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

Nov 15, 2023 – 09:22 PM JST

| | | |
|---|---|---|
| PDB ID | : | 6JWV |
| Title | : | Crystal structure of Plasmodium falciparum HPPK-DHPS A437G with STZ-DHP |
| Authors | : | Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y. |
| Deposited on | : | 2019-04-21 |
| Resolution | : | 2.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

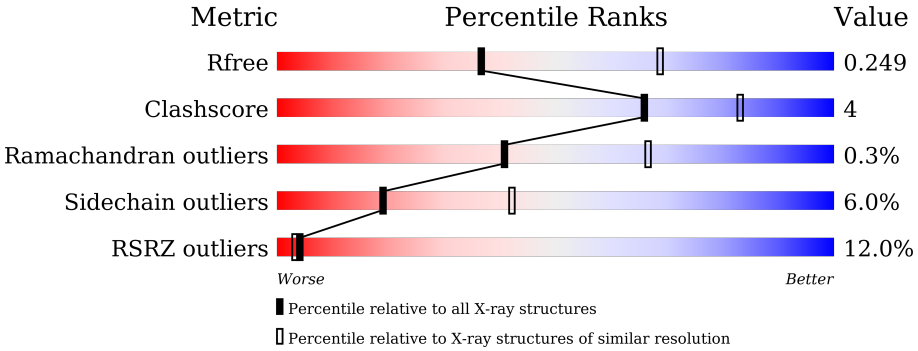
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2808 (2.70-2.70) |
| Clashscore | 141614 | 3122 (2.70-2.70) |
| Ramachandran outliers | 138981 | 3069 (2.70-2.70) |
| Sidechain outliers | 138945 | 3069 (2.70-2.70) |
| RSRZ outliers | 127900 | 2737 (2.70-2.70) |

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 | 728 | 4% 63% 10% • 25% |
| 1 | B | 728 | 14% 63% 10% • 26% |

# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9403 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihyd ropteroate synthase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 543 | 4501 | 2897 | 741 | 841 | 22 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 1 | B | 540 | 4454 | 2864 | 733 | 836 | 21 | 0 | 0 | 0 |

There are 46 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 437 | GLY | ALA | engineered mutation | UNP Q25704 |
| A | 707 | LYS | - | expression tag | UNP Q25704 |
| A | 708 | ASP | - | expression tag | UNP Q25704 |
| A | 709 | PRO | - | expression tag | UNP Q25704 |
| A | 710 | ASN | - | expression tag | UNP Q25704 |
| A | 711 | SER | - | expression tag | UNP Q25704 |
| A | 712 | SER | - | expression tag | UNP Q25704 |
| A | 713 | SER | - | expression tag | UNP Q25704 |
| A | 714 | VAL | - | expression tag | UNP Q25704 |
| A | 715 | ASP | - | expression tag | UNP Q25704 |
| A | 716 | LYS | - | expression tag | UNP Q25704 |
| A | 717 | LEU | - | expression tag | UNP Q25704 |
| A | 718 | ALA | - | expression tag | UNP Q25704 |
| A | 719 | ALA | - | expression tag | UNP Q25704 |
| A | 720 | ALA | - | expression tag | UNP Q25704 |
| A | 721 | LEU | - | expression tag | UNP Q25704 |
| A | 722 | GLU | - | expression tag | UNP Q25704 |
| A | 723 | HIS | - | expression tag | UNP Q25704 |
| A | 724 | HIS | - | expression tag | UNP Q25704 |
| A | 725 | HIS | - | expression tag | UNP Q25704 |
| A | 726 | HIS | - | expression tag | UNP Q25704 |
| A | 727 | HIS | - | expression tag | UNP Q25704 |
| A | 728 | HIS | - | expression tag | UNP Q25704 |
| B | 437 | GLY | ALA | engineered mutation | UNP Q25704 |

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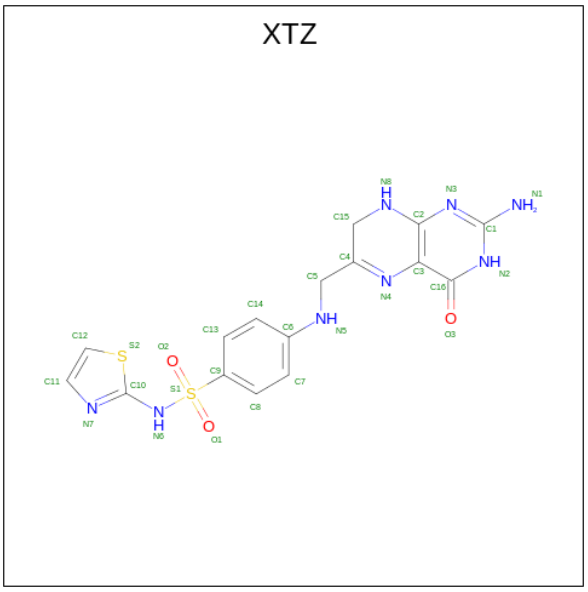
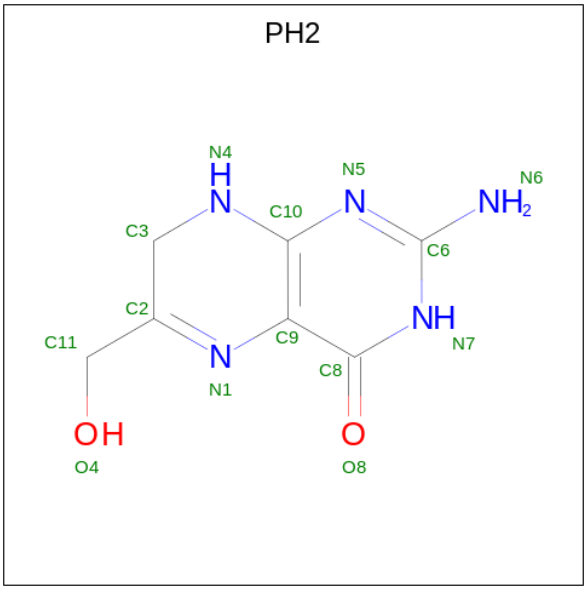
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 707 | LYS | - | expression tag | UNP Q25704 |
| B | 708 | ASP | - | expression tag | UNP Q25704 |
| B | 709 | PRO | - | expression tag | UNP Q25704 |
| B | 710 | ASN | - | expression tag | UNP Q25704 |
| B | 711 | SER | - | expression tag | UNP Q25704 |
| B | 712 | SER | - | expression tag | UNP Q25704 |
| B | 713 | SER | - | expression tag | UNP Q25704 |
| B | 714 | VAL | - | expression tag | UNP Q25704 |
| B | 715 | ASP | - | expression tag | UNP Q25704 |
| B | 716 | LYS | - | expression tag | UNP Q25704 |
| B | 717 | LEU | - | expression tag | UNP Q25704 |
| B | 718 | ALA | - | expression tag | UNP Q25704 |
| B | 719 | ALA | - | expression tag | UNP Q25704 |
| B | 720 | ALA | - | expression tag | UNP Q25704 |
| B | 721 | LEU | - | expression tag | UNP Q25704 |
| B | 722 | GLU | - | expression tag | UNP Q25704 |
| B | 723 | HIS | - | expression tag | UNP Q25704 |
| B | 724 | HIS | - | expression tag | UNP Q25704 |
| B | 725 | HIS | - | expression tag | UNP Q25704 |
| B | 726 | HIS | - | expression tag | UNP Q25704 |
| B | 727 | HIS | - | expression tag | UNP Q25704 |
| B | 728 | HIS | - | expression tag | UNP Q25704 |

- Molecule 2 is 4-{[(2-amino-4-oxo-3,4,7,8-tetrahydropteridin-6-yl)methyl]amino}-N-(1,3-thiazol-2-yl)benzenesulfonamide (three-letter code: XTZ) (formula: $C_{16}H_{16}N_8O_3S_2$).



