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

Dec 10, 2023 – 09:26 pm GMT

PDB ID : 1OGP

Title : The crystal structure of plant sulfite oxidase provides insight into sulfite oxidation in plants and animals

Authors : Schrader, N.; Fischer, K.; Theis, K.; Mendel, R.R.; Schwarz, G.; Kisker, C.

Deposited on : 2003-05-08

Resolution : 2.60 Å(reported)

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

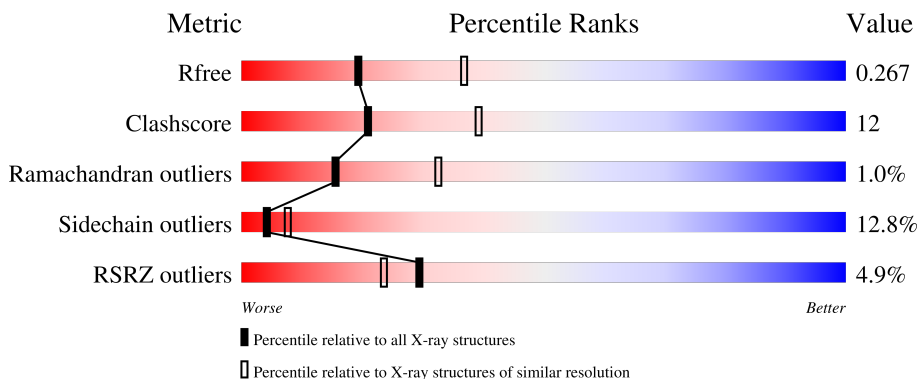|  |  |  |
| --- | --- | --- |
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 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　ⓘ

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

The reported resolution of this entry is 2.60 Å.

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

| Metric | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.267 |
| Clashscore | | 12 |
| Ramachandran outliers | | 1.0% |
| Sidechain outliers | | 12.8% |
| RSRZ outliers | | 4.9% |

*Worse*　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|----------------------------------------------------|
| $R_{free}$ | 130704 | 3163 (2.60-2.60) |
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (2.60-2.60) |

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 | 393 | 5%　68%　24%　5% ·· |
| 1 | B | 393 | 3%　70%　22%　5% ·· |
| 1 | C | 393 | 5%　66%　25%　6% ·· |
| 1 | D | 393 | 9%　56%　30%　10% ·· |
| 1 | E | 393 | 4%　68%　25%　5% ·· |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 393 | 3% ▌ 69% 23% 6% •• |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4 | MTQ | D | 1394 | - | - | X | - |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18888 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 SULFITE OXIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |
| 1 | B | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |
| 1 | C | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |
| 1 | D | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |
| 1 | E | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |
| 1 | F | 388 | Total 3014 | C 1902 | N 538 | O 565 | S 9 | 0 | 0 | 0 |

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 2 | Total 2 | Cs 2 | 0 | 0 |
| 2 | B | 2 | Total 2 | Cs 2 | 0 | 0 |
| 2 | C | 2 | Total 2 | Cs 2 | 0 | 0 |
| 2 | D | 2 | Total 2 | Cs 2 | 0 | 0 |
| 2 | E | 2 | Total 2 | Cs 2 | 0 | 0 |
| 2 | F | 2 | Total 2 | Cs 2 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

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

- Molecule 4 is (MOLYBDOPTERIN-S,S)-DIOXO-THIO-MOLYBDENUM(VI) (three-letter code: MTQ) (formula: $C_{10}H_8MoN_5O_8PS_2$).

MTQ

| Mol | Chain | Residues | Atoms | | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |
| 4 | B | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |
| 4 | C | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |
| 4 | D | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |
| 4 | E | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |
| 4 | F | 1 | Total | C | Mo | N | O | P | S | 0 | 0 |
| | | | 27 | 10 | 1 | 5 | 8 | 1 | 2 | | |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 5 | A | 105 | Total | O | 0 | 0 |
| | | | 105 | 105 | | |
| 5 | B | 95 | Total | O | 0 | 1 |
| | | | 95 | 95 | | |
| 5 | C | 86 | Total | O | 0 | 1 |
| | | | 86 | 86 | | |
| 5 | D | 90 | Total | O | 0 | 0 |
| | | | 90 | 90 | | |
| 5 | E | 107 | Total | O | 0 | 0 |
| | | | 107 | 107 | | |
| 5 | F | 111 | Total | O | 0 | 1 |
| | | | 111 | 111 | | |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises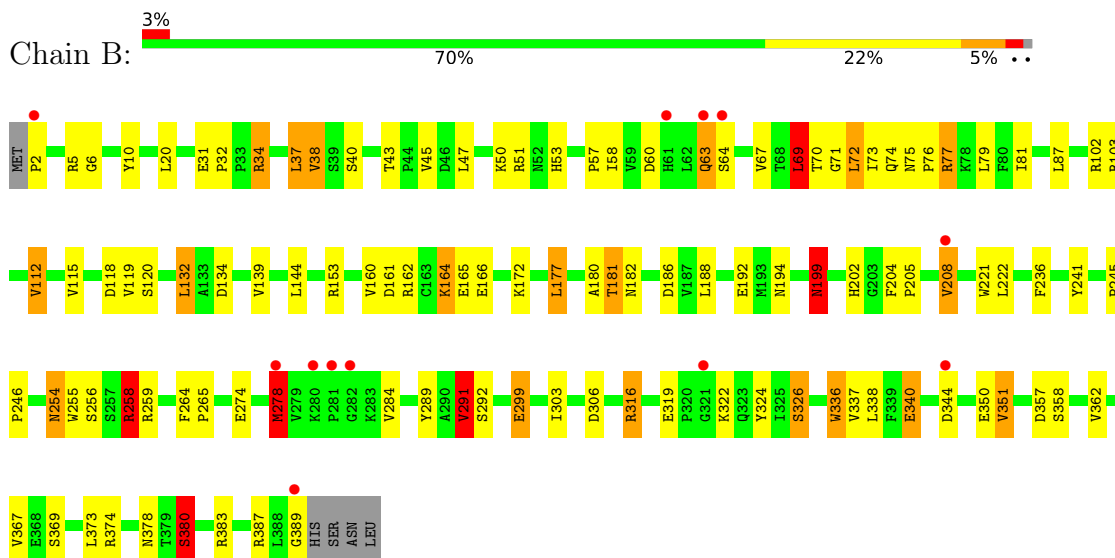 the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: 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.
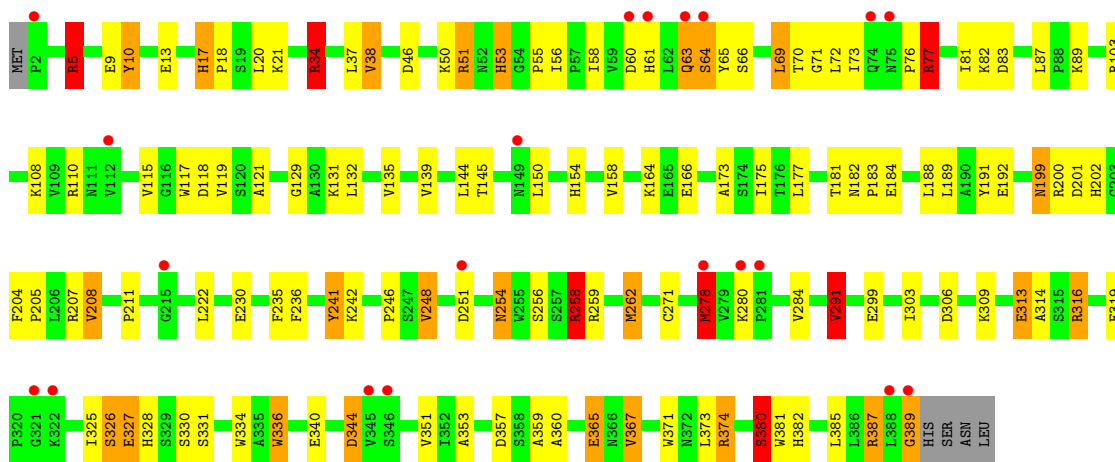
- Molecule 1: SULFITE OXIDASE
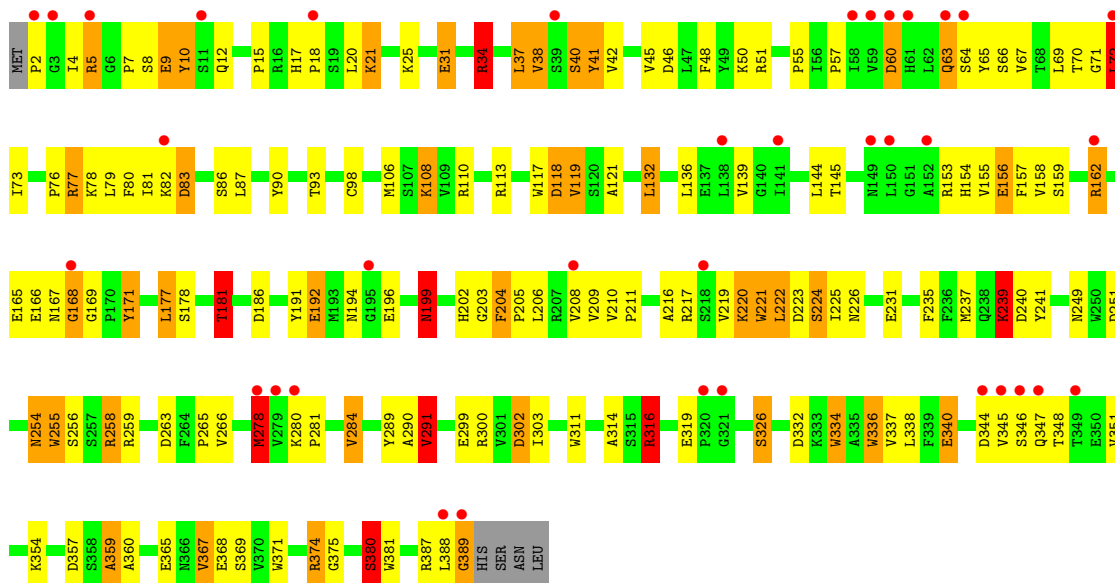
Chain A:



- Molecule 1: SULFITE OXIDASE

Chain B:



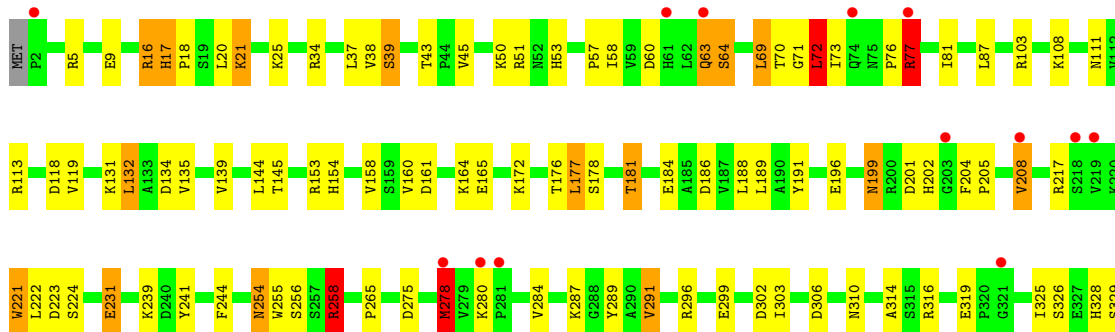- Molecule 1: SULFITE OXIDASE

Chain C:

MET P2 R5 E9 Y10 E13 H17 P18 S19 L20 K21 R34 L37 V38 D46 K50 R51 N52 H53 G54 P55 I56 P57 I58 V59 D60 H61 L62 Q63 S64 Y65 S66 L69 T70 G71 L72 I73 Q74 N75 P76 R77 I81 K82 D83 L87 P88 K89 R103

K108 V109 R110 N111 V112 V115 G116 W117 D118 V119 S120 A121 G129 A130 K131 L132 V135 V139 L144 T145 N149 L150 H154 V158 K164 E165 E166 A173 S174 I175 I176 L177 T181 N182 P183 E184 L188 L189 A190 Y191 E192 N199 R200 D201 H202 G203

F204 P205 L206 R207 V208 P211 G215 L222 E230 F235 F236 Y241 K242 P246 S247 V248 D251 N254 W255 S256 S257 R258 R259 M262 C271 M278 V279 K280 P281 V284 V291 E299 I303 D306 K309 E313 A314 S315 R316 E319

P320 G321 K322 I325 S326 E327 H328 S329 S330 S331 W334 A335 W336 E340 D344 V345 S346 V351 I352 A353 D357 S358 A359 A360 E365 N366 V367 W371 N372 L373 R374 S380 W381 H382 L385 L386 R387 L388 G389 HIS SER ASN LEU

● Molecule 1: SULFITE OXIDASE

Chain D:

Molecule 1: SULFITE OXIDASE bar diagram showing 9%, 56%, 30%, 10%

MET P2 G3 I4 R5 G6 P7 S8 E9 Y10 S11 Q12 P15 R16 H17 P18 S19 L20 K21 K25 E31 R34 L37 V38 S39 S40 Y41 Y42 V45 D46 L47 F48 Y49 K50 R51 P55 I56 P57 I58 V59 D60 H61 L62 Q63 S64 Y65 S66 V67 T68 L69 T70 G71 L72

I73 P76 R77 K78 L79 F80 I81 K82 D83 S86 L87 Y90 T93 C98 M106 S107 K108 V109 R110 R113 W117 D118 V119 S120 A121 L132 L136 E137 L138 V139 G140 I141 L144 T145 N149 L150 G151 A152 R153 H154 V155 E156 F157 V158 S159 R162

E165 E166 N167 G168 G169 P170 Y171 L177 S178 T181 D186 Y191 E192 M193 N194 G195 E196 N199 H202 G203 F204 P205 L206 R207 V208 V209 V210 P211 A216 R217 S218 V219 K220 W221 L222 D223 S224 I225 N226 E231 F235 F236 M237 Q238 K239 D240 Y241 N249 W250 D251

N254 W255 S256 S257 R258 R259 D263 F264 P265 V266 M278 V279 K280 P281 V284 Y289 A290 V291 E299 R300 V301 D302 I303 W311 A314 S315 R316 E319 P320 G321 S326 D332 K333 W334 A335 W336 V337 L338 F339 E340 D344 V345 S346 Q347 T348 T349 E350 V351

K354 D357 S358 A359 A360 E365 N366 V367 E368 S369 V370 W371 R374 G375 S380 W381 R387 L388 G389 HIS SER ASN LEU

● Molecule 1: SULFITE OXIDASE

Chain E:

Molecule 1: SULFITE OXIDASE bar diagram showing 4%, 68%, 25%, 5%

MET P2 R5 E9 R16 H17 P18 S19 L20 K21 K25 R34 L37 V38 S39 T43 P44 V45 K50 R51 N52 H53 P57 I58 V59 D60 H61 L62 Q63 S64 L69 T70 G71 L72 I73 Q74 N75 P76 R77 I81 L87 R103 K108 N111 V112

R113 D118 V119 K131 L132 A133 D134 V135 V139 K144 L132? V160? D161? -- transcribe labels: R113 D118 V119 K131 L132 A133 D134 V135 V139 L144 T145 R153 H154 V158 S159 V160 D161 K164 E165 K172 T176 L177 S178 T181 E184 A185 D186 V187 L188 L189 A190 Y191 E196 N199 R200 D201 H202 G203 F204 P205 V208 R217 S218 V219 K220

W221 L222 D223 S224 E231 K239 D240 Y241 F244 N254 W255 S256 S257 R258 P265 D275 M278 V279 K280 P281 V284 K287 G288 Y289 A290 V291 R296 E299 D302 I303 D306 N310 A314 S315 R316 E319 P320 G321 I325 S326 E327 H328 S329

S330 S331 W336 E340 D344 V345 S346 Q347 T348 T349 E350 V351 D357 N361 E365 N366 V367 L373 R374 S380 W381 R387 L388 G389 HIS SER ASN LEU

• Molecule 1: SULFITE OXIDASE

Chain F:

MET P2 R5 E9 H17 P18 S19 L20 K21 E31 R34 S35 A36 L37 V38 S39 S40 F48 Y49 K50 R51 N52 H53 P57 I58 H61 L62 Q63 S64 L69 T70 G71 L72 I73 P76 R77 I81 K82 D83 L87 L96 V112 D118 V119 S120

K131 L132 A133 D134 L144 R153 H154 V155 E156 F157 V158 S159 V160 K164 E165 Y171 K172 L177 T181 N182 P183 L188 Y191 E196 N199 R200 D201 H202 G203 F204 P205 L206 R207 V208 A216 W221 L222 D223 N226 E230 E231 F244 W250

D251 N254 W255 S256 S257 R258 R259 D263 F264 P265 M278 V279 K280 V284 V291 S292 E299 I303 D306 K309 N310 W311 A314 S315 R316 G321 K322 Q323 Y324 I325 S326 W334 A335 W336 V337 L338 F339 E340 D344 T349 E350 V351 K354 A355

V362 V367 E368 L373 R374 G375 V376 L377 S380 W381 V384 R387 L388 G389 HIS SER ASN LEU

# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 222.92Å　351.27Å　158.28Å<br>90.00°　　90.00°　　90.00° | Depositor |
| Resolution (Å) | 182.57　–　2.60<br>29.93　–　2.60 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.0 (182.57-2.60)<br>99.0 (29.93-2.60) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.38 (at 2.61Å) | Xtriage |
| Refinement program | REFMAC 5.1.24 | Depositor |
| R, $R_{free}$ | 0.235　,　0.266<br>0.241　,　0.267 | Depositor<br>DCC |
| $R_{free}$ test set | 9369 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 53.8 | Xtriage |
| Anisotropy | 0.022 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 63.5 | EDS |
| L-test for twinning[2] | $< |L| > = 0.47, < L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 18888 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 56.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CS, MTQ, GOL

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 | 1.51 | 27/3085 (0.9%) | 1.39 | 40/4196 (1.0%) |
| 1 | B | 1.52 | 27/3085 (0.9%) | 1.39 | 33/4196 (0.8%) |
| 1 | C | 1.61 | 27/3085 (0.9%) | 1.32 | 27/4196 (0.6%) |
| 1 | D | 1.77 | 62/3085 (2.0%) | 1.49 | 45/4196 (1.1%) |
| 1 | E | 1.56 | 19/3085 (0.6%) | 1.43 | 41/4196 (1.0%) |
| 1 | F | 1.52 | 21/3085 (0.7%) | 1.39 | 30/4196 (0.7%) |
| All | All | 1.58 | 183/18510 (1.0%) | 1.40 | 216/25176 (0.9%) |

