



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 3, 2021 – 10:05 AM EST

PDB ID : 6U1L  
Title : Structure of two-domain translational regulator Yih1 reveals a possible mechanism of action  
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Deposited on : 2019-08-16

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	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

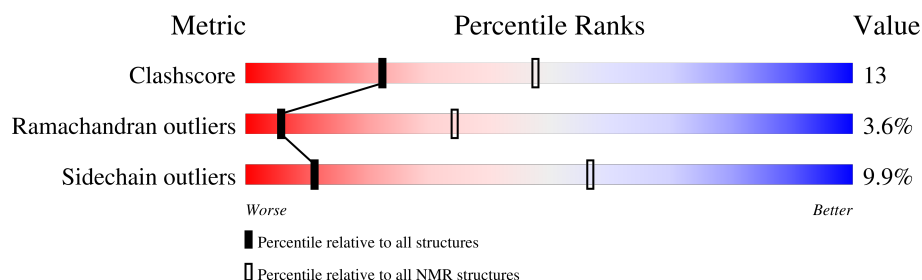
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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	258	<div> <div>55%</div> <div>33%</div> <div>• 10%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:68, A:76-A:93, A:97-A:112 (99)	0.52	1
2	A:126-A:258 (133)	0.58	6

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

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

The models can be grouped into 1 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 8, 9, 10
Single-model clusters	4; 5; 7

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3995 atoms, of which 1955 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein IMPACT homolog.

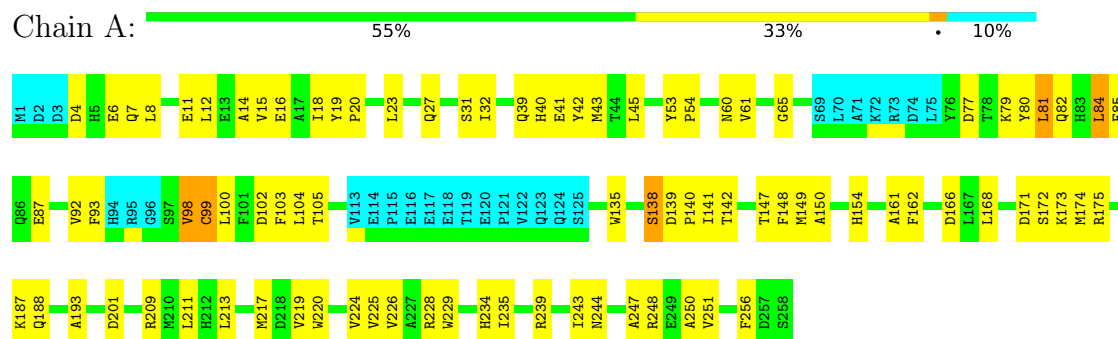
Mol	Chain	Residues	Atoms						Trace
1	A	258	Total	C	H	N	O	S	0
			3995	1286	1955	337	406	11	