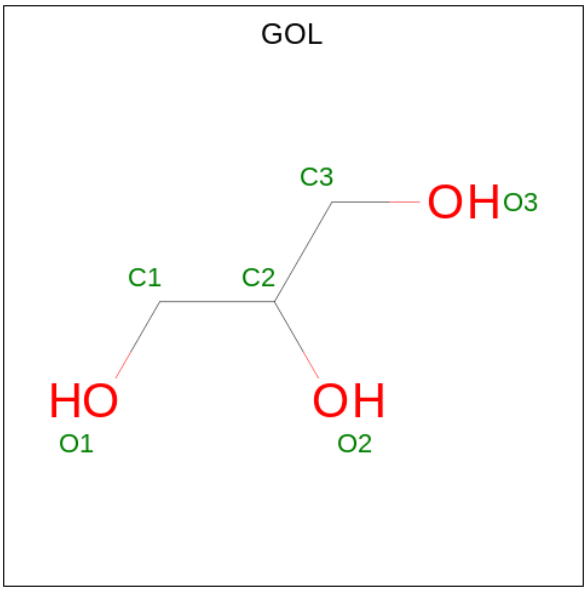
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | A | 1 | 29 | 16 | 8 | 3 | 2 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 2 | B | 1 | 29 | 16 | 8 | 3 | 2 | 0 | 0 |

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: $C_7H_9N_5O_2$).



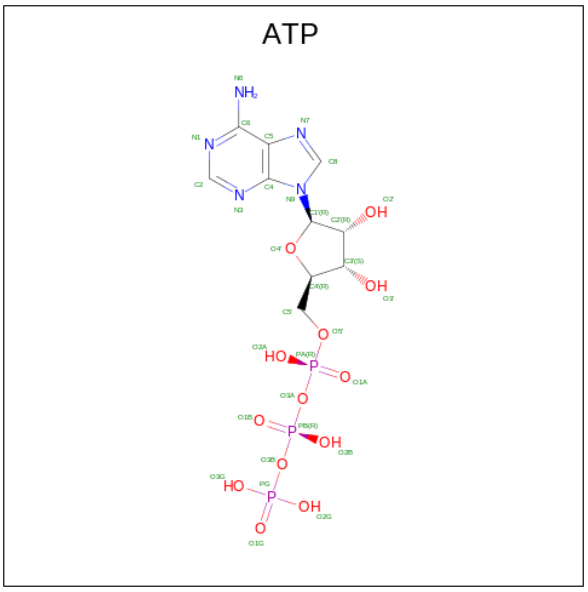

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | A | 1 | 14 | 7 | 5 | 2 | 0 | 0 |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 4 | A | 1 | 6 | 3 | 3 | 0 | 0 |
| | | | Total | C | O | | |
| 4 | B | 1 | 6 | 3 | 3 | 0 | 0 |

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | A | 1 | 31 | 10 | 5 | 13 | 3 | 0 | 0 |

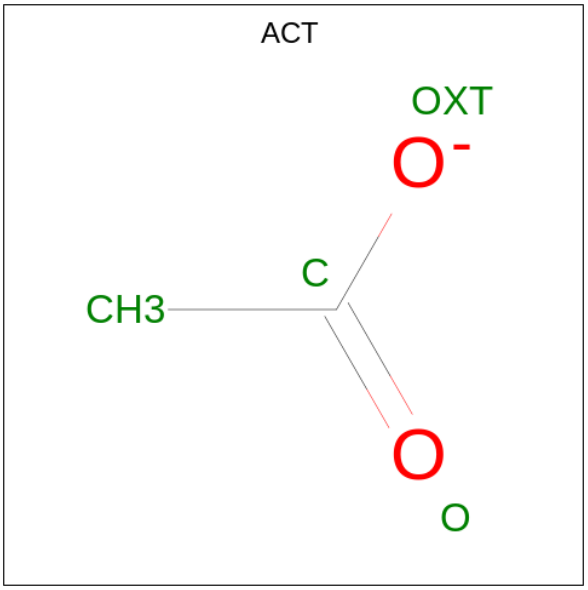
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | A | 2 | Total Mg<br>2 2 | 0 | 0 |
| 6 | B | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 7 | A | 1 | Total Ca<br>1 1 | 0 | 0 |
| 7 | B | 1 | Total Ca<br>1 1 | 0 | 0 |

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 8 | A | 1 | Total C O<br>4 2 2 | 0 | 0 |
| 8 | A | 1 | Total C O<br>4 2 2 | 0 | 0 |
| 8 | B | 1 | Total C O<br>4 2 2 | 0 | 0 |
| 8 | B | 1 | Total C O<br>4 2 2 | 0 | 0 |

- Molecule 9 is water.

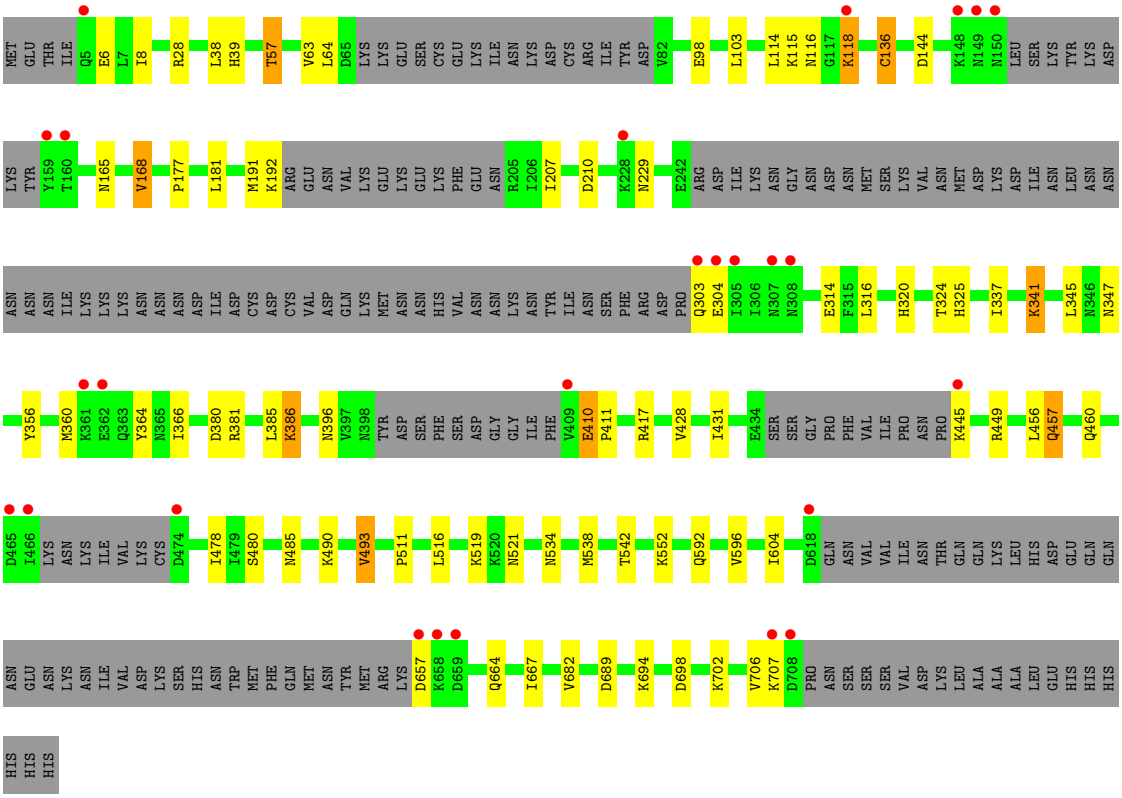
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 9 | A | 210 | 210 | 210 | 0 | 0 |
| | | | Total | O | | |
| 9 | B | 102 | 102 | 102 | 0 | 0 |

# 3 Residue-property plots (i)

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.