All (183) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | D | 389 | GLY | C-O | 11.27 | 1.41 | 1.23 |
| 1 | D | 156 | GLU | CD-OE1 | 10.77 | 1.37 | 1.25 |
| 1 | A | 278 | MET | CG-SD | 10.02 | 2.07 | 1.81 |
| 1 | B | 278 | MET | CG-SD | 9.57 | 2.06 | 1.81 |
| 1 | C | 241 | TYR | CD2-CE2 | 9.55 | 1.53 | 1.39 |
| 1 | D | 192 | GLU | CD-OE1 | 9.29 | 1.35 | 1.25 |
| 1 | E | 278 | MET | SD-CE | 9.19 | 2.29 | 1.77 |
| 1 | D | 10 | TYR | CD1-CE1 | -9.16 | 1.25 | 1.39 |
| 1 | F | 355 | ALA | CA-CB | -9.10 | 1.33 | 1.52 |
| 1 | B | 350 | GLU | CD-OE2 | 8.94 | 1.35 | 1.25 |
| 1 | C | 262 | MET | CG-SD | 8.63 | 2.03 | 1.81 |
| 1 | E | 380 | SER | CB-OG | -8.52 | 1.31 | 1.42 |
| 1 | D | 368 | GLU | CD-OE1 | 8.05 | 1.34 | 1.25 |
| 1 | C | 248 | VAL | CB-CG2 | 8.00 | 1.69 | 1.52 |
| 1 | A | 371 | TRP | CB-CG | 8.00 | 1.64 | 1.50 |
| 1 | F | 278 | MET | CG-SD | 7.98 | 2.01 | 1.81 |
| 1 | B | 316 | ARG | CB-CG | -7.76 | 1.31 | 1.52 |
| 1 | C | 327 | GLU | CD-OE1 | 7.66 | 1.34 | 1.25 |
| 1 | D | 359 | ALA | CA-CB | -7.55 | 1.36 | 1.52 |
| 1 | B | 324 | TYR | CD1-CE1 | -7.54 | 1.28 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | B | 278 | MET | CB-CG | 7.53 | 1.75 | 1.51 |
| 1 | C | 389 | GLY | C-O | 7.51 | 1.35 | 1.23 |
| 1 | B | 45 | VAL | CB-CG2 | 7.42 | 1.68 | 1.52 |
| 1 | B | 192 | GLU | CD-OE1 | 7.42 | 1.33 | 1.25 |
| 1 | A | 380 | SER | CB-OG | -7.38 | 1.32 | 1.42 |
| 1 | B | 362 | VAL | CB-CG2 | -7.33 | 1.37 | 1.52 |
| 1 | D | 278 | MET | SD-CE | 7.32 | 2.18 | 1.77 |
| 1 | B | 350 | GLU | CD-OE1 | 7.21 | 1.33 | 1.25 |
| 1 | D | 221 | TRP | CG-CD1 | 7.20 | 1.46 | 1.36 |
| 1 | E | 108 | LYS | CD-CE | 7.15 | 1.69 | 1.51 |
| 1 | F | 191 | TYR | CD1-CE1 | 7.13 | 1.50 | 1.39 |
| 1 | B | 241 | TYR | CD1-CE1 | -7.07 | 1.28 | 1.39 |
| 1 | D | 65 | TYR | CG-CD1 | 7.02 | 1.48 | 1.39 |
| 1 | E | 278 | MET | CG-SD | 6.98 | 1.99 | 1.81 |
| 1 | E | 221 | TRP | CG-CD1 | -6.96 | 1.27 | 1.36 |
| 1 | D | 10 | TYR | CD2-CE2 | -6.92 | 1.28 | 1.39 |
| 1 | F | 316 | ARG | CB-CG | -6.88 | 1.33 | 1.52 |
| 1 | D | 380 | SER | CB-OG | -6.88 | 1.33 | 1.42 |
| 1 | D | 21 | LYS | CD-CE | 6.86 | 1.68 | 1.51 |
| 1 | C | 353 | ALA | CA-CB | -6.81 | 1.38 | 1.52 |
| 1 | C | 65 | TYR | CD1-CE1 | -6.76 | 1.29 | 1.39 |
| 1 | A | 316 | ARG | CB-CG | -6.70 | 1.34 | 1.52 |
| 1 | B | 274 | GLU | CD-OE1 | 6.69 | 1.33 | 1.25 |
| 1 | C | 173 | ALA | CA-CB | 6.67 | 1.66 | 1.52 |
| 1 | D | 204 | PHE | CD2-CE2 | 6.66 | 1.52 | 1.39 |
| 1 | F | 244 | PHE | CD2-CE2 | -6.65 | 1.25 | 1.39 |
| 1 | F | 230 | GLU | CD-OE1 | 6.64 | 1.32 | 1.25 |
| 1 | C | 66 | SER | CB-OG | 6.57 | 1.50 | 1.42 |
| 1 | A | 367 | VAL | CB-CG1 | -6.57 | 1.39 | 1.52 |
| 1 | B | 351 | VAL | CB-CG1 | -6.54 | 1.39 | 1.52 |
| 1 | D | 41 | TYR | CD2-CE2 | 6.54 | 1.49 | 1.39 |
| 1 | A | 235 | PHE | CE1-CZ | 6.53 | 1.49 | 1.37 |
| 1 | A | 34 | ARG | CB-CG | -6.44 | 1.35 | 1.52 |
| 1 | C | 166 | GLU | CD-OE1 | 6.42 | 1.32 | 1.25 |
| 1 | F | 221 | TRP | CB-CG | -6.42 | 1.38 | 1.50 |
| 1 | E | 191 | TYR | CE2-CZ | 6.41 | 1.46 | 1.38 |
| 1 | C | 200 | ARG | NE-CZ | 6.41 | 1.41 | 1.33 |
| 1 | D | 239 | LYS | CD-CE | 6.39 | 1.67 | 1.51 |
| 1 | A | 278 | MET | CB-CG | 6.36 | 1.71 | 1.51 |
| 1 | E | 39 | SER | CB-OG | -6.36 | 1.33 | 1.42 |
| 1 | B | 199 | ASN | CB-CG | -6.32 | 1.36 | 1.51 |
| 1 | B | 115 | VAL | CA-CB | -6.30 | 1.41 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | C | 365 | GLU | CG-CD | 6.30 | 1.61 | 1.51 |
| 1 | D | 191 | TYR | CD2-CE2 | 6.28 | 1.48 | 1.39 |
| 1 | D | 368 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 1 | F | 250 | TRP | CB-CG | -6.24 | 1.39 | 1.50 |
| 1 | D | 108 | LYS | CG-CD | 6.23 | 1.73 | 1.52 |
| 1 | D | 31 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | F | 165 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 1 | D | 235 | PHE | CD2-CE2 | 6.20 | 1.51 | 1.39 |
| 1 | E | 231 | GLU | CD-OE1 | -6.19 | 1.18 | 1.25 |
| 1 | D | 311 | TRP | CB-CG | 6.19 | 1.61 | 1.50 |
| 1 | C | 166 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | C | 65 | TYR | CE2-CZ | -6.15 | 1.30 | 1.38 |
| 1 | D | 258 | ARG | CD-NE | -6.14 | 1.36 | 1.46 |
| 1 | C | 316 | ARG | CB-CG | -6.14 | 1.35 | 1.52 |
| 1 | D | 65 | TYR | CE2-CZ | 6.11 | 1.46 | 1.38 |
| 1 | C | 313 | GLU | CD-OE2 | 6.09 | 1.32 | 1.25 |
| 1 | D | 159 | SER | CB-OG | 6.09 | 1.50 | 1.42 |
| 1 | A | 165 | GLU | CD-OE2 | 6.09 | 1.32 | 1.25 |
| 1 | E | 165 | GLU | CD-OE1 | 6.08 | 1.32 | 1.25 |
| 1 | E | 45 | VAL | CB-CG2 | 6.06 | 1.65 | 1.52 |
| 1 | A | 365 | GLU | CG-CD | 6.05 | 1.61 | 1.51 |
| 1 | D | 354 | LYS | CB-CG | -6.05 | 1.36 | 1.52 |
| 1 | A | 300 | ARG | CB-CG | -6.04 | 1.36 | 1.52 |
| 1 | C | 184 | GLU | CG-CD | 6.02 | 1.60 | 1.51 |
| 1 | D | 239 | LYS | CE-NZ | 6.01 | 1.64 | 1.49 |
| 1 | E | 256 | SER | CB-OG | -6.00 | 1.34 | 1.42 |
| 1 | B | 112 | VAL | CA-CB | 5.97 | 1.67 | 1.54 |
| 1 | D | 255 | TRP | CB-CG | -5.97 | 1.39 | 1.50 |
| 1 | E | 111 | ASN | CB-CG | -5.96 | 1.37 | 1.51 |
| 1 | D | 311 | TRP | CG-CD1 | 5.93 | 1.45 | 1.36 |
| 1 | A | 230 | GLU | CD-OE1 | 5.89 | 1.32 | 1.25 |
| 1 | F | 9 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | A | 178 | SER | CB-OG | -5.87 | 1.34 | 1.42 |
| 1 | D | 93 | THR | C-O | 5.86 | 1.34 | 1.23 |
| 1 | E | 165 | GLU | CG-CD | 5.86 | 1.60 | 1.51 |
| 1 | F | 230 | GLU | CG-CD | 5.86 | 1.60 | 1.51 |
| 1 | D | 9 | GLU | CD-OE2 | 5.85 | 1.32 | 1.25 |
| 1 | D | 168 | GLY | C-O | 5.84 | 1.33 | 1.23 |
| 1 | D | 108 | LYS | CD-CE | 5.79 | 1.65 | 1.51 |
| 1 | B | 40 | SER | CB-OG | -5.78 | 1.34 | 1.42 |
| 1 | E | 241 | TYR | CB-CG | -5.75 | 1.43 | 1.51 |
| 1 | B | 303 | ILE | CA-CB | -5.73 | 1.41 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | A | 221 | TRP | CG-CD1 | -5.72 | 1.28 | 1.36 |
| 1 | B | 166 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | D | 290 | ALA | CA-CB | -5.72 | 1.40 | 1.52 |
| 1 | D | 374 | ARG | CZ-NH1 | 5.72 | 1.40 | 1.33 |
| 1 | E | 184 | GLU | CD-OE1 | 5.71 | 1.31 | 1.25 |
| 1 | C | 365 | GLU | CD-OE1 | 5.68 | 1.31 | 1.25 |
| 1 | A | 191 | TYR | CB-CG | 5.68 | 1.60 | 1.51 |
| 1 | C | 278 | MET | SD-CE | 5.68 | 2.09 | 1.77 |
| 1 | A | 139 | VAL | CB-CG2 | -5.67 | 1.41 | 1.52 |
| 1 | B | 337 | VAL | CB-CG1 | -5.67 | 1.41 | 1.52 |
| 1 | C | 235 | PHE | CD2-CE2 | 5.64 | 1.50 | 1.39 |
| 1 | A | 365 | GLU | CD-OE1 | 5.62 | 1.31 | 1.25 |
| 1 | D | 220 | LYS | CD-CE | 5.61 | 1.65 | 1.51 |
| 1 | B | 6 | GLY | C-O | -5.59 | 1.14 | 1.23 |
| 1 | B | 358 | SER | C-O | -5.59 | 1.12 | 1.23 |
| 1 | B | 241 | TYR | CB-CG | 5.57 | 1.60 | 1.51 |
| 1 | D | 9 | GLU | CD-OE1 | 5.57 | 1.31 | 1.25 |
| 1 | D | 113 | ARG | CB-CG | -5.57 | 1.37 | 1.52 |
| 1 | F | 278 | MET | CB-CG | 5.56 | 1.69 | 1.51 |
| 1 | B | 10 | TYR | CE1-CZ | 5.55 | 1.45 | 1.38 |
| 1 | D | 340 | GLU | CG-CD | 5.55 | 1.60 | 1.51 |
| 1 | D | 204 | PHE | CE1-CZ | 5.55 | 1.47 | 1.37 |
| 1 | D | 171 | TYR | CD2-CE2 | 5.55 | 1.47 | 1.39 |
| 1 | D | 5 | ARG | CZ-NH1 | 5.49 | 1.40 | 1.33 |
| 1 | D | 15 | PRO | CG-CD | 5.47 | 1.68 | 1.50 |
| 1 | D | 231 | GLU | CD-OE1 | 5.47 | 1.31 | 1.25 |
| 1 | F | 258 | ARG | CG-CD | 5.46 | 1.65 | 1.51 |
| 1 | A | 127 | TRP | CG-CD1 | -5.45 | 1.29 | 1.36 |
| 1 | F | 368 | GLU | CD-OE1 | 5.45 | 1.31 | 1.25 |
| 1 | D | 258 | ARG | NE-CZ | -5.45 | 1.25 | 1.33 |
| 1 | F | 324 | TYR | CB-CG | 5.45 | 1.59 | 1.51 |
| 1 | A | 299 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | D | 199 | ASN | CB-CG | -5.43 | 1.38 | 1.51 |
| 1 | D | 156 | GLU | CG-CD | 5.40 | 1.60 | 1.51 |
| 1 | C | 82 | LYS | CD-CE | 5.39 | 1.64 | 1.51 |
| 1 | D | 371 | TRP | CB-CG | 5.39 | 1.59 | 1.50 |
| 1 | D | 209 | VAL | CB-CG2 | 5.38 | 1.64 | 1.52 |
| 1 | D | 235 | PHE | CD1-CE1 | 5.37 | 1.50 | 1.39 |
| 1 | F | 334 | TRP | CB-CG | -5.37 | 1.40 | 1.50 |
| 1 | C | 291 | VAL | CA-CB | 5.37 | 1.66 | 1.54 |
| 1 | A | 165 | GLU | CD-OE1 | 5.36 | 1.31 | 1.25 |
| 1 | C | 230 | GLU | CG-CD | 5.35 | 1.59 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | F | 48 | PHE | CD1-CE1 | -5.35 | 1.28 | 1.39 |
| 1 | E | 21 | LYS | CD-CE | 5.32 | 1.64 | 1.51 |
| 1 | A | 294 | GLY | C-O | -5.31 | 1.15 | 1.23 |
| 1 | D | 220 | LYS | CE-NZ | 5.30 | 1.62 | 1.49 |
| 1 | B | 289 | TYR | CE1-CZ | 5.29 | 1.45 | 1.38 |
| 1 | E | 244 | PHE | CD1-CE1 | -5.29 | 1.28 | 1.39 |
| 1 | B | 383 | ARG | CD-NE | 5.28 | 1.55 | 1.46 |
| 1 | D | 316 | ARG | NE-CZ | 5.28 | 1.40 | 1.33 |
| 1 | F | 2 | PRO | CB-CG | 5.28 | 1.76 | 1.50 |
| 1 | A | 278 | MET | SD-CE | 5.23 | 2.07 | 1.77 |
| 1 | D | 166 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | F | 157 | PHE | CD1-CE1 | -5.22 | 1.28 | 1.39 |
| 1 | A | 271 | CYS | CB-SG | -5.21 | 1.73 | 1.81 |
| 1 | D | 192 | GLU | CG-CD | 5.19 | 1.59 | 1.51 |
| 1 | D | 266 | VAL | CA-CB | -5.17 | 1.43 | 1.54 |
| 1 | D | 334 | TRP | CE3-CZ3 | 5.15 | 1.47 | 1.38 |
| 1 | C | 184 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | A | 230 | GLU | CG-CD | 5.14 | 1.59 | 1.51 |
| 1 | C | 316 | ARG | CG-CD | 5.14 | 1.64 | 1.51 |
| 1 | D | 10 | TYR | CE1-CZ | -5.13 | 1.31 | 1.38 |
| 1 | D | 241 | TYR | CD1-CE1 | -5.11 | 1.31 | 1.39 |
| 1 | D | 369 | SER | CB-OG | 5.11 | 1.48 | 1.42 |
| 1 | F | 384 | VAL | CB-CG1 | -5.10 | 1.42 | 1.52 |
| 1 | E | 131 | LYS | CD-CE | 5.10 | 1.64 | 1.51 |
| 1 | C | 278 | MET | CB-CG | 5.09 | 1.67 | 1.51 |
| 1 | A | 98 | CYS | CB-SG | 5.08 | 1.90 | 1.82 |
| 1 | F | 351 | VAL | CB-CG2 | -5.07 | 1.42 | 1.52 |
| 1 | D | 162 | ARG | CZ-NH1 | 5.06 | 1.39 | 1.33 |
| 1 | C | 10 | TYR | CD1-CE1 | 5.06 | 1.47 | 1.39 |
| 1 | D | 300 | ARG | CZ-NH1 | 5.05 | 1.39 | 1.33 |
| 1 | E | 365 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |
| 1 | A | 354 | LYS | CD-CE | 5.04 | 1.63 | 1.51 |
| 1 | B | 258 | ARG | NE-CZ | -5.03 | 1.26 | 1.33 |
| 1 | D | 12 | GLN | CG-CD | 5.03 | 1.62 | 1.51 |
| 1 | D | 316 | ARG | CZ-NH1 | 5.03 | 1.39 | 1.33 |
| 1 | A | 389 | GLY | C-O | 5.02 | 1.31 | 1.23 |
| 1 | B | 299 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |

All (216) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | F | 258 | ARG | NE-CZ-NH1 | 19.98 | 130.29 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | E | 258 | ARG | NE-CZ-NH2 | -18.19 | 111.20 | 120.30 |
| 1 | F | 258 | ARG | NE-CZ-NH2 | -17.91 | 111.34 | 120.30 |
| 1 | E | 258 | ARG | NE-CZ-NH1 | 15.58 | 128.09 | 120.30 |
| 1 | F | 259 | ARG | NE-CZ-NH2 | -14.73 | 112.93 | 120.30 |
| 1 | D | 258 | ARG | NE-CZ-NH2 | -13.19 | 113.71 | 120.30 |
| 1 | A | 258 | ARG | NE-CZ-NH2 | -12.91 | 113.84 | 120.30 |
| 1 | B | 258 | ARG | NE-CZ-NH2 | -12.72 | 113.94 | 120.30 |
| 1 | A | 258 | ARG | NE-CZ-NH1 | 11.72 | 126.16 | 120.30 |
| 1 | B | 259 | ARG | NE-CZ-NH2 | -11.30 | 114.65 | 120.30 |
| 1 | D | 60 | ASP | CB-CG-OD2 | 11.27 | 128.44 | 118.30 |
| 1 | E | 275 | ASP | CB-CG-OD2 | 11.16 | 128.34 | 118.30 |
| 1 | E | 302 | ASP | CB-CG-OD2 | 11.15 | 128.33 | 118.30 |
| 1 | A | 201 | ASP | CB-CG-OD2 | 11.00 | 128.20 | 118.30 |
| 1 | A | 186 | ASP | CB-CG-OD2 | 10.97 | 128.18 | 118.30 |
| 1 | A | 51 | ARG | NE-CZ-NH1 | 10.55 | 125.58 | 120.30 |
| 1 | D | 34 | ARG | NE-CZ-NH2 | -10.31 | 115.15 | 120.30 |
| 1 | B | 389 | GLY | CA-C-O | 10.02 | 138.64 | 120.60 |
| 1 | C | 258 | ARG | NE-CZ-NH2 | -9.91 | 115.34 | 120.30 |
| 1 | F | 263 | ASP | CB-CG-OD2 | 9.85 | 127.17 | 118.30 |
| 1 | B | 199 | ASN | CB-CA-C | -9.70 | 91.01 | 110.40 |
| 1 | B | 278 | MET | CG-SD-CE | 9.39 | 115.22 | 100.20 |
| 1 | C | 60 | ASP | CB-CG-OD2 | 9.34 | 126.70 | 118.30 |
| 1 | A | 208 | VAL | CB-CA-C | -9.31 | 93.71 | 111.40 |
| 1 | D | 258 | ARG | NE-CZ-NH1 | 9.22 | 124.91 | 120.30 |
| 1 | A | 118 | ASP | CB-CG-OD2 | 9.21 | 126.59 | 118.30 |
| 1 | D | 186 | ASP | CB-CG-OD2 | 9.17 | 126.56 | 118.30 |
| 1 | A | 223 | ASP | CB-CG-OD2 | 9.09 | 126.48 | 118.30 |
| 1 | B | 258 | ARG | NE-CZ-NH1 | 9.04 | 124.82 | 120.30 |
| 1 | D | 110 | ARG | NE-CZ-NH1 | 8.93 | 124.76 | 120.30 |
| 1 | D | 259 | ARG | NE-CZ-NH2 | -8.90 | 115.85 | 120.30 |
| 1 | F | 118 | ASP | CB-CG-OD2 | 8.83 | 126.25 | 118.30 |
| 1 | E | 374 | ARG | NE-CZ-NH1 | 8.73 | 124.67 | 120.30 |
| 1 | D | 217 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 |
| 1 | D | 223 | ASP | CB-CG-OD2 | 8.62 | 126.06 | 118.30 |
| 1 | A | 316 | ARG | NE-CZ-NH1 | 8.57 | 124.59 | 120.30 |
| 1 | F | 291 | VAL | CB-CA-C | -8.55 | 95.16 | 111.40 |
| 1 | B | 60 | ASP | CB-CG-OD2 | 8.52 | 125.97 | 118.30 |
| 1 | A | 199 | ASN | CB-CA-C | -8.48 | 93.44 | 110.40 |
| 1 | E | 316 | ARG | CG-CD-NE | -8.39 | 94.17 | 111.80 |
| 1 | E | 296 | ARG | NE-CZ-NH1 | 8.36 | 124.48 | 120.30 |
| 1 | B | 208 | VAL | CB-CA-C | -8.32 | 95.59 | 111.40 |
| 1 | D | 259 | ARG | NE-CZ-NH1 | 8.25 | 124.42 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | E | 291 | VAL | CB-CA-C | -8.21 | 95.79 | 111.40 |
| 1 | E | 199 | ASN | CB-CA-C | -8.16 | 94.08 | 110.40 |
| 1 | E | 380 | SER | CB-CA-C | -8.12 | 94.68 | 110.10 |
| 1 | A | 380 | SER | CB-CA-C | -8.00 | 94.90 | 110.10 |
| 1 | E | 275 | ASP | CB-CG-OD1 | -7.90 | 111.19 | 118.30 |
| 1 | A | 77 | ARG | NE-CZ-NH1 | 7.89 | 124.24 | 120.30 |
| 1 | B | 291 | VAL | CB-CA-C | -7.84 | 96.50 | 111.40 |
| 1 | A | 291 | VAL | CB-CA-C | -7.83 | 96.53 | 111.40 |
| 1 | D | 291 | VAL | CB-CA-C | -7.76 | 96.65 | 111.40 |
| 1 | B | 350 | GLU | OE1-CD-OE2 | 7.74 | 132.59 | 123.30 |
| 1 | E | 316 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 1 | E | 208 | VAL | CB-CA-C | -7.67 | 96.83 | 111.40 |
| 1 | E | 389 | GLY | CA-C-O | 7.62 | 134.33 | 120.60 |
| 1 | B | 316 | ARG | NE-CZ-NH1 | 7.50 | 124.05 | 120.30 |
| 1 | A | 302 | ASP | CB-CG-OD2 | 7.49 | 125.04 | 118.30 |
| 1 | D | 199 | ASN | CB-CA-C | -7.49 | 95.41 | 110.40 |
| 1 | E | 357 | ASP | CB-CG-OD2 | 7.45 | 125.00 | 118.30 |
| 1 | A | 258 | ARG | CG-CD-NE | -7.40 | 96.27 | 111.80 |
| 1 | A | 200 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 1 | E | 134 | ASP | CB-CG-OD2 | 7.22 | 124.80 | 118.30 |
| 1 | D | 217 | ARG | NE-CZ-NH1 | 7.21 | 123.90 | 120.30 |
| 1 | F | 77 | ARG | NE-CZ-NH2 | -7.21 | 116.70 | 120.30 |
| 1 | D | 5 | ARG | NE-CZ-NH2 | -7.10 | 116.75 | 120.30 |
| 1 | A | 316 | ARG | CG-CD-NE | -7.09 | 96.91 | 111.80 |
| 1 | A | 162 | ARG | NE-CZ-NH1 | 7.09 | 123.84 | 120.30 |
| 1 | C | 327 | GLU | N-CA-CB | 7.08 | 123.35 | 110.60 |
| 1 | E | 103 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 1 | A | 200 | ARG | NE-CZ-NH2 | -7.03 | 116.79 | 120.30 |
| 1 | D | 46 | ASP | CB-CG-OD2 | 6.98 | 124.58 | 118.30 |
| 1 | A | 51 | ARG | NE-CZ-NH2 | -6.96 | 116.82 | 120.30 |
| 1 | D | 113 | ARG | CB-CA-C | -6.92 | 96.56 | 110.40 |
| 1 | F | 258 | ARG | CD-NE-CZ | 6.90 | 133.26 | 123.60 |
| 1 | F | 223 | ASP | CB-CG-OD2 | 6.89 | 124.50 | 118.30 |
| 1 | C | 291 | VAL | CB-CA-C | -6.85 | 98.39 | 111.40 |
| 1 | C | 357 | ASP | CB-CG-OD2 | 6.80 | 124.42 | 118.30 |
| 1 | E | 316 | ARG | NE-CZ-NH2 | -6.76 | 116.92 | 120.30 |
| 1 | F | 77 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 1 | F | 207 | ARG | NE-CZ-NH2 | 6.72 | 123.66 | 120.30 |
| 1 | D | 60 | ASP | CB-CG-OD1 | -6.69 | 112.28 | 118.30 |
| 1 | F | 380 | SER | CB-CA-C | -6.68 | 97.41 | 110.10 |
| 1 | E | 16 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | C | 344 | ASP | CB-CG-OD2 | 6.66 | 124.29 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | B | 259 | ARG | NE-CZ-NH1 | 6.59 | 123.59 | 120.30 |
| 1 | A | 251 | ASP | CB-CG-OD1 | 6.58 | 124.23 | 118.30 |
| 1 | C | 200 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | B | 134 | ASP | CB-CG-OD2 | 6.54 | 124.19 | 118.30 |
| 1 | D | 83 | ASP | CB-CG-OD2 | 6.54 | 124.19 | 118.30 |
| 1 | D | 258 | ARG | CG-CD-NE | -6.54 | 98.06 | 111.80 |
| 1 | B | 186 | ASP | CB-CG-OD1 | 6.51 | 124.16 | 118.30 |
| 1 | F | 134 | ASP | CB-CG-OD2 | 6.49 | 124.14 | 118.30 |
| 1 | D | 302 | ASP | CB-CG-OD2 | 6.46 | 124.11 | 118.30 |
| 1 | C | 118 | ASP | CB-CG-OD2 | 6.41 | 124.07 | 118.30 |
| 1 | F | 387 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 1 | C | 306 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 1 | F | 306 | ASP | CB-CG-OD1 | 6.36 | 124.02 | 118.30 |
| 1 | B | 69 | LEU | CA-CB-CG | -6.32 | 100.76 | 115.30 |
| 1 | B | 103 | ARG | NE-CZ-NH2 | -6.32 | 117.14 | 120.30 |
| 1 | D | 389 | GLY | CA-C-O | 6.29 | 131.92 | 120.60 |
| 1 | E | 161 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | E | 34 | ARG | NE-CZ-NH1 | 6.27 | 123.43 | 120.30 |
| 1 | D | 316 | ARG | NE-CZ-NH2 | -6.26 | 117.17 | 120.30 |
| 1 | C | 83 | ASP | CB-CG-OD2 | 6.25 | 123.93 | 118.30 |
| 1 | E | 153 | ARG | NE-CZ-NH1 | 6.25 | 123.42 | 120.30 |
| 1 | D | 237 | MET | CG-SD-CE | -6.24 | 90.22 | 100.20 |
| 1 | A | 240 | ASP | CB-CG-OD1 | 6.20 | 123.88 | 118.30 |
| 1 | D | 240 | ASP | CB-CG-OD1 | 6.19 | 123.87 | 118.30 |
| 1 | D | 302 | ASP | CB-CA-C | -6.19 | 98.02 | 110.40 |
| 1 | E | 217 | ARG | NE-CZ-NH2 | -6.15 | 117.22 | 120.30 |
| 1 | F | 316 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | E | 69 | LEU | CA-CB-CG | -6.08 | 101.32 | 115.30 |
| 1 | C | 158 | VAL | CB-CA-C | -6.07 | 99.86 | 111.40 |
| 1 | E | 357 | ASP | OD1-CG-OD2 | -6.07 | 111.76 | 123.30 |
| 1 | C | 5 | ARG | NE-CZ-NH2 | -6.05 | 117.28 | 120.30 |
| 1 | D | 153 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | F | 208 | VAL | CB-CA-C | -6.02 | 99.96 | 111.40 |
| 1 | F | 278 | MET | CG-SD-CE | 6.00 | 109.80 | 100.20 |
| 1 | E | 201 | ASP | CB-CG-OD2 | 6.00 | 123.70 | 118.30 |
| 1 | B | 67 | VAL | CB-CA-C | -5.98 | 100.04 | 111.40 |
| 1 | C | 77 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 1 | A | 77 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 1 | A | 344 | ASP | CB-CG-OD2 | 5.96 | 123.67 | 118.30 |
| 1 | B | 161 | ASP | CB-CG-OD2 | 5.96 | 123.67 | 118.30 |
| 1 | F | 326 | SER | C-N-CA | -5.96 | 106.80 | 121.70 |
| 1 | D | 110 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | E | 118 | ASP | CB-CG-OD2 | 5.94 | 123.64 | 118.30 |
| 1 | C | 326 | SER | C-N-CA | -5.92 | 106.89 | 121.70 |
| 1 | F | 83 | ASP | CB-CG-OD2 | 5.92 | 123.63 | 118.30 |
| 1 | E | 5 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 1 | E | 132 | LEU | CB-CG-CD2 | 5.90 | 121.03 | 111.00 |
| 1 | E | 60 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | E | 77 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | B | 344 | ASP | CB-CG-OD2 | 5.86 | 123.57 | 118.30 |
| 1 | A | 134 | ASP | CB-CG-OD2 | 5.85 | 123.57 | 118.30 |
| 1 | E | 186 | ASP | CB-CG-OD2 | 5.84 | 123.56 | 118.30 |
| 1 | E | 113 | ARG | CB-CA-C | -5.82 | 98.76 | 110.40 |
| 1 | C | 316 | ARG | CB-CA-C | 5.81 | 122.03 | 110.40 |
| 1 | D | 374 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | C | 208 | VAL | CB-CA-C | -5.79 | 100.41 | 111.40 |
| 1 | E | 326 | SER | C-N-CA | -5.75 | 107.32 | 121.70 |
| 1 | D | 239 | LYS | CA-CB-CG | 5.75 | 126.04 | 113.40 |
| 1 | A | 34 | ARG | N-CA-CB | -5.71 | 100.31 | 110.60 |
| 1 | D | 8 | SER | CB-CA-C | -5.70 | 99.27 | 110.10 |
| 1 | E | 388 | LEU | CB-CG-CD1 | -5.68 | 101.34 | 111.00 |
| 1 | E | 72 | LEU | CB-CG-CD1 | 5.67 | 120.64 | 111.00 |
| 1 | C | 77 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | F | 263 | ASP | OD1-CG-OD2 | -5.64 | 112.58 | 123.30 |
| 1 | A | 306 | ASP | CB-CG-OD2 | 5.63 | 123.37 | 118.30 |
| 1 | C | 259 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | A | 326 | SER | C-N-CA | -5.62 | 107.66 | 121.70 |
| 1 | B | 102 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | B | 278 | MET | CB-CG-SD | 5.57 | 129.12 | 112.40 |
| 1 | B | 326 | SER | C-N-CA | -5.54 | 107.84 | 121.70 |
| 1 | E | 223 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |
| 1 | F | 201 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |
| 1 | B | 387 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 1 | E | 43 | THR | OG1-CB-CG2 | -5.51 | 97.33 | 110.00 |
| 1 | E | 357 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | B | 153 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | F | 326 | SER | O-C-N | -5.46 | 113.97 | 122.70 |
| 1 | B | 188 | LEU | CB-CG-CD1 | -5.45 | 101.74 | 111.00 |
| 1 | F | 316 | ARG | CG-CD-NE | -5.44 | 100.37 | 111.80 |
| 1 | C | 69 | LEU | CA-CB-CG | -5.44 | 102.80 | 115.30 |
| 1 | B | 357 | ASP | CB-CG-OD1 | 5.43 | 123.18 | 118.30 |
| 1 | B | 118 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 1 | C | 380 | SER | CB-CA-C | -5.38 | 99.88 | 110.10 |
| 1 | A | 113 | ARG | NE-CZ-NH1 | -5.37 | 117.61 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | B | 258 | ARG | CG-CD-NE | -5.36 | 100.54 | 111.80 |
| 1 | C | 258 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | A | 46 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | F | 389 | GLY | CA-C-O | -5.33 | 111.01 | 120.60 |
| 1 | D | 387 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 1 | F | 251 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | D | 118 | ASP | CB-CG-OD2 | 5.30 | 123.08 | 118.30 |
| 1 | D | 326 | SER | C-N-CA | -5.30 | 108.44 | 121.70 |
| 1 | A | 296 | ARG | NE-CZ-NH2 | -5.29 | 117.66 | 120.30 |
| 1 | A | 332 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | A | 357 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | F | 34 | ARG | N-CA-CB | -5.26 | 101.14 | 110.60 |
| 1 | D | 108 | LYS | CD-CE-NZ | 5.25 | 123.79 | 111.70 |
| 1 | D | 181 | THR | N-CA-CB | -5.25 | 100.33 | 110.30 |
| 1 | C | 34 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 1 | E | 258 | ARG | CG-CD-NE | -5.24 | 100.80 | 111.80 |
| 1 | A | 326 | SER | O-C-N | -5.23 | 114.33 | 122.70 |
| 1 | D | 162 | ARG | CG-CD-NE | -5.23 | 100.82 | 111.80 |
| 1 | D | 357 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | D | 34 | ARG | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 1 | B | 326 | SER | O-C-N | -5.21 | 114.36 | 122.70 |
| 1 | C | 46 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | F | 362 | VAL | CG1-CB-CG2 | -5.19 | 102.59 | 110.90 |
| 1 | A | 37 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 1 | E | 258 | ARG | CD-NE-CZ | 5.18 | 130.85 | 123.60 |
| 1 | D | 263 | ASP | CB-CG-OD1 | 5.15 | 122.94 | 118.30 |
| 1 | A | 243 | MET | CG-SD-CE | 5.15 | 108.44 | 100.20 |
| 1 | C | 326 | SER | O-C-N | -5.14 | 114.48 | 122.70 |
| 1 | A | 259 | ARG | NE-CZ-NH2 | -5.13 | 117.73 | 120.30 |
| 1 | A | 278 | MET | CB-CG-SD | 5.13 | 127.80 | 112.40 |
| 1 | A | 258 | ARG | CD-NE-CZ | 5.12 | 130.77 | 123.60 |
| 1 | C | 199 | ASN | CB-CA-C | 5.12 | 120.64 | 110.40 |
| 1 | C | 201 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 1 | D | 162 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | F | 316 | ARG | CB-CA-C | 5.10 | 120.60 | 110.40 |
| 1 | C | 382 | HIS | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | D | 326 | SER | O-C-N | -5.08 | 114.57 | 122.70 |
| 1 | B | 258 | ARG | CD-NE-CZ | 5.07 | 130.70 | 123.60 |
| 1 | A | 162 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | D | 166 | GLU | CB-CA-C | 5.06 | 120.51 | 110.40 |
| 1 | D | 4 | ILE | CB-CA-C | -5.04 | 101.51 | 111.60 |
| 1 | D | 110 | ARG | N-CA-CB | 5.03 | 119.66 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | B | 306 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | D | 316 | ARG | CA-CB-CG | 5.03 | 124.45 | 113.40 |
| 1 | F | 119 | VAL | CG1-CB-CG2 | 5.02 | 118.94 | 110.90 |
| 1 | B | 316 | ARG | CG-CD-NE | -5.01 | 101.27 | 111.80 |
| 1 | B | 162 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |

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 | 3014 | 0 | 2998 | 61 | 0 |
| 1 | B | 3014 | 0 | 2998 | 58 | 0 |
| 1 | C | 3014 | 0 | 2998 | 84 | 0 |
| 1 | D | 3014 | 0 | 2999 | 128 | 0 |
| 1 | E | 3014 | 0 | 2998 | 48 | 0 |
| 1 | F | 3014 | 0 | 2997 | 66 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 2 | E | 2 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 6 | 0 | 8 | 0 | 0 |
| 3 | B | 6 | 0 | 7 | 0 | 0 |
| 3 | C | 6 | 0 | 8 | 2 | 0 |
| 3 | D | 6 | 0 | 8 | 2 | 0 |
| 3 | E | 6 | 0 | 8 | 1 | 0 |
| 3 | F | 6 | 0 | 8 | 0 | 0 |
| 4 | A | 27 | 0 | 6 | 2 | 0 |
| 4 | B | 27 | 0 | 6 | 2 | 0 |
| 4 | C | 27 | 0 | 6 | 3 | 0 |
| 4 | D | 27 | 0 | 6 | 9 | 0 |
| 4 | E | 27 | 0 | 6 | 1 | 0 |
| 4 | F | 27 | 0 | 6 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | A | 105 | 0 | 0 | 9 | 0 |
| 5 | B | 95 | 0 | 0 | 16 | 0 |
| 5 | C | 86 | 0 | 0 | 17 | 0 |
| 5 | D | 90 | 0 | 0 | 54 | 0 |
| 5 | E | 107 | 0 | 0 | 8 | 0 |
| 5 | F | 111 | 0 | 0 | 11 | 0 |
| All | All | 18888 | 0 | 18071 | 439 | 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 (439) 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:278:MET:CG | 1:B:278:MET:CB | 1.75 | 1.59 |
| 1:B:2:PRO:CB | 1:B:2:PRO:CG | 1.74 | 1.52 |
| 1:F:2:PRO:CG | 1:F:2:PRO:CB | 1.76 | 1.50 |
| 1:F:278:MET:CG | 1:F:278:MET:SD | 2.01 | 1.48 |
| 1:F:278:MET:SD | 1:F:278:MET:CE | 2.03 | 1.47 |
| 1:C:262:MET:CG | 1:C:262:MET:SD | 2.03 | 1.46 |
| 1:B:278:MET:CG | 1:B:278:MET:SD | 2.06 | 1.44 |
| 1:A:278:MET:SD | 1:A:278:MET:CE | 2.07 | 1.43 |
| 1:A:278:MET:SD | 1:A:278:MET:CG | 2.07 | 1.42 |
| 1:C:278:MET:SD | 1:C:278:MET:CE | 2.09 | 1.40 |
| 1:D:278:MET:SD | 1:D:278:MET:CE | 2.18 | 1.30 |
| 1:E:278:MET:CE | 1:E:278:MET:SD | 2.29 | 1.20 |
| 1:D:162:ARG:HD3 | 5:D:2036:HOH:O | 1.39 | 1.17 |
| 1:D:136:LEU:HA | 5:D:2029:HOH:O | 1.55 | 1.05 |
| 1:D:98:CYS:SG | 4:D:1394:MTQ:OM1 | 2.18 | 1.02 |
| 1:C:144:LEU:HD11 | 1:D:144:LEU:HD11 | 1.36 | 1.01 |
| 1:A:98:CYS:SG | 4:A:1394:MTQ:OM1 | 2.24 | 0.96 |
| 1:F:77:ARG:HG3 | 1:F:77:ARG:HH11 | 1.28 | 0.94 |
| 1:B:53:HIS:HE1 | 5:B:2053:HOH:O | 1.51 | 0.93 |
| 1:E:17:HIS:ND1 | 1:E:18:PRO:HD2 | 1.86 | 0.90 |
| 1:C:17:HIS:ND1 | 1:C:18:PRO:HD2 | 1.86 | 0.89 |
| 1:C:77:ARG:HG3 | 1:C:77:ARG:HH11 | 1.34 | 0.88 |
| 1:D:17:HIS:CD2 | 1:D:18:PRO:HD2 | 2.11 | 0.86 |
| 1:D:80:PHE:HB2 | 1:D:83:ASP:OD2 | 1.77 | 0.85 |
| 1:C:144:LEU:CD1 | 1:D:144:LEU:HD11 | 2.07 | 0.84 |
| 1:C:73:ILE:CG1 | 1:C:139:VAL:HG12 | 2.07 | 0.84 |
| 1:E:154:HIS:HD2 | 1:E:176:THR:HA | 1.41 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:77:ARG:HG3 | 1:E:77:ARG:HH11 | 1.41 | 0.84 |
| 1:D:21:LYS:HE2 | 5:E:2028:HOH:O | 1.77 | 0.83 |
| 1:C:73:ILE:HG12 | 1:C:139:VAL:HG12 | 1.61 | 0.82 |
| 1:A:202:HIS:CE1 | 5:A:2061:HOH:O | 2.30 | 0.82 |
| 1:D:157:PHE:CD1 | 5:D:2033:HOH:O | 2.31 | 0.82 |
| 1:C:278:MET:HB2 | 5:C:2085:HOH:O | 1.80 | 0.81 |
| 1:E:299:GLU:OE2 | 1:F:258:ARG:HD3 | 1.80 | 0.81 |
| 1:B:278:MET:HB3 | 5:B:2062:HOH:O | 1.80 | 0.81 |
| 1:C:73:ILE:HG12 | 1:C:139:VAL:CG1 | 2.10 | 0.81 |
| 1:C:51:ARG:NH2 | 1:C:53:HIS:HE1 | 1.78 | 0.80 |
| 1:A:77:ARG:HG3 | 1:A:77:ARG:HH11 | 1.47 | 0.79 |
| 1:D:254:ASN:C | 1:D:254:ASN:HD22 | 1.86 | 0.79 |
| 1:D:67:VAL:HG21 | 1:D:206:LEU:HD23 | 1.66 | 0.78 |
| 1:D:303:ILE:HD12 | 1:D:314:ALA:HB2 | 1.64 | 0.78 |
| 1:C:77:ARG:HG3 | 1:C:77:ARG:NH1 | 1.97 | 0.78 |
| 1:E:177:LEU:O | 1:E:181:THR:HB | 1.85 | 0.77 |
| 1:C:371:TRP:HA | 5:C:2082:HOH:O | 1.85 | 0.76 |
| 1:D:79:LEU:N | 5:D:2013:HOH:O | 2.17 | 0.76 |
| 1:F:50:LYS:HE3 | 1:F:202:HIS:CE1 | 2.21 | 0.76 |
| 1:F:199:ASN:C | 1:F:199:ASN:HD22 | 1.88 | 0.75 |
| 1:D:72:LEU:HD13 | 5:D:2056:HOH:O | 1.86 | 0.75 |
| 1:A:254:ASN:C | 1:A:254:ASN:HD22 | 1.88 | 0.74 |
| 1:A:202:HIS:CD2 | 5:A:2061:HOH:O | 2.39 | 0.74 |
| 1:A:258:ARG:HD3 | 1:B:299:GLU:OE2 | 1.87 | 0.74 |
| 1:C:131:LYS:NZ | 1:C:183:PRO:O | 2.20 | 0.74 |
| 1:F:389:GLY:HA3 | 5:F:2110:HOH:O | 1.87 | 0.74 |
| 1:A:299:GLU:OE2 | 1:B:258:ARG:HD3 | 1.88 | 0.73 |
| 1:C:89:LYS:NZ | 1:C:192:GLU:OE1 | 2.20 | 0.73 |
| 1:D:192:GLU:HB3 | 5:D:2048:HOH:O | 1.89 | 0.73 |
| 1:D:78:LYS:HG2 | 5:D:2011:HOH:O | 1.90 | 0.71 |
| 1:D:98:CYS:SG | 4:D:1394:MTQ:S2' | 2.89 | 0.70 |
| 1:D:108:LYS:HD2 | 5:E:2005:HOH:O | 1.91 | 0.70 |
| 1:C:389:GLY:HA3 | 5:C:2085:HOH:O | 1.91 | 0.70 |
| 1:D:177:LEU:O | 1:D:181:THR:HB | 1.92 | 0.70 |
| 1:F:77:ARG:HG3 | 1:F:77:ARG:NH1 | 1.96 | 0.69 |
| 1:E:63:GLN:O | 1:E:64:SER:HB3 | 1.90 | 0.69 |
| 1:C:144:LEU:HD11 | 1:D:144:LEU:CD1 | 2.19 | 0.69 |
| 1:F:50:LYS:HE3 | 1:F:202:HIS:HE1 | 1.58 | 0.69 |
| 1:B:53:HIS:CE1 | 5:B:2053:HOH:O | 2.32 | 0.69 |
| 1:E:144:LEU:HD11 | 1:F:144:LEU:HD11 | 1.74 | 0.68 |
| 1:C:51:ARG:NH2 | 1:C:53:HIS:CE1 | 2.61 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:258:ARG:HD3 | 1:D:299:GLU:OE2 | 1.92 | 0.68 |
| 1:B:340:GLU:HG3 | 5:B:2070:HOH:O | 1.94 | 0.68 |
| 1:F:322:LYS:NZ | 5:F:2082:HOH:O | 2.26 | 0.68 |
| 1:D:162:ARG:HG2 | 1:D:168:GLY:O | 1.93 | 0.68 |
| 1:D:157:PHE:CG | 5:D:2033:HOH:O | 2.47 | 0.68 |
| 4:C:1394:MTQ:OM2 | 4:C:1394:MTQ:MOM1 | 1.65 | 0.67 |
| 1:C:254:ASN:HD22 | 1:C:254:ASN:C | 1.96 | 0.67 |
| 1:A:202:HIS:CG | 5:A:2061:HOH:O | 2.47 | 0.67 |
| 1:D:157:PHE:C | 5:D:2034:HOH:O | 2.33 | 0.66 |
| 1:F:50:LYS:CE | 1:F:202:HIS:HE1 | 2.08 | 0.66 |
| 4:E:1394:MTQ:MOM1 | 4:E:1394:MTQ:OM2 | 1.67 | 0.66 |
| 1:C:371:TRP:CA | 5:C:2082:HOH:O | 2.43 | 0.66 |
| 1:F:50:LYS:NZ | 1:F:202:HIS:HE1 | 1.94 | 0.66 |
| 1:C:303:ILE:HD12 | 1:C:314:ALA:HB2 | 1.77 | 0.65 |
| 1:C:262:MET:CG | 1:C:262:MET:CE | 2.74 | 0.65 |
| 1:E:254:ASN:C | 1:E:254:ASN:HD22 | 1.99 | 0.65 |
| 1:A:202:HIS:NE2 | 5:A:2061:HOH:O | 2.29 | 0.64 |
| 4:F:1394:MTQ:OM2 | 4:F:1394:MTQ:MOM1 | 1.66 | 0.64 |
| 1:C:154:HIS:HD2 | 3:C:1393:GOL:O3 | 1.81 | 0.64 |
| 1:D:90:TYR:OH | 5:D:2015:HOH:O | 2.15 | 0.64 |
| 1:A:254:ASN:ND2 | 1:A:256:SER:H | 1.96 | 0.64 |
| 1:C:103:ARG:HD2 | 1:C:115:VAL:O | 1.97 | 0.64 |
| 4:A:1394:MTQ:OM1 | 4:A:1394:MTQ:MOM1 | 1.69 | 0.64 |
| 1:A:177:LEU:O | 1:A:181:THR:HB | 1.98 | 0.63 |
| 1:D:225:ILE:C | 5:D:2055:HOH:O | 2.36 | 0.63 |
| 1:D:225:ILE:N | 5:D:2055:HOH:O | 2.31 | 0.63 |
| 1:B:73:ILE:CG1 | 1:B:139:VAL:HG12 | 2.28 | 0.63 |
| 1:E:63:GLN:O | 1:E:64:SER:CB | 2.45 | 0.63 |
| 1:C:365:GLU:HG3 | 1:C:381:TRP:CZ3 | 2.34 | 0.63 |
| 1:B:73:ILE:HG12 | 1:B:139:VAL:CG1 | 2.29 | 0.63 |
| 4:B:1394:MTQ:OM2 | 4:B:1394:MTQ:MOM1 | 1.70 | 0.63 |
| 1:F:177:LEU:O | 1:F:181:THR:HB | 1.99 | 0.62 |
| 1:C:5:ARG:HD3 | 5:C:2001:HOH:O | 1.99 | 0.62 |
| 1:D:346:SER:HA | 5:D:2078:HOH:O | 1.98 | 0.62 |
| 1:F:53:HIS:HD2 | 1:F:171:TYR:CE1 | 2.17 | 0.62 |
| 1:A:17:HIS:CD2 | 1:A:18:PRO:HD2 | 2.34 | 0.62 |
| 4:D:1394:MTQ:OM1 | 4:D:1394:MTQ:MOM1 | 1.70 | 0.62 |
| 1:C:10:TYR:CE2 | 1:C:55:PRO:HG3 | 2.34 | 0.62 |
| 1:B:322:LYS:NZ | 5:B:2073:HOH:O | 2.32 | 0.62 |
| 1:E:328:HIS:HD2 | 1:E:329:SER:H | 1.47 | 0.62 |
| 1:A:254:ASN:HD22 | 1:A:255:TRP:N | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:53:HIS:HD2 | 1:F:171:TYR:CD1 | 2.18 | 0.62 |
| 1:F:303:ILE:HD12 | 1:F:314:ALA:HB2 | 1.81 | 0.62 |
| 1:A:144:LEU:HD11 | 1:B:144:LEU:HD11 | 1.82 | 0.62 |
| 1:C:387:ARG:CG | 1:C:387:ARG:HH11 | 2.12 | 0.62 |
| 1:C:13:GLU:OE1 | 1:C:56:ILE:HG12 | 2.00 | 0.62 |
| 1:C:246:PRO:HD2 | 5:D:2069:HOH:O | 2.00 | 0.61 |
| 1:C:299:GLU:OE2 | 1:D:258:ARG:HD3 | 2.01 | 0.61 |
| 1:B:77:ARG:HH11 | 1:B:77:ARG:HG3 | 1.64 | 0.61 |
| 1:A:57:PRO:HD2 | 1:A:221:TRP:CE2 | 2.36 | 0.61 |
| 1:D:78:LYS:HE3 | 5:D:2011:HOH:O | 2.01 | 0.60 |
| 1:A:254:ASN:C | 1:A:254:ASN:ND2 | 2.51 | 0.60 |
| 4:D:1394:MTQ:MOM1 | 4:D:1394:MTQ:OM2 | 1.72 | 0.60 |
| 1:E:258:ARG:HD3 | 1:F:299:GLU:OE2 | 2.01 | 0.60 |
| 1:C:248:VAL:HG12 | 1:C:373:LEU:HD22 | 1.82 | 0.60 |
| 1:D:2:PRO:HA | 5:D:2001:HOH:O | 2.01 | 0.60 |
| 1:D:82:LYS:HD3 | 5:D:2014:HOH:O | 2.00 | 0.60 |
| 1:A:48:PHE:HB3 | 1:A:202:HIS:HE1 | 1.66 | 0.60 |
| 1:F:71:GLY:O | 1:F:73:ILE:N | 2.33 | 0.60 |
| 1:F:254:ASN:C | 1:F:254:ASN:HD22 | 2.02 | 0.60 |
| 1:D:158:VAL:N | 5:D:2034:HOH:O | 2.34 | 0.60 |
| 1:F:311:TRP:CZ2 | 1:F:354:LYS:HE3 | 2.37 | 0.60 |
| 1:A:25:LYS:HE2 | 1:D:239:LYS:NZ | 2.17 | 0.59 |
| 1:D:21:LYS:CE | 5:E:2028:HOH:O | 2.42 | 0.59 |
| 1:E:77:ARG:HH11 | 1:E:77:ARG:CG | 2.13 | 0.59 |
| 1:E:154:HIS:CD2 | 1:E:176:THR:HA | 2.32 | 0.59 |
| 1:F:53:HIS:CD2 | 1:F:171:TYR:CE1 | 2.90 | 0.59 |
| 1:F:17:HIS:HD2 | 1:F:19:SER:OG | 1.86 | 0.59 |
| 1:C:387:ARG:HH11 | 1:C:387:ARG:HG2 | 1.67 | 0.59 |
| 1:D:66:SER:HB2 | 5:D:2013:HOH:O | 2.01 | 0.59 |
| 1:D:203:GLY:HA2 | 1:D:221:TRP:CD1 | 2.38 | 0.59 |
| 1:C:254:ASN:C | 1:C:254:ASN:ND2 | 2.56 | 0.59 |
| 1:A:50:LYS:HE3 | 1:A:202:HIS:NE2 | 2.17 | 0.58 |
| 1:F:63:GLN:O | 1:F:64:SER:CB | 2.49 | 0.58 |
| 1:D:224:SER:HB2 | 5:D:2055:HOH:O | 2.04 | 0.58 |
| 1:B:73:ILE:HG12 | 1:B:139:VAL:HG11 | 1.85 | 0.58 |
| 1:C:367:VAL:HG13 | 1:C:380:SER:OG | 2.03 | 0.58 |
| 1:D:139:VAL:HB | 5:D:2029:HOH:O | 2.03 | 0.58 |
| 4:D:1394:MTQ:OM1 | 4:D:1394:MTQ:S1' | 2.62 | 0.58 |
| 1:C:71:GLY:O | 1:C:73:ILE:N | 2.36 | 0.57 |
| 1:B:278:MET:HA | 5:B:2062:HOH:O | 2.02 | 0.57 |
| 1:E:328:HIS:HD2 | 1:E:329:SER:N | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:63:GLN:O | 1:D:64:SER:CB | 2.53 | 0.57 |
| 1:E:77:ARG:HG3 | 1:E:77:ARG:NH1 | 2.08 | 0.57 |
| 1:A:63:GLN:O | 1:A:64:SER:CB | 2.51 | 0.57 |
| 1:C:53:HIS:CD2 | 1:C:236:PHE:CZ | 2.93 | 0.57 |
| 1:E:53:HIS:HE1 | 5:E:2066:HOH:O | 1.86 | 0.57 |
| 1:D:77:ARG:NH1 | 1:D:77:ARG:HG3 | 2.20 | 0.56 |
| 1:A:25:LYS:HE2 | 1:D:239:LYS:HZ3 | 1.71 | 0.56 |
| 1:B:57:PRO:HD2 | 1:B:221:TRP:CE2 | 2.40 | 0.56 |
| 1:D:79:LEU:C | 5:D:2013:HOH:O | 2.43 | 0.56 |
| 1:E:365:GLU:HG3 | 1:E:381:TRP:CZ3 | 2.41 | 0.56 |
| 1:B:63:GLN:O | 1:B:64:SER:CB | 2.52 | 0.56 |
| 1:A:204:PHE:CD1 | 1:A:205:PRO:HA | 2.41 | 0.56 |
| 1:D:67:VAL:HG21 | 1:D:206:LEU:CD2 | 2.36 | 0.56 |
| 1:B:278:MET:CB | 5:B:2062:HOH:O | 2.48 | 0.56 |
| 1:D:204:PHE:CD1 | 1:D:205:PRO:HA | 2.40 | 0.56 |
| 1:D:389:GLY:C | 5:D:2088:HOH:O | 2.43 | 0.56 |
| 1:A:325:ILE:HG21 | 1:A:328:HIS:HD2 | 1.70 | 0.55 |
| 1:D:156:GLU:HB3 | 1:D:226:ASN:HB3 | 1.88 | 0.55 |
| 1:F:199:ASN:C | 1:F:199:ASN:ND2 | 2.57 | 0.55 |
| 1:D:156:GLU:C | 5:D:2033:HOH:O | 2.44 | 0.55 |
| 1:F:77:ARG:HH11 | 1:F:77:ARG:CG | 2.10 | 0.55 |
| 1:D:63:GLN:O | 1:D:64:SER:OG | 2.17 | 0.55 |
| 1:B:254:ASN:C | 1:B:254:ASN:HD22 | 2.09 | 0.55 |
| 1:B:278:MET:CA | 5:B:2062:HOH:O | 2.54 | 0.55 |
| 1:D:254:ASN:C | 1:D:254:ASN:ND2 | 2.55 | 0.55 |
| 1:D:157:PHE:CE1 | 5:D:2033:HOH:O | 2.57 | 0.55 |
| 1:C:63:GLN:O | 1:C:64:SER:CB | 2.54 | 0.54 |
| 1:D:78:LYS:C | 5:D:2013:HOH:O | 2.43 | 0.54 |
| 1:D:254:ASN:ND2 | 1:D:256:SER:H | 2.06 | 0.54 |
| 1:E:366:ASN:HB2 | 5:E:2100:HOH:O | 2.06 | 0.54 |
| 1:F:153:ARG:C | 1:F:154:HIS:ND1 | 2.60 | 0.54 |
| 1:C:145:THR:O | 1:C:181:THR:HG21 | 2.08 | 0.54 |
| 1:E:254:ASN:C | 1:E:254:ASN:ND2 | 2.61 | 0.54 |
| 1:F:311:TRP:CH2 | 1:F:354:LYS:HE3 | 2.43 | 0.54 |
| 1:D:171:TYR:CZ | 5:D:2090:HOH:O | 2.52 | 0.53 |
| 1:D:332:ASP:C | 5:D:2077:HOH:O | 2.46 | 0.53 |
| 1:F:388:LEU:C | 5:F:2109:HOH:O | 2.46 | 0.53 |
| 1:C:387:ARG:CG | 1:C:387:ARG:NH1 | 2.70 | 0.53 |
| 1:D:281:PRO:HG3 | 5:D:2078:HOH:O | 2.07 | 0.53 |
| 1:F:131:LYS:NZ | 1:F:183:PRO:O | 2.35 | 0.53 |
| 1:C:34:ARG:HB2 | 5:C:2024:HOH:O | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:326:SER:HB3 | 5:C:2067:HOH:O | 2.08 | 0.53 |
| 1:B:71:GLY:O | 1:B:73:ILE:N | 2.41 | 0.53 |
| 1:D:154:HIS:HD2 | 3:D:1393:GOL:O3 | 1.91 | 0.53 |
| 1:B:246:PRO:HD2 | 5:B:2056:HOH:O | 2.07 | 0.53 |
| 1:F:291:VAL:HG13 | 1:F:336:TRP:HA | 1.91 | 0.53 |
| 1:D:34:ARG:HB2 | 5:D:2027:HOH:O | 2.07 | 0.52 |
| 1:D:203:GLY:HA2 | 1:D:221:TRP:NE1 | 2.24 | 0.52 |
| 1:A:154:HIS:ND1 | 1:A:231:GLU:CA | 2.72 | 0.52 |
| 1:D:136:LEU:CA | 5:D:2029:HOH:O | 2.33 | 0.52 |
| 1:D:17:HIS:HD2 | 1:D:18:PRO:HD2 | 1.69 | 0.52 |
| 1:D:117:TRP:N | 5:D:2019:HOH:O | 2.43 | 0.52 |
| 1:A:113:ARG:NH1 | 5:A:2039:HOH:O | 2.21 | 0.52 |
| 1:A:77:ARG:HG3 | 1:A:77:ARG:NH1 | 2.14 | 0.52 |
| 1:C:328:HIS:HD2 | 1:C:330:SER:H | 1.58 | 0.52 |
| 1:E:328:HIS:CD2 | 1:E:329:SER:N | 2.77 | 0.52 |
| 1:D:77:ARG:HG3 | 1:D:77:ARG:HH11 | 1.74 | 0.51 |
| 1:B:202:HIS:ND1 | 4:B:1394:MTQ:O2P | 2.33 | 0.51 |
| 1:D:73:ILE:HG13 | 1:D:139:VAL:HG12 | 1.92 | 0.51 |
| 1:E:357:ASP:OD1 | 1:E:361:ASN:HB2 | 2.10 | 0.51 |
| 1:A:12:GLN:HE21 | 1:D:167:ASN:ND2 | 2.09 | 0.51 |
| 1:C:77:ARG:HH11 | 1:C:77:ARG:CG | 2.14 | 0.51 |
| 1:D:367:VAL:HG22 | 5:D:2083:HOH:O | 2.10 | 0.51 |
| 1:A:154:HIS:ND1 | 1:A:231:GLU:HA | 2.26 | 0.51 |
| 1:B:139:VAL:HG12 | 1:B:139:VAL:O | 2.10 | 0.51 |
| 1:F:278:MET:HB3 | 5:F:2110:HOH:O | 2.09 | 0.51 |
| 1:C:291:VAL:HG13 | 1:C:336:TRP:HA | 1.92 | 0.51 |
| 4:D:1394:MTQ:C6 | 5:D:2090:HOH:O | 2.59 | 0.51 |
| 1:D:71:GLY:O | 1:D:73:ILE:N | 2.43 | 0.50 |
| 1:B:69:LEU:CD1 | 1:B:79:LEU:HD12 | 2.42 | 0.50 |
| 1:B:278:MET:CG | 1:B:278:MET:CA | 2.83 | 0.50 |
| 1:C:73:ILE:HG12 | 1:C:139:VAL:HG11 | 1.91 | 0.50 |
| 1:D:45:VAL:O | 1:D:50:LYS:NZ | 2.42 | 0.50 |
| 1:A:202:HIS:ND1 | 5:A:2061:HOH:O | 2.40 | 0.50 |
| 1:B:53:HIS:O | 5:B:2016:HOH:O | 2.19 | 0.50 |
| 1:B:254:ASN:C | 1:B:254:ASN:ND2 | 2.64 | 0.50 |
| 1:A:154:HIS:ND1 | 1:A:231:GLU:N | 2.60 | 0.50 |
| 1:D:38:VAL:HG22 | 1:D:338:LEU:HD22 | 1.93 | 0.49 |
| 1:A:37:LEU:HD22 | 1:A:336:TRP:HH2 | 1.77 | 0.49 |
| 1:A:145:THR:O | 1:A:181:THR:HG21 | 2.12 | 0.49 |
| 1:A:193:MET:CE | 1:A:202:HIS:HD1 | 2.25 | 0.49 |
| 1:B:165:GLU:O | 5:B:2033[A]:HOH:O | 2.20 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:50:LYS:HE3 | 1:C:202:HIS:HE1 | 1.77 | 0.49 |
| 1:C:21:LYS:HE3 | 5:C:2005:HOH:O | 2.12 | 0.49 |
| 1:F:254:ASN:C | 1:F:254:ASN:ND2 | 2.64 | 0.49 |
| 1:B:278:MET:H | 1:B:278:MET:HG3 | 1.77 | 0.49 |
| 1:C:38:VAL:HG13 | 1:C:38:VAL:O | 2.11 | 0.49 |
| 1:D:265:PRO:HD2 | 5:D:2065:HOH:O | 2.12 | 0.49 |
| 1:E:204:PHE:CD1 | 1:E:205:PRO:HA | 2.48 | 0.49 |
| 1:F:349:THR:CG2 | 5:F:2094:HOH:O | 2.61 | 0.49 |
| 1:F:367:VAL:HG13 | 1:F:380:SER:OG | 2.13 | 0.49 |
| 1:E:135:VAL:HG21 | 1:E:189:LEU:HD12 | 1.94 | 0.49 |
| 1:C:181:THR:HG23 | 5:C:2037:HOH:O | 2.12 | 0.49 |
| 1:D:73:ILE:CG1 | 1:D:139:VAL:HG12 | 2.43 | 0.49 |
| 1:D:157:PHE:HB3 | 5:D:2034:HOH:O | 2.12 | 0.49 |
| 1:D:165:GLU:HA | 5:D:2037:HOH:O | 2.13 | 0.49 |
| 1:A:25:LYS:CE | 1:D:239:LYS:NZ | 2.75 | 0.48 |
| 1:C:262:MET:CG | 1:C:262:MET:HE2 | 2.43 | 0.48 |
| 1:D:157:PHE:CG | 1:D:208:VAL:HG21 | 2.47 | 0.48 |
| 1:A:67:VAL:HG21 | 1:A:206:LEU:HD23 | 1.95 | 0.48 |
| 1:C:242:LYS:NZ | 5:C:2049:HOH:O | 2.47 | 0.48 |
| 1:B:164:LYS:HD3 | 5:B:2003:HOH:O | 2.13 | 0.48 |
| 1:D:281:PRO:HB3 | 5:D:2078:HOH:O | 2.12 | 0.48 |
| 1:E:21:LYS:HE2 | 5:E:2005:HOH:O | 2.13 | 0.48 |
| 1:E:139:VAL:HG12 | 1:E:139:VAL:O | 2.14 | 0.48 |
| 1:F:374:ARG:HD2 | 1:F:374:ARG:HA | 1.58 | 0.48 |
| 1:C:254:ASN:ND2 | 1:C:256:SER:H | 2.12 | 0.48 |
| 1:A:153:ARG:O | 1:A:154:HIS:CD2 | 2.66 | 0.48 |
| 1:D:289:TYR:CD1 | 1:D:289:TYR:C | 2.86 | 0.48 |
| 1:A:303:ILE:HD12 | 1:A:314:ALA:HB2 | 1.94 | 0.48 |
| 1:E:154:HIS:ND1 | 1:E:231:GLU:HA | 2.29 | 0.48 |
| 1:F:373:LEU:HA | 1:F:373:LEU:HD12 | 1.56 | 0.48 |
| 1:E:145:THR:O | 1:E:181:THR:HG21 | 2.14 | 0.47 |
| 1:F:204:PHE:CD1 | 1:F:205:PRO:HA | 2.48 | 0.47 |
| 1:A:71:GLY:O | 1:A:73:ILE:N | 2.46 | 0.47 |
| 1:E:71:GLY:O | 1:E:73:ILE:N | 2.46 | 0.47 |
| 1:F:389:GLY:N | 5:F:2109:HOH:O | 2.47 | 0.47 |
| 1:B:132:LEU:HD13 | 1:B:180:ALA:HB1 | 1.96 | 0.47 |
| 1:B:172:LYS:HE2 | 5:B:2040:HOH:O | 2.14 | 0.47 |
| 5:A:2012:HOH:O | 1:D:239:LYS:HG2 | 2.13 | 0.47 |
| 1:C:150:LEU:HD12 | 5:C:2014:HOH:O | 2.13 | 0.47 |
| 1:D:106:MET:SD | 1:D:375:GLY:HA2 | 2.54 | 0.47 |
| 1:C:202:HIS:O | 1:C:207:ARG:HD2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:377:LEU:HA | 5:F:2017:HOH:O | 2.13 | 0.47 |
| 1:B:73:ILE:HG13 | 1:B:139:VAL:HG12 | 1.95 | 0.47 |
| 1:B:43:THR:O | 1:B:194:ASN:ND2 | 2.48 | 0.47 |
| 1:D:136:LEU:C | 5:D:2029:HOH:O | 2.53 | 0.47 |
| 1:D:284:VAL:HG12 | 1:D:345:VAL:HG22 | 1.97 | 0.47 |
| 1:F:38:VAL:HG22 | 1:F:338:LEU:HD22 | 1.96 | 0.47 |
| 1:B:74:GLN:HB3 | 5:B:2018:HOH:O | 2.15 | 0.47 |
| 1:F:156:GLU:HB3 | 1:F:226:ASN:HB3 | 1.97 | 0.47 |
| 1:C:182:ASN:N | 5:C:2037:HOH:O | 2.47 | 0.47 |
| 1:D:210:VAL:HB | 5:D:2053:HOH:O | 2.15 | 0.47 |
| 1:F:51:ARG:CZ | 1:F:53:HIS:CE1 | 2.97 | 0.47 |
| 1:D:73:ILE:HG12 | 1:D:139:VAL:CG1 | 2.45 | 0.46 |
| 1:B:177:LEU:O | 1:B:181:THR:HB | 2.15 | 0.46 |
| 1:D:211:PRO:HB2 | 1:D:334:TRP:CD2 | 2.50 | 0.46 |
| 1:F:254:ASN:ND2 | 1:F:256:SER:H | 2.13 | 0.46 |
| 1:A:78:LYS:CE | 5:A:2025:HOH:O | 2.63 | 0.46 |
| 1:B:77:ARG:HG3 | 1:B:77:ARG:NH1 | 2.29 | 0.46 |
| 1:C:51:ARG:CZ | 1:C:53:HIS:CE1 | 2.98 | 0.46 |
| 1:C:135:VAL:HG21 | 1:C:189:LEU:HD12 | 1.97 | 0.46 |
| 1:C:326:SER:CB | 5:C:2067:HOH:O | 2.63 | 0.46 |
| 1:D:249:ASN:OD1 | 1:D:251:ASP:N | 2.45 | 0.46 |
| 1:E:239:LYS:HA | 1:E:255:TRP:CE3 | 2.51 | 0.46 |
| 1:E:303:ILE:HD12 | 1:E:314:ALA:HB2 | 1.96 | 0.46 |
| 1:A:25:LYS:CE | 1:D:239:LYS:HZ1 | 2.29 | 0.46 |
| 1:D:64:SER:HA | 1:D:80:PHE:HE2 | 1.81 | 0.46 |
| 1:F:38:VAL:O | 1:F:38:VAL:HG13 | 2.14 | 0.46 |
| 1:A:367:VAL:HG13 | 1:A:380:SER:OG | 2.14 | 0.46 |
| 1:D:45:VAL:HG21 | 5:D:2047:HOH:O | 2.16 | 0.46 |
| 1:D:48:PHE:CD1 | 1:D:202:HIS:HE1 | 2.34 | 0.46 |
| 1:D:347:GLN:HG2 | 1:D:348:THR:N | 2.29 | 0.46 |
| 1:D:169:GLY:C | 5:D:2040:HOH:O | 2.52 | 0.46 |
| 1:D:359:ALA:O | 1:D:360:ALA:HB3 | 2.16 | 0.46 |
| 1:E:154:HIS:CE1 | 1:E:231:GLU:HB3 | 2.51 | 0.46 |
| 1:B:378:ASN:OD1 | 1:B:380:SER:HB2 | 2.16 | 0.46 |
| 1:D:119:VAL:O | 1:D:119:VAL:HG13 | 2.16 | 0.46 |
| 1:B:291:VAL:HG13 | 1:B:336:TRP:HA | 1.97 | 0.46 |
| 1:F:51:ARG:NH2 | 1:F:53:HIS:HE1 | 2.14 | 0.45 |
| 1:F:154:HIS:CD2 | 1:F:231:GLU:HA | 2.51 | 0.45 |
| 1:B:326:SER:HB3 | 5:B:2075:HOH:O | 2.15 | 0.45 |
| 1:C:129:GLY:HA2 | 1:C:191:TYR:CE2 | 2.51 | 0.45 |
| 1:B:254:ASN:ND2 | 1:B:256:SER:H | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:31:GLU:OE1 | 1:F:120:SER:HB2 | 2.16 | 0.45 |
| 1:A:77:ARG:HH11 | 1:A:77:ARG:CG | 2.21 | 0.45 |
| 1:C:50:LYS:HE3 | 1:C:202:HIS:CE1 | 2.51 | 0.45 |
| 1:C:117:TRP:CE3 | 1:C:121:ALA:HB2 | 2.52 | 0.45 |
| 1:E:158:VAL:HG22 | 1:E:172:LYS:HD3 | 1.98 | 0.45 |
| 1:F:158:VAL:HG22 | 1:F:172:LYS:HD3 | 1.98 | 0.45 |
| 1:A:63:GLN:O | 1:A:64:SER:HB3 | 2.15 | 0.45 |
| 1:A:374:ARG:HD2 | 1:A:374:ARG:HA | 1.75 | 0.45 |
| 1:D:139:VAL:HG12 | 1:D:139:VAL:O | 2.17 | 0.45 |
| 1:A:347:GLN:HA | 1:A:388:LEU:HD11 | 1.98 | 0.45 |
| 1:B:32:PRO:HG3 | 1:B:47:LEU:O | 2.16 | 0.45 |
| 1:A:260:PRO:HB3 | 5:A:2070:HOH:O | 2.15 | 0.45 |
| 1:D:7:PRO:HD3 | 1:D:57:PRO:HA | 1.98 | 0.44 |
| 1:D:45:VAL:HG23 | 1:D:194:ASN:HD22 | 1.81 | 0.44 |
| 1:D:157:PHE:CB | 5:D:2034:HOH:O | 2.66 | 0.44 |
| 1:D:216:ALA:HA | 4:D:1394:MTQ:S1' | 2.58 | 0.44 |
| 1:C:110:ARG:HB3 | 1:C:371:TRP:CE2 | 2.52 | 0.44 |
| 3:D:1393:GOL:H12 | 5:D:2089:HOH:O | 2.16 | 0.44 |
| 1:C:50:LYS:CE | 1:C:202:HIS:HE1 | 2.31 | 0.44 |
| 1:D:132:LEU:HD22 | 1:D:132:LEU:O | 2.18 | 0.44 |
| 1:A:103:ARG:HD2 | 1:A:115:VAL:O | 2.18 | 0.44 |
| 1:B:204:PHE:CD1 | 1:B:205:PRO:HA | 2.52 | 0.44 |
| 1:C:34:ARG:HG2 | 1:C:271:CYS:O | 2.17 | 0.44 |
| 1:B:373:LEU:HD12 | 1:B:373:LEU:HA | 1.64 | 0.44 |
| 1:C:204:PHE:CD1 | 1:C:205:PRO:HA | 2.53 | 0.44 |
| 1:A:373:LEU:HA | 1:A:373:LEU:HD12 | 1.70 | 0.44 |
| 1:D:18:PRO:HG2 | 5:D:2006:HOH:O | 2.18 | 0.44 |
| 1:D:37:LEU:HD22 | 1:D:336:TRP:HH2 | 1.83 | 0.43 |
| 1:D:41:TYR:HA | 1:D:338:LEU:HD11 | 1.99 | 0.43 |
| 1:D:281:PRO:CB | 5:D:2078:HOH:O | 2.65 | 0.43 |
| 1:E:325:ILE:O | 1:E:331:SER:HB3 | 2.18 | 0.43 |
| 1:F:58:ILE:HD11 | 5:F:2004:HOH:O | 2.18 | 0.43 |
| 1:E:154:HIS:ND1 | 1:E:231:GLU:CA | 2.81 | 0.43 |
| 1:A:58:ILE:HG13 | 1:A:59:VAL:N | 2.32 | 0.43 |
| 1:A:129:GLY:HA2 | 1:A:191:TYR:CE2 | 2.53 | 0.43 |
| 1:C:110:ARG:HB3 | 1:C:371:TRP:NE1 | 2.33 | 0.43 |
| 1:D:10:TYR:CZ | 1:D:55:PRO:HG3 | 2.53 | 0.43 |
| 1:D:40:SER:OG | 1:D:42:VAL:O | 2.36 | 0.43 |
| 1:D:220:LYS:NZ | 4:D:1394:MTQ:O1P | 2.49 | 0.43 |
| 1:B:374:ARG:HD2 | 1:B:374:ARG:HA | 1.66 | 0.43 |
| 1:F:53:HIS:CD2 | 1:F:171:TYR:HE1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:57:PRO:HD2 | 1:D:221:TRP:CD2 | 2.54 | 0.43 |
| 1:E:347:GLN:HG2 | 1:E:348:THR:N | 2.34 | 0.43 |
| 1:F:153:ARG:O | 1:F:154:HIS:ND1 | 2.51 | 0.43 |
| 1:A:153:ARG:O | 1:A:154:HIS:HD2 | 2.02 | 0.43 |
| 1:C:182:ASN:CA | 5:C:2037:HOH:O | 2.67 | 0.43 |
| 1:D:222:LEU:HD12 | 5:D:2034:HOH:O | 2.18 | 0.43 |
| 1:C:241:TYR:OH | 4:C:1394:MTQ:OM1 | 2.33 | 0.43 |
| 1:C:359:ALA:O | 1:C:360:ALA:HB3 | 2.19 | 0.43 |
| 1:D:254:ASN:HD22 | 1:D:256:SER:H | 1.66 | 0.43 |
| 1:F:17:HIS:CD2 | 1:F:19:SER:OG | 2.68 | 0.43 |
| 1:F:254:ASN:HD22 | 1:F:255:TRP:N | 2.16 | 0.43 |
| 1:A:62:LEU:HD12 | 1:A:62:LEU:O | 2.19 | 0.43 |
| 1:C:164:LYS:HG2 | 5:C:2031:HOH:O | 2.17 | 0.43 |
| 1:E:231:GLU:OE2 | 3:E:1393:GOL:O2 | 2.37 | 0.43 |
| 1:D:365:GLU:HA | 1:D:381:TRP:CE2 | 2.54 | 0.43 |
| 1:A:316:ARG:HB2 | 1:A:337:VAL:CG1 | 2.49 | 0.42 |
| 1:B:37:LEU:HD22 | 1:B:336:TRP:HH2 | 1.83 | 0.42 |
| 1:E:347:GLN:HA | 1:E:388:LEU:HD11 | 2.01 | 0.42 |
| 1:F:354:LYS:HD3 | 1:F:381:TRP:CE2 | 2.54 | 0.42 |
| 1:B:31:GLU:OE1 | 1:B:120:SER:HB2 | 2.19 | 0.42 |
| 1:B:132:LEU:HD22 | 1:B:132:LEU:O | 2.19 | 0.42 |
| 1:D:255:TRP:HH2 | 1:D:374:ARG:HD3 | 1.83 | 0.42 |
| 1:C:175:ILE:HA | 3:C:1393:GOL:H31 | 2.01 | 0.42 |
| 1:C:211:PRO:HB2 | 1:C:334:TRP:CD2 | 2.54 | 0.42 |
| 1:E:373:LEU:HA | 1:E:373:LEU:HD12 | 1.71 | 0.42 |
| 1:E:306:ASP:OD2 | 1:E:310:ASN:HB2 | 2.18 | 0.42 |
| 1:F:51:ARG:NH2 | 1:F:53:HIS:CE1 | 2.88 | 0.42 |
| 1:B:254:ASN:HD22 | 1:B:255:TRP:N | 2.17 | 0.42 |
| 1:D:155:VAL:HG12 | 5:D:2033:HOH:O | 2.20 | 0.42 |
| 1:D:347:GLN:HA | 1:D:388:LEU:HD11 | 2.02 | 0.42 |
| 1:C:53:HIS:CD2 | 1:C:236:PHE:CE2 | 3.08 | 0.42 |
| 1:A:315:SER:O | 1:A:339:PHE:HA | 2.20 | 0.42 |
| 1:C:182:ASN:HB2 | 5:C:2037:HOH:O | 2.20 | 0.42 |
| 1:E:154:HIS:ND1 | 1:E:231:GLU:N | 2.68 | 0.42 |
| 1:A:26:GLU:HA | 1:A:27:PRO:HA | 1.87 | 0.41 |
| 1:B:53:HIS:CE1 | 1:B:236:PHE:CE2 | 3.09 | 0.41 |
| 1:C:291:VAL:HG13 | 1:C:336:TRP:CA | 2.50 | 0.41 |
| 1:C:387:ARG:HD3 | 5:C:2084:HOH:O | 2.19 | 0.41 |
| 1:E:21:LYS:CE | 5:E:2005:HOH:O | 2.68 | 0.41 |
| 1:E:73:ILE:HG12 | 1:E:139:VAL:HG11 | 2.02 | 0.41 |
| 1:F:349:THR:HA | 5:F:2094:HOH:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:F:367:VAL:HG22 | 5:F:2101:HOH:O | 2.20 | 0.41 |
| 1:D:77:ARG:HH11 | 1:D:77:ARG:CG | 2.32 | 0.41 |
| 1:E:57:PRO:HD2 | 1:E:221:TRP:CE2 | 2.56 | 0.41 |
| 1:C:51:ARG:HD2 | 4:C:1394:MTQ:S1' | 2.61 | 0.41 |
| 1:A:201:ASP:HB3 | 1:A:202:HIS:HD2 | 1.86 | 0.41 |
| 1:D:291:VAL:HG13 | 1:D:336:TRP:HA | 2.02 | 0.41 |
| 1:F:63:GLN:O | 1:F:64:SER:HB3 | 2.20 | 0.41 |
| 1:C:63:GLN:O | 1:C:64:SER:HB3 | 2.20 | 0.41 |
| 1:F:315:SER:O | 1:F:339:PHE:HA | 2.21 | 0.41 |
| 1:D:31:GLU:OE1 | 1:D:118:ASP:HB3 | 2.21 | 0.41 |
| 1:A:306:ASP:OD2 | 1:A:310:ASN:HB2 | 2.20 | 0.41 |
| 1:C:38:VAL:O | 1:C:38:VAL:CG1 | 2.69 | 0.41 |
| 1:D:367:VAL:HG13 | 1:D:380:SER:OG | 2.20 | 0.41 |
| 1:A:154:HIS:CE1 | 1:A:231:GLU:HB3 | 2.56 | 0.41 |
| 1:A:328:HIS:ND1 | 1:A:329:SER:N | 2.68 | 0.41 |
| 1:B:182:ASN:OD1 | 1:B:182:ASN:C | 2.59 | 0.41 |
| 1:B:199:ASN:HD22 | 1:B:199:ASN:HA | 1.45 | 0.41 |
| 1:D:117:TRP:CE3 | 1:D:121:ALA:HB2 | 2.55 | 0.41 |
| 1:D:162:ARG:CD | 5:D:2036:HOH:O | 2.24 | 0.41 |
| 1:D:165:GLU:CA | 5:D:2037:HOH:O | 2.69 | 0.41 |
| 1:D:199:ASN:HB2 | 5:D:2050:HOH:O | 2.20 | 0.41 |
| 1:F:112:VAL:HG21 | 1:F:375:GLY:HA3 | 2.02 | 0.41 |
| 1:F:349:THR:HG23 | 5:F:2094:HOH:O | 2.20 | 0.41 |
| 1:B:38:VAL:HG22 | 1:B:338:LEU:HD22 | 2.03 | 0.41 |
| 1:E:289:TYR:CD1 | 1:E:289:TYR:C | 2.94 | 0.41 |
| 1:B:264:PHE:HB2 | 1:B:265:PRO:HD2 | 2.04 | 0.40 |
| 1:C:325:ILE:O | 1:C:331:SER:HB3 | 2.21 | 0.40 |
| 1:D:316:ARG:HB2 | 1:D:337:VAL:CG1 | 2.51 | 0.40 |
| 1:E:50:LYS:HE3 | 1:E:202:HIS:NE2 | 2.36 | 0.40 |
| 1:D:157:PHE:CD1 | 1:D:208:VAL:HG21 | 2.56 | 0.40 |
| 1:D:216:ALA:HB2 | 4:D:1394:MTQ:OM2 | 2.21 | 0.40 |
| 1:F:57:PRO:HD2 | 1:F:221:TRP:CE2 | 2.56 | 0.40 |
| 1:F:388:LEU:HD23 | 1:F:388:LEU:HA | 1.91 | 0.40 |
| 1:D:219:VAL:HG11 | 5:D:2034:HOH:O | 2.21 | 0.40 |
| 1:D:326:SER:CB | 5:D:2068:HOH:O | 2.69 | 0.40 |
| 5:D:2084:HOH:O | 1:E:25:LYS:HE2 | 2.21 | 0.40 |
| 1:F:50:LYS:CE | 1:F:202:HIS:CE1 | 2.90 | 0.40 |
| 1:B:77:ARG:HH11 | 1:B:77:ARG:CG | 2.30 | 0.40 |
| 1:B:245:PRO:HB2 | 5:B:2056:HOH:O | 2.20 | 0.40 |
| 1:C:374:ARG:HA | 1:C:374:ARG:HD2 | 1.49 | 0.40 |
| 1:C:385:LEU:HD12 | 1:C:385:LEU:HA | 1.95 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:254:ASN:HD22 | 1:D:255:TRP:N | 2.17 | 0.40 |
| 1:E:164:LYS:HE2 | 5:E:2041:HOH:O | 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 | 386/393 (98%) | 369 (96%) | 13 (3%) | 4 (1%) | 15 | 32 |
| 1 | B | 386/393 (98%) | 371 (96%) | 11 (3%) | 4 (1%) | 15 | 32 |
| 1 | C | 386/393 (98%) | 369 (96%) | 13 (3%) | 4 (1%) | 15 | 32 |
| 1 | D | 386/393 (98%) | 370 (96%) | 12 (3%) | 4 (1%) | 15 | 32 |
| 1 | E | 386/393 (98%) | 370 (96%) | 13 (3%) | 3 (1%) | 19 | 39 |
| 1 | F | 386/393 (98%) | 368 (95%) | 14 (4%) | 4 (1%) | 15 | 32 |
| All | All | 2316/2358 (98%) | 2217 (96%) | 76 (3%) | 23 (1%) | 15 | 32 |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 72 | LEU |
| 1 | A | 380 | SER |
| 1 | B | 72 | LEU |
| 1 | C | 72 | LEU |
| 1 | C | 380 | SER |
| 1 | D | 72 | LEU |
| 1 | E | 72 | LEU |
| 1 | F | 72 | LEU |
| 1 | B | 380 | SER |
| 1 | C | 34 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 380 | SER |
| 1 | E | 380 | SER |
| 1 | F | 380 | SER |
| 1 | A | 76 | PRO |
| 1 | B | 76 | PRO |
| 1 | C | 76 | PRO |
| 1 | D | 34 | ARG |
| 1 | D | 76 | PRO |
| 1 | E | 76 | PRO |
| 1 | B | 34 | ARG |
| 1 | F | 76 | PRO |
| 1 | A | 378 | ASN |
| 1 | F | 34 | ARG |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 331/336 (98%) | 294 (89%) | 37 (11%) | 6 | 10 |
| 1 | B | 331/336 (98%) | 291 (88%) | 40 (12%) | 5 | 9 |
| 1 | C | 331/336 (98%) | 286 (86%) | 45 (14%) | 3 | 6 |
| 1 | D | 331/336 (98%) | 290 (88%) | 41 (12%) | 4 | 8 |
| 1 | E | 331/336 (98%) | 287 (87%) | 44 (13%) | 4 | 7 |
| 1 | F | 331/336 (98%) | 284 (86%) | 47 (14%) | 3 | 5 |
| All | All | 1986/2016 (98%) | 1732 (87%) | 254 (13%) | 4 | 8 |

