



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 02:29 PM EST

PDB ID : 1RW5  
Title : Solution structure of human prolactin  
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Deposited on : 2003-12-16

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:

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 : 2.26  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

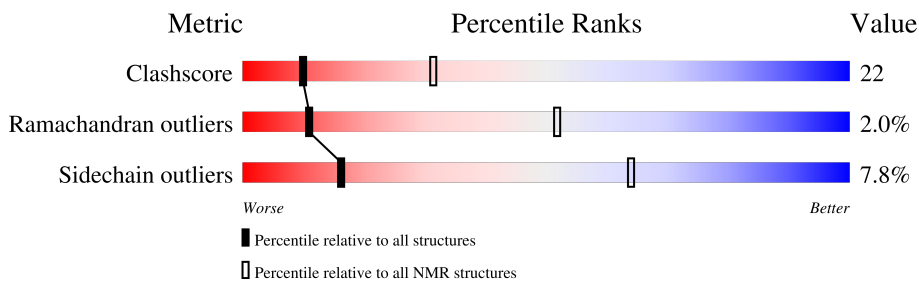
# 1 Overall quality at a glance

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	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	199	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 15 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:14-A:51, A:58-A:67, A:78-A:138, A:146-A:194 (158)	0.34	15

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 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3196 atoms, of which 1590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Prolactin.

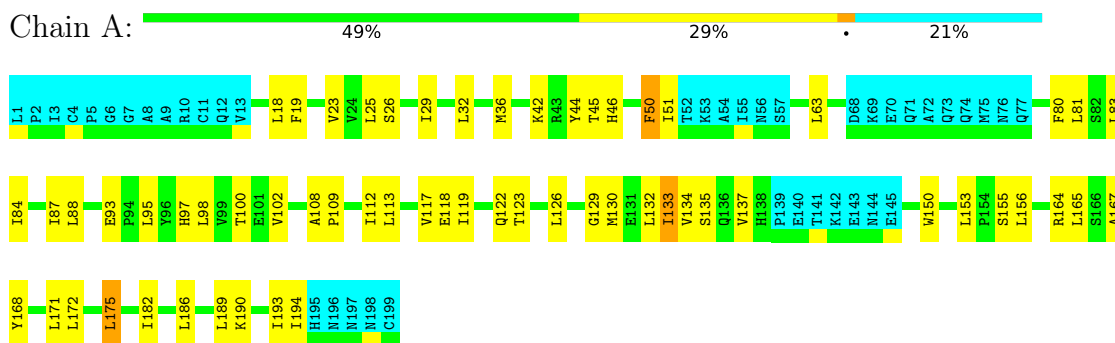
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	199	3196	1008	1590	284	303	11	0

## 4 Residue-property plots

### 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: Prolactin

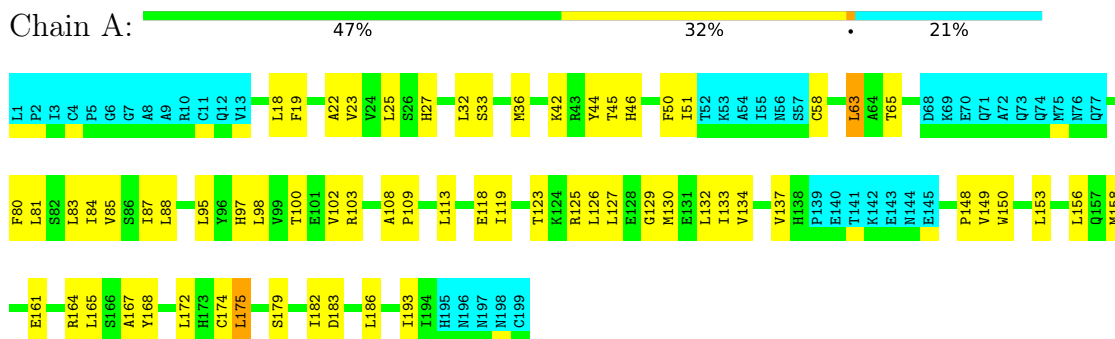


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

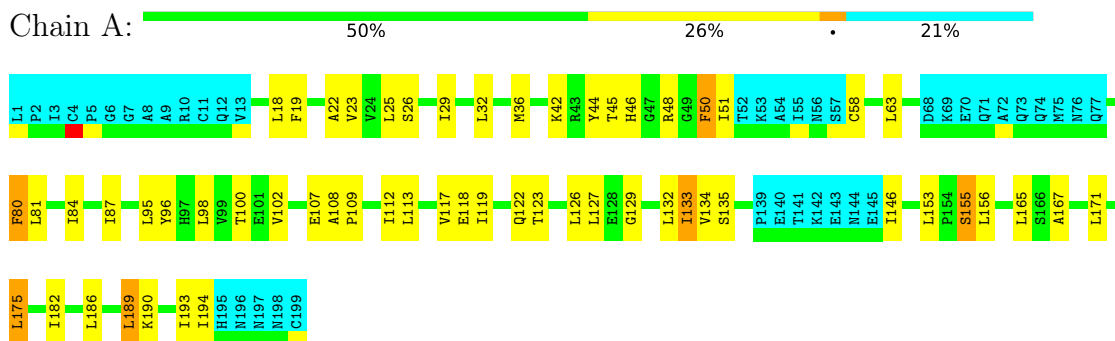
#### 4.2.1 Score per residue for model 1

- Molecule 1: Prolactin



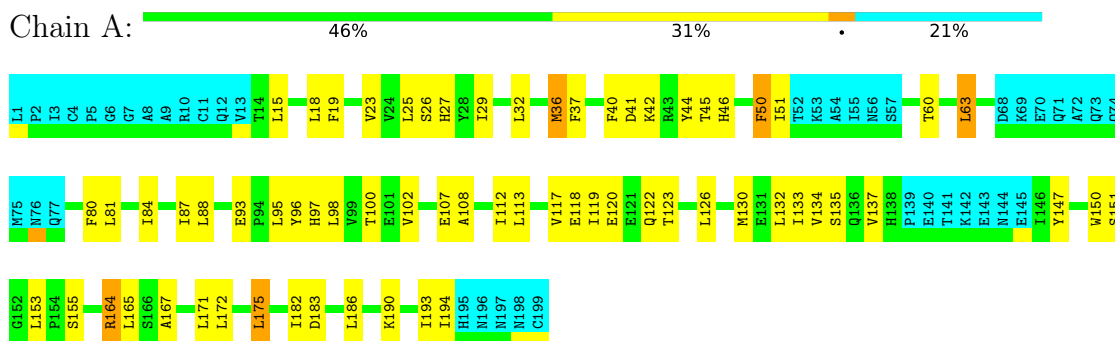
### 4.2.2 Score per residue for model 2

- Molecule 1: Prolactin



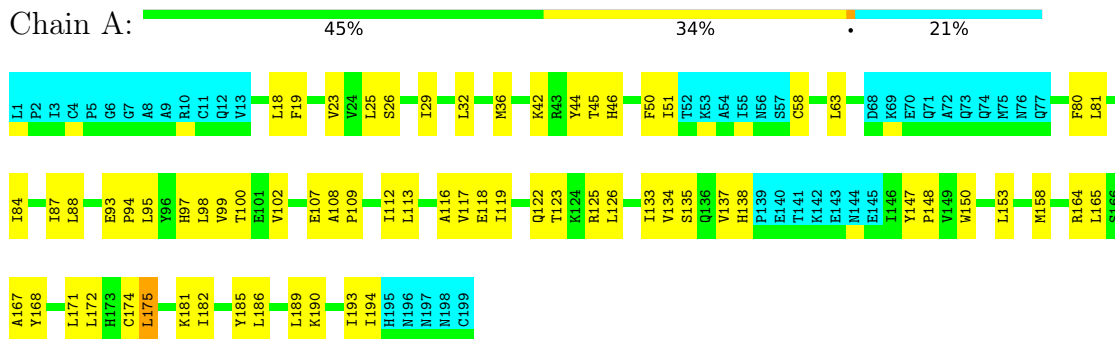
### 4.2.3 Score per residue for model 3

- Molecule 1: Prolactin



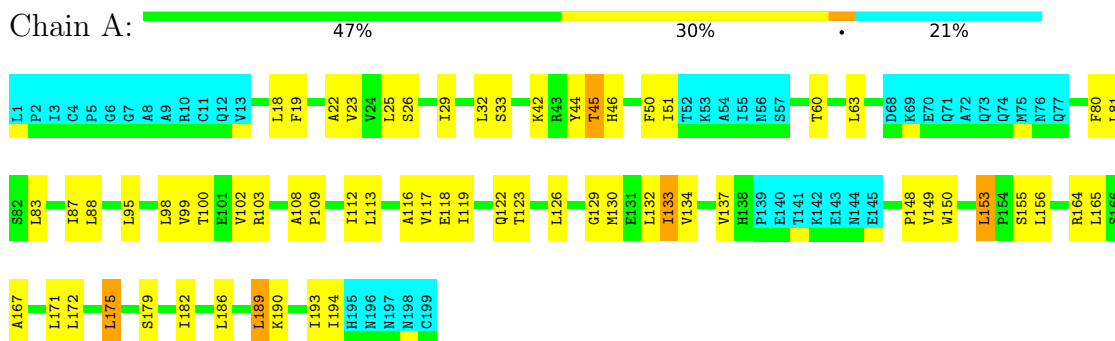
### 4.2.4 Score per residue for model 4

- Molecule 1: Prolactin



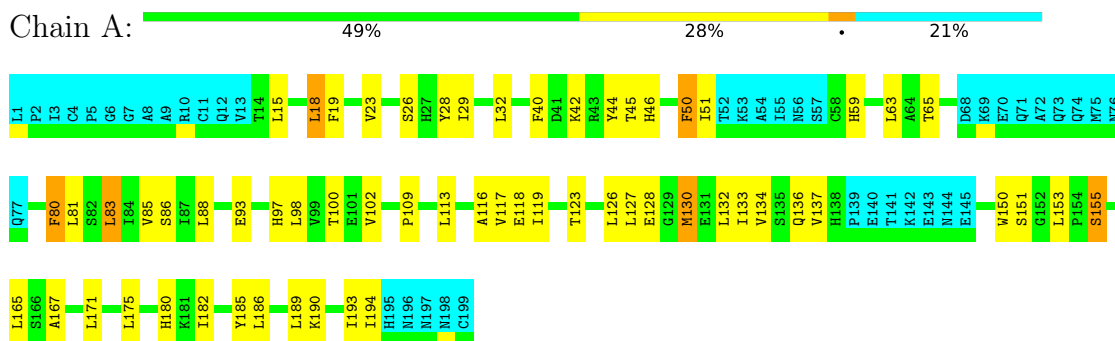
### 4.2.5 Score per residue for model 5

- Molecule 1: Prolactin



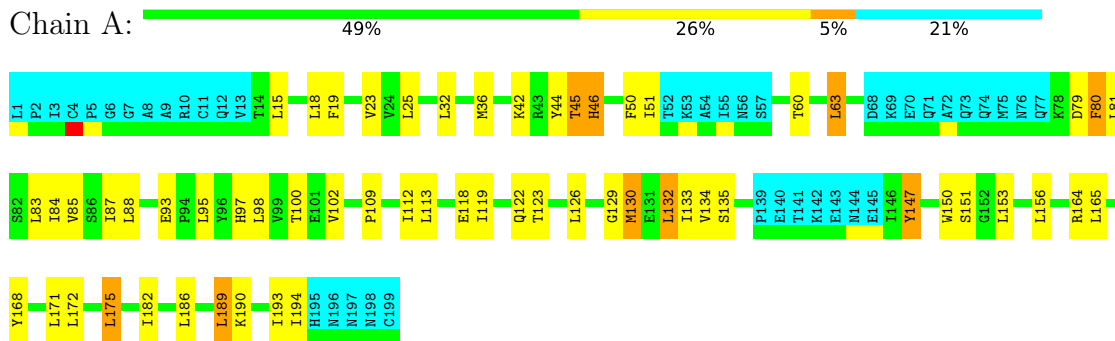
### 4.2.6 Score per residue for model 6

- Molecule 1: Prolactin



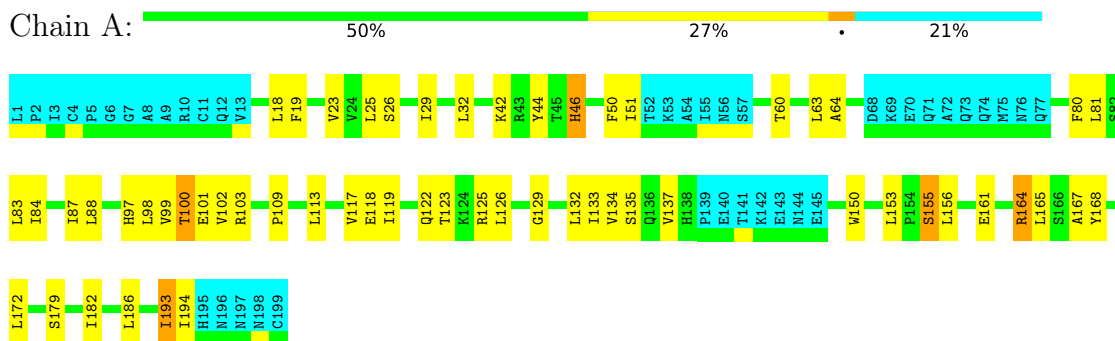
### 4.2.7 Score per residue for model 7

- Molecule 1: Prolactin



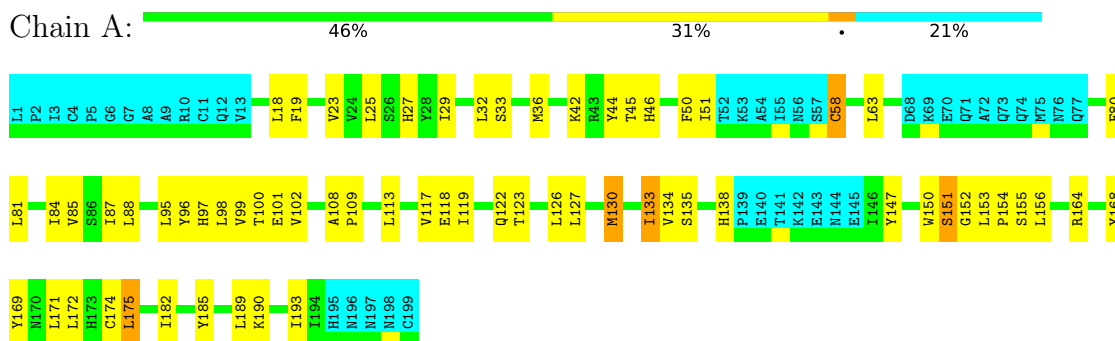
### 4.2.8 Score per residue for model 8

- Molecule 1: Prolactin