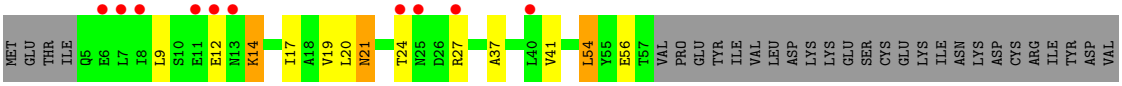
• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase

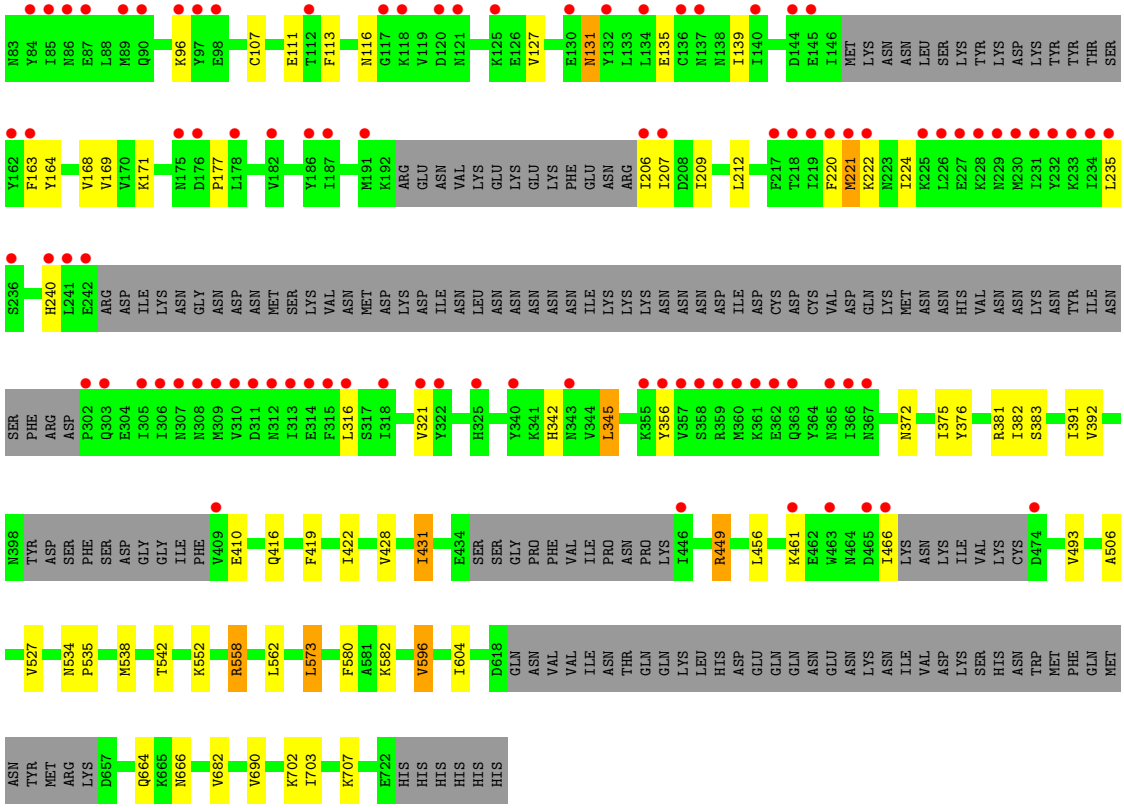
Chain A:




• Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase

Chain B:




N83 Y84 I85 N86 E87 L88 M89 Q90 K96 Y97 E98 C107 E111 T112 F113 N116 G117 K118 V119 D120 N121 K125 E126 V127 E130 N131 Y132 L133 L134 E135 C136 N137 N138 I139 I140 D144 E145 I146 MET LYS ASN ASN LEU SER LYS TYR LYS ASP LYS TYR TYR THR SER
Y162 F163 Y164 V168 V169 V170 K171 N176 D176 P177 L178 V182 Y186 I187 M191 K192 ARG GLU ASN VAL LYS GLU LYS GLU LYS PHE GLU ASN ARG I206 I207 D208 I209 L212 F217 T218 I219 F220 M221 K222 N223 I224 K225 L226 E227 K228 M229 M230 I231 Y232 K233 I234 L235
S236 H240 L241 E242 ARG ASP ILE LYS ASN GLY ASN ASP ASN MET SER LYS VAL ASN MET ASP LYS ASP ILE ASN LEU ASN ASN ASN ASN ASN ILE LYS LYS LYS ASN ASN ASN ASP ILE ASP CYS ASP CYS VAL ASP GLN LYS MET ASN ASN HIS VAL ASN ASN LYS ASN TYR ILE ASN
SER PHE ARG ASP P302 Q303 E304 I305 I306 N307 N308 M309 V310 D311 N312 I313 E314 F315 L316 S317 I318 V321 Y322 H325 Y340 K341 H342 N343 V344 L345 K355 Y356 V357 S358 R359 M360 K361 E362 Q363 Y364 N365 I366 N367 N372 I375 Y376 R381 I382 S383 I391 V392
N398 TYR ASP SER PHE SER ASP GLY GLY ILE PHE Y409 E410 Q416 F419 I422 V428 I431 E434 SER SER GLY PRO PHE VAL ILE PRO ASN PRO LYS I446 R449 L456 K461 E462 W463 N464 D465 I466 LYS ASN LYS ILE VAL LYS CYS D474 V493 A506
V527 N534 P535 M538 T542 K552 R558 L562 L573 F580 A581 K582 V596 I604 D618 GLN ASN VAL VAL ILE ASN THR GLN GLN LYS LEU HIS ASP GLU GLN GLN ASN GLU ASN LYS ASN ILE VAL ASP LYS SER HIS ASN TRP MET PHE GLN MET
ASN TYR MET ARG LYS D657 Q664 K665 N666 V682 V690 K702 I703 K707 E722 HIS HIS HIS HIS HIS HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 98.89Å 136.72Å 138.70Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.70<br>41.88 – 2.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 90.3 (30.00-2.70)<br>90.4 (41.88-2.70) | Depositor<br>EDS |
| $R_{merge}$ | 0.04 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 8.14 (at 2.69Å) | Xtriage |
| Refinement program | REFMAC 5.8.0135 | Depositor |
| R, $R_{free}$ | 0.206 , 0.257<br>0.202 , 0.249 | Depositor<br>DCC |
| $R_{free}$ test set | 4716 reflections (10.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 29.7 | Xtriage |
| Anisotropy | 0.387 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 54.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.007 for -h,l,k | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 9403 | 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 3.47% 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 (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PH2, GOL, ATP, XTZ, ACT, MG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | A | 0.49 | 0/4568 | 0.70 | 0/6159 |
| 1 | B | 0.48 | 0/4520 | 0.69 | 0/6095 |
| All | All | 0.49 | 0/9088 | 0.70 | 0/12254 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (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 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 | 4501 | 0 | 4589 | 37 | 0 |
| 1 | B | 4454 | 0 | 4538 | 35 | 0 |
| 2 | A | 29 | 0 | 16 | 2 | 0 |
| 2 | B | 29 | 0 | 16 | 0 | 0 |
| 3 | A | 14 | 0 | 9 | 0 | 0 |
| 4 | A | 6 | 0 | 8 | 2 | 0 |
| 4 | B | 6 | 0 | 8 | 0 | 0 |
| 5 | A | 31 | 0 | 12 | 2 | 0 |
| 6 | A | 2 | 0 | 0 | 0 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 7 | B | 1 | 0 | 0 | 0 | 0 |
| 8 | A | 8 | 0 | 6 | 0 | 0 |
| 8 | B | 8 | 0 | 6 | 0 | 0 |
| 9 | A | 210 | 0 | 0 | 3 | 0 |
| 9 | B | 102 | 0 | 0 | 0 | 0 |
| All | All | 9403 | 0 | 9208 | 73 | 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 4.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:552:LYS:HD2 | 1:B:596:VAL:HG13 | 1.58 | 0.84 |
| 1:B:527:VAL:HG22 | 1:B:573:LEU:HD12 | 1.63 | 0.80 |
| 2:A:801:XTZ:H5 | 4:A:803:GOL:H11 | 1.65 | 0.79 |
| 1:A:552:LYS:HD2 | 1:A:596:VAL:HG13 | 1.66 | 0.77 |
| 1:A:57:THR:HG21 | 1:A:165:ASN:OD1 | 1.91 | 0.71 |
| 2:A:801:XTZ:N7 | 2:A:801:XTZ:H9 | 2.05 | 0.70 |
| 1:B:375:ILE:HG21 | 1:B:382:ILE:HD13 | 1.75 | 0.69 |
| 1:A:396:ASN:OD1 | 4:A:803:GOL:H2 | 1.97 | 0.64 |
| 1:B:56:GLU:O | 1:B:372:ASN:HA | 1.97 | 0.64 |
| 1:B:534:ASN:HB2 | 1:B:535:PRO:CD | 2.28 | 0.64 |
| 1:A:63:VAL:HG11 | 1:A:325:HIS:HB3 | 1.81 | 0.61 |
| 1:A:177:PRO:HB2 | 1:A:316:LEU:HD21 | 1.82 | 0.61 |
| 1:B:534:ASN:HB2 | 1:B:535:PRO:HD2 | 1.83 | 0.61 |
| 1:A:431:ILE:HG21 | 1:A:456:LEU:HD21 | 1.82 | 0.60 |
| 1:B:221:MET:HB3 | 1:B:224:ILE:HD11 | 1.82 | 0.60 |
| 1:A:6:GLU:HB3 | 1:A:8:ILE:HG22 | 1.83 | 0.60 |
| 1:B:419:PHE:HA | 1:B:422:ILE:HD12 | 1.83 | 0.59 |
| 1:A:118:LYS:HD2 | 1:A:118:LYS:H | 1.67 | 0.58 |
| 1:B:392:VAL:HG22 | 1:B:428:VAL:HB | 1.85 | 0.58 |
| 1:A:485:ASN:HB2 | 9:A:1092:HOH:O | 2.05 | 0.57 |
| 1:A:364:TYR:HB3 | 1:A:366:ILE:HG12 | 1.88 | 0.56 |
| 1:A:490:LYS:HD3 | 1:A:516:LEU:HD22 | 1.87 | 0.55 |
| 1:B:506:ALA:HB1 | 1:B:558:ARG:HG2 | 1.88 | 0.55 |
| 1:B:449:ARG:HH11 | 1:B:449:ARG:HG3 | 1.71 | 0.54 |
| 1:B:376:TYR:O | 1:B:383:SER:HB2 | 2.07 | 0.53 |
| 1:B:20:LEU:HB2 | 1:B:168:VAL:HG22 | 1.90 | 0.53 |
| 1:B:206:ILE:HG23 | 1:B:207:ILE:HG22 | 1.90 | 0.52 |
| 1:A:39:HIS:NE2 | 1:A:521:ASN:O | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:177:PRO:HB2 | 1:B:316:LEU:HD11 | 1.92 | 0.52 |
| 1:B:127:VAL:HB | 1:B:131:ASN:HB3 | 1.92 | 0.51 |
| 1:A:534:ASN:O | 1:A:538:MET:HB2 | 2.10 | 0.51 |
| 1:A:181:LEU:HD21 | 5:A:804:ATP:H2' | 1.92 | 0.50 |
| 1:A:191:MET:HE1 | 1:A:207:ILE:HG12 | 1.94 | 0.50 |
| 1:B:342:HIS:HB3 | 1:B:345:LEU:HG | 1.93 | 0.50 |
| 1:B:431:ILE:HG21 | 1:B:456:LEU:HD21 | 1.93 | 0.49 |
| 1:B:375:ILE:HG12 | 1:B:382:ILE:HG23 | 1.95 | 0.49 |
| 1:A:103:LEU:CD1 | 1:A:511:PRO:HB2 | 2.44 | 0.48 |
| 1:A:592:GLN:HG2 | 1:B:703:ILE:O | 2.14 | 0.47 |
| 1:A:385:LEU:HG | 1:A:386:LYS:HD3 | 1.95 | 0.47 |
| 1:A:694:LYS:HE3 | 1:A:698:ASP:OD1 | 2.16 | 0.46 |
| 1:A:410:GLU:N | 1:A:411:PRO:CD | 2.78 | 0.46 |
| 1:A:667:ILE:HG13 | 1:A:689:ASP:OD2 | 2.16 | 0.46 |
| 1:A:493:VAL:HG13 | 1:A:519:LYS:HE3 | 1.97 | 0.46 |
| 1:B:54:LEU:HB3 | 1:B:375:ILE:HB | 1.98 | 0.46 |
| 1:B:107:CYS:SG | 1:B:171:LYS:HD3 | 2.56 | 0.44 |
| 1:B:24:THR:HG23 | 1:B:164:TYR:HB2 | 1.99 | 0.44 |
| 1:B:391:ILE:HG21 | 1:B:690:VAL:HG13 | 1.99 | 0.44 |
| 1:A:428:VAL:HG22 | 1:A:478:ILE:HB | 2.01 | 0.43 |
| 1:B:96:LYS:HG2 | 1:B:240:HIS:CD2 | 2.54 | 0.43 |
| 1:A:457:GLN:HG3 | 9:A:1029:HOH:O | 2.19 | 0.43 |
| 1:A:114:LEU:HD21 | 1:A:337:ILE:HG22 | 2.01 | 0.42 |
| 1:A:604:ILE:HG12 | 1:A:682:VAL:HG11 | 2.01 | 0.42 |
| 1:A:210:ASP:HB3 | 1:A:320:HIS:CD2 | 2.54 | 0.42 |
| 1:A:38:LEU:HD21 | 1:A:168:VAL:HG11 | 2.01 | 0.42 |
| 1:A:118:LYS:H | 1:A:118:LYS:CD | 2.32 | 0.41 |
| 1:B:604:ILE:HG12 | 1:B:682:VAL:HG11 | 2.01 | 0.41 |
| 1:A:316:LEU:HA | 5:A:804:ATP:C8 | 2.56 | 0.41 |
| 1:B:19:VAL:HG22 | 1:B:169:VAL:HG22 | 2.03 | 0.41 |
| 1:B:580:PHE:O | 1:B:582:LYS:HD2 | 2.20 | 0.41 |
| 1:A:115:LYS:O | 1:A:116:ASN:HB2 | 2.19 | 0.41 |
| 1:A:136:CYS:SG | 9:A:961:HOH:O | 2.62 | 0.41 |
| 1:B:17:ILE:HG13 | 1:B:113:PHE:HB2 | 2.03 | 0.41 |
| 1:A:324:THR:CG2 | 1:A:345:LEU:HD22 | 2.51 | 0.41 |
| 1:B:21:ASN:HB2 | 1:B:212:LEU:HD21 | 2.03 | 0.41 |
| 1:B:135:GLU:O | 1:B:139:ILE:HG12 | 2.21 | 0.41 |
| 1:A:356:TYR:O | 1:A:360:MET:HG2 | 2.21 | 0.41 |
| 1:A:341:LYS:HE2 | 1:A:345:LEU:O | 2.21 | 0.40 |
| 1:A:385:LEU:O | 1:A:386:LYS:HB2 | 2.21 | 0.40 |
| 1:A:38:LEU:CD2 | 1:A:168:VAL:HG11 | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:12:GLU:O | 1:B:14:LYS:HE3 | 2.21 | 0.40 |
| 1:B:37:ALA:O | 1:B:41:VAL:HG23 | 2.22 | 0.40 |
| 1:B:116:ASN:HD22 | 1:B:116:ASN:HA | 1.64 | 0.40 |
| 1:B:21:ASN:O | 1:B:209:ILE:HA | 2.21 | 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 | 525/728 (72%) | 502 (96%) | 22 (4%) | 1 (0%) | 47 | 73 |
| 1 | B | 522/728 (72%) | 496 (95%) | 24 (5%) | 2 (0%) | 34 | 60 |
| All | All | 1047/1456 (72%) | 998 (95%) | 46 (4%) | 3 (0%) | 41 | 66 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 222 | LYS |
| 1 | B | 538 | MET |
| 1 | A | 410 | GLU |