All (254) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | ARG |
| 1 | A | 9 | GLU |
| 1 | A | 20 | LEU |
| 1 | A | 37 | LEU |
| 1 | A | 38 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 51 | ARG |
| 1 | A | 58 | ILE |
| 1 | A | 63 | GLN |
| 1 | A | 64 | SER |
| 1 | A | 70 | THR |
| 1 | A | 72 | LEU |
| 1 | A | 77 | ARG |
| 1 | A | 81 | ILE |
| 1 | A | 87 | LEU |
| 1 | A | 110 | ARG |
| 1 | A | 119 | VAL |
| 1 | A | 132 | LEU |
| 1 | A | 177 | LEU |
| 1 | A | 178 | SER |
| 1 | A | 181 | THR |
| 1 | A | 184 | GLU |
| 1 | A | 199 | ASN |
| 1 | A | 208 | VAL |
| 1 | A | 222 | LEU |
| 1 | A | 254 | ASN |
| 1 | A | 258 | ARG |
| 1 | A | 265 | PRO |
| 1 | A | 278 | MET |
| 1 | A | 280 | LYS |
| 1 | A | 284 | VAL |
| 1 | A | 291 | VAL |
| 1 | A | 312 | VAL |
| 1 | A | 316 | ARG |
| 1 | A | 336 | TRP |
| 1 | A | 340 | GLU |
| 1 | A | 351 | VAL |
| 1 | A | 367 | VAL |
| 1 | B | 5 | ARG |
| 1 | B | 20 | LEU |
| 1 | B | 34 | ARG |
| 1 | B | 37 | LEU |
| 1 | B | 38 | VAL |
| 1 | B | 50 | LYS |
| 1 | B | 51 | ARG |
| 1 | B | 58 | ILE |
| 1 | B | 63 | GLN |
| 1 | B | 69 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 70 | THR |
| 1 | B | 72 | LEU |
| 1 | B | 75 | ASN |
| 1 | B | 77 | ARG |
| 1 | B | 81 | ILE |
| 1 | B | 87 | LEU |
| 1 | B | 112 | VAL |
| 1 | B | 119 | VAL |
| 1 | B | 132 | LEU |
| 1 | B | 160 | VAL |
| 1 | B | 164 | LYS |
| 1 | B | 177 | LEU |
| 1 | B | 181 | THR |
| 1 | B | 199 | ASN |
| 1 | B | 208 | VAL |
| 1 | B | 222 | LEU |
| 1 | B | 254 | ASN |
| 1 | B | 258 | ARG |
| 1 | B | 278 | MET |
| 1 | B | 284 | VAL |
| 1 | B | 291 | VAL |
| 1 | B | 292 | SER |
| 1 | B | 316 | ARG |
| 1 | B | 319 | GLU |
| 1 | B | 336 | TRP |
| 1 | B | 340 | GLU |
| 1 | B | 351 | VAL |
| 1 | B | 367 | VAL |
| 1 | B | 369 | SER |
| 1 | B | 380 | SER |
| 1 | C | 5 | ARG |
| 1 | C | 9 | GLU |
| 1 | C | 17 | HIS |
| 1 | C | 20 | LEU |
| 1 | C | 37 | LEU |
| 1 | C | 38 | VAL |
| 1 | C | 51 | ARG |
| 1 | C | 53 | HIS |
| 1 | C | 58 | ILE |
| 1 | C | 61 | HIS |
| 1 | C | 63 | GLN |
| 1 | C | 64 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 69 | LEU |
| 1 | C | 70 | THR |
| 1 | C | 77 | ARG |
| 1 | C | 81 | ILE |
| 1 | C | 87 | LEU |
| 1 | C | 108 | LYS |
| 1 | C | 119 | VAL |
| 1 | C | 132 | LEU |
| 1 | C | 177 | LEU |
| 1 | C | 188 | LEU |
| 1 | C | 199 | ASN |
| 1 | C | 208 | VAL |
| 1 | C | 222 | LEU |
| 1 | C | 251 | ASP |
| 1 | C | 254 | ASN |
| 1 | C | 258 | ARG |
| 1 | C | 278 | MET |
| 1 | C | 280 | LYS |
| 1 | C | 284 | VAL |
| 1 | C | 291 | VAL |
| 1 | C | 309 | LYS |
| 1 | C | 313 | GLU |
| 1 | C | 316 | ARG |
| 1 | C | 319 | GLU |
| 1 | C | 327 | GLU |
| 1 | C | 336 | TRP |
| 1 | C | 340 | GLU |
| 1 | C | 344 | ASP |
| 1 | C | 351 | VAL |
| 1 | C | 367 | VAL |
| 1 | C | 374 | ARG |
| 1 | C | 380 | SER |
| 1 | C | 387 | ARG |
| 1 | D | 5 | ARG |
| 1 | D | 9 | GLU |
| 1 | D | 20 | LEU |
| 1 | D | 25 | LYS |
| 1 | D | 37 | LEU |
| 1 | D | 38 | VAL |
| 1 | D | 40 | SER |
| 1 | D | 51 | ARG |
| 1 | D | 60 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 63 | GLN |
| 1 | D | 69 | LEU |
| 1 | D | 70 | THR |
| 1 | D | 72 | LEU |
| 1 | D | 77 | ARG |
| 1 | D | 81 | ILE |
| 1 | D | 86 | SER |
| 1 | D | 87 | LEU |
| 1 | D | 119 | VAL |
| 1 | D | 132 | LEU |
| 1 | D | 145 | THR |
| 1 | D | 177 | LEU |
| 1 | D | 178 | SER |
| 1 | D | 181 | THR |
| 1 | D | 196 | GLU |
| 1 | D | 199 | ASN |
| 1 | D | 222 | LEU |
| 1 | D | 224 | SER |
| 1 | D | 239 | LYS |
| 1 | D | 254 | ASN |
| 1 | D | 278 | MET |
| 1 | D | 280 | LYS |
| 1 | D | 284 | VAL |
| 1 | D | 291 | VAL |
| 1 | D | 302 | ASP |
| 1 | D | 316 | ARG |
| 1 | D | 319 | GLU |
| 1 | D | 336 | TRP |
| 1 | D | 340 | GLU |
| 1 | D | 344 | ASP |
| 1 | D | 351 | VAL |
| 1 | D | 367 | VAL |
| 1 | E | 9 | GLU |
| 1 | E | 16 | ARG |
| 1 | E | 17 | HIS |
| 1 | E | 20 | LEU |
| 1 | E | 37 | LEU |
| 1 | E | 38 | VAL |
| 1 | E | 39 | SER |
| 1 | E | 51 | ARG |
| 1 | E | 58 | ILE |
| 1 | E | 63 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 64 | SER |
| 1 | E | 69 | LEU |
| 1 | E | 70 | THR |
| 1 | E | 72 | LEU |
| 1 | E | 77 | ARG |
| 1 | E | 81 | ILE |
| 1 | E | 87 | LEU |
| 1 | E | 119 | VAL |
| 1 | E | 132 | LEU |
| 1 | E | 160 | VAL |
| 1 | E | 177 | LEU |
| 1 | E | 178 | SER |
| 1 | E | 181 | THR |
| 1 | E | 188 | LEU |
| 1 | E | 196 | GLU |
| 1 | E | 199 | ASN |
| 1 | E | 208 | VAL |
| 1 | E | 222 | LEU |
| 1 | E | 224 | SER |
| 1 | E | 254 | ASN |
| 1 | E | 258 | ARG |
| 1 | E | 265 | PRO |
| 1 | E | 278 | MET |
| 1 | E | 280 | LYS |
| 1 | E | 284 | VAL |
| 1 | E | 287 | LYS |
| 1 | E | 291 | VAL |
| 1 | E | 319 | GLU |
| 1 | E | 336 | TRP |
| 1 | E | 340 | GLU |
| 1 | E | 344 | ASP |
| 1 | E | 351 | VAL |
| 1 | E | 367 | VAL |
| 1 | E | 387 | ARG |
| 1 | F | 5 | ARG |
| 1 | F | 9 | GLU |
| 1 | F | 20 | LEU |
| 1 | F | 21 | LYS |
| 1 | F | 35 | SER |
| 1 | F | 37 | LEU |
| 1 | F | 38 | VAL |
| 1 | F | 40 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 51 | ARG |
| 1 | F | 58 | ILE |
| 1 | F | 61 | HIS |
| 1 | F | 63 | GLN |
| 1 | F | 64 | SER |
| 1 | F | 69 | LEU |
| 1 | F | 70 | THR |
| 1 | F | 72 | LEU |
| 1 | F | 77 | ARG |
| 1 | F | 81 | ILE |
| 1 | F | 87 | LEU |
| 1 | F | 119 | VAL |
| 1 | F | 132 | LEU |
| 1 | F | 160 | VAL |
| 1 | F | 164 | LYS |
| 1 | F | 177 | LEU |
| 1 | F | 181 | THR |
| 1 | F | 188 | LEU |
| 1 | F | 196 | GLU |
| 1 | F | 199 | ASN |
| 1 | F | 205 | PRO |
| 1 | F | 208 | VAL |
| 1 | F | 222 | LEU |
| 1 | F | 226 | ASN |
| 1 | F | 254 | ASN |
| 1 | F | 258 | ARG |
| 1 | F | 265 | PRO |
| 1 | F | 278 | MET |
| 1 | F | 280 | LYS |
| 1 | F | 284 | VAL |
| 1 | F | 291 | VAL |
| 1 | F | 292 | SER |
| 1 | F | 309 | LYS |
| 1 | F | 336 | TRP |
| 1 | F | 340 | GLU |
| 1 | F | 344 | ASP |
| 1 | F | 351 | VAL |
| 1 | F | 367 | VAL |
| 1 | F | 387 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 17 | HIS |
| 1 | A | 63 | GLN |
| 1 | A | 74 | GLN |
| 1 | A | 91 | ASN |
| 1 | A | 254 | ASN |
| 1 | A | 323 | GLN |
| 1 | A | 382 | HIS |
| 1 | B | 91 | ASN |
| 1 | B | 199 | ASN |
| 1 | B | 254 | ASN |
| 1 | B | 323 | GLN |
| 1 | B | 328 | HIS |
| 1 | C | 53 | HIS |
| 1 | C | 91 | ASN |
| 1 | C | 149 | ASN |
| 1 | C | 154 | HIS |
| 1 | C | 202 | HIS |
| 1 | C | 254 | ASN |
| 1 | C | 323 | GLN |
| 1 | C | 328 | HIS |
| 1 | D | 17 | HIS |
| 1 | D | 154 | HIS |
| 1 | D | 167 | ASN |
| 1 | D | 199 | ASN |
| 1 | D | 202 | HIS |
| 1 | D | 254 | ASN |
| 1 | D | 382 | HIS |
| 1 | E | 53 | HIS |
| 1 | E | 199 | ASN |
| 1 | E | 254 | ASN |
| 1 | E | 323 | GLN |
| 1 | F | 17 | HIS |
| 1 | F | 53 | HIS |
| 1 | F | 199 | ASN |
| 1 | F | 202 | HIS |
| 1 | F | 254 | ASN |
| 1 | F | 323 | GLN |