## 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: Protein IMPACT homolog

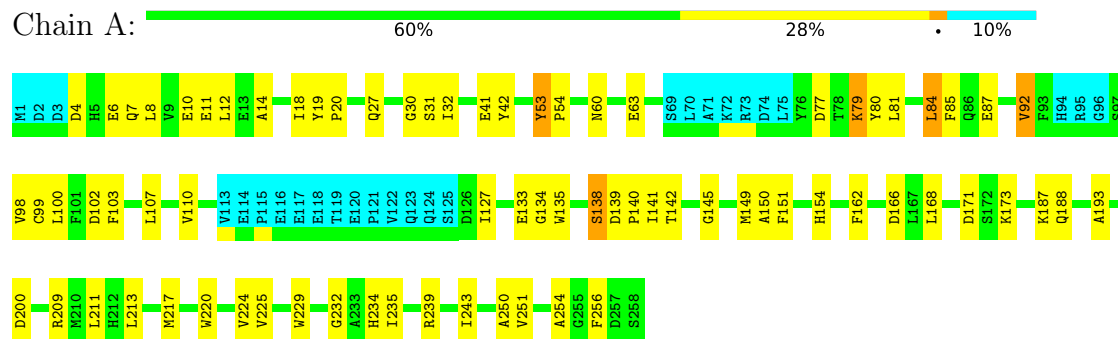


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

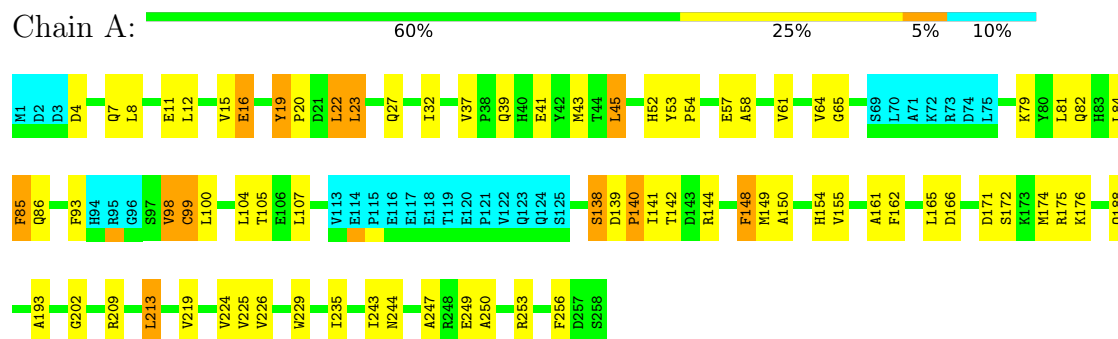
#### 4.2.1 Score per residue for model 1

