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

Feb 28, 2024 – 10:48 PM EST

| | | |
|---|---|---|
| PDB ID | : | 5S51 |
| Title | : | Tubulin-Z1251207602-complex |
| Authors | : | Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O. |
| Deposited on | : | 2020-11-08 |
| Resolution | : | 2.40 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:

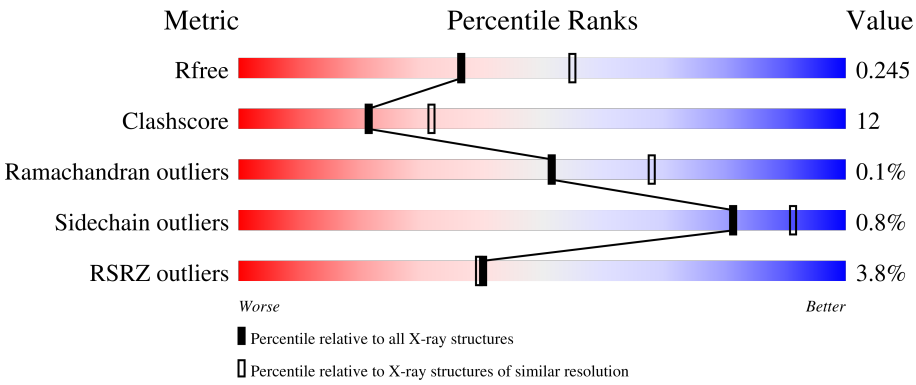
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 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 2.40 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 | 3907 (2.40-2.40) |
| Clashscore | 141614 | 4398 (2.40-2.40) |
| Ramachandran outliers | 138981 | 4318 (2.40-2.40) |
| Sidechain outliers | 138945 | 4319 (2.40-2.40) |
| RSRZ outliers | 127900 | 3811 (2.40-2.40) |

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 | 451 | 2%, 72%, 25%, • |
| 1 | C | 451 | 2%, 75%, 22%, • |
| 2 | B | 445 | %, 70%, 25%, • |
| 2 | D | 445 | 4%, 69%, 28%, • |
| 3 | E | 143 | 7%, 66%, 20%, 14% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | F | 384 | 8% 67% 25% 8% |

# 2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17944 atoms, of which 26 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 Tubulin alpha-1B chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 438 | 3424 | 2167 | 582 | 653 | 22 | 0 | 0 | 0 |
| 1 | C | 440 | 3443 | 2178 | 585 | 657 | 23 | 0 | 1 | 0 |

- Molecule 2 is a protein called Tubulin beta-2B chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 425 | 3359 | 2109 | 577 | 646 | 27 | 13 | 1 | 0 |
| 2 | D | 431 | 3368 | 2113 | 575 | 653 | 27 | 6 | 0 | 0 |

- Molecule 3 is a protein called Stathmin-4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | E | 123 | 1014 | 625 | 183 | 201 | 5 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 3 | MET | - | initiating methionine | UNP P63043 |
| E | 4 | ALA | - | expression tag | UNP P63043 |

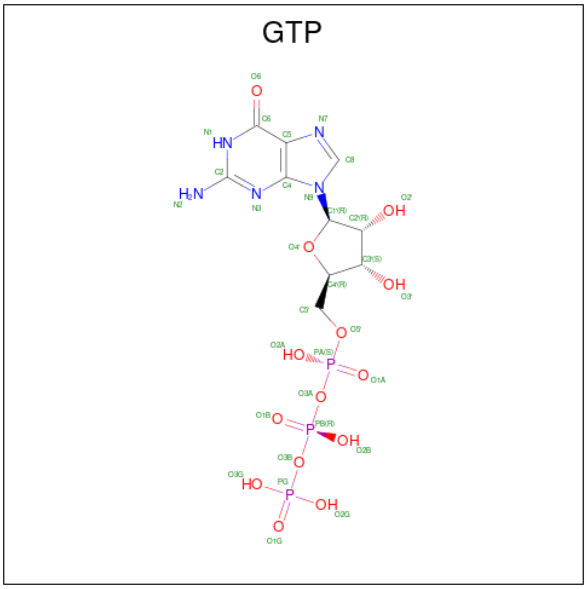
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | F | 352 | 2877 | 1843 | 495 | 525 | 14 | 0 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 379 | HIS | - | expression tag | UNP E1BQ43 |
| F | 380 | HIS | - | expression tag | UNP E1BQ43 |
| F | 381 | HIS | - | expression tag | UNP E1BQ43 |
| F | 382 | HIS | - | expression tag | UNP E1BQ43 |
| F | 383 | HIS | - | expression tag | UNP E1BQ43 |
| F | 384 | HIS | - | expression tag | UNP E1BQ43 |

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | A | 1 | 32 | 10 | 5 | 14 | 3 | 0 | 0 |
| | | | Total | C | N | O | P | | |
| 5 | C | 1 | 32 | 10 | 5 | 14 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 6 | A | 1 | 1 | 1 | 0 | 0 |
| | | | Total | Mg | | |
| 6 | B | 1 | 1 | 1 | 0 | 0 |
| | | | Total | Mg | | |
| 6 | C | 1 | 1 | 1 | 0 | 0 |
| | | | Total | Mg | | |
| 6 | D | 1 | 1 | 1 | 0 | 0 |

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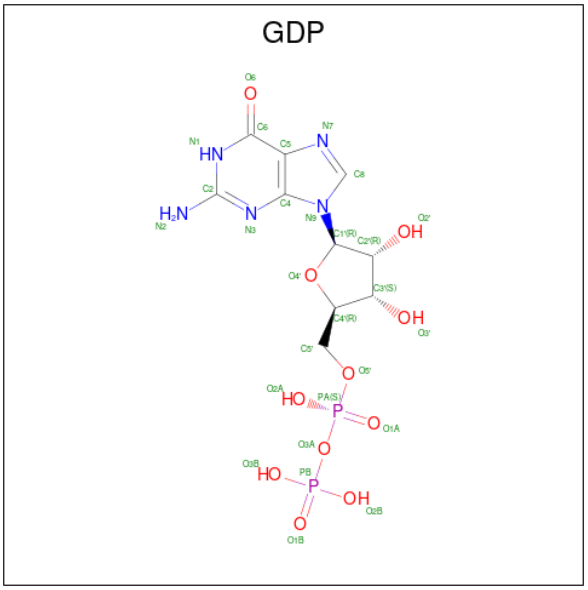
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 6 | F | 1 | 1 | 1 | 0 | 0 |

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

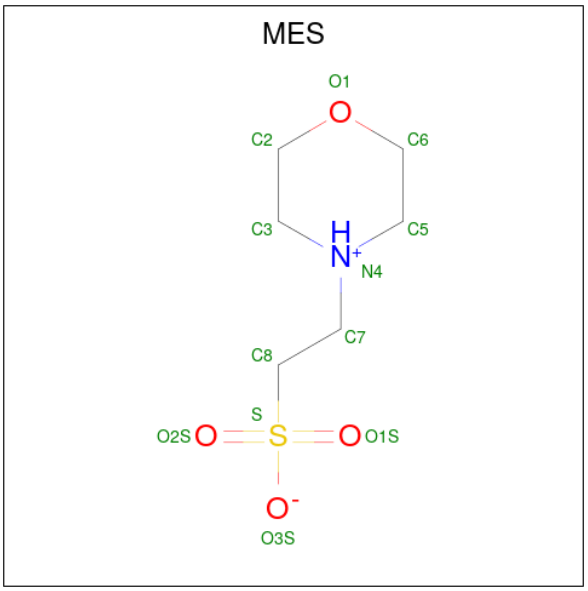
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Ca | | |
| 7 | A | 2 | 2 | 2 | 0 | 0 |
| | | | Total | Ca | | |
| 7 | B | 1 | 1 | 1 | 0 | 0 |
| | | | Total | Ca | | |
| 7 | C | 1 | 1 | 1 | 0 | 0 |

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



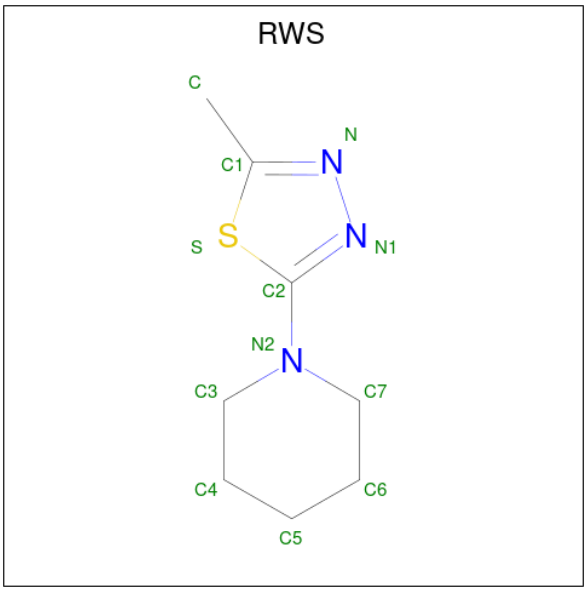

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 8 | B | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |
| | | | Total | C | N | O | P | | |
| 8 | D | 1 | 28 | 10 | 5 | 11 | 2 | 0 | 0 |

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



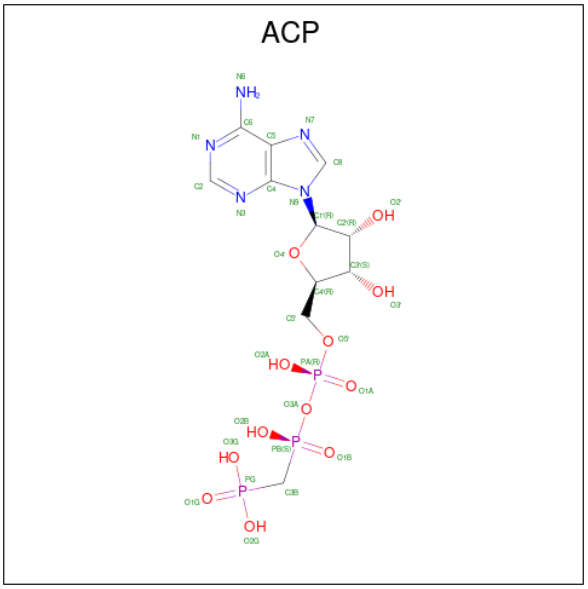

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | B | 1 | 12 | 6 | 1 | 4 | 1 | 0 | 0 |

- Molecule 10 is 1-(5-methyl-1,3,4-thiadiazol-2-yl)piperidine (three-letter code: RWS) (formula: $C_8H_{13}N_3S$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | S | | |
| 10 | B | 1 | 25 | 8 | 13 | 3 | 1 | 0 | 0 |
| | | | Total | C | H | N | S | | |
| 10 | B | 1 | 25 | 8 | 13 | 3 | 1 | 0 | 0 |

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 11 | F | 1 | 31 | 11 | 5 | 12 | 3 | 0 | 0 |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 12 | A | 42 | 42 | 42 | 0 | 0 |
| 12 | B | 43 | 43 | 43 | 0 | 0 |
| 12 | C | 120 | 120 | 120 | 0 | 0 |
| 12 | D | 22 | 22 | 22 | 0 | 0 |
| 12 | E | 6 | 6 | 6 | 0 | 0 |
| 12 | F | 4 | 4 | 4 | 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: Tubulin alpha-1B chain

Chain A: 2% 72% 25%

M1 R2 E3 A12 W21 M36 D39 H61 V62 P63 D69 L70 E71 P72 T73 D76 R79 L86 F87 H88 P89 E90 Q91 L92 I93 T94 D98 N101 N102 Y103 L119 D120 R121 C129 Q133 G134 S140 F141 G142 S147 G148 S151

R156 Y161 K164 S165 K166 S170 I171 Y172 P175 T179 A180 E183 S187 I188 T193 E196 H197 D205 I209 Y210 D211 R214 I219 E220 R221 P222 N226 L227 L230 I231 S232 Q233 I234 V235 I238 A247 Y262 I265 T271

P274 A278 Y282 H283 E284 Q285 L286 A289 N293 A294 C295 N300 K304 K311 C315 N329 A330 A331 I335 K336 R339 S340 I341 Q342 F343 V344 D345 W346 C347 P348 T349 G350 F351 Y357 D367 L368 A369 T381 T382 A383 L391 F395 K401

S419 E423 K430 D431 Y432 E433 E434 V435 G436 V437 D438 SER VAL GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU TYR

• Molecule 1: Tubulin alpha-1B chain

Chain C: 2% 75% 22%

M1 C4 I5 S6 I7 Q11 Q15 I16 W21 M36 S48 H61 V62 P63 R64 A65 V68 E71 I75 D76 T80 I93 T94 A100 N101 N102 Y103 Y108 K112 E113 I114 L117 V118 R121 L136 H139 S140 G148 F149 T150

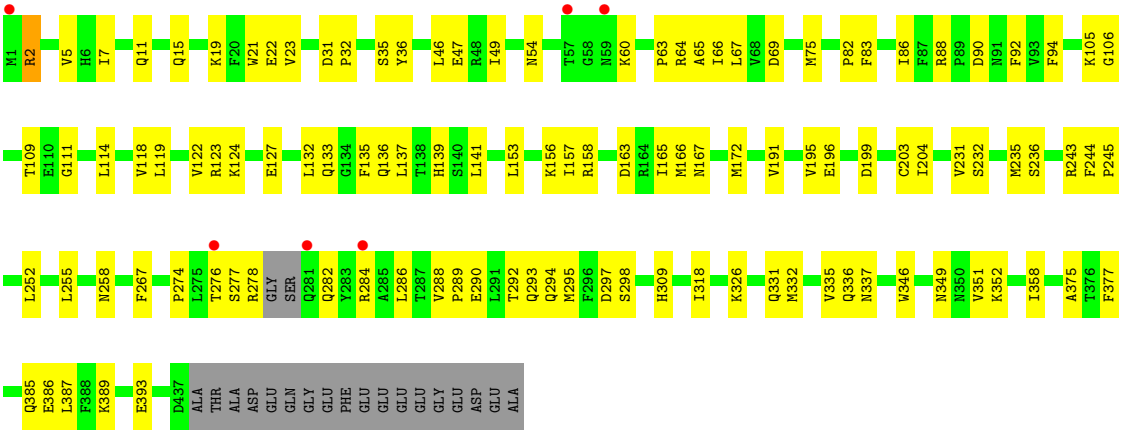
S151 L152 L153 K163 K164 S165 K166 L167 I171 Y172 P173 A174 V177 S178 T179 A180 S187 I188 H192 T193 T194 L195 E196 D199 C200 D205 N206 E207 A208 I209 Y210 R214 I219 E220 R221 P222 N226 L227 N228 R229 L230 I231 S232 Q233 I234 D245 N249

E254 F255 A270 T271 I276 A281 Y282 H283 L286 E290 I291 T292 E297 P298 A299 N300 Q301 M302 R308 Y312 C316 R320 D327 I335 I341 G350 F351 K352 N356 Y357 T361 D367 L368 L391 E414 E417 A421 M425

