# WORLDWIDE wwPDB PROTEIN DATA BANK

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

Oct 28, 2024 – 05:20 pm GMT

|  |  |  |
|---|---|---|
| PDB ID | : | 6QF7 |
| Title | : | Crystal structures of the recombinant beta-Factor XIIa protease with bound Thr-Arg and Pro-Arg substrate mimetics |
| Authors | : | Pathak, M.; Mannal, R.; Li, C.; Bubacarr, G.K.; Badraldin, K.H.; Belviso, B.D.; Camila, R.B.; Dreveny, I.; Fischer, P.M.; Dekker, L.V.; Oliva, M.L.V.; Emsley, J. |
| Deposited on | : | 2019-01-09 |
| Resolution | : | 4.00 Å(reported) |

The following versions of software and data (see references ①) were used in the production of this report:

| | | |
|---:|:---:|:---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 3.0 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.003 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1    Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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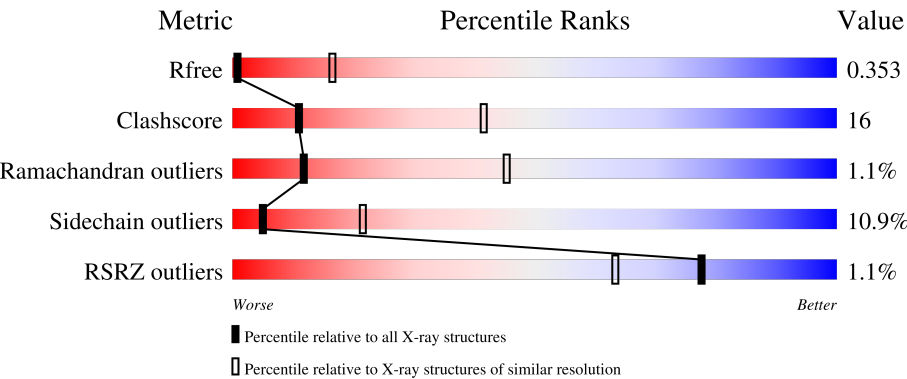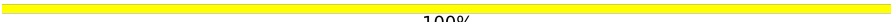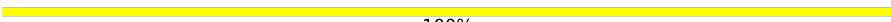


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 164625 | 1028 (4.22-3.78) |
| Clashscore | 180529 | 1055 (4.20-3.80) |
| Ramachandran outliers | 177936 | 1004 (4.20-3.80) |
| Sidechain outliers | 177891 | 1027 (4.22-3.78) |
| RSRZ outliers | 164620 | 1029 (4.22-3.78) |

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 | 374 |  |
| 1 | C | 374 |  |
| 2 | B | 254 |  |
| 2 | D | 254 |  |
| 3 | E | 2 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | F | 2 | 100% |
| 4 | G | 2 | 100% |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | NAG | E | 2 | X | - | - | - |
| 4 | GLC | F | 2 | - | - | X | - |
| 5 | NAG | B | 701 | X | - | - | - |
| 6 | 0G6 | D | 703 | - | - | X | - |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9512 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 Maltodextrin-binding protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 369 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 2839 | 1830 | 462 | 541 | 6 | | | |
| 1 | C | 370 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 2845 | 1834 | 463 | 542 | 6 | | | |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | -1 | ARG | - | expression tag | UNP A0A376KDN7 |
| A | 0 | SER | ALA | conflict | UNP A0A376KDN7 |
| A | 82 | ALA | ASP | conflict | UNP A0A376KDN7 |
| A | 83 | ALA | LYS | conflict | UNP A0A376KDN7 |
| A | 172 | ALA | GLU | conflict | UNP A0A376KDN7 |
| A | 173 | ALA | ASN | conflict | UNP A0A376KDN7 |
| A | 239 | ALA | LYS | conflict | UNP A0A376KDN7 |
| A | 362 | ALA | LYS | conflict | UNP A0A376KDN7 |
| A | 363 | ALA | ASP | conflict | UNP A0A376KDN7 |
| A | 367 | ASN | ARG | conflict | UNP A0A376KDN7 |
| A | 368 | ALA | - | expression tag | UNP A0A376KDN7 |
| A | 369 | ALA | - | expression tag | UNP A0A376KDN7 |
| A | 370 | ALA | - | expression tag | UNP A0A376KDN7 |
| A | 371 | ALA | - | expression tag | UNP A0A376KDN7 |
| A | 372 | SER | - | expression tag | UNP A0A376KDN7 |
| C | -1 | ARG | - | expression tag | UNP A0A376KDN7 |
| C | 0 | SER | ALA | conflict | UNP A0A376KDN7 |
| C | 82 | ALA | ASP | conflict | UNP A0A376KDN7 |
| C | 83 | ALA | LYS | conflict | UNP A0A376KDN7 |
| C | 172 | ALA | GLU | conflict | UNP A0A376KDN7 |
| C | 173 | ALA | ASN | conflict | UNP A0A376KDN7 |
| C | 239 | ALA | LYS | conflict | UNP A0A376KDN7 |
| C | 362 | ALA | LYS | conflict | UNP A0A376KDN7 |
| C | 363 | ALA | ASP | conflict | UNP A0A376KDN7 |
| C | 367 | ASN | ARG | conflict | UNP A0A376KDN7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| C | 368 | ALA | - | expression tag | UNP A0A376KDN7 |
| C | 369 | ALA | - | expression tag | UNP A0A376KDN7 |
| C | 370 | ALA | - | expression tag | UNP A0A376KDN7 |
| C | 371 | ALA | - | expression tag | UNP A0A376KDN7 |
| C | 372 | SER | - | expression tag | UNP A0A376KDN7 |

- Molecule 2 is a protein called Coagulation factor XII.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|---------|---------|-------|
| 2 | B | 244 | Total | C | N | O | S | 3 | 0 | 0 |
| | | | 1840 | 1153 | 325 | 347 | 15 | | | |
| 2 | D | 244 | Total | C | N | O | S | 3 | 0 | 0 |
| | | | 1840 | 1153 | 325 | 347 | 15 | | | |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| B | 330 | ALA | - | expression tag | UNP P00748 |
| B | 331 | ALA | - | expression tag | UNP P00748 |
| B | 332 | ALA | - | expression tag | UNP P00748 |
| B | 333 | ALA | - | expression tag | UNP P00748 |
| B | 334 | SER | THR | conflict | UNP P00748 |
| B | 335 | GLU | ARG | conflict | UNP P00748 |
| B | 336 | PHE | ASN | conflict | UNP P00748 |
| B | ? | - | LEU | deletion | UNP P00748 |
| B | ? | - | ARG | deletion | UNP P00748 |
| B | ? | - | LYS | deletion | UNP P00748 |
| B | ? | - | SER | deletion | UNP P00748 |
| B | ? | - | LEU | deletion | UNP P00748 |
| B | ? | - | SER | deletion | UNP P00748 |
| B | ? | - | SER | deletion | UNP P00748 |
| B | ? | - | MET | deletion | UNP P00748 |
| B | ? | - | THR | deletion | UNP P00748 |
| B | ? | - | ARG | deletion | UNP P00748 |
| B | ? | - | GLN | deletion | UNP P00748 |
| B | ? | - | ALA | deletion | UNP P00748 |
| B | ? | - | ALA | deletion | UNP P00748 |
| B | ? | - | GLU | deletion | UNP P00748 |
| D | 329 | ALA | - | expression tag | UNP P00748 |
| D | 330 | ALA | - | expression tag | UNP P00748 |
| D | 331 | ALA | - | expression tag | UNP P00748 |
| D | 332 | ALA | - | expression tag | UNP P00748 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| D | 333 | SER | THR | conflict | UNP P00748 |
| D | 334 | GLU | ARG | conflict | UNP P00748 |
| D | 335 | PHE | ASN | conflict | UNP P00748 |
| D | ? | - | LEU | deletion | UNP P00748 |
| D | ? | - | ARG | deletion | UNP P00748 |
| D | ? | - | LYS | deletion | UNP P00748 |
| D | ? | - | SER | deletion | UNP P00748 |
| D | ? | - | LEU | deletion | UNP P00748 |
| D | ? | - | SER | deletion | UNP P00748 |
| D | ? | - | SER | deletion | UNP P00748 |
| D | ? | - | MET | deletion | UNP P00748 |
| D | ? | - | THR | deletion | UNP P00748 |
| D | ? | - | ARG | deletion | UNP P00748 |
| D | ? | - | GLN | deletion | UNP P00748 |
| D | ? | - | ALA | deletion | UNP P00748 |
| D | ? | - | ALA | deletion | UNP P00748 |
| D | ? | - | GLU | deletion | UNP P00748 |