- Molecule 1: Protein IMPACT homolog



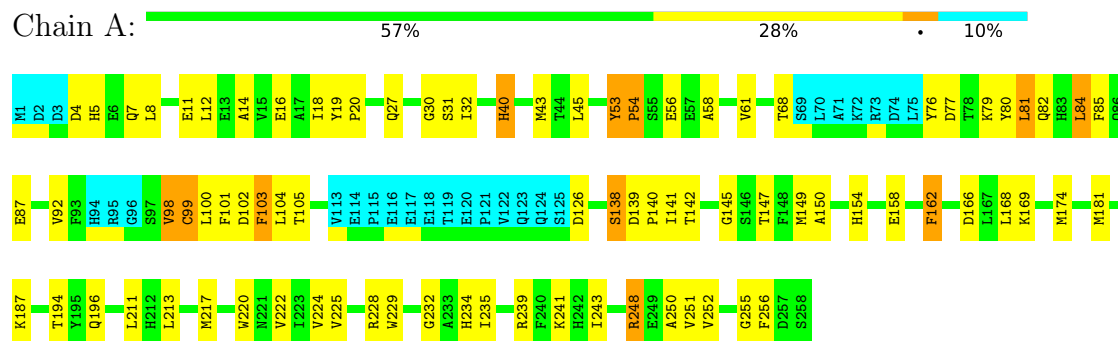
## 4.2.2 Score per residue for model 2

- Molecule 1: Protein IMPACT homolog



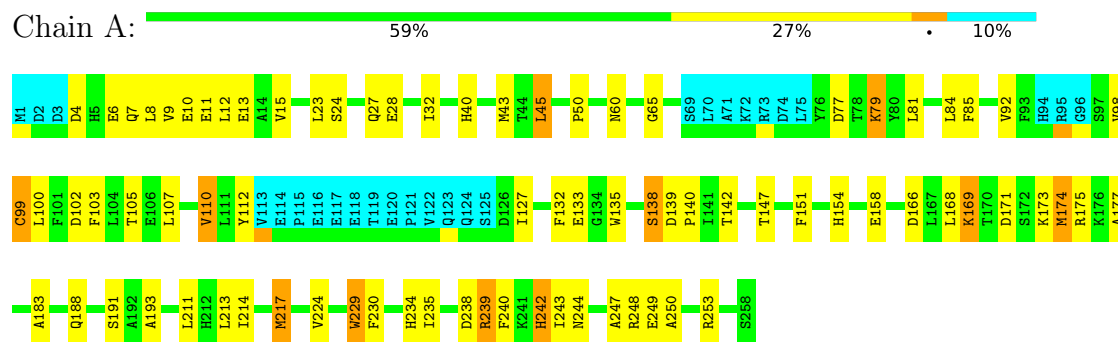
## 4.2.3 Score per residue for model 3

- Molecule 1: Protein IMPACT homolog



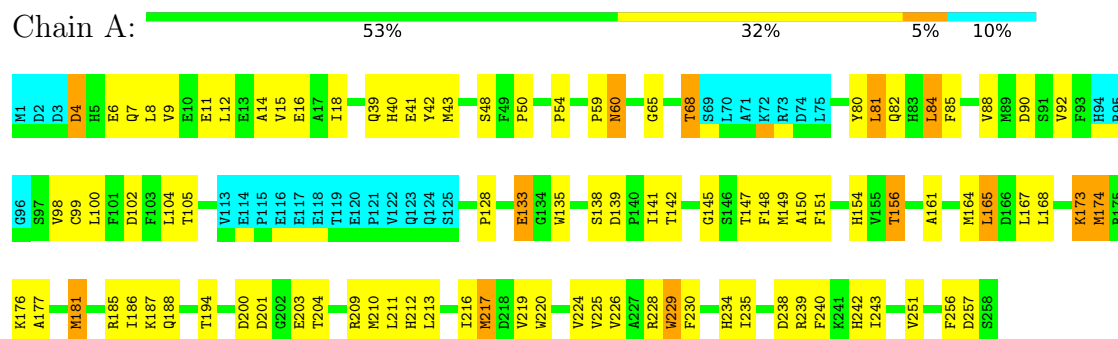
## 4.2.4 Score per residue for model 4

- Molecule 1: Protein IMPACT homolog



### 4.2.5 Score per residue for model 5

- Molecule 1: Protein IMPACT homolog



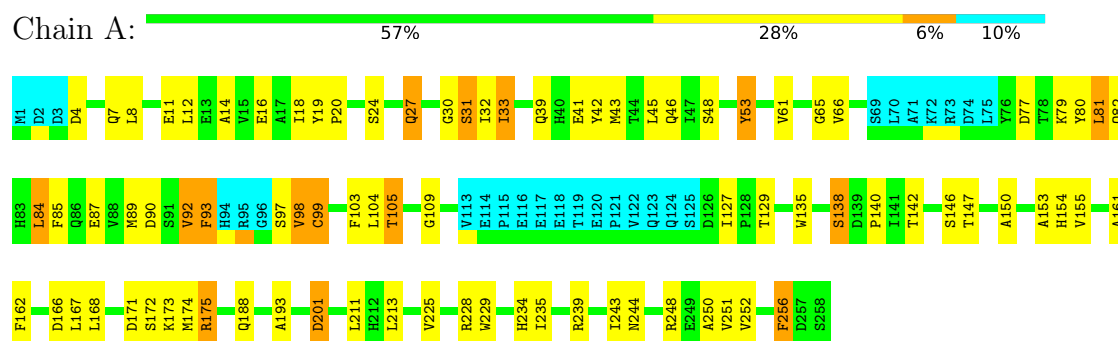
### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Protein IMPACT homolog



