



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:24 pm BST

PDB ID : 2LTV  
Title : YAP WW2 in complex with a Smad7 derived peptide  
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Deposited on : 2012-06-04

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

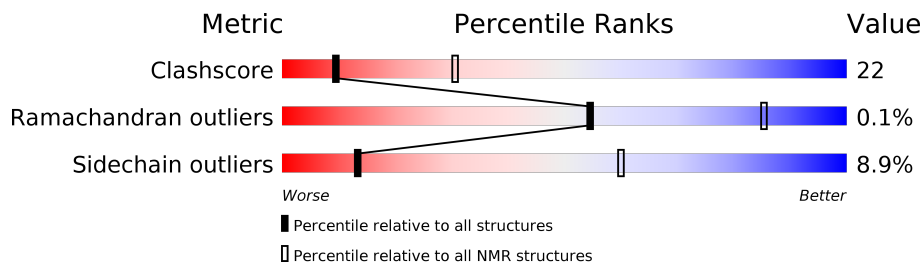
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 45%.

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  $\geq 3$ , 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	36	
2	B	12	

## 2 Ensemble composition and analysis i

This entry contains 40 models. Model 25 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:230-A:265, B:206-B:215 (46)	0.31	25

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 6 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 7, 9, 10, 14, 21, 23, 25, 27, 30, 32, 38
2	4, 5, 13, 15, 19, 22, 28, 33
3	8, 11, 17, 24, 29, 31, 37
4	20, 34, 35
5	3, 16
6	18, 36
Single-model clusters	12; 26; 39; 40

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 761 atoms, of which 366 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Yorkie homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	36	571	187	275	49	59	1	0

- Molecule 2 is a protein called Smad7 derived peptide.

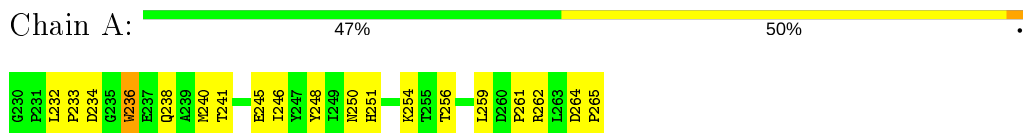
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	12	190	64	91	15	19	1	0

