# Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 09:08 PM EST

| | | |
|---|---|---|
| PDB ID | : | 2KWB |
| Title | : | Minimal Constraint Solution NMR Structure of Translationally-controlled tumor protein (TCTP) from C.elegans, Northeast Structural Genomics Consortium Target WR73 |
| Authors | : | Aramini, J.M.; Rossi, P.; Cort, J.R.; Cooper, B.; Maglaqui, M.; Janjua, H.; Xiao, R.; Acton, T.B.; Everett, J.K.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG) |
| Deposited on | : | 2010-04-02 |

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 (i) symbol.

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

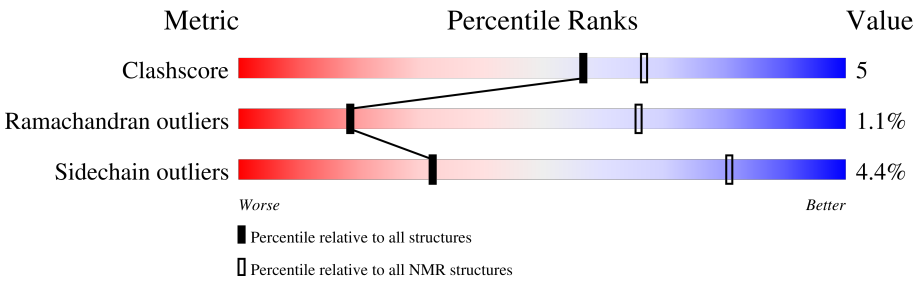
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.27 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.27 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 189 | 76% 5% 16% . |

# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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:1-A:37, A:65-A:180 (153) | 0.78 | 6 |

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 4 clusters and 7 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2902 atoms, of which 1445 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translationally-controlled tumor protein homolog.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 183 | 2902 | 922 | 1445 | 239 | 287 | 9 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 182 | LEU | - | expression tag | UNP Q93573 |
| A | 183 | GLU | - | expression tag | UNP Q93573 |
| A | 184 | HIS | - | expression tag | UNP Q93573 |
| A | 185 | HIS | - | expression tag | UNP Q93573 |
| A | 186 | HIS | - | expression tag | UNP Q93573 |
| A | 187 | HIS | - | expression tag | UNP Q93573 |
| A | 188 | HIS | - | expression tag | UNP Q93573 |
| A | 189 | HIS | - | expression tag | UNP Q93573 |

# 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: Translationally-controlled tumor protein homolog

Chain A: 76% 5% 16% •

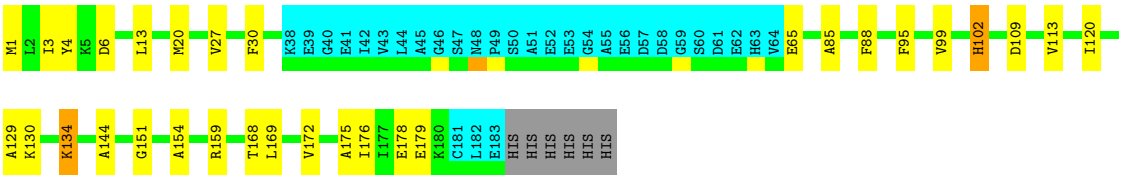
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Translationally-controlled tumor protein homolog

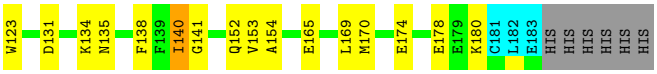
Chain A: 65% 15% • 16% •




### 4.2.2 Score per residue for model 2

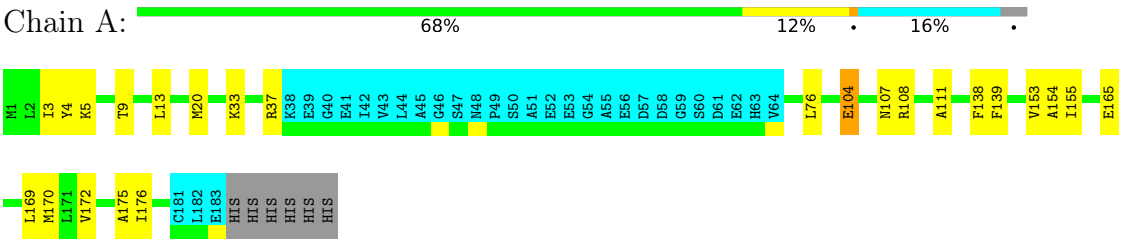
• Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 63% 15% • 16% •