### 5.3.3  RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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 | #$|Z| > 2$ |
| 4 | MTQ | D | 1394 | 1 | 20,30,30 | 3.71 | 14 (70%) | 21,48,48 | 5.64 | 12 (57%) |
| 3 | GOL | A | 1393 | - | 5,5,5 | 0.78 | 0 | 5,5,5 | 1.67 | 1 (20%) |
| 4 | MTQ | C | 1394 | 1 | 20,30,30 | 4.60 | 11 (55%) | 21,48,48 | 5.41 | 13 (61%) |
| 4 | MTQ | F | 1394 | 1 | 20,30,30 | 3.93 | 10 (50%) | 21,48,48 | 4.92 | 9 (42%) |
| 4 | MTQ | E | 1394 | 1 | 20,30,30 | 4.26 | 10 (50%) | 21,48,48 | 5.94 | 15 (71%) |
| 4 | MTQ | A | 1394 | 1 | 20,30,30 | 4.07 | 13 (65%) | 21,48,48 | 6.52 | 14 (66%) |
| 4 | MTQ | B | 1394 | 1 | 20,30,30 | 4.46 | 10 (50%) | 21,48,48 | 5.23 | 13 (61%) |
| 3 | GOL | E | 1393 | - | 5,5,5 | 0.58 | 0 | 5,5,5 | 1.30 | 0 |
| 3 | GOL | C | 1393 | - | 5,5,5 | 0.56 | 0 | 5,5,5 | 1.30 | 1 (20%) |
| 3 | GOL | B | 1393 | - | 5,5,5 | 0.97 | 0 | 5,5,5 | 0.91 | 0 |
| 3 | GOL | D | 1393 | - | 5,5,5 | 0.68 | 0 | 5,5,5 | 1.40 | 1 (20%) |
| 3 | GOL | F | 1393 | - | 5,5,5 | 0.63 | 0 | 5,5,5 | 0.71 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4 | MTQ | D | 1394 | 1 | - | 1/4/60/60 | 0/4/4/4 |