K430 E434 V440 GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU TYR

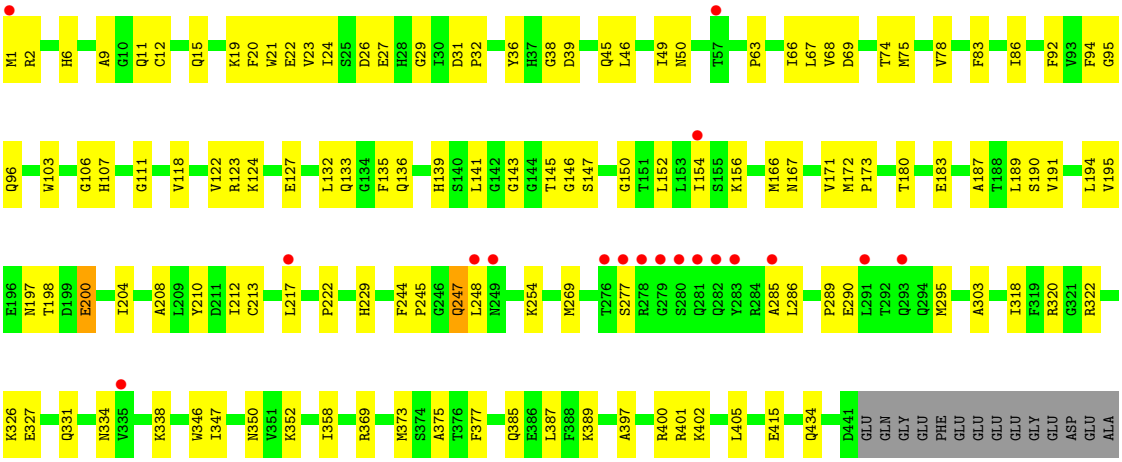
• Molecule 2: Tubulin beta-2B chain

Chain B: % 70% 25%



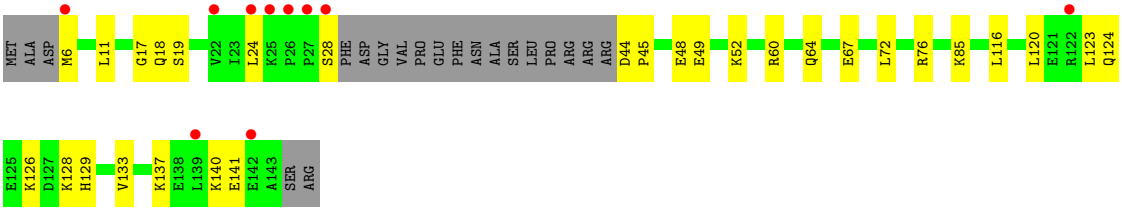

- Molecule 2: Tubulin beta-2B chain

Chain D:



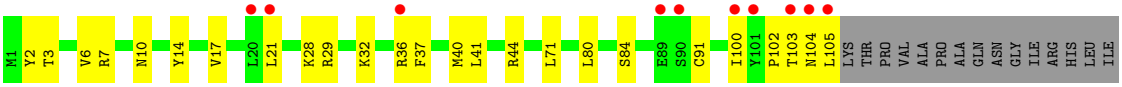

- Molecule 3: Stathmin-4

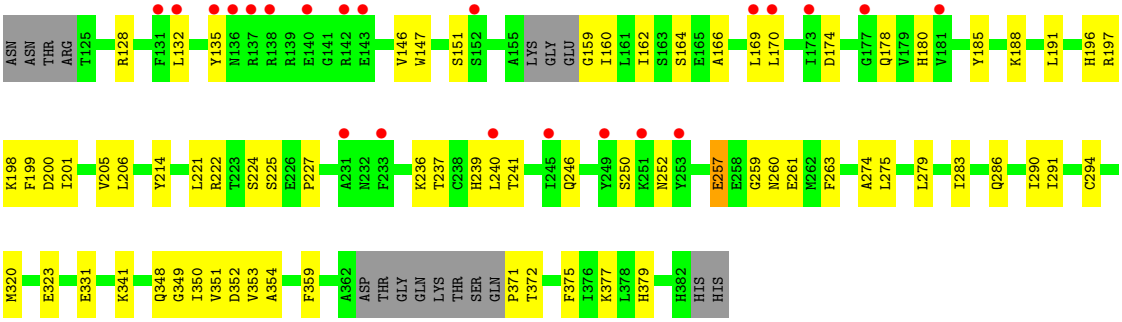
Chain E:




- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




ASN ASN THR ARG T125 R128 F131 L132 Y135 N136 R137 R138 R139 E140 G141 R142 E143 V146 W147 S151 S152 A155 LYS GLY GLU G159 I160 L161 I162 S163 S164 E165 A166 L169 L170 I173 D174 G177 Q178 V179 H180 V181 Y185 K188 L191 H196 R197
K198 F199 D200 I201 V205 L206 Y214 L221 R222 T223 S224 S225 E226 P227 A231 N232 F233 K236 T237 C238 H239 L240 T241 I245 Q246 Y249 S250 K251 N252 Y253 E257 E258 G259 N260 E261 M262 F263 A274 L275 L279 I283 Q286 I290 I291 C294
M320 E323 E331 K341 Q348 G349 I350 V351 D352 V353 A354 F359 A362 ASP THR GLY GLN LYS THR SER GLN P371 T372 F375 I376 K377 L378 H379 H382 HIS HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 104.42Å 157.45Å 179.36Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 78.73 – 2.40<br>118.33 – 2.40 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.8 (78.73-2.40)<br>99.9 (118.33-2.40) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.15 (at 2.40Å) | Xtriage |
| Refinement program | PHENIX 1.18.2_3874 | Depositor |
| R, $R_{free}$ | 0.203 , 0.245<br>0.203 , 0.245 | Depositor<br>DCC |
| $R_{free}$ test set | 5771 reflections (4.98%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 70.4 | Xtriage |
| Anisotropy | 0.202 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 58.9 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.51$, $< L^2 > = 0.34$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.96 | EDS |
| Total number of atoms | 17944 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 87.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: RWS, MES, MG, CA, GDP, GTP, ACP

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 | 0.25 | 0/3502 | 0.41 | 0/4754 |
| 1 | C | 0.26 | 0/3521 | 0.42 | 0/4780 |
| 2 | B | 0.26 | 0/3433 | 0.42 | 0/4647 |
| 2 | D | 0.25 | 0/3442 | 0.41 | 0/4664 |
| 3 | E | 0.24 | 0/1022 | 0.35 | 0/1356 |
| 4 | F | 0.24 | 0/2944 | 0.40 | 0/3978 |
| All | All | 0.25 | 0/17864 | 0.41 | 0/24179 |

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 | 3424 | 0 | 3334 | 87 | 0 |
| 1 | C | 3443 | 0 | 3352 | 66 | 0 |
| 2 | B | 3359 | 0 | 3235 | 89 | 0 |
| 2 | D | 3368 | 0 | 3236 | 92 | 0 |
| 3 | E | 1014 | 0 | 1029 | 24 | 0 |
| 4 | F | 2877 | 0 | 2839 | 71 | 0 |
| 5 | A | 32 | 0 | 12 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | C | 32 | 0 | 12 | 0 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 6 | C | 1 | 0 | 0 | 0 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 6 | F | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 2 | 0 | 0 | 0 | 0 |
| 7 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | C | 1 | 0 | 0 | 0 | 0 |
| 8 | B | 28 | 0 | 12 | 0 | 0 |
| 8 | D | 28 | 0 | 12 | 5 | 0 |
| 9 | B | 12 | 0 | 12 | 2 | 0 |
| 10 | B | 24 | 26 | 0 | 2 | 0 |
| 11 | F | 31 | 0 | 14 | 3 | 0 |
| 12 | A | 42 | 0 | 0 | 1 | 0 |
| 12 | B | 43 | 0 | 0 | 3 | 0 |
| 12 | C | 120 | 0 | 0 | 5 | 0 |
| 12 | D | 22 | 0 | 0 | 2 | 0 |
| 12 | E | 6 | 0 | 0 | 1 | 0 |
| 12 | F | 4 | 0 | 0 | 1 | 0 |
| All | All | 17918 | 26 | 17099 | 415 | 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 12.