## 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: Yorkie homolog



- Molecule 2: Smad7 derived peptide

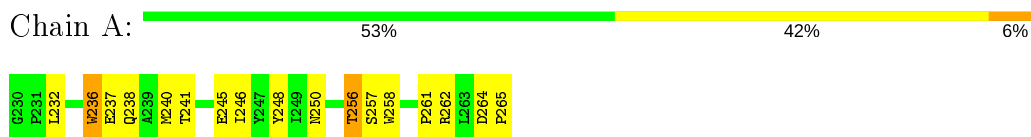


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Yorkie homolog

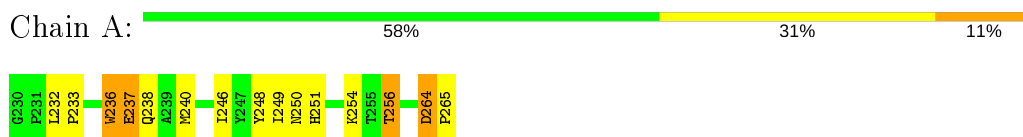


- Molecule 2: Smad7 derived peptide



### 4.2.2 Score per residue for model 2

- Molecule 1: Yorkie homolog

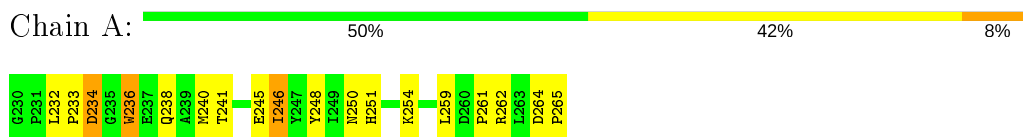


- Molecule 2: Smad7 derived peptide



### 4.2.3 Score per residue for model 3

- Molecule 1: Yorkie homolog

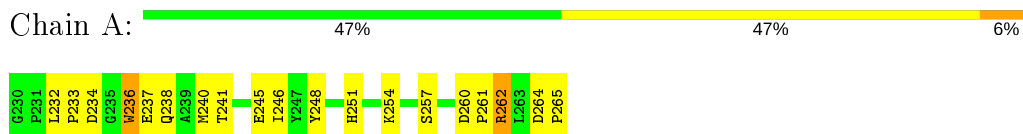


- Molecule 2: Smad7 derived peptide



### 4.2.4 Score per residue for model 4

- Molecule 1: Yorkie homolog

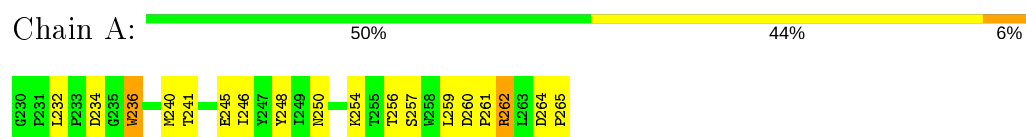


- Molecule 2: Smad7 derived peptide



### 4.2.5 Score per residue for model 5

- Molecule 1: Yorkie homolog

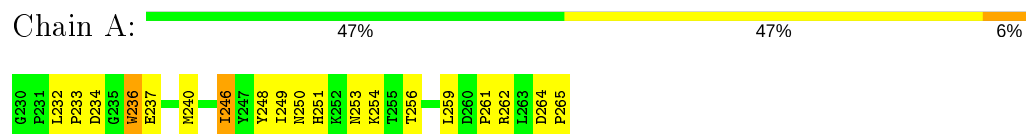


- Molecule 2: Smad7 derived peptide

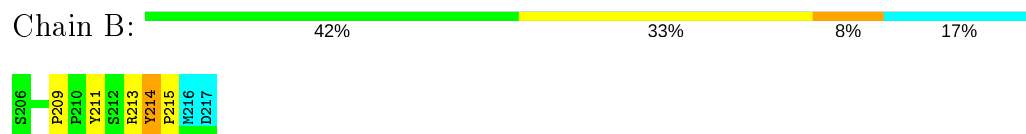


### 4.2.6 Score per residue for model 6

- Molecule 1: Yorkie homolog

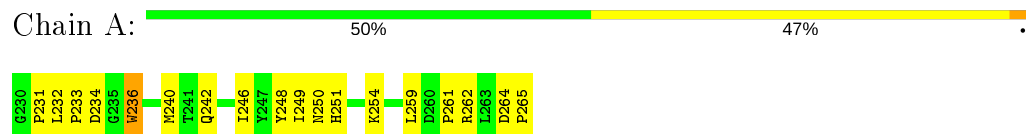


- Molecule 2: Smad7 derived peptide



### 4.2.7 Score per residue for model 7

- Molecule 1: Yorkie homolog

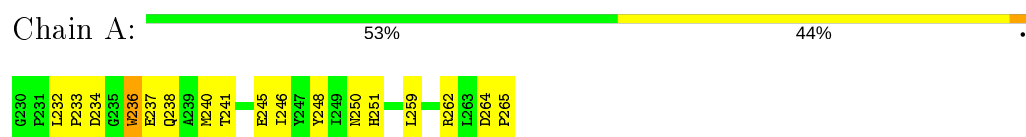


- Molecule 2: Smad7 derived peptide

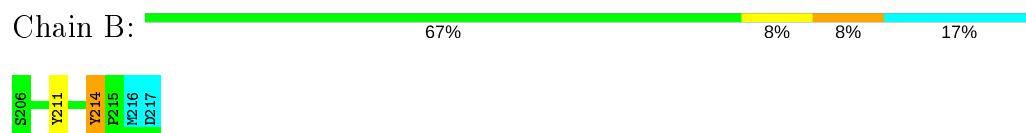


### 4.2.8 Score per residue for model 8

- Molecule 1: Yorkie homolog

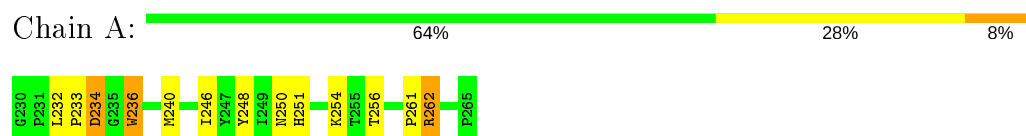


- Molecule 2: Smad7 derived peptide

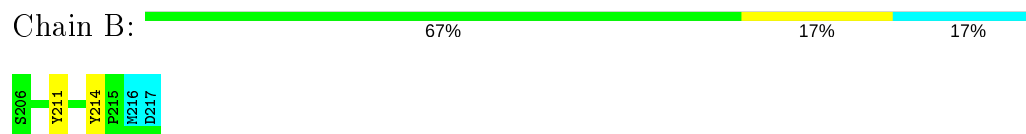


### 4.2.9 Score per residue for model 9

- Molecule 1: Yorkie homolog

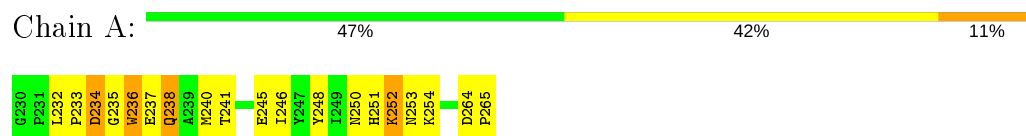


- Molecule 2: Smad7 derived peptide

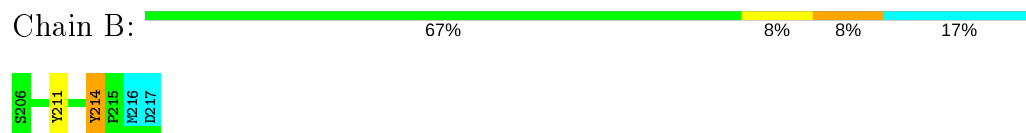


### 4.2.10 Score per residue for model 10

- Molecule 1: Yorkie homolog



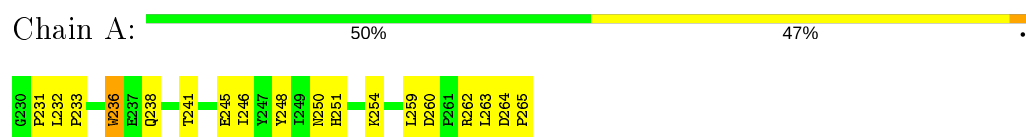
- Molecule 2: Smad7 derived peptide





### 4.2.11 Score per residue for model 11

- Molecule 1: Yorkie homolog

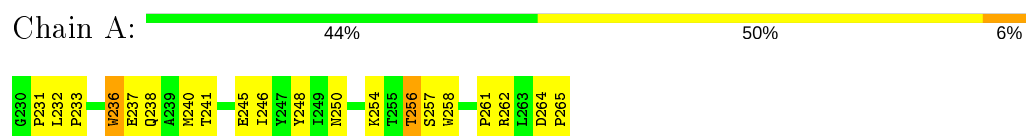


- Molecule 2: Smad7 derived peptide



### 4.2.12 Score per residue for model 12

- Molecule 1: Yorkie homolog

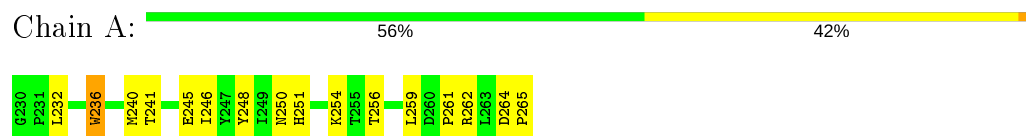


- Molecule 2: Smad7 derived peptide



### 4.2.13 Score per residue for model 13

- Molecule 1: Yorkie homolog

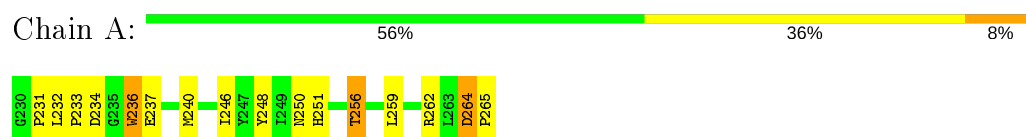


- Molecule 2: Smad7 derived peptide



#### 4.2.14 Score per residue for model 14

- Molecule 1: Yorkie homolog

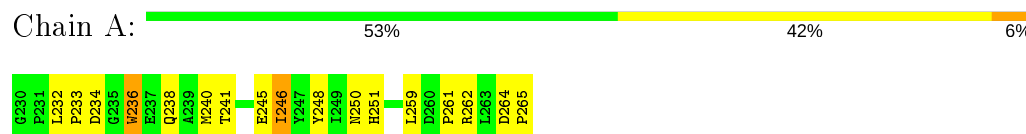


- Molecule 2: Smad7 derived peptide



#### 4.2.15 Score per residue for model 15

- Molecule 1: Yorkie homolog



- Molecule 2: Smad7 derived peptide



#### 4.2.16 Score per residue for model 16

- Molecule 1: Yorkie homolog

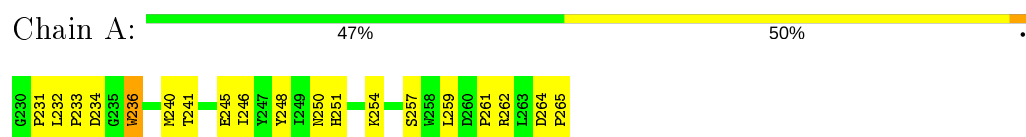


- Molecule 2: Smad7 derived peptide

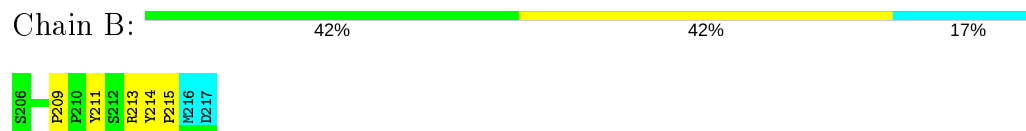


### 4.2.17 Score per residue for model 17

- Molecule 1: Yorkie homolog

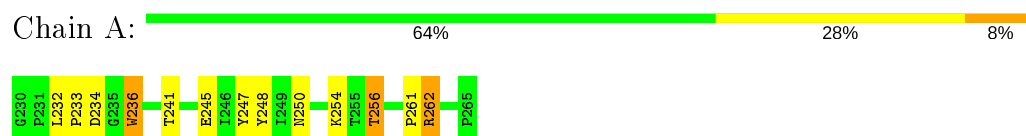