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 3 | E | 2 | 28 | 16 | 2 | 10 | 0 | 0 | 0 |

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---------|---------|-------|
| | | | Total | C | O | | | |
| 4 | F | 2 | 23 | 12 | 11 | 0 | 0 | 0 |
| 4 | G | 2 | 23 | 12 | 11 | 0 | 0 | 0 |

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | B | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

- Molecule 6 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



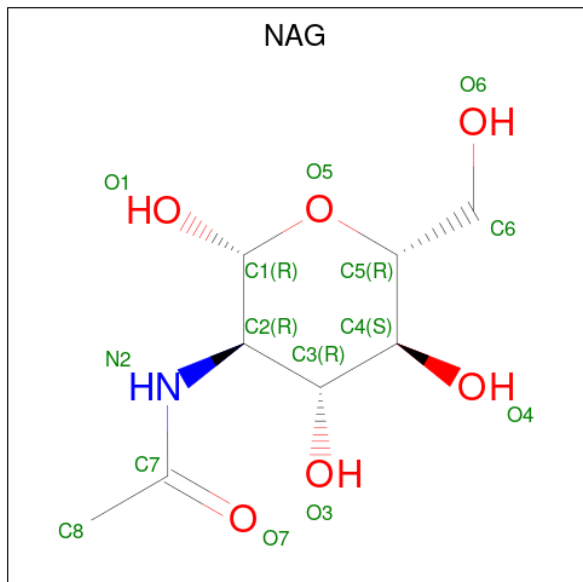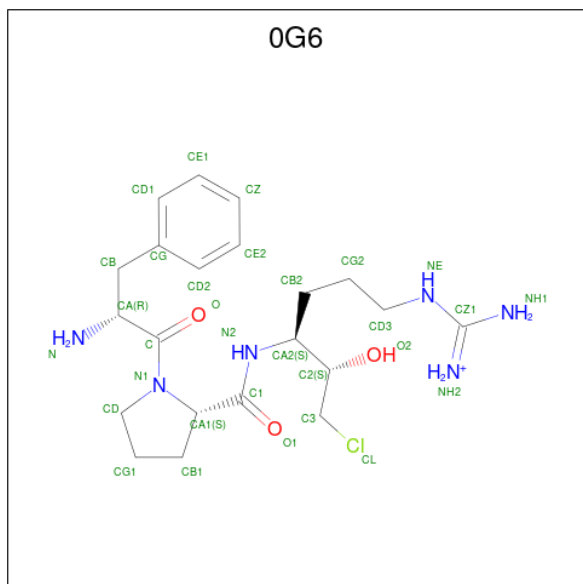| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 6 | B | 1 | 30 | 21 | 6 | 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| | | | Total | C | N | O | | |
| 6 | D | 1 | 30 | 21 | 6 | 3 | 0 | 0 |

# 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: Maltodextrin-binding protein
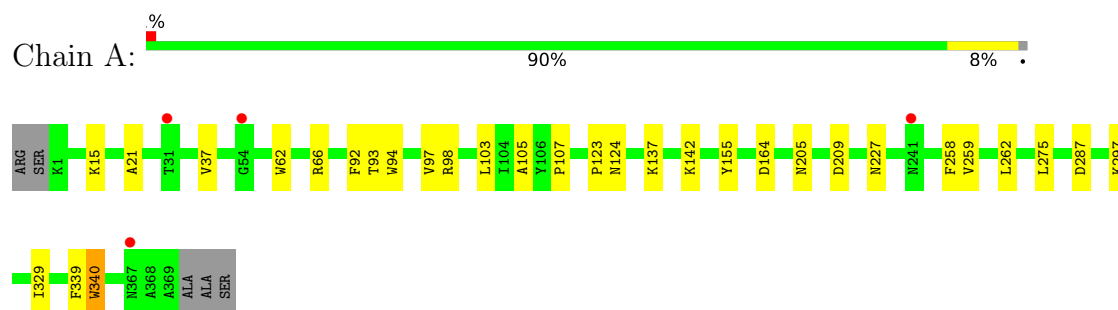


• Molecule 1: Maltodextrin-binding protein
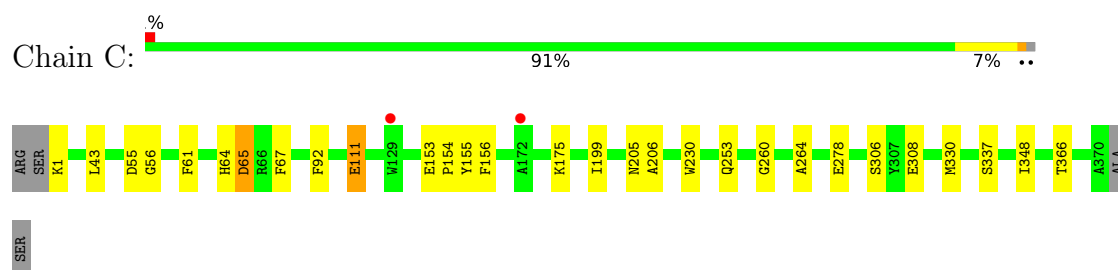


• Molecule 2: Coagulation factor XII



• Molecule 2: Coagulation factor XII

ALA ALA ALA ALA SER GLU PHE GLY PRO LEU S339 C340 G341 Q342 R343 L361 R362 H365 P366 Y367 I368 A369 A370 L371 Y372 W373 G374 F377 C378 C386 W387 H393 C394 L395 A400 P401 E402 V406 Q410 E411 R412 R413 N414 H415 S416 C417 E418 P419 C420 L423

R426 S427 Y428 R429 E432 Y439 D442 L443 L446 Q449 E450 D451 A452 D453 G454 S455 Y462 V463 Q464 P465 V466 C467 L468 P475 S476 E477 T478 T479 L480 C481 Q482 G487 H488 E491 E495 S498 F499 L500 Q501 E502 F507 L508 S509 L510 E511 V518 H519

S522 M527 A539 D543 V549 R557 R558 L559 T560 L561 I562 S563 W564 C568 Y582 H590 T591 V592 S593

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
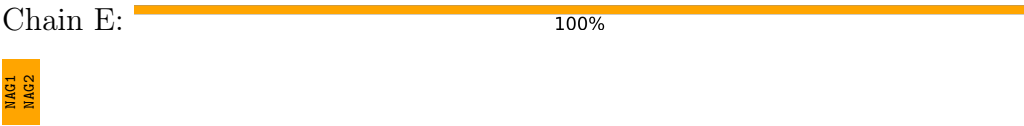
Chain E:    100%