All (415) 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) |
|---|---|---|---|
| 4:F:102:PRO:HG2 | 4:F:105:LEU:HD13 | 1.52 | 0.91 |
| 2:B:2:ARG:HB2 | 2:B:133:GLN:HG3 | 1.53 | 0.88 |
| 1:C:209:ILE:HD11 | 1:C:302:MET:HE3 | 1.56 | 0.87 |
| 1:A:71:GLU:OE2 | 1:A:73:THR:OG1 | 1.94 | 0.86 |
| 1:C:93:ILE:HD11 | 1:C:121:ARG:HG3 | 1.58 | 0.86 |
| 2:D:334:ASN:HD21 | 2:D:338:LYS:HE3 | 1.43 | 0.81 |
| 2:D:217:LEU:HA | 2:D:277:SER:HB3 | 1.63 | 0.81 |
| 2:D:397:ALA:O | 2:D:401:ARG:NH1 | 2.13 | 0.80 |
| 1:A:336:LYS:HG3 | 3:E:24:LEU:HD13 | 1.65 | 0.79 |
| 1:A:336:LYS:HD2 | 1:A:341:ILE:HD12 | 1.65 | 0.77 |
| 4:F:128:ARG:NH2 | 4:F:174:ASP:OD1 | 2.18 | 0.76 |
| 2:D:295:MET:HE2 | 2:D:377:PHE:HB2 | 1.67 | 0.76 |
| 4:F:241:THR:OG1 | 11:F:401:ACP:O3' | 1.99 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:274:PRO:HB3 | 2:B:286:LEU:HD22 | 1.69 | 0.74 |
| 1:A:175:PRO:HA | 1:A:179:THR:HG21 | 1.69 | 0.74 |
| 1:C:76:ASP:O | 1:C:80:THR:HG22 | 1.88 | 0.72 |
| 4:F:147:TRP:HB2 | 4:F:169:LEU:HD11 | 1.71 | 0.72 |
| 1:A:71:GLU:HG2 | 1:A:72:PRO:HD2 | 1.72 | 0.72 |
| 2:D:83:PHE:O | 2:D:86:ILE:HG22 | 1.90 | 0.71 |
| 4:F:102:PRO:HG2 | 4:F:105:LEU:CD1 | 2.21 | 0.71 |
| 4:F:10:ASN:HB2 | 4:F:44:ARG:HH22 | 1.55 | 0.71 |
| 2:D:136:GLN:HA | 2:D:167:ASN:O | 1.91 | 0.70 |
| 1:C:270:ALA:O | 1:C:302:MET:HG2 | 1.91 | 0.69 |
| 2:D:397:ALA:HA | 2:D:400:ARG:NH1 | 2.07 | 0.69 |
| 1:C:327:ASP:OD2 | 12:C:601:HOH:O | 2.09 | 0.69 |
| 2:B:2:ARG:HB2 | 2:B:133:GLN:CG | 2.22 | 0.68 |
| 1:C:4[A]:CYS:SG | 1:C:136:LEU:HG | 2.34 | 0.68 |
| 2:B:69:ASP:O | 2:B:94:PHE:HA | 1.95 | 0.67 |
| 1:A:210:TYR:CE1 | 1:A:222:PRO:HD2 | 2.30 | 0.67 |
| 2:D:434:GLN:OE1 | 12:D:601:HOH:O | 2.11 | 0.67 |
| 1:C:320:ARG:HA | 1:C:356:ASN:O | 1.94 | 0.67 |
| 1:A:175:PRO:HA | 1:A:179:THR:CG2 | 2.26 | 0.66 |
| 4:F:205:VAL:HG21 | 4:F:291:ILE:HD13 | 1.77 | 0.66 |
| 2:B:389:LYS:O | 2:B:393:GLU:HG3 | 1.95 | 0.66 |
| 2:B:11:GLN:OE1 | 12:B:601:HOH:O | 2.13 | 0.66 |
| 4:F:348:GLN:NE2 | 4:F:352:ASP:OD1 | 2.28 | 0.65 |
| 1:A:271:THR:HG21 | 1:A:295:CYS:HA | 1.78 | 0.65 |
| 1:A:101:ASN:HD22 | 2:B:258:ASN:HD21 | 1.44 | 0.65 |
| 8:D:501:GDP:O1A | 12:D:602:HOH:O | 2.15 | 0.65 |
| 4:F:197:ARG:NH1 | 4:F:257:GLU:OE2 | 2.26 | 0.65 |
| 2:B:82:PRO:O | 12:B:602:HOH:O | 2.13 | 0.64 |
| 1:A:226:ASN:ND2 | 1:A:367:ASP:OD2 | 2.29 | 0.64 |
| 2:D:1:MET:CE | 2:D:50:ASN:HB2 | 2.27 | 0.64 |
| 4:F:371:PRO:HA | 4:F:372:THR:O | 1.98 | 0.64 |
| 2:D:2:ARG:HB3 | 2:D:133:GLN:HG2 | 1.79 | 0.64 |
| 4:F:236:LYS:HB3 | 4:F:240:LEU:HD13 | 1.78 | 0.64 |
| 2:B:274:PRO:HB3 | 2:B:286:LEU:CD2 | 2.28 | 0.64 |
| 2:D:194:LEU:HD22 | 2:D:198:THR:HG21 | 1.79 | 0.64 |
| 1:C:108:TYR:O | 1:C:112:LYS:HG2 | 1.98 | 0.63 |
| 2:D:67:LEU:HD22 | 2:D:92:PHE:CE2 | 2.33 | 0.63 |
| 4:F:91:CYS:HA | 12:F:504:HOH:O | 1.98 | 0.63 |
| 1:A:278:ALA:HA | 1:A:369:ALA:HB2 | 1.81 | 0.62 |
| 1:A:36:MET:HB3 | 1:A:61:HIS:CE1 | 2.34 | 0.62 |
| 1:C:174:ALA:HB1 | 1:C:207:GLU:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:371:PRO:HA | 4:F:372:THR:HB | 1.80 | 0.62 |
| 1:A:166:LYS:HE2 | 1:A:197:HIS:O | 1.99 | 0.62 |
| 2:B:35:SER:OG | 2:B:60:LYS:NZ | 2.18 | 0.62 |
| 1:A:187:SER:CB | 1:A:391:LEU:HD21 | 2.29 | 0.62 |
| 2:D:334:ASN:ND2 | 2:D:338:LYS:HE3 | 2.12 | 0.62 |
| 2:B:2:ARG:HB2 | 2:B:133:GLN:HE21 | 1.64 | 0.62 |
| 2:B:278:ARG:HG2 | 2:B:282:GLN:NE2 | 2.15 | 0.62 |
| 1:C:414:GLU:OE2 | 12:C:602:HOH:O | 2.16 | 0.62 |
| 1:A:351:PHE:HE1 | 3:E:24:LEU:HD11 | 1.63 | 0.62 |
| 1:C:234:ILE:HG12 | 1:C:302:MET:HE2 | 1.82 | 0.61 |
| 1:C:254:GLU:HG2 | 1:C:352:LYS:HE2 | 1.83 | 0.61 |
| 1:C:220:GLU:HB3 | 2:D:326:LYS:HD2 | 1.82 | 0.61 |
| 2:D:69:ASP:O | 2:D:94:PHE:HA | 2.01 | 0.61 |
| 2:B:141:LEU:HD12 | 2:B:172:MET:SD | 2.41 | 0.61 |
| 1:C:187:SER:HB3 | 1:C:391:LEU:HD21 | 1.82 | 0.61 |
| 2:D:248:LEU:HD21 | 2:D:352:LYS:HB3 | 1.81 | 0.61 |
| 4:F:132:LEU:HD21 | 4:F:170:LEU:HD11 | 1.81 | 0.61 |
| 1:A:88:HIS:HB2 | 1:A:89:PRO:HD2 | 1.83 | 0.61 |
| 1:A:180:ALA:HB1 | 2:B:258:ASN:OD1 | 2.01 | 0.60 |
| 1:A:293:ASN:OD1 | 1:A:339:ARG:NH2 | 2.25 | 0.60 |
| 2:B:67:LEU:HD22 | 2:B:92:PHE:CE2 | 2.36 | 0.60 |
| 2:B:83:PHE:O | 2:B:86:ILE:HG22 | 2.00 | 0.60 |
| 2:D:46:LEU:HA | 2:D:49:ILE:HB | 1.82 | 0.60 |
| 2:D:347:ILE:HG22 | 2:D:350:ASN:HB3 | 1.82 | 0.60 |
| 3:E:120:LEU:O | 3:E:124:GLN:HG3 | 2.01 | 0.60 |
| 4:F:371:PRO:CA | 4:F:372:THR:HB | 2.31 | 0.60 |
| 4:F:146:VAL:HG22 | 4:F:164:SER:HB3 | 1.83 | 0.60 |
| 4:F:147:TRP:HB2 | 4:F:169:LEU:CD1 | 2.31 | 0.60 |
| 2:D:2:ARG:HB3 | 2:D:133:GLN:CG | 2.31 | 0.60 |
| 1:C:117:LEU:HD11 | 1:C:121:ARG:NH2 | 2.17 | 0.60 |
| 2:B:123:ARG:O | 2:B:127:GLU:HG3 | 2.01 | 0.60 |
| 1:C:286:LEU:HA | 1:C:290:GLU:OE1 | 2.02 | 0.60 |
| 2:D:143:GLY:O | 2:D:147:SER:OG | 2.20 | 0.59 |
| 1:C:226:ASN:ND2 | 1:C:367:ASP:OD2 | 2.35 | 0.59 |
| 2:D:154:ILE:HG23 | 2:D:166:MET:HG2 | 1.84 | 0.59 |
| 2:D:208:ALA:O | 2:D:212:ILE:HG13 | 2.03 | 0.59 |
| 4:F:178:GLN:N | 4:F:178:GLN:OE1 | 2.36 | 0.59 |
| 4:F:331:GLU:OE2 | 11:F:401:ACP:O3G | 2.21 | 0.59 |
| 4:F:188:LYS:HD3 | 4:F:323:GLU:OE2 | 2.03 | 0.59 |
| 1:A:247:ALA:N | 12:A:603:HOH:O | 2.35 | 0.58 |
| 1:C:188:ILE:HG13 | 1:C:425:MET:HG3 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:295:MET:SD | 2:B:375:ALA:HB1 | 2.44 | 0.58 |
| 3:E:60:ARG:O | 3:E:64:GLN:HG3 | 2.04 | 0.58 |
| 2:B:284:ARG:NH2 | 2:B:290:GLU:OE2 | 2.37 | 0.58 |
| 1:A:187:SER:HB3 | 1:A:391:LEU:HD21 | 1.85 | 0.57 |
| 2:B:21:TRP:CZ3 | 2:B:63:PRO:HB3 | 2.39 | 0.57 |
| 2:B:119:LEU:HD11 | 2:B:156:LYS:HB3 | 1.86 | 0.57 |
| 1:A:71:GLU:HG2 | 1:A:72:PRO:CD | 2.35 | 0.57 |
| 2:B:258:ASN:HB3 | 10:B:506:RWS:C3 | 2.34 | 0.57 |
| 2:D:167:ASN:OD1 | 2:D:200:GLU:HG3 | 2.05 | 0.57 |
| 1:A:142:GLY:CA | 1:A:183:GLU:HG2 | 2.35 | 0.57 |
| 2:B:292:THR:HG22 | 2:B:335:VAL:HG21 | 1.87 | 0.57 |
| 1:C:214:ARG:HG2 | 1:C:219:ILE:O | 2.04 | 0.56 |
| 4:F:200:ASP:OD1 | 4:F:222:ARG:HB2 | 2.04 | 0.56 |
| 1:C:233:GLN:HG3 | 1:C:368:LEU:CD1 | 2.35 | 0.56 |
| 1:C:100:ALA:HA | 2:D:254:LYS:HG3 | 1.88 | 0.56 |
| 2:B:133:GLN:OE1 | 2:B:252:LEU:HG | 2.05 | 0.56 |
| 3:E:48:GLU:HG2 | 3:E:52:LYS:HE3 | 1.87 | 0.56 |
| 4:F:263:PHE:CZ | 4:F:341:LYS:HE2 | 2.39 | 0.56 |
| 1:A:142:GLY:HA3 | 1:A:183:GLU:HG2 | 1.86 | 0.56 |
| 2:B:295:MET:CG | 2:B:377:PHE:HB2 | 2.35 | 0.56 |
| 12:B:625:HOH:O | 1:C:163:LYS:HD2 | 2.05 | 0.56 |
| 1:A:172:TYR:HB3 | 1:A:205:ASP:HA | 1.87 | 0.56 |
| 1:C:93:ILE:HG22 | 1:C:114:ILE:HD11 | 1.87 | 0.55 |
| 2:B:172:MET:HG3 | 2:B:387:LEU:HD11 | 1.88 | 0.55 |
| 2:D:152:LEU:O | 2:D:156:LYS:HG2 | 2.06 | 0.55 |
| 1:C:249:ASN:OD1 | 1:C:356:ASN:ND2 | 2.34 | 0.55 |
| 1:C:36:MET:HB3 | 1:C:61:HIS:CE1 | 2.42 | 0.55 |
| 1:A:381:THR:HG22 | 1:A:383:ALA:H | 1.70 | 0.55 |
| 3:E:11:LEU:HD11 | 3:E:18:GLN:OE1 | 2.07 | 0.55 |
| 1:A:234:ILE:O | 1:A:238:ILE:HG13 | 2.07 | 0.55 |
| 2:D:141:LEU:HD12 | 2:D:172:MET:SD | 2.47 | 0.55 |
| 1:A:88:HIS:CD2 | 1:A:91:GLN:HG3 | 2.42 | 0.54 |
| 1:C:165:SER:HA | 1:C:199:ASP:OD2 | 2.07 | 0.54 |
| 2:B:136:GLN:HA | 2:B:167:ASN:O | 2.07 | 0.54 |
| 2:B:47:GLU:OE1 | 2:B:245:PRO:HG3 | 2.06 | 0.54 |
| 1:A:180:ALA:N | 1:A:183:GLU:OE1 | 2.33 | 0.54 |
| 4:F:198:LYS:HG2 | 4:F:199:PHE:H | 1.72 | 0.54 |
| 4:F:205:VAL:CG2 | 4:F:291:ILE:HD13 | 2.38 | 0.54 |
| 4:F:17:VAL:O | 4:F:21:LEU:HG | 2.08 | 0.54 |
| 2:D:295:MET:CE | 2:D:377:PHE:HB2 | 2.35 | 0.54 |
| 2:B:309:HIS:ND1 | 2:B:386:GLU:OE2 | 2.35 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:337:ASN:OD1 | 4:F:36:ARG:HD3 | 2.07 | 0.54 |
| 4:F:100:ILE:HD12 | 4:F:128:ARG:HA | 1.89 | 0.53 |
| 1:A:79:ARG:HG2 | 1:A:92:LEU:HD12 | 1.90 | 0.53 |
| 1:A:315:CYS:HG | 1:A:351:PHE:HD2 | 1.54 | 0.53 |
| 2:D:23:VAL:O | 2:D:27:GLU:HG3 | 2.09 | 0.53 |
| 2:D:191:VAL:O | 2:D:195:VAL:HG23 | 2.09 | 0.53 |
| 2:D:289:PRO:HG3 | 2:D:331:GLN:NE2 | 2.24 | 0.53 |
| 1:C:174:ALA:CB | 1:C:207:GLU:HB2 | 2.39 | 0.52 |
| 1:A:151:SER:HB2 | 1:A:193:THR:OG1 | 2.10 | 0.52 |
| 1:A:274:PRO:HB3 | 1:A:286:LEU:HD12 | 1.91 | 0.52 |
| 2:D:1:MET:HE2 | 2:D:50:ASN:HB2 | 1.90 | 0.52 |
| 1:A:343:PHE:CD1 | 1:A:349:THR:HG23 | 2.44 | 0.52 |
| 1:A:196:GLU:OE1 | 1:A:196:GLU:HA | 2.10 | 0.52 |
| 1:C:11:GLN:O | 1:C:15:GLN:HG3 | 2.10 | 0.52 |
| 1:A:209:ILE:HG23 | 1:A:230:LEU:HD23 | 1.92 | 0.52 |
| 1:C:103:TYR:CE2 | 1:C:148:GLY:HA2 | 2.45 | 0.52 |
| 4:F:135:TYR:CE1 | 4:F:166:ALA:HB2 | 2.45 | 0.51 |
| 4:F:371:PRO:HA | 4:F:372:THR:C | 2.29 | 0.51 |
| 2:B:118:VAL:HG11 | 2:B:153:LEU:HD11 | 1.91 | 0.51 |
| 2:D:19:LYS:O | 2:D:23:VAL:HG23 | 2.10 | 0.51 |
| 2:D:171:VAL:HA | 2:D:204:ILE:O | 2.11 | 0.51 |
| 4:F:10:ASN:CB | 4:F:44:ARG:HH22 | 2.22 | 0.51 |
| 4:F:259:GLY:O | 4:F:261:GLU:HG3 | 2.11 | 0.51 |
| 1:C:430:LYS:HE2 | 1:C:434:GLU:OE2 | 2.11 | 0.51 |
| 1:A:227:LEU:O | 1:A:231:ILE:HG13 | 2.11 | 0.51 |
| 3:E:128:LYS:O | 3:E:128:LYS:HD3 | 2.10 | 0.51 |
| 2:D:124:LYS:C | 2:D:124:LYS:HD3 | 2.30 | 0.51 |
| 2:D:213:CYS:HA | 2:D:217:LEU:HB2 | 1.93 | 0.51 |
| 2:D:402:LYS:HE2 | 2:D:415:GLU:OE1 | 2.11 | 0.51 |
| 2:D:141:LEU:HD22 | 2:D:190:SER:HB3 | 1.92 | 0.51 |
| 1:A:271:THR:CG2 | 1:A:295:CYS:HA | 2.41 | 0.51 |
| 1:A:329:ASN:HB3 | 3:E:6:MET:HE3 | 1.92 | 0.51 |
| 1:C:209:ILE:CD1 | 1:C:302:MET:HE3 | 2.36 | 0.51 |
| 1:A:214:ARG:HG2 | 1:A:219:ILE:O | 2.11 | 0.50 |
| 2:D:26:ASP:OD2 | 2:D:369:ARG:HD2 | 2.12 | 0.50 |
| 1:A:233:GLN:HG3 | 1:A:368:LEU:CD1 | 2.40 | 0.50 |
| 1:A:289:ALA:HA | 1:A:331:ALA:CB | 2.41 | 0.50 |
| 2:D:46:LEU:O | 2:D:49:ILE:HG22 | 2.12 | 0.50 |
| 1:A:2:ARG:HB2 | 1:A:133:GLN:HE21 | 1.77 | 0.50 |
| 2:B:276:THR:HG22 | 2:B:277:SER:O | 2.12 | 0.50 |
| 2:D:107:HIS:O | 2:D:152:LEU:HD22 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:201:ILE:HG12 | 4:F:221:LEU:HG | 1.94 | 0.50 |
| 1:C:151:SER:HB2 | 1:C:193:THR:CG2 | 2.41 | 0.50 |
| 1:A:336:LYS:HG3 | 3:E:24:LEU:CD1 | 2.40 | 0.50 |
| 2:B:191:VAL:O | 2:B:195:VAL:HG23 | 2.11 | 0.50 |
| 2:D:11:GLN:O | 2:D:15:GLN:HG2 | 2.11 | 0.50 |
| 2:B:46:LEU:HA | 2:B:49:ILE:HB | 1.94 | 0.49 |
| 2:D:244:PHE:CE1 | 2:D:358:ILE:HD12 | 2.47 | 0.49 |
| 2:B:199:ASP:OD1 | 9:B:504:MES:H62 | 2.12 | 0.49 |
| 2:B:318:ILE:N | 2:B:318:ILE:HD12 | 2.27 | 0.49 |
| 2:B:385:GLN:OE1 | 2:B:389:LYS:HE3 | 2.12 | 0.49 |
| 1:C:312:TYR:CE2 | 1:C:341:ILE:HG23 | 2.46 | 0.49 |
| 1:A:93:ILE:HD11 | 1:A:121:ARG:HG3 | 1.95 | 0.49 |
| 1:A:265:ILE:HG23 | 1:A:432:TYR:CE1 | 2.47 | 0.49 |
| 2:D:346:TRP:CE3 | 2:D:347:ILE:HG13 | 2.47 | 0.49 |
| 4:F:17:VAL:HG13 | 4:F:351:VAL:HG22 | 1.93 | 0.49 |
| 2:D:145:THR:HB | 8:D:501:GDP:O2B | 2.13 | 0.49 |
| 3:E:67:GLU:OE1 | 3:E:67:GLU:HA | 2.12 | 0.49 |
| 2:B:5:VAL:HG23 | 2:B:132:LEU:HD11 | 1.94 | 0.49 |
| 2:B:31:ASP:HB2 | 2:B:32:PRO:CD | 2.43 | 0.49 |
| 2:D:387:LEU:HD23 | 2:D:387:LEU:O | 2.12 | 0.49 |
| 2:D:106:GLY:O | 2:D:111:GLY:HA3 | 2.13 | 0.49 |
| 1:A:335:ILE:HG23 | 1:A:339:ARG:HG3 | 1.95 | 0.49 |
| 1:A:233:GLN:HG3 | 1:A:368:LEU:HD12 | 1.95 | 0.48 |
| 1:A:311:LYS:HA | 1:A:342:GLN:O | 2.13 | 0.48 |
| 3:E:129:HIS:O | 3:E:133:VAL:HG23 | 2.13 | 0.48 |
| 1:C:417:GLU:OE2 | 12:C:603:HOH:O | 2.20 | 0.48 |
| 2:D:103:TRP:CE3 | 2:D:189:LEU:HD13 | 2.48 | 0.48 |
| 1:C:297:GLU:HG3 | 1:C:299:ALA:H | 1.79 | 0.48 |
| 4:F:159:GLY:C | 4:F:160:ILE:HD12 | 2.34 | 0.48 |
| 4:F:191:LEU:HD12 | 4:F:196:HIS:CE1 | 2.48 | 0.48 |
| 1:C:234:ILE:HD12 | 1:C:234:ILE:H | 1.79 | 0.48 |
| 2:D:75:MET:HE3 | 2:D:92:PHE:HD2 | 1.79 | 0.48 |
| 2:D:141:LEU:HA | 2:D:147:SER:HB3 | 1.95 | 0.48 |
| 2:B:67:LEU:N | 2:B:67:LEU:HD12 | 2.29 | 0.48 |
| 2:B:75:MET:HE3 | 2:B:92:PHE:HD2 | 1.78 | 0.48 |
| 2:B:88:ARG:NH1 | 2:B:90:ASP:HB2 | 2.28 | 0.48 |
| 2:D:385:GLN:O | 2:D:389:LYS:HG3 | 2.13 | 0.48 |
| 1:A:134:GLY:HA3 | 1:A:165:SER:O | 2.13 | 0.48 |
| 1:A:289:ALA:HA | 1:A:331:ALA:HB1 | 1.95 | 0.48 |
| 1:A:336:LYS:NZ | 1:A:341:ILE:HB | 2.29 | 0.48 |
| 4:F:162:ILE:HD13 | 4:F:185:TYR:CE2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:119:LEU:HD12 | 1:A:156:ARG:NH2 | 2.29 | 0.48 |
| 1:A:335:ILE:HG23 | 1:A:339:ARG:CG | 2.44 | 0.48 |
| 1:C:21:TRP:CZ3 | 1:C:63:PRO:HB3 | 2.49 | 0.48 |
| 1:C:227:LEU:O | 1:C:231:ILE:HG13 | 2.14 | 0.48 |
| 3:E:48:GLU:CG | 3:E:52:LYS:HE3 | 2.43 | 0.48 |
| 1:A:119:LEU:HD11 | 1:A:156:ARG:HB3 | 1.96 | 0.48 |
| 1:C:48:SER:OG | 1:C:245:ASP:HB2 | 2.13 | 0.48 |
| 2:D:12:CYS:HB2 | 8:D:501:GDP:C8 | 2.49 | 0.48 |
| 2:D:21:TRP:CZ3 | 2:D:63:PRO:HB3 | 2.49 | 0.48 |
| 2:B:332:MET:O | 2:B:336:GLN:HG3 | 2.14 | 0.47 |
| 3:E:44:ASP:HB3 | 3:E:45:PRO:HD2 | 1.95 | 0.47 |
| 2:D:132:LEU:HD21 | 2:D:135:PHE:CZ | 2.49 | 0.47 |
| 2:B:46:LEU:O | 2:B:49:ILE:HG22 | 2.15 | 0.47 |
| 1:C:292:THR:HG22 | 1:C:335:ILE:HD12 | 1.96 | 0.47 |
| 4:F:7:ARG:NH1 | 4:F:32:LYS:O | 2.48 | 0.47 |
| 4:F:102:PRO:HB2 | 4:F:104:ASN:OD1 | 2.14 | 0.47 |
| 1:A:21:TRP:CZ3 | 1:A:63:PRO:HB3 | 2.49 | 0.47 |
| 1:A:329:ASN:HB3 | 3:E:6:MET:CE | 2.44 | 0.47 |
| 2:D:269:MET:HG3 | 2:D:303:ALA:HB3 | 1.95 | 0.47 |
| 4:F:274:ALA:HB3 | 4:F:275:LEU:HD22 | 1.95 | 0.47 |
| 1:A:419:SER:O | 1:A:423:GLU:HG3 | 2.14 | 0.47 |
| 2:B:15:GLN:O | 2:B:19:LYS:HG2 | 2.15 | 0.47 |
| 2:B:31:ASP:HB2 | 2:B:32:PRO:HD2 | 1.96 | 0.47 |
| 1:A:98:ASP:HB2 | 5:A:501:GTP:O2G | 2.15 | 0.47 |
| 2:D:95:GLY:O | 2:D:96:GLN:NE2 | 2.48 | 0.47 |
| 3:E:85:LYS:NZ | 12:E:202:HOH:O | 2.48 | 0.47 |
| 4:F:246:GLN:O | 4:F:250:SER:HB3 | 2.15 | 0.47 |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:HG13 | 1.97 | 0.47 |
| 2:B:278:ARG:HG2 | 2:B:282:GLN:CD | 2.36 | 0.47 |
| 1:C:11:GLN:HE22 | 2:D:247:GLN:NE2 | 2.13 | 0.47 |
| 2:D:74:THR:O | 2:D:78:VAL:HG23 | 2.15 | 0.47 |
| 2:B:75:MET:HE3 | 2:B:92:PHE:CD2 | 2.50 | 0.47 |
| 1:A:231:ILE:O | 1:A:235:VAL:HG23 | 2.15 | 0.46 |
| 1:C:187:SER:CB | 1:C:391:LEU:HD21 | 2.45 | 0.46 |
| 2:B:22:GLU:HG3 | 2:B:83:PHE:CE1 | 2.50 | 0.46 |
| 2:B:36:TYR:CD1 | 2:B:46:LEU:HD21 | 2.49 | 0.46 |
| 1:C:139:HIS:CD2 | 1:C:150:THR:HG21 | 2.50 | 0.46 |
| 4:F:100:ILE:CD1 | 4:F:128:ARG:HA | 2.45 | 0.46 |
| 1:A:234:ILE:HD12 | 1:A:234:ILE:N | 2.31 | 0.46 |
| 2:B:75:MET:HE1 | 2:B:94:PHE:HD1 | 1.81 | 0.46 |
| 2:D:6:HIS:CD2 | 2:D:21:TRP:HE1 | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:180:THR:O | 2:D:183:GLU:HG3 | 2.16 | 0.46 |
| 2:D:286:LEU:HD12 | 2:D:290:GLU:OE1 | 2.15 | 0.46 |
| 4:F:103:THR:HG23 | 4:F:128:ARG:NH2 | 2.31 | 0.46 |
| 1:A:431:ASP:O | 1:A:435:VAL:HG23 | 2.16 | 0.46 |
| 2:B:236:SER:O | 2:B:243:ARG:NH2 | 2.49 | 0.46 |
| 2:D:67:LEU:N | 2:D:67:LEU:HD12 | 2.30 | 0.46 |
| 2:B:23:VAL:HG21 | 2:B:232:SER:HB3 | 1.98 | 0.46 |
| 2:B:124:LYS:HD3 | 2:B:124:LYS:C | 2.36 | 0.46 |
| 2:B:331:GLN:O | 2:B:335:VAL:HG23 | 2.15 | 0.46 |
| 2:D:9:ALA:HA | 2:D:68:VAL:O | 2.16 | 0.46 |
| 4:F:237:THR:HG21 | 4:F:250:SER:HA | 1.98 | 0.46 |
| 1:C:75:ILE:HD12 | 1:C:94:THR:HG22 | 1.97 | 0.46 |
| 4:F:198:LYS:O | 4:F:199:PHE:HB3 | 2.14 | 0.46 |
| 1:A:346:TRP:HZ2 | 1:A:435:VAL:HG13 | 1.81 | 0.45 |
| 4:F:286:GLN:O | 4:F:290:ILE:HG13 | 2.17 | 0.45 |
| 1:C:276:ILE:HD13 | 1:C:281:ALA:HB2 | 1.98 | 0.45 |
| 2:B:21:TRP:CE3 | 2:B:63:PRO:HB3 | 2.52 | 0.45 |
| 2:B:244:PHE:CD1 | 2:B:358:ILE:HD12 | 2.51 | 0.45 |
| 1:C:172:TYR:HB3 | 1:C:205:ASP:HA | 1.98 | 0.45 |
| 2:D:387:LEU:HD23 | 2:D:387:LEU:C | 2.36 | 0.45 |
| 1:A:188:ILE:HD12 | 1:A:395:PHE:CD2 | 2.52 | 0.45 |
| 2:B:289:PRO:O | 2:B:293:GLN:HG3 | 2.15 | 0.45 |
| 2:D:146:GLY:O | 2:D:150:GLY:HA3 | 2.16 | 0.45 |
| 1:A:220:GLU:OE1 | 2:B:326:LYS:HD2 | 2.17 | 0.45 |
| 2:B:132:LEU:HD21 | 2:B:135:PHE:CZ | 2.52 | 0.45 |
| 1:C:7:ILE:HG21 | 1:C:153:LEU:HD21 | 1.98 | 0.45 |
| 4:F:2:TYR:CE1 | 4:F:359:PHE:HB3 | 2.51 | 0.45 |
| 1:C:192:HIS:CG | 1:C:421:ALA:HA | 2.52 | 0.45 |
| 2:D:327:GLU:O | 2:D:331:GLN:HG2 | 2.15 | 0.45 |
| 2:B:114:LEU:O | 2:B:114:LEU:HG | 2.16 | 0.45 |
| 2:D:20:PHE:CZ | 2:D:24:ILE:HD13 | 2.52 | 0.45 |
| 4:F:71:LEU:HD11 | 4:F:294:CYS:HB3 | 1.99 | 0.45 |
| 2:B:2:ARG:CB | 2:B:133:GLN:HE21 | 2.30 | 0.45 |
| 2:B:231:VAL:O | 2:B:235:MET:HG3 | 2.17 | 0.45 |
| 1:C:210:TYR:CZ | 1:C:222:PRO:HD2 | 2.52 | 0.45 |
| 4:F:246:GLN:HB3 | 4:F:260:ASN:ND2 | 2.32 | 0.45 |
| 1:A:401:LYS:HG3 | 2:B:346:TRP:CE3 | 2.52 | 0.44 |
| 2:D:385:GLN:OE1 | 2:D:389:LYS:NZ | 2.40 | 0.44 |
| 4:F:237:THR:O | 4:F:246:GLN:NE2 | 2.48 | 0.44 |
| 1:A:161:TYR:HB3 | 1:A:164:LYS:HD3 | 1.99 | 0.44 |
| 2:B:2:ARG:HB2 | 2:B:133:GLN:NE2 | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:101:ASN:ND2 | 1:C:180:ALA:HB2 | 2.32 | 0.44 |
| 4:F:80:LEU:O | 4:F:84:SER:OG | 2.20 | 0.44 |
| 1:A:141:PHE:O | 1:A:147:SER:HB3 | 2.18 | 0.44 |
| 1:C:292:THR:HG22 | 1:C:335:ILE:CD1 | 2.48 | 0.44 |
| 1:C:271:THR:HG23 | 1:C:300:ASN:O | 2.17 | 0.44 |
| 4:F:14:TYR:HB3 | 4:F:41:LEU:HD13 | 2.00 | 0.44 |
| 1:C:196:GLU:HG2 | 12:C:646:HOH:O | 2.17 | 0.44 |
| 4:F:196:HIS:O | 4:F:227:PRO:HA | 2.17 | 0.44 |
| 4:F:350:ILE:O | 4:F:354:ALA:HB3 | 2.17 | 0.44 |
| 1:A:357:TYR:CE2 | 3:E:17:GLY:HA2 | 2.53 | 0.44 |
| 2:D:244:PHE:CD1 | 2:D:358:ILE:HD12 | 2.53 | 0.44 |
| 2:D:402:LYS:HB3 | 2:D:405:LEU:HD12 | 2.00 | 0.44 |
| 1:A:12:ALA:HB3 | 1:A:140:SER:HB3 | 2.00 | 0.43 |
| 2:B:105:LYS:HA | 2:B:109:THR:OG1 | 2.17 | 0.43 |
| 1:C:282:TYR:O | 1:C:283:HIS:HB2 | 2.18 | 0.43 |
| 2:D:295:MET:HE2 | 2:D:295:MET:HB2 | 1.85 | 0.43 |
| 3:E:72:LEU:O | 3:E:76:ARG:HG2 | 2.18 | 0.43 |
| 1:A:265:ILE:HG23 | 1:A:432:TYR:CZ | 2.52 | 0.43 |
| 2:B:22:GLU:HG3 | 2:B:83:PHE:CD1 | 2.53 | 0.43 |
| 2:D:210:TYR:CE1 | 2:D:222:PRO:HG2 | 2.54 | 0.43 |
| 4:F:225:SER:HB2 | 4:F:252:ASN:O | 2.18 | 0.43 |
| 1:A:437:VAL:HG12 | 1:A:438:ASP:N | 2.33 | 0.43 |
| 1:A:315:CYS:SG | 1:A:351:PHE:HD2 | 2.41 | 0.43 |
| 2:B:278:ARG:HG2 | 2:B:282:GLN:HE22 | 1.82 | 0.43 |
| 2:D:22:GLU:HG2 | 2:D:83:PHE:CD1 | 2.54 | 0.43 |
| 2:D:75:MET:HE3 | 2:D:92:PHE:CD2 | 2.53 | 0.43 |
| 11:F:401:ACP:O3G | 11:F:401:ACP:O1B | 2.37 | 0.43 |
| 2:B:349:ASN:O | 2:B:352:LYS:HE2 | 2.19 | 0.43 |
| 1:C:68:VAL:HG11 | 1:C:118:VAL:HG21 | 2.00 | 0.43 |
| 2:D:318:ILE:O | 2:D:375:ALA:HA | 2.19 | 0.43 |
| 4:F:151:SER:HB3 | 4:F:180:HIS:CG | 2.54 | 0.43 |
| 4:F:279:LEU:HD12 | 4:F:283:ILE:HB | 2.00 | 0.43 |
| 1:A:345:ASP:O | 3:E:28:SER:HB2 | 2.17 | 0.43 |
| 2:B:7:ILE:O | 2:B:137:LEU:HA | 2.18 | 0.43 |
| 2:B:106:GLY:O | 2:B:111:GLY:HA3 | 2.19 | 0.43 |
| 3:E:137:LYS:HE2 | 3:E:141:GLU:OE2 | 2.19 | 0.43 |
| 1:C:16:ILE:CD1 | 1:C:171:ILE:HD11 | 2.49 | 0.43 |
| 1:C:255:PHE:CD1 | 1:C:316:CYS:HB3 | 2.54 | 0.43 |
| 4:F:6:VAL:HB | 4:F:29:ARG:NH2 | 2.34 | 0.43 |
| 4:F:199:PHE:CD1 | 4:F:221:LEU:HD23 | 2.54 | 0.43 |
| 2:B:54:ASN:OD1 | 2:B:64:ARG:NH2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:140:SER:HA | 1:C:171:ILE:HB | 2.01 | 0.42 |
| 2:D:11:GLN:HB3 | 8:D:501:GDP:O2A | 2.18 | 0.42 |
| 4:F:37:PHE:CE1 | 4:F:40:MET:HB2 | 2.53 | 0.42 |
| 4:F:214:TYR:HB3 | 4:F:375:PHE:HB3 | 2.01 | 0.42 |
| 1:C:234:ILE:HD12 | 1:C:234:ILE:N | 2.34 | 0.42 |
| 2:D:31:ASP:HB2 | 2:D:32:PRO:HD2 | 2.01 | 0.42 |
| 1:C:167:LEU:HG | 1:C:200:CYS:HB3 | 2.02 | 0.42 |
| 1:C:312:TYR:CD2 | 1:C:341:ILE:HG23 | 2.55 | 0.42 |
| 4:F:240:LEU:HD12 | 4:F:240:LEU:N | 2.35 | 0.42 |
| 1:A:211:ASP:OD2 | 1:A:304:LYS:NZ | 2.44 | 0.42 |
| 2:D:123:ARG:O | 2:D:127:GLU:HG3 | 2.19 | 0.42 |
| 1:A:3:GLU:OE1 | 1:A:129:CYS:HB3 | 2.20 | 0.42 |
| 1:A:76:ASP:OD1 | 1:A:79:ARG:NH1 | 2.46 | 0.42 |
| 2:B:290:GLU:O | 2:B:294:GLN:HG3 | 2.20 | 0.42 |
| 2:D:69:ASP:HA | 2:D:145:THR:HG21 | 2.01 | 0.42 |
| 4:F:135:TYR:CZ | 4:F:166:ALA:HB2 | 2.54 | 0.42 |
| 1:A:188:ILE:HD12 | 1:A:395:PHE:CG | 2.55 | 0.42 |
| 2:B:158:ARG:NH1 | 2:B:196:GLU:O | 2.53 | 0.42 |
| 1:A:188:ILE:HD12 | 1:A:395:PHE:CB | 2.50 | 0.42 |
| 1:C:229:ARG:NH1 | 12:C:615:HOH:O | 2.51 | 0.42 |
| 2:D:145:THR:N | 8:D:501:GDP:O2B | 2.53 | 0.42 |
| 2:B:66:ILE:HD12 | 2:B:122:VAL:HG22 | 2.02 | 0.42 |
| 2:D:118:VAL:O | 2:D:122:VAL:HG23 | 2.19 | 0.42 |
| 4:F:160:ILE:HD12 | 4:F:160:ILE:N | 2.34 | 0.42 |
| 1:A:430:LYS:HE2 | 1:A:434:GLU:OE2 | 2.19 | 0.42 |
| 1:C:6:SER:O | 1:C:65:ALA:HA | 2.19 | 0.42 |
| 1:C:194:THR:O | 1:C:194:THR:HG22 | 2.19 | 0.42 |
| 2:D:154:ILE:HG22 | 2:D:197:ASN:HB3 | 2.02 | 0.42 |
| 4:F:197:ARG:HB2 | 4:F:224:SER:O | 2.20 | 0.42 |
| 1:A:247:ALA:HB3 | 3:E:19:SER:OG | 2.20 | 0.42 |
| 2:B:21:TRP:CZ2 | 2:B:65:ALA:HB2 | 2.55 | 0.42 |
| 4:F:185:TYR:OH | 4:F:239:HIS:HB3 | 2.20 | 0.42 |
| 2:B:255:LEU:HD13 | 10:B:505:RWS:C1 | 2.49 | 0.41 |
| 2:D:20:PHE:O | 2:D:24:ILE:HG12 | 2.20 | 0.41 |
| 2:D:21:TRP:CE3 | 2:D:63:PRO:HB3 | 2.54 | 0.41 |
| 1:A:69:ASP:O | 1:A:94:THR:HA | 2.20 | 0.41 |
| 1:C:167:LEU:HA | 1:C:200:CYS:O | 2.19 | 0.41 |
| 2:D:320:ARG:O | 2:D:373:MET:HA | 2.20 | 0.41 |
| 2:D:322:ARG:NH1 | 2:D:322:ARG:HB3 | 2.34 | 0.41 |
| 4:F:3:THR:HA | 4:F:28:LYS:O | 2.20 | 0.41 |
| 4:F:320:MET:HE3 | 4:F:320:MET:HB3 | 1.95 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:66:ILE:CD1 | 2:B:122:VAL:HG22 | 2.50 | 0.41 |
| 1:C:254:GLU:HG2 | 1:C:352:LYS:CE | 2.49 | 0.41 |
| 2:B:288:VAL:N | 2:B:289:PRO:CD | 2.84 | 0.41 |
| 2:D:173:PRO:HB3 | 2:D:183:GLU:OE1 | 2.19 | 0.41 |
| 3:E:45:PRO:HA | 3:E:49:GLU:OE1 | 2.20 | 0.41 |
| 2:B:2:ARG:CB | 2:B:133:GLN:HG3 | 2.38 | 0.41 |
| 2:B:88:ARG:NH2 | 2:B:124:LYS:HE3 | 2.35 | 0.41 |
| 4:F:377:LYS:HD3 | 4:F:379:HIS:CE1 | 2.55 | 0.41 |
| 1:A:336:LYS:HZ2 | 1:A:341:ILE:HB | 1.85 | 0.41 |
| 1:A:39:ASP:OD2 | 1:A:61:HIS:NE2 | 2.53 | 0.41 |
| 2:B:203:CYS:SG | 2:B:267:PHE:HB3 | 2.61 | 0.41 |
| 2:B:351:VAL:O | 2:B:352:LYS:HD2 | 2.21 | 0.41 |
| 2:D:38:GLY:HA3 | 2:D:45:GLN:OE1 | 2.20 | 0.41 |
| 2:D:66:ILE:HD12 | 2:D:122:VAL:HG22 | 2.02 | 0.41 |
| 3:E:116:LEU:HD23 | 3:E:116:LEU:HA | 1.95 | 0.41 |
| 3:E:123:LEU:HD23 | 3:E:126:LYS:HD3 | 2.03 | 0.41 |
| 4:F:151:SER:HB3 | 4:F:180:HIS:CD2 | 2.56 | 0.41 |
| 4:F:349:GLY:O | 4:F:353:VAL:HG22 | 2.21 | 0.41 |
| 2:B:163:ASP:HA | 9:B:504:MES:O1S | 2.21 | 0.41 |
| 2:B:157:ILE:HG21 | 2:B:166:MET:CE | 2.50 | 0.40 |
| 2:B:165:ILE:HG21 | 2:B:252:LEU:HB3 | 2.03 | 0.40 |
| 4:F:206:LEU:HD21 | 4:F:354:ALA:HB2 | 2.03 | 0.40 |
| 1:A:284:GLU:CD | 1:A:284:GLU:H | 2.25 | 0.40 |
| 2:B:297:ASP:OD1 | 2:B:298:SER:N | 2.54 | 0.40 |
| 1:A:103:TYR:CE2 | 1:A:148:GLY:HA2 | 2.56 | 0.40 |
| 3:E:140:LYS:HE2 | 3:E:140:LYS:HB3 | 1.90 | 0.40 |
| 1:A:141:PHE:CE1 | 1:A:170:SER:HB3 | 2.55 | 0.40 |
| 1:A:344:VAL:HG23 | 1:A:347:CYS:HB2 | 2.03 | 0.40 |
| 2:B:5:VAL:HG23 | 2:B:132:LEU:CD1 | 2.51 | 0.40 |
| 2:D:29:GLY:O | 2:D:36:TYR:HA | 2.21 | 0.40 |
| 2:D:66:ILE:CD1 | 2:D:122:VAL:HG22 | 2.51 | 0.40 |
| 2:D:154:ILE:HD13 | 2:D:198:THR:HG22 | 2.03 | 0.40 |
| 2:D:173:PRO:HG3 | 2:D:187:ALA:HB2 | 2.02 | 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 | 436/451 (97%) | 412 (94%) | 24 (6%) | 0 | 100 | 100 |
| 1 | C | 439/451 (97%) | 430 (98%) | 9 (2%) | 0 | 100 | 100 |
| 2 | B | 422/445 (95%) | 411 (97%) | 11 (3%) | 0 | 100 | 100 |
| 2 | D | 429/445 (96%) | 414 (96%) | 13 (3%) | 2 (0%) | 29 | 41 |
| 3 | E | 119/143 (83%) | 119 (100%) | 0 | 0 | 100 | 100 |
| 4 | F | 344/384 (90%) | 323 (94%) | 21 (6%) | 0 | 100 | 100 |
| All | All | 2189/2319 (94%) | 2109 (96%) | 78 (4%) | 2 (0%) | 51 | 68 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 285 | ALA |
| 2 | D | 245 | PRO |