- Molecule 2: Smad7 derived peptide

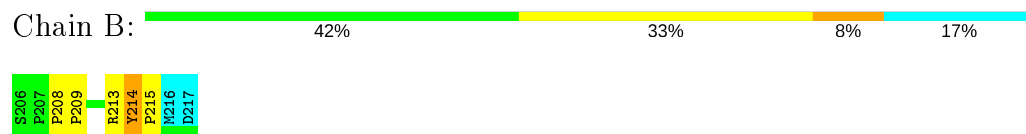


### 4.2.18 Score per residue for model 18

- Molecule 1: Yorkie homolog

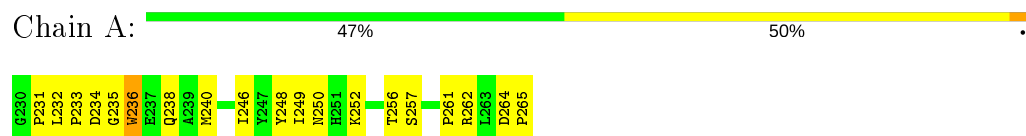


- Molecule 2: Smad7 derived peptide

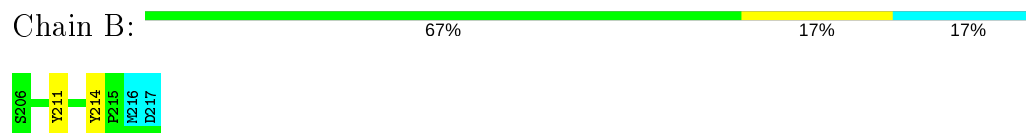


### 4.2.19 Score per residue for model 19

- Molecule 1: Yorkie homolog

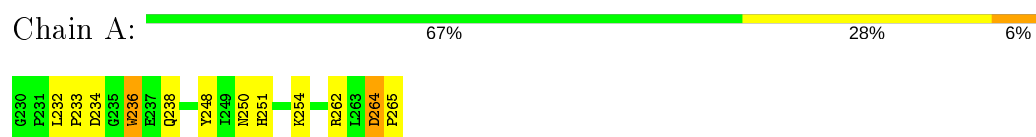


- Molecule 2: Smad7 derived peptide

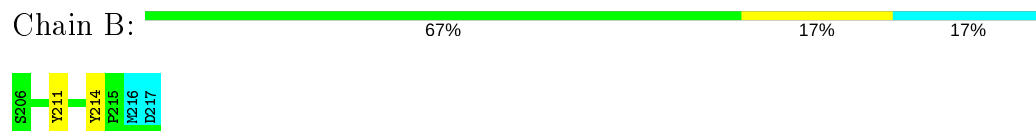


#### 4.2.20 Score per residue for model 20

- Molecule 1: Yorkie homolog

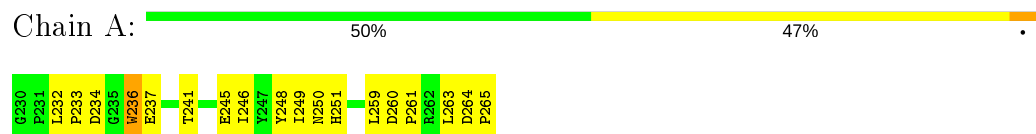


- Molecule 2: Smad7 derived peptide



#### 4.2.21 Score per residue for model 21

- Molecule 1: Yorkie homolog

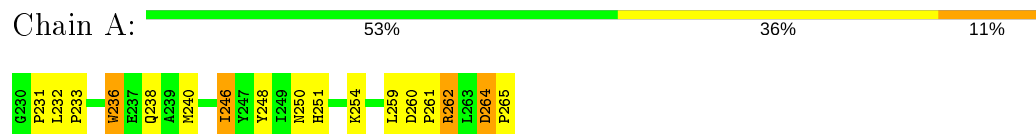


- Molecule 2: Smad7 derived peptide

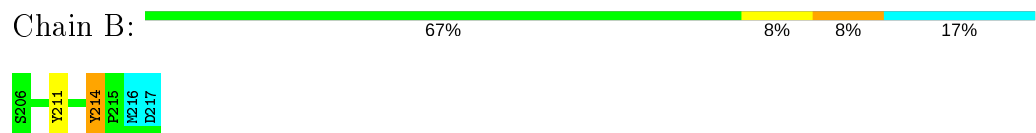


#### 4.2.22 Score per residue for model 22

- Molecule 1: Yorkie homolog

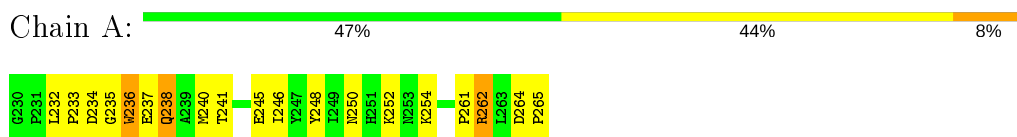


- Molecule 2: Smad7 derived peptide



### 4.2.23 Score per residue for model 23

- Molecule 1: Yorkie homolog

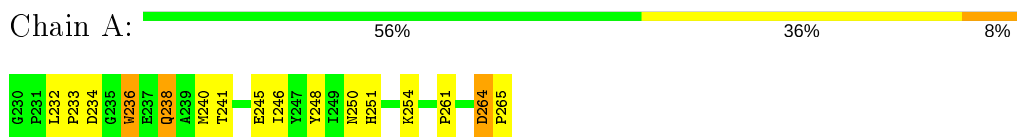


- Molecule 2: Smad7 derived peptide

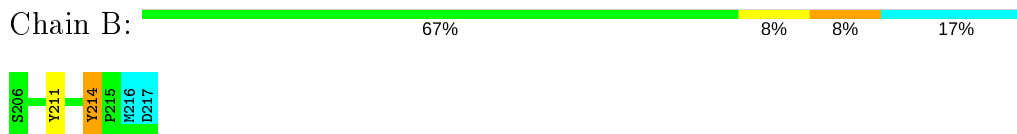


### 4.2.24 Score per residue for model 24

- Molecule 1: Yorkie homolog

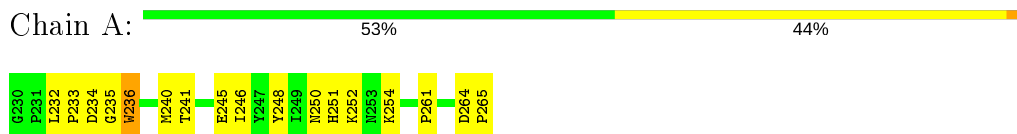


- Molecule 2: Smad7 derived peptide



### 4.2.25 Score per residue for model 25 (medoid)

- Molecule 1: Yorkie homolog

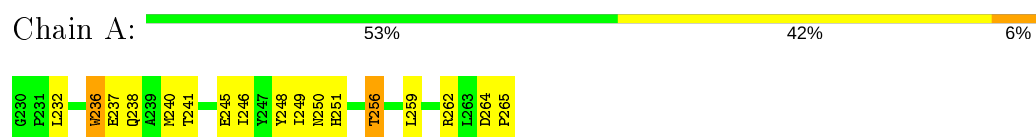