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | GOL | A | 1393 | - | - | 2/4/4/4 | - |
| 4 | MTQ | C | 1394 | 1 | - | 0/4/60/60 | 0/4/4/4 |
| 4 | MTQ | F | 1394 | 1 | - | 0/4/60/60 | 0/4/4/4 |
| 4 | MTQ | E | 1394 | 1 | - | 1/4/60/60 | 0/4/4/4 |
| 4 | MTQ | A | 1394 | 1 | - | 1/4/60/60 | 0/4/4/4 |
| 4 | MTQ | B | 1394 | 1 | - | 0/4/60/60 | 0/4/4/4 |
| 3 | GOL | E | 1393 | - | - | 0/4/4/4 | - |
| 3 | GOL | C | 1393 | - | - | 1/4/4/4 | - |
| 3 | GOL | B | 1393 | - | - | 2/4/4/4 | - |
| 3 | GOL | D | 1393 | - | - | 0/4/4/4 | - |
| 3 | GOL | F | 1393 | - | - | 0/4/4/4 | - |

All (68) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 4 | B | 1394 | MTQ | O4'-C4' | 11.23 | 1.50 | 1.43 |
| 4 | E | 1394 | MTQ | O4'-C4' | 10.95 | 1.50 | 1.43 |
| 4 | C | 1394 | MTQ | O4'-C4' | 8.87 | 1.49 | 1.43 |
| 4 | F | 1394 | MTQ | O3'-C3' | 8.36 | 1.51 | 1.36 |
| 4 | F | 1394 | MTQ | C4'-C3' | -8.24 | 1.35 | 1.48 |
| 4 | C | 1394 | MTQ | O3'-C3' | 8.05 | 1.51 | 1.36 |
| 4 | C | 1394 | MTQ | O4-C4 | 8.02 | 1.37 | 1.23 |
| 4 | B | 1394 | MTQ | O3'-C3' | 7.90 | 1.50 | 1.36 |
| 4 | D | 1394 | MTQ | O3'-C3' | 7.57 | 1.50 | 1.36 |
| 4 | C | 1394 | MTQ | P-O4' | -7.42 | 1.36 | 1.60 |
| 4 | E | 1394 | MTQ | C4'-C3' | -7.33 | 1.36 | 1.48 |
| 4 | F | 1394 | MTQ | P-O4' | -6.94 | 1.37 | 1.60 |
| 4 | C | 1394 | MTQ | C9-N5 | 6.80 | 1.50 | 1.32 |
| 4 | E | 1394 | MTQ | P-O4' | -6.73 | 1.38 | 1.60 |
| 4 | A | 1394 | MTQ | O3'-C3' | 6.71 | 1.48 | 1.36 |
| 4 | A | 1394 | MTQ | C4'-C3' | -6.58 | 1.38 | 1.48 |
| 4 | A | 1394 | MTQ | O4'-C4' | 6.51 | 1.47 | 1.43 |
| 4 | B | 1394 | MTQ | O4-C4 | 6.29 | 1.34 | 1.23 |
| 4 | B | 1394 | MTQ | P-O4' | -6.09 | 1.40 | 1.60 |
| 4 | A | 1394 | MTQ | C6-N5 | 5.99 | 1.54 | 1.36 |
| 4 | A | 1394 | MTQ | P-O4' | -5.96 | 1.41 | 1.60 |
| 4 | D | 1394 | MTQ | P-O4' | -5.89 | 1.41 | 1.60 |
| 4 | D | 1394 | MTQ | C4'-C3' | -5.86 | 1.39 | 1.48 |
| 4 | A | 1394 | MTQ | C9-N5 | 5.71 | 1.47 | 1.32 |
| 4 | E | 1394 | MTQ | C9-N5 | 5.69 | 1.47 | 1.32 |
| 4 | E | 1394 | MTQ | C6-N5 | 5.66 | 1.53 | 1.36 |
| 4 | F | 1394 | MTQ | C6-N5 | 5.54 | 1.52 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | D | 1394 | MTQ | C6-N5 | 5.46 | 1.52 | 1.36 |
| 4 | E | 1394 | MTQ | O3'-C3' | 5.43 | 1.46 | 1.36 |
| 4 | B | 1394 | MTQ | C4'-C3' | -5.39 | 1.39 | 1.48 |
| 4 | C | 1394 | MTQ | C6-N5 | 4.95 | 1.51 | 1.36 |
| 4 | B | 1394 | MTQ | C9-N5 | 4.82 | 1.45 | 1.32 |
| 4 | C | 1394 | MTQ | C4'-C3' | -4.80 | 1.40 | 1.48 |
| 4 | A | 1394 | MTQ | O4-C4 | 4.75 | 1.31 | 1.23 |
| 4 | C | 1394 | MTQ | P-O1P | -4.67 | 1.35 | 1.50 |
| 4 | D | 1394 | MTQ | O4'-C4' | 4.61 | 1.46 | 1.43 |
| 4 | B | 1394 | MTQ | C6-N5 | 4.56 | 1.50 | 1.36 |
| 4 | D | 1394 | MTQ | C9-N5 | 4.54 | 1.44 | 1.32 |
| 4 | F | 1394 | MTQ | C9-N5 | 4.52 | 1.44 | 1.32 |
| 4 | D | 1394 | MTQ | O4-C4 | 4.42 | 1.31 | 1.23 |
| 4 | F | 1394 | MTQ | P-O1P | -4.41 | 1.36 | 1.50 |
| 4 | A | 1394 | MTQ | P-O1P | -4.30 | 1.36 | 1.50 |
| 4 | A | 1394 | MTQ | C9-C10 | 4.14 | 1.55 | 1.43 |
| 4 | B | 1394 | MTQ | P-O1P | -4.06 | 1.37 | 1.50 |
| 4 | B | 1394 | MTQ | C9-C10 | 4.05 | 1.54 | 1.43 |
| 4 | A | 1394 | MTQ | P-O2P | -3.77 | 1.40 | 1.54 |
| 4 | E | 1394 | MTQ | P-O1P | -3.72 | 1.38 | 1.50 |
| 4 | C | 1394 | MTQ | O3'-C7 | 3.71 | 1.51 | 1.45 |
| 4 | F | 1394 | MTQ | O3'-C7 | 3.56 | 1.50 | 1.45 |
| 4 | C | 1394 | MTQ | C10-N8 | 3.55 | 1.39 | 1.35 |
| 4 | E | 1394 | MTQ | C9-C10 | 3.30 | 1.52 | 1.43 |
| 4 | D | 1394 | MTQ | P-O1P | -3.22 | 1.40 | 1.50 |
| 4 | D | 1394 | MTQ | C9-C10 | 3.19 | 1.52 | 1.43 |
| 4 | C | 1394 | MTQ | C9-C10 | 3.17 | 1.52 | 1.43 |
| 4 | E | 1394 | MTQ | C2-N3 | -2.94 | 1.28 | 1.35 |
| 4 | E | 1394 | MTQ | C1'-C6 | 2.94 | 1.43 | 1.36 |
| 4 | D | 1394 | MTQ | C1'-C6 | 2.87 | 1.42 | 1.36 |
| 4 | F | 1394 | MTQ | O4-C4 | 2.80 | 1.28 | 1.23 |
| 4 | A | 1394 | MTQ | C1'-C6 | 2.79 | 1.42 | 1.36 |
| 4 | F | 1394 | MTQ | C9-C10 | 2.77 | 1.51 | 1.43 |
| 4 | D | 1394 | MTQ | C10-N1 | 2.77 | 1.38 | 1.32 |
| 4 | B | 1394 | MTQ | P-O2P | -2.75 | 1.44 | 1.54 |
| 4 | A | 1394 | MTQ | C2-N3 | -2.67 | 1.29 | 1.35 |
| 4 | D | 1394 | MTQ | O3'-C7 | 2.64 | 1.49 | 1.45 |
| 4 | D | 1394 | MTQ | C4-N3 | -2.53 | 1.33 | 1.38 |
| 4 | A | 1394 | MTQ | C2-N2 | -2.45 | 1.28 | 1.34 |
| 4 | F | 1394 | MTQ | P-O2P | -2.32 | 1.45 | 1.54 |
| 4 | D | 1394 | MTQ | P-O2P | -2.14 | 1.46 | 1.54 |

All (79) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 1394 | MTQ | C2'-C1'-C6 | -25.18 | 98.04 | 123.96 |
| 4 | E | 1394 | MTQ | C2'-C1'-C6 | -22.23 | 101.08 | 123.96 |
| 4 | D | 1394 | MTQ | C2'-C1'-C6 | -20.79 | 102.56 | 123.96 |
| 4 | B | 1394 | MTQ | C2'-C1'-C6 | -19.57 | 103.82 | 123.96 |
| 4 | F | 1394 | MTQ | C2'-C1'-C6 | -17.80 | 105.64 | 123.96 |
| 4 | C | 1394 | MTQ | C2'-C1'-C6 | -14.44 | 109.09 | 123.96 |
| 4 | E | 1394 | MTQ | C4-C9-N5 | 9.83 | 128.97 | 118.01 |
| 4 | C | 1394 | MTQ | O3'-C7-N8 | -8.35 | 99.69 | 108.43 |
| 4 | C | 1394 | MTQ | N2-C2-N3 | 7.96 | 129.59 | 117.06 |
| 4 | C | 1394 | MTQ | C4-C9-N5 | 7.08 | 125.91 | 118.01 |
| 4 | A | 1394 | MTQ | O3'-C7-N8 | -7.05 | 101.05 | 108.43 |
| 4 | D | 1394 | MTQ | C4-C9-N5 | 7.03 | 125.85 | 118.01 |
| 4 | F | 1394 | MTQ | O3'-C7-N8 | 6.89 | 115.64 | 108.43 |
| 4 | B | 1394 | MTQ | C2'-C1'-S1' | 6.47 | 129.57 | 115.81 |
| 4 | A | 1394 | MTQ | C2'-C1'-S1' | 6.24 | 129.09 | 115.81 |
| 4 | A | 1394 | MTQ | O3'-C7-C6 | -6.12 | 87.17 | 112.10 |
| 4 | F | 1394 | MTQ | C4-C9-N5 | 6.10 | 124.81 | 118.01 |
| 4 | D | 1394 | MTQ | O3'-C7-N8 | -5.77 | 102.39 | 108.43 |
| 4 | C | 1394 | MTQ | C1'-C2'-C3' | -5.61 | 117.23 | 123.82 |
| 4 | C | 1394 | MTQ | C2'-C1'-S1' | 5.51 | 127.53 | 115.81 |
| 4 | C | 1394 | MTQ | O3'-C7-C6 | -5.42 | 90.04 | 112.10 |
| 4 | C | 1394 | MTQ | O3P-P-O1P | -5.36 | 89.70 | 110.68 |
| 4 | C | 1394 | MTQ | O2P-P-O4' | 5.31 | 120.87 | 106.73 |
| 4 | A | 1394 | MTQ | O4'-P-O1P | 5.29 | 121.31 | 106.47 |
| 4 | F | 1394 | MTQ | C2'-C1'-S1' | 5.22 | 126.91 | 115.81 |
| 4 | C | 1394 | MTQ | N1-C2-N3 | -5.05 | 118.23 | 126.43 |
| 4 | A | 1394 | MTQ | C4-C9-N5 | 5.04 | 123.63 | 118.01 |
| 4 | B | 1394 | MTQ | O3'-C7-C6 | -5.04 | 91.57 | 112.10 |
| 4 | E | 1394 | MTQ | O3'-C7-C6 | -4.88 | 92.22 | 112.10 |
| 4 | E | 1394 | MTQ | N1-C2-N3 | -4.84 | 118.58 | 126.43 |
| 4 | D | 1394 | MTQ | N2-C2-N3 | 4.82 | 124.64 | 117.06 |
| 4 | D | 1394 | MTQ | C2'-C1'-S1' | 4.52 | 125.42 | 115.81 |
| 4 | B | 1394 | MTQ | O3'-C7-N8 | -4.51 | 103.71 | 108.43 |
| 4 | A | 1394 | MTQ | O4-C4-N3 | 4.46 | 127.83 | 120.23 |
| 4 | B | 1394 | MTQ | N1-C2-N3 | -4.21 | 119.59 | 126.43 |
| 4 | D | 1394 | MTQ | O3'-C7-C6 | -4.10 | 95.39 | 112.10 |
| 4 | D | 1394 | MTQ | N1-C2-N3 | -4.10 | 119.77 | 126.43 |
| 4 | F | 1394 | MTQ | O3'-C7-C6 | -4.09 | 95.46 | 112.10 |
| 4 | B | 1394 | MTQ | O4-C4-N3 | 4.06 | 127.14 | 120.23 |
| 4 | E | 1394 | MTQ | C2'-C1'-S1' | 4.00 | 124.32 | 115.81 |
| 4 | D | 1394 | MTQ | C1'-C2'-C3' | -3.98 | 119.14 | 123.82 |
| 4 | D | 1394 | MTQ | O3P-P-O1P | 3.90 | 125.94 | 110.68 |
| 4 | C | 1394 | MTQ | C10-C9-N5 | -3.78 | 115.75 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 4 | B | 1394 | MTQ | O2P-P-O4' | 3.77 | 116.76 | 106.73 |
| 4 | B | 1394 | MTQ | C4-C9-N5 | 3.69 | 122.12 | 118.01 |
| 4 | E | 1394 | MTQ | C10-C9-N5 | -3.68 | 115.97 | 124.48 |
| 4 | F | 1394 | MTQ | C10-C9-N5 | -3.60 | 116.16 | 124.48 |
| 4 | D | 1394 | MTQ | O2P-P-O4' | -3.53 | 97.34 | 106.73 |
| 4 | C | 1394 | MTQ | O4-C4-N3 | 3.52 | 126.23 | 120.23 |
| 4 | E | 1394 | MTQ | O3P-P-O2P | 3.45 | 120.81 | 107.64 |
| 4 | A | 1394 | MTQ | C1'-C2'-C3' | -3.42 | 119.81 | 123.82 |
| 4 | E | 1394 | MTQ | O4'-P-O1P | 3.34 | 115.83 | 106.47 |
| 4 | F | 1394 | MTQ | C1'-C2'-S2' | -3.27 | 108.85 | 115.81 |
| 4 | F | 1394 | MTQ | O4'-C4'-C3' | -3.26 | 105.90 | 110.64 |
| 4 | F | 1394 | MTQ | O4'-P-O1P | 3.23 | 115.53 | 106.47 |
| 4 | D | 1394 | MTQ | C10-C9-N5 | -3.11 | 117.29 | 124.48 |
| 4 | D | 1394 | MTQ | O2P-P-O1P | -3.10 | 98.53 | 110.68 |
| 4 | E | 1394 | MTQ | C1'-C2'-S2' | -3.05 | 109.33 | 115.81 |
| 4 | E | 1394 | MTQ | O2P-P-O1P | -2.93 | 99.21 | 110.68 |
| 3 | A | 1393 | GOL | C3-C2-C1 | -2.92 | 100.33 | 111.70 |
| 4 | A | 1394 | MTQ | O2P-P-O1P | -2.87 | 99.43 | 110.68 |
| 4 | E | 1394 | MTQ | N2-C2-N1 | 2.75 | 121.04 | 116.57 |
| 4 | C | 1394 | MTQ | N2-C2-N1 | -2.70 | 112.18 | 116.57 |
| 4 | B | 1394 | MTQ | C10-C9-N5 | -2.70 | 118.25 | 124.48 |
| 4 | B | 1394 | MTQ | C1'-C2'-S2' | -2.62 | 110.24 | 115.81 |
| 4 | A | 1394 | MTQ | N1-C2-N3 | -2.60 | 122.21 | 126.43 |
| 4 | A | 1394 | MTQ | O3P-P-O2P | 2.55 | 117.37 | 107.64 |
| 4 | A | 1394 | MTQ | N2-C2-N1 | 2.51 | 120.64 | 116.57 |
| 4 | A | 1394 | MTQ | C1'-C2'-S2' | -2.49 | 110.51 | 115.81 |
| 4 | A | 1394 | MTQ | C10-C9-N5 | -2.45 | 118.82 | 124.48 |
| 4 | B | 1394 | MTQ | N2-C2-N1 | 2.36 | 120.39 | 116.57 |
| 4 | E | 1394 | MTQ | O3P-P-O4' | -2.35 | 100.48 | 106.73 |
| 4 | E | 1394 | MTQ | O4-C4-N3 | 2.27 | 124.10 | 120.23 |
| 4 | B | 1394 | MTQ | C1'-C2'-C3' | -2.19 | 121.25 | 123.82 |
| 4 | E | 1394 | MTQ | N2-C2-N3 | 2.07 | 120.33 | 117.06 |
| 3 | C | 1393 | GOL | O3-C3-C2 | 2.07 | 120.12 | 110.20 |
| 4 | B | 1394 | MTQ | O3P-P-O2P | 2.07 | 115.54 | 107.64 |
| 3 | D | 1393 | GOL | C3-C2-C1 | -2.04 | 103.77 | 111.70 |
| 4 | E | 1394 | MTQ | C4-C9-C10 | -2.04 | 115.06 | 117.40 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | A | 1393 | GOL | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 3 | B | 1393 | GOL | C1-C2-C3-O3 |
| 4 | A | 1394 | MTQ | C4'-O4'-P-O2P |
| 3 | A | 1393 | GOL | O1-C1-C2-O2 |
| 3 | B | 1393 | GOL | O2-C2-C3-O3 |
| 4 | D | 1394 | MTQ | C4'-O4'-P-O3P |
| 4 | E | 1394 | MTQ | C4'-O4'-P-O2P |
| 3 | C | 1393 | GOL | O2-C2-C3-O3 |

There are no ring outliers.