### 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 | 369/379 (97%) | 364 (99%) | 5 (1%) | 67 | 82 |
| 1 | C | 372/379 (98%) | 369 (99%) | 3 (1%) | 81 | 91 |
| 2 | B | 368/383 (96%) | 366 (100%) | 2 (0%) | 88 | 95 |
| 2 | D | 368/383 (96%) | 363 (99%) | 5 (1%) | 67 | 82 |
| 3 | E | 110/127 (87%) | 110 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | F | 315/342 (92%) | 314 (100%) | 1 (0%) | 92 97 |
| All | All | 1902/1993 (95%) | 1886 (99%) | 16 (1%) | 81 91 |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 71 | GLU |
| 1 | A | 221 | ARG |
| 1 | A | 282 | TYR |
| 1 | A | 284 | GLU |
| 1 | A | 300 | ASN |
| 2 | B | 2 | ARG |
| 2 | B | 139 | HIS |
| 1 | C | 71 | GLU |
| 1 | C | 221 | ARG |
| 1 | C | 361 | THR |
| 2 | D | 39 | ASP |
| 2 | D | 139 | HIS |
| 2 | D | 200 | GLU |
| 2 | D | 229 | HIS |
| 2 | D | 247 | GLN |
| 4 | F | 257 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 88 | HIS |
| 1 | A | 101 | ASN |
| 1 | A | 300 | ASN |
| 1 | A | 301 | GLN |
| 2 | B | 15 | GLN |
| 2 | B | 167 | ASN |
| 2 | B | 282 | GLN |
| 2 | B | 294 | GLN |
| 2 | B | 424 | ASN |
| 1 | C | 11 | GLN |
| 2 | D | 96 | GLN |
| 2 | D | 197 | ASN |
| 2 | D | 294 | GLN |
| 2 | D | 336 | GLN |
| 4 | F | 229 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | F | 269 | GLN |
| 4 | F | 333 | ASN |
| 4 | F | 348 | GLN |

### 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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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 | $\#\|Z\| > 2$ |
| 10 | RWS | B | 506 | - | 10,13,13 | 1.68 | 2 (20%) | 8,17,17 | 2.14 | 2 (25%) |
| 9 | MES | B | 504 | - | 12,12,12 | 2.25 | 1 (8%) | 14,16,16 | 2.01 | 6 (42%) |
| 5 | GTP | A | 501 | 6 | 26,34,34 | 1.14 | 1 (3%) | 32,54,54 | 1.39 | 5 (15%) |
| 8 | GDP | D | 501 | 6 | 24,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.18 | 3 (10%) |
| 10 | RWS | B | 505 | - | 10,13,13 | 1.64 | 2 (20%) | 8,17,17 | 1.83 | 2 (25%) |
| 5 | GTP | C | 501 | 6 | 26,34,34 | 1.16 | 2 (7%) | 32,54,54 | 1.42 | 6 (18%) |
| 8 | GDP | B | 501 | 6 | 24,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.16 | 4 (13%) |
| 11 | ACP | F | 401 | 6 | 27,33,33 | 1.40 | 5 (18%) | 32,52,52 | 1.50 | 4 (12%) |

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 |
|---|---|---|---|---|---|---|---|
| 10 | RWS | B | 506 | - | - | 1/2/12/12 | 0/2/2/2 |
| 9 | MES | B | 504 | - | - | 4/6/14/14 | 0/1/1/1 |
| 5 | GTP | A | 501 | 6 | - | 7/18/38/38 | 0/3/3/3 |
| 8 | GDP | D | 501 | 6 | - | 2/12/32/32 | 0/3/3/3 |
| 10 | RWS | B | 505 | - | - | 1/2/12/12 | 0/2/2/2 |
| 5 | GTP | C | 501 | 6 | - | 5/18/38/38 | 0/3/3/3 |
| 8 | GDP | B | 501 | 6 | - | 3/12/32/32 | 0/3/3/3 |
| 11 | ACP | F | 401 | 6 | - | 10/15/38/38 | 0/3/3/3 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | B | 504 | MES | C8-S | -7.49 | 1.66 | 1.77 |
| 5 | C | 501 | GTP | C5-C6 | -4.14 | 1.39 | 1.47 |
| 5 | A | 501 | GTP | C5-C6 | -3.94 | 1.39 | 1.47 |
| 10 | B | 506 | RWS | C2-N2 | 3.83 | 1.38 | 1.32 |
| 10 | B | 505 | RWS | C2-N2 | 3.68 | 1.37 | 1.32 |
| 11 | F | 401 | ACP | PG-O2G | 2.99 | 1.61 | 1.54 |
| 11 | F | 401 | ACP | PG-O3G | 2.94 | 1.61 | 1.54 |
| 11 | F | 401 | ACP | PB-O3A | 2.86 | 1.61 | 1.58 |
| 10 | B | 506 | RWS | N-N1 | 2.61 | 1.42 | 1.37 |
| 10 | B | 505 | RWS | N-N1 | 2.60 | 1.42 | 1.37 |
| 11 | F | 401 | ACP | C5-C4 | 2.56 | 1.47 | 1.40 |
| 8 | D | 501 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 11 | F | 401 | ACP | PB-O2B | 2.25 | 1.61 | 1.56 |
| 5 | C | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 8 | B | 501 | GDP | C6-N1 | -2.12 | 1.34 | 1.37 |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | B | 506 | RWS | C-C1-S | 4.56 | 126.25 | 120.12 |
| 10 | B | 505 | RWS | C-C1-S | 4.35 | 125.96 | 120.12 |
| 11 | F | 401 | ACP | PB-O3A-PA | -4.15 | 119.41 | 132.56 |
| 9 | B | 504 | MES | C5-N4-C3 | 3.91 | 117.62 | 108.83 |
| 11 | F | 401 | ACP | C3'-C2'-C1' | 3.58 | 106.37 | 100.98 |
| 8 | D | 501 | GDP | PA-O3A-PB | -3.34 | 121.38 | 132.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | F | 401 | ACP | N3-C2-N1 | -3.19 | 123.69 | 128.68 |
| 5 | C | 501 | GTP | PA-O3A-PB | -3.10 | 122.18 | 132.83 |
| 5 | C | 501 | GTP | C8-N7-C5 | 3.08 | 108.86 | 102.99 |
| 5 | A | 501 | GTP | C5-C6-N1 | 3.06 | 119.36 | 113.95 |
| 5 | C | 501 | GTP | C5-C6-N1 | 3.05 | 119.34 | 113.95 |
| 5 | A | 501 | GTP | C8-N7-C5 | 3.05 | 108.81 | 102.99 |
| 9 | B | 504 | MES | C6-C5-N4 | -3.05 | 105.48 | 110.10 |
| 10 | B | 506 | RWS | C3-N2-C7 | 2.99 | 118.12 | 111.52 |
| 9 | B | 504 | MES | O1S-S-C8 | 2.86 | 110.36 | 106.92 |
| 5 | A | 501 | GTP | PA-O3A-PB | -2.84 | 123.06 | 132.83 |
| 5 | C | 501 | GTP | C2-N1-C6 | -2.72 | 120.08 | 125.10 |
| 5 | C | 501 | GTP | PB-O3B-PG | -2.67 | 123.68 | 132.83 |
| 5 | A | 501 | GTP | C2-N1-C6 | -2.62 | 120.27 | 125.10 |
| 11 | F | 401 | ACP | C4-C5-N7 | -2.57 | 106.72 | 109.40 |
| 8 | B | 501 | GDP | C5-C6-N1 | 2.54 | 118.44 | 113.95 |
| 8 | B | 501 | GDP | PA-O3A-PB | -2.54 | 124.11 | 132.83 |
| 5 | A | 501 | GTP | PB-O3B-PG | -2.51 | 124.20 | 132.83 |
| 8 | B | 501 | GDP | C8-N7-C5 | 2.41 | 107.58 | 102.99 |
| 9 | B | 504 | MES | O2S-S-C8 | 2.41 | 109.81 | 106.92 |
| 8 | D | 501 | GDP | C8-N7-C5 | 2.36 | 107.48 | 102.99 |
| 8 | B | 501 | GDP | O6-C6-C5 | -2.21 | 120.06 | 124.37 |
| 8 | D | 501 | GDP | C5-C6-N1 | 2.20 | 117.83 | 113.95 |
| 5 | C | 501 | GTP | O6-C6-C5 | -2.14 | 120.19 | 124.37 |
| 9 | B | 504 | MES | C7-N4-C5 | 2.13 | 116.67 | 111.23 |
| 9 | B | 504 | MES | O3S-S-C8 | 2.08 | 109.14 | 105.77 |
| 10 | B | 505 | RWS | C3-N2-C7 | 2.01 | 115.96 | 111.52 |