NAG1 NAG2

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:    100%

GLC1 GLC2

• Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:    100%

GLC1 GLC2
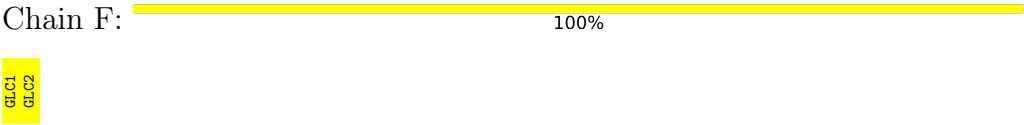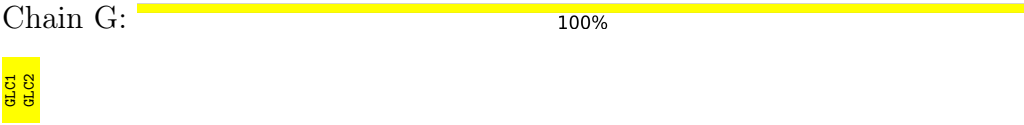
# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants <br> a, b, c, $\alpha$, $\beta$, $\gamma$ | 131.45Å   131.45Å   238.35Å <br> 90.00°    90.00°     90.00° | Depositor |
| Resolution (Å) | 115.11  –  4.00 <br> 115.11  –  4.00 | Depositor <br> EDS |
| % Data completeness <br> (in resolution range) | 93.1 (115.11-4.00) <br> 93.1 (115.11-4.00) | Depositor <br> EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.93 (at 3.98Å) | Xtriage |
| Refinement program | REFMAC 5.8.0189 | Depositor |
| R, $R_{free}$ | 0.297  ,  0.356 <br> 0.298  ,  0.353 | Depositor <br> DCC |
| $R_{free}$ test set | 15371 reflections (10.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 39.9 | Xtriage |
| Anisotropy | 0.033 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.25 , 0.0 | EDS |
| L-test for twinning[2] | $< |L| > = 0.39, < L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.74 | EDS |
| Total number of atoms | 9512 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 39.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: NAG, 0G6, GLC

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|------|------|------|------|
| | | RMSZ | #$|Z|$>5 | RMSZ | #$|Z|$>5 |
| 1 | A | 0.42 | 0/2914 | 0.57 | 0/3962 |
| 1 | C | 0.43 | 0/2920 | 0.56 | 0/3971 |
| 2 | B | 0.55 | 0/1886 | 0.82 | 2/2569 (0.1%) |
| 2 | D | 0.58 | 0/1886 | 0.81 | 0/2569 |
| All | All | 0.49 | 0/9606 | 0.67 | 2/13071 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|------------|---------|
| 2 | B | 499 | PHE | CB-CA-C | 7.09 | 124.59 | 110.40 |
| 2 | B | 360 | ALA | N-CA-C | 6.29 | 127.98 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2839 | 0 | 2817 | 32 | 0 |
| 1 | C | 2845 | 0 | 2824 | 20 | 0 |
| 2 | B | 1840 | 0 | 1741 | 129 | 0 |
| 2 | D | 1840 | 0 | 1742 | 117 | 0 |
| 3 | E | 28 | 0 | 25 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | F | 23 | 0 | 21 | 16 | 0 |
| 4 | G | 23 | 0 | 21 | 5 | 0 |
| 5 | B | 14 | 0 | 13 | 1 | 0 |
| 6 | B | 30 | 0 | 31 | 1 | 0 |
| 6 | D | 30 | 0 | 31 | 21 | 0 |
| All | All | 9512 | 0 | 9266 | 304 | 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 16.

The worst 5 of 304 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) |
|--------|--------|--------------------------|-------------------|
| 2:D:377:PHE:HD1 | 2:D:378:CYS:N | 1.32 | 1.25 |
| 2:B:362:ARG:HG3 | 2:B:363:GLY:N | 1.37 | 1.23 |
| 2:B:360:ALA:HB2 | 2:B:500:LEU:O | 1.42 | 1.17 |
| 2:B:367:TYR:HD2 | 2:B:466:VAL:CG1 | 1.58 | 1.15 |
| 2:B:367:TYR:CD2 | 2:B:466:VAL:HG11 | 1.82 | 1.14 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 | 369/374 (99%) | 337 (91%) | 31 (8%) | 1 (0%) | 37 | 71 |
| 1 | C | 370/374 (99%) | 344 (93%) | 25 (7%) | 1 (0%) | 37 | 71 |
| 2 | B | 238/254 (94%) | 199 (84%) | 32 (13%) | 7 (3%) | 3 | 27 |
| 2 | D | 238/254 (94%) | 206 (87%) | 28 (12%) | 4 (2%) | 7 | 37 |
| All | All | 1215/1256 (97%) | 1086 (89%) | 116 (10%) | 13 (1%) | 12 | 45 |

5 of 13 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 466 | VAL |
| 2 | B | 453 | ASP |
| 2 | B | 465 | PRO |
| 2 | B | 581 | ALA |
| 1 | C | 67 | PHE |

### 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 | 288/289 (100%) | 276 (96%) | 12 (4%) | 25 | 48 |
| 1 | C | 288/289 (100%) | 275 (96%) | 13 (4%) | 23 | 46 |
| 2 | B | 194/199 (98%) | 154 (79%) | 40 (21%) | 1 | 6 |
| 2 | D | 194/199 (98%) | 154 (79%) | 40 (21%) | 1 | 6 |
| All | All | 964/976 (99%) | 859 (89%) | 105 (11%) | 5 | 21 |

5 of 105 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 175 | LYS |
| 2 | D | 368 | ILE |
| 2 | D | 558 | ARG |
| 1 | C | 253 | GLN |
| 2 | D | 342 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 482 | GLN |
| 2 | D | 501 | GLN |
| 2 | D | 519 | HIS |
| 1 | C | 253 | GLN |
| 2 | D | 342 | GLN |

#### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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 | $\#|Z| > 2$ |
| 3 | NAG | E | 1 | 3 | 14,14,15 | 0.95 | 0 | 17,19,21 | 1.37 | 3 (17%) |
| 3 | NAG | E | 2 | 3 | 14,14,15 | 1.01 | 1 (7%) | 17,19,21 | 1.33 | 4 (23%) |
| 4 | GLC | F | 1 | 4 | 12,12,12 | 0.44 | 0 | 17,17,17 | 0.53 | 0 |
| 4 | GLC | F | 2 | 4 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.62 | 0 |
| 4 | GLC | G | 1 | 4 | 12,12,12 | 0.44 | 0 | 17,17,17 | 0.56 | 0 |
| 4 | GLC | G | 2 | 4 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.64 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3 | NAG | E | 1 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | E | 2 | 3 | 1/1/5/7 | 2/6/23/26 | 0/1/1/1 |
| 4 | GLC | F | 1 | 4 | - | 0/2/22/22 | 0/1/1/1 |
| 4 | GLC | F | 2 | 4 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | GLC | G | 1 | 4 | - | 0/2/22/22 | 0/1/1/1 |
| 4 | GLC | G | 2 | 4 | - | 1/2/19/22 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | E | 2 | NAG | C1-C2 | 3.00 | 1.56 | 1.52 |

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 3 | E | 1 | NAG | O4-C4-C3 | -2.89 | 103.66 | 110.35 |
| 3 | E | 1 | NAG | C3-C4-C5 | -2.82 | 105.21 | 110.24 |
| 3 | E | 2 | NAG | C4-C3-C2 | 2.72 | 115.00 | 111.02 |
| 3 | E | 2 | NAG | O5-C5-C6 | 2.64 | 111.34 | 107.20 |
| 3 | E | 1 | NAG | C2-N2-C7 | -2.18 | 119.80 | 122.90 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 3 | E | 2 | NAG | C1 |