9 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | D | 1394 | MTQ | 9 | 0 |
| 4 | C | 1394 | MTQ | 3 | 0 |
| 4 | F | 1394 | MTQ | 1 | 0 |
| 4 | E | 1394 | MTQ | 1 | 0 |
| 4 | A | 1394 | MTQ | 2 | 0 |
| 4 | B | 1394 | MTQ | 2 | 0 |
| 3 | E | 1393 | GOL | 1 | 0 |
| 3 | C | 1393 | GOL | 2 | 0 |
| 3 | D | 1393 | 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 MTQ D 1394



Bond lengths



Bond angles



Torsions



Rings

## Ligand MTQ C 1394



Bond lengths



Bond angles



Torsions



Rings

## Ligand MTQ F 1394



Bond lengths



Bond angles



Torsions



Rings

## Ligand MTQ E 1394



Bond lengths



Bond angles



Torsions



Rings

## Ligand MTQ A 1394

**Bond lengths**

**Bond angles**

**Torsions**

**Rings**

## Ligand MTQ B 1394



**Bond lengths**

**Bond angles**

**Torsions**

**Rings**
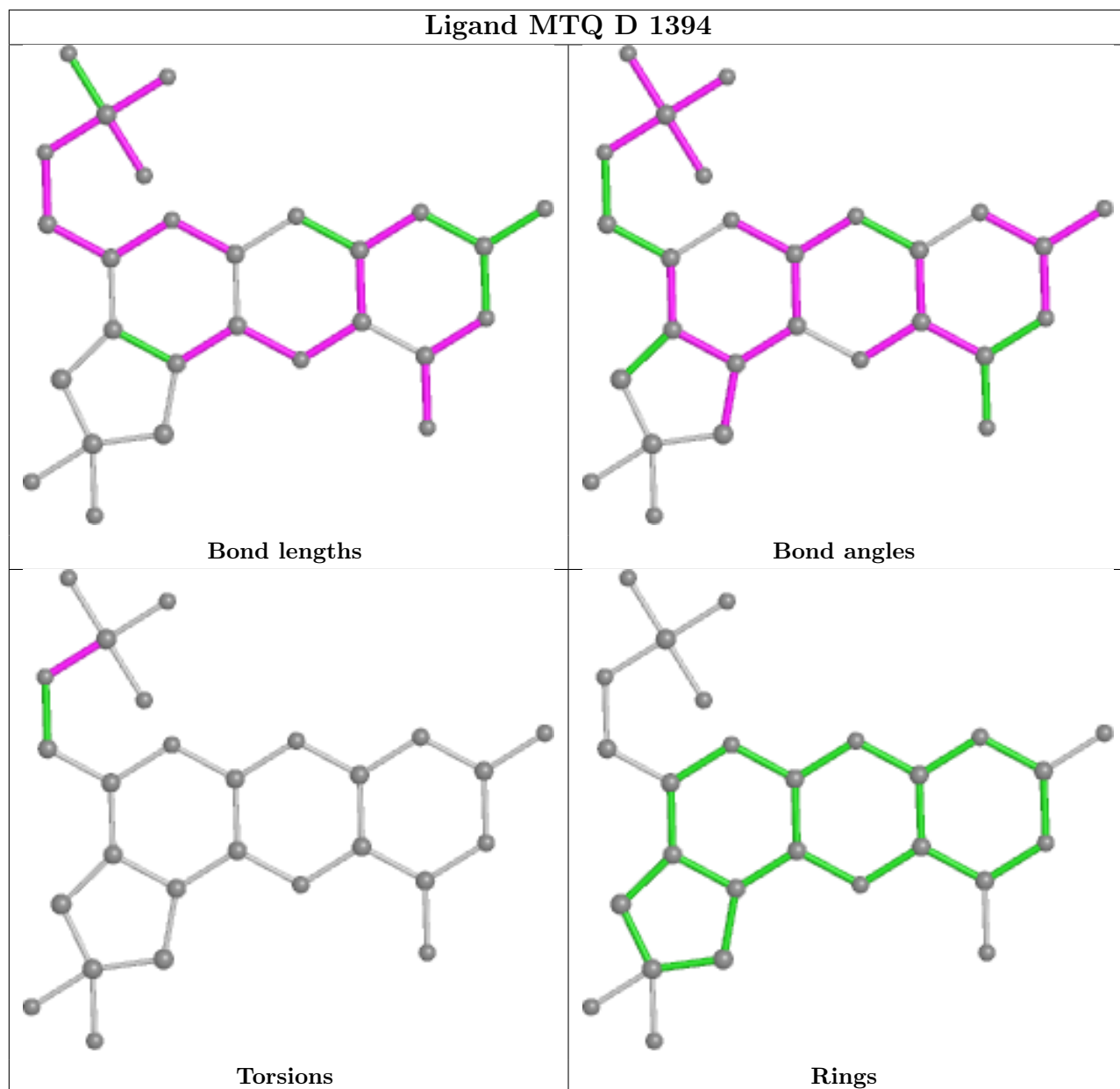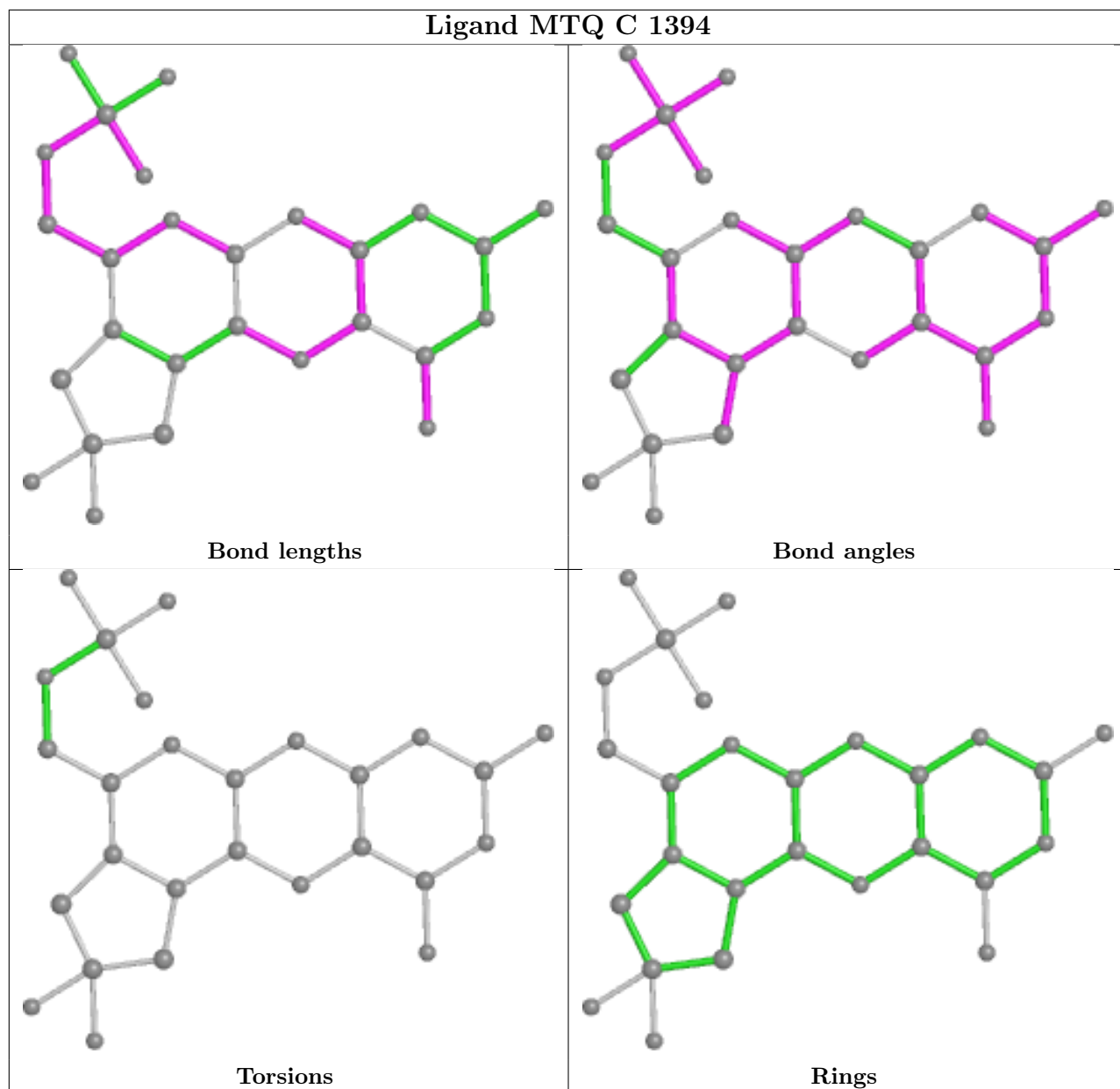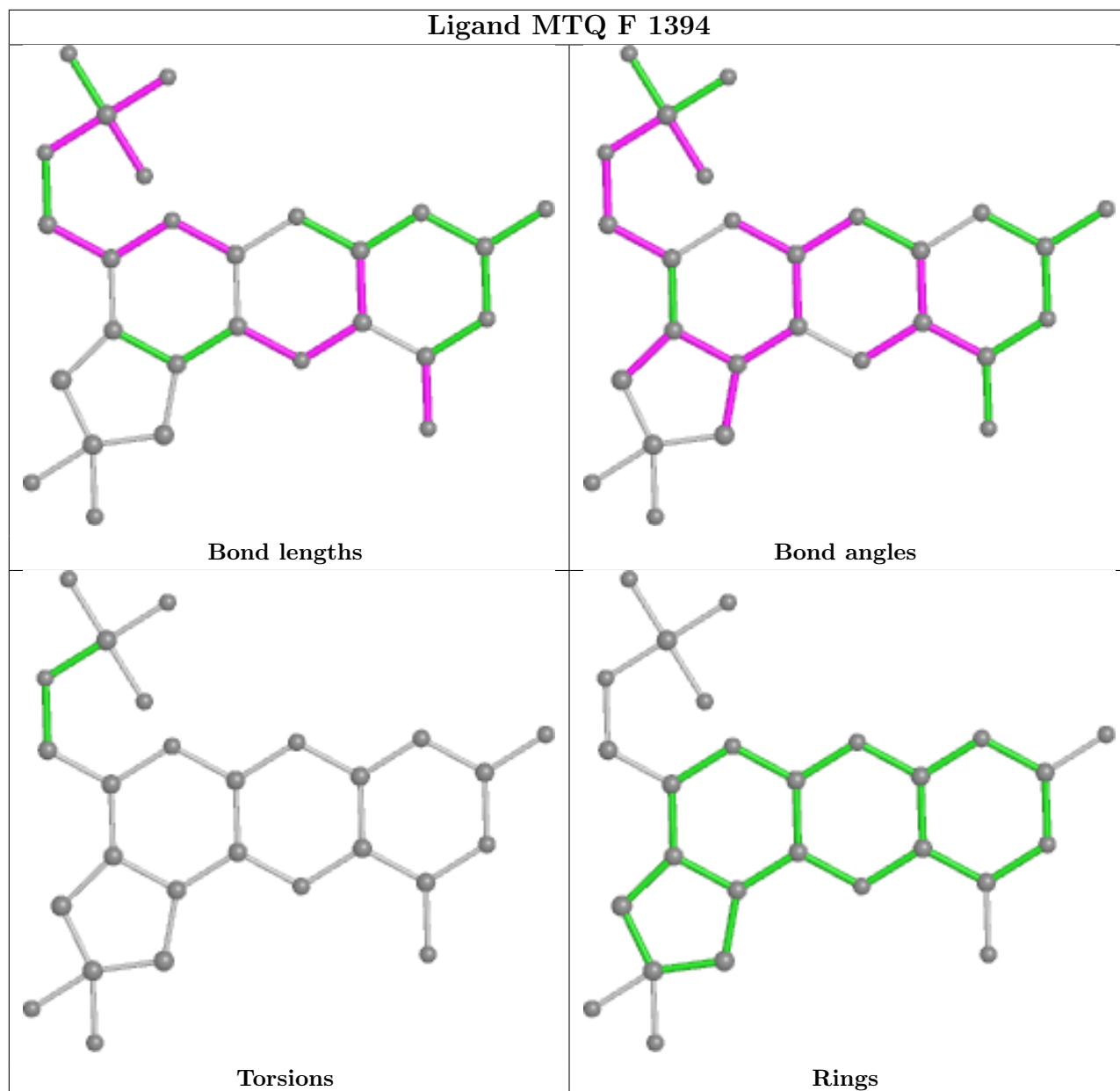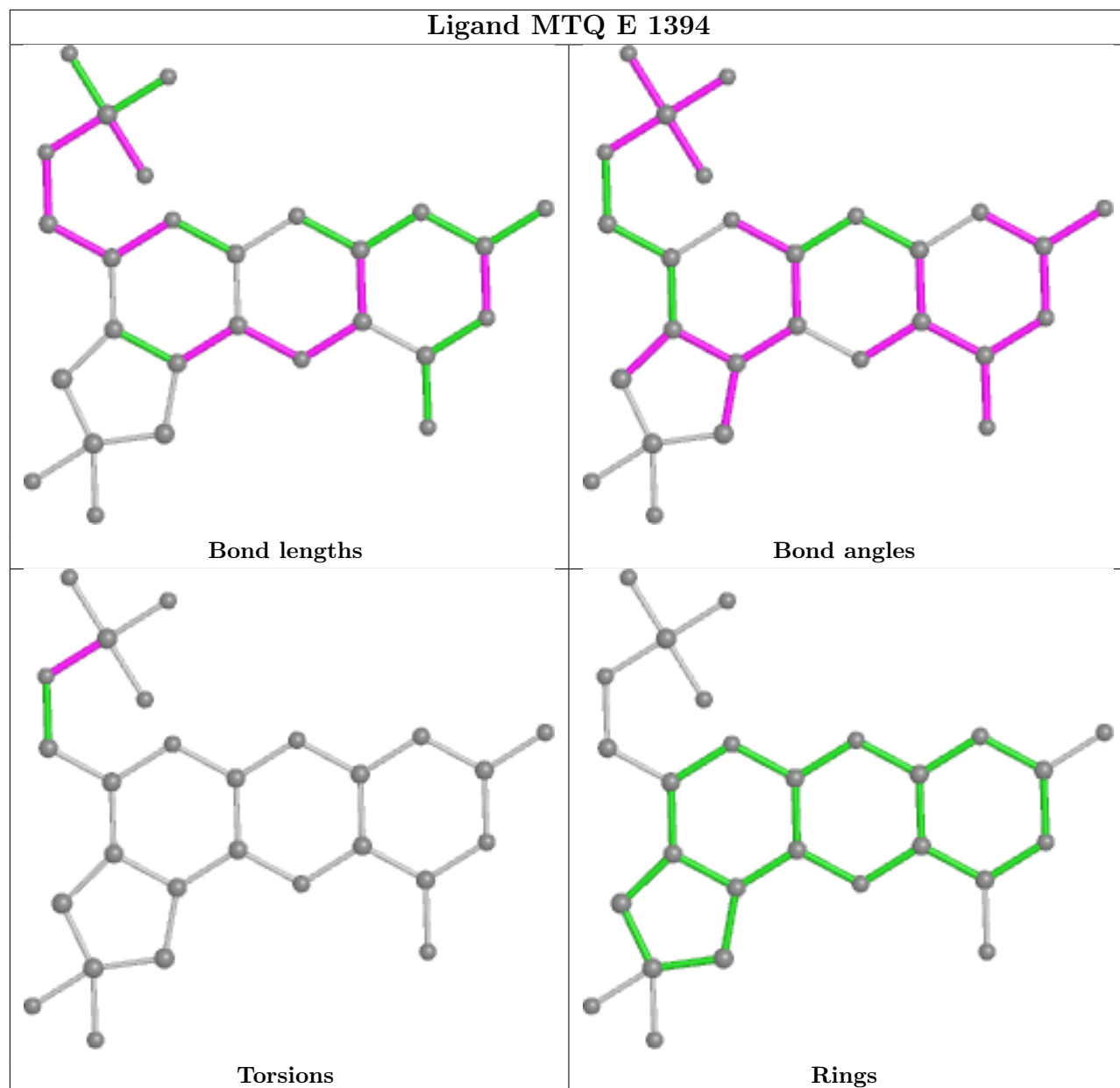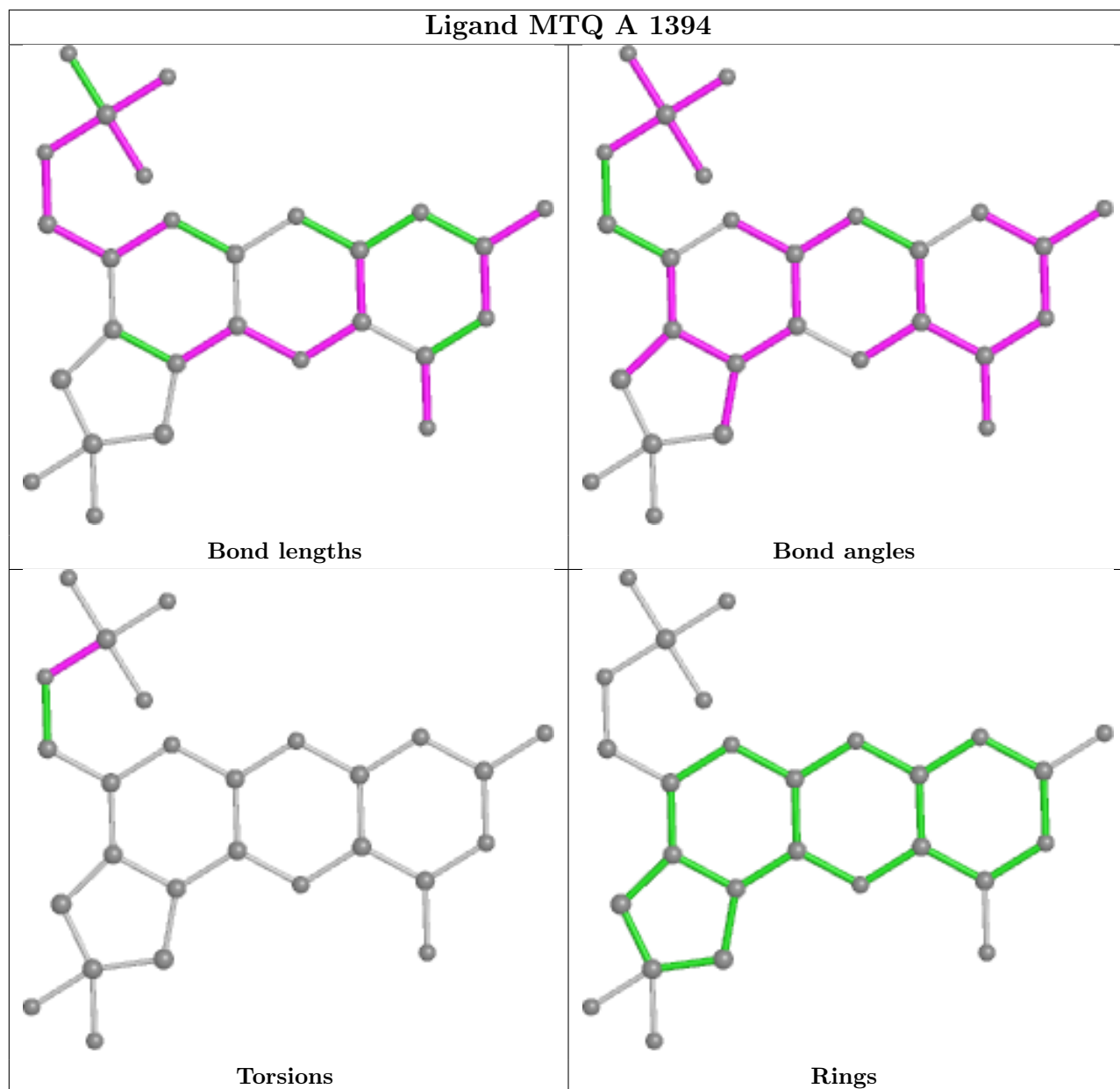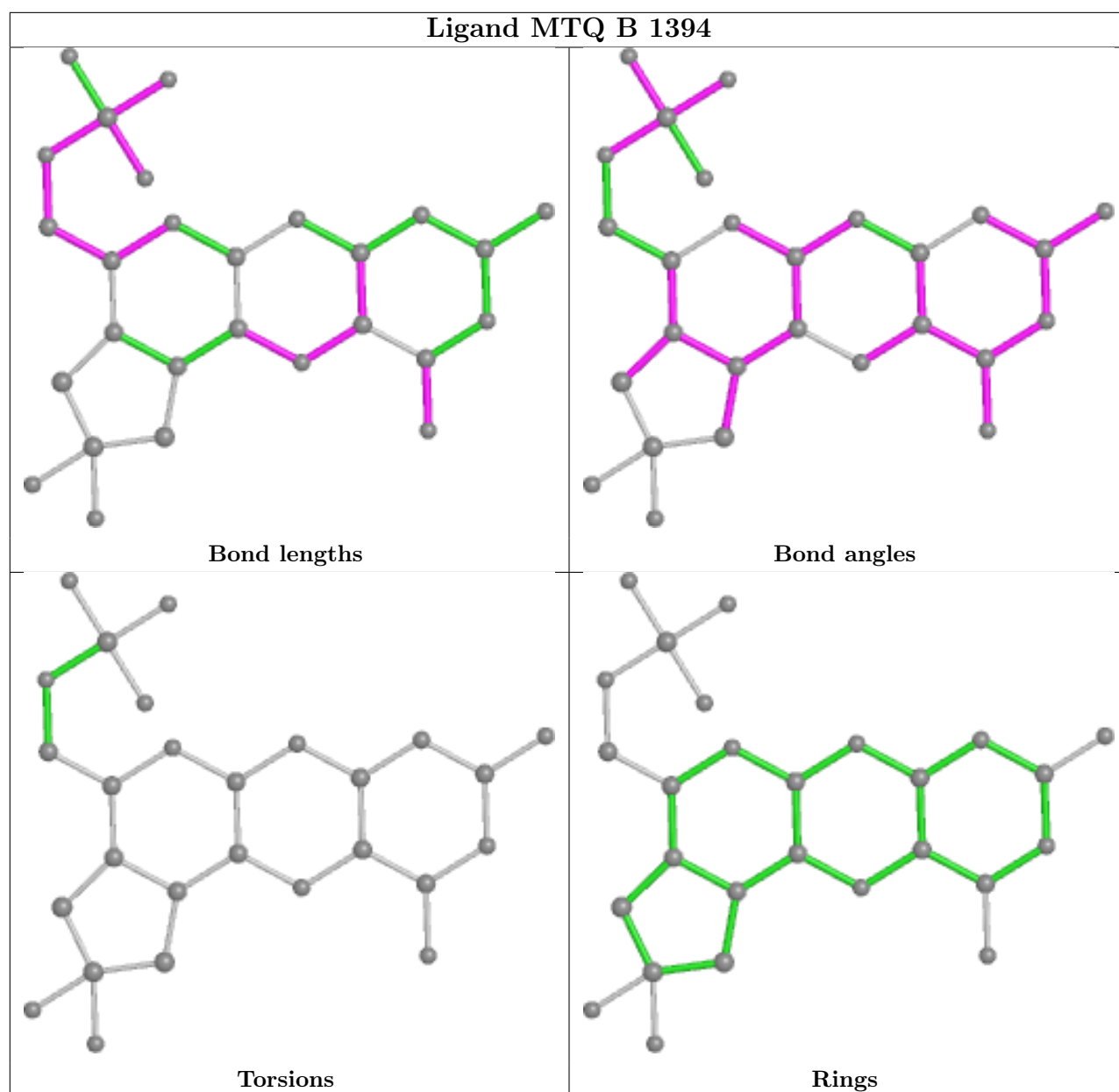
## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|----------|-------|
| 1 | A | 388/393 (98%) | 0.01 | 18 (4%) | 32 | 26 | 39, 54, 78, 90 | 0 |
| 1 | B | 388/393 (98%) | -0.02 | 12 (3%) | 49 | 42 | 39, 54, 78, 90 | 0 |
| 1 | C | 388/393 (98%) | 0.09 | 20 (5%) | 27 | 21 | 40, 55, 78, 90 | 0 |
| 1 | D | 388/393 (98%) | 0.28 | 36 (9%) | 8 | 6 | 39, 55, 78, 90 | 0 |
| 1 | E | 388/393 (98%) | 0.08 | 17 (4%) | 34 | 27 | 39, 54, 78, 90 | 0 |
| 1 | F | 388/393 (98%) | 0.08 | 12 (3%) | 49 | 42 | 39, 54, 78, 90 | 0 |
| All | All | 2328/2358 (98%) | 0.09 | 115 (4%) | 29 | 23 | 39, 54, 78, 90 | 0 |

All (115) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 389 | GLY | 8.7 |
| 1 | B | 389 | GLY | 7.7 |
| 1 | F | 2 | PRO | 6.7 |
| 1 | D | 2 | PRO | 6.5 |
| 1 | F | 389 | GLY | 6.2 |
| 1 | B | 2 | PRO | 5.8 |
| 1 | D | 389 | GLY | 5.8 |
| 1 | C | 2 | PRO | 5.8 |
| 1 | A | 2 | PRO | 4.7 |
| 1 | A | 389 | GLY | 4.5 |
| 1 | D | 388 | LEU | 4.4 |
| 1 | D | 3 | GLY | 4.4 |
| 1 | E | 2 | PRO | 4.3 |
| 1 | D | 344 | ASP | 4.0 |
| 1 | D | 63 | GLN | 3.9 |
| 1 | D | 321 | GLY | 3.7 |
| 1 | D | 280 | LYS | 3.7 |
| 1 | A | 280 | LYS | 3.6 |
| 1 | D | 82 | LYS | 3.6 |

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Full wwPDB X-ray Structure Validation Report

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 346 | SER | 3.5 |
| 1 | F | 64 | SER | 3.5 |
| 1 | C | 61 | HIS | 3.5 |
| 1 | D | 64 | SER | 3.4 |
| 1 | C | 388 | LEU | 3.4 |
| 1 | E | 321 | GLY | 3.4 |
| 1 | D | 61 | HIS | 3.3 |
| 1 | D | 149 | ASN | 3.3 |
| 1 | A | 279 | VAL | 3.2 |
| 1 | E | 63 | GLN | 3.1 |
| 1 | E | 389 | GLY | 3.1 |
| 1 | D | 195 | GLY | 3.1 |
| 1 | A | 278 | MET | 3.0 |
| 1 | C | 278 | MET | 3.0 |
| 1 | D | 320 | PRO | 3.0 |
| 1 | C | 280 | LYS | 3.0 |
| 1 | B | 278 | MET | 3.0 |
| 1 | D | 278 | MET | 3.0 |
| 1 | C | 346 | SER | 2.9 |
| 1 | F | 321 | GLY | 2.9 |
| 1 | E | 349 | THR | 2.9 |
| 1 | D | 18 | PRO | 2.9 |
| 1 | D | 168 | GLY | 2.8 |
| 1 | D | 5 | ARG | 2.8 |
| 1 | B | 281 | PRO | 2.8 |
| 1 | C | 281 | PRO | 2.8 |
| 1 | D | 347 | GLN | 2.8 |
| 1 | F | 278 | MET | 2.7 |
| 1 | A | 321 | GLY | 2.7 |
| 1 | D | 39 | SER | 2.7 |
| 1 | C | 321 | GLY | 2.7 |
| 1 | D | 152 | ALA | 2.7 |
| 1 | C | 149 | ASN | 2.7 |
| 1 | E | 388 | LEU | 2.7 |
| 1 | C | 345 | VAL | 2.6 |
| 1 | D | 208 | VAL | 2.6 |
| 1 | A | 215 | GLY | 2.6 |
| 1 | E | 61 | HIS | 2.6 |
| 1 | B | 280 | LYS | 2.6 |
| 1 | E | 218 | SER | 2.6 |
| 1 | D | 279 | VAL | 2.6 |
| 1 | C | 64 | SER | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 60 | ASP | 2.5 |
| 1 | E | 208 | VAL | 2.5 |
| 1 | D | 72 | LEU | 2.5 |
| 1 | B | 64 | SER | 2.5 |
| 1 | A | 61 | HIS | 2.5 |
| 1 | D | 349 | THR | 2.5 |
| 1 | A | 219 | VAL | 2.4 |
| 1 | D | 11 | SER | 2.4 |
| 1 | A | 388 | LEU | 2.4 |
| 1 | B | 282 | GLY | 2.4 |
| 1 | F | 61 | HIS | 2.4 |
| 1 | A | 96 | LEU | 2.4 |
| 1 | A | 218 | SER | 2.4 |
| 1 | C | 75 | ASN | 2.4 |
| 1 | E | 219 | VAL | 2.4 |
| 1 | F | 96 | LEU | 2.3 |
| 1 | B | 321 | GLY | 2.3 |
| 1 | E | 281 | PRO | 2.3 |
| 1 | B | 344 | ASP | 2.3 |
| 1 | E | 278 | MET | 2.3 |
| 1 | D | 162 | ARG | 2.3 |
| 1 | D | 150 | LEU | 2.3 |
| 1 | C | 74 | GLN | 2.3 |
| 1 | D | 59 | VAL | 2.3 |
| 1 | D | 345 | VAL | 2.3 |
| 1 | E | 203 | GLY | 2.3 |
| 1 | C | 251 | ASP | 2.2 |
| 1 | B | 208 | VAL | 2.2 |
| 1 | B | 63 | GLN | 2.2 |
| 1 | F | 280 | LYS | 2.2 |
| 1 | D | 60 | ASP | 2.2 |
| 1 | C | 215 | GLY | 2.2 |
| 1 | E | 77 | ARG | 2.2 |
| 1 | A | 74 | GLN | 2.2 |
| 1 | A | 208 | VAL | 2.2 |
| 1 | D | 141 | ILE | 2.2 |
| 1 | F | 63 | GLN | 2.2 |
| 1 | D | 218 | SER | 2.1 |
| 1 | C | 112 | VAL | 2.1 |
| 1 | C | 322 | LYS | 2.1 |
| 1 | F | 207 | ARG | 2.1 |
| 1 | A | 207 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 61 | HIS | 2.1 |
| 1 | D | 138 | LEU | 2.1 |
| 1 | D | 58 | ILE | 2.1 |
| 1 | F | 202 | HIS | 2.1 |
| 1 | E | 74 | GLN | 2.0 |
| 1 | A | 209 | VAL | 2.0 |
| 1 | F | 216 | ALA | 2.0 |
| 1 | C | 63 | GLN | 2.0 |
| 1 | A | 346 | SER | 2.0 |
| 1 | E | 346 | SER | 2.0 |
| 1 | A | 222 | LEU | 2.0 |
| 1 | E | 280 | LYS | 2.0 |

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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 |
|-----|------|-------|-----|-------|------|-----|------------------|-------|
| 3 | GOL | A | 1393 | 6/6 | 0.91 | 0.22 | 47,57,62,62 | 0 |
| 3 | GOL | C | 1393 | 6/6 | 0.92 | 0.18 | 52,57,60,64 | 0 |
| 3 | GOL | D | 1393 | 6/6 | 0.92 | 0.16 | 52,58,63,64 | 0 |
| 3 | GOL | E | 1393 | 6/6 | 0.94 | 0.19 | 47,56,62,63 | 0 |
| 3 | GOL | B | 1393 | 6/6 | 0.96 | 0.18 | 51,57,62,62 | 0 |
| 2 | CS | D | 1391 | 1/1 | 0.96 | 0.19 | 106,106,106,106 | 0 |
| 2 | CS | F | 1392 | 1/1 | 0.97 | 0.04 | 70,70,70,70 | 1 |
| 2 | CS | C | 1392 | 1/1 | 0.97 | 0.05 | 79,79,79,79 | 1 |
| 2 | CS | E | 1392 | 1/1 | 0.97 | 0.05 | 73,73,73,73 | 1 |
| 3 | GOL | F | 1393 | 6/6 | 0.97 | 0.17 | 45,57,61,63 | 0 |
| 2 | CS | D | 1392 | 1/1 | 0.98 | 0.11 | 81,81,81,81 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors($\text{Å}^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | CS | B | 1392 | 1/1 | 0.98 | 0.03 | 67,67,67,67 | 1 |
| 2 | CS | C | 1391 | 1/1 | 0.98 | 0.04 | 80,80,80,80 | 0 |
| 4 | MTQ | D | 1394 | 27/27 | 0.98 | 0.15 | 35,42,51,56 | 0 |
| 2 | CS | B | 1391 | 1/1 | 0.99 | 0.04 | 73,73,73,73 | 0 |
| 2 | CS | F | 1391 | 1/1 | 0.99 | 0.05 | 73,73,73,73 | 0 |
| 2 | CS | A | 1391 | 1/1 | 0.99 | 0.07 | 67,67,67,67 | 0 |
| 2 | CS | A | 1392 | 1/1 | 0.99 | 0.04 | 69,69,69,69 | 1 |
| 4 | MTQ | A | 1394 | 27/27 | 0.99 | 0.19 | 33,40,44,49 | 0 |
| 4 | MTQ | B | 1394 | 27/27 | 0.99 | 0.18 | 33,40,46,51 | 0 |
| 4 | MTQ | C | 1394 | 27/27 | 0.99 | 0.15 | 34,42,50,51 | 0 |
| 2 | CS | E | 1391 | 1/1 | 0.99 | 0.06 | 68,68,68,68 | 0 |
| 4 | MTQ | E | 1394 | 27/27 | 0.99 | 0.19 | 29,39,44,47 | 0 |
| 4 | MTQ | F | 1394 | 27/27 | 0.99 | 0.20 | 32,39,44,49 | 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.
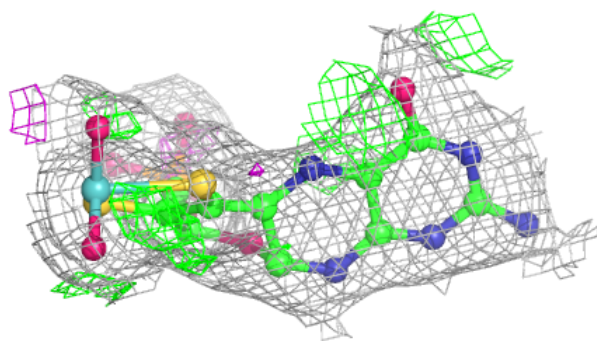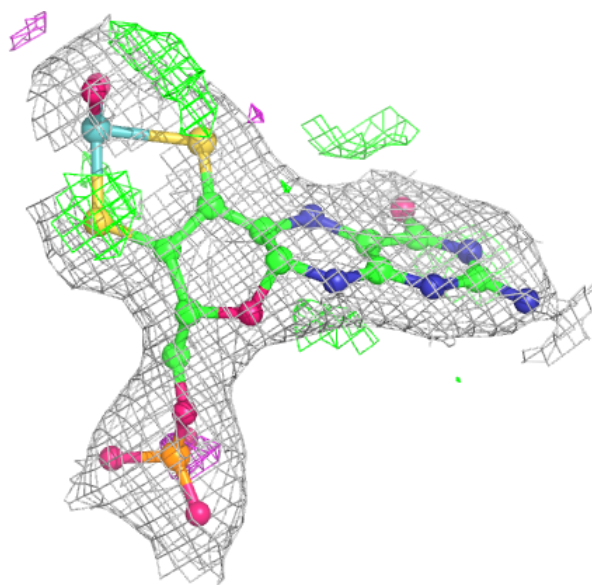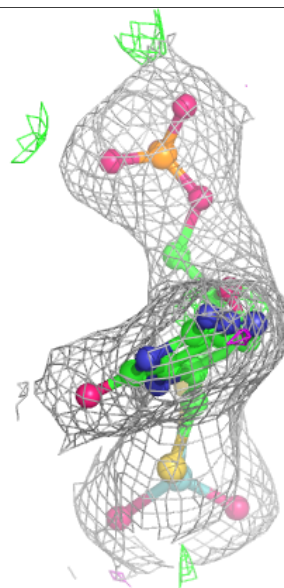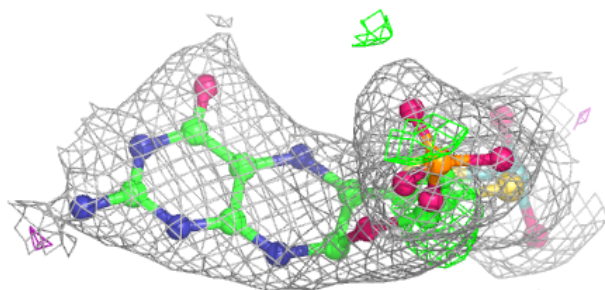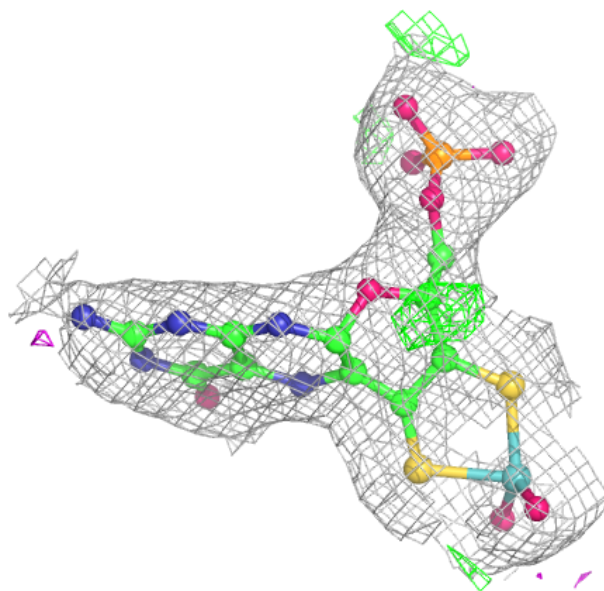
**Electron density around MTQ D 1394:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
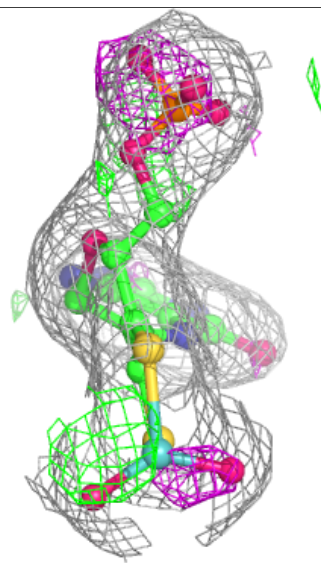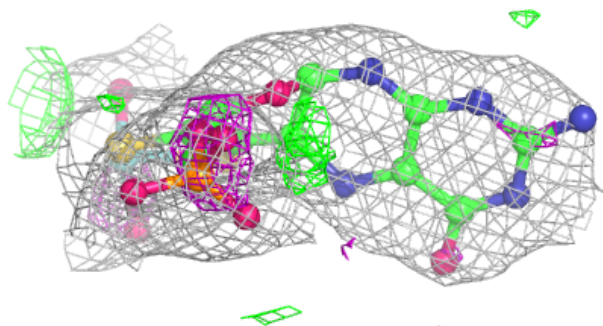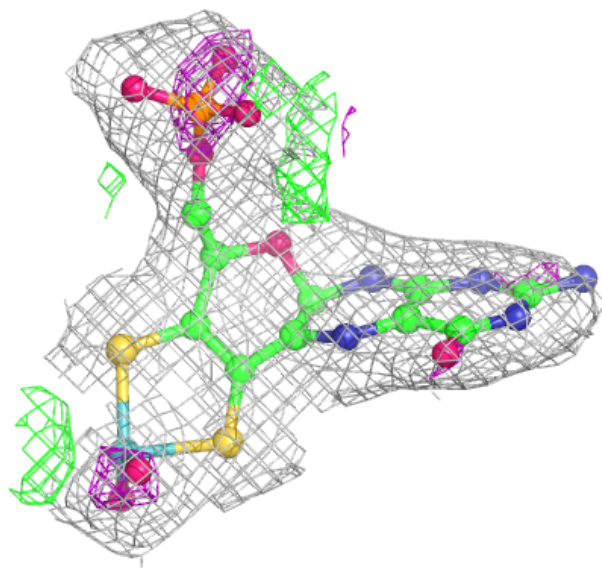
**Electron density around MTQ A 1394:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
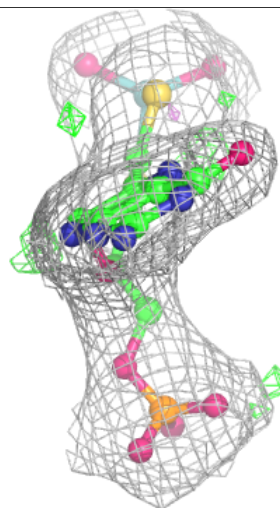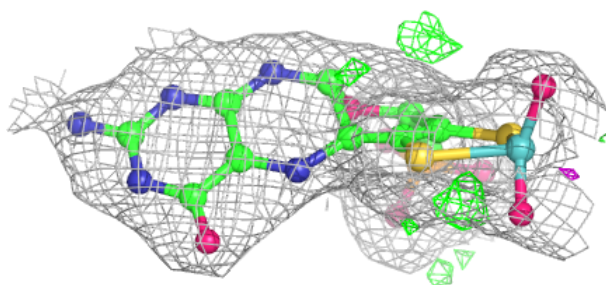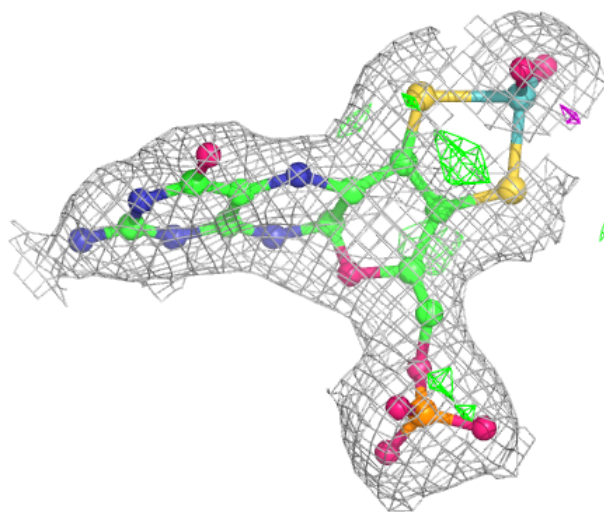
**Electron density around MTQ B 1394:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
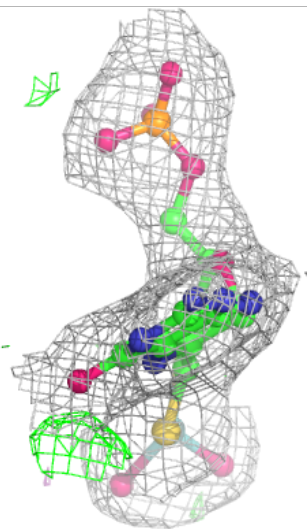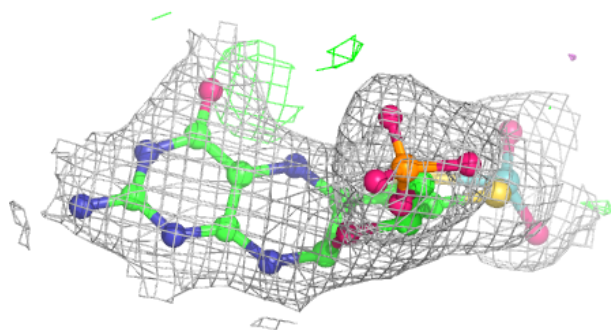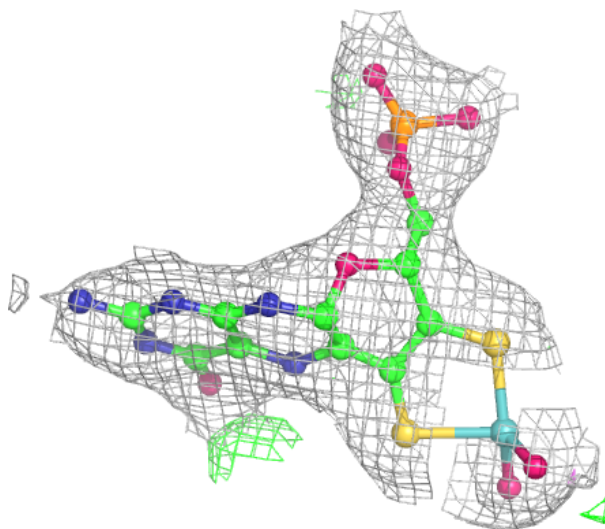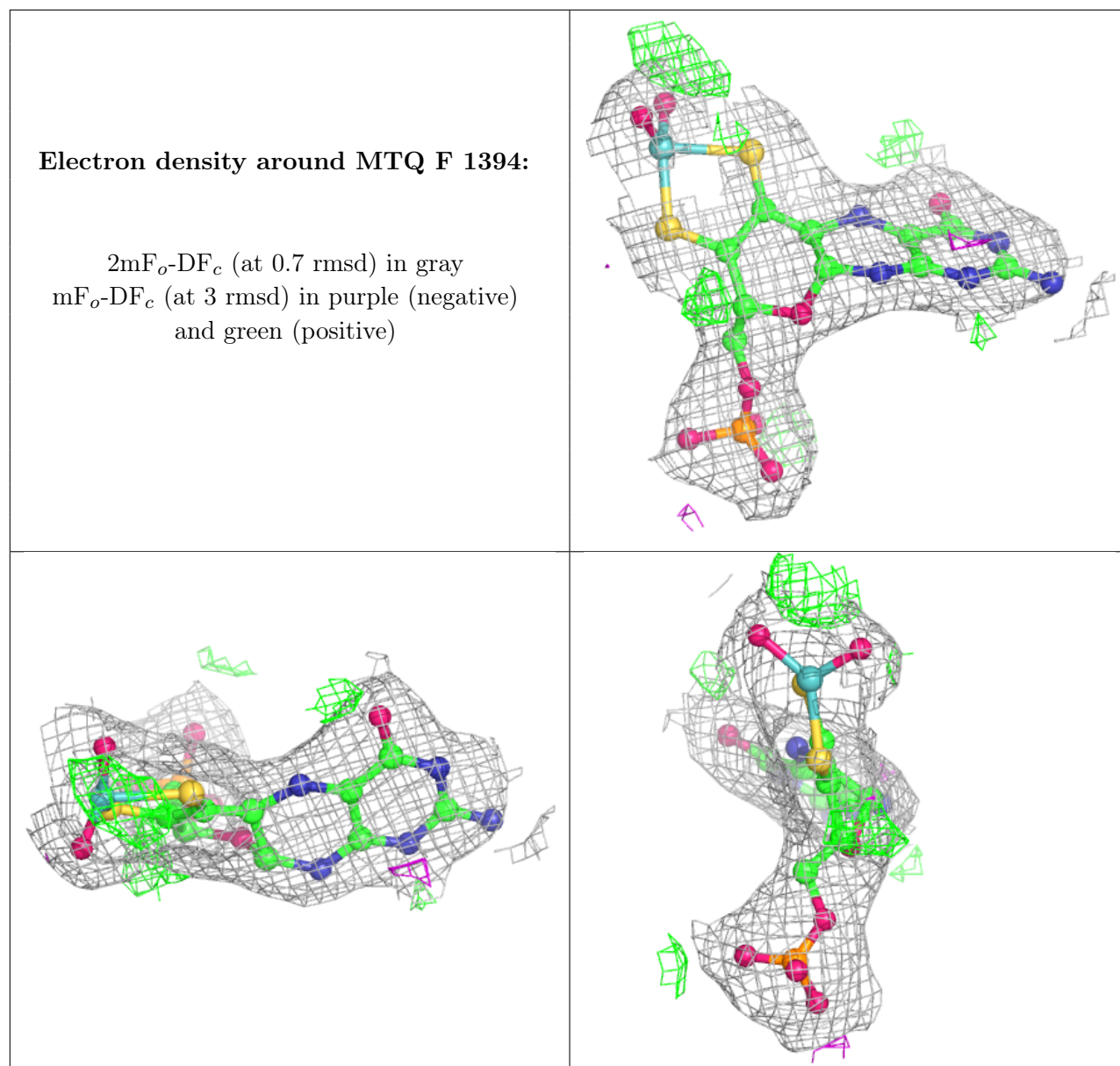
**Electron density around MTQ C 1394:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
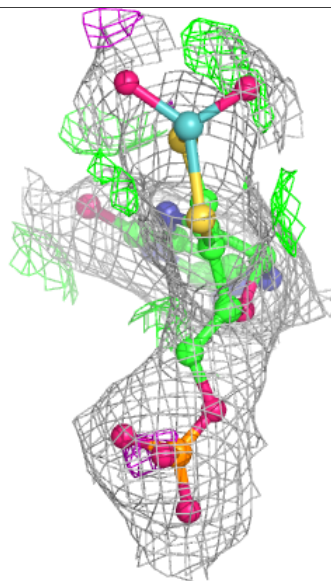
**Electron density around MTQ E 1394:**

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

**Electron density around MTQ F 1394:**

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 ⓘ

There are no such residues in this entry.