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | A | 501 | GTP | C5'-O5'-PA-O1A |
| 5 | A | 501 | GTP | C5'-O5'-PA-O2A |
| 5 | C | 501 | GTP | C5'-O5'-PA-O1A |
| 5 | C | 501 | GTP | C5'-O5'-PA-O2A |
| 8 | B | 501 | GDP | C5'-O5'-PA-O1A |
| 8 | B | 501 | GDP | C5'-O5'-PA-O2A |
| 8 | D | 501 | GDP | C5'-O5'-PA-O3A |
| 9 | B | 504 | MES | C8-C7-N4-C5 |
| 9 | B | 504 | MES | C7-C8-S-O2S |
| 9 | B | 504 | MES | C7-C8-S-O3S |
| 10 | B | 505 | RWS | S-C2-N2-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 10 | B | 506 | RWS | S-C2-N2-C3 |
| 11 | F | 401 | ACP | PB-C3B-PG-O1G |
| 11 | F | 401 | ACP | PB-C3B-PG-O2G |
| 11 | F | 401 | ACP | PB-C3B-PG-O3G |
| 11 | F | 401 | ACP | PG-C3B-PB-O1B |
| 11 | F | 401 | ACP | PG-C3B-PB-O3A |
| 11 | F | 401 | ACP | C5'-O5'-PA-O1A |
| 11 | F | 401 | ACP | C5'-O5'-PA-O2A |
| 5 | C | 501 | GTP | PB-O3B-PG-O2G |
| 8 | B | 501 | GDP | C5'-O5'-PA-O3A |
| 8 | D | 501 | GDP | C5'-O5'-PA-O2A |
| 9 | B | 504 | MES | C7-C8-S-O1S |
| 11 | F | 401 | ACP | PG-C3B-PB-O2B |
| 5 | A | 501 | GTP | C4'-C5'-O5'-PA |
| 5 | A | 501 | GTP | PB-O3A-PA-O2A |
| 5 | C | 501 | GTP | C4'-C5'-O5'-PA |
| 5 | A | 501 | GTP | PB-O3B-PG-O2G |
| 11 | F | 401 | ACP | PB-O3A-PA-O2A |
| 5 | A | 501 | GTP | C5'-O5'-PA-O3A |
| 5 | C | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | F | 401 | ACP | C5'-O5'-PA-O3A |
| 5 | A | 501 | GTP | PB-O3A-PA-O1A |

There are no ring outliers.

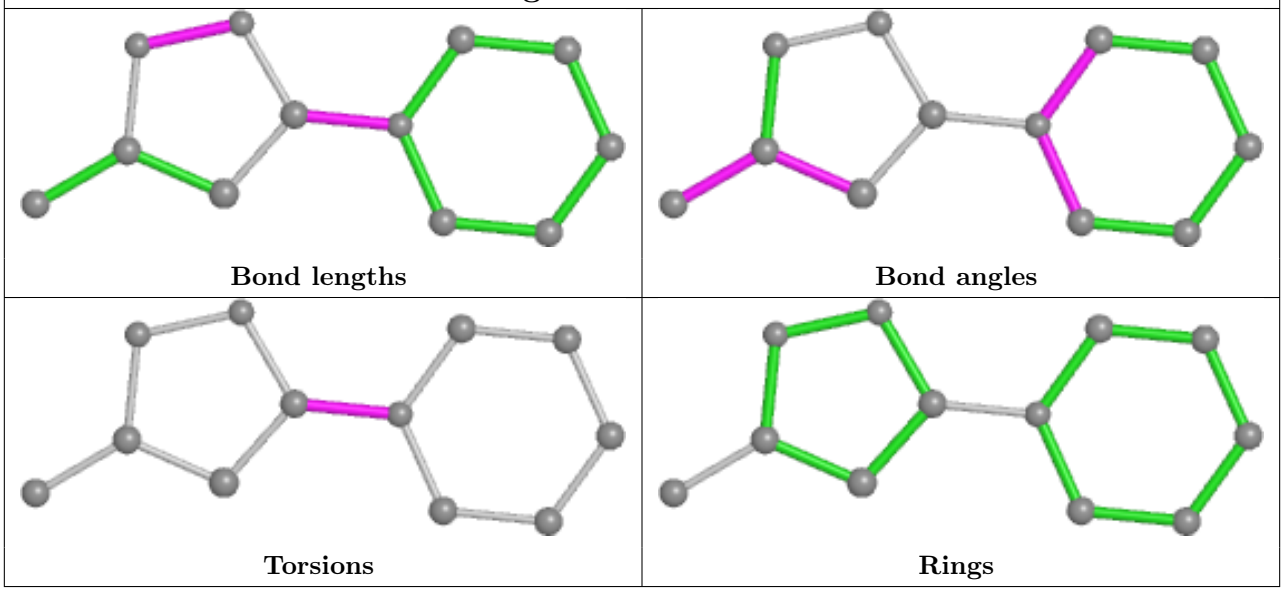
6 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 10 | B | 506 | RWS | 1 | 0 |
| 9 | B | 504 | MES | 2 | 0 |
| 5 | A | 501 | GTP | 1 | 0 |
| 8 | D | 501 | GDP | 5 | 0 |
| 10 | B | 505 | RWS | 1 | 0 |
| 11 | F | 401 | ACP | 3 | 0 |

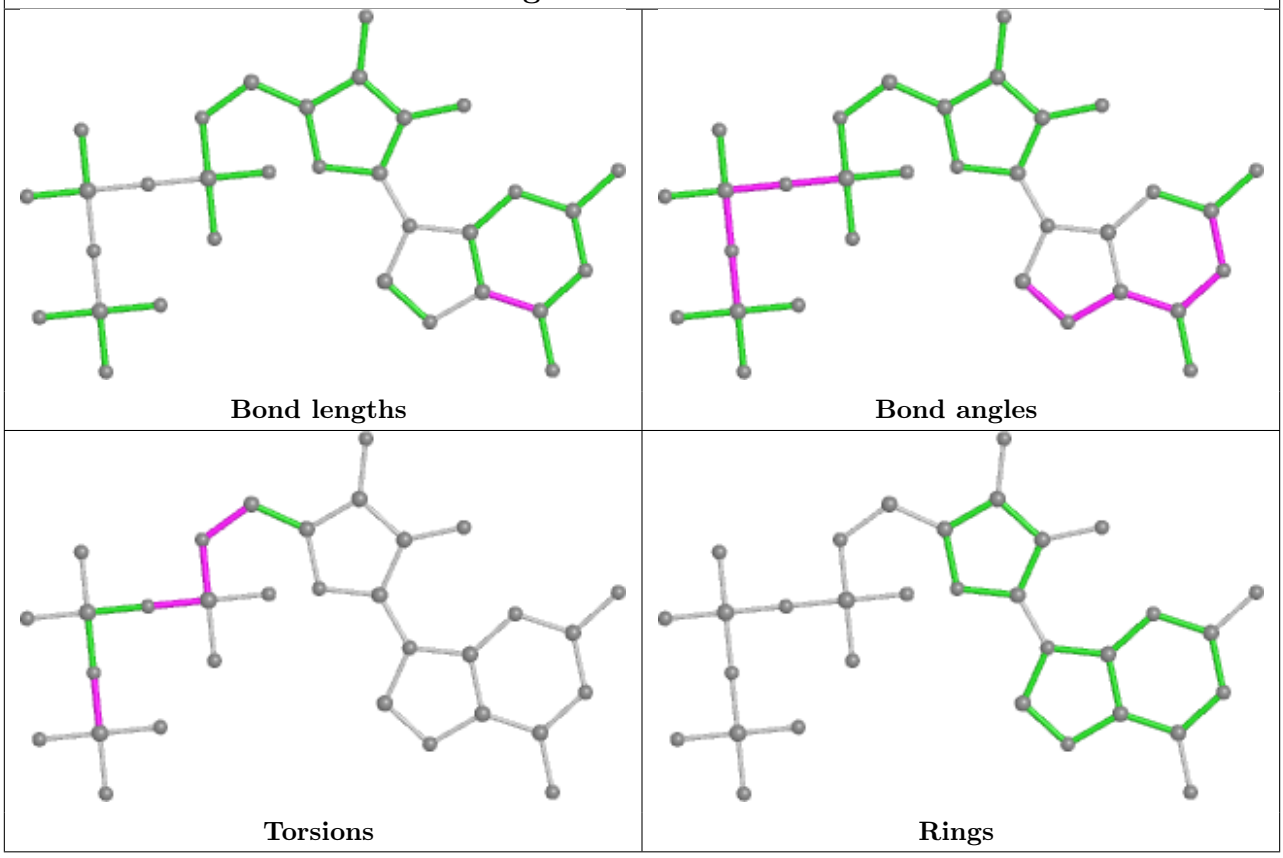
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

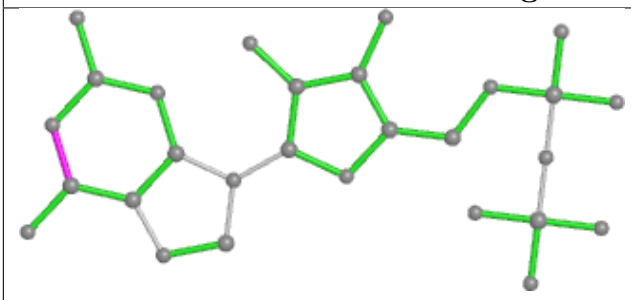
**Ligand RWS B 506**



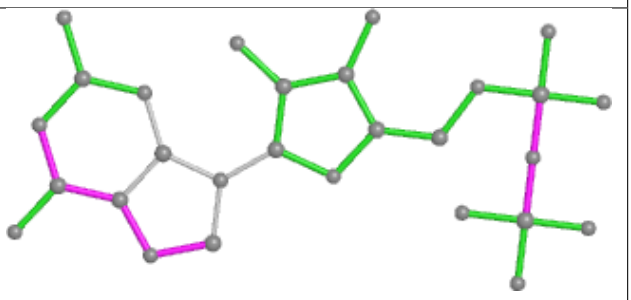

**Ligand GTP A 501**



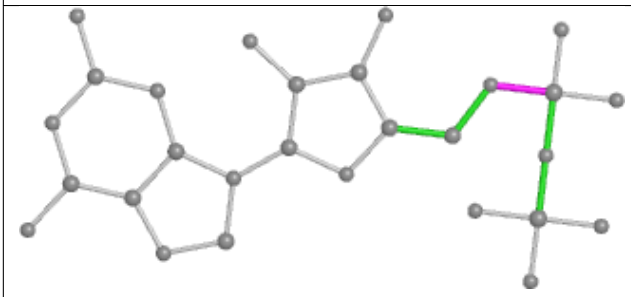
## Ligand GDP D 501



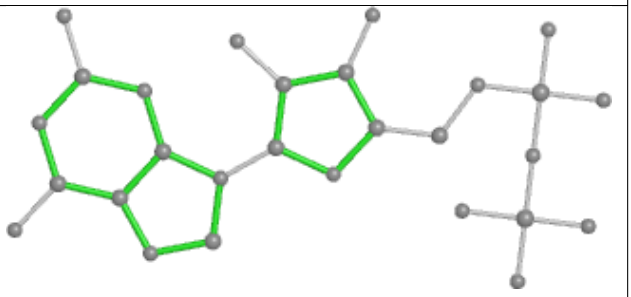
Bond lengths



Bond angles

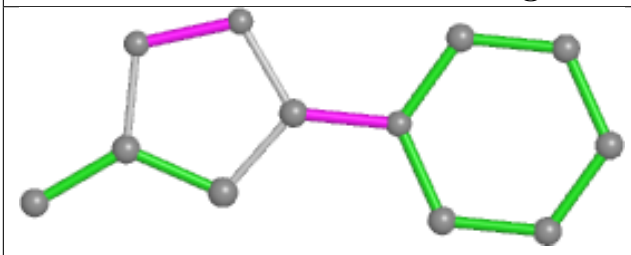


Torsions

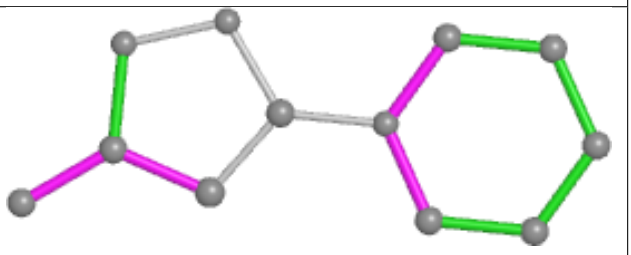


Rings

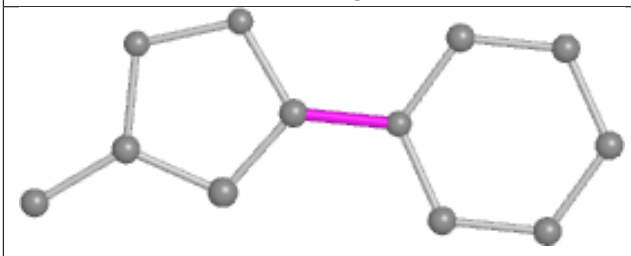
## Ligand RWS B 505



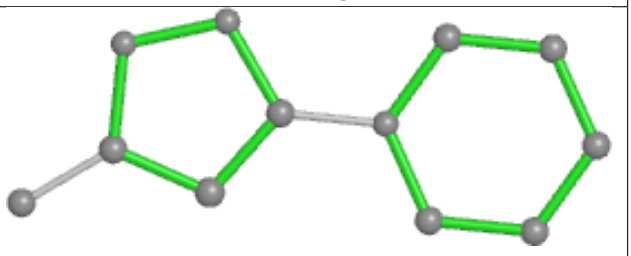
Bond lengths



Bond angles

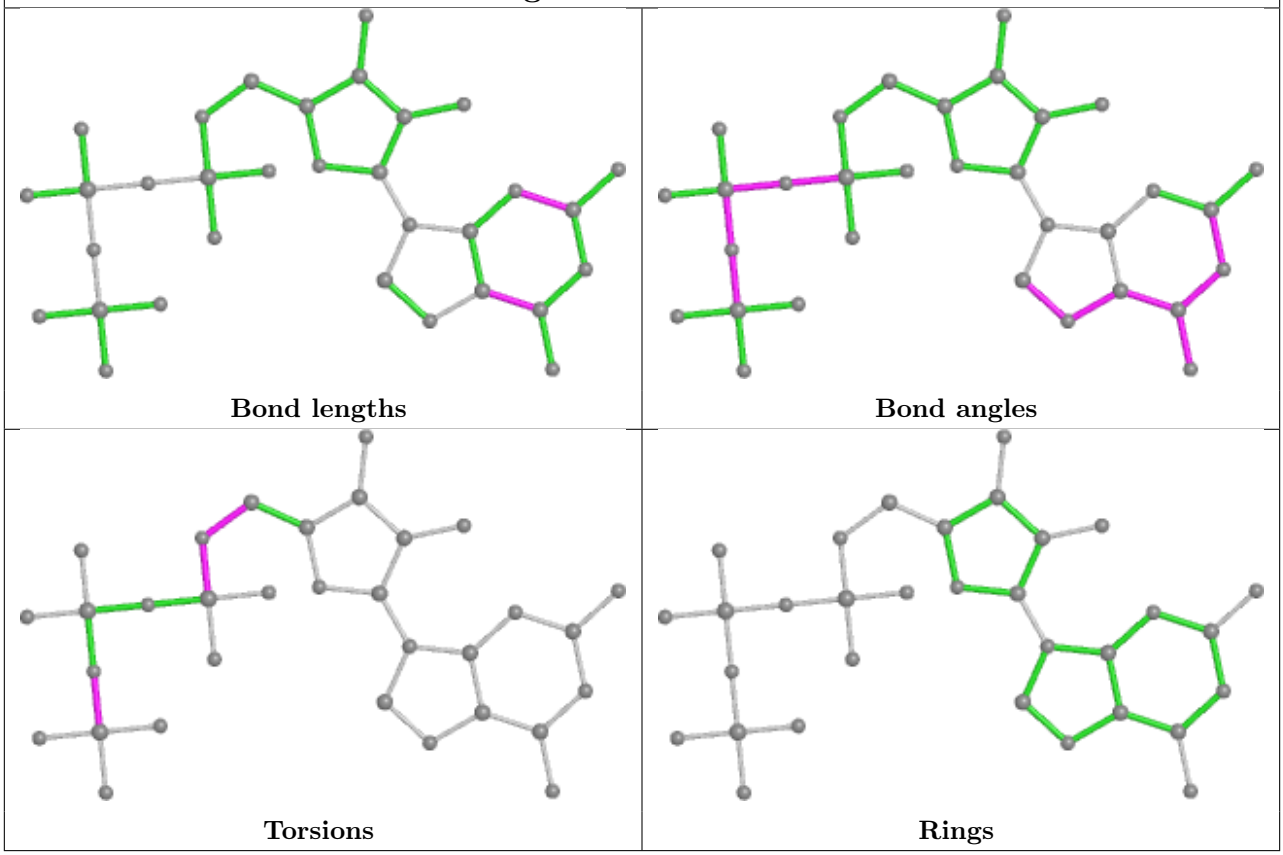


Torsions

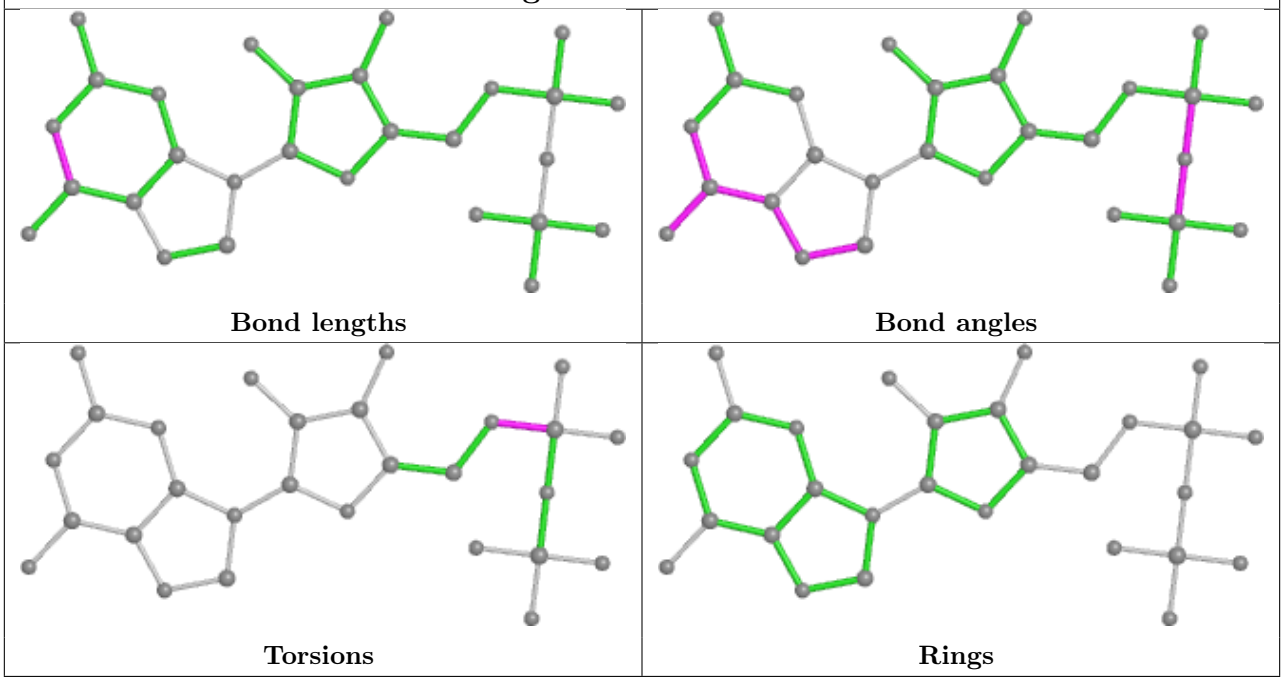


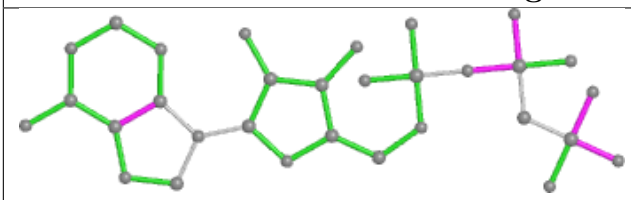
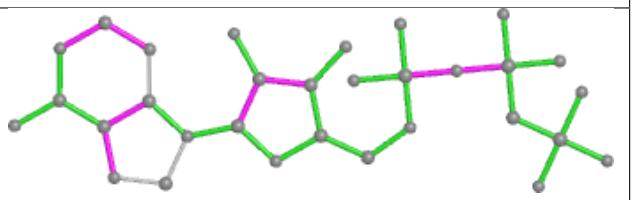
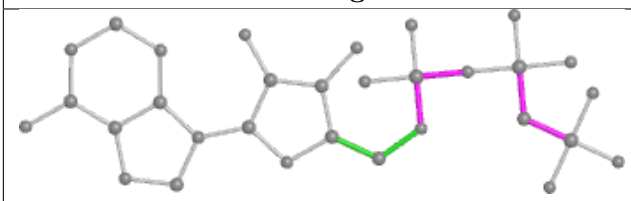
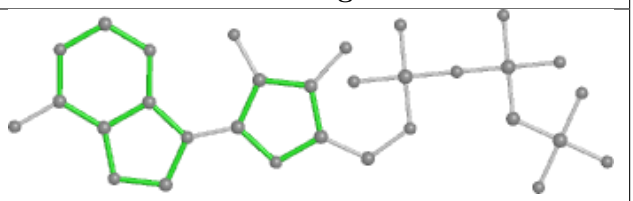
Rings

## Ligand GTP C 501




## Ligand GDP B 501



| Ligand ACP F 401 | |
|---|---|
|  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 | 438/451 (97%) | 0.32 | 10 (2%) | 60 | 58 | 56, 80, 124, 180 | 0 |
| 1 | C | 440/451 (97%) | 0.29 | 8 (1%) | 68 | 66 | 52, 66, 98, 163 | 0 |
| 2 | B | 425/445 (95%) | 0.37 | 6 (1%) | 75 | 73 | 50, 72, 115, 166 | 3 (0%) |
| 2 | D | 431/445 (96%) | 0.37 | 18 (4%) | 36 | 35 | 63, 89, 132, 198 | 5 (1%) |
| 3 | E | 123/143 (86%) | 0.72 | 10 (8%) | 12 | 11 | 62, 93, 143, 197 | 0 |
| 4 | F | 352/384 (91%) | 0.59 | 32 (9%) | 9 | 8 | 69, 108, 172, 239 | 0 |
| All | All | 2209/2319 (95%) | 0.40 | 84 (3%) | 40 | 39 | 50, 82, 141, 239 | 8 (0%) |

All (84) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | E | 27 | PRO | 8.9 |
| 3 | E | 24 | LEU | 8.7 |
| 1 | A | 341 | ILE | 8.5 |
| 2 | D | 281 | GLN | 8.0 |
| 1 | A | 349 | THR | 7.5 |
| 1 | C | 179 | THR | 7.2 |
| 3 | E | 26 | PRO | 7.0 |
| 4 | F | 103 | THR | 6.3 |
| 4 | F | 173 | ILE | 6.1 |
| 4 | F | 89 | GLU | 5.6 |
| 4 | F | 90 | SER | 5.4 |
| 2 | D | 276 | THR | 5.3 |
| 1 | A | 339 | ARG | 5.3 |
| 3 | E | 28 | SER | 5.2 |
| 2 | D | 279 | GLY | 5.1 |
| 2 | B | 1 | MET | 5.0 |
| 2 | D | 278 | ARG | 4.9 |
| 3 | E | 25 | LYS | 4.9 |
| 2 | D | 282 | GLN | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | F | 104 | ASN | 4.7 |
| 2 | B | 284 | ARG | 4.6 |
| 2 | D | 280 | SER | 4.6 |
| 2 | B | 281 | GLN | 4.1 |
| 4 | F | 169 | LEU | 4.0 |
| 4 | F | 131 | PHE | 3.9 |
| 2 | B | 59 | ASN | 3.8 |
| 4 | F | 233 | PHE | 3.8 |
| 2 | B | 276 | THR | 3.8 |
| 1 | C | 341 | ILE | 3.7 |
| 2 | D | 248 | LEU | 3.7 |
| 1 | A | 351 | PHE | 3.6 |
| 4 | F | 143 | GLU | 3.5 |
| 4 | F | 132 | LEU | 3.5 |
| 4 | F | 137 | ARG | 3.5 |
| 1 | A | 346 | TRP | 3.5 |
| 2 | D | 249 | ASN | 3.4 |
| 4 | F | 140 | GLU | 3.3 |
| 4 | F | 101 | TYR | 3.2 |
| 4 | F | 253 | TYR | 3.2 |
| 4 | F | 100 | ILE | 3.1 |
| 3 | E | 142 | GLU | 3.1 |
| 4 | F | 240 | LEU | 3.1 |
| 4 | F | 251 | LYS | 3.0 |
| 1 | A | 335 | ILE | 2.9 |
| 4 | F | 105 | LEU | 2.9 |
| 3 | E | 6 | MET | 2.9 |
| 4 | F | 249 | TYR | 2.9 |
| 1 | A | 262 | TYR | 2.8 |
| 2 | D | 285 | ALA | 2.8 |
| 1 | A | 282 | TYR | 2.7 |
| 1 | C | 335 | ILE | 2.7 |
| 4 | F | 135 | TYR | 2.7 |
| 4 | F | 231 | ALA | 2.6 |
| 4 | F | 36 | ARG | 2.5 |
| 2 | D | 283 | TYR | 2.5 |
| 2 | D | 1 | MET | 2.4 |
| 1 | A | 86 | LEU | 2.4 |
| 4 | F | 142 | ARG | 2.4 |
| 2 | D | 293 | GLN | 2.4 |
| 3 | E | 22 | VAL | 2.4 |
| 2 | D | 277 | SER | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 308 | ARG | 2.3 |
| 4 | F | 245 | ILE | 2.3 |
| 3 | E | 139 | LEU | 2.3 |
| 1 | C | 286 | LEU | 2.3 |
| 2 | D | 335 | VAL | 2.3 |
| 2 | D | 57 | THR | 2.2 |
| 4 | F | 152 | SER | 2.2 |
| 4 | F | 181 | VAL | 2.2 |
| 4 | F | 177 | GLY | 2.2 |
| 3 | E | 122 | ARG | 2.2 |
| 1 | C | 177 | VAL | 2.2 |
| 1 | C | 357 | TYR | 2.1 |
| 4 | F | 138 | ARG | 2.1 |
| 2 | D | 217 | LEU | 2.1 |
| 4 | F | 20 | LEU | 2.1 |
| 4 | F | 170 | LEU | 2.1 |
| 2 | B | 57 | THR | 2.1 |
| 4 | F | 21 | LEU | 2.1 |
| 2 | D | 154 | ILE | 2.1 |
| 2 | D | 291 | LEU | 2.1 |
| 4 | F | 136 | ASN | 2.1 |
| 1 | A | 344 | VAL | 2.0 |
| 1 | C | 350 | GLY | 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.