5 of 7 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | E | 1 | NAG | C1-C2-N2-C7 |
| 3 | E | 1 | NAG | C8-C7-N2-C2 |
| 3 | E | 1 | NAG | O7-C7-N2-C2 |
| 3 | E | 2 | NAG | O5-C5-C6-O6 |
| 3 | E | 2 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

6 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | G | 2 | GLC | 1 | 0 |
| 4 | F | 2 | GLC | 16 | 0 |
| 3 | E | 1 | NAG | 2 | 0 |
| 3 | E | 2 | NAG | 1 | 0 |
| 4 | G | 1 | GLC | 4 | 0 |
| 4 | F | 1 | GLC | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain E

**Bond lengths**

**Bond angles**

**Torsions**

**Rings**

## Oligosaccharide Chain F


Bond lengths


Bond angles


Torsions


Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
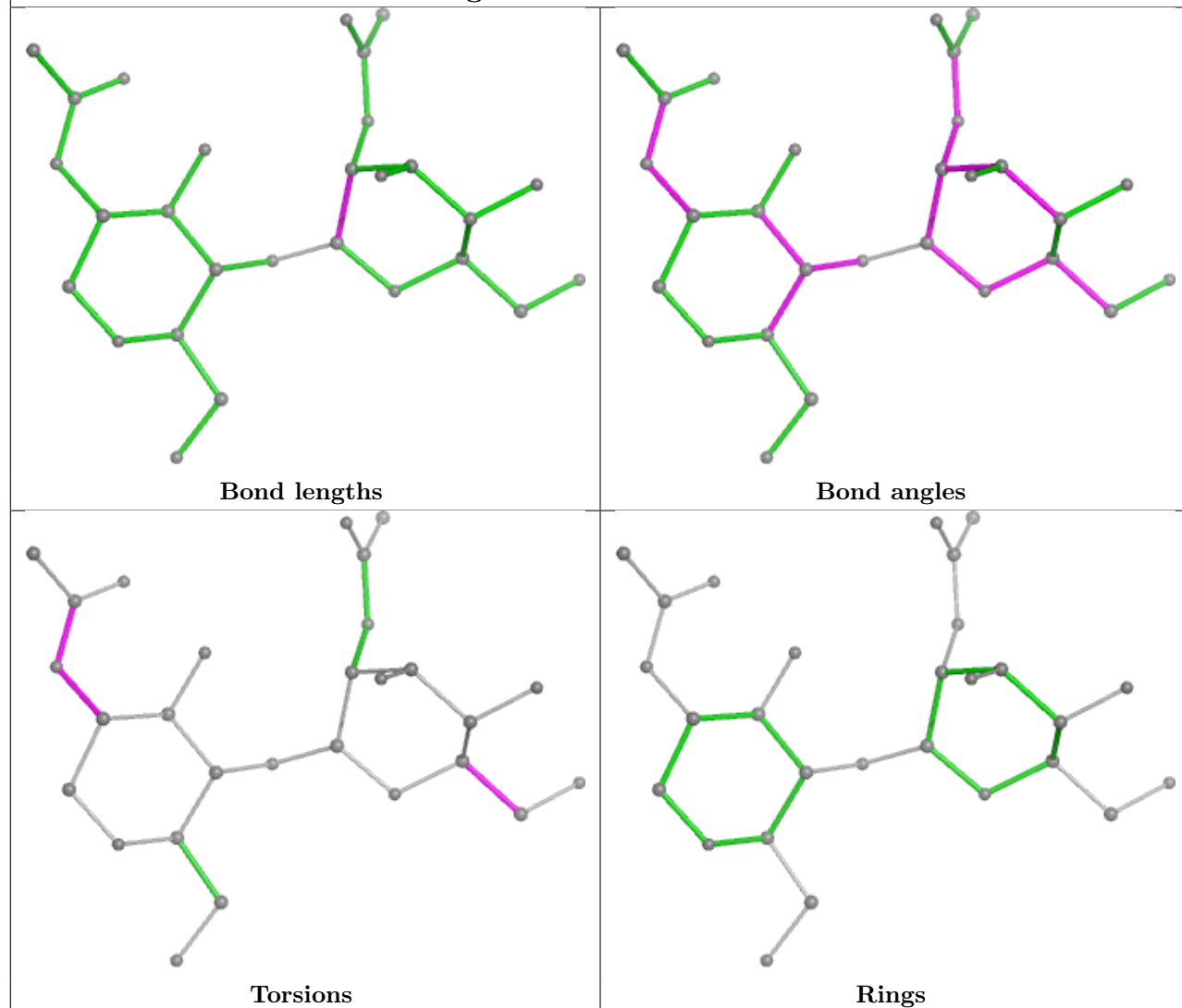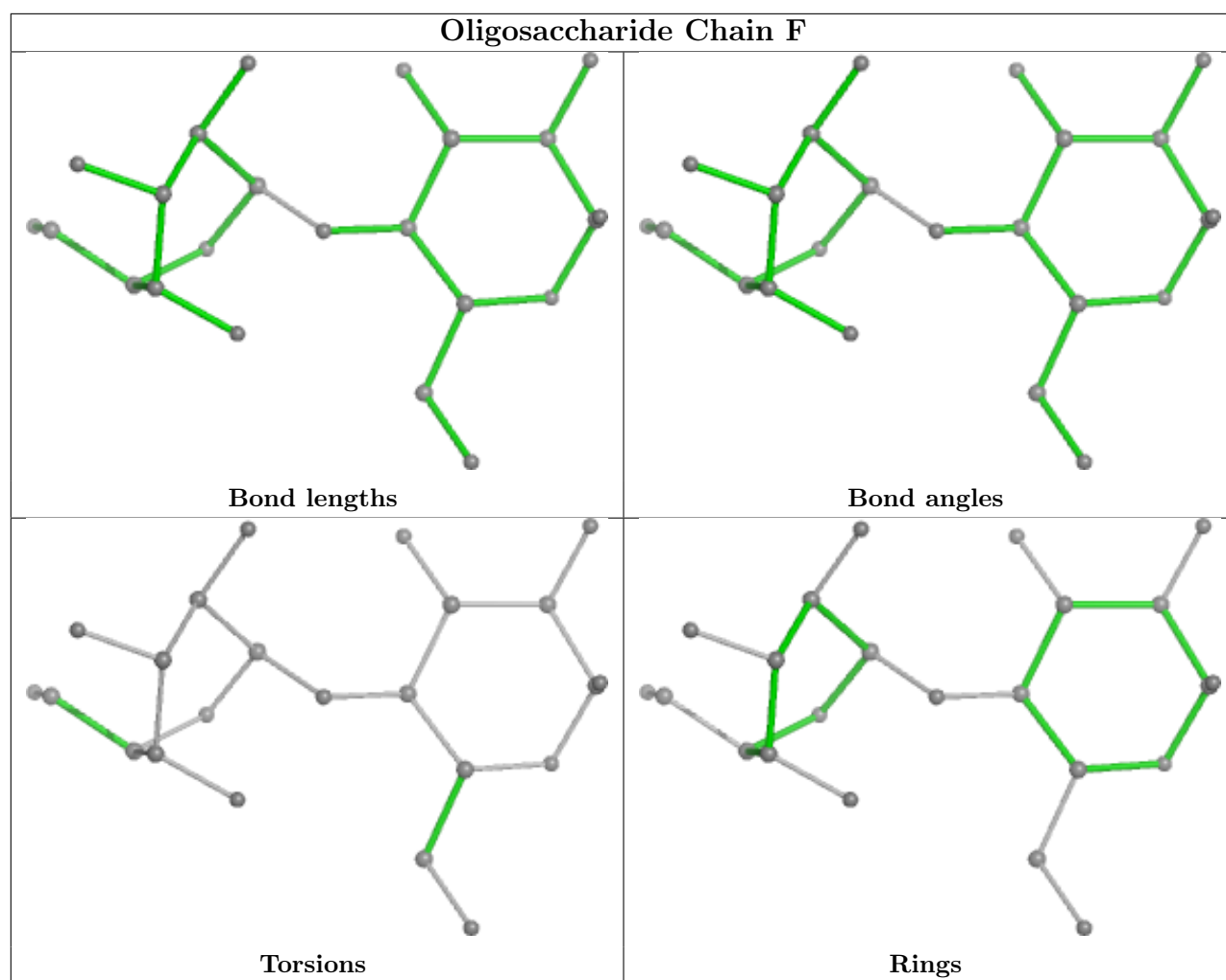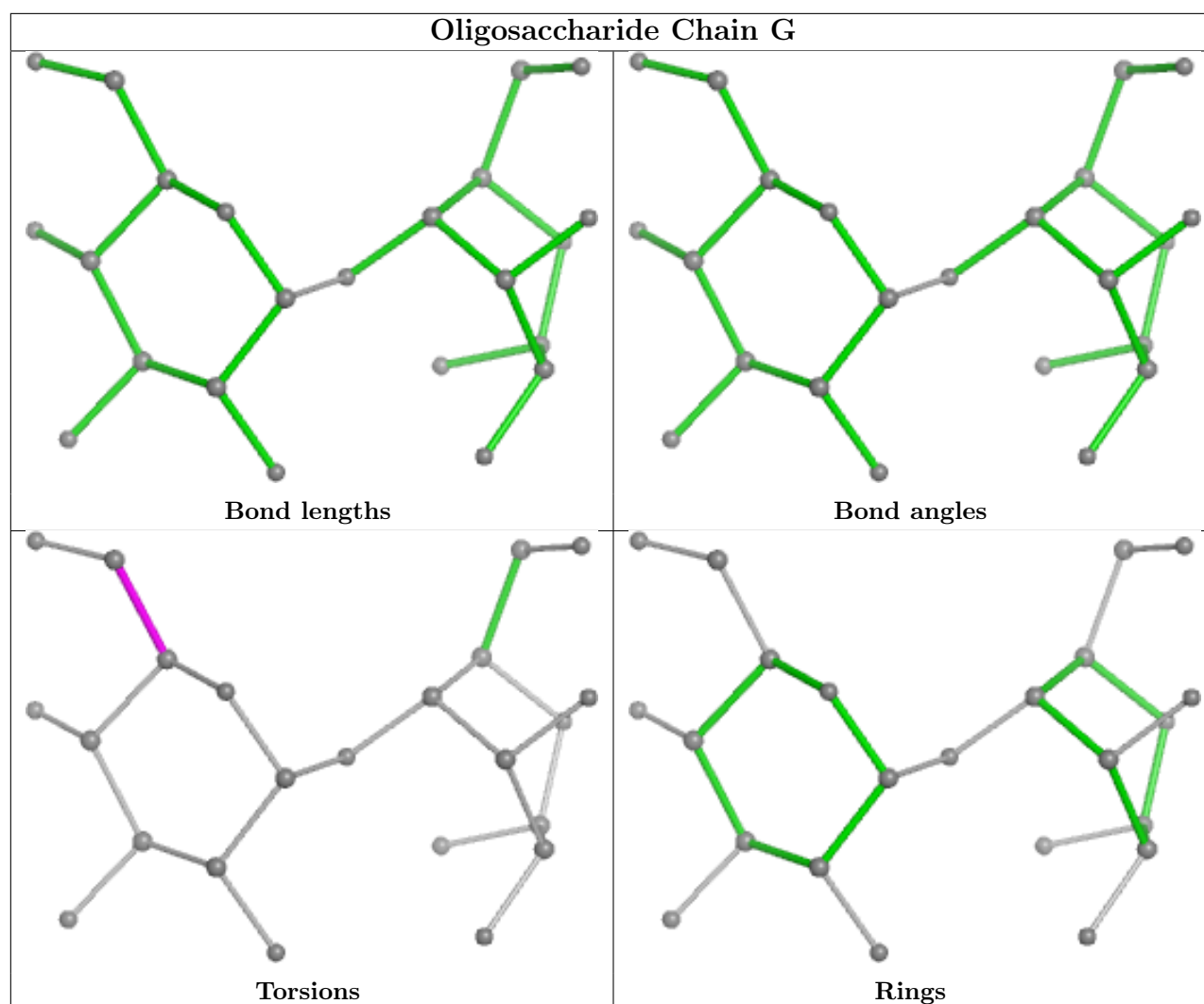
## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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 | #$|Z| > 2$ |
| 5 | NAG | B | 701 | 2 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.64 | 0 |
| 6 | 0G6 | D | 703 | 2 | 30,31,32 | 0.39 | 0 | 37,41,42 | 0.78 | 1 (2%) |
| 6 | 0G6 | B | 702 | 2 | 30,31,32 | 0.40 | 0 | 37,41,42 | 0.78 | 1 (2%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 5 | NAG | B | 701 | 2 | 1/1/5/7 | 4/6/23/26 | 0/1/1/1 |
| 6 | 0G6 | D | 703 | 2 | - | 20/31/41/43 | 0/2/2/2 |
| 6 | 0G6 | B | 702 | 2 | - | 20/31/41/43 | 0/2/2/2 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------|--------|
| 6 | B | 702 | 0G6 | CG-CB-CA | -2.26 | 109.42 | 114.13 |
| 6 | D | 703 | 0G6 | CG-CB-CA | -2.25 | 109.45 | 114.13 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 5 | B | 701 | NAG | C1 |

5 of 44 torsion outliers are listed below:

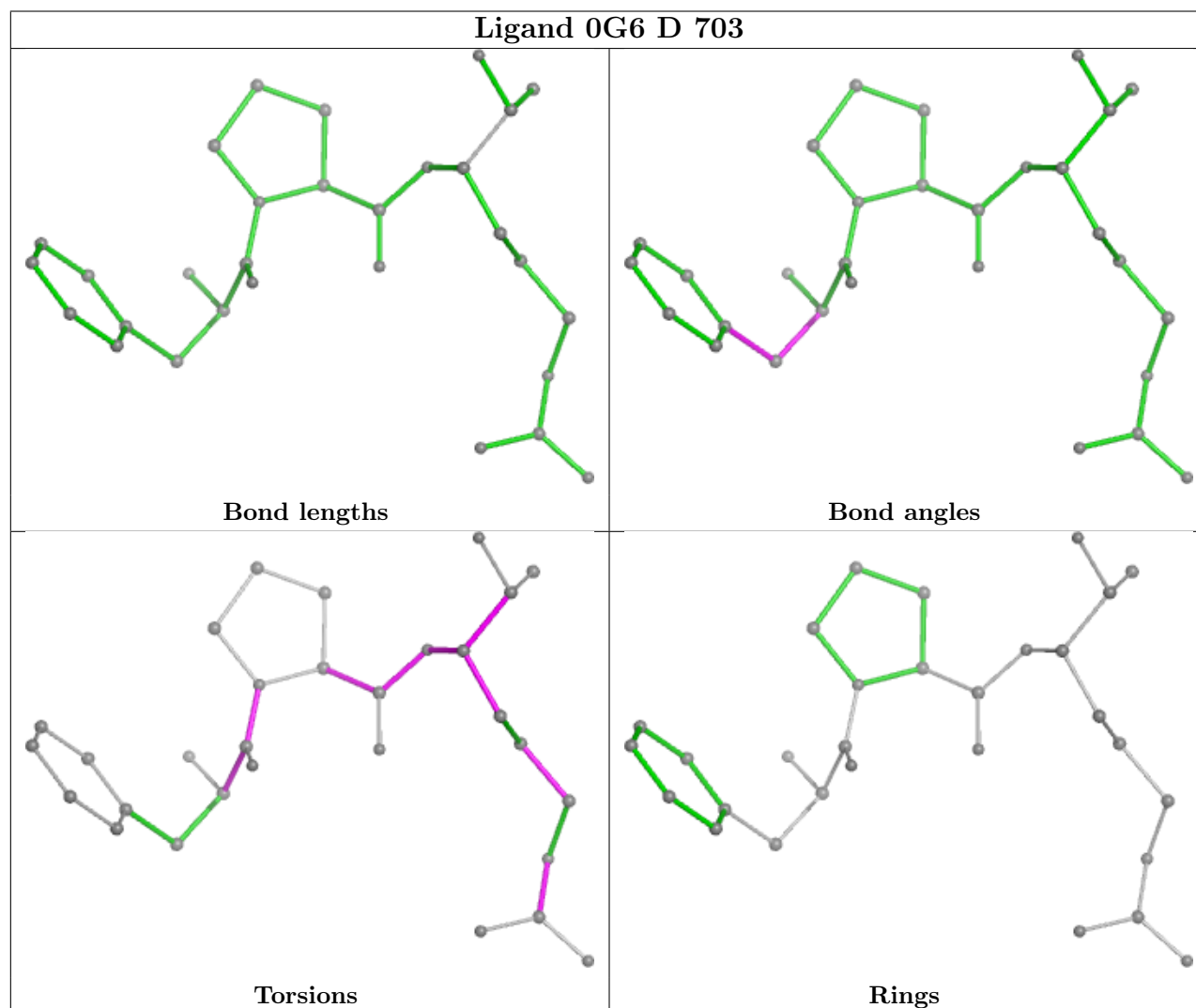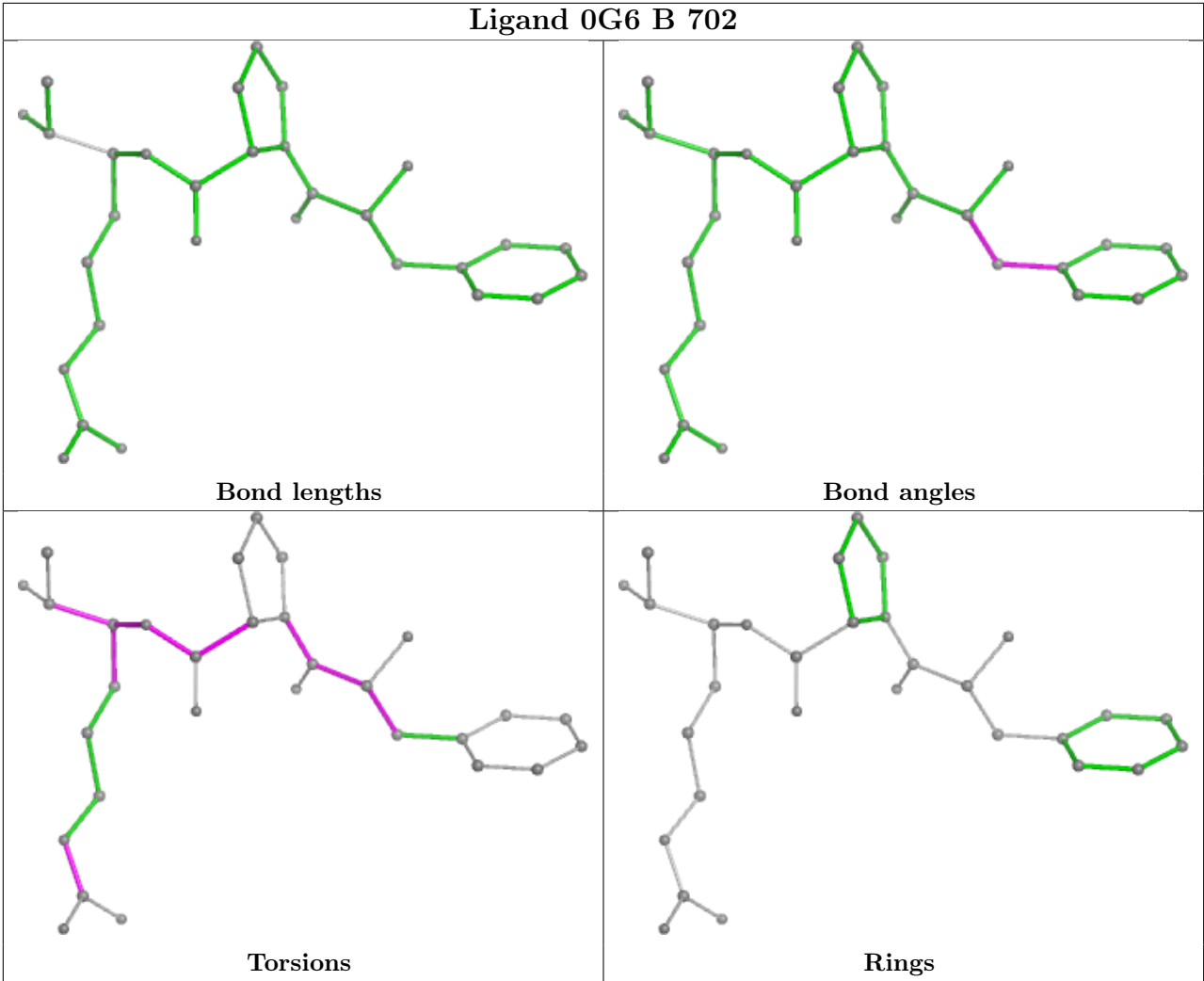| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 5 | B | 701 | NAG | C3-C2-N2-C7 |
| 5 | B | 701 | NAG | C8-C7-N2-C2 |
| 5 | B | 701 | NAG | O7-C7-N2-C2 |
| 6 | B | 702 | 0G6 | N1-C-CA-N |
| 6 | B | 702 | 0G6 | N-CA-CB-CG |

There are no ring outliers.

3 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | B | 701 | NAG | 1 | 0 |
| 6 | D | 703 | 0G6 | 21 | 0 |
| 6 | B | 702 | 0G6 | 1 | 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 0G6 D 703**



Bond lengths

Bond angles

Torsions

Rings

Ligand 0G6 B 702



Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | B     | 2                |
| 2   | D     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 344:ARG   | C      | 354:VAL   | N      | 22.66        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | D | 343:ARG | C | 354:VAL | N | 22.36 |
| 1 | D | 552:ASP | C | 557:ARG | N | 6.48 |
| 1 | B | 552:ASP | C | 557:ARG | N | 5.00 |

# 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 | 369/374 (98%) | 0.29 | 4 (1%) | 77 | 63 | 13, 35, 68, 94 | 2 (0%) |
| 1 | C | 370/374 (98%) | 0.32 | 2 (0%) | 87 | 76 | 12, 40, 61, 75 | 2 (0%) |
| 2 | B | 244/254 (96%) | 0.55 | 2 (0%) | 82 | 69 | 20, 38, 72, 94 | 1 (0%) |
| 2 | D | 244/254 (96%) | 0.51 | 5 (2%) | 64 | 49 | 18, 29, 74, 107 | 1 (0%) |
| All | All | 1227/1256 (97%) | 0.40 | 13 (1%) | 77 | 63 | 12, 36, 67, 107 | 6 (0%) |

The worst 5 of 13 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 172 | ALA | 3.9 |
| 2 | D | 478 | THR | 3.6 |
| 1 | A | 31 | THR | 3.0 |
| 2 | D | 593 | SER | 2.8 |
| 1 | A | 54 | GLY | 2.4 |

## 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 ⓘ

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.
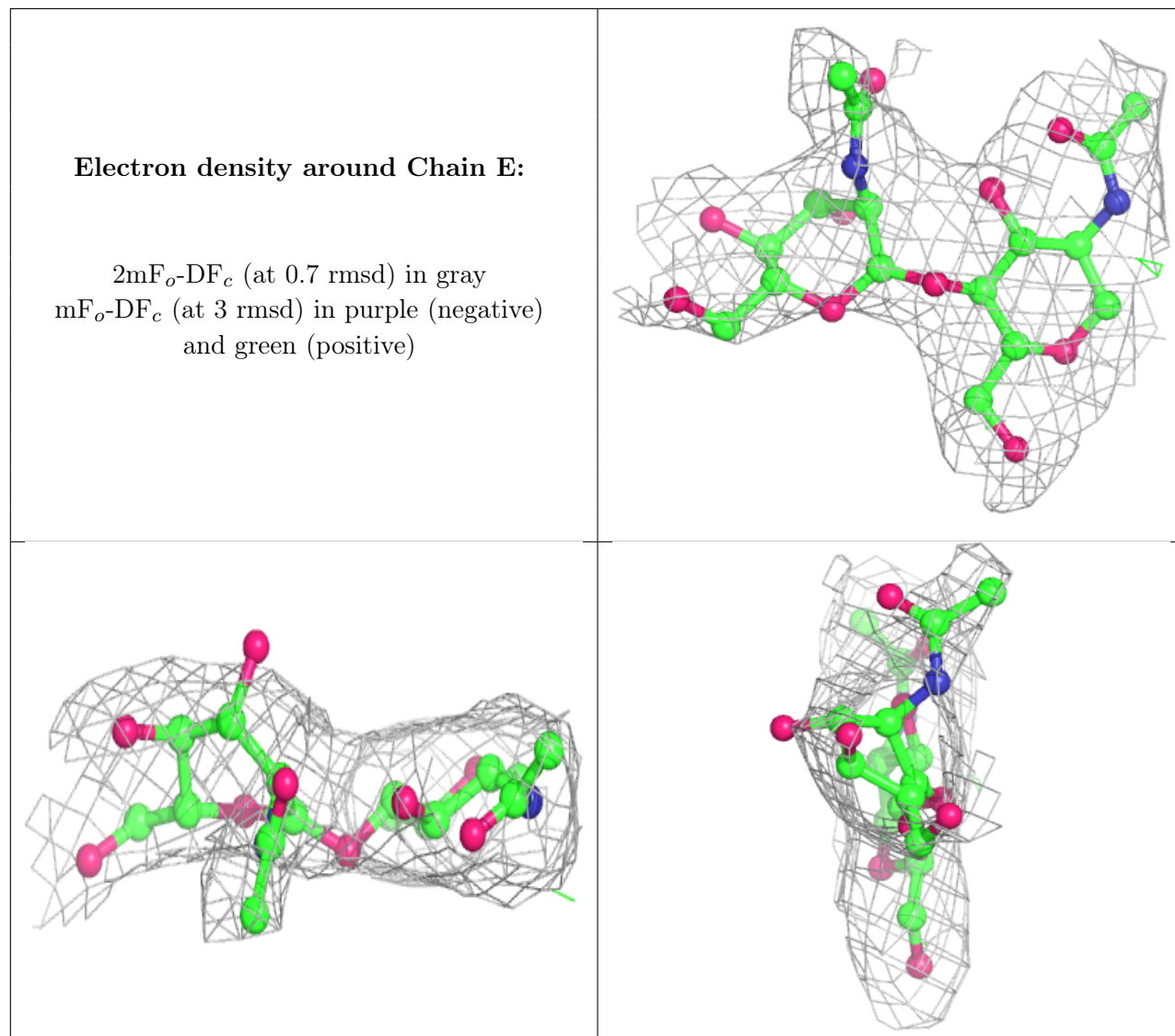
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|---------------|-------|
| 3 | NAG | E | 2 | 14/15 | 0.72 | 0.14 | 30,30,31,31 | 0 |
| 3 | NAG | E | 1 | 14/15 | 0.75 | 0.17 | 27,28,29,29 | 0 |

*Continued on next page...*
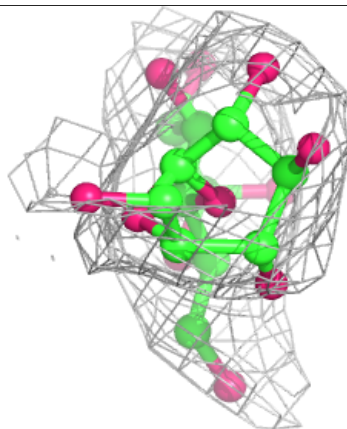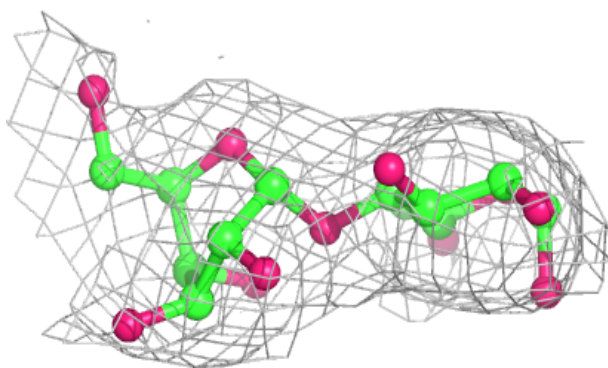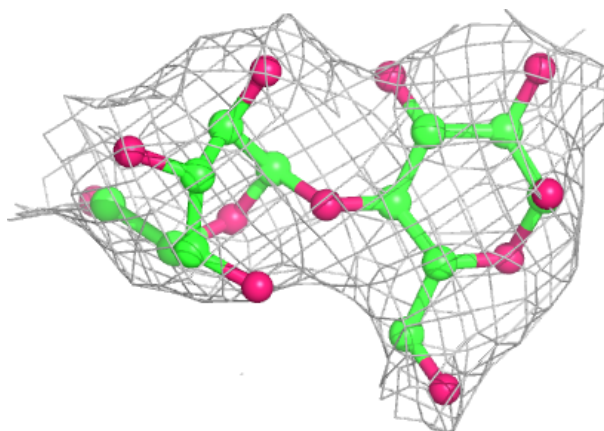
*Continued from previous page...*

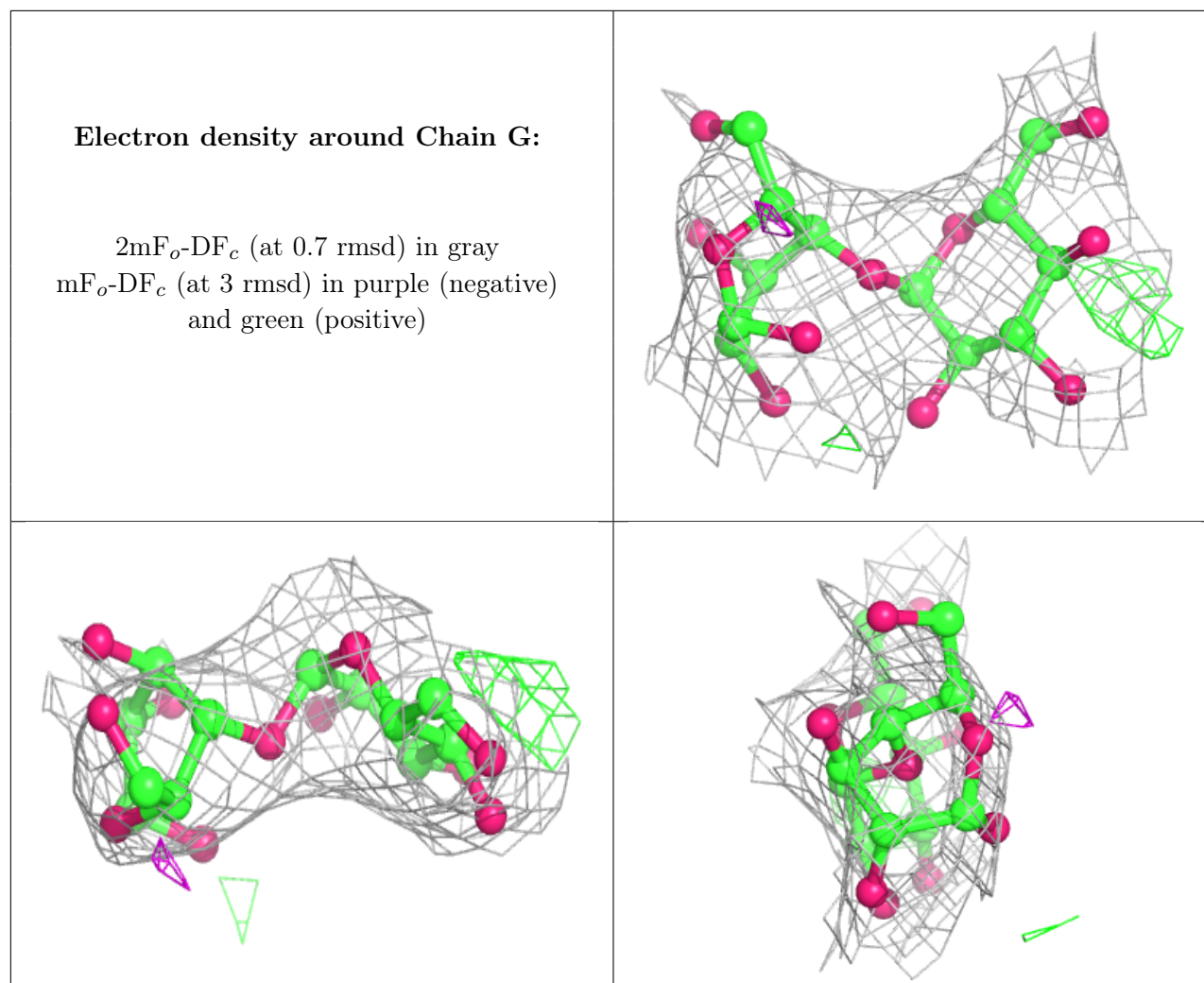| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------------------|-------|
| 4 | GLC | G | 2 | 11/12 | 0.85 | 0.17 | 19,19,19,20 | 0 |
| 4 | GLC | G | 1 | 12/12 | 0.90 | 0.20 | 19,19,19,19 | 3 |
| 4 | GLC | F | 2 | 11/12 | 0.91 | 0.15 | 19,19,19,20 | 2 |
| 4 | GLC | F | 1 | 12/12 | 0.92 | 0.12 | 19,19,19,20 | 0 |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

**Electron density around Chain F:**

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

**Electron density around Chain G:**

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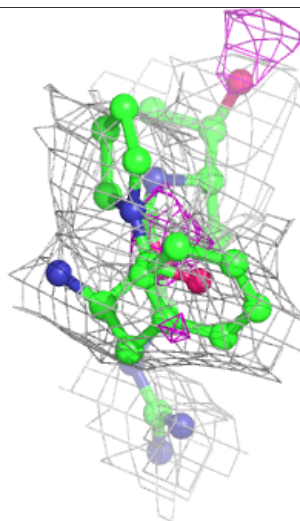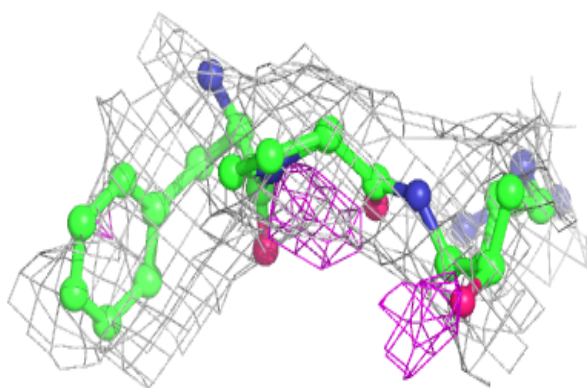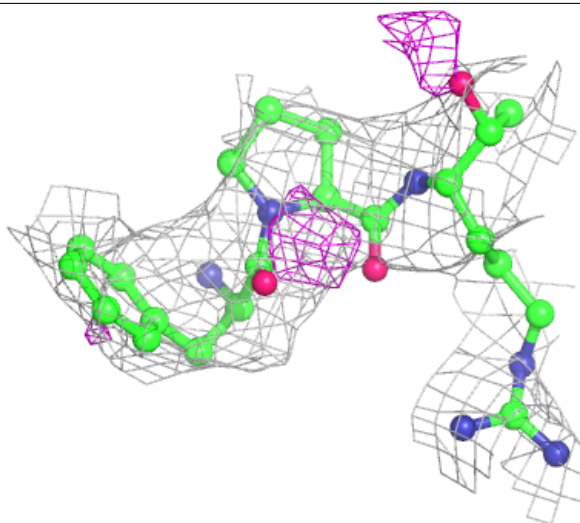and green (positive)



## 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($\mathring{A}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------------------------------|-------|
| 5 | NAG | B | 701 | 14/15 | 0.18 | 0.36 | 40,42,42,42 | 6 |
| 6 | 0G6 | D | 703 | 30/31 | 0.87 | 0.17 | 14,18,19,19 | 3 |
| 6 | 0G6 | B | 702 | 30/31 | 0.90 | 0.17 | 27,28,29,29 | 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.
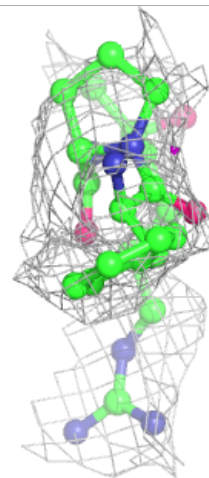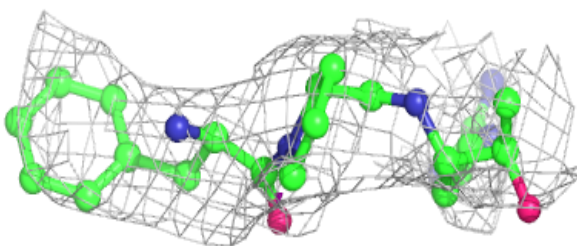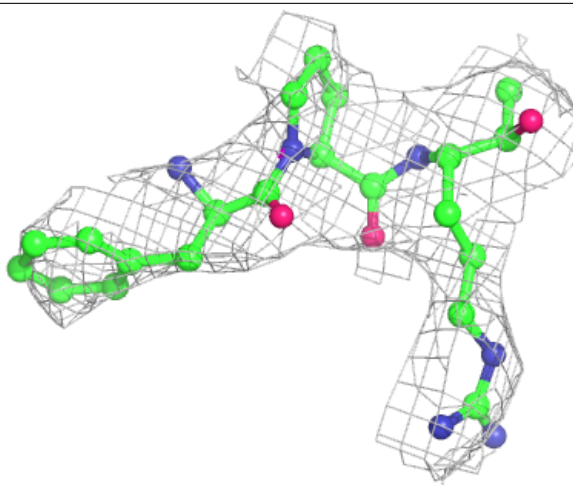
**Electron density around 0G6 D 703:**

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

**Electron density around 0G6 B 702:**

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.