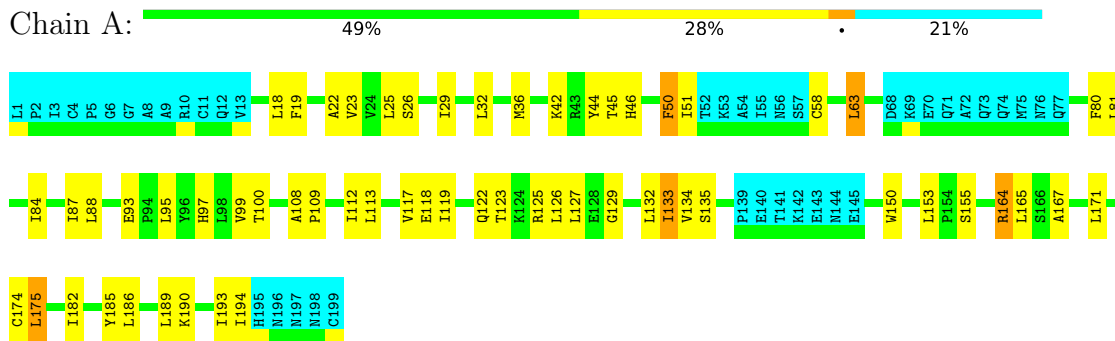
### 4.2.9 Score per residue for model 9

- Molecule 1: Prolactin



### 4.2.10 Score per residue for model 10

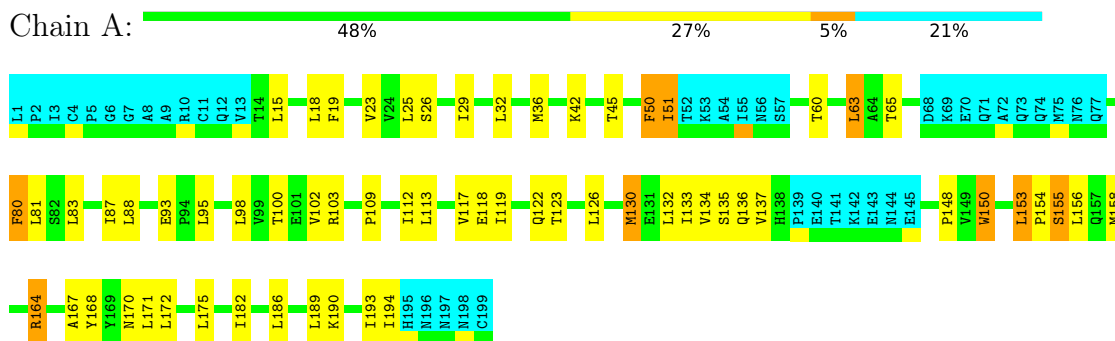
- Molecule 1: Prolactin





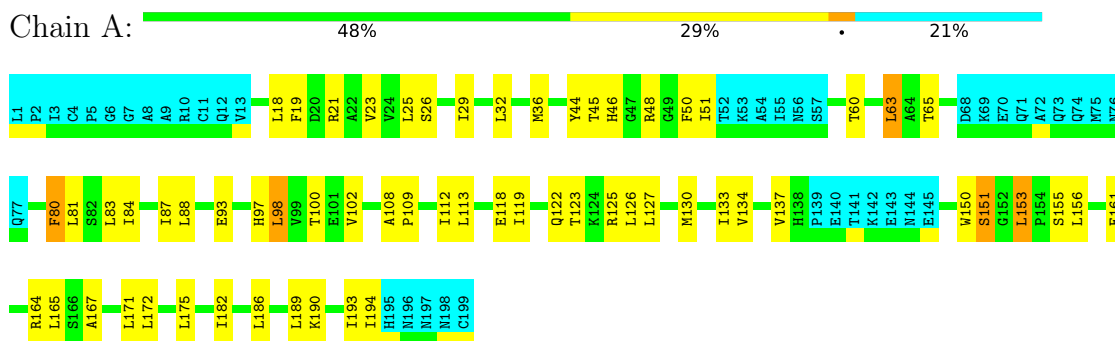
### 4.2.11 Score per residue for model 11

- Molecule 1: Prolactin



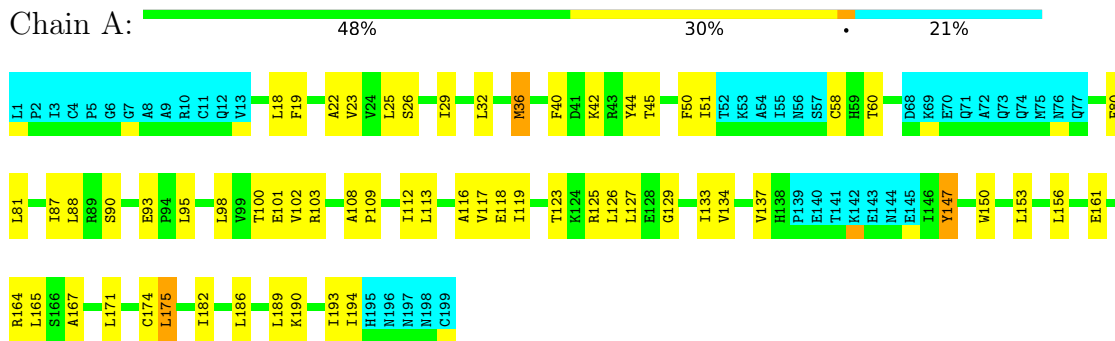
### 4.2.12 Score per residue for model 12

- Molecule 1: Prolactin



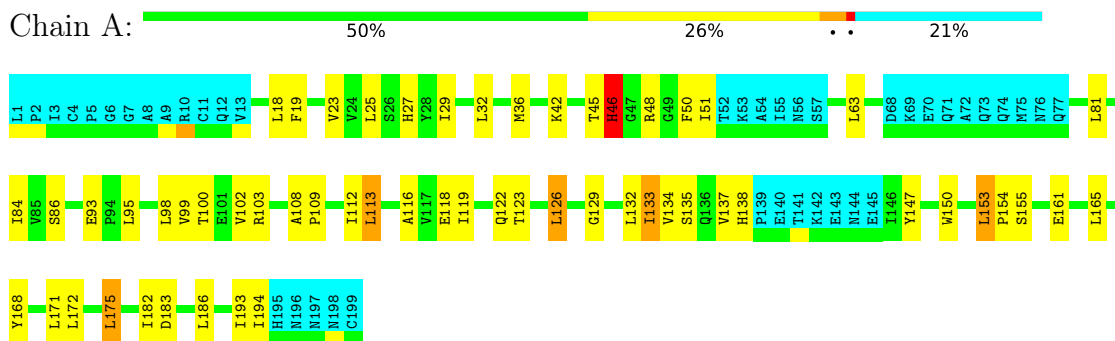
### 4.2.13 Score per residue for model 13

- Molecule 1: Prolactin



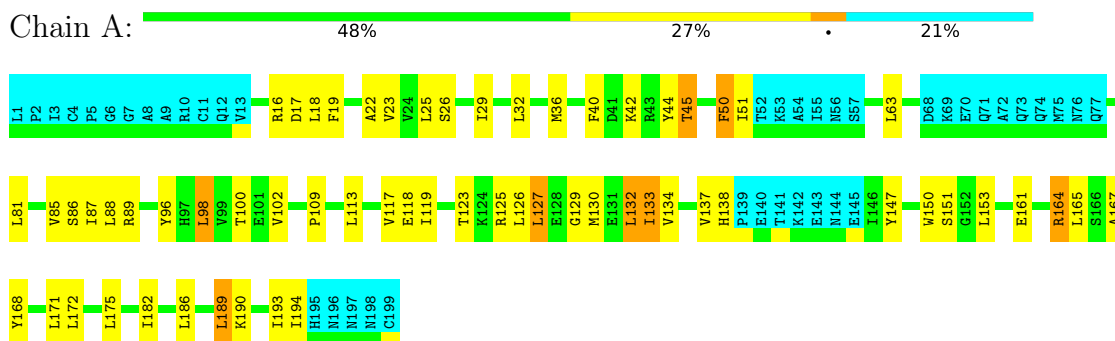
## 4.2.14 Score per residue for model 14

- Molecule 1: Prolactin



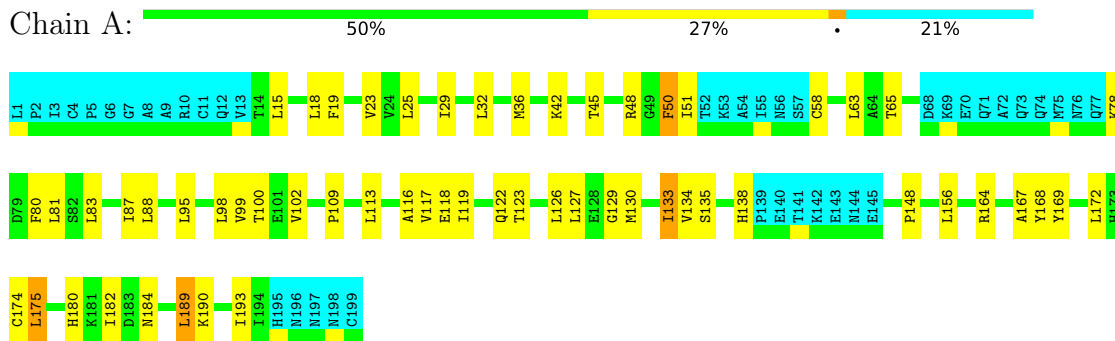
## 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Prolactin



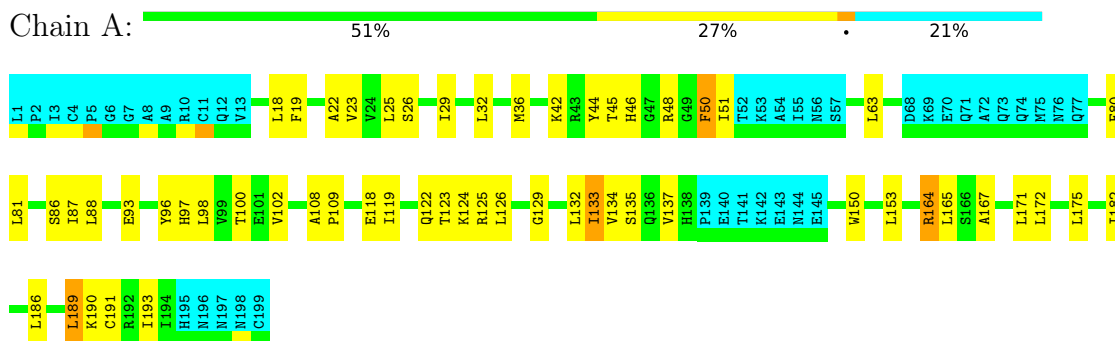
## 4.2.16 Score per residue for model 16

- Molecule 1: Prolactin



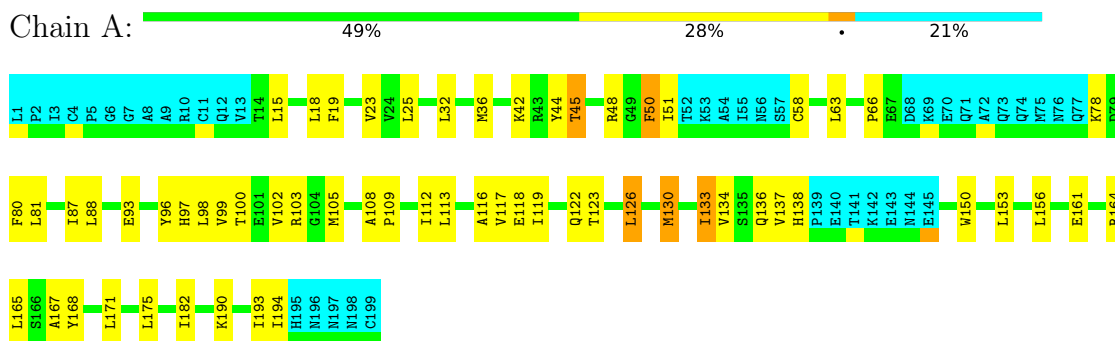
## 4.2.17 Score per residue for model 17

- Molecule 1: Prolactin



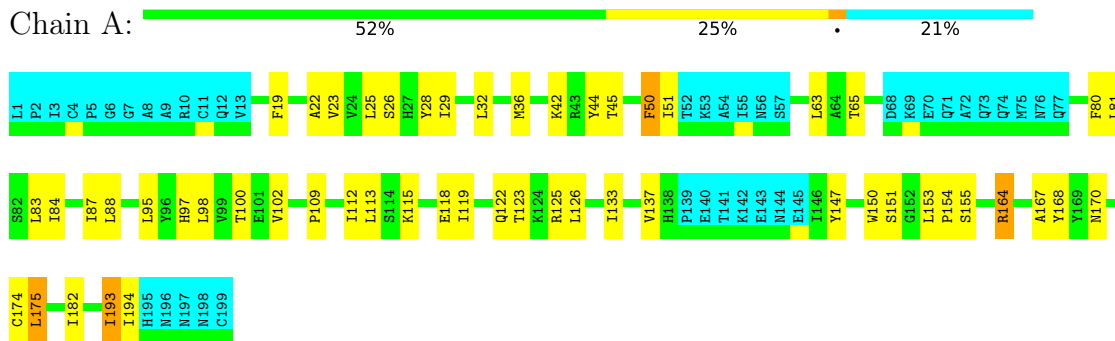
## 4.2.18 Score per residue for model 18

- Molecule 1: Prolactin



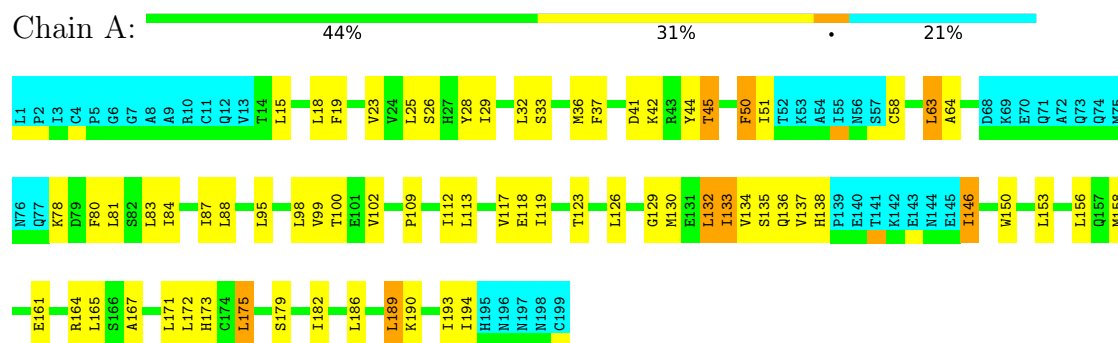
## 4.2.19 Score per residue for model 19

- Molecule 1: Prolactin



## 4.2.20 Score per residue for model 20

## ● Molecule 1: Prolactin



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models are the 20 with the lowest energy of the structures with no restraint violations larger than 0.4 Å, 5 deg, and 1 Hz for noe's, torsion angles and rdc's respectively.*

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

Software name	Classification	Version
CYANA	structure solution	1.0.6
XPLOR-NIH	structure solution	2.9
XPLOR-NIH	refinement	2.9

No chemical shift data was provided.