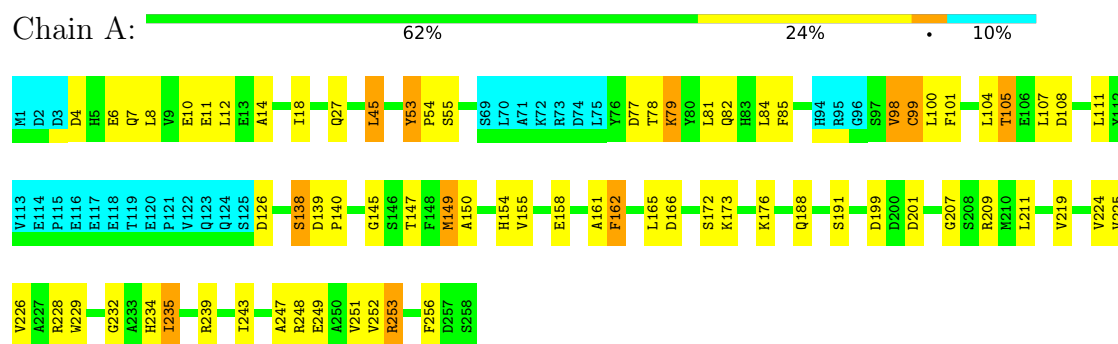
### 4.2.7 Score per residue for model 7

- Molecule 1: Protein IMPACT homolog



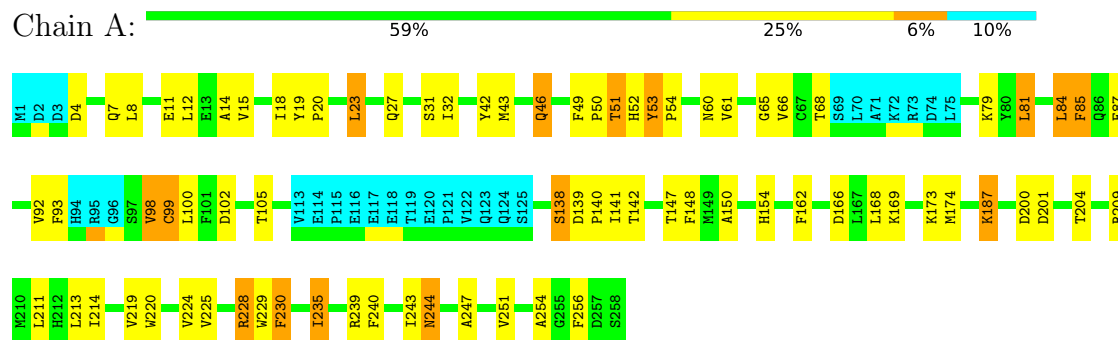
### 4.2.8 Score per residue for model 8

- Molecule 1: Protein IMPACT homolog



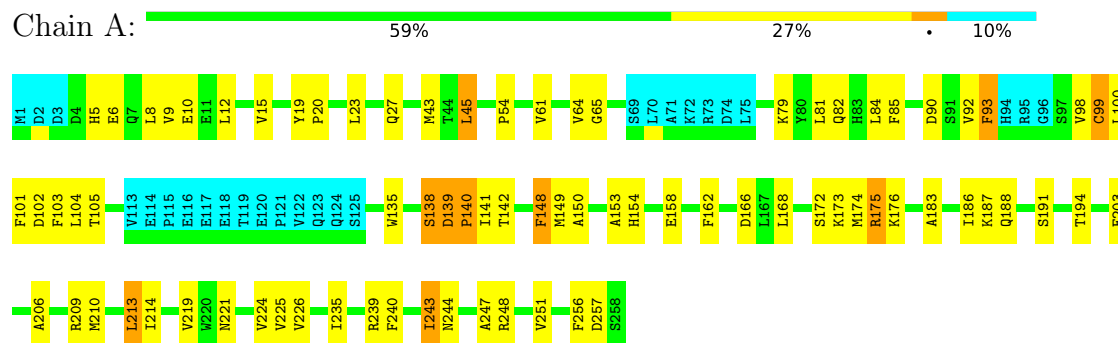
### 4.2.9 Score per residue for model 9

- Molecule 1: Protein IMPACT homolog



### 4.2.10 Score per residue for model 10

- Molecule 1: Protein IMPACT homolog





## 5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 10 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	structure calculation	
X-PLOR NIH	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2682
Number of shifts mapped to atoms	2682
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