### 5.3.2 Protein sidechains (i)

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 | 518/696 (74%) | 487 (94%) | 31 (6%) | 19 | 42 |
| 1 | B | 512/696 (74%) | 481 (94%) | 31 (6%) | 18 | 41 |
| All | All | 1030/1392 (74%) | 968 (94%) | 62 (6%) | 19 | 42 |

All (62) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 28 | ARG |
| 1 | A | 57 | THR |
| 1 | A | 64 | LEU |
| 1 | A | 98 | GLU |
| 1 | A | 118 | LYS |
| 1 | A | 136 | CYS |
| 1 | A | 144 | ASP |
| 1 | A | 168 | VAL |
| 1 | A | 192 | LYS |
| 1 | A | 229 | ASN |
| 1 | A | 303 | GLN |
| 1 | A | 304 | GLU |
| 1 | A | 314 | GLU |
| 1 | A | 341 | LYS |
| 1 | A | 347 | ASN |
| 1 | A | 380 | ASP |
| 1 | A | 381 | ARG |
| 1 | A | 386 | LYS |
| 1 | A | 417 | ARG |
| 1 | A | 445 | LYS |
| 1 | A | 449 | ARG |
| 1 | A | 457 | GLN |
| 1 | A | 460 | GLN |
| 1 | A | 480 | SER |
| 1 | A | 493 | VAL |
| 1 | A | 542 | THR |
| 1 | A | 657 | ASP |
| 1 | A | 664 | GLN |
| 1 | A | 702 | LYS |
| 1 | A | 706 | VAL |
| 1 | A | 707 | LYS |
| 1 | B | 9 | LEU |
| 1 | B | 14 | LYS |
| 1 | B | 21 | ASN |
| 1 | B | 27 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 54 | LEU |
| 1 | B | 111 | GLU |
| 1 | B | 131 | ASN |
| 1 | B | 163 | PHE |
| 1 | B | 220 | PHE |
| 1 | B | 221 | MET |
| 1 | B | 235 | LEU |
| 1 | B | 321 | VAL |
| 1 | B | 345 | LEU |
| 1 | B | 356 | TYR |
| 1 | B | 381 | ARG |
| 1 | B | 410 | GLU |
| 1 | B | 416 | GLN |
| 1 | B | 431 | ILE |
| 1 | B | 449 | ARG |
| 1 | B | 461 | LYS |
| 1 | B | 466 | ILE |
| 1 | B | 493 | VAL |
| 1 | B | 542 | THR |
| 1 | B | 558 | ARG |
| 1 | B | 562 | LEU |
| 1 | B | 573 | LEU |
| 1 | B | 596 | VAL |
| 1 | B | 664 | GLN |
| 1 | B | 666 | ASN |
| 1 | B | 702 | LYS |
| 1 | B | 707 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 460 | GLN |
| 1 | A | 557 | GLN |
| 1 | B | 25 | ASN |
| 1 | B | 116 | ASN |
| 1 | B | 240 | HIS |
| 1 | B | 307 | ASN |
| 1 | B | 495 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | XTZ | B | 801 | - | 26,32,32 | 2.24 | 2 (7%) | 28,46,46 | 2.24 | 7 (25%) |
| 2 | XTZ | A | 801 | - | 26,32,32 | 2.25 | 3 (11%) | 28,46,46 | 2.66 | 6 (21%) |
| 5 | ATP | A | 804 | 6 | 26,33,33 | 0.91 | 1 (3%) | 31,52,52 | 1.44 | 5 (16%) |
| 3 | PH2 | A | 802 | 6 | 10,15,15 | 1.12 | 1 (10%) | 10,21,21 | 2.28 | 4 (40%) |
| 4 | GOL | B | 802 | - | 5,5,5 | 0.40 | 0 | 5,5,5 | 0.42 | 0 |
| 8 | ACT | B | 805 | - | 3,3,3 | 0.82 | 0 | 3,3,3 | 0.78 | 0 |
| 4 | GOL | A | 803 | - | 5,5,5 | 0.55 | 0 | 5,5,5 | 0.82 | 0 |
| 8 | ACT | A | 808 | - | 3,3,3 | 0.75 | 0 | 3,3,3 | 0.93 | 0 |
| 8 | ACT | B | 804 | - | 3,3,3 | 0.76 | 0 | 3,3,3 | 0.80 | 0 |
| 8 | ACT | A | 807 | - | 3,3,3 | 0.87 | 0 | 3,3,3 | 0.21 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | XTZ | B | 801 | - | - | 6/12/25/25 | 0/4/4/4 |
| 2 | XTZ | A | 801 | - | - | 5/12/25/25 | 0/4/4/4 |
| 5 | ATP | A | 804 | 6 | - | 4/18/38/38 | 0/3/3/3 |
| 3 | PH2 | A | 802 | 6 | - | 0/0/11/11 | 0/2/2/2 |
| 4 | GOL | B | 802 | - | - | 0/4/4/4 | - |
| 4 | GOL | A | 803 | - | - | 2/4/4/4 | - |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 801 | XTZ | C9-S1 | -9.65 | 1.61 | 1.76 |
| 2 | A | 801 | XTZ | C9-S1 | -9.64 | 1.61 | 1.76 |
| 2 | A | 801 | XTZ | C3-C2 | 3.87 | 1.49 | 1.40 |
| 2 | B | 801 | XTZ | C3-C2 | 3.14 | 1.47 | 1.40 |
| 3 | A | 802 | PH2 | C9-C10 | 2.57 | 1.48 | 1.41 |
| 5 | A | 804 | ATP | C5-C4 | 2.40 | 1.47 | 1.40 |
| 2 | A | 801 | XTZ | C16-N2 | -2.32 | 1.34 | 1.38 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 801 | XTZ | O2-S1-O1 | -10.99 | 106.04 | 119.55 |
| 2 | B | 801 | XTZ | O2-S1-O1 | -8.11 | 109.58 | 119.55 |
| 2 | A | 801 | XTZ | O1-S1-C9 | 4.71 | 113.78 | 107.97 |
| 2 | B | 801 | XTZ | C9-S1-N6 | 4.35 | 112.30 | 106.83 |
| 3 | A | 802 | PH2 | C6-N7-C8 | 4.17 | 122.55 | 115.93 |
| 2 | B | 801 | XTZ | C1-N3-C2 | 4.06 | 120.76 | 113.43 |
| 2 | A | 801 | XTZ | C1-N3-C2 | 3.95 | 120.56 | 113.43 |
| 5 | A | 804 | ATP | N3-C2-N1 | -3.95 | 122.50 | 128.68 |
| 5 | A | 804 | ATP | PA-O3A-PB | -3.62 | 120.39 | 132.83 |
| 3 | A | 802 | PH2 | C9-C8-N7 | -3.53 | 118.61 | 123.43 |
| 3 | A | 802 | PH2 | C6-N5-C10 | 3.12 | 121.53 | 114.54 |
| 2 | B | 801 | XTZ | C3-N4-C4 | 3.05 | 122.30 | 116.24 |
| 5 | A | 804 | ATP | C4-C5-N7 | -2.68 | 106.61 | 109.40 |
| 2 | A | 801 | XTZ | C8-C9-S1 | 2.63 | 122.63 | 119.77 |
| 2 | B | 801 | XTZ | O3-C16-C3 | -2.48 | 120.02 | 126.60 |
| 3 | A | 802 | PH2 | C10-C9-C8 | 2.21 | 115.97 | 114.53 |
| 2 | B | 801 | XTZ | C10-N6-S1 | 2.21 | 128.18 | 124.16 |
| 2 | B | 801 | XTZ | C3-C16-N2 | 2.20 | 118.79 | 113.19 |
| 2 | A | 801 | XTZ | O2-S1-N6 | 2.20 | 112.25 | 106.73 |
| 5 | A | 804 | ATP | C2-N1-C6 | 2.13 | 122.40 | 118.75 |
| 5 | A | 804 | ATP | PB-O3B-PG | -2.03 | 125.86 | 132.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 801 | XTZ | C14-C13-C9 | 2.02 | 121.54 | 119.45 |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | A | 804 | ATP | C5'-O5'-PA-O3A |
| 4 | A | 803 | GOL | C1-C2-C3-O3 |
| 2 | B | 801 | XTZ | C7-C6-N5-C5 |
| 2 | A | 801 | XTZ | C7-C6-N5-C5 |
| 2 | B | 801 | XTZ | C14-C6-N5-C5 |
| 2 | A | 801 | XTZ | C14-C6-N5-C5 |
| 4 | A | 803 | GOL | O2-C2-C3-O3 |
| 5 | A | 804 | ATP | C5'-O5'-PA-O1A |
| 5 | A | 804 | ATP | C5'-O5'-PA-O2A |
| 2 | A | 801 | XTZ | C13-C9-S1-O1 |
| 2 | B | 801 | XTZ | C10-N6-S1-O1 |
| 5 | A | 804 | ATP | O4'-C4'-C5'-O5' |
| 2 | A | 801 | XTZ | C8-C9-S1-O1 |
| 2 | A | 801 | XTZ | C4-C5-N5-C6 |
| 2 | B | 801 | XTZ | C4-C5-N5-C6 |
| 2 | B | 801 | XTZ | C8-C9-S1-O2 |
| 2 | B | 801 | XTZ | C13-C9-S1-O2 |

There are no ring outliers.