## 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	1294	1296	1296	56±8
All	All	25880	25920	25920	1127

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:153:LEU:HD11	1:A:171:LEU:HD11	1.06	1.26	15	7
1:A:15:LEU:HD21	1:A:193:ILE:HD11	0.99	1.33	16	1
1:A:45:THR:HG22	1:A:165:LEU:HD13	0.95	1.39	2	3
1:A:65:THR:HG22	1:A:83:LEU:HD13	0.89	1.39	6	1
1:A:153:LEU:HD21	1:A:171:LEU:HD11	0.87	1.47	18	2
1:A:81:LEU:HD21	1:A:189:LEU:HD21	0.87	1.44	6	1
1:A:18:LEU:HD21	1:A:132:LEU:HD13	0.84	1.45	20	1
1:A:153:LEU:HD23	1:A:156:LEU:HD11	0.83	1.48	8	1
1:A:25:LEU:HD11	1:A:122:GLN:NE2	0.82	1.90	16	4
1:A:88:LEU:CD2	1:A:182:ILE:HD13	0.82	2.05	9	12
1:A:18:LEU:HD23	1:A:132:LEU:CD2	0.81	2.05	8	1
1:A:150:TRP:CH2	1:A:153:LEU:HD13	0.79	2.11	12	4
1:A:96:TYR:O	1:A:100:THR:HG23	0.77	1.79	3	6
1:A:85:VAL:HG23	1:A:127:LEU:HD11	0.77	1.56	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:O	1:A:23:VAL:HG23	0.77	1.80	3	16
1:A:129:GLY:O	1:A:133:ILE:HD12	0.76	1.79	10	10
1:A:45:THR:HB	1:A:51:ILE:HD13	0.76	1.57	3	18
1:A:19:PHE:CD2	1:A:193:ILE:HD13	0.76	2.16	3	2
1:A:25:LEU:HD11	1:A:122:GLN:OE1	0.75	1.81	5	8
1:A:19:PHE:CE2	1:A:193:ILE:HG21	0.74	2.17	18	7
1:A:119:ILE:O	1:A:123:THR:HG23	0.74	1.82	4	20
1:A:44:TYR:O	1:A:165:LEU:HD21	0.74	1.82	15	4
1:A:153:LEU:HD12	1:A:171:LEU:CD1	0.74	2.12	5	1
1:A:98:LEU:HD13	1:A:172:LEU:HD21	0.73	1.59	16	8
1:A:129:GLY:O	1:A:132:LEU:HD12	0.72	1.84	20	1
1:A:95:LEU:HD21	1:A:175:LEU:HD11	0.72	1.61	1	13
1:A:161:GLU:O	1:A:165:LEU:HD13	0.72	1.85	18	8
1:A:153:LEU:HD23	1:A:167:ALA:HB1	0.71	1.61	3	3
1:A:19:PHE:CD1	1:A:193:ILE:HD13	0.71	2.20	13	14
1:A:19:PHE:CG	1:A:193:ILE:HD13	0.71	2.21	15	14
1:A:18:LEU:HD21	1:A:132:LEU:CD1	0.71	2.15	20	1
1:A:18:LEU:CD2	1:A:132:LEU:HD22	0.71	2.15	20	1
1:A:88:LEU:HD23	1:A:182:ILE:HD13	0.71	1.63	9	11
1:A:153:LEU:HD12	1:A:156:LEU:CD2	0.70	2.15	9	1
1:A:18:LEU:CD2	1:A:132:LEU:HD13	0.70	2.16	20	1
1:A:88:LEU:HD21	1:A:182:ILE:HG21	0.70	1.60	10	8
1:A:63:LEU:HD21	1:A:148:PRO:HD3	0.70	1.63	5	3
1:A:81:LEU:HD23	1:A:134:VAL:HA	0.69	1.64	9	15
1:A:153:LEU:CD1	1:A:171:LEU:HD11	0.69	2.13	15	6
1:A:87:ILE:HG22	1:A:182:ILE:HD11	0.69	1.63	7	17
1:A:81:LEU:HD11	1:A:189:LEU:HD21	0.69	1.61	20	6
1:A:193:ILE:HG23	1:A:194:ILE:HG12	0.69	1.64	15	1
1:A:126:LEU:HD23	1:A:126:LEU:O	0.69	1.87	16	7
1:A:18:LEU:HD23	1:A:132:LEU:HD21	0.69	1.64	8	1
1:A:50:PHE:CZ	1:A:51:ILE:HG23	0.68	2.23	8	1
1:A:18:LEU:HD21	1:A:132:LEU:HD22	0.68	1.64	20	1
1:A:153:LEU:HD11	1:A:171:LEU:CD1	0.68	2.18	3	5
1:A:98:LEU:HD21	1:A:172:LEU:HD21	0.68	1.65	8	2
1:A:29:ILE:CD1	1:A:126:LEU:HD12	0.68	2.19	19	16
1:A:153:LEU:CD2	1:A:156:LEU:HD11	0.68	2.20	8	1
1:A:25:LEU:HD11	1:A:122:GLN:HG3	0.67	1.66	12	1
1:A:101:GLU:HG3	1:A:156:LEU:HD12	0.67	1.64	8	2
1:A:89:ARG:HG3	1:A:127:LEU:HD21	0.67	1.65	15	1
1:A:84:ILE:HG23	1:A:182:ILE:HG23	0.67	1.67	3	8
1:A:50:PHE:CE1	1:A:51:ILE:HG23	0.67	2.23	15	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE2	1:A:23:VAL:HG21	0.66	2.26	12	13
1:A:45:THR:CB	1:A:51:ILE:HD13	0.65	2.21	1	9
1:A:103:ARG:HA	1:A:113:LEU:HD13	0.65	1.68	14	1
1:A:153:LEU:HD12	1:A:156:LEU:CD1	0.65	2.22	18	1
1:A:25:LEU:HD23	1:A:126:LEU:HG	0.64	1.69	19	13
1:A:153:LEU:HG	1:A:171:LEU:HD11	0.64	1.69	2	2
1:A:85:VAL:HG23	1:A:130:MET:SD	0.64	2.32	7	3
1:A:153:LEU:HD12	1:A:156:LEU:HD11	0.64	1.67	18	1
1:A:25:LEU:HD21	1:A:125:ARG:HB2	0.63	1.69	19	8
1:A:63:LEU:HD23	1:A:86:SER:OG	0.63	1.93	6	1
1:A:137:VAL:HG12	1:A:138:HIS:CD2	0.63	2.28	18	2
1:A:22:ALA:O	1:A:126:LEU:HD21	0.63	1.94	15	8
1:A:81:LEU:HD21	1:A:137:VAL:HG21	0.63	1.69	14	5
1:A:81:LEU:HD11	1:A:137:VAL:HG21	0.63	1.69	1	1
1:A:88:LEU:HD13	1:A:126:LEU:HB3	0.63	1.71	4	5
1:A:153:LEU:CD2	1:A:167:ALA:HB1	0.62	2.24	6	3
1:A:98:LEU:O	1:A:102:VAL:HG23	0.62	1.94	19	19
1:A:36:MET:HG2	1:A:112:ILE:HG23	0.62	1.71	11	10
1:A:179:SER:HA	1:A:182:ILE:HD12	0.62	1.71	1	4
1:A:23:VAL:HA	1:A:186:LEU:HD23	0.62	1.71	14	1
1:A:88:LEU:HB2	1:A:127:LEU:HD21	0.62	1.72	6	3
1:A:130:MET:HA	1:A:133:ILE:HD12	0.62	1.70	11	2
1:A:63:LEU:HD11	1:A:86:SER:CB	0.62	2.25	15	1
1:A:81:LEU:CD2	1:A:189:LEU:HD21	0.62	2.25	6	1
1:A:81:LEU:HD11	1:A:189:LEU:HD11	0.61	1.70	17	2
1:A:81:LEU:HD21	1:A:137:VAL:HG11	0.61	1.72	11	1
1:A:44:TYR:HB3	1:A:165:LEU:HD11	0.61	1.71	18	6
1:A:87:ILE:CG2	1:A:182:ILE:HD11	0.61	2.25	7	6
1:A:36:MET:SD	1:A:172:LEU:HD22	0.61	2.36	17	7
1:A:65:THR:CG2	1:A:83:LEU:HD22	0.61	2.25	11	3
1:A:99:VAL:HG22	1:A:116:ALA:HB1	0.60	1.73	5	5
1:A:26:SER:HA	1:A:126:LEU:HD11	0.60	1.72	12	10
1:A:81:LEU:HD22	1:A:138:HIS:CE1	0.60	2.32	20	2
1:A:133:ILE:O	1:A:137:VAL:HG23	0.60	1.96	3	8
1:A:44:TYR:HB3	1:A:165:LEU:HD21	0.60	1.73	3	3
1:A:153:LEU:HG	1:A:167:ALA:HB1	0.60	1.74	5	1
1:A:15:LEU:HD21	1:A:193:ILE:CD1	0.60	2.20	16	1
1:A:88:LEU:HD11	1:A:182:ILE:HG21	0.60	1.72	19	4
1:A:44:TYR:OH	1:A:108:ALA:HB2	0.59	1.96	9	6
1:A:130:MET:SD	1:A:186:LEU:HD21	0.59	2.37	3	1
1:A:18:LEU:HD12	1:A:19:PHE:N	0.59	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:HD23	1:A:132:LEU:HD22	0.59	1.74	8	1
1:A:81:LEU:CD1	1:A:189:LEU:HD21	0.58	2.28	10	3
1:A:18:LEU:HD21	1:A:132:LEU:CD2	0.58	2.28	20	1
1:A:88:LEU:CG	1:A:182:ILE:HG21	0.58	2.28	4	4
1:A:133:ILE:O	1:A:137:VAL:HG12	0.58	1.98	11	1
1:A:32:LEU:CB	1:A:119:ILE:HD12	0.58	2.28	5	18
1:A:26:SER:OG	1:A:186:LEU:HD12	0.58	1.99	6	3
1:A:88:LEU:HD21	1:A:182:ILE:HD12	0.58	1.76	6	1
1:A:18:LEU:HD13	1:A:132:LEU:HB2	0.58	1.75	7	1
1:A:81:LEU:CD1	1:A:189:LEU:HD11	0.58	2.28	17	2
1:A:98:LEU:HD21	1:A:172:LEU:CD2	0.57	2.28	8	2
1:A:23:VAL:HG22	1:A:186:LEU:HB3	0.57	1.75	2	7
1:A:18:LEU:HD23	1:A:18:LEU:O	0.57	2.00	15	3
1:A:60:THR:O	1:A:63:LEU:HD22	0.57	2.00	11	4
1:A:15:LEU:HD13	1:A:136:GLN:HG3	0.57	1.76	6	2
1:A:32:LEU:HD22	1:A:118:GLU:OE2	0.57	1.99	16	6
1:A:98:LEU:HD13	1:A:172:LEU:CD2	0.57	2.30	16	4
1:A:193:ILE:HG23	1:A:194:ILE:HG13	0.57	1.77	20	1
1:A:23:VAL:HG21	1:A:190:LYS:HE3	0.57	1.75	4	1
1:A:132:LEU:HD12	1:A:133:ILE:N	0.56	2.15	14	2
1:A:50:PHE:CD1	1:A:51:ILE:HG23	0.56	2.36	10	10
1:A:108:ALA:CB	1:A:112:ILE:HD12	0.56	2.31	4	6
1:A:29:ILE:HD11	1:A:126:LEU:HD12	0.56	1.76	15	10
1:A:25:LEU:HD23	1:A:126:LEU:CA	0.56	2.31	7	4
1:A:153:LEU:HD21	1:A:171:LEU:CD1	0.56	2.31	10	3
1:A:153:LEU:HD12	1:A:171:LEU:HD11	0.55	1.78	5	1
1:A:153:LEU:HD11	1:A:167:ALA:HB1	0.55	1.77	20	1
1:A:194:ILE:HG22	1:A:194:ILE:O	0.55	2.02	20	10
1:A:84:ILE:HD12	1:A:130:MET:HE1	0.55	1.77	3	1
1:A:32:LEU:HD13	1:A:118:GLU:HG3	0.55	1.79	9	20
1:A:95:LEU:HD21	1:A:175:LEU:CD1	0.55	2.31	9	8
1:A:88:LEU:CD1	1:A:182:ILE:HG21	0.55	2.32	19	3
1:A:63:LEU:HD21	1:A:86:SER:OG	0.55	2.02	17	1
1:A:164:ARG:O	1:A:167:ALA:HB3	0.54	2.02	11	15
1:A:81:LEU:HB3	1:A:134:VAL:HG23	0.54	1.80	13	2
1:A:63:LEU:HD11	1:A:86:SER:HB3	0.54	1.80	15	1
1:A:101:GLU:OE2	1:A:156:LEU:HD13	0.53	2.03	9	1
1:A:103:ARG:CA	1:A:113:LEU:HD13	0.53	2.32	14	1
1:A:153:LEU:CG	1:A:167:ALA:HB1	0.53	2.34	5	1
1:A:80:PHE:HA	1:A:83:LEU:HD23	0.53	1.81	6	1
1:A:63:LEU:HD11	1:A:86:SER:OG	0.53	2.03	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:CD2	1:A:193:ILE:HD11	0.53	2.23	16	1
1:A:23:VAL:HG22	1:A:186:LEU:HD12	0.53	1.80	10	3
1:A:15:LEU:HD23	1:A:136:GLN:HG2	0.53	1.79	20	1
1:A:45:THR:HG22	1:A:165:LEU:HD22	0.53	1.80	3	3
1:A:45:THR:HB	1:A:51:ILE:HG21	0.52	1.80	7	3
1:A:65:THR:HA	1:A:83:LEU:HD13	0.52	1.81	19	2
1:A:99:VAL:HG21	1:A:117:VAL:HA	0.52	1.81	8	1
1:A:113:LEU:HD23	1:A:113:LEU:O	0.52	2.05	18	12
1:A:25:LEU:HD23	1:A:126:LEU:CB	0.51	2.36	11	2
1:A:25:LEU:HD21	1:A:125:ARG:HB3	0.51	1.82	12	1
1:A:153:LEU:HD12	1:A:156:LEU:HD21	0.51	1.82	9	1
1:A:153:LEU:CG	1:A:171:LEU:HD11	0.51	2.36	2	2
1:A:153:LEU:HD11	1:A:167:ALA:CA	0.51	2.36	1	1
1:A:84:ILE:HD13	1:A:186:LEU:HD21	0.51	1.82	12	3
1:A:99:VAL:HG22	1:A:116:ALA:CB	0.50	2.36	4	1
1:A:153:LEU:HB3	1:A:156:LEU:HD21	0.50	1.83	1	3
1:A:26:SER:CA	1:A:126:LEU:HD11	0.50	2.37	19	9
1:A:153:LEU:HD13	1:A:171:LEU:HD11	0.50	1.84	20	1
1:A:95:LEU:HD13	1:A:119:ILE:HG23	0.50	1.83	3	3
1:A:153:LEU:N	1:A:153:LEU:HD23	0.50	2.20	4	2
1:A:97:HIS:CD2	1:A:150:TRP:CZ3	0.50	3.00	7	9
1:A:150:TRP:CZ3	1:A:153:LEU:HD13	0.50	2.40	12	1
1:A:189:LEU:O	1:A:193:ILE:HG22	0.50	2.07	4	7
1:A:40:PHE:CD1	1:A:44:TYR:CD1	0.50	3.00	15	4
1:A:130:MET:O	1:A:134:VAL:HG12	0.50	2.06	1	1
1:A:97:HIS:CD2	1:A:150:TRP:CH2	0.50	3.00	4	3
1:A:81:LEU:HD12	1:A:81:LEU:N	0.50	2.22	4	7
1:A:190:LYS:HA	1:A:193:ILE:HG22	0.50	1.83	12	15
1:A:113:LEU:C	1:A:113:LEU:HD13	0.49	2.28	4	1
1:A:18:LEU:CD1	1:A:132:LEU:HD22	0.49	2.36	17	4
1:A:79:ASP:OD2	1:A:83:LEU:HD11	0.49	2.07	7	1
1:A:83:LEU:HD11	1:A:185:TYR:CE2	0.49	2.42	6	1
1:A:40:PHE:CE1	1:A:44:TYR:CD1	0.49	3.00	6	3
1:A:185:TYR:O	1:A:189:LEU:HD12	0.49	2.08	10	2
1:A:130:MET:HA	1:A:133:ILE:HD13	0.49	1.85	18	1
1:A:50:PHE:CZ	1:A:165:LEU:HD12	0.49	2.43	7	1
1:A:133:ILE:O	1:A:137:VAL:HG22	0.48	2.08	14	1
1:A:19:PHE:CD2	1:A:194:ILE:HD11	0.48	2.42	20	1
1:A:88:LEU:CD2	1:A:182:ILE:HG21	0.48	2.38	17	2
1:A:88:LEU:HD11	1:A:182:ILE:CG2	0.48	2.38	19	2
1:A:26:SER:HA	1:A:29:ILE:HD12	0.48	1.85	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LEU:HD22	1:A:156:LEU:HD13	0.48	1.85	5	1
1:A:18:LEU:HB2	1:A:132:LEU:HD13	0.48	1.84	7	1
1:A:25:LEU:HD11	1:A:122:GLN:CD	0.48	2.29	10	3
1:A:116:ALA:O	1:A:119:ILE:HG22	0.48	2.09	6	2
1:A:150:TRP:CH2	1:A:153:LEU:HD12	0.48	2.44	7	1
1:A:23:VAL:HA	1:A:186:LEU:HD13	0.48	1.85	13	3
1:A:133:ILE:HG22	1:A:134:VAL:N	0.48	2.23	2	5
1:A:97:HIS:HB3	1:A:156:LEU:HD11	0.48	1.84	7	1
1:A:18:LEU:HD22	1:A:132:LEU:HD21	0.48	1.86	15	1
1:A:19:PHE:CE1	1:A:23:VAL:HG21	0.47	2.44	8	2
1:A:153:LEU:CD1	1:A:171:LEU:HD13	0.47	2.39	11	1
1:A:88:LEU:HD21	1:A:182:ILE:HD13	0.47	1.83	12	3
1:A:133:ILE:O	1:A:137:VAL:HG13	0.47	2.10	14	1
1:A:15:LEU:O	1:A:15:LEU:HD23	0.47	2.10	16	1
1:A:19:PHE:CE2	1:A:23:VAL:CG2	0.47	2.98	5	13
1:A:19:PHE:CE1	1:A:23:VAL:CG2	0.47	2.97	3	4
1:A:60:THR:HG22	1:A:90:SER:CB	0.47	2.39	13	1
1:A:108:ALA:HB1	1:A:112:ILE:HD12	0.47	1.86	4	3
1:A:95:LEU:HD23	1:A:98:LEU:HD12	0.47	1.85	9	2
1:A:65:THR:HG22	1:A:83:LEU:HD22	0.47	1.86	11	1
1:A:81:LEU:HD11	1:A:137:VAL:CG2	0.47	2.40	1	1
1:A:113:LEU:C	1:A:113:LEU:HD23	0.47	2.30	8	9
1:A:113:LEU:HD23	1:A:113:LEU:C	0.47	2.30	20	4
1:A:65:THR:CG2	1:A:83:LEU:HD13	0.47	2.27	6	1
1:A:45:THR:O	1:A:51:ILE:HD11	0.47	2.10	16	2
1:A:50:PHE:CE1	1:A:51:ILE:CG2	0.47	2.98	7	15
1:A:130:MET:O	1:A:130:MET:HE3	0.47	2.10	11	1
1:A:25:LEU:HD23	1:A:126:LEU:HA	0.47	1.87	20	3
1:A:63:LEU:HD21	1:A:148:PRO:CG	0.46	2.40	11	1
1:A:81:LEU:CD2	1:A:137:VAL:HG21	0.46	2.40	14	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.46	2.25	9	4
1:A:134:VAL:HG13	1:A:135:SER:N	0.46	2.25	11	9
1:A:19:PHE:CD2	1:A:194:ILE:HD12	0.46	2.45	14	1
1:A:25:LEU:HD11	1:A:122:GLN:HE21	0.46	1.71	19	1
1:A:19:PHE:HD2	1:A:194:ILE:HD11	0.46	1.70	20	1
1:A:153:LEU:HD22	1:A:153:LEU:N	0.46	2.26	18	1
1:A:85:VAL:HG23	1:A:127:LEU:CD1	0.46	2.34	15	1
1:A:50:PHE:CE2	1:A:51:ILE:CG2	0.46	2.99	3	1
1:A:19:PHE:CZ	1:A:23:VAL:CG2	0.46	2.99	6	5
1:A:32:LEU:HB3	1:A:119:ILE:HD12	0.46	1.88	1	3
1:A:81:LEU:HD13	1:A:134:VAL:HG23	0.46	1.88	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:HD12	1:A:168:TYR:CD1	0.46	2.46	8	1
1:A:19:PHE:CZ	1:A:193:ILE:HG21	0.46	2.45	18	1
1:A:81:LEU:HD22	1:A:138:HIS:HE1	0.46	1.66	20	1
1:A:65:THR:HG23	1:A:83:LEU:HD22	0.46	1.87	1	2
1:A:60:THR:HA	1:A:63:LEU:HD23	0.46	1.88	5	1
1:A:147:TYR:CD1	1:A:147:TYR:N	0.45	2.84	4	2
1:A:81:LEU:HD21	1:A:137:VAL:CG1	0.45	2.39	11	1
1:A:88:LEU:CB	1:A:127:LEU:HD21	0.45	2.41	12	2
1:A:81:LEU:HD21	1:A:137:VAL:CG2	0.45	2.41	14	1
1:A:98:LEU:CD1	1:A:168:TYR:CD1	0.45	3.00	8	1
1:A:33:SER:OG	1:A:119:ILE:HD11	0.45	2.11	5	4
1:A:193:ILE:HG22	1:A:194:ILE:N	0.45	2.27	8	2
1:A:15:LEU:HD23	1:A:136:GLN:OE1	0.45	2.12	11	1
1:A:50:PHE:CZ	1:A:51:ILE:CG2	0.45	2.99	8	3
1:A:168:TYR:CD1	1:A:168:TYR:N	0.45	2.84	18	8
1:A:37:PHE:CD1	1:A:172:LEU:CB	0.45	3.00	20	1
1:A:50:PHE:CG	1:A:51:ILE:N	0.44	2.85	8	1
1:A:132:LEU:HD12	1:A:132:LEU:C	0.44	2.32	14	2
1:A:19:PHE:CD1	1:A:193:ILE:CD1	0.44	3.00	12	3
1:A:45:THR:HG22	1:A:165:LEU:CD2	0.44	2.43	18	1
1:A:87:ILE:HG21	1:A:182:ILE:CG1	0.44	2.42	5	5
1:A:81:LEU:HD23	1:A:130:MET:HE1	0.44	1.89	1	1
1:A:64:ALA:HB3	1:A:83:LEU:HD21	0.44	1.89	8	1
1:A:84:ILE:O	1:A:84:ILE:HG22	0.44	2.12	20	1
1:A:46:HIS:CD2	1:A:46:HIS:N	0.44	2.85	14	1
1:A:45:THR:CG2	1:A:165:LEU:HD22	0.44	2.42	3	1
1:A:103:ARG:HA	1:A:113:LEU:HD12	0.44	1.88	13	3
1:A:63:LEU:N	1:A:63:LEU:HD13	0.44	2.28	11	4
1:A:97:HIS:NE2	1:A:150:TRP:CZ3	0.44	2.86	10	1
1:A:113:LEU:O	1:A:117:VAL:HG13	0.43	2.12	9	1
1:A:18:LEU:HD13	1:A:132:LEU:HD22	0.43	1.88	5	1
1:A:99:VAL:CG2	1:A:116:ALA:HB1	0.43	2.41	4	1
1:A:18:LEU:HG	1:A:132:LEU:HD21	0.43	1.90	6	1
1:A:15:LEU:HA	1:A:18:LEU:HD21	0.43	1.90	7	1
1:A:84:ILE:HD13	1:A:186:LEU:CD2	0.43	2.44	10	1
1:A:96:TYR:O	1:A:99:VAL:HG22	0.43	2.14	9	1
1:A:64:ALA:O	1:A:83:LEU:HD21	0.43	2.13	20	1
1:A:94:PRO:HA	1:A:97:HIS:CD2	0.43	2.49	4	1
1:A:15:LEU:HD23	1:A:15:LEU:C	0.43	2.34	16	1
1:A:19:PHE:CD2	1:A:193:ILE:CD1	0.43	3.02	4	1
1:A:88:LEU:CG	1:A:182:ILE:HD13	0.43	2.44	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE1	1:A:186:LEU:HD13	0.43	2.49	7	1
1:A:153:LEU:HD11	1:A:171:LEU:HD12	0.42	1.89	4	1
1:A:95:LEU:HD22	1:A:119:ILE:CG2	0.42	2.44	11	1
1:A:18:LEU:HD13	1:A:132:LEU:CD2	0.42	2.45	17	2
1:A:105:MET:HG2	1:A:108:ALA:HB3	0.42	1.90	18	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.42	2.83	1	3
1:A:137:VAL:CG1	1:A:138:HIS:CE1	0.42	3.02	20	1
1:A:129:GLY:HA2	1:A:132:LEU:HD21	0.42	1.90	2	1
1:A:63:LEU:HD21	1:A:148:PRO:CD	0.42	2.41	5	1
1:A:103:ARG:N	1:A:113:LEU:HD13	0.42	2.29	11	1
1:A:128:GLU:O	1:A:132:LEU:HD23	0.42	2.15	6	1
1:A:19:PHE:CD2	1:A:193:ILE:HG21	0.42	2.49	15	2
1:A:103:ARG:HG2	1:A:113:LEU:HD11	0.42	1.90	18	1
1:A:81:LEU:CD1	1:A:137:VAL:HG21	0.42	2.42	1	1
1:A:50:PHE:O	1:A:50:PHE:CG	0.42	2.73	11	5
1:A:156:LEU:HD22	1:A:156:LEU:N	0.42	2.29	16	2
1:A:37:PHE:CD1	1:A:172:LEU:HB2	0.42	2.50	20	1
1:A:50:PHE:HE1	1:A:165:LEU:HD12	0.42	1.73	6	2
1:A:117:VAL:HG13	1:A:118:GLU:N	0.42	2.29	2	6
1:A:81:LEU:CD1	1:A:81:LEU:N	0.42	2.83	10	3
1:A:161:GLU:O	1:A:165:LEU:HD22	0.42	2.15	20	1
1:A:99:VAL:HG13	1:A:100:THR:N	0.42	2.30	8	1
1:A:81:LEU:N	1:A:81:LEU:HD22	0.42	2.30	19	1
1:A:19:PHE:CD1	1:A:193:ILE:HG21	0.41	2.49	19	2
1:A:78:LYS:NZ	1:A:138:HIS:CG	0.41	2.88	18	1
1:A:37:PHE:CE1	1:A:41:ASP:OD1	0.41	2.74	20	2
1:A:150:TRP:HE1	1:A:171:LEU:HD21	0.41	1.75	5	1
1:A:18:LEU:HD23	1:A:18:LEU:C	0.41	2.36	15	1
1:A:88:LEU:HD21	1:A:123:THR:O	0.41	2.14	18	1
1:A:88:LEU:HG	1:A:182:ILE:HG21	0.41	1.92	4	1
1:A:81:LEU:N	1:A:81:LEU:CD2	0.41	2.84	19	1
1:A:44:TYR:CD1	1:A:44:TYR:N	0.41	2.88	20	6
1:A:16:ARG:CG	1:A:17:ASP:N	0.41	2.84	15	1
1:A:168:TYR:N	1:A:168:TYR:CD1	0.41	2.86	19	1
1:A:94:PRO:O	1:A:97:HIS:CD2	0.41	2.73	4	1
1:A:81:LEU:HD12	1:A:130:MET:HE3	0.41	1.91	6	1
1:A:46:HIS:CD2	1:A:46:HIS:O	0.41	2.73	7	1
1:A:117:VAL:CG1	1:A:118:GLU:N	0.41	2.84	20	11
1:A:81:LEU:N	1:A:81:LEU:CD1	0.41	2.84	14	4
1:A:96:TYR:CE2	1:A:100:THR:HG21	0.41	2.51	3	1
1:A:85:VAL:CG1	1:A:86:SER:N	0.41	2.84	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:TYR:CZ	1:A:107:GLU:OE1	0.41	2.74	4	1
1:A:134:VAL:CG1	1:A:135:SER:N	0.41	2.84	7	5
1:A:23:VAL:HG13	1:A:186:LEU:HB3	0.41	1.91	5	1
1:A:134:VAL:HA	1:A:137:VAL:HG22	0.41	1.92	6	1
1:A:44:TYR:CB	1:A:165:LEU:HD21	0.41	2.45	7	1
1:A:88:LEU:CD1	1:A:126:LEU:HD22	0.41	2.46	7	1
1:A:156:LEU:N	1:A:156:LEU:CD2	0.41	2.84	20	4
1:A:84:ILE:HG22	1:A:88:LEU:HD12	0.41	1.92	9	1
1:A:150:TRP:O	1:A:150:TRP:CG	0.41	2.73	10	1
1:A:98:LEU:HD11	1:A:171:LEU:HD13	0.41	1.92	18	1
1:A:153:LEU:CD1	1:A:156:LEU:HD11	0.41	2.42	18	1
1:A:18:LEU:CD1	1:A:132:LEU:CD2	0.41	2.99	1	2
1:A:27:HIS:CE1	1:A:183:ASP:OD2	0.41	2.74	14	2
1:A:181:LYS:O	1:A:185:TYR:CD2	0.41	2.74	4	1
1:A:63:LEU:N	1:A:63:LEU:CD2	0.41	2.84	15	2
1:A:15:LEU:H	1:A:15:LEU:HD12	0.41	1.76	20	1
1:A:27:HIS:CD2	1:A:183:ASP:OD2	0.40	2.74	1	1
1:A:113:LEU:CD2	1:A:117:VAL:CG1	0.40	2.99	3	1
1:A:103:ARG:CA	1:A:113:LEU:HD12	0.40	2.46	5	1
1:A:186:LEU:N	1:A:186:LEU:CD2	0.40	2.84	11	2
1:A:81:LEU:HD21	1:A:189:LEU:CD2	0.40	2.32	6	1
1:A:150:TRP:HH2	1:A:153:LEU:HD12	0.40	1.76	7	1
1:A:18:LEU:N	1:A:18:LEU:CD2	0.40	2.84	12	2
1:A:46:HIS:O	1:A:46:HIS:CG	0.40	2.74	2	2
1:A:15:LEU:HD12	1:A:15:LEU:H	0.40	1.77	3	1
1:A:119:ILE:CG2	1:A:120:GLU:N	0.40	2.84	3	1
1:A:87:ILE:CG2	1:A:182:ILE:CG1	0.40	3.00	5	1
1:A:129:GLY:HA2	1:A:132:LEU:HD12	0.40	1.93	7	1
1:A:50:PHE:O	1:A:50:PHE:CD2	0.40	2.74	9	1
1:A:153:LEU:N	1:A:154:PRO:CD	0.40	2.85	11	1
1:A:37:PHE:CE2	1:A:41:ASP:OD2	0.40	2.74	20	1
1:A:113:LEU:HD21	1:A:117:VAL:CG1	0.40	2.47	3	1
1:A:19:PHE:CD1	1:A:194:ILE:HD12	0.40	2.51	8	1
1:A:60:THR:CG2	1:A:90:SER:CB	0.40	3.00	13	1
1:A:81:LEU:CD2	1:A:137:VAL:CG2	0.40	3.00	14	1
1:A:28:TYR:CD2	1:A:122:GLN:OE1	0.40	2.75	19	1
1:A:44:TYR:CE2	1:A:107:GLU:OE1	0.40	2.74	3	1
1:A:98:LEU:CD2	1:A:168:TYR:CD1	0.40	3.04	11	1
1:A:180:HIS:CD2	1:A:184:ASN:OD1	0.40	2.75	16	1
1:A:44:TYR:CE1	1:A:107:GLU:OE1	0.40	2.74	2	1
1:A:40:PHE:CE1	1:A:44:TYR:CG	0.40	3.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LEU:HD12	1:A:171:LEU:HD12	0.40	1.88	5	1
1:A:59:HIS:CE1	1:A:151:SER:OG	0.40	2.75	6	1
1:A:83:LEU:C	1:A:83:LEU:HD12	0.40	2.37	6	1
1:A:194:ILE:O	1:A:194:ILE:HG22	0.40	2.17	6	1
1:A:19:PHE:HA	1:A:133:ILE:HD11	0.40	1.94	8	1
1:A:150:TRP:O	1:A:150:TRP:CD1	0.40	2.74	11	1
1:A:21:ARG:NH2	1:A:125:ARG:NH2	0.40	2.70	12	1
1:A:167:ALA:O	1:A:171:LEU:HD12	0.40	2.17	12	1
1:A:19:PHE:CE2	1:A:193:ILE:CG2	0.40	2.99	18	1
1:A:88:LEU:HB2	1:A:182:ILE:HD13	0.40	1.93	18	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	158/199 (79%)	147±2 (93±1%)	8±2 (5±1%)	3±1 (2±1%)	11	52
All	All	3160/3980 (79%)	2932 (93%)	164 (5%)	64 (2%)	11	52

All 12 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	109	PRO	19
1	A	46	HIS	12
1	A	155	SER	11
1	A	158	MET	4
1	A	151	SER	4
1	A	58	CYS	3
1	A	154	PRO	3
1	A	146	ILE	2
1	A	63	LEU	2
1	A	150	TRP	2
1	A	152	GLY	1
1	A	148	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	146/181 (81%)	135±2 (92±1%)	11±2 (8±1%)	16 64
All	All	2920/3620 (81%)	2693 (92%)	227 (8%)	16 64

All 43 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	42	LYS	19
1	A	175	LEU	19
1	A	80	PHE	17
1	A	100	THR	14
1	A	133	ILE	12
1	A	50	PHE	11
1	A	93	GLU	11
1	A	189	LEU	10
1	A	130	MET	10
1	A	164	ARG	9
1	A	63	LEU	7
1	A	174	CYS	7
1	A	58	CYS	7
1	A	48	ARG	6
1	A	127	LEU	5
1	A	132	LEU	5
1	A	147	TYR	5
1	A	45	THR	5
1	A	193	ILE	4
1	A	155	SER	4
1	A	18	LEU	4
1	A	153	LEU	4
1	A	151	SER	4
1	A	138	HIS	3
1	A	149	VAL	2
1	A	36	MET	2
1	A	28	TYR	2
1	A	99	VAL	2
1	A	98	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	126	LEU	2
1	A	83	LEU	1
1	A	180	HIS	1
1	A	60	THR	1
1	A	27	HIS	1
1	A	51	ILE	1
1	A	156	LEU	1
1	A	46	HIS	1
1	A	113	LEU	1
1	A	78	LYS	1
1	A	124	LYS	1
1	A	191	CYS	1
1	A	190	LYS	1
1	A	115	LYS	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

No chemical shift data were provided