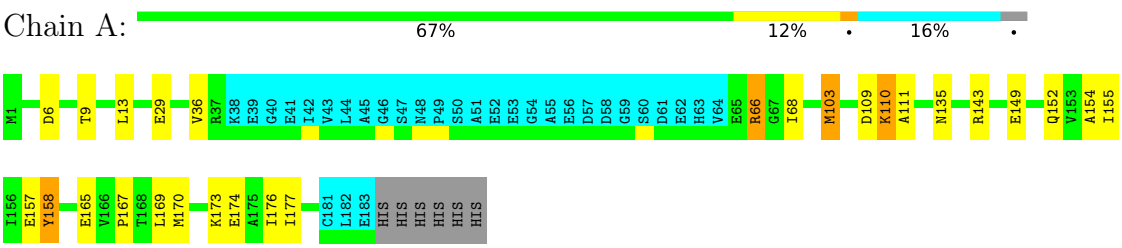

### 4.2.3 Score per residue for model 3

- Molecule 1: Translationally-controlled tumor protein homolog



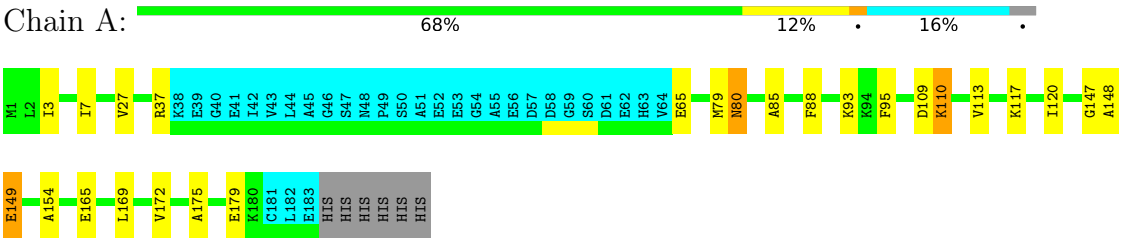

### 4.2.4 Score per residue for model 4

- Molecule 1: Translationally-controlled tumor protein homolog



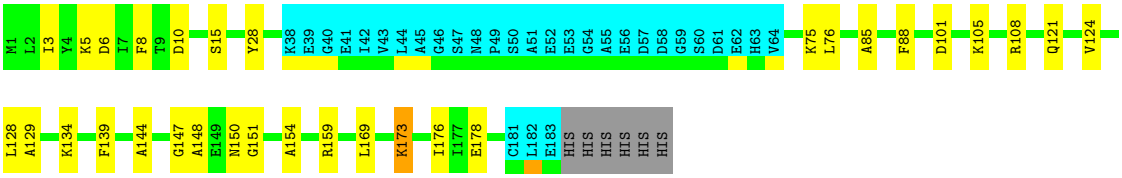

### 4.2.5 Score per residue for model 5

- Molecule 1: Translationally-controlled tumor protein homolog




### 4.2.6 Score per residue for model 6 (medoid)

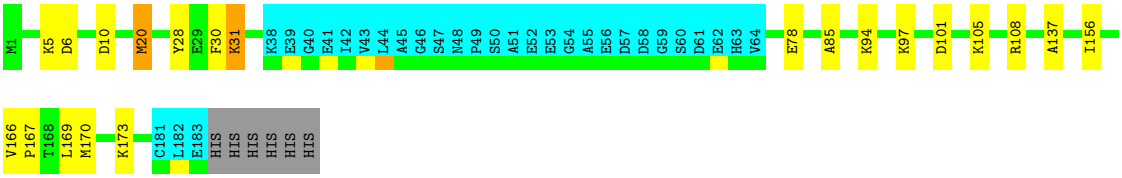
- Molecule 1: Translationally-controlled tumor protein homolog




### 4.2.7 Score per residue for model 7

- Molecule 1: Translationally-controlled tumor protein homolog

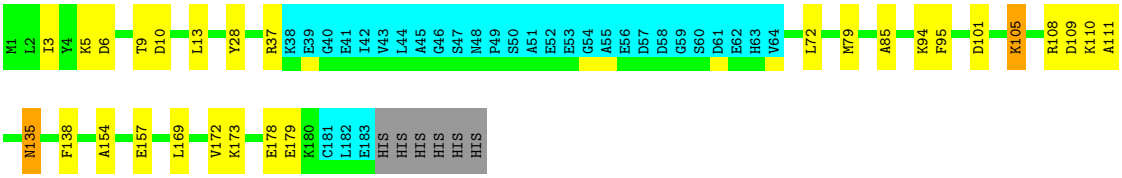
Chain A:




### 4.2.8 Score per residue for model 8

- Molecule 1: Translationally-controlled tumor protein homolog

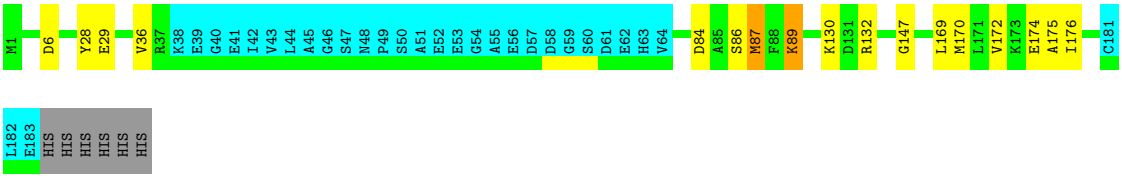
Chain A:




### 4.2.9 Score per residue for model 9

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A:




### 4.2.10 Score per residue for model 10

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 65% 16% 16% •

M1 K5 D6 T9 D10 L13 F30 K31 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 L72 N80 D84 M87 F95 E104 R108 V113 K130

G147 A148 E149 A154 I155 R159 D160 V161 D162 G163 T164 E165 L169 M170 A175 I176 I177 C181 L182 E183 HIS HIS HIS HIS HIS

### 4.2.11 Score per residue for model 11

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 69% 11% • 16% •

M1 K5 D6 T9 L13 L22 D25 E29 H34 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 K75 K97 D109 V113 Q121 A144 G151

I155 I156 E157 E165 V166 P167 T168 L169 M170 C181 L182 E183 HIS HIS HIS HIS HIS

### 4.2.12 Score per residue for model 12

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 67% 14% 16% •

M1 D16 V27 F30 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 L72 L76 A85 F88 F95 E104 K105 N106 D109 V113 Q121 V124

L128 A129 K130 F139 A144 A148 E157 L169 M170 L171 V172 I176 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.13 Score per residue for model 13

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 66% 14% • 16% •

M1 L2 I3 Y4 K5 D6 D10 L13 Y28 E29 F30 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 R66 I70 M103 N106 N107 R108 D109 V113 D114 K117 K118

Q121 V125 K130 E142 A154 L169 M170 K173 K180 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.14 Score per residue for model 14

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 66% 15% 16% •

M1 L2 S15 M20 K31 H34 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 D84 A85 F88 K93 D109 V113 A129 F133 L136 A137 F138

R143 A144 A145 E146 G147 A148 Q152 V153 A154 D160 E165 L169 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.15 Score per residue for model 15

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 59% 18% • 16% •

M1 L2 I3 Y4 K5 D6 L13 D16 M20 K21 D24 E29 F30 V36 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 R66 A85 F88 Y91 I100 E104

K105 N106 N107 K110 V113 D114 Q121 F133 K134 N135 L136 A137 E149 N150 A154 I155 I156 E157 D160 E165 L169 M170 E174 A175 I176 I177 E178 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.16 Score per residue for model 16

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 70% 10% • 16% •

M1 D6 D10 L13 Y28 V36 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 L72 N106 K130 F133 K134 N135 L136 A137 F138 G147 V153 A154 R159

E165 L169 M170 K173 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.17 Score per residue for model 17

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 69% 11% • 16% •

M1 K5 F8 L13 M20 Y28 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 I68 D69 I70 N80 F95 V99 N106 N107 R108 A129 K130 D131 E142

G147 A154 R159 E165 L169 V172 K173 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.18 Score per residue for model 18

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 69% 10% • 16% •

M1 L13 M20 K21 E29 F30 K31 G32 V36 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 R66 G67 I68 D69 I70 K75 E78 F95 A129 K130 D131 R132 A144

G151 L169 V172 E178 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.19 Score per residue for model 19

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 66% 14% • 16% •

M1 L2 D6 T9 D10 D11 E12 V27 V36 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 Y82 E83 D84 A85 S86 M87 F88 F95 N98 N107 R108 D109 V124

L128 A129 Q152 R159 D160 V161 V172 K173 E178 E179 K180 C181 L182 E183 HIS HIS HIS HIS HIS HIS

### 4.2.20 Score per residue for model 20

- Molecule 1: Translationally-controlled tumor protein homolog

Chain A: 72% 9% 16% •

M1 E12 K21 Y28 E29 R37 K38 E39 G40 E41 I42 V43 L44 A45 G46 S47 N48 P49 S50 A51 E52 E53 G54 A55 E56 D57 D58 G59 S60 D61 E62 H63 V64 E65 M79 K97 K130 F138 R143 A144 A154 I155 L169 M170 K173 C181 L182

E183 HIS HIS HIS HIS HIS HIS

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 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 |
|---|---|---|
| CNS | refinement | 1.2 |
| CNS | structure solution | 1.2 |
| CNS | geometry optimization | 1.2 |
| CYANA | structure solution | 3.0 |

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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 | 1243 | 1259 | 1256 | 13±4 |
| All | All | 24860 | 25180 | 25120 | 256 |

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 5.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:154:ALA:HB1 | 1:A:169:LEU:HD11 | 0.77 | 1.56 | 3 | 14 |
| 1:A:37:ARG:HB3 | 1:A:65:GLU:HB2 | 0.77 | 1.56 | 14 | 2 |
| 1:A:37:ARG:HB3 | 1:A:65:GLU:HB3 | 0.71 | 1.62 | 18 | 3 |
| 1:A:4:TYR:HB2 | 1:A:176:ILE:HD11 | 0.67 | 1.66 | 1 | 1 |
| 1:A:87:MET:SD | 1:A:87:MET:N | 0.67 | 2.68 | 9 | 1 |
| 1:A:173:LYS:HZ3 | 1:A:173:LYS:HB3 | 0.64 | 1.52 | 13 | 1 |
| 1:A:160:ASP:HA | 1:A:165:GLU:HA | 0.64 | 1.69 | 14 | 2 |
| 1:A:30:PHE:HB3 | 1:A:169:LEU:HB3 | 0.63 | 1.68 | 12 | 6 |
| 1:A:37:ARG:HB2 | 1:A:65:GLU:HB2 | 0.62 | 1.70 | 15 | 3 |
| 1:A:6:ASP:HB3 | 1:A:176:ILE:HG22 | 0.62 | 1.70 | 15 | 1 |
| 1:A:20:MET:SD | 1:A:20:MET:N | 0.61 | 2.73 | 7 | 4 |
| 1:A:7:ILE:HD11 | 1:A:175:ALA:HB1 | 0.59 | 1.73 | 5 | 1 |
| 1:A:76:LEU:HB3 | 1:A:139:PHE:HB3 | 0.59 | 1.75 | 12 | 3 |
| 1:A:6:ASP:HB3 | 1:A:9:THR:HB | 0.58 | 1.75 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:27:VAL:HB | 1:A:170:MET:SD | 0.57 | 2.39 | 12 | 1 |
| 1:A:155:ILE:HB | 1:A:170:MET:HB2 | 0.57 | 1.76 | 3 | 4 |
| 1:A:84:ASP:HA | 1:A:87:MET:SD | 0.56 | 2.40 | 9 | 1 |
| 1:A:3:ILE:HG13 | 1:A:179:GLU:HB3 | 0.56 | 1.76 | 5 | 1 |
| 1:A:31:LYS:HG3 | 1:A:166:VAL:HB | 0.56 | 1.77 | 7 | 1 |
| 1:A:104:GLU:HA | 1:A:113:VAL:HG11 | 0.55 | 1.78 | 10 | 2 |
| 1:A:3:ILE:HB | 1:A:179:GLU:HB3 | 0.55 | 1.79 | 1 | 2 |
| 1:A:84:ASP:HA | 1:A:87:MET:HB3 | 0.55 | 1.78 | 10 | 1 |
| 1:A:20:MET:SD | 1:A:30:PHE:HB2 | 0.55 | 2.42 | 15 | 1 |
| 1:A:32:GLY:HA3 | 1:A:70:ILE:HG13 | 0.55 | 1.78 | 18 | 1 |
| 1:A:3:ILE:HB | 1:A:13:LEU:HD21 | 0.54 | 1.80 | 13 | 1 |
| 1:A:12:GLU:HG3 | 1:A:144:ALA:HB2 | 0.54 | 1.77 | 20 | 1 |
| 1:A:5:LYS:HB2 | 1:A:10:ASP:HB2 | 0.54 | 1.80 | 13 | 1 |
| 1:A:155:ILE:HB | 1:A:170:MET:HB3 | 0.54 | 1.79 | 15 | 2 |
| 1:A:28:TYR:O | 1:A:170:MET:HA | 0.53 | 2.03 | 13 | 5 |
| 1:A:159:ARG:NH2 | 1:A:168:THR:HG21 | 0.52 | 2.20 | 1 | 1 |
| 1:A:109:ASP:O | 1:A:113:VAL:HG22 | 0.51 | 2.06 | 12 | 6 |
| 1:A:37:ARG:HB3 | 1:A:72:LEU:HD22 | 0.51 | 1.81 | 8 | 1 |
| 1:A:21:LYS:HB2 | 1:A:29:GLU:HB3 | 0.51 | 1.81 | 18 | 1 |
| 1:A:6:ASP:O | 1:A:10:ASP:HB3 | 0.51 | 2.03 | 8 | 5 |
| 1:A:138:PHE:HB3 | 1:A:153:VAL:HG11 | 0.51 | 1.83 | 2 | 2 |
| 1:A:85:ALA:HA | 1:A:88:PHE:CE2 | 0.51 | 2.40 | 12 | 7 |
| 1:A:29:GLU:HA | 1:A:169:LEU:O | 0.51 | 2.06 | 13 | 5 |
| 1:A:101:ASP:O | 1:A:105:LYS:HG2 | 0.50 | 2.05 | 6 | 2 |
| 1:A:36:VAL:HG12 | 1:A:66:ARG:HG3 | 0.50 | 1.83 | 18 | 1 |
| 1:A:110:LYS:HD3 | 1:A:110:LYS:H | 0.50 | 1.65 | 5 | 1 |
| 1:A:132:ARG:HD2 | 1:A:132:ARG:H | 0.50 | 1.66 | 18 | 1 |
| 1:A:97:LYS:HA | 1:A:97:LYS:HE2 | 0.50 | 1.83 | 11 | 1 |
| 1:A:79:MET:HB2 | 1:A:138:PHE:HB2 | 0.50 | 1.82 | 8 | 2 |
| 1:A:144:ALA:HB2 | 1:A:151:GLY:HA3 | 0.50 | 1.83 | 1 | 1 |
| 1:A:5:LYS:HG3 | 1:A:10:ASP:HB2 | 0.49 | 1.84 | 7 | 2 |
| 1:A:144:ALA:HA | 1:A:148:ALA:HB3 | 0.49 | 1.84 | 6 | 3 |
| 1:A:107:ASN:O | 1:A:108:ARG:HG2 | 0.49 | 2.07 | 13 | 2 |
| 1:A:130:LYS:H | 1:A:130:LYS:HD2 | 0.49 | 1.68 | 9 | 1 |
| 1:A:99:VAL:O | 1:A:103:MET:SD | 0.49 | 2.71 | 2 | 1 |
| 1:A:135:ASN:N | 1:A:135:ASN:HD22 | 0.49 | 2.06 | 8 | 1 |
| 1:A:114:ASP:O | 1:A:118:LYS:HG2 | 0.49 | 2.08 | 13 | 1 |
| 1:A:109:ASP:O | 1:A:111:ALA:N | 0.48 | 2.46 | 4 | 2 |
| 1:A:107:ASN:HD21 | 1:A:111:ALA:HB3 | 0.48 | 1.68 | 3 | 1 |
| 1:A:95:PHE:CZ | 1:A:172:VAL:HG11 | 0.48 | 2.44 | 8 | 5 |
| 1:A:68:ILE:HD12 | 1:A:70:ILE:HD12 | 0.48 | 1.84 | 17 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:144:ALA:HB1 | 1:A:151:GLY:HA2 | 0.48 | 1.84 | 18 | 1 |
| 1:A:105:LYS:HE3 | 1:A:105:LYS:HA | 0.48 | 1.86 | 15 | 1 |
| 1:A:9:THR:HG22 | 1:A:9:THR:O | 0.47 | 2.09 | 3 | 1 |
| 1:A:6:ASP:HA | 1:A:176:ILE:HG22 | 0.47 | 1.86 | 6 | 1 |
| 1:A:5:LYS:HB3 | 1:A:13:LEU:HD13 | 0.47 | 1.86 | 11 | 1 |
| 1:A:5:LYS:HB2 | 1:A:13:LEU:HD13 | 0.47 | 1.85 | 10 | 2 |
| 1:A:103:MET:HA | 1:A:106:ASN:ND2 | 0.47 | 2.24 | 13 | 1 |
| 1:A:75:LYS:NZ | 1:A:75:LYS:HB2 | 0.47 | 2.24 | 11 | 1 |
| 1:A:4:TYR:HE1 | 1:A:16:ASP:HB2 | 0.47 | 1.68 | 15 | 1 |
| 1:A:27:VAL:HG12 | 1:A:172:VAL:HA | 0.47 | 1.86 | 12 | 4 |
| 1:A:148:ALA:O | 1:A:149:GLU:HG2 | 0.47 | 2.10 | 5 | 1 |
| 1:A:144:ALA:HB1 | 1:A:151:GLY:H | 0.47 | 1.70 | 11 | 1 |
| 1:A:91:TYR:OH | 1:A:150:ASN:HB3 | 0.46 | 2.09 | 15 | 1 |
| 1:A:6:ASP:HA | 1:A:175:ALA:O | 0.46 | 2.10 | 9 | 2 |
| 1:A:152:GLN:HE22 | 1:A:176:ILE:HG23 | 0.46 | 1.69 | 4 | 1 |
| 1:A:150:ASN:N | 1:A:150:ASN:HD22 | 0.46 | 2.09 | 15 | 1 |
| 1:A:130:LYS:O | 1:A:134:LYS:HB2 | 0.46 | 2.09 | 16 | 1 |
| 1:A:173:LYS:HZ2 | 1:A:173:LYS:HB3 | 0.46 | 1.70 | 17 | 1 |
| 1:A:130:LYS:H | 1:A:130:LYS:HD3 | 0.46 | 1.69 | 18 | 1 |
| 1:A:2:LEU:O | 1:A:15:SER:HA | 0.46 | 2.10 | 14 | 1 |
| 1:A:80:ASN:N | 1:A:80:ASN:HD22 | 0.46 | 2.08 | 5 | 1 |
| 1:A:137:ALA:HB3 | 1:A:156:ILE:HB | 0.46 | 1.86 | 7 | 2 |
| 1:A:88:PHE:HA | 1:A:91:TYR:HD2 | 0.46 | 1.71 | 15 | 1 |
| 1:A:6:ASP:HB2 | 1:A:9:THR:HG22 | 0.46 | 1.86 | 19 | 1 |
| 1:A:37:ARG:HB2 | 1:A:72:LEU:HD13 | 0.46 | 1.87 | 12 | 1 |
| 1:A:138:PHE:HB3 | 1:A:153:VAL:HG13 | 0.46 | 1.85 | 3 | 2 |
| 1:A:28:TYR:CE2 | 1:A:173:LYS:HA | 0.46 | 2.46 | 17 | 2 |
| 1:A:130:LYS:HD2 | 1:A:131:ASP:N | 0.46 | 2.25 | 17 | 1 |
| 1:A:5:LYS:HB3 | 1:A:177:ILE:HB | 0.46 | 1.88 | 10 | 1 |
| 1:A:133:PHE:O | 1:A:136:LEU:HG | 0.46 | 2.11 | 16 | 3 |
| 1:A:30:PHE:CZ | 1:A:169:LEU:HD23 | 0.45 | 2.47 | 7 | 2 |
| 1:A:5:LYS:HG2 | 1:A:13:LEU:HD12 | 0.45 | 1.86 | 17 | 1 |
| 1:A:2:LEU:HD11 | 1:A:178:GLU:HB2 | 0.45 | 1.88 | 15 | 2 |
| 1:A:157:GLU:O | 1:A:167:PRO:HA | 0.45 | 2.11 | 11 | 1 |
| 1:A:87:MET:SD | 1:A:87:MET:C | 0.45 | 2.95 | 19 | 1 |
| 1:A:103:MET:SD | 1:A:103:MET:N | 0.45 | 2.90 | 2 | 1 |
| 1:A:116:PHE:HE1 | 1:A:174:GLU:HG3 | 0.45 | 1.71 | 2 | 1 |
| 1:A:95:PHE:HZ | 1:A:120:ILE:HD11 | 0.45 | 1.70 | 5 | 1 |
| 1:A:95:PHE:HZ | 1:A:172:VAL:HG11 | 0.45 | 1.72 | 8 | 3 |
| 1:A:143:ARG:HD2 | 1:A:143:ARG:H | 0.44 | 1.71 | 4 | 1 |
| 1:A:172:VAL:O | 1:A:176:ILE:HG22 | 0.44 | 2.12 | 12 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:143:ARG:HD2 | 1:A:143:ARG:N | 0.44 | 2.27 | 4 | 1 |
| 1:A:21:LYS:HB3 | 1:A:21:LYS:NZ | 0.44 | 2.27 | 15 | 1 |
| 1:A:143:ARG:HA | 1:A:143:ARG:NE | 0.44 | 2.27 | 20 | 1 |
| 1:A:104:GLU:O | 1:A:108:ARG:HB2 | 0.44 | 2.12 | 3 | 1 |
| 1:A:135:ASN:HB3 | 1:A:158:TYR:OH | 0.44 | 2.12 | 4 | 1 |
| 1:A:110:LYS:HD3 | 1:A:110:LYS:N | 0.44 | 2.28 | 5 | 1 |
| 1:A:117:LYS:HA | 1:A:120:ILE:HG22 | 0.44 | 1.90 | 5 | 1 |
| 1:A:8:PHE:HB3 | 1:A:150:ASN:O | 0.44 | 2.13 | 6 | 1 |
| 1:A:31:LYS:HG2 | 1:A:167:PRO:O | 0.44 | 2.13 | 7 | 1 |
| 1:A:101:ASP:O | 1:A:105:LYS:HB2 | 0.44 | 2.12 | 7 | 1 |
| 1:A:157:GLU:HG2 | 1:A:158:TYR:N | 0.44 | 2.26 | 4 | 1 |
| 1:A:21:LYS:HB2 | 1:A:29:GLU:O | 0.44 | 2.13 | 20 | 1 |
| 1:A:99:VAL:HA | 1:A:102:HIS:HD2 | 0.43 | 1.73 | 1 | 1 |
| 1:A:66:ARG:O | 1:A:66:ARG:HD2 | 0.43 | 2.13 | 4 | 2 |
| 1:A:20:MET:SD | 1:A:20:MET:C | 0.43 | 2.96 | 2 | 1 |
| 1:A:161:VAL:O | 1:A:163:GLY:N | 0.43 | 2.52 | 10 | 1 |
| 1:A:36:VAL:O | 1:A:36:VAL:HG23 | 0.43 | 2.14 | 9 | 1 |
| 1:A:110:LYS:O | 1:A:114:ASP:HB3 | 0.43 | 2.13 | 15 | 1 |
| 1:A:1:MET:SD | 1:A:1:MET:N | 0.43 | 2.76 | 1 | 1 |
| 1:A:131:ASP:O | 1:A:134:LYS:NZ | 0.43 | 2.49 | 2 | 1 |
| 1:A:5:LYS:HE2 | 1:A:13:LEU:HD13 | 0.43 | 1.90 | 10 | 1 |
| 1:A:103:MET:HA | 1:A:103:MET:HE2 | 0.43 | 1.91 | 4 | 1 |
| 1:A:124:VAL:O | 1:A:128:LEU:HG | 0.42 | 2.15 | 12 | 3 |
| 1:A:65:GLU:HG2 | 1:A:72:LEU:HD22 | 0.42 | 1.91 | 10 | 2 |
| 1:A:121:GLN:HE21 | 1:A:121:GLN:HA | 0.42 | 1.74 | 15 | 1 |
| 1:A:140:ILE:HD13 | 1:A:141:GLY:N | 0.42 | 2.29 | 2 | 1 |
| 1:A:36:VAL:HA | 1:A:66:ARG:HA | 0.42 | 1.92 | 4 | 1 |
| 1:A:95:PHE:CZ | 1:A:120:ILE:HD11 | 0.42 | 2.49 | 5 | 1 |
| 1:A:28:TYR:CE2 | 1:A:173:LYS:HB3 | 0.42 | 2.49 | 6 | 2 |
| 1:A:154:ALA:CB | 1:A:169:LEU:HD11 | 0.42 | 2.44 | 10 | 1 |
| 1:A:123:TRP:NE1 | 1:A:170:MET:SD | 0.42 | 2.89 | 2 | 1 |
| 1:A:80:ASN:HB2 | 1:A:82:TYR:CE1 | 0.42 | 2.50 | 2 | 1 |
| 1:A:95:PHE:CE1 | 1:A:175:ALA:HB2 | 0.42 | 2.49 | 10 | 1 |
| 1:A:100:ILE:O | 1:A:104:GLU:HG3 | 0.42 | 2.15 | 15 | 1 |
| 1:A:172:VAL:HB | 1:A:175:ALA:HB3 | 0.42 | 1.92 | 3 | 1 |
| 1:A:158:TYR:HB2 | 1:A:165:GLU:HB3 | 0.42 | 1.91 | 4 | 1 |
| 1:A:30:PHE:CE2 | 1:A:70:ILE:HD13 | 0.42 | 2.50 | 13 | 1 |
| 1:A:108:ARG:HD2 | 1:A:109:ASP:N | 0.41 | 2.30 | 2 | 1 |
| 1:A:6:ASP:HB3 | 1:A:9:THR:HG22 | 0.41 | 1.91 | 10 | 1 |
| 1:A:177:ILE:HD12 | 1:A:177:ILE:N | 0.41 | 2.29 | 10 | 1 |
| 1:A:22:LEU:HG | 1:A:25:ASP:HA | 0.41 | 1.92 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:117:LYS:O | 1:A:121:GLN:HB3 | 0.41 | 2.14 | 13 | 1 |
| 1:A:107:ASN:O | 1:A:113:VAL:HG13 | 0.41 | 2.14 | 15 | 1 |
| 1:A:130:LYS:O | 1:A:134:LYS:N | 0.41 | 2.53 | 1 | 1 |
| 1:A:6:ASP:HB2 | 1:A:9:THR:H | 0.41 | 1.75 | 4 | 1 |
| 1:A:172:VAL:O | 1:A:176:ILE:HG12 | 0.41 | 2.16 | 3 | 1 |
| 1:A:68:ILE:HG21 | 1:A:167:PRO:HB3 | 0.41 | 1.92 | 4 | 1 |
| 1:A:3:ILE:HG22 | 1:A:15:SER:HB3 | 0.41 | 1.92 | 6 | 1 |
| 1:A:176:ILE:HG13 | 1:A:176:ILE:O | 0.41 | 2.16 | 15 | 1 |
| 1:A:173:LYS:NZ | 1:A:173:LYS:HB2 | 0.41 | 2.31 | 16 | 1 |
| 1:A:95:PHE:CE1 | 1:A:172:VAL:HG11 | 0.41 | 2.51 | 17 | 1 |
| 1:A:6:ASP:O | 1:A:10:ASP:HB2 | 0.41 | 2.15 | 6 | 1 |
| 1:A:34:HIS:O | 1:A:34:HIS:ND1 | 0.41 | 2.54 | 14 | 1 |
| 1:A:95:PHE:O | 1:A:99:VAL:HG22 | 0.41 | 2.16 | 17 | 1 |
| 1:A:82:TYR:CG | 1:A:83:GLU:N | 0.41 | 2.88 | 19 | 1 |
| 1:A:94:LYS:HA | 1:A:97:LYS:HD2 | 0.41 | 1.92 | 7 | 1 |
| 1:A:159:ARG:NH2 | 1:A:161:VAL:HG22 | 0.41 | 2.31 | 19 | 1 |
| 1:A:3:ILE:HB | 1:A:13:LEU:HD11 | 0.41 | 1.93 | 3 | 1 |
| 1:A:110:LYS:HG3 | 1:A:111:ALA:N | 0.41 | 2.31 | 4 | 1 |
| 1:A:144:ALA:HB1 | 1:A:151:GLY:HA3 | 0.41 | 1.92 | 6 | 1 |
| 1:A:86:SER:O | 1:A:89:LYS:HG2 | 0.41 | 2.16 | 9 | 1 |
| 1:A:143:ARG:HA | 1:A:146:GLU:HB3 | 0.40 | 1.92 | 14 | 1 |
| 1:A:91:TYR:HE2 | 1:A:152:GLN:HG3 | 0.40 | 1.76 | 2 | 1 |
| 1:A:121:GLN:O | 1:A:125:VAL:HG23 | 0.40 | 2.16 | 13 | 1 |
| 1:A:2:LEU:HD13 | 1:A:180:LYS:HB3 | 0.40 | 1.93 | 19 | 1 |
| 1:A:36:VAL:HA | 1:A:65:GLU:O | 0.40 | 2.16 | 19 | 1 |
| 1:A:95:PHE:HE2 | 1:A:120:ILE:HG12 | 0.40 | 1.76 | 1 | 1 |
| 1:A:170:MET:N | 1:A:170:MET:SD | 0.40 | 2.95 | 9 | 1 |
| 1:A:66:ARG:O | 1:A:66:ARG:HD3 | 0.40 | 2.16 | 15 | 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 | 152/189 (80%) | 136±4 (90±2%) | 14±4 (9±3%) | 2±1 (1±1%) | 18 66 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 3040/3780 (80%) | 2730 (90%) | 276 (9%) | 34 (1%) | 18 66 |

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 147 | GLY | 7 |
| 1 | A | 129 | ALA | 6 |
| 1 | A | 13 | LEU | 6 |
| 1 | A | 134 | LYS | 3 |
| 1 | A | 108 | ARG | 3 |
| 1 | A | 110 | LYS | 2 |
| 1 | A | 149 | GLU | 2 |
| 1 | A | 85 | ALA | 2 |
| 1 | A | 65 | GLU | 1 |
| 1 | A | 16 | ASP | 1 |
| 1 | A | 10 | ASP | 1 |

### 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 | 135/164 (82%) | 129±2 (96±1%) | 6±2 (4±1%) | 32 81 |
| All | All | 2700/3280 (82%) | 2581 (96%) | 119 (4%) | 32 81 |

All 53 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 | 165 | GLU | 7 |
| 1 | A | 173 | LYS | 7 |
| 1 | A | 178 | GLU | 6 |
| 1 | A | 130 | LYS | 6 |
| 1 | A | 20 | MET | 5 |
| 1 | A | 121 | GLN | 5 |
| 1 | A | 159 | ARG | 4 |
| 1 | A | 106 | ASN | 4 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 13 | LEU | 3 |
| 1 | A | 66 | ARG | 3 |
| 1 | A | 174 | GLU | 3 |
| 1 | A | 80 | ASN | 3 |
| 1 | A | 75 | LYS | 3 |
| 1 | A | 108 | ARG | 3 |
| 1 | A | 31 | LYS | 3 |
| 1 | A | 157 | GLU | 3 |
| 1 | A | 103 | MET | 2 |
| 1 | A | 135 | ASN | 2 |
| 1 | A | 180 | LYS | 2 |
| 1 | A | 5 | LYS | 2 |
| 1 | A | 104 | GLU | 2 |
| 1 | A | 149 | GLU | 2 |
| 1 | A | 93 | LYS | 2 |
| 1 | A | 78 | GLU | 2 |
| 1 | A | 105 | LYS | 2 |
| 1 | A | 87 | MET | 2 |
| 1 | A | 132 | ARG | 2 |
| 1 | A | 97 | LYS | 2 |
| 1 | A | 142 | GLU | 2 |
| 1 | A | 152 | GLN | 2 |
| 1 | A | 102 | HIS | 1 |
| 1 | A | 140 | ILE | 1 |
| 1 | A | 4 | TYR | 1 |
| 1 | A | 33 | LYS | 1 |
| 1 | A | 37 | ARG | 1 |
| 1 | A | 158 | TYR | 1 |
| 1 | A | 177 | ILE | 1 |
| 1 | A | 79 | MET | 1 |
| 1 | A | 110 | LYS | 1 |
| 1 | A | 134 | LYS | 1 |
| 1 | A | 9 | THR | 1 |
| 1 | A | 94 | LYS | 1 |
| 1 | A | 89 | LYS | 1 |
| 1 | A | 34 | HIS | 1 |
| 1 | A | 16 | ASP | 1 |
| 1 | A | 84 | ASP | 1 |
| 1 | A | 21 | LYS | 1 |
| 1 | A | 24 | ASP | 1 |
| 1 | A | 150 | ASN | 1 |
| 1 | A | 8 | PHE | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 12 | GLU | 1 |
| 1 | A | 98 | ASN | 1 |
| 1 | A | 109 | ASP | 1 |

#### 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)

There are no ligands in this entry.

### 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)

No chemical shift data were provided