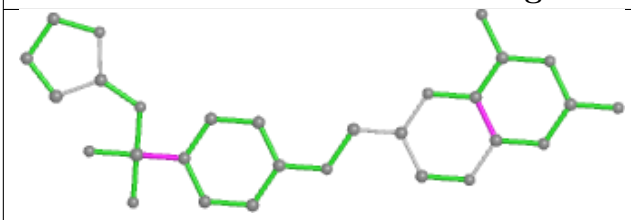
3 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | A | 801 | XTZ | 2 | 0 |
| 5 | A | 804 | ATP | 2 | 0 |
| 4 | A | 803 | GOL | 2 | 0 |

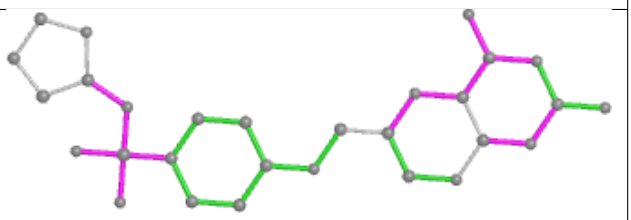
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

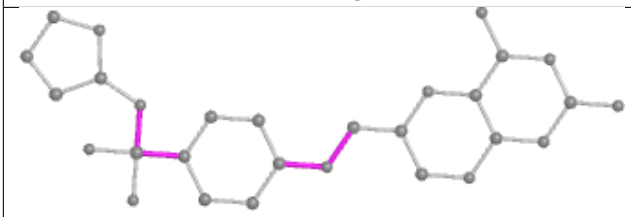
**Ligand XTZ B 801**



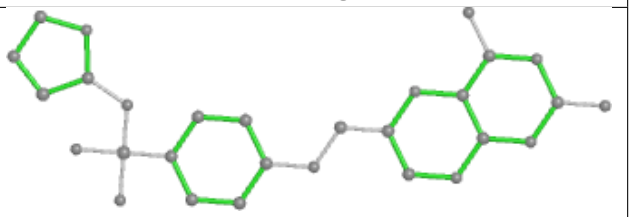
**Bond lengths**



**Bond angles**

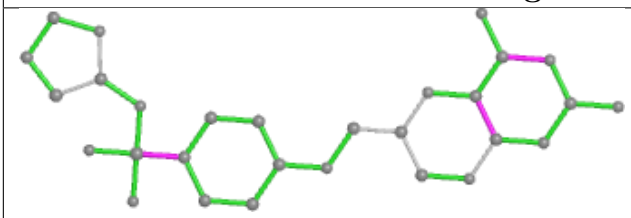


**Torsions**

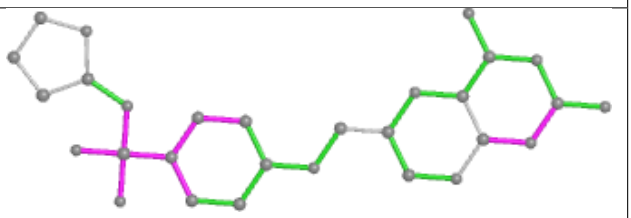


**Rings**

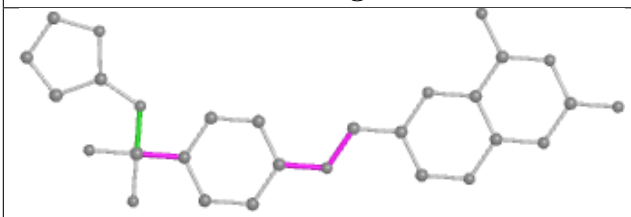
**Ligand XTZ A 801**



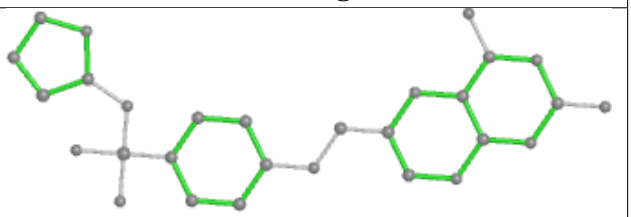
**Bond lengths**



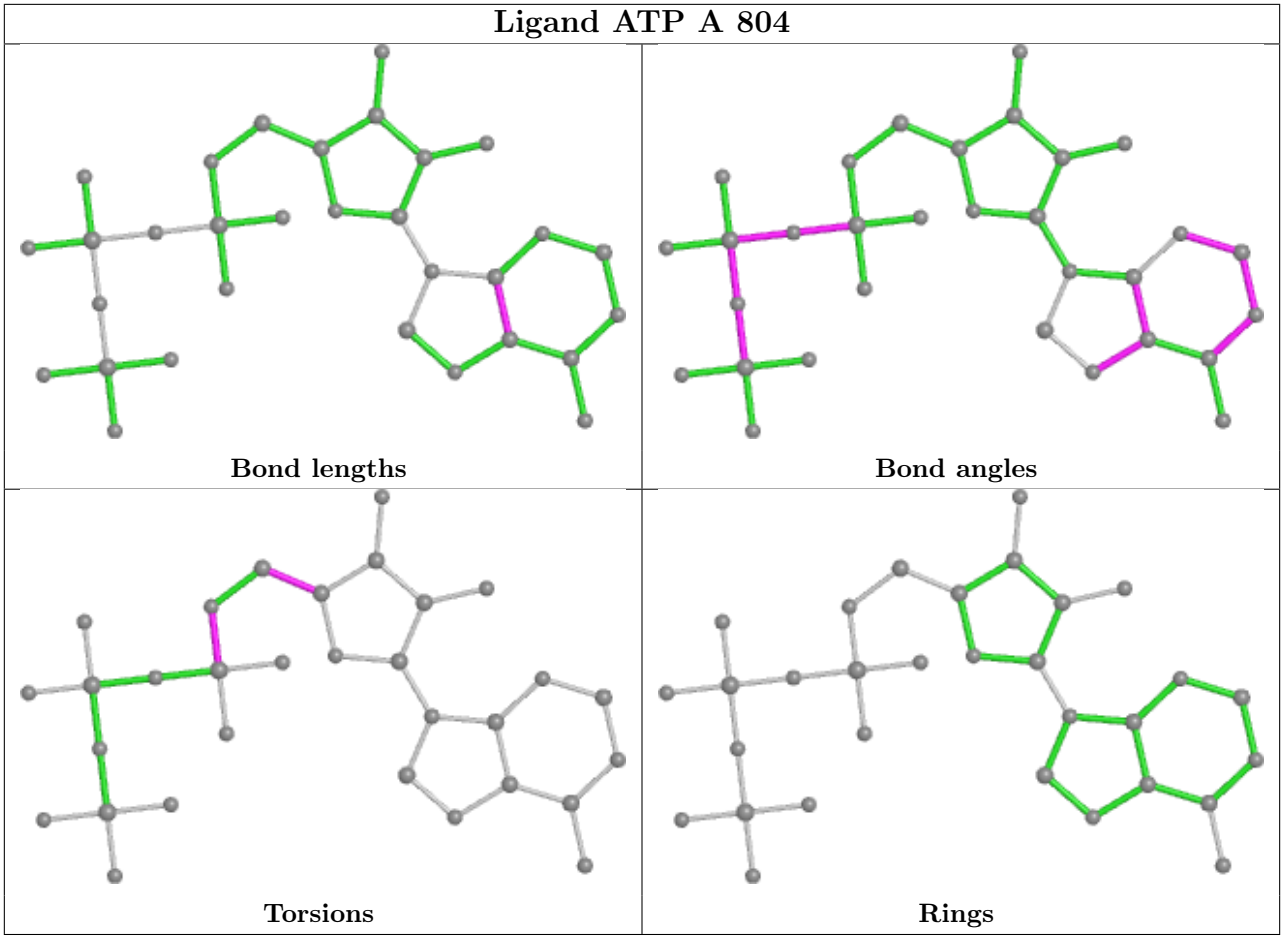
**Bond angles**



**Torsions**



**Rings**




## 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, $95^{th}$ 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 | 543/728 (74%) | -0.02 | 26 (4%) | 30 | 28 | 7, 25, 84, 120 | 0 |
| 1 | B | 540/728 (74%) | 0.80 | 104 (19%) | 1 | 0 | 8, 58, 120, 120 | 0 |
| All | All | 1083/1456 (74%) | 0.38 | 130 (12%) | 4 | 3 | 7, 34, 117, 120 | 0 |

All (130) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 8 | ILE | 8.7 |
| 1 | B | 233 | LYS | 6.4 |
| 1 | B | 140 | ILE | 6.4 |
| 1 | B | 305 | ILE | 6.0 |
| 1 | B | 366 | ILE | 5.9 |
| 1 | A | 708 | ASP | 5.7 |
| 1 | B | 357 | VAL | 5.7 |
| 1 | B | 231 | ILE | 5.7 |
| 1 | B | 228 | LYS | 5.5 |
| 1 | B | 229 | ASN | 5.4 |
| 1 | B | 90 | GLN | 5.2 |
| 1 | B | 118 | LYS | 5.2 |
| 1 | B | 134 | LEU | 5.0 |
| 1 | A | 305 | ILE | 4.9 |
| 1 | B | 125 | LYS | 4.9 |
| 1 | B | 240 | HIS | 4.8 |
| 1 | A | 308 | ASN | 4.8 |
| 1 | B | 191 | MET | 4.7 |
| 1 | B | 220 | PHE | 4.7 |
| 1 | B | 311 | ASP | 4.7 |
| 1 | B | 136 | CYS | 4.6 |
| 1 | A | 304 | GLU | 4.6 |
| 1 | A | 5 | GLN | 4.5 |
| 1 | B | 316 | LEU | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 221 | MET | 4.4 |
| 1 | B | 361 | LYS | 4.4 |
| 1 | B | 96 | LYS | 4.4 |
| 1 | B | 206 | ILE | 4.3 |
| 1 | B | 162 | TYR | 4.2 |
| 1 | A | 148 | LYS | 4.2 |
| 1 | B | 227 | GLU | 4.1 |
| 1 | B | 7 | LEU | 4.1 |
| 1 | B | 132 | TYR | 4.1 |
| 1 | B | 25 | ASN | 4.0 |
| 1 | B | 225 | LYS | 4.0 |
| 1 | B | 222 | LYS | 4.0 |
| 1 | B | 307 | ASN | 4.0 |
| 1 | B | 178 | LEU | 3.9 |
| 1 | A | 659 | ASP | 3.9 |
| 1 | B | 27 | ARG | 3.9 |
| 1 | B | 343 | ASN | 3.8 |
| 1 | B | 219 | ILE | 3.8 |
| 1 | B | 6 | GLU | 3.8 |
| 1 | B | 86 | ASN | 3.7 |
| 1 | B | 234 | ILE | 3.7 |
| 1 | A | 409 | VAL | 3.7 |
| 1 | B | 446 | ILE | 3.6 |
| 1 | B | 187 | ILE | 3.5 |
| 1 | B | 98 | GLU | 3.5 |
| 1 | B | 218 | THR | 3.5 |
| 1 | B | 365 | ASN | 3.5 |
| 1 | A | 303 | GLN | 3.4 |
| 1 | B | 84 | TYR | 3.4 |
| 1 | A | 149 | ASN | 3.4 |
| 1 | B | 12 | GLU | 3.4 |
| 1 | B | 359 | ARG | 3.4 |
| 1 | B | 363 | GLN | 3.3 |
| 1 | B | 207 | ILE | 3.3 |
| 1 | A | 445 | LYS | 3.3 |
| 1 | B | 309 | MET | 3.3 |
| 1 | B | 310 | VAL | 3.3 |
| 1 | B | 367 | ASN | 3.2 |
| 1 | B | 318 | ILE | 3.2 |
| 1 | B | 145 | GLU | 3.2 |
| 1 | A | 160 | THR | 3.2 |
| 1 | A | 228 | LYS | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 150 | ASN | 3.2 |
| 1 | B | 144 | ASP | 3.1 |
| 1 | A | 474 | ASP | 3.1 |
| 1 | B | 232 | TYR | 3.0 |
| 1 | B | 409 | VAL | 3.0 |
| 1 | B | 137 | ASN | 3.0 |
| 1 | B | 461 | LYS | 3.0 |
| 1 | A | 466 | ILE | 3.0 |
| 1 | B | 465 | ASP | 2.9 |
| 1 | B | 226 | LEU | 2.9 |
| 1 | B | 130 | GLU | 2.9 |
| 1 | B | 87 | GLU | 2.9 |
| 1 | B | 13 | ASN | 2.9 |
| 1 | B | 362 | GLU | 2.8 |
| 1 | B | 306 | ILE | 2.8 |
| 1 | B | 315 | PHE | 2.8 |
| 1 | A | 618 | ASP | 2.8 |
| 1 | B | 121 | ASN | 2.7 |
| 1 | B | 175 | ASN | 2.7 |
| 1 | B | 325 | HIS | 2.7 |
| 1 | B | 358 | SER | 2.7 |
| 1 | B | 186 | TYR | 2.6 |
| 1 | B | 182 | VAL | 2.6 |
| 1 | A | 118 | LYS | 2.6 |
| 1 | B | 11 | GLU | 2.6 |
| 1 | B | 322 | TYR | 2.6 |
| 1 | A | 657 | ASP | 2.5 |
| 1 | B | 313 | ILE | 2.5 |
| 1 | A | 361 | LYS | 2.5 |
| 1 | A | 465 | ASP | 2.5 |
| 1 | B | 355 | LYS | 2.5 |
| 1 | B | 120 | ASP | 2.5 |
| 1 | B | 241 | LEU | 2.5 |
| 1 | B | 176 | ASP | 2.5 |
| 1 | A | 707 | LYS | 2.5 |
| 1 | B | 230 | MET | 2.4 |
| 1 | B | 303 | GLN | 2.4 |
| 1 | B | 24 | THR | 2.4 |
| 1 | A | 307 | ASN | 2.4 |
| 1 | B | 163 | PHE | 2.4 |
| 1 | B | 85 | ILE | 2.4 |
| 1 | B | 312 | ASN | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 89 | MET | 2.4 |
| 1 | B | 340 | TYR | 2.4 |
| 1 | B | 112 | THR | 2.4 |
| 1 | B | 314 | GLU | 2.3 |
| 1 | B | 40 | LEU | 2.3 |
| 1 | B | 235 | LEU | 2.3 |
| 1 | A | 658 | LYS | 2.3 |
| 1 | B | 474 | ASP | 2.3 |
| 1 | B | 117 | GLY | 2.3 |
| 1 | B | 302 | PRO | 2.3 |
| 1 | B | 321 | VAL | 2.3 |
| 1 | B | 236 | SER | 2.3 |
| 1 | A | 159 | TYR | 2.2 |
| 1 | B | 217 | PHE | 2.2 |
| 1 | B | 466 | ILE | 2.2 |
| 1 | B | 97 | TYR | 2.2 |
| 1 | A | 362 | GLU | 2.2 |
| 1 | B | 308 | ASN | 2.2 |
| 1 | B | 242 | GLU | 2.1 |
| 1 | B | 360 | MET | 2.1 |
| 1 | B | 356 | TYR | 2.0 |
| 1 | B | 463 | TRP | 2.0 |

## 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 monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | GOL | B | 802 | 6/6 | 0.83 | 0.26 | 32,39,43,45 | 0 |

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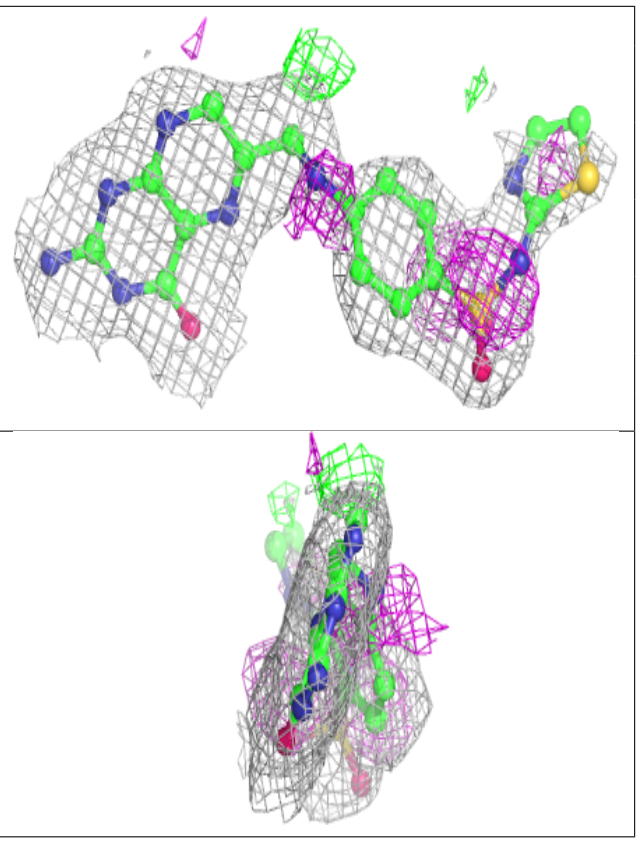
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | GOL | A | 803 | 6/6 | 0.86 | 0.21 | 28,30,35,36 | 0 |
| 2 | XTZ | A | 801 | 29/29 | 0.89 | 0.25 | 14,36,100,104 | 0 |
| 6 | MG | B | 806 | 1/1 | 0.89 | 0.20 | 74,74,74,74 | 0 |
| 7 | CA | B | 803 | 1/1 | 0.89 | 0.15 | 83,83,83,83 | 0 |
| 6 | MG | A | 805 | 1/1 | 0.91 | 0.13 | 15,15,15,15 | 0 |
| 8 | ACT | A | 808 | 4/4 | 0.91 | 0.20 | 60,60,60,61 | 0 |
| 5 | ATP | A | 804 | 31/31 | 0.92 | 0.15 | 31,52,86,88 | 0 |
| 2 | XTZ | B | 801 | 29/29 | 0.93 | 0.19 | 13,25,48,50 | 0 |
| 8 | ACT | A | 807 | 4/4 | 0.95 | 0.21 | 26,26,26,27 | 0 |
| 8 | ACT | B | 805 | 4/4 | 0.95 | 0.21 | 37,37,38,38 | 0 |
| 6 | MG | A | 809 | 1/1 | 0.96 | 0.10 | 55,55,55,55 | 0 |
| 3 | PH2 | A | 802 | 14/14 | 0.96 | 0.12 | 31,34,35,36 | 0 |
| 8 | ACT | B | 804 | 4/4 | 0.97 | 0.13 | 14,14,14,15 | 0 |
| 7 | CA | A | 806 | 1/1 | 0.98 | 0.10 | 19,19,19,19 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

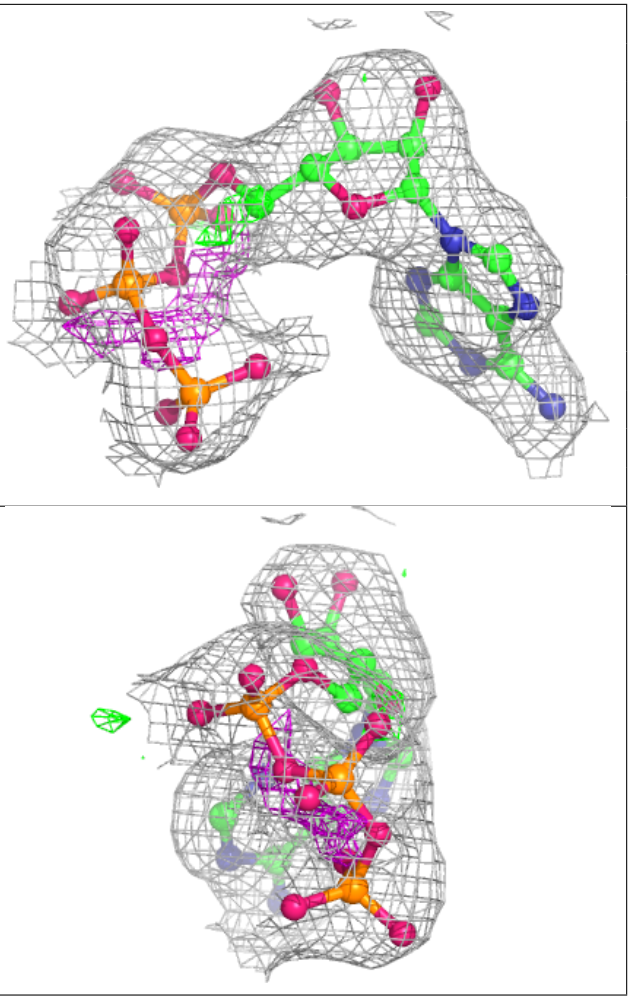
**Electron density around XTZ A 801:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



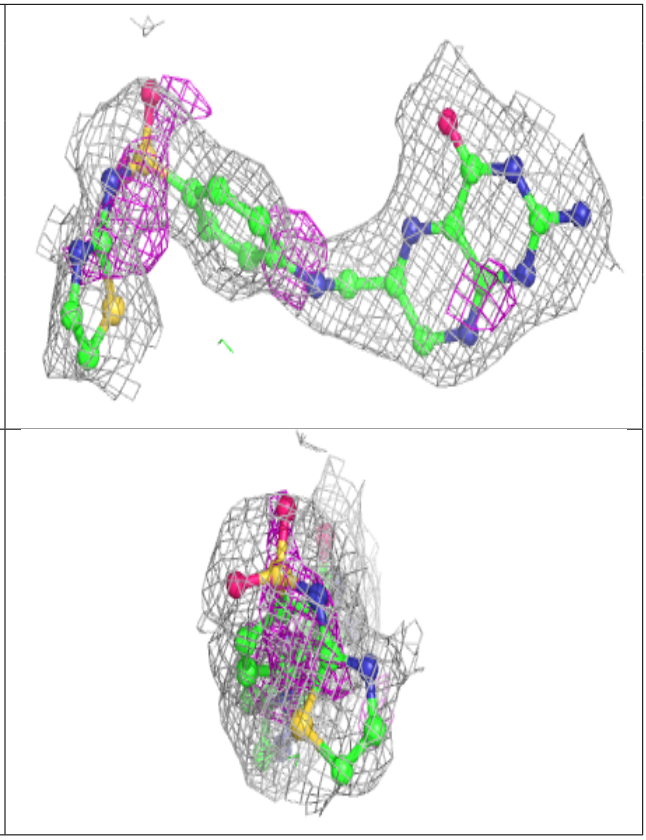
**Electron density around ATP A 804:**

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



**Electron density around XTZ B 801:**

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



## 6.5 Other polymers (i)

There are no such residues in this entry.