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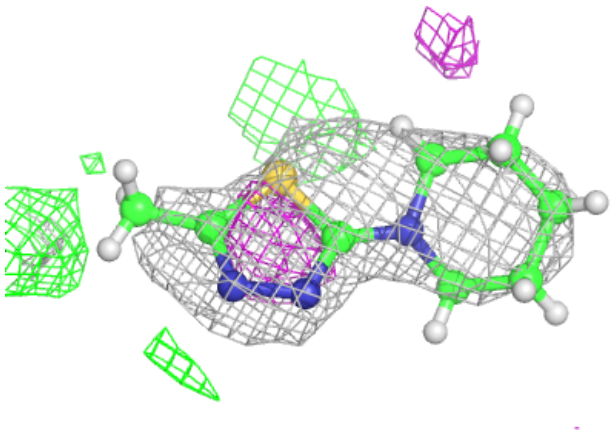
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|

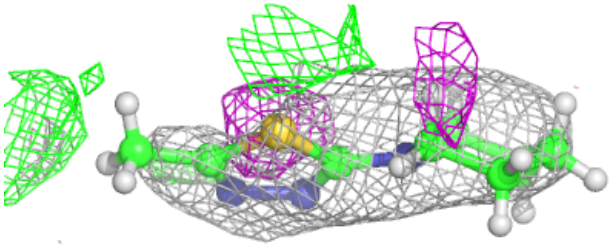
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 10 | RWS | B | 505 | 12/12 | 0.68 | 0.37 | 117,137,150,153 | 0 |
| 10 | RWS | B | 506 | 12/12 | 0.78 | 0.28 | 64,82,99,99 | 25 |
| 7 | CA | A | 503 | 1/1 | 0.84 | 0.11 | 112,112,112,112 | 0 |
| 11 | ACP | F | 401 | 31/31 | 0.84 | 0.14 | 105,115,130,134 | 0 |
| 7 | CA | A | 504 | 1/1 | 0.88 | 0.10 | 106,106,106,106 | 0 |
| 6 | MG | D | 502 | 1/1 | 0.89 | 0.14 | 82,82,82,82 | 0 |
| 7 | CA | B | 503 | 1/1 | 0.90 | 0.09 | 112,112,112,112 | 0 |
| 9 | MES | B | 504 | 12/12 | 0.95 | 0.18 | 82,87,99,110 | 0 |
| 6 | MG | F | 402 | 1/1 | 0.95 | 0.15 | 106,106,106,106 | 0 |
| 6 | MG | B | 502 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 8 | GDP | D | 501 | 28/28 | 0.95 | 0.17 | 75,81,92,99 | 0 |
| 7 | CA | C | 503 | 1/1 | 0.97 | 0.15 | 82,82,82,82 | 0 |
| 6 | MG | C | 502 | 1/1 | 0.98 | 0.17 | 61,61,61,61 | 0 |
| 5 | GTP | C | 501 | 32/32 | 0.98 | 0.18 | 48,56,64,71 | 0 |
| 6 | MG | A | 502 | 1/1 | 0.98 | 0.16 | 59,59,59,59 | 0 |
| 5 | GTP | A | 501 | 32/32 | 0.98 | 0.17 | 50,60,66,68 | 0 |
| 8 | GDP | B | 501 | 28/28 | 0.99 | 0.18 | 49,55,64,71 | 0 |

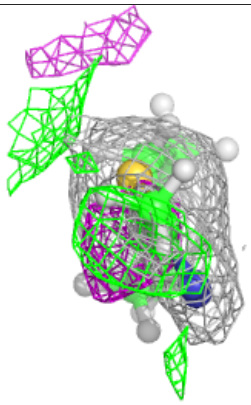
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RWS B 505:**

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

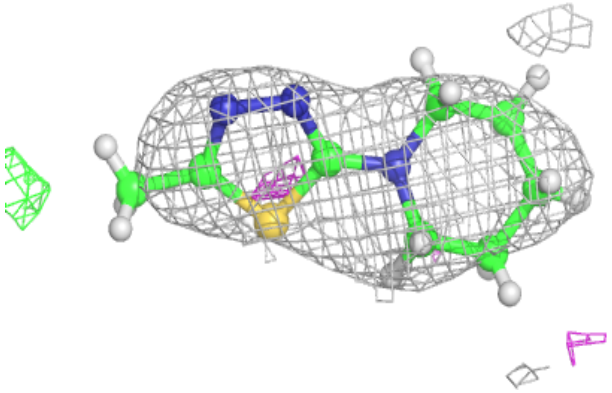


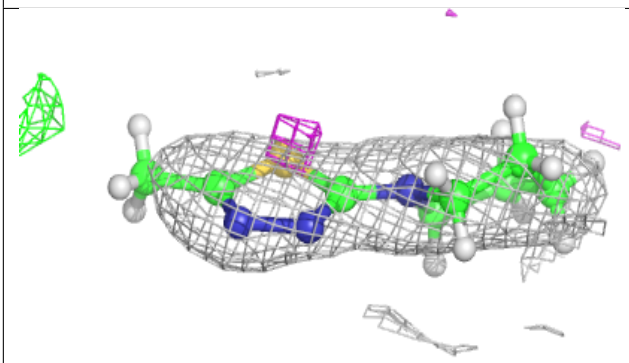


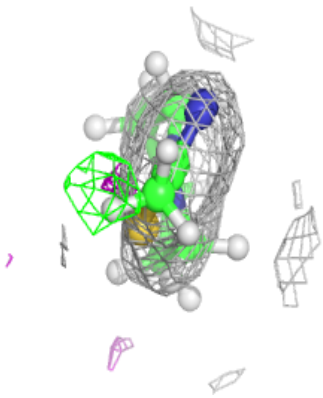


**Electron density around RWS B 506:**

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

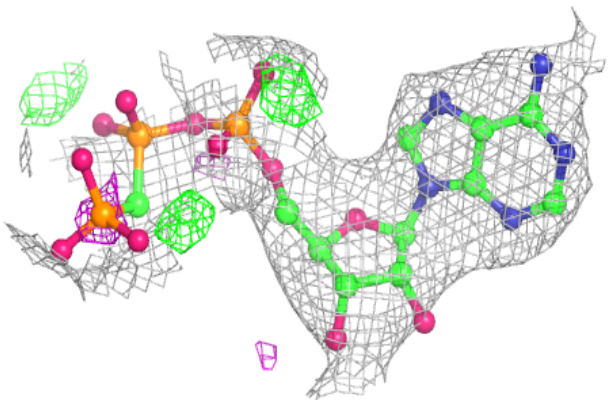


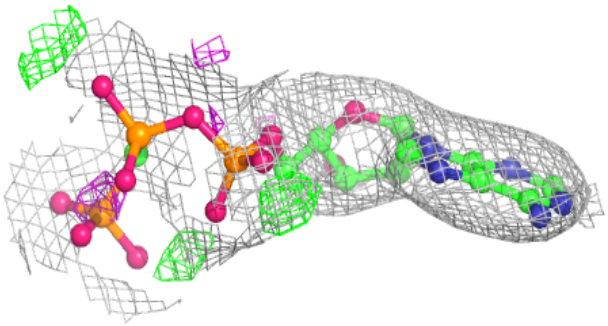


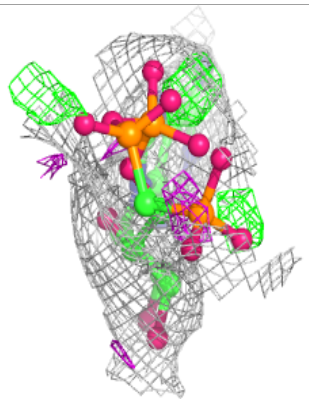


**Electron density around ACP F 401:**

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

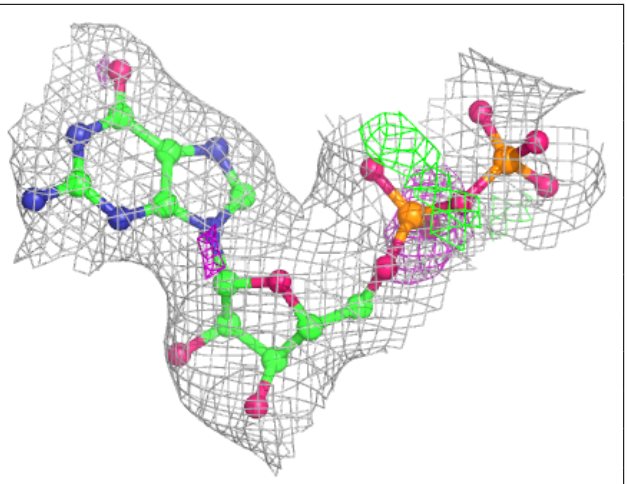


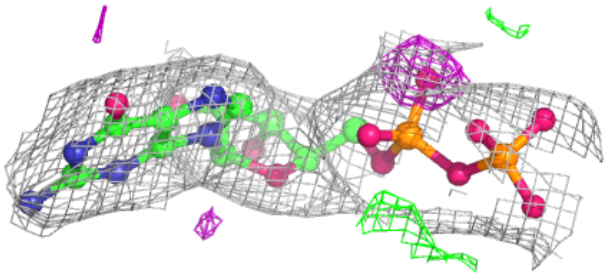


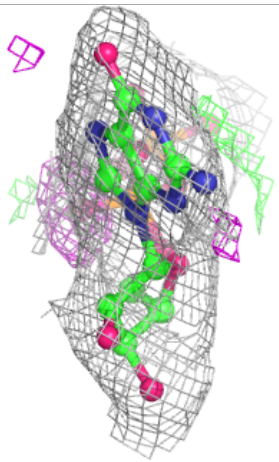


**Electron density around GDP D 501:**

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

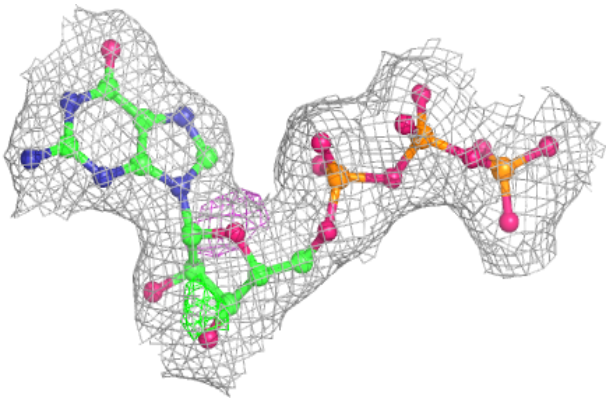


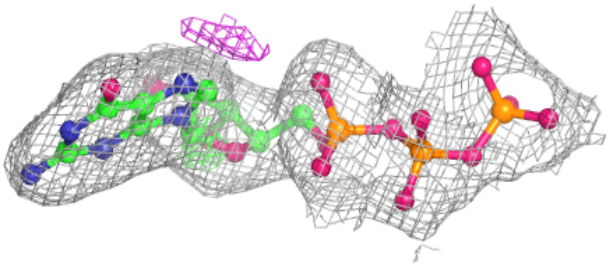


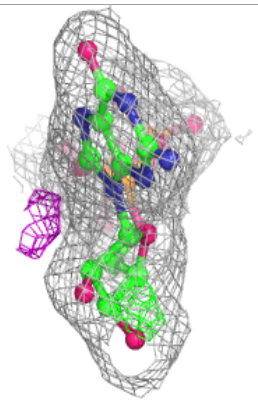


**Electron density around GTP C 501:**

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

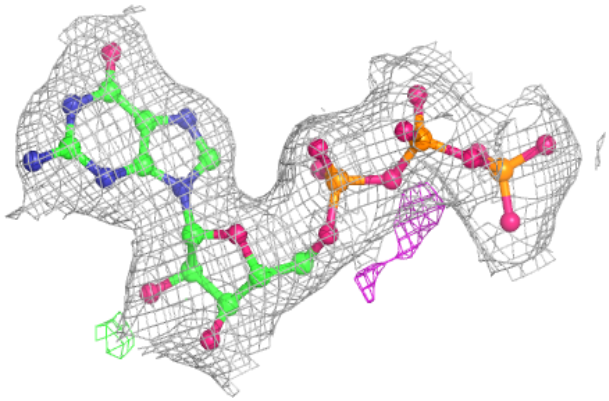


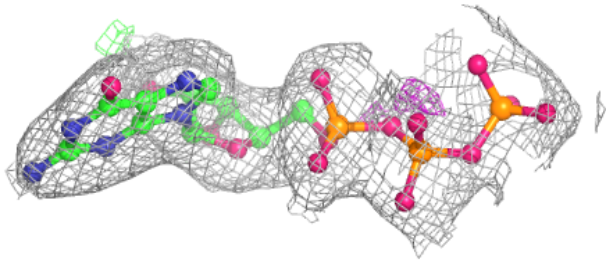


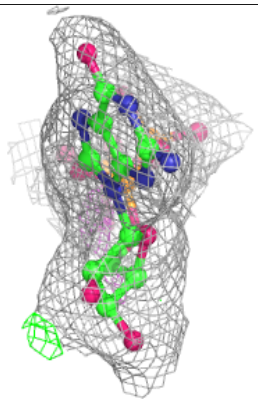


**Electron density around GTP A 501:**

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

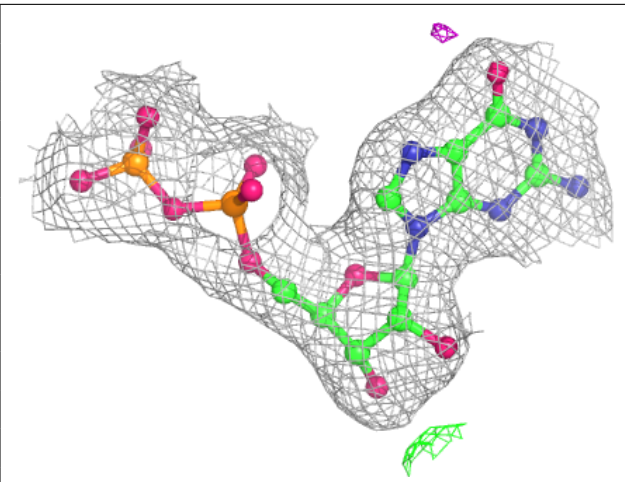


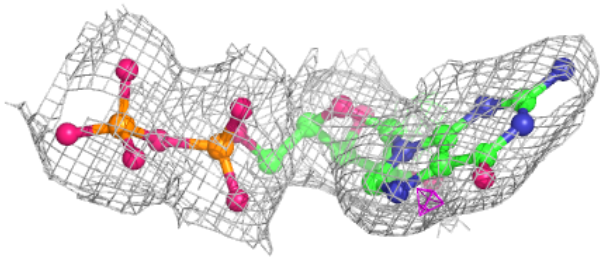


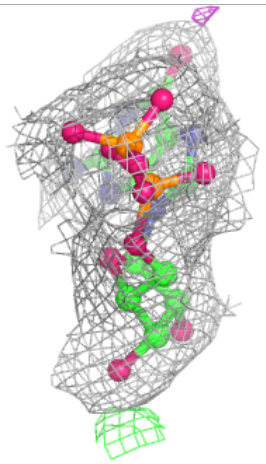


**Electron density around GDP B 501:**

$2mF_o$-$DF_c$ (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.