## 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	1832	1760	1751	45±5
All	All	18320	17600	17510	450

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:MET:SD	1:A:81:LEU:HG	0.76	2.21	2	7
1:A:141:ILE:HB	1:A:148:PHE:CE1	0.72	2.19	10	2
1:A:142:THR:HG23	1:A:235:ILE:HD12	0.68	1.64	2	8
1:A:187:LYS:HG3	1:A:220:TRP:CD1	0.68	2.24	9	3
1:A:82:GLN:HG2	1:A:85:PHE:CE2	0.66	2.26	2	1
1:A:52:HIS:O	1:A:57:GLU:HB3	0.65	1.91	2	1
1:A:6:GLU:O	1:A:10:GLU:HB2	0.65	1.91	10	2
1:A:85:PHE:HD1	1:A:86:GLN:N	0.65	1.90	2	1
1:A:82:GLN:HA	1:A:85:PHE:CD2	0.64	2.27	2	1
1:A:4:ASP:HA	1:A:7:GLN:NE2	0.64	2.08	6	9
1:A:100:LEU:H	1:A:100:LEU:HD23	0.63	1.53	10	3
1:A:82:GLN:HA	1:A:85:PHE:CE2	0.62	2.30	2	1
1:A:102:ASP:O	1:A:105:THR:HG22	0.62	1.94	3	4
1:A:8:LEU:O	1:A:12:LEU:HG	0.60	1.97	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HG	1:A:85:PHE:CE1	0.60	2.31	10	3
1:A:173:LYS:HG3	1:A:174:MET:SD	0.60	2.37	4	1
1:A:240:PHE:O	1:A:244:ASN:HB2	0.59	1.97	9	2
1:A:84:LEU:O	1:A:87:GLU:HG2	0.59	1.97	7	4
1:A:206:ALA:O	1:A:210:MET:HG2	0.59	1.97	10	1
1:A:8:LEU:O	1:A:11:GLU:HG2	0.59	1.97	6	8
1:A:102:ASP:O	1:A:105:THR:HB	0.59	1.98	9	1
1:A:171:ASP:OD1	1:A:173:LYS:HG2	0.59	1.97	1	3
1:A:150:ALA:HA	1:A:225:VAL:O	0.59	1.97	7	9
1:A:147:THR:HB	1:A:229:TRP:O	0.59	1.97	4	1
1:A:213:LEU:O	1:A:217:MET:HB2	0.59	1.98	5	2
1:A:41:GLU:O	1:A:42:TYR:HB2	0.58	1.97	7	1
1:A:43:MET:HA	1:A:65:GLY:O	0.58	1.98	7	6
1:A:61:VAL:HG12	1:A:89:MET:SD	0.58	2.37	7	1
1:A:171:ASP:O	1:A:175:ARG:HB2	0.58	1.97	4	1
1:A:172:SER:O	1:A:176:LYS:HG2	0.58	1.99	2	2
1:A:188:GLN:HB2	1:A:193:ALA:O	0.58	1.99	2	1
1:A:219:VAL:HG21	1:A:256:PHE:HA	0.57	1.77	9	4
1:A:145:GLY:HA2	1:A:232:GLY:O	0.57	1.98	8	3
1:A:251:VAL:O	1:A:256:PHE:HB2	0.57	2.00	8	5
1:A:89:MET:HA	1:A:92:VAL:CG1	0.57	2.29	7	1
1:A:142:THR:HG21	1:A:234:HIS:O	0.57	1.99	1	3
1:A:176:LYS:HB2	1:A:229:TRP:CZ2	0.57	2.35	8	1
1:A:45:LEU:HG	1:A:85:PHE:CZ	0.56	2.34	6	2
1:A:140:PRO:O	1:A:243:ILE:HG21	0.56	2.00	4	1
1:A:138:SER:C	1:A:140:PRO:HD3	0.56	2.21	6	8
1:A:209:ARG:O	1:A:213:LEU:HB2	0.56	2.00	10	6
1:A:155:VAL:HG21	1:A:161:ALA:HB2	0.55	1.78	6	4
1:A:30:GLY:O	1:A:32:ILE:N	0.55	2.40	3	4
1:A:239:ARG:NE	1:A:239:ARG:HA	0.55	2.17	4	1
1:A:85:PHE:CD1	1:A:86:GLN:N	0.55	2.74	2	1
1:A:107:LEU:HA	1:A:110:VAL:HG12	0.55	1.78	4	2
1:A:50:PRO:C	1:A:52:HIS:H	0.55	2.04	9	1
1:A:15:VAL:HB	1:A:100:LEU:CD1	0.54	2.31	9	3
1:A:224:VAL:HB	1:A:256:PHE:CZ	0.54	2.37	2	8
1:A:162:PHE:O	1:A:166:ASP:HB2	0.54	2.02	6	8
1:A:133:GLU:C	1:A:135:TRP:H	0.54	2.06	5	2
1:A:14:ALA:O	1:A:18:ILE:HG13	0.54	2.02	8	7
1:A:138:SER:O	1:A:140:PRO:HD3	0.54	2.03	3	7
1:A:12:LEU:O	1:A:16:GLU:HB2	0.54	2.03	6	5
1:A:140:PRO:HD2	1:A:243:ILE:HG21	0.54	1.79	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LYS:HG2	1:A:174:MET:SD	0.54	2.43	5	1
1:A:248:ARG:O	1:A:252:VAL:HG22	0.54	2.02	8	1
1:A:200:ASP:HB2	1:A:204:THR:HA	0.53	1.79	9	1
1:A:239:ARG:O	1:A:243:ILE:HG12	0.53	2.04	3	4
1:A:151:PHE:O	1:A:224:VAL:HA	0.53	2.04	5	4
1:A:244:ASN:O	1:A:248:ARG:HG3	0.53	2.03	4	2
1:A:15:VAL:HG13	1:A:23:LEU:HG	0.53	1.80	4	1
1:A:77:ASP:OD1	1:A:79:LYS:HG2	0.53	2.04	8	1
1:A:92:VAL:HG12	1:A:102:ASP:HB3	0.53	1.81	6	2
1:A:183:ALA:HB1	1:A:214:ILE:HD13	0.53	1.81	4	2
1:A:199:ASP:OD2	1:A:207:GLY:HA3	0.53	2.04	8	1
1:A:139:ASP:HA	1:A:247:ALA:CB	0.53	2.34	9	5
1:A:12:LEU:O	1:A:15:VAL:HG12	0.52	2.04	5	4
1:A:138:SER:O	1:A:247:ALA:HA	0.52	2.05	2	2
1:A:147:THR:O	1:A:228:ARG:HA	0.52	2.05	9	5
1:A:42:TYR:O	1:A:66:VAL:HA	0.52	2.04	9	2
1:A:142:THR:HG23	1:A:234:HIS:O	0.52	2.04	7	1
1:A:81:LEU:O	1:A:85:PHE:HB2	0.52	2.05	4	2
1:A:61:VAL:HG22	1:A:82:GLN:OE1	0.52	2.05	10	2
1:A:128:PRO:HD3	1:A:149:MET:SD	0.51	2.45	5	1
1:A:252:VAL:HA	1:A:256:PHE:O	0.51	2.05	7	1
1:A:135:TRP:CE3	1:A:153:ALA:HB2	0.51	2.40	7	3
1:A:142:THR:HG21	1:A:234:HIS:CD2	0.51	2.41	3	1
1:A:212:HIS:O	1:A:216:ILE:HG13	0.51	2.06	5	1
1:A:133:GLU:O	1:A:133:GLU:HG3	0.51	2.04	4	1
1:A:147:THR:OG1	1:A:235:ILE:HD11	0.51	2.06	4	2
1:A:98:VAL:O	1:A:99:CYS:HB3	0.51	2.06	7	4
1:A:181:MET:CG	1:A:226:VAL:HB	0.51	2.36	5	1
1:A:84:LEU:O	1:A:88:VAL:HG23	0.50	2.05	5	1
1:A:104:LEU:HD12	1:A:105:THR:N	0.50	2.22	7	4
1:A:5:HIS:O	1:A:9:VAL:HG13	0.50	2.06	10	1
1:A:27:GLN:HG2	1:A:32:ILE:HB	0.50	1.83	1	6
1:A:238:ASP:O	1:A:242:HIS:HB2	0.50	2.06	5	2
1:A:39:GLN:O	1:A:40:HIS:HB3	0.50	2.06	5	1
1:A:229:TRP:CE3	1:A:229:TRP:HA	0.50	2.42	5	1
1:A:141:ILE:HB	1:A:148:PHE:CD1	0.49	2.42	2	2
1:A:149:MET:O	1:A:226:VAL:HA	0.49	2.07	2	5
1:A:249:GLU:O	1:A:253:ARG:HB2	0.49	2.07	8	3
1:A:39:GLN:OE1	1:A:39:GLN:HA	0.49	2.07	7	1
1:A:140:PRO:HG2	1:A:243:ILE:CD1	0.49	2.37	10	2
1:A:85:PHE:CE1	1:A:107:LEU:HD21	0.49	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LYS:HD3	1:A:80:TYR:N	0.49	2.23	6	2
1:A:166:ASP:O	1:A:169:LYS:HG3	0.49	2.08	4	1
1:A:140:PRO:HD2	1:A:243:ILE:CG2	0.48	2.38	4	1
1:A:88:VAL:O	1:A:92:VAL:HG13	0.48	2.07	5	1
1:A:51:THR:HA	1:A:53:TYR:CE1	0.48	2.43	9	1
1:A:92:VAL:HG21	1:A:99:CYS:SG	0.48	2.49	3	2
1:A:219:VAL:HG21	1:A:256:PHE:CD2	0.48	2.43	5	2
1:A:79:LYS:HD2	1:A:79:LYS:C	0.48	2.29	4	1
1:A:15:VAL:CG1	1:A:23:LEU:HG	0.48	2.39	9	1
1:A:61:VAL:HB	1:A:85:PHE:CE2	0.48	2.43	9	1
1:A:142:THR:H	1:A:240:PHE:HB3	0.48	1.68	4	1
1:A:251:VAL:HG22	1:A:256:PHE:CB	0.48	2.39	5	2
1:A:158:GLU:O	1:A:162:PHE:HB2	0.48	2.09	8	1
1:A:127:ILE:HD13	1:A:239:ARG:HE	0.48	1.69	1	1
1:A:92:VAL:HG11	1:A:103:PHE:CB	0.48	2.39	3	1
1:A:45:LEU:HD12	1:A:64:VAL:CG1	0.48	2.38	10	1
1:A:188:GLN:HG2	1:A:193:ALA:O	0.48	2.09	1	2
1:A:9:VAL:O	1:A:13:GLU:HG3	0.48	2.08	4	1
1:A:8:LEU:HD11	1:A:49:PHE:CD1	0.48	2.44	9	1
1:A:140:PRO:HD2	1:A:243:ILE:HD13	0.47	1.86	1	1
1:A:138:SER:HB2	1:A:250:ALA:CB	0.47	2.39	4	5
1:A:15:VAL:HG21	1:A:23:LEU:HD13	0.47	1.86	10	1
1:A:145:GLY:O	1:A:230:PHE:HA	0.47	2.10	5	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.47	2.09	6	1
1:A:100:LEU:HD23	1:A:100:LEU:N	0.47	2.23	9	5
1:A:222:VAL:HG11	1:A:255:GLY:O	0.47	2.09	3	1
1:A:171:ASP:O	1:A:175:ARG:HG3	0.47	2.08	2	1
1:A:80:TYR:O	1:A:84:LEU:HD23	0.47	2.10	3	2
1:A:50:PRO:HG3	1:A:60:ASN:OD1	0.47	2.10	4	1
1:A:188:GLN:HA	1:A:188:GLN:OE1	0.47	2.10	5	3
1:A:173:LYS:H	1:A:173:LYS:HD2	0.47	1.68	5	1
1:A:239:ARG:HA	1:A:239:ARG:CZ	0.47	2.39	4	1
1:A:229:TRP:HA	1:A:229:TRP:CE3	0.47	2.43	4	1
1:A:54:PRO:HB3	1:A:98:VAL:O	0.47	2.10	8	2
1:A:141:ILE:HG22	1:A:142:THR:N	0