



Full wwPDB NMR Structure Validation Report ⓘ

Jun 10, 2021 – 12:18 PM BST

PDB ID : 7ND1
Title : First-in-class small molecule inhibitors of Polycomb Repressive Complex 1 (PRC1) RING domain
Authors : Cierpicki, T.; Lund, G.; Jaremko, L.
Deposited on : 2021-01-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.20
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

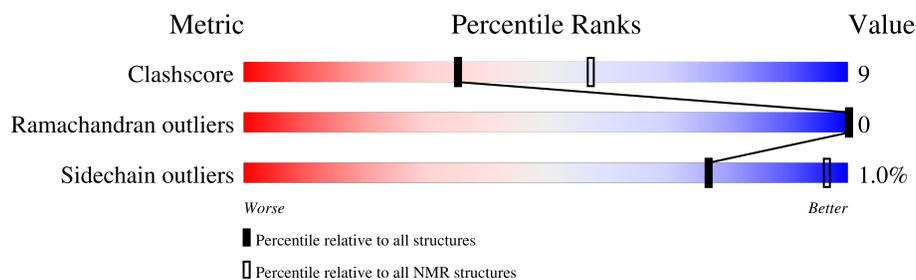
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 14%.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 112 | |
| 2 | H | 101 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:16-A:77, A:89-A:103, H:1004-H:1102 (176) | 0.07 | 9 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 4 single-model clusters were found.

| Cluster number | Models |
|-----------------------|---|
| 1 | 1, 3, 4, 5, 7, 8, 9, 11, 14, 15, 16, 17, 18 |
| 2 | 10, 13, 19 |
| Single-model clusters | 2; 6; 12; 20 |

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3280 atoms, of which 1651 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase RING2.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|---|
| | | | Total | C | H | N | O | | S |
| 1 | A | 100 | 1603 | 498 | 810 | 138 | 147 | 10 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 8 | GLY | - | expression tag | UNP Q99496 |
| A | 9 | PRO | - | expression tag | UNP Q99496 |
| A | 117 | MET | - | expression tag | UNP Q99496 |
| A | 118 | HIS | - | expression tag | UNP Q99496 |
| A | 119 | ARG | - | expression tag | UNP Q99496 |

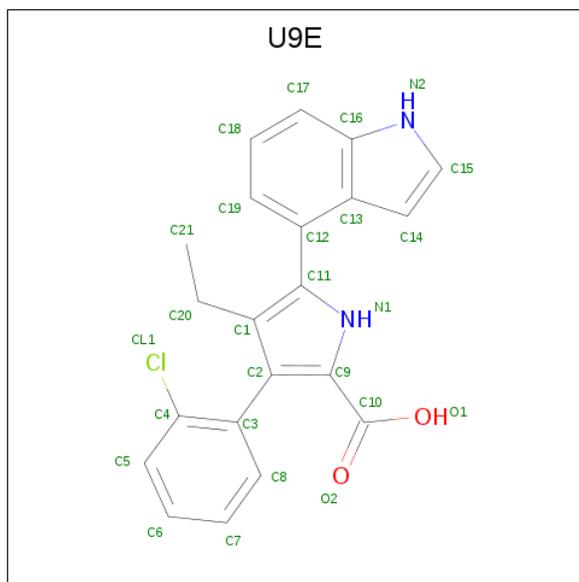
- Molecule 2 is a protein called Polycomb complex protein BMI-1.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|---|
| | | | Total | C | H | N | O | | S |
| 2 | H | 99 | 1631 | 517 | 825 | 141 | 139 | 9 | 0 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| | | | Total | Zn |
| 3 | A | 2 | 2 | 2 |
| 3 | H | 2 | 2 | 2 |

- Molecule 4 is 3-(2-chlorophenyl)-4-ethyl-5-(1 {H}-indol-4-yl)-1 {H}-pyrrole-2-carboxylic acid (three-letter code: U9E) (formula: C₂₁H₁₇ClN₂O₂) (labeled as "Ligand of Interest" by depositor).



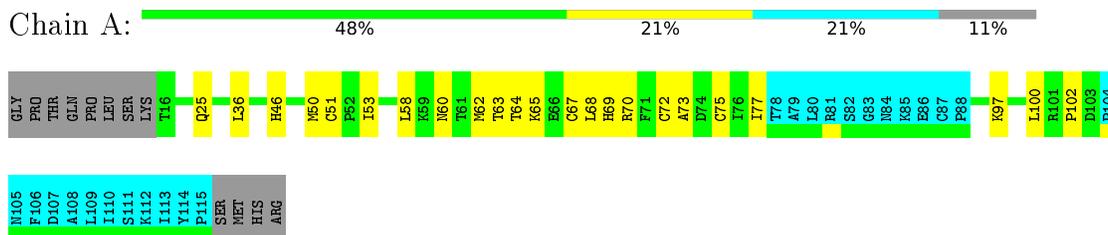
| Mol | Chain | Residues | Atoms | | | | | |
|-----|-------|----------|-------|----|----|----|---|---|
| | | | Total | C | Cl | H | N | O |
| 4 | A | 1 | 42 | 21 | 1 | 16 | 2 | 2 |

4 Residue-property plots [i](#)

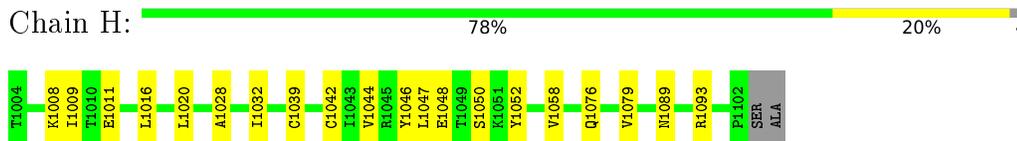
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 2: Polycomb complex protein BMI-1

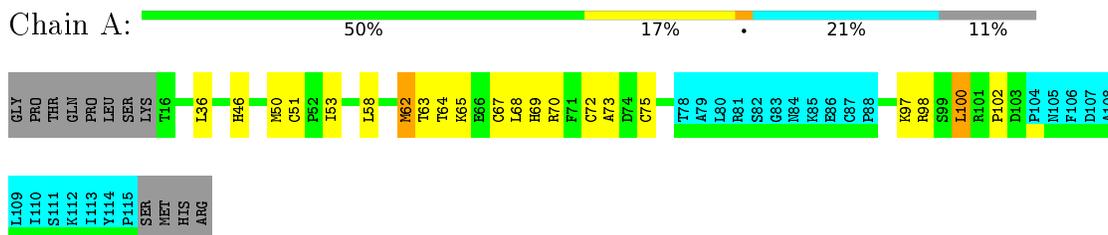


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 2: Polycomb complex protein BMI-1

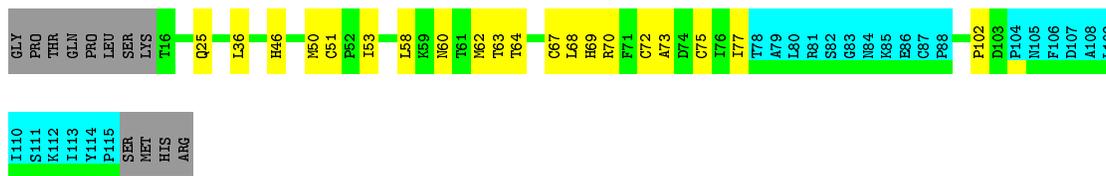
Chain H: 



4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase RING2

Chain A: 



- Molecule 2: Polycomb complex protein BMI-1

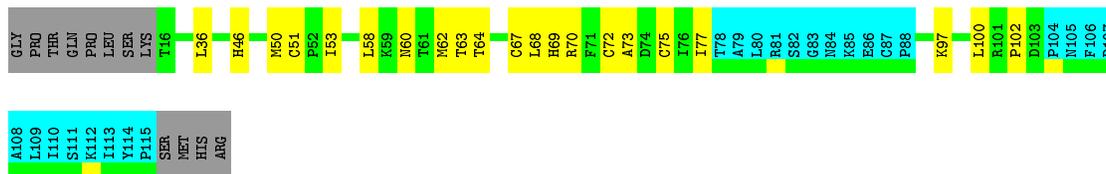
Chain H: 



4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase RING2

Chain A: 



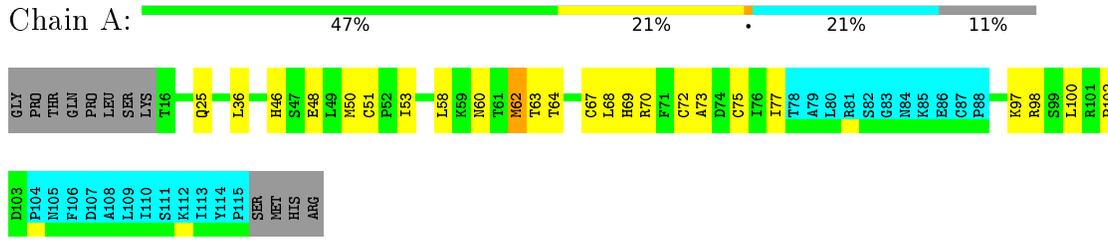
- Molecule 2: Polycomb complex protein BMI-1

Chain H: 

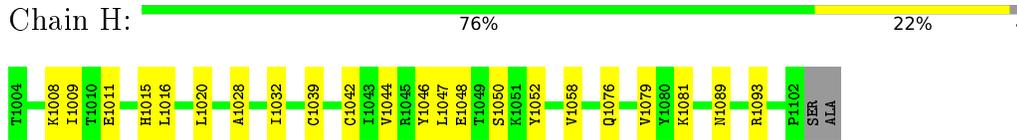


4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase RING2

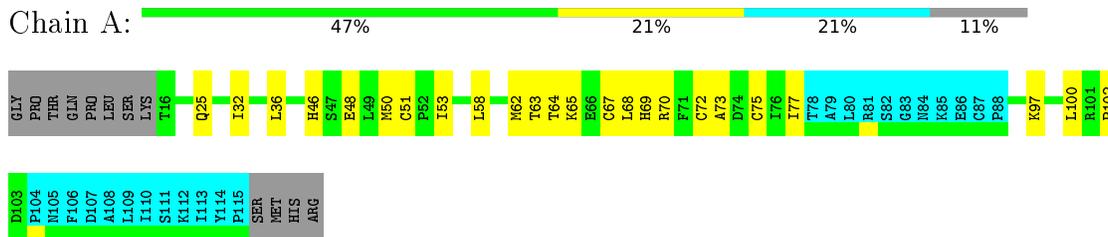


- Molecule 2: Polycomb complex protein BMI-1

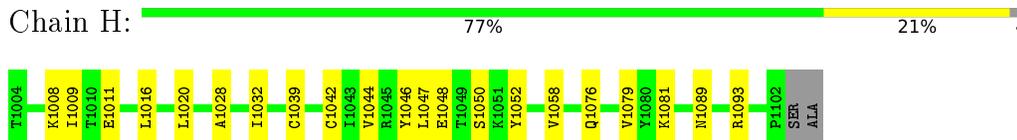


4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase RING2

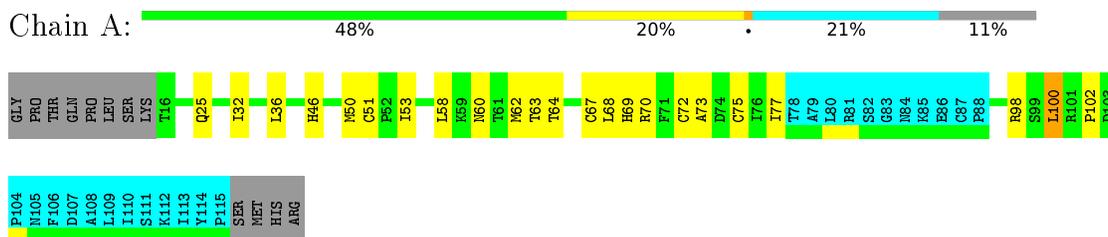


- Molecule 2: Polycomb complex protein BMI-1

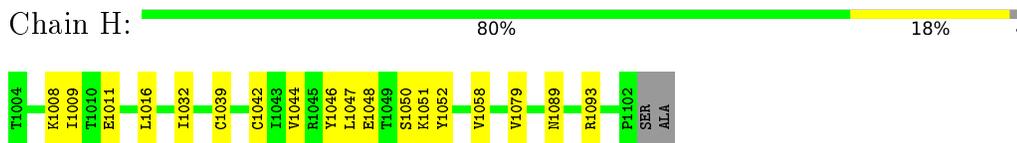


4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase RING2

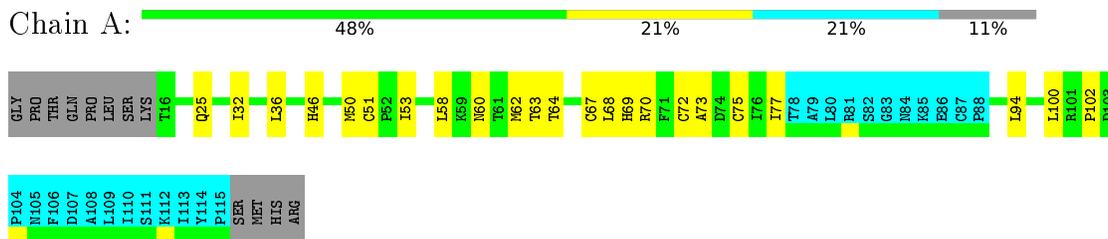


- Molecule 2: Polycomb complex protein BMI-1

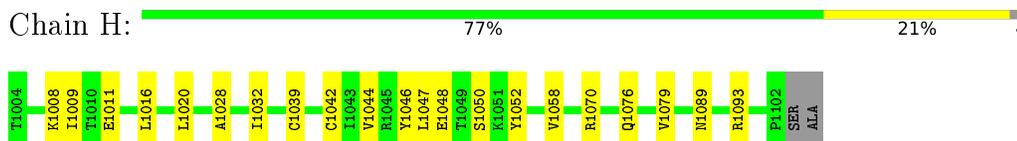


4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase RING2

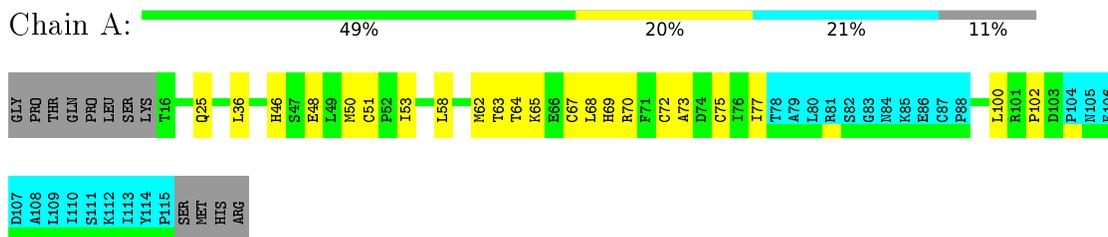


- Molecule 2: Polycomb complex protein BMI-1

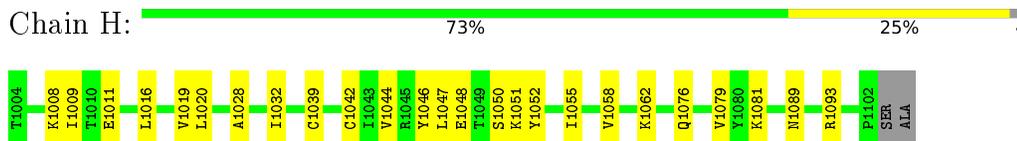


4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 2: Polycomb complex protein BMI-1



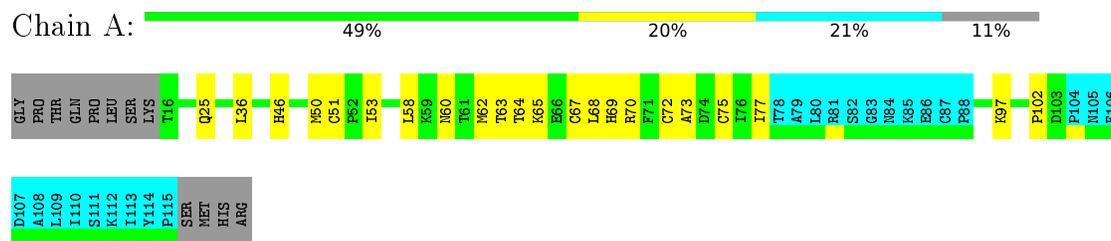
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase RING2

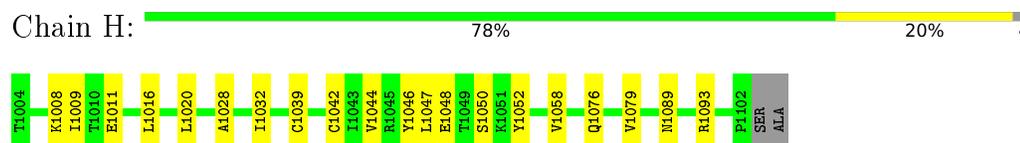


4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase RING2

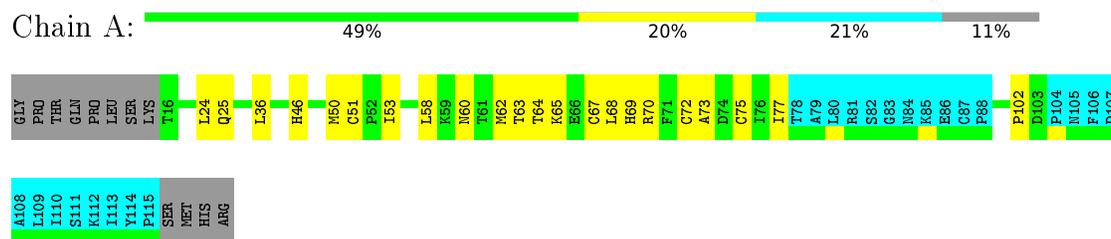


- Molecule 2: Polycomb complex protein BMI-1

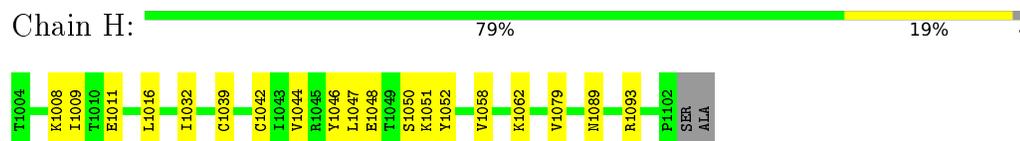


4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase RING2



- Molecule 2: Polycomb complex protein BMI-1



4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase RING2

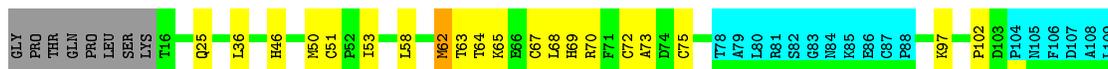
Chain H:  77% 21%



4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase RING2

Chain A:  51% 17% 21% 11%



- Molecule 2: Polycomb complex protein BMI-1

Chain H:  78% 20%



4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase RING2

Chain A:  50% 19% 21% 11%



- Molecule 2: Polycomb complex protein BMI-1

Chain H:  78% 20%



4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase RING2

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| HADDOCK | refinement | 2.4 |
| HADDOCK | structure calculation | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 378 |
| Number of shifts mapped to atoms | 370 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 8 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 14% |

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U9E

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 616 | 632 | 632 | 14±1 |
| 2 | H | 806 | 825 | 828 | 13±1 |
| 4 | A | 26 | 16 | 0 | 2±1 |
| All | All | 29040 | 29460 | 29202 | 503 |

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 9.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:LEU:HD21 | 2:H:1032:ILE:HG22 | 0.79 | 1.55 | 1 | 20 |
| 1:A:64:THR:OG1 | 1:A:67:CYS:SG | 0.68 | 2.52 | 5 | 20 |
| 4:A:203:U9E:C21 | 4:A:203:U9E:C3 | 0.64 | 2.75 | 6 | 11 |
| 1:A:36:LEU:O | 2:H:1009:ILE:HG12 | 0.59 | 1.96 | 8 | 20 |
| 2:H:1039:CYS:HB2 | 2:H:1042:CYS:SG | 0.57 | 2.39 | 13 | 20 |
| 2:H:1044:VAL:O | 2:H:1048:GLU:HG3 | 0.57 | 2.00 | 4 | 20 |
| 1:A:72:CYS:HB2 | 1:A:75:CYS:SG | 0.56 | 2.40 | 1 | 16 |
| 1:A:51:CYS:SG | 1:A:53:ILE:HB | 0.55 | 2.42 | 13 | 20 |
| 1:A:100:LEU:HD23 | 4:A:203:U9E:C19 | 0.55 | 2.32 | 1 | 5 |
| 1:A:97:LYS:HA | 4:A:203:U9E:C19 | 0.53 | 2.33 | 4 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-------------------|-------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:62:MET:HG3 | 1:A:73:ALA:HA | 0.52 | 1.80 | 9 | 18 |
| 1:A:65:LYS:HG2 | 2:H:1032:ILE:O | 0.51 | 2.05 | 18 | 10 |
| 1:A:46:HIS:O | 1:A:50:MET:HG2 | 0.51 | 2.06 | 11 | 20 |
| 1:A:72:CYS:O | 1:A:76:ILE:HG22 | 0.50 | 2.05 | 9 | 1 |
| 4:A:203:U9E:C8 | 4:A:203:U9E:C21 | 0.50 | 2.89 | 10 | 2 |
| 1:A:62:MET:O | 1:A:70:ARG:HA | 0.50 | 2.07 | 5 | 20 |
| 4:A:203:U9E:C21 | 4:A:203:U9E:C8 | 0.49 | 2.90 | 13 | 1 |
| 1:A:62:MET:CG | 1:A:73:ALA:HA | 0.48 | 2.38 | 15 | 11 |
| 1:A:63:THR:HA | 1:A:69:HIS:O | 0.48 | 2.09 | 5 | 20 |
| 1:A:60:ASN:O | 1:A:73:ALA:N | 0.48 | 2.44 | 2 | 12 |
| 2:H:1046:TYR:CE1 | 2:H:1050:SER:HB3 | 0.48 | 2.44 | 19 | 20 |
| 2:H:1052:TYR:HA | 2:H:1058:VAL:O | 0.48 | 2.09 | 10 | 20 |
| 1:A:72:CYS:HB2 | 1:A:75:CYS:HB2 | 0.47 | 1.85 | 12 | 10 |
| 2:H:1051:LYS:NZ | 2:H:1062:LYS:O | 0.47 | 2.37 | 11 | 6 |
| 1:A:48:GLU:OE2 | 2:H:1081:LYS:NZ | 0.46 | 2.44 | 16 | 4 |
| 2:H:1046:TYR:HD1 | 2:H:1047:LEU:HD23 | 0.45 | 1.72 | 5 | 20 |
| 1:A:51:CYS:HB2 | 1:A:58:LEU:HD23 | 0.45 | 1.89 | 2 | 20 |
| 2:H:1008:LYS:O | 2:H:1011:GLU:HB2 | 0.44 | 2.13 | 10 | 20 |
| 1:A:97:LYS:HA | 4:A:203:U9E:C18 | 0.44 | 2.42 | 4 | 1 |
| 1:A:62:MET:HB3 | 1:A:100:LEU:HD12 | 0.43 | 1.89 | 1 | 1 |
| 1:A:65:LYS:HD3 | 1:A:98:ARG:O | 0.43 | 2.13 | 15 | 2 |
| 2:H:1016:LEU:HD22 | 2:H:1079:VAL:HG22 | 0.43 | 1.90 | 6 | 20 |
| 1:A:98:ARG:NH1 | 1:A:100:LEU:O | 0.43 | 2.52 | 4 | 4 |
| 1:A:32:ILE:HB | 2:H:1009:ILE:HD12 | 0.43 | 1.91 | 20 | 5 |
| 1:A:94:LEU:HD21 | 1:A:100:LEU:HD21 | 0.43 | 1.90 | 10 | 1 |
| 1:A:72:CYS:HB2 | 1:A:75:CYS:CB | 0.43 | 2.44 | 1 | 5 |
| 2:H:1089:ASN:O | 2:H:1093:ARG:HG3 | 0.42 | 2.15 | 3 | 20 |
| 1:A:68:LEU:CD1 | 2:H:1070:ARG:HB2 | 0.42 | 2.44 | 7 | 1 |
| 1:A:77:ILE:HD13 | 4:A:203:U9E:CL1 | 0.42 | 2.52 | 13 | 1 |
| 2:H:1028:ALA:N | 2:H:1076:GLN:OE1 | 0.42 | 2.53 | 16 | 15 |
| 2:H:1051:LYS:HE2 | 2:H:1051:LYS:HB3 | 0.41 | 1.68 | 10 | 2 |
| 1:A:24:LEU:HD23 | 1:A:24:LEU:HA | 0.41 | 1.74 | 13 | 2 |
| 1:A:69:HIS:HE1 | 1:A:90:CYS:SG | 0.41 | 2.38 | 16 | 2 |
| 2:H:1020:LEU:HD12 | 2:H:1042:CYS:HB3 | 0.41 | 1.93 | 5 | 16 |
| 1:A:77:ILE:HD11 | 4:A:203:U9E:CL1 | 0.41 | 2.53 | 2 | 1 |
| 4:A:203:U9E:C10 | 4:A:203:U9E:CL1 | 0.41 | 3.06 | 11 | 1 |
| 2:H:1019:VAL:HG21 | 2:H:1055:ILE:HD11 | 0.40 | 1.93 | 8 | 4 |
| 1:A:65:LYS:HD3 | 1:A:99:SER:HA | 0.40 | 1.92 | 11 | 1 |

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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 | 76/112 (68%) | 70±0 (92±0%) | 6±0 (8±0%) | 0±0 (0±0%) | 100 | 100 |
| 2 | H | 97/101 (96%) | 91±0 (94±0%) | 6±0 (6±0%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 3460/4260 (81%) | 3220 (93%) | 240 (7%) | 0 (0%) | 100 | 100 |

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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 | 74/105 (70%) | 72±1 (98±1%) | 2±1 (2±1%) | 54 | 92 |
| 2 | H | 93/94 (99%) | 93±0 (100±0%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 3340/3980 (84%) | 3308 (99%) | 32 (1%) | 77 | 96 |

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 25 | GLN | 18 |
| 1 | A | 100 | LEU | 6 |
| 1 | A | 62 | MET | 5 |
| 1 | A | 94 | LEU | 3 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | U9E | A | 203 | - | 22,29,29 | 3.78±0.01 | 6±0 (27±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | U9E | A | 203 | - | 23,42,42 | 1.08±0.02 | 3±1 (12±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 |
|-----|------|-------|-----|------|---------|-------------|-----------|
| 4 | U9E | A | 203 | - | - | 0±0,9,20,20 | 0±0,4,4,4 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 203 | U9E | C3-C2 | 14.04 | 1.33 | 1.50 | 14 | 20 |
| 4 | A | 203 | U9E | C2-C9 | 6.71 | 1.33 | 1.41 | 1 | 20 |
| 4 | A | 203 | U9E | C17-C16 | 4.97 | 1.33 | 1.41 | 18 | 20 |
| 4 | A | 203 | U9E | C12-C13 | 4.21 | 1.33 | 1.42 | 7 | 20 |
| 4 | A | 203 | U9E | C2-C1 | 4.06 | 1.33 | 1.41 | 8 | 20 |
| 4 | A | 203 | U9E | C13-C16 | 3.43 | 1.33 | 1.42 | 17 | 20 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | A | 203 | U9E | C2-C3-C4 | 2.30 | 119.72 | 122.32 | 6 | 18 |
| 4 | A | 203 | U9E | C14-C13-C16 | 2.26 | 108.10 | 106.18 | 6 | 20 |
| 4 | A | 203 | U9E | C8-C3-C4 | 2.21 | 120.08 | 117.63 | 4 | 18 |

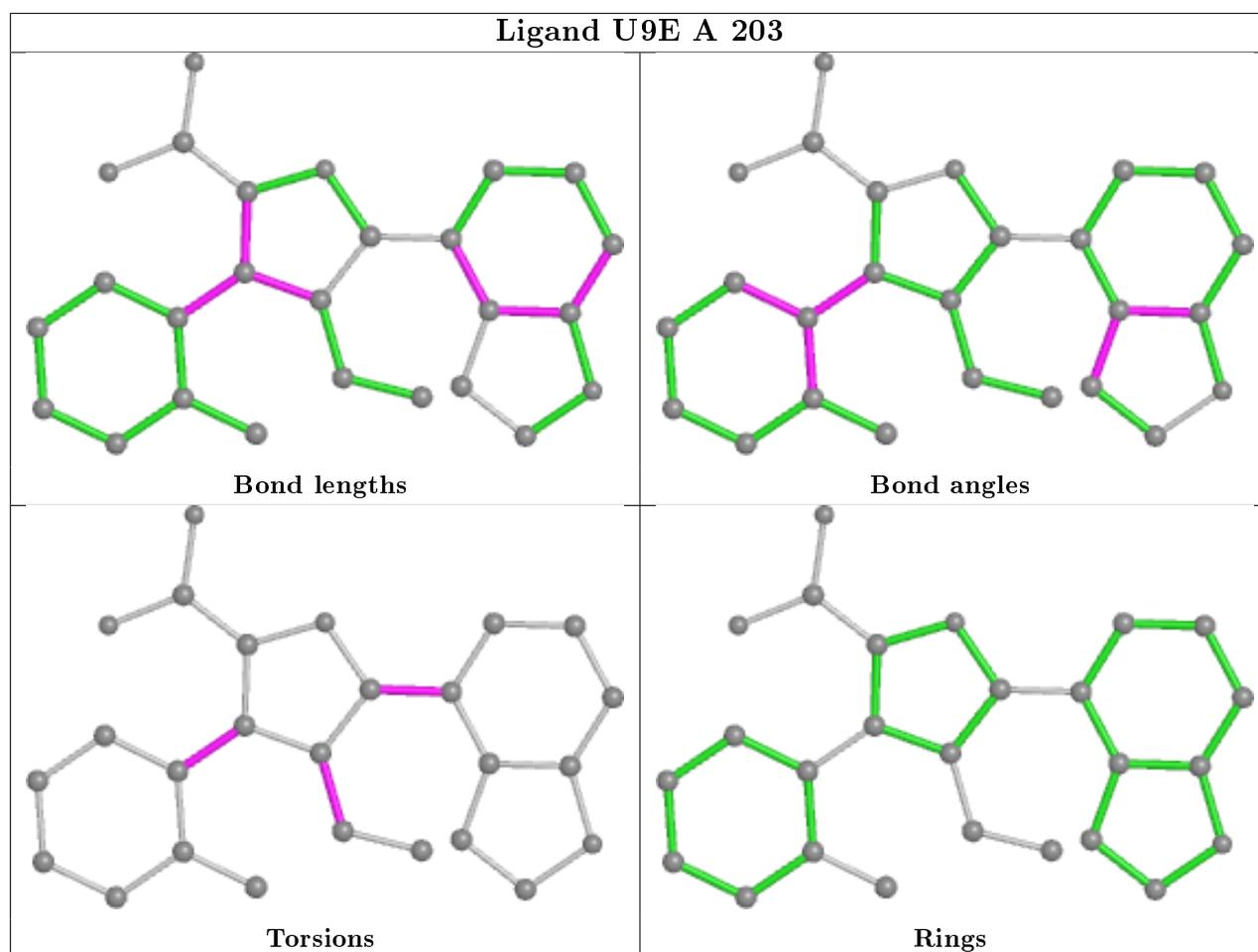
There are no chirality outliers.

All unique torsion outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|---------------|----------------|
| 4 | A | 203 | U9E | C2-C1-C20-C21 | 1 |

There are no ring outliers.

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 than 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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 14% for the well-defined parts and 14% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS_RingBMI1b_R2_full.tab*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|-----|
| Total number of shifts | 378 |
| Number of shifts mapped to atoms | 370 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 8 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 8 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| H | 116 | SER | H | 7.879 | 0.02 | 1 |
| H | 116 | SER | N | 112.204 | 0.2 | 1 |
| H | 117 | MET | H | 8.142 | 0.02 | 1 |
| H | 117 | MET | N | 119.308 | 0.2 | 1 |
| H | 118 | HIS | H | 7.964 | 0.02 | 1 |
| H | 118 | HIS | N | 115.271 | 0.2 | 1 |
| H | 119 | ARG | H | 7.869 | 0.02 | 1 |
| H | 119 | ARG | N | 118.321 | 0.2 | 1 |

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}_\beta$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 189 | 1.00 ± 0.18 | Should be applied |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 14%, i.e. 318 atoms were assigned a chemical shift out of a possible 2268. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 318/862 (37%) | 159/343 (46%) | 0/352 (0%) | 159/167 (95%) |
| Sidechain | 0/1261 (0%) | 0/743 (0%) | 0/458 (0%) | 0/60 (0%) |
| Aromatic | 0/145 (0%) | 0/79 (0%) | 0/61 (0%) | 0/5 (0%) |
| Overall | 318/2268 (14%) | 159/1165 (14%) | 0/871 (0%) | 159/232 (69%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 14%, i.e. 356 atoms were assigned a chemical shift out of a possible 2549. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone | 356/971 (37%) | 178/386 (46%) | 0/398 (0%) | 178/187 (95%) |
| Sidechain | 0/1416 (0%) | 0/836 (0%) | 0/513 (0%) | 0/67 (0%) |
| Aromatic | 0/162 (0%) | 0/88 (0%) | 0/69 (0%) | 0/5 (0%) |
| Overall | 356/2549 (14%) | 178/1310 (14%) | 0/980 (0%) | 178/259 (69%) |

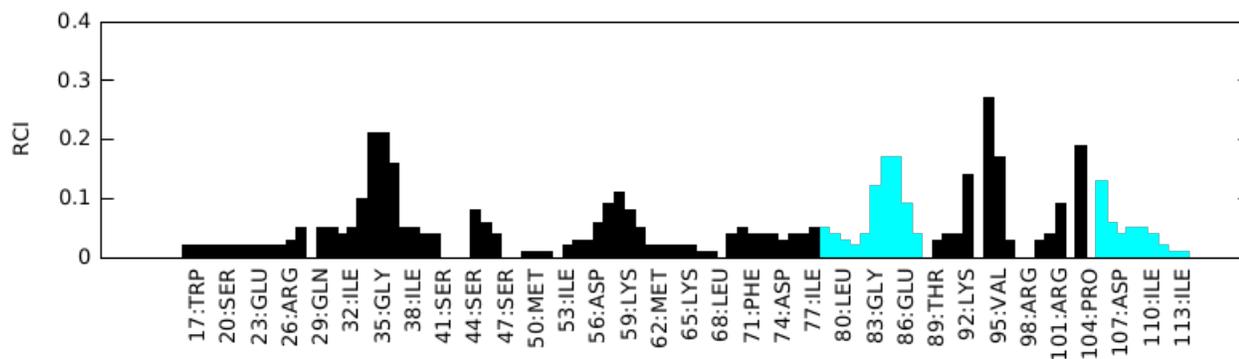
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain H:

