# Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:34 PM BST

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|---|---|---|
| PDB ID | : | 2KGL |
| Title | : | NMR solution structure of MESD |
| Authors | : | Chen, J.; Wang, J. |
| Deposited on | : | 2009-03-12 |

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
http://wwpdb.org/validation/2016/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:

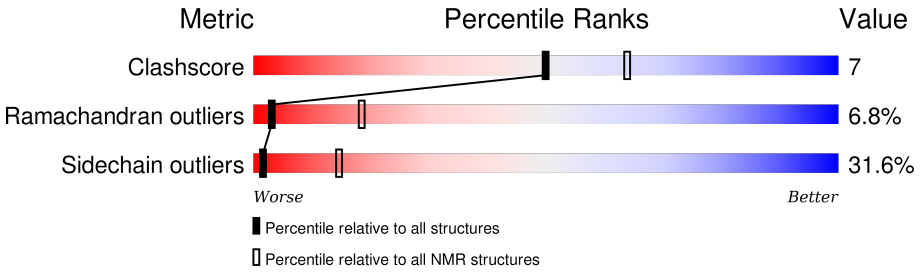
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | rb-20027457 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20027457 |

# 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 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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 195 | 53% 39% • 7% |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:11-A:59, A:64-A:195 (181) | 0.73 | 4 |

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 3 clusters and 6 single-model clusters were found.

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3073 atoms, of which 1527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mesoderm development candidate 2.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 195 | 3073 | 960 | 1527 | 271 | 308 | 7 | 0 |

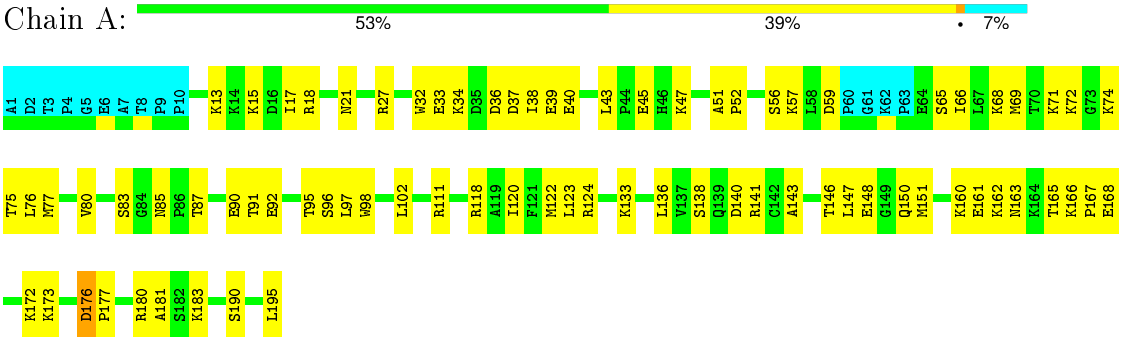
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Mesoderm development candidate 2

Chain A:



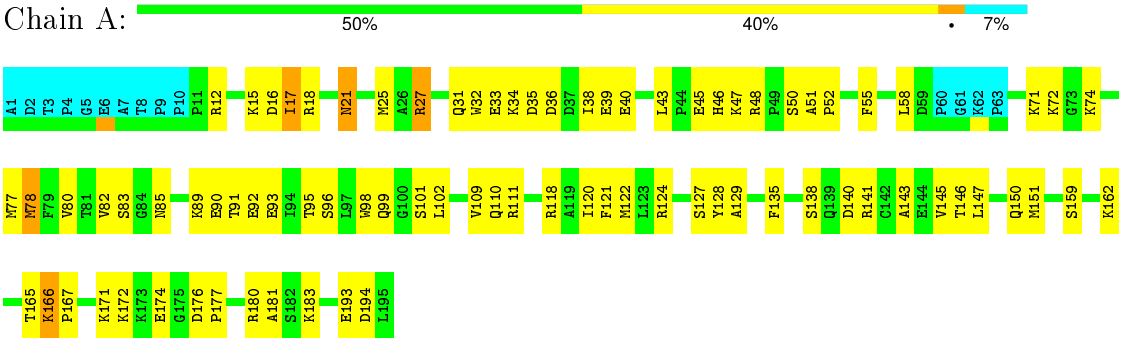

## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

- Molecule 1: Mesoderm development candidate 2

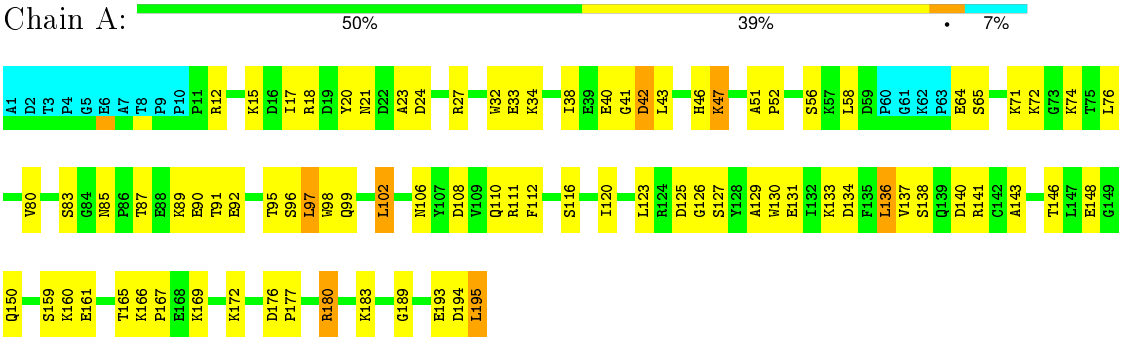
Chain A:



### 4.2.2 Score per residue for model 2

• Molecule 1: Mesoderm development candidate 2

Chain A:




### 4.2.3 Score per residue for model 3

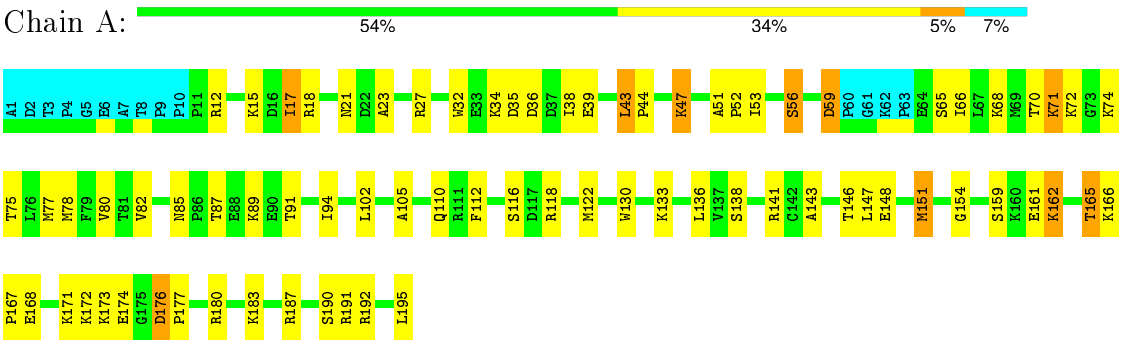
• Molecule 1: Mesoderm development candidate 2

Chain A:


### 4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Mesoderm development candidate 2

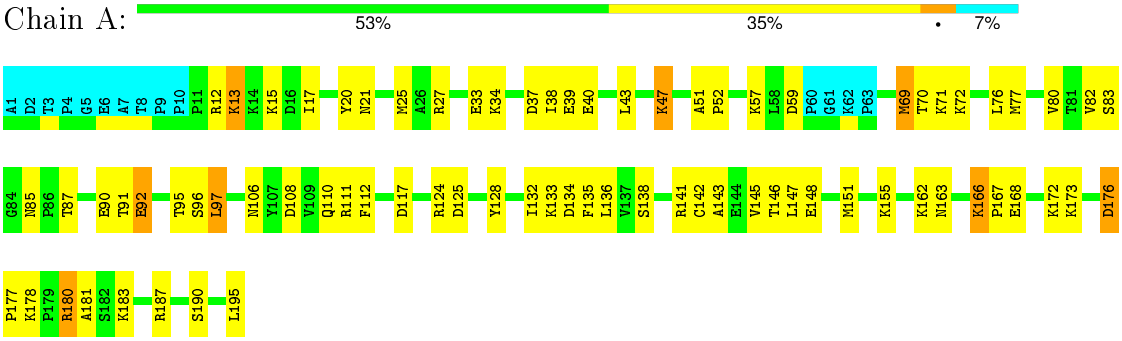
Chain A:



### 4.2.5 Score per residue for model 5

• Molecule 1: Mesoderm development candidate 2

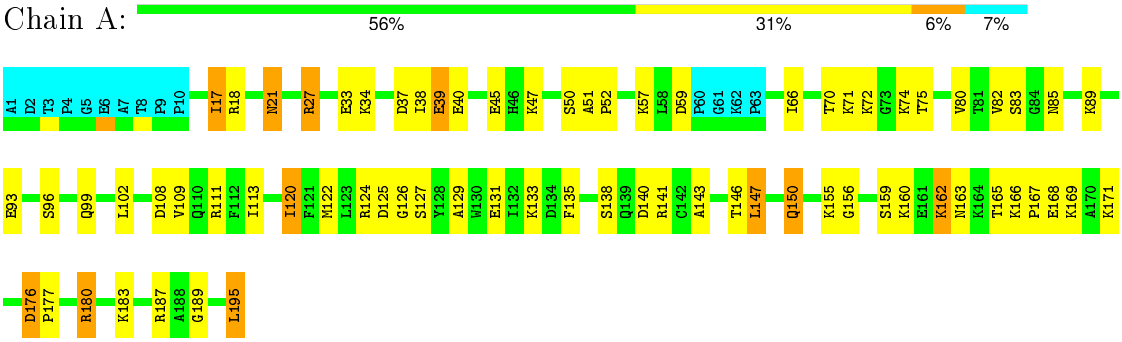
Chain A:




### 4.2.6 Score per residue for model 6

• Molecule 1: Mesoderm development candidate 2

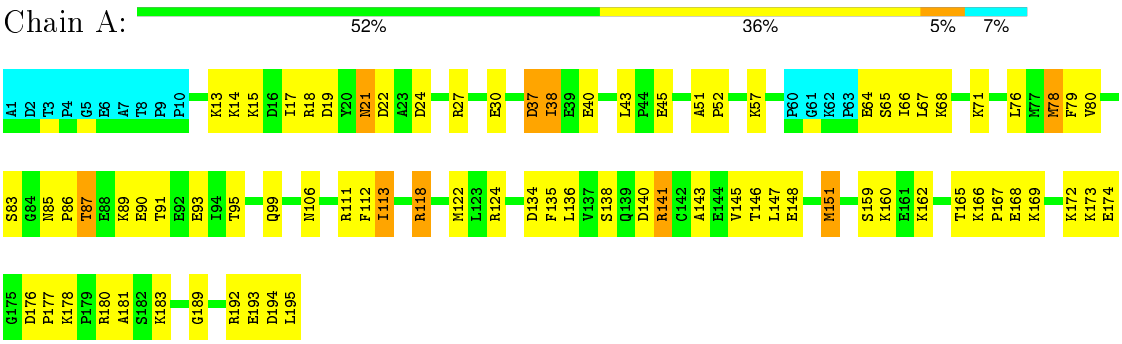
Chain A:




### 4.2.7 Score per residue for model 7

• Molecule 1: Mesoderm development candidate 2

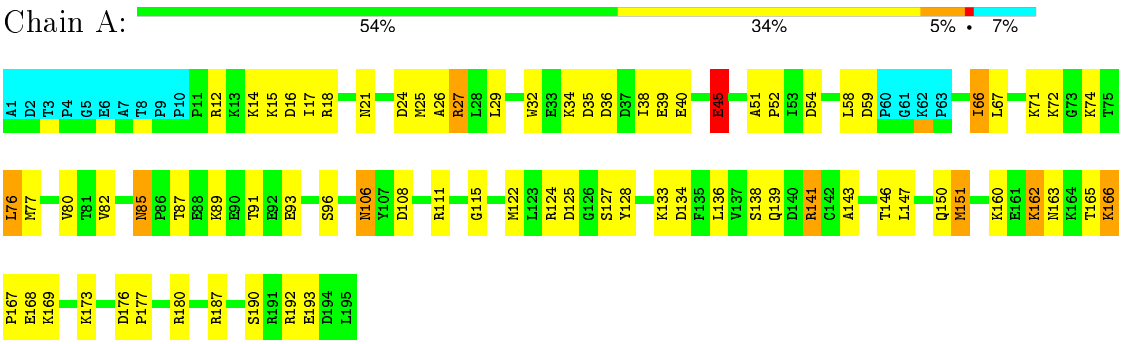
Chain A:



### 4.2.8 Score per residue for model 8

• Molecule 1: Mesoderm development candidate 2

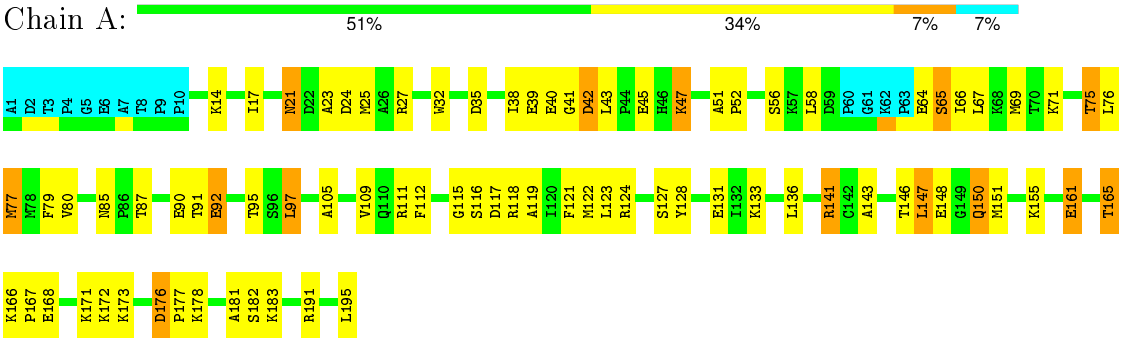
Chain A:




### 4.2.9 Score per residue for model 9

• Molecule 1: Mesoderm development candidate 2

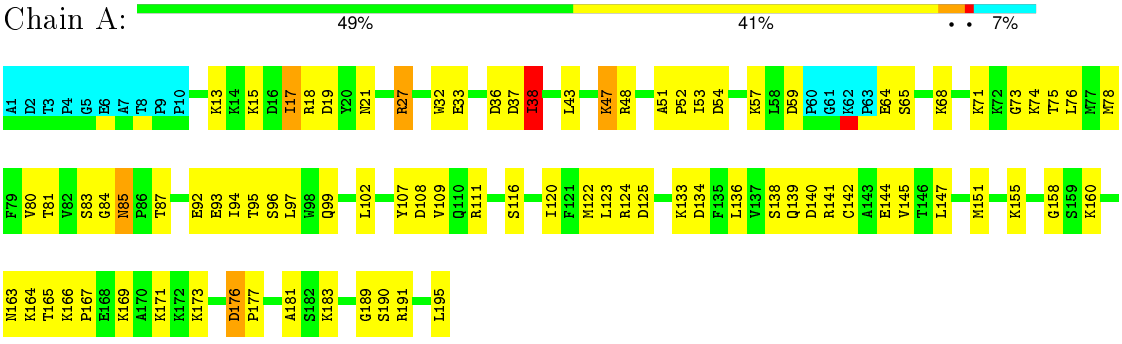
Chain A:




### 4.2.10 Score per residue for model 10

• Molecule 1: Mesoderm development candidate 2

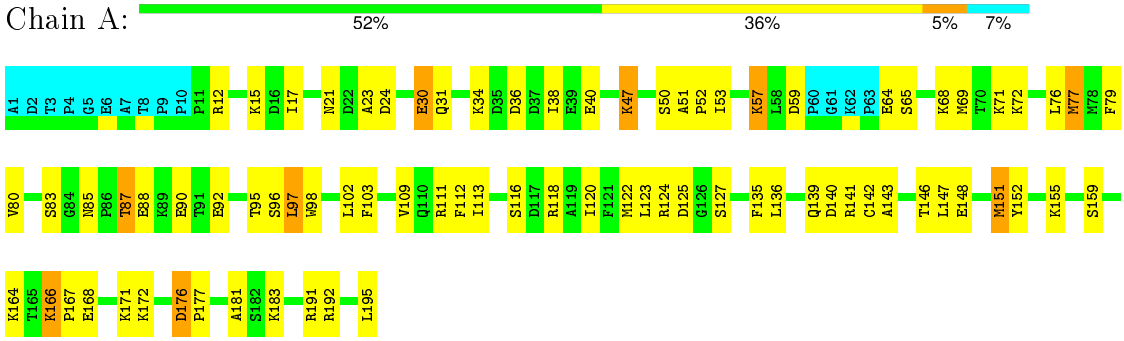
Chain A:



### 4.2.11 Score per residue for model 11

• Molecule 1: Mesoderm development candidate 2

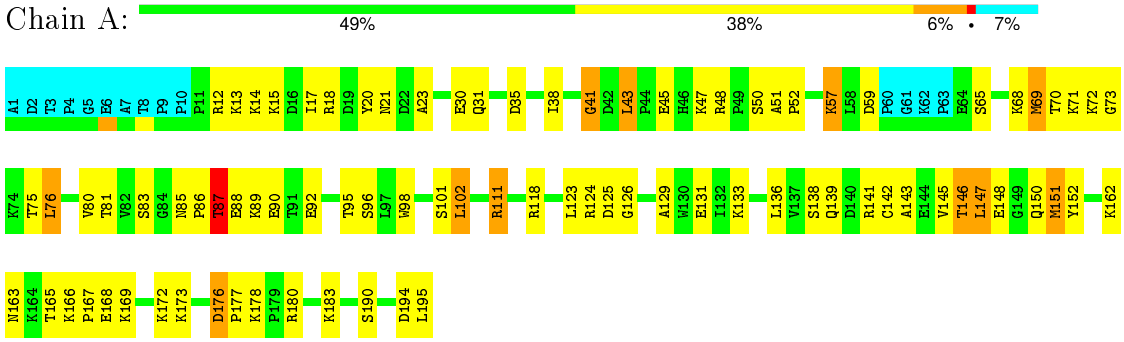
Chain A:




### 4.2.12 Score per residue for model 12

• Molecule 1: Mesoderm development candidate 2

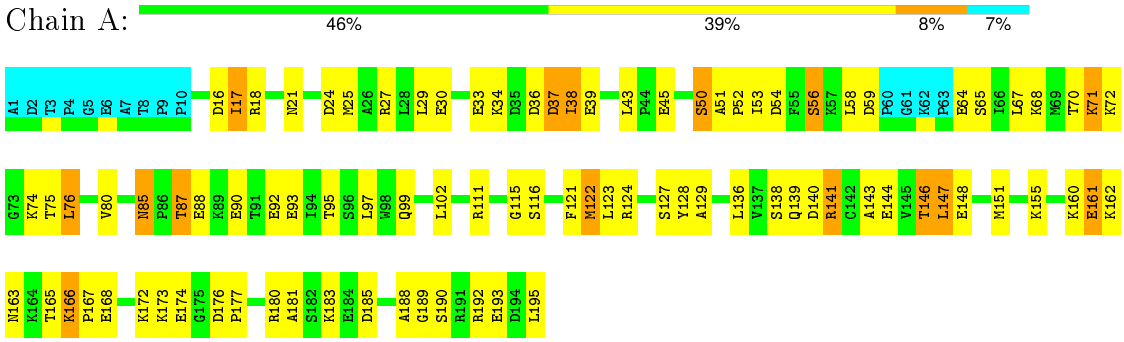
Chain A:




### 4.2.13 Score per residue for model 13

• Molecule 1: Mesoderm development candidate 2

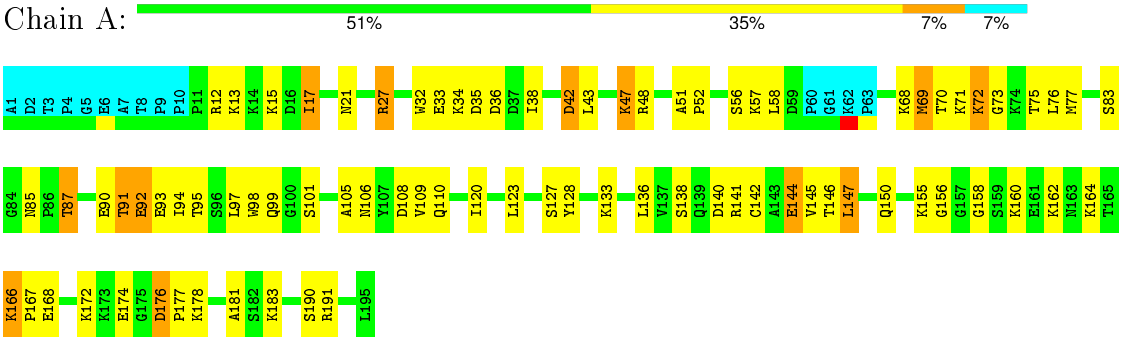
Chain A:



### 4.2.14 Score per residue for model 14

• Molecule 1: Mesoderm development candidate 2

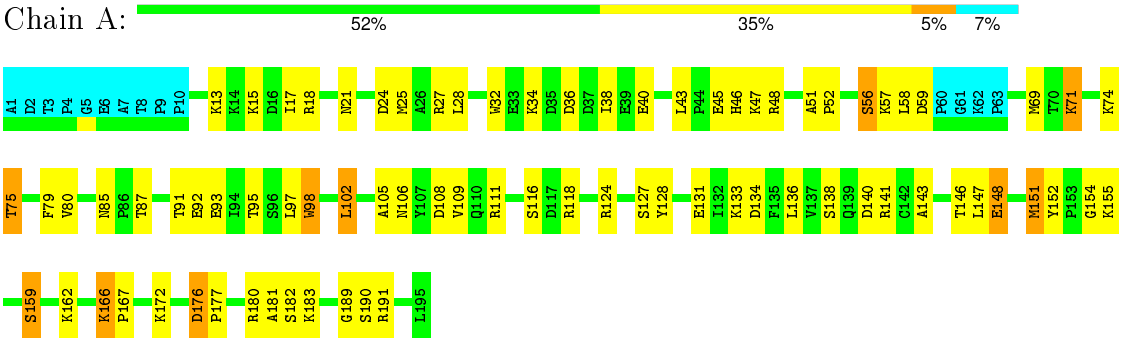
Chain A:




### 4.2.15 Score per residue for model 15

• Molecule 1: Mesoderm development candidate 2

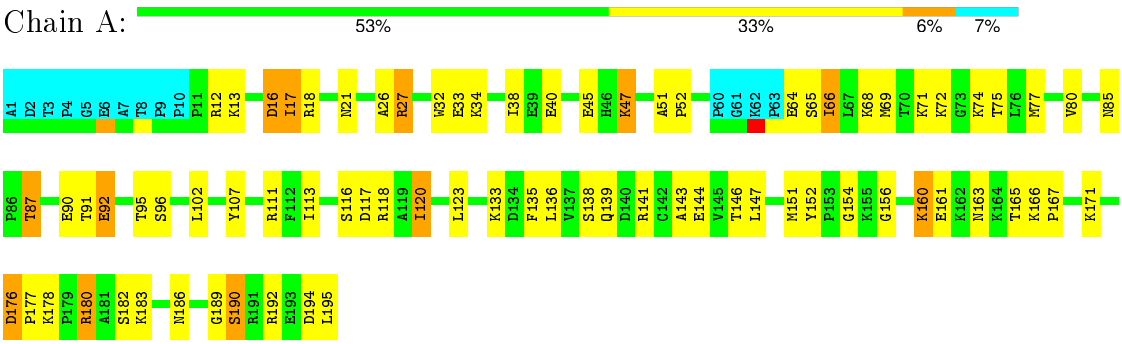
Chain A:




### 4.2.16 Score per residue for model 16

• Molecule 1: Mesoderm development candidate 2

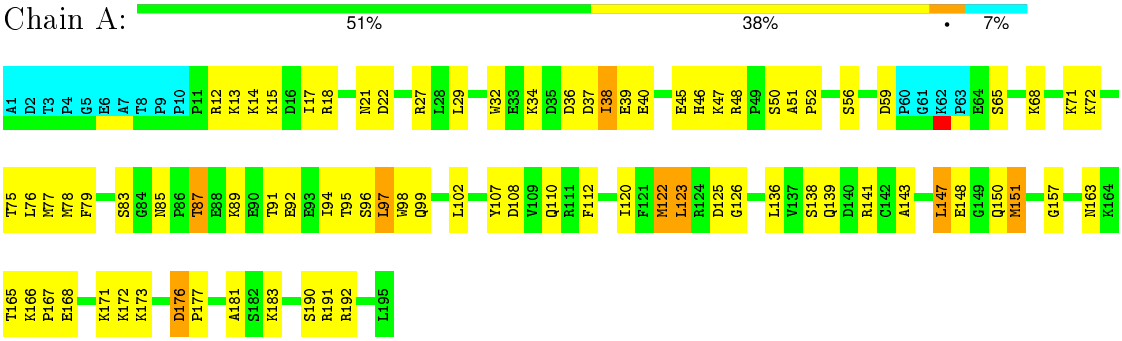
Chain A:



### 4.2.17 Score per residue for model 17

• Molecule 1: Mesoderm development candidate 2

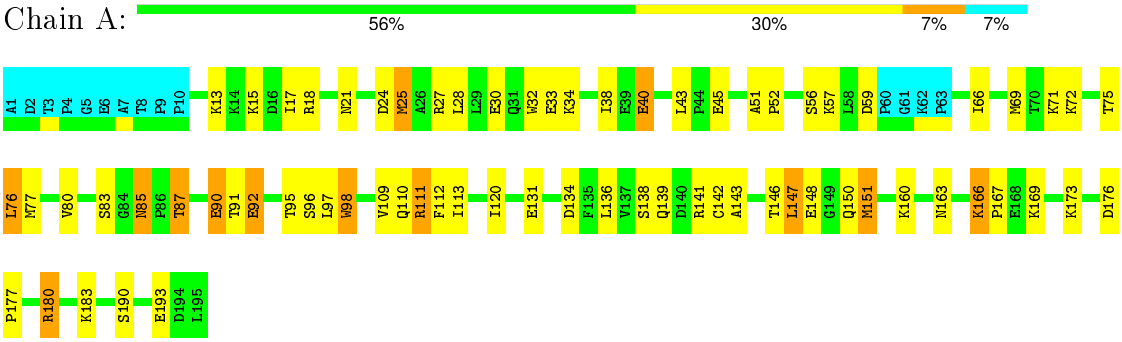
Chain A:




### 4.2.18 Score per residue for model 18

• Molecule 1: Mesoderm development candidate 2

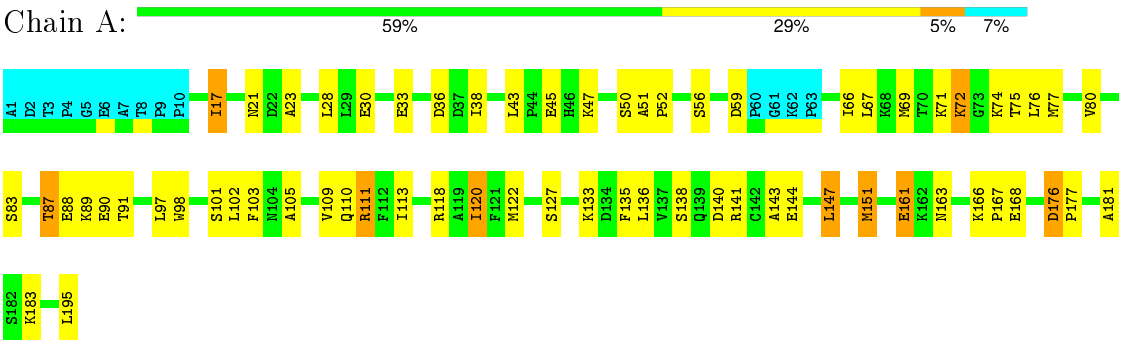
Chain A:




### 4.2.19 Score per residue for model 19

• Molecule 1: Mesoderm development candidate 2

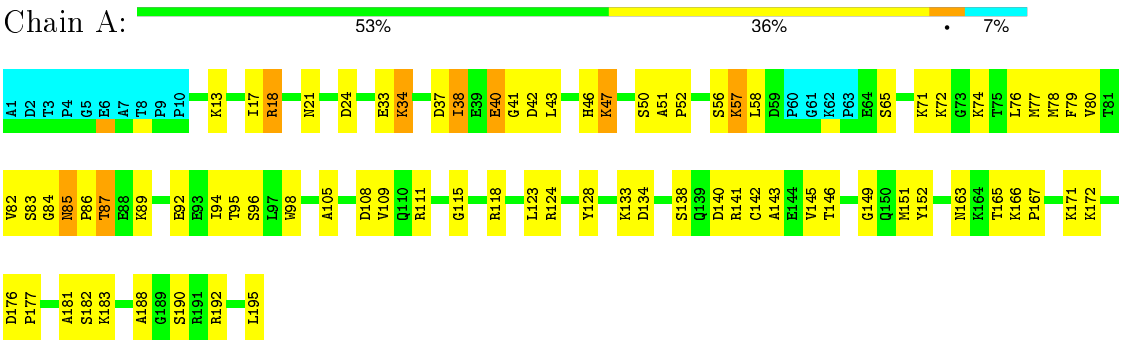
Chain A:



### 4.2.20 Score per residue for model 20

- Molecule 1: Mesoderm development candidate 2

Chain A:



# 5 Refinement protocol and experimental data overview

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

Of the 500 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 |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

# 6 Model quality

## 6.1 Standard geometry

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

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 | 1453 | 1439 | 1439 | 21±3 |
| All | All | 29060 | 28780 | 28780 | 425 |

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 7.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:76:LEU:HD23 | 1:A:97:LEU:HD13 | 0.86 | 1.46 | 11 | 3 |
| 1:A:97:LEU:HD13 | 1:A:147:LEU:HD21 | 0.81 | 1.52 | 17 | 1 |
| 1:A:123:LEU:HD23 | 1:A:129:ALA:HB2 | 0.81 | 1.52 | 12 | 1 |
| 1:A:76:LEU:HD23 | 1:A:97:LEU:HD12 | 0.77 | 1.56 | 19 | 1 |
| 1:A:76:LEU:C | 1:A:76:LEU:HD22 | 0.72 | 2.05 | 12 | 1 |
| 1:A:76:LEU:HD22 | 1:A:76:LEU:C | 0.70 | 2.06 | 18 | 1 |
| 1:A:97:LEU:HD11 | 1:A:147:LEU:HD23 | 0.69 | 1.64 | 15 | 1 |
| 1:A:147:LEU:C | 1:A:147:LEU:HD22 | 0.68 | 2.10 | 19 | 2 |
| 1:A:147:LEU:HD22 | 1:A:147:LEU:C | 0.67 | 2.10 | 13 | 2 |
| 1:A:27:ARG:HB3 | 1:A:91:THR:HG21 | 0.67 | 1.67 | 14 | 5 |
| 1:A:87:THR:O | 1:A:91:THR:HG23 | 0.65 | 1.92 | 4 | 7 |
| 1:A:76:LEU:HD11 | 1:A:122:MET:CG | 0.64 | 2.22 | 8 | 1 |
| 1:A:41:GLY:O | 1:A:145:VAL:HG12 | 0.64 | 1.93 | 20 | 2 |
| 1:A:87:THR:HG21 | 1:A:145:VAL:HG21 | 0.63 | 1.68 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:76:LEU:CD2 | 1:A:97:LEU:HD13 | 0.63 | 2.24 | 9 | 1 |
| 1:A:87:THR:HG22 | 1:A:90:GLU:HB2 | 0.62 | 1.71 | 14 | 6 |
| 1:A:98:TRP:CZ2 | 1:A:109:VAL:HG21 | 0.61 | 2.30 | 14 | 3 |
| 1:A:40:GLU:HB3 | 1:A:143:ALA:HB3 | 0.61 | 1.71 | 15 | 4 |
| 1:A:87:THR:HG22 | 1:A:90:GLU:CG | 0.61 | 2.25 | 12 | 1 |
| 1:A:78:MET:CG | 1:A:145:VAL:HG13 | 0.61 | 2.26 | 7 | 1 |
| 1:A:147:LEU:HD13 | 1:A:147:LEU:N | 0.61 | 2.11 | 12 | 1 |
| 1:A:76:LEU:HD13 | 1:A:77:MET:N | 0.60 | 2.12 | 19 | 4 |
| 1:A:29:LEU:HD22 | 1:A:192:ARG:HA | 0.60 | 1.73 | 8 | 2 |
| 1:A:97:LEU:HD21 | 1:A:147:LEU:HD11 | 0.60 | 1.72 | 17 | 1 |
| 1:A:23:ALA:HB1 | 1:A:111:ARG:NE | 0.60 | 2.12 | 9 | 1 |
| 1:A:76:LEU:HD11 | 1:A:122:MET:HG3 | 0.59 | 1.74 | 8 | 1 |
| 1:A:27:ARG:CB | 1:A:91:THR:HG21 | 0.59 | 2.27 | 14 | 4 |
| 1:A:85:ASN:OD1 | 1:A:143:ALA:HB1 | 0.59 | 1.98 | 20 | 3 |
| 1:A:92:GLU:O | 1:A:95:THR:HG22 | 0.58 | 1.98 | 13 | 15 |
| 1:A:98:TRP:NE1 | 1:A:102:LEU:HD23 | 0.58 | 2.14 | 3 | 2 |
| 1:A:79:PHE:CE1 | 1:A:123:LEU:HD12 | 0.58 | 2.34 | 17 | 1 |
| 1:A:132:ILE:HG22 | 1:A:136:LEU:HD23 | 0.58 | 1.73 | 5 | 1 |
| 1:A:80:VAL:HG23 | 1:A:143:ALA:HA | 0.57 | 1.75 | 1 | 15 |
| 1:A:76:LEU:HD13 | 1:A:122:MET:CE | 0.57 | 2.29 | 7 | 1 |
| 1:A:67:LEU:HD13 | 1:A:163:ASN:HB2 | 0.57 | 1.76 | 8 | 1 |
| 1:A:40:GLU:CB | 1:A:143:ALA:HB3 | 0.57 | 2.30 | 17 | 3 |
| 1:A:93:GLU:HB3 | 1:A:147:LEU:HD11 | 0.57 | 1.77 | 10 | 1 |
| 1:A:87:THR:HG22 | 1:A:90:GLU:HG3 | 0.57 | 1.77 | 12 | 1 |
| 1:A:78:MET:CG | 1:A:145:VAL:HG23 | 0.56 | 2.29 | 1 | 3 |
| 1:A:75:THR:O | 1:A:97:LEU:HD22 | 0.56 | 2.01 | 13 | 1 |
| 1:A:97:LEU:HD11 | 1:A:147:LEU:HD21 | 0.56 | 1.77 | 14 | 2 |
| 1:A:68:LYS:O | 1:A:70:THR:HG23 | 0.56 | 2.00 | 3 | 1 |
| 1:A:45:GLU:HG2 | 1:A:146:THR:HG23 | 0.56 | 1.76 | 8 | 1 |
| 1:A:98:TRP:CZ2 | 1:A:102:LEU:HD12 | 0.56 | 2.36 | 17 | 2 |
| 1:A:17:ILE:HD11 | 1:A:109:VAL:O | 0.56 | 2.01 | 14 | 2 |
| 1:A:56:SER:OG | 1:A:105:ALA:HB3 | 0.56 | 1.99 | 15 | 1 |
| 1:A:80:VAL:HG21 | 1:A:85:ASN:CG | 0.56 | 2.20 | 10 | 3 |
| 1:A:59:ASP:CB | 1:A:105:ALA:HB1 | 0.56 | 2.30 | 4 | 1 |
| 1:A:29:LEU:HD12 | 1:A:192:ARG:HG2 | 0.56 | 1.76 | 17 | 1 |
| 1:A:67:LEU:HD22 | 1:A:159:SER:CB | 0.56 | 2.30 | 7 | 1 |
| 1:A:81:THR:HG21 | 1:A:139:GLN:HB2 | 0.56 | 1.77 | 10 | 1 |
| 1:A:74:LYS:O | 1:A:97:LEU:HD22 | 0.55 | 2.00 | 19 | 2 |
| 1:A:67:LEU:HD22 | 1:A:161:GLU:HG3 | 0.55 | 1.79 | 3 | 2 |
| 1:A:23:ALA:HB1 | 1:A:111:ARG:CD | 0.55 | 2.32 | 2 | 4 |
| 1:A:90:GLU:OE2 | 1:A:147:LEU:HD21 | 0.55 | 2.02 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:98:TRP:CH2 | 1:A:109:VAL:HG21 | 0.55 | 2.36 | 14 | 2 |
| 1:A:97:LEU:CD1 | 1:A:147:LEU:HD23 | 0.54 | 2.32 | 15 | 1 |
| 1:A:76:LEU:HD21 | 1:A:122:MET:HB2 | 0.54 | 1.79 | 13 | 1 |
| 1:A:25:MET:HG3 | 1:A:28:LEU:HD12 | 0.54 | 1.80 | 18 | 1 |
| 1:A:27:ARG:CZ | 1:A:120:ILE:HG21 | 0.54 | 2.32 | 16 | 1 |
| 1:A:94:ILE:HD12 | 1:A:122:MET:CE | 0.54 | 2.33 | 3 | 2 |
| 1:A:75:THR:HG22 | 1:A:154:GLY:CA | 0.54 | 2.33 | 15 | 1 |
| 1:A:76:LEU:HD22 | 1:A:97:LEU:CB | 0.54 | 2.32 | 2 | 1 |
| 1:A:43:LEU:HD11 | 1:A:144:GLU:CG | 0.54 | 2.31 | 14 | 1 |
| 1:A:48:ARG:CZ | 1:A:146:THR:HG21 | 0.53 | 2.33 | 12 | 1 |
| 1:A:70:THR:HG23 | 1:A:162:LYS:HB3 | 0.53 | 1.78 | 13 | 1 |
| 1:A:78:MET:HG3 | 1:A:145:VAL:HG13 | 0.53 | 1.79 | 7 | 1 |
| 1:A:58:LEU:HD23 | 1:A:105:ALA:O | 0.53 | 2.03 | 14 | 1 |
| 1:A:26:ALA:HB2 | 1:A:190:SER:CB | 0.53 | 2.34 | 16 | 1 |
| 1:A:29:LEU:HD13 | 1:A:192:ARG:HB3 | 0.53 | 1.81 | 8 | 1 |
| 1:A:121:PHE:CE1 | 1:A:129:ALA:HB1 | 0.53 | 2.37 | 13 | 2 |
| 1:A:147:LEU:HD22 | 1:A:148:GLU:N | 0.53 | 2.19 | 11 | 2 |
| 1:A:67:LEU:HD13 | 1:A:163:ASN:CB | 0.53 | 2.34 | 8 | 1 |
| 1:A:146:THR:C | 1:A:147:LEU:HD13 | 0.52 | 2.24 | 12 | 1 |
| 1:A:39:GLU:HG2 | 1:A:82:VAL:HG21 | 0.52 | 1.80 | 6 | 3 |
| 1:A:102:LEU:HD23 | 1:A:102:LEU:O | 0.52 | 2.04 | 16 | 1 |
| 1:A:97:LEU:CD2 | 1:A:147:LEU:HD11 | 0.52 | 2.34 | 17 | 1 |
| 1:A:166:LYS:CB | 1:A:167:PRO:CD | 0.52 | 2.87 | 15 | 17 |
| 1:A:70:THR:HG23 | 1:A:162:LYS:CB | 0.52 | 2.34 | 13 | 2 |
| 1:A:147:LEU:HD22 | 1:A:147:LEU:O | 0.52 | 2.05 | 13 | 2 |
| 1:A:29:LEU:HD13 | 1:A:192:ARG:CB | 0.52 | 2.35 | 8 | 1 |
| 1:A:113:ILE:HG22 | 1:A:118:ARG:CZ | 0.52 | 2.35 | 7 | 1 |
| 1:A:26:ALA:HB2 | 1:A:190:SER:HB3 | 0.52 | 1.82 | 16 | 1 |
| 1:A:147:LEU:O | 1:A:147:LEU:HD22 | 0.51 | 2.05 | 6 | 2 |
| 1:A:76:LEU:CD2 | 1:A:76:LEU:C | 0.51 | 2.79 | 18 | 1 |
| 1:A:102:LEU:O | 1:A:102:LEU:HD13 | 0.51 | 2.05 | 12 | 2 |
| 1:A:45:GLU:HG3 | 1:A:146:THR:HG22 | 0.51 | 1.82 | 13 | 1 |
| 1:A:27:ARG:NE | 1:A:120:ILE:HD13 | 0.51 | 2.21 | 6 | 1 |
| 1:A:70:THR:HG23 | 1:A:162:LYS:HB2 | 0.51 | 1.83 | 4 | 2 |
| 1:A:166:LYS:N | 1:A:167:PRO:HD2 | 0.51 | 2.21 | 19 | 15 |
| 1:A:76:LEU:O | 1:A:76:LEU:HD22 | 0.51 | 2.06 | 18 | 2 |
| 1:A:102:LEU:HD11 | 1:A:176:ASP:OD2 | 0.51 | 2.06 | 11 | 1 |
| 1:A:109:VAL:HG22 | 1:A:122:MET:CB | 0.51 | 2.36 | 19 | 2 |
| 1:A:28:LEU:HG | 1:A:91:THR:HG21 | 0.51 | 1.83 | 19 | 3 |
| 1:A:67:LEU:HD13 | 1:A:161:GLU:HG2 | 0.50 | 1.82 | 9 | 1 |
| 1:A:109:VAL:HG22 | 1:A:122:MET:HB2 | 0.50 | 1.82 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:97:LEU:HD21 | 1:A:147:LEU:HD21 | 0.49 | 1.83 | 18 | 2 |
| 1:A:17:ILE:HG23 | 1:A:23:ALA:HB2 | 0.49 | 1.84 | 4 | 1 |
| 1:A:39:GLU:CG | 1:A:82:VAL:HG21 | 0.49 | 2.37 | 8 | 1 |
| 1:A:111:ARG:HA | 1:A:120:ILE:HD12 | 0.49 | 1.84 | 19 | 2 |
| 1:A:109:VAL:HG13 | 1:A:122:MET:HB3 | 0.49 | 1.83 | 19 | 2 |
| 1:A:87:THR:HG21 | 1:A:145:VAL:HG11 | 0.49 | 1.84 | 14 | 2 |
| 1:A:75:THR:HG21 | 1:A:124:ARG:NH2 | 0.49 | 2.23 | 10 | 1 |
| 1:A:51:ALA:HB1 | 1:A:52:PRO:HD2 | 0.49 | 1.85 | 15 | 20 |
| 1:A:78:MET:SD | 1:A:145:VAL:HG23 | 0.49 | 2.48 | 10 | 2 |
| 1:A:16:ASP:C | 1:A:17:ILE:HD12 | 0.49 | 2.28 | 16 | 2 |
| 1:A:108:ASP:OD2 | 1:A:129:ALA:HB3 | 0.49 | 2.07 | 2 | 1 |
| 1:A:43:LEU:HB3 | 1:A:145:VAL:HG13 | 0.49 | 1.85 | 12 | 1 |
| 1:A:29:LEU:HD13 | 1:A:192:ARG:HB2 | 0.48 | 1.84 | 13 | 1 |
| 1:A:147:LEU:C | 1:A:147:LEU:CD2 | 0.48 | 2.82 | 6 | 2 |
| 1:A:80:VAL:CG2 | 1:A:82:VAL:HG12 | 0.48 | 2.38 | 20 | 1 |
| 1:A:27:ARG:HD3 | 1:A:120:ILE:HD12 | 0.48 | 1.84 | 3 | 1 |
| 1:A:147:LEU:HD13 | 1:A:148:GLU:N | 0.48 | 2.24 | 17 | 1 |
| 1:A:102:LEU:HD13 | 1:A:102:LEU:O | 0.48 | 2.08 | 3 | 1 |
| 1:A:18:ARG:NH1 | 1:A:188:ALA:HB1 | 0.48 | 2.24 | 20 | 1 |
| 1:A:76:LEU:C | 1:A:76:LEU:CD2 | 0.48 | 2.78 | 12 | 1 |
| 1:A:23:ALA:HB1 | 1:A:111:ARG:HG2 | 0.48 | 1.85 | 11 | 1 |
| 1:A:17:ILE:HG23 | 1:A:23:ALA:CB | 0.48 | 2.38 | 4 | 2 |
| 1:A:97:LEU:HD21 | 1:A:147:LEU:CD2 | 0.48 | 2.39 | 15 | 1 |
| 1:A:39:GLU:HG2 | 1:A:82:VAL:HG11 | 0.47 | 1.85 | 1 | 3 |
| 1:A:98:TRP:CE2 | 1:A:102:LEU:HD23 | 0.47 | 2.44 | 2 | 1 |
| 1:A:27:ARG:CD | 1:A:120:ILE:HD12 | 0.47 | 2.38 | 3 | 1 |
| 1:A:58:LEU:HD23 | 1:A:106:ASN:OD1 | 0.47 | 2.09 | 8 | 1 |
| 1:A:27:ARG:HB2 | 1:A:91:THR:HG21 | 0.47 | 1.86 | 9 | 1 |
| 1:A:86:PRO:O | 1:A:87:THR:HG23 | 0.47 | 2.09 | 12 | 3 |
| 1:A:78:MET:SD | 1:A:94:ILE:HD11 | 0.47 | 2.49 | 4 | 2 |
| 1:A:50:SER:HB3 | 1:A:75:THR:HG21 | 0.47 | 1.86 | 13 | 1 |
| 1:A:147:LEU:CD2 | 1:A:147:LEU:C | 0.47 | 2.82 | 19 | 2 |
| 1:A:27:ARG:CZ | 1:A:120:ILE:HD13 | 0.47 | 2.39 | 6 | 1 |
| 1:A:27:ARG:NE | 1:A:120:ILE:HG21 | 0.47 | 2.23 | 16 | 2 |
| 1:A:67:LEU:HD22 | 1:A:159:SER:HB3 | 0.47 | 1.87 | 7 | 1 |
| 1:A:23:ALA:HB1 | 1:A:111:ARG:HD2 | 0.47 | 1.86 | 2 | 1 |
| 1:A:176:ASP:N | 1:A:177:PRO:HD2 | 0.47 | 2.25 | 16 | 20 |
| 1:A:65:SER:HA | 1:A:165:THR:HG21 | 0.47 | 1.87 | 9 | 1 |
| 1:A:34:LYS:CE | 1:A:38:ILE:HD12 | 0.47 | 2.40 | 20 | 1 |
| 1:A:79:PHE:HB3 | 1:A:136:LEU:HD13 | 0.47 | 1.87 | 11 | 4 |
| 1:A:97:LEU:HD11 | 1:A:147:LEU:CD2 | 0.47 | 2.40 | 14 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:176:ASP:CB | 1:A:177:PRO:CD | 0.46 | 2.94 | 13 | 20 |
| 1:A:109:VAL:HG23 | 1:A:122:MET:HB3 | 0.46 | 1.84 | 9 | 1 |
| 1:A:66:ILE:HG12 | 1:A:102:LEU:HD23 | 0.46 | 1.86 | 4 | 1 |
| 1:A:111:ARG:NH1 | 1:A:113:ILE:HD12 | 0.46 | 2.26 | 18 | 1 |
| 1:A:147:LEU:HD13 | 1:A:147:LEU:C | 0.46 | 2.32 | 11 | 5 |
| 1:A:30:GLU:OE2 | 1:A:113:ILE:HG23 | 0.46 | 2.11 | 11 | 1 |
| 1:A:24:ASP:O | 1:A:91:THR:HG23 | 0.46 | 2.11 | 3 | 1 |
| 1:A:17:ILE:HG12 | 1:A:109:VAL:HG23 | 0.46 | 1.86 | 10 | 1 |
| 1:A:66:ILE:HD11 | 1:A:99:GLN:O | 0.46 | 2.11 | 7 | 1 |
| 1:A:76:LEU:HD13 | 1:A:94:ILE:HD12 | 0.46 | 1.87 | 10 | 1 |
| 1:A:165:THR:HG22 | 1:A:167:PRO:HD2 | 0.45 | 1.88 | 4 | 1 |
| 1:A:147:LEU:HD13 | 1:A:147:LEU:O | 0.45 | 2.11 | 11 | 1 |
| 1:A:17:ILE:HD13 | 1:A:109:VAL:CG1 | 0.45 | 2.42 | 6 | 1 |
| 1:A:76:LEU:HD23 | 1:A:147:LEU:HD23 | 0.45 | 1.89 | 5 | 1 |
| 1:A:136:LEU:HD23 | 1:A:137:VAL:N | 0.44 | 2.26 | 2 | 1 |
| 1:A:43:LEU:N | 1:A:43:LEU:HD22 | 0.44 | 2.27 | 19 | 1 |
| 1:A:75:THR:HG22 | 1:A:154:GLY:N | 0.44 | 2.27 | 4 | 3 |
| 1:A:80:VAL:HG21 | 1:A:85:ASN:OD1 | 0.44 | 2.12 | 18 | 1 |
| 1:A:34:LYS:HE3 | 1:A:38:ILE:HD12 | 0.44 | 1.89 | 20 | 1 |
| 1:A:27:ARG:CD | 1:A:120:ILE:HG21 | 0.44 | 2.42 | 10 | 2 |
| 1:A:21:ASN:OD1 | 1:A:95:THR:HG23 | 0.44 | 2.13 | 7 | 1 |
| 1:A:98:TRP:CZ2 | 1:A:102:LEU:HD13 | 0.44 | 2.48 | 11 | 1 |
| 1:A:94:ILE:HD12 | 1:A:122:MET:HE2 | 0.43 | 1.90 | 3 | 1 |
| 1:A:43:LEU:HD12 | 1:A:144:GLU:HA | 0.43 | 1.89 | 13 | 1 |
| 1:A:45:GLU:CG | 1:A:146:THR:HG23 | 0.43 | 2.43 | 8 | 1 |
| 1:A:126:GLY:O | 1:A:129:ALA:HB3 | 0.43 | 2.13 | 6 | 1 |
| 1:A:75:THR:HG21 | 1:A:124:ARG:CD | 0.43 | 2.43 | 9 | 1 |
| 1:A:98:TRP:CH2 | 1:A:109:VAL:HG11 | 0.43 | 2.49 | 14 | 2 |
| 1:A:78:MET:HG2 | 1:A:145:VAL:HG23 | 0.43 | 1.90 | 1 | 1 |
| 1:A:76:LEU:C | 1:A:76:LEU:HD13 | 0.43 | 2.34 | 11 | 2 |
| 1:A:147:LEU:CD1 | 1:A:147:LEU:N | 0.43 | 2.82 | 13 | 5 |
| 1:A:29:LEU:HD22 | 1:A:192:ARG:CA | 0.43 | 2.43 | 13 | 1 |
| 1:A:147:LEU:C | 1:A:147:LEU:HD13 | 0.42 | 2.34 | 1 | 3 |
| 1:A:82:VAL:HG13 | 1:A:84:GLY:O | 0.42 | 2.14 | 20 | 1 |
| 1:A:121:PHE:HE1 | 1:A:129:ALA:HB1 | 0.42 | 1.73 | 13 | 1 |
| 1:A:76:LEU:HD12 | 1:A:94:ILE:HG23 | 0.42 | 1.91 | 14 | 1 |
| 1:A:79:PHE:CZ | 1:A:123:LEU:HD13 | 0.42 | 2.49 | 9 | 1 |
| 1:A:76:LEU:HD12 | 1:A:77:MET:N | 0.42 | 2.30 | 8 | 1 |
| 1:A:66:ILE:HD13 | 1:A:103:PHE:CE2 | 0.42 | 2.50 | 19 | 1 |
| 1:A:76:LEU:HD13 | 1:A:122:MET:HE3 | 0.42 | 1.88 | 7 | 1 |
| 1:A:76:LEU:HD22 | 1:A:97:LEU:C | 0.42 | 2.35 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:39:GLU:CG | 1:A:82:VAL:HG11 | 0.42 | 2.44 | 4 | 1 |
| 1:A:40:GLU:HB2 | 1:A:143:ALA:HB3 | 0.42 | 1.90 | 17 | 1 |
| 1:A:98:TRP:CZ3 | 1:A:102:LEU:HD23 | 0.42 | 2.49 | 15 | 1 |
| 1:A:37:ASP:O | 1:A:38:ILE:C | 0.42 | 2.58 | 3 | 6 |
| 1:A:98:TRP:CZ2 | 1:A:109:VAL:HG11 | 0.42 | 2.49 | 15 | 1 |
| 1:A:78:MET:CE | 1:A:94:ILE:HD11 | 0.42 | 2.44 | 10 | 2 |
| 1:A:26:ALA:HB3 | 1:A:27:ARG:NH2 | 0.41 | 2.30 | 8 | 1 |
| 1:A:17:ILE:HG13 | 1:A:109:VAL:HG23 | 0.41 | 1.91 | 1 | 1 |
| 1:A:166:LYS:CB | 1:A:167:PRO:HD3 | 0.41 | 2.45 | 15 | 2 |
| 1:A:166:LYS:N | 1:A:167:PRO:CD | 0.41 | 2.84 | 11 | 1 |
| 1:A:193:GLU:OE2 | 1:A:195:LEU:HD23 | 0.41 | 2.14 | 2 | 1 |
| 1:A:185:ASP:O | 1:A:188:ALA:HB3 | 0.41 | 2.15 | 13 | 1 |
| 1:A:87:THR:HG22 | 1:A:90:GLU:CB | 0.41 | 2.46 | 16 | 1 |
| 1:A:76:LEU:HD11 | 1:A:122:MET:HG2 | 0.41 | 1.90 | 8 | 1 |
| 1:A:80:VAL:HG23 | 1:A:143:ALA:CB | 0.41 | 2.46 | 4 | 2 |
| 1:A:27:ARG:HH22 | 1:A:119:ALA:N | 0.41 | 2.14 | 9 | 1 |
| 1:A:78:MET:HE2 | 1:A:147:LEU:HB2 | 0.40 | 1.92 | 17 | 1 |
| 1:A:69:MET:O | 1:A:70:THR:C | 0.40 | 2.59 | 5 | 3 |
| 1:A:136:LEU:HD13 | 1:A:136:LEU:C | 0.40 | 2.36 | 4 | 1 |
| 1:A:39:GLU:HG3 | 1:A:82:VAL:HG21 | 0.40 | 1.94 | 5 | 1 |
| 1:A:195:LEU:O | 1:A:195:LEU:HD23 | 0.40 | 2.15 | 6 | 1 |
| 1:A:67:LEU:HD22 | 1:A:161:GLU:CB | 0.40 | 2.46 | 19 | 1 |
| 1:A:58:LEU:HD22 | 1:A:105:ALA:O | 0.40 | 2.15 | 20 | 1 |
| 1:A:43:LEU:HD23 | 1:A:44:PRO:HD2 | 0.40 | 1.92 | 4 | 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 | 180/195 (92%) | 131±4 (73±2%) | 37±4 (20±2%) | 12±2 (7±1%) | 3 | 18 |
| All | All | 3600/3900 (92%) | 2620 (73%) | 735 (20%) | 245 (7%) | 3 | 18 |

All 38 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 | 21 | ASN | 20 |
| 1 | A | 17 | ILE | 20 |
| 1 | A | 38 | ILE | 20 |
| 1 | A | 71 | LYS | 20 |
| 1 | A | 141 | ARG | 20 |
| 1 | A | 47 | LYS | 15 |
| 1 | A | 151 | MET | 15 |
| 1 | A | 181 | ALA | 13 |
| 1 | A | 160 | LYS | 9 |
| 1 | A | 75 | THR | 8 |
| 1 | A | 45 | GLU | 8 |
| 1 | A | 56 | SER | 7 |
| 1 | A | 180 | ARG | 7 |
| 1 | A | 189 | GLY | 7 |
| 1 | A | 57 | LYS | 6 |
| 1 | A | 150 | GLN | 4 |
| 1 | A | 115 | GLY | 4 |
| 1 | A | 53 | ILE | 3 |
| 1 | A | 41 | GLY | 3 |
| 1 | A | 73 | GLY | 3 |
| 1 | A | 156 | GLY | 3 |
| 1 | A | 194 | ASP | 3 |
| 1 | A | 72 | LYS | 3 |
| 1 | A | 126 | GLY | 3 |
| 1 | A | 107 | TYR | 3 |
| 1 | A | 42 | ASP | 3 |
| 1 | A | 159 | SER | 2 |
| 1 | A | 162 | LYS | 2 |
| 1 | A | 158 | GLY | 2 |
| 1 | A | 157 | GLY | 1 |
| 1 | A | 83 | SER | 1 |
| 1 | A | 55 | PHE | 1 |
| 1 | A | 191 | ARG | 1 |
| 1 | A | 149 | GLY | 1 |
| 1 | A | 87 | THR | 1 |
| 1 | A | 58 | LEU | 1 |
| 1 | A | 84 | GLY | 1 |
| 1 | A | 13 | LYS | 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 | 158/168 (94%) | 108±5 (68±3%) | 50±5 (32±3%) | 1 14 |
| All | All | 3160/3360 (94%) | 2163 (68%) | 997 (32%) | 1 14 |

All 130 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 | 85 | ASN | 19 |
| 1 | A | 183 | LYS | 18 |
| 1 | A | 138 | SER | 18 |
| 1 | A | 72 | LYS | 15 |
| 1 | A | 18 | ARG | 15 |
| 1 | A | 146 | THR | 15 |
| 1 | A | 172 | LYS | 14 |
| 1 | A | 34 | LYS | 14 |
| 1 | A | 133 | LYS | 14 |
| 1 | A | 165 | THR | 14 |
| 1 | A | 15 | LYS | 13 |
| 1 | A | 83 | SER | 13 |
| 1 | A | 168 | GLU | 13 |
| 1 | A | 176 | ASP | 13 |
| 1 | A | 195 | LEU | 13 |
| 1 | A | 190 | SER | 13 |
| 1 | A | 59 | ASP | 13 |
| 1 | A | 87 | THR | 13 |
| 1 | A | 111 | ARG | 13 |
| 1 | A | 96 | SER | 12 |
| 1 | A | 151 | MET | 12 |
| 1 | A | 140 | ASP | 12 |
| 1 | A | 36 | ASP | 11 |
| 1 | A | 173 | LYS | 11 |
| 1 | A | 65 | SER | 11 |
| 1 | A | 124 | ARG | 11 |
| 1 | A | 32 | TRP | 11 |
| 1 | A | 27 | ARG | 11 |
| 1 | A | 13 | LYS | 11 |
| 1 | A | 43 | LEU | 11 |
| 1 | A | 136 | LEU | 11 |
| 1 | A | 180 | ARG | 11 |
| 1 | A | 33 | GLU | 11 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 118 | ARG | 10 |
| 1 | A | 40 | GLU | 10 |
| 1 | A | 163 | ASN | 10 |
| 1 | A | 77 | MET | 10 |
| 1 | A | 171 | LYS | 10 |
| 1 | A | 68 | LYS | 10 |
| 1 | A | 127 | SER | 10 |
| 1 | A | 69 | MET | 10 |
| 1 | A | 74 | LYS | 10 |
| 1 | A | 12 | ARG | 10 |
| 1 | A | 89 | LYS | 10 |
| 1 | A | 155 | LYS | 9 |
| 1 | A | 134 | ASP | 9 |
| 1 | A | 148 | GLU | 9 |
| 1 | A | 50 | SER | 9 |
| 1 | A | 162 | LYS | 9 |
| 1 | A | 24 | ASP | 9 |
| 1 | A | 112 | PHE | 9 |
| 1 | A | 123 | LEU | 9 |
| 1 | A | 110 | GLN | 9 |
| 1 | A | 128 | TYR | 9 |
| 1 | A | 47 | LYS | 9 |
| 1 | A | 108 | ASP | 9 |
| 1 | A | 120 | ILE | 8 |
| 1 | A | 142 | CYS | 8 |
| 1 | A | 150 | GLN | 8 |
| 1 | A | 116 | SER | 8 |
| 1 | A | 166 | LYS | 8 |
| 1 | A | 102 | LEU | 8 |
| 1 | A | 93 | GLU | 8 |
| 1 | A | 57 | LYS | 8 |
| 1 | A | 147 | LEU | 8 |
| 1 | A | 64 | GLU | 8 |
| 1 | A | 125 | ASP | 8 |
| 1 | A | 178 | LYS | 7 |
| 1 | A | 139 | GLN | 7 |
| 1 | A | 169 | LYS | 7 |
| 1 | A | 25 | MET | 7 |
| 1 | A | 191 | ARG | 7 |
| 1 | A | 99 | GLN | 7 |
| 1 | A | 135 | PHE | 7 |
| 1 | A | 122 | MET | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 131 | GLU | 6 |
| 1 | A | 106 | ASN | 6 |
| 1 | A | 90 | GLU | 6 |
| 1 | A | 193 | GLU | 6 |
| 1 | A | 30 | GLU | 6 |
| 1 | A | 161 | GLU | 6 |
| 1 | A | 192 | ARG | 6 |
| 1 | A | 35 | ASP | 6 |
| 1 | A | 92 | GLU | 5 |
| 1 | A | 46 | HIS | 5 |
| 1 | A | 174 | GLU | 5 |
| 1 | A | 76 | LEU | 5 |
| 1 | A | 48 | ARG | 5 |
| 1 | A | 45 | GLU | 5 |
| 1 | A | 101 | SER | 5 |
| 1 | A | 14 | LYS | 5 |
| 1 | A | 159 | SER | 5 |
| 1 | A | 144 | GLU | 5 |
| 1 | A | 182 | SER | 5 |
| 1 | A | 39 | GLU | 5 |
| 1 | A | 97 | LEU | 5 |
| 1 | A | 56 | SER | 5 |
| 1 | A | 152 | TYR | 5 |
| 1 | A | 113 | ILE | 4 |
| 1 | A | 141 | ARG | 4 |
| 1 | A | 88 | GLU | 4 |
| 1 | A | 16 | ASP | 4 |
| 1 | A | 37 | ASP | 4 |
| 1 | A | 187 | ARG | 4 |
| 1 | A | 58 | LEU | 4 |
| 1 | A | 42 | ASP | 4 |
| 1 | A | 31 | GLN | 3 |
| 1 | A | 21 | ASN | 3 |
| 1 | A | 54 | ASP | 3 |
| 1 | A | 66 | ILE | 3 |
| 1 | A | 20 | TYR | 3 |
| 1 | A | 19 | ASP | 3 |
| 1 | A | 117 | ASP | 3 |
| 1 | A | 71 | LYS | 3 |
| 1 | A | 130 | TRP | 3 |
| 1 | A | 164 | LYS | 3 |
| 1 | A | 22 | ASP | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 78 | MET | 2 |
| 1 | A | 98 | TRP | 2 |
| 1 | A | 91 | THR | 2 |
| 1 | A | 194 | ASP | 2 |
| 1 | A | 160 | LYS | 2 |
| 1 | A | 53 | ILE | 1 |
| 1 | A | 79 | PHE | 1 |
| 1 | A | 28 | LEU | 1 |
| 1 | A | 186 | ASN | 1 |
| 1 | A | 103 | PHE | 1 |
| 1 | A | 38 | ILE | 1 |
| 1 | A | 81 | THR | 1 |
| 1 | A | 121 | PHE | 1 |

#### 6.3.3 RNA

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains

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

### 6.5 Carbohydrates

There are no carbohydrates in this entry.

### 6.6 Ligand geometry

There are no ligands in this entry.

### 6.7 Other polymers

There are no such molecules in this entry.

### 6.8 Polymer linkage issues

There are no chain breaks in this entry.

# 7 Chemical shift validation

No chemical shift data were provided