- Molecule 2: Smad7 derived peptide



#### 4.2.26 Score per residue for model 26

- Molecule 1: Yorkie homolog

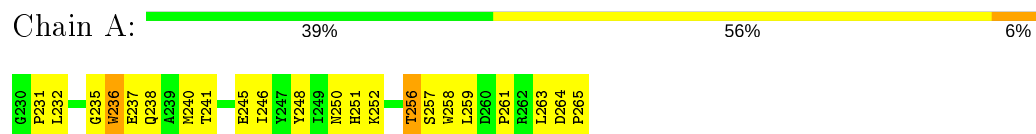


- Molecule 2: Smad7 derived peptide



#### 4.2.27 Score per residue for model 27

- Molecule 1: Yorkie homolog

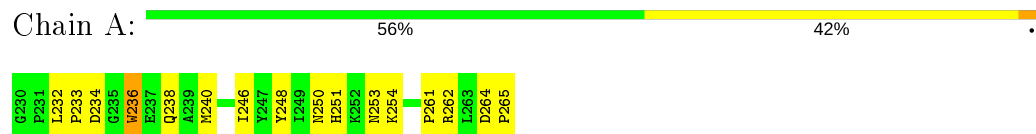


- Molecule 2: Smad7 derived peptide

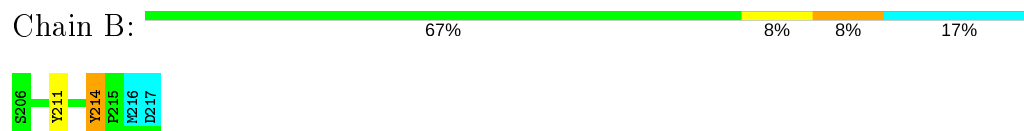


#### 4.2.28 Score per residue for model 28

- Molecule 1: Yorkie homolog

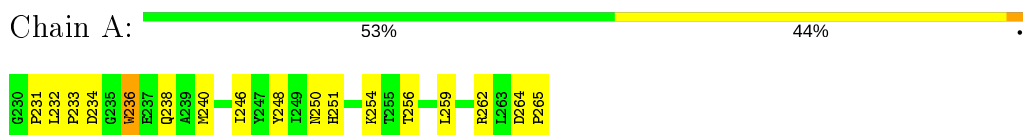


- Molecule 2: Smad7 derived peptide



#### 4.2.29 Score per residue for model 29

- Molecule 1: Yorkie homolog

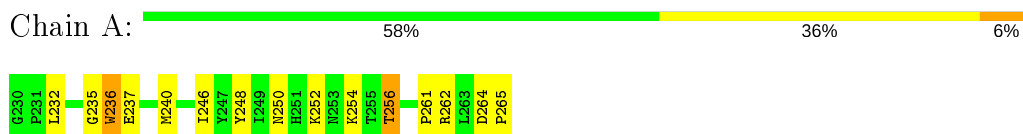


- Molecule 2: Smad7 derived peptide



#### 4.2.30 Score per residue for model 30

- Molecule 1: Yorkie homolog

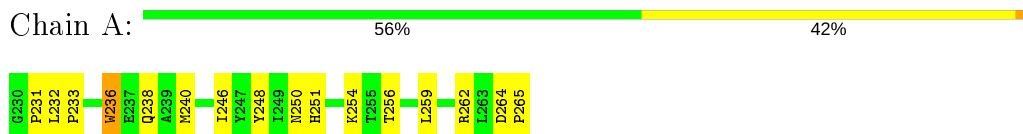


- Molecule 2: Smad7 derived peptide

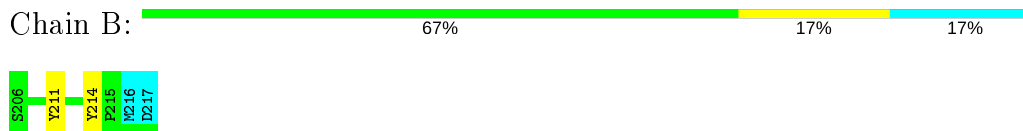


#### 4.2.31 Score per residue for model 31

- Molecule 1: Yorkie homolog

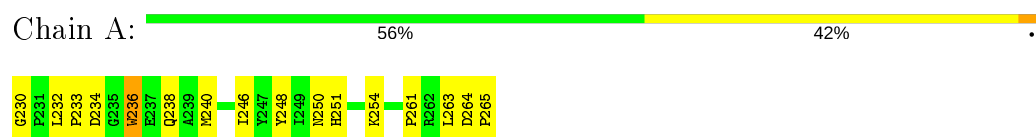


- Molecule 2: Smad7 derived peptide



### 4.2.32 Score per residue for model 32

- Molecule 1: Yorkie homolog



- Molecule 2: Smad7 derived peptide

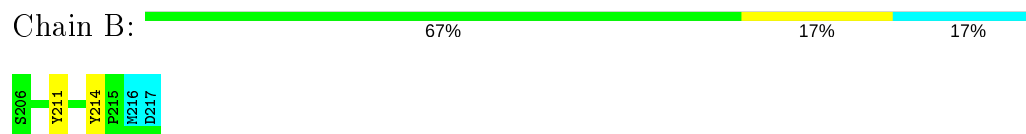


### 4.2.33 Score per residue for model 33

- Molecule 1: Yorkie homolog

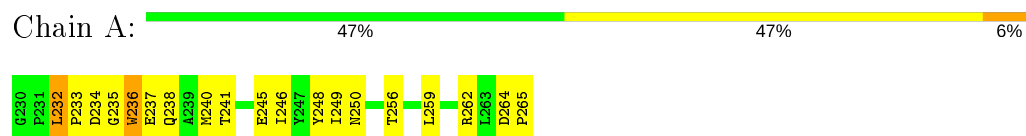


- Molecule 2: Smad7 derived peptide



### 4.2.34 Score per residue for model 34

- Molecule 1: Yorkie homolog



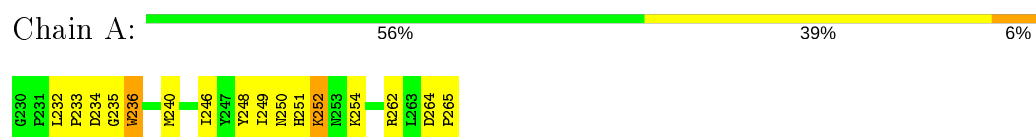
- Molecule 2: Smad7 derived peptide





### 4.2.35 Score per residue for model 35

- Molecule 1: Yorkie homolog

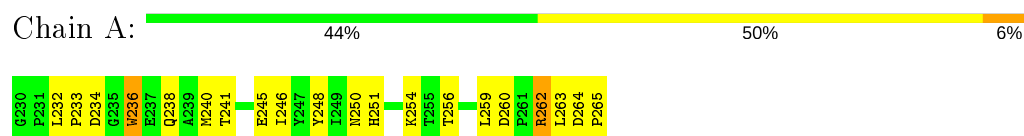


- Molecule 2: Smad7 derived peptide



### 4.2.36 Score per residue for model 36

- Molecule 1: Yorkie homolog

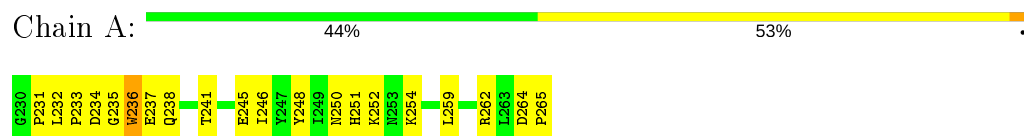


- Molecule 2: Smad7 derived peptide



### 4.2.37 Score per residue for model 37

- Molecule 1: Yorkie homolog

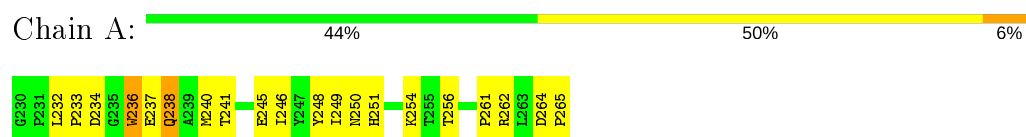


- Molecule 2: Smad7 derived peptide



### 4.2.38 Score per residue for model 38

- Molecule 1: Yorkie homolog

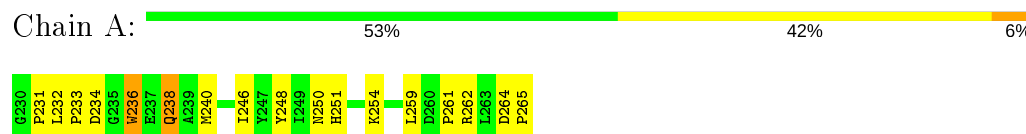


- Molecule 2: Smad7 derived peptide

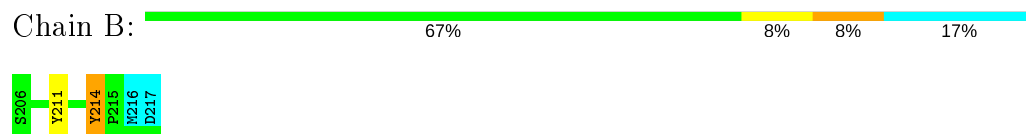


### 4.2.39 Score per residue for model 39

- Molecule 1: Yorkie homolog



- Molecule 2: Smad7 derived peptide



### 4.2.40 Score per residue for model 40

- Molecule 1: Yorkie homolog



- Molecule 2: Smad7 derived peptide



## 5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 40 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
CNSSOLVE	structure solution	
CNSSOLVE	refinement	

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)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	279
Number of shifts mapped to atoms	279
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

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	296	275	271	14±3
2	B	82	78	75	4±2
All	All	15120	14120	13840	648

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:ILE:HB	2:B:211:TYR:HD1	0.92	1.25	38	7
1:A:240:MET:HG3	1:A:246:ILE:HG22	0.80	1.54	28	8
1:A:233:PRO:HD2	1:A:236:TRP:HE1	0.78	1.37	29	18
1:A:256:THR:HB	2:B:208:PRO:HB2	0.77	1.56	30	8
1:A:249:ILE:HB	2:B:211:TYR:CD1	0.75	2.14	38	8
1:A:240:MET:HG2	1:A:246:ILE:HG22	0.74	1.58	10	25
1:A:232:LEU:HG	1:A:248:TYR:CE1	0.71	2.20	34	12
1:A:246:ILE:HD11	1:A:259:LEU:HD23	0.71	1.60	39	1
1:A:254:LYS:HG3	2:B:211:TYR:CD2	0.71	2.21	38	8
1:A:238:GLN:HE21	1:A:246:ILE:HG13	0.68	1.48	3	1
2:B:209:PRO:HG3	2:B:215:PRO:HG3	0.67	1.65	18	2
1:A:236:TRP:HB2	1:A:248:TYR:HB3	0.66	1.65	16	13
1:A:254:LYS:HG3	2:B:211:TYR:HD2	0.66	1.51	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:ILE:HD11	1:A:259:LEU:HD21	0.65	1.67	6	18
1:A:235:GLY:HA2	1:A:252:LYS:HD3	0.64	1.70	27	7
2:B:213:ARG:HA	2:B:213:ARG:HE	0.64	1.53	36	1
1:A:236:TRP:CE3	1:A:250:ASN:HB2	0.63	2.29	11	39
1:A:233:PRO:HD2	1:A:236:TRP:NE1	0.63	2.08	29	13
1:A:231:PRO:HD2	1:A:263:LEU:HD21	0.61	1.72	27	1
1:A:238:GLN:HB2	1:A:248:TYR:CE1	0.61	2.31	16	7
1:A:231:PRO:O	1:A:262:ARG:HD2	0.60	1.96	39	2
1:A:260:ASP:OD1	1:A:262:ARG:HG3	0.60	1.97	5	4
1:A:238:GLN:HB2	1:A:248:TYR:CZ	0.60	2.32	4	15
1:A:262:ARG:O	1:A:262:ARG:HD2	0.58	1.98	36	2
1:A:232:LEU:HG	1:A:248:TYR:CE2	0.58	2.34	23	28
1:A:254:LYS:HG3	2:B:211:TYR:CE2	0.57	2.34	11	10
2:B:214:TYR:CD1	2:B:214:TYR:N	0.57	2.68	3	22
1:A:237:GLU:HB3	1:A:251:HIS:NE2	0.57	2.15	38	1
1:A:231:PRO:O	1:A:262:ARG:HD3	0.57	1.99	11	4
1:A:251:HIS:HA	2:B:211:TYR:CZ	0.56	2.35	38	2
1:A:233:PRO:O	1:A:234:ASP:HB2	0.56	2.00	20	28
1:A:237:GLU:HB2	1:A:251:HIS:NE2	0.55	2.17	2	1
2:B:214:TYR:N	2:B:214:TYR:CD1	0.55	2.73	7	18
2:B:213:ARG:HG3	2:B:214:TYR:H	0.55	1.62	18	20
2:B:213:ARG:HA	2:B:213:ARG:NE	0.55	2.17	25	2
1:A:251:HIS:HA	2:B:211:TYR:OH	0.55	2.02	15	29
1:A:254:LYS:NZ	1:A:254:LYS:HB3	0.54	2.17	18	1
1:A:232:LEU:HD21	1:A:248:TYR:OH	0.54	2.01	20	11
1:A:241:THR:HG22	1:A:245:GLU:O	0.54	2.02	13	22
1:A:264:ASP:N	1:A:265:PRO:HD2	0.53	2.19	34	38
1:A:246:ILE:H	1:A:246:ILE:HD13	0.52	1.64	3	2
1:A:254:LYS:HA	2:B:211:TYR:CE2	0.52	2.40	23	14
1:A:236:TRP:HB3	1:A:250:ASN:HA	0.52	1.82	13	10
1:A:254:LYS:HG2	2:B:211:TYR:CD2	0.51	2.41	33	1
1:A:262:ARG:HA	1:A:262:ARG:HE	0.51	1.65	20	1
1:A:233:PRO:CD	1:A:236:TRP:HE1	0.51	2.16	29	4
1:A:254:LYS:HA	2:B:211:TYR:CE1	0.50	2.42	30	1
1:A:262:ARG:HH21	1:A:265:PRO:HG3	0.50	1.65	3	2
1:A:256:THR:HG21	2:B:209:PRO:O	0.50	2.07	38	3
1:A:232:LEU:CD1	1:A:261:PRO:HD2	0.49	2.38	13	25
1:A:231:PRO:O	1:A:262:ARG:HG2	0.48	2.08	14	3
1:A:238:GLN:NE2	1:A:246:ILE:HG13	0.48	2.23	22	2
1:A:250:ASN:ND2	1:A:253:ASN:HB2	0.48	2.24	6	1
1:A:236:TRP:CE2	1:A:261:PRO:HG3	0.48	2.43	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:LYS:HB3	1:A:254:LYS:NZ	0.48	2.23	37	1
1:A:262:ARG:NE	1:A:262:ARG:HA	0.47	2.25	30	2
1:A:262:ARG:HA	1:A:262:ARG:NE	0.46	2.24	20	3
1:A:235:GLY:HA2	1:A:252:LYS:HG3	0.46	1.85	23	1
1:A:238:GLN:HG3	1:A:246:ILE:HB	0.46	1.86	39	1
1:A:235:GLY:O	1:A:250:ASN:HA	0.46	2.10	34	3
1:A:233:PRO:HA	1:A:262:ARG:NH2	0.46	2.25	38	1
2:B:214:TYR:HD1	2:B:214:TYR:N	0.46	2.09	1	2
1:A:232:LEU:HD12	1:A:261:PRO:HD2	0.46	1.86	24	3
1:A:246:ILE:HD13	1:A:246:ILE:H	0.46	1.71	22	2
1:A:262:ARG:HE	1:A:262:ARG:HA	0.46	1.71	30	1
1:A:251:HIS:HA	2:B:211:TYR:CE1	0.45	2.47	38	1
1:A:236:TRP:CZ2	1:A:261:PRO:HG3	0.45	2.46	19	3
1:A:238:GLN:OE1	1:A:246:ILE:HD12	0.45	2.11	33	2
1:A:248:TYR:HB2	1:A:257:SER:O	0.45	2.10	1	8
1:A:236:TRP:HE3	1:A:250:ASN:HB2	0.45	1.70	5	2
1:A:232:LEU:HG	1:A:248:TYR:HE2	0.44	1.71	1	21
1:A:254:LYS:HG3	2:B:211:TYR:HE2	0.44	1.72	22	2
1:A:238:GLN:HB2	1:A:248:TYR:CE2	0.44	2.48	3	2
1:A:254:LYS:O	1:A:254:LYS:HG2	0.44	2.13	39	1
1:A:256:THR:HG23	2:B:211:TYR:HB2	0.44	1.90	26	1
1:A:247:TYR:OH	2:B:214:TYR:HB3	0.44	2.13	18	1
1:A:262:ARG:O	1:A:265:PRO:HD2	0.43	2.13	34	1
1:A:238:GLN:OE1	1:A:246:ILE:HG13	0.43	2.13	15	1
1:A:260:ASP:OD2	1:A:263:LEU:HG	0.43	2.14	11	2
2:B:213:ARG:CA	2:B:213:ARG:HE	0.43	2.23	36	1
1:A:238:GLN:CD	1:A:246:ILE:HB	0.43	2.34	27	1
2:B:213:ARG:HG3	2:B:214:TYR:N	0.43	2.28	3	3
1:A:262:ARG:HD3	1:A:262:ARG:O	0.43	2.13	23	2
1:A:256:THR:CG2	2:B:208:PRO:HB2	0.43	2.44	13	2
1:A:254:LYS:HA	2:B:211:TYR:CD2	0.43	2.48	38	3
1:A:230:GLY:HA3	1:A:263:LEU:HD21	0.43	1.91	32	1
2:B:209:PRO:CB	2:B:215:PRO:HG3	0.43	2.44	23	3
1:A:236:TRP:CD1	1:A:236:TRP:N	0.43	2.87	17	5
1:A:232:LEU:CG	1:A:248:TYR:CE1	0.42	3.00	16	3
1:A:238:GLN:OE1	1:A:246:ILE:HB	0.42	2.14	27	1
1:A:262:ARG:HD3	1:A:262:ARG:C	0.42	2.35	18	1
1:A:245:GLU:HB3	1:A:258:TRP:CZ3	0.42	2.50	12	1
1:A:260:ASP:CG	1:A:263:LEU:HG	0.42	2.35	21	1
1:A:240:MET:SD	1:A:246:ILE:HG22	0.42	2.54	35	1
1:A:236:TRP:HA	1:A:249:ILE:O	0.42	2.15	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:248:TYR:HB2	1:A:257:SER:OG	0.42	2.15	16	1
1:A:246:ILE:O	1:A:258:TRP:HE3	0.42	1.98	27	2
1:A:236:TRP:N	1:A:236:TRP:CD1	0.42	2.87	24	2
1:A:231:PRO:HD2	1:A:262:ARG:HH21	0.41	1.75	19	1
1:A:246:ILE:HD11	1:A:259:LEU:CD2	0.41	2.45	15	3
1:A:236:TRP:HB3	1:A:250:ASN:CA	0.41	2.43	11	2
1:A:264:ASP:N	1:A:265:PRO:CD	0.41	2.83	2	2
1:A:259:LEU:HA	1:A:259:LEU:HD23	0.41	1.80	5	1
1:A:232:LEU:HG	1:A:248:TYR:HE1	0.40	1.75	12	1
1:A:259:LEU:HD23	1:A:259:LEU:HA	0.40	1.79	13	1
1:A:254:LYS:HG2	2:B:211:TYR:HD2	0.40	1.77	33	1
2:B:207:PRO:HA	2:B:208:PRO:HD3	0.40	1.82	37	1
1:A:254:LYS:HG2	1:A:254:LYS:O	0.40	2.16	20	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	34/36 (94%)	32±1 (94±2%)	2±1 (6±2%)	0±0 (0±0%)	100	100
2	B	9/12 (75%)	9±0 (96±5%)	0±0 (4±5%)	0±0 (0±2%)	44	80
All	All	1720/1920 (90%)	1619 (94%)	100 (6%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	215	PRO	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	32/32 (100%)	29±1 (91±4%)	3±1 (9±4%)	13	59
2	B	10/12 (83%)	9±1 (92±8%)	1±1 (8±8%)	14	61
All	All	1680/1760 (95%)	1530 (91%)	150 (9%)	13	60

All 16 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	236	TRP	40
2	B	214	TYR	24
1	A	237	GLU	17
1	A	256	THR	16
1	A	262	ARG	14
1	A	238	GLN	10
2	B	213	ARG	7
1	A	264	ASP	5
1	A	234	ASP	4
1	A	246	ILE	4
1	A	252	LYS	2
1	A	253	ASN	2
2	B	211	TYR	2
1	A	232	LEU	1
1	A	231	PRO	1
2	B	212	SER	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 carbohydrates 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](#)

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 44% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *Smad*

#### 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	37
Number of shifts mapped to atoms	37
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

#### 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 8%, i.e. 44 atoms were assigned a chemical shift out of a possible 580. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	10/212 (5%)	10/83 (12%)	0/92 (0%)	0/37 (0%)
Sidechain	26/304 (9%)	26/185 (14%)	0/107 (0%)	0/12 (0%)
Aromatic	8/64 (12%)	8/32 (25%)	0/28 (0%)	0/4 (0%)
Overall	44/580 (8%)	44/300 (15%)	0/227 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 44 atoms were assigned a chemical shift out of a possible 602. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	10/222 (5%)	10/87 (11%)	0/96 (0%)	0/39 (0%)
Sidechain	26/316 (8%)	26/192 (14%)	0/112 (0%)	0/12 (0%)
Aromatic	8/64 (12%)	8/32 (25%)	0/28 (0%)	0/4 (0%)
Overall	44/602 (7%)	44/311 (14%)	0/236 (0%)	0/55 (0%)

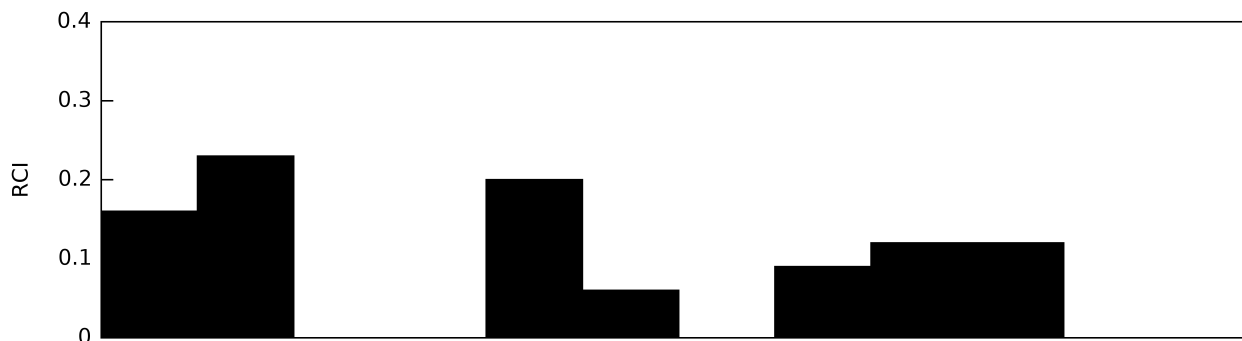
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *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 B:



## 7.2 Chemical shift list 2

File name: input\_cs.cif

Chemical shift list name: YAPWW2

### 7.2.1 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	242
Number of shifts mapped to atoms	242

Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

### 7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 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 38%, i.e. 219 atoms were assigned a chemical shift out of a possible 580. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	68/212 (32%)	68/83 (82%)	0/92 (0%)	0/37 (0%)
Sidechain	129/304 (42%)	129/185 (70%)	0/107 (0%)	0/12 (0%)
Aromatic	22/64 (34%)	22/32 (69%)	0/28 (0%)	0/4 (0%)
Overall	219/580 (38%)	219/300 (73%)	0/227 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 36%, i.e. 219 atoms were assigned a chemical shift out of a possible 602. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	68/222 (31%)	68/87 (78%)	0/96 (0%)	0/39 (0%)
Sidechain	129/316 (41%)	129/192 (67%)	0/112 (0%)	0/12 (0%)
Aromatic	22/64 (34%)	22/32 (69%)	0/28 (0%)	0/4 (0%)
Overall	219/602 (36%)	219/311 (70%)	0/236 (0%)	0/55 (0%)

### 7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	250	ASN	HB3	-0.39	4.41 – 1.11	-9.5
1	A	260	ASP	HA	2.67	6.15 – 3.05	-6.2
1	A	261	PRO	HG3	0.09	3.56 – 0.26	-5.5

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

The image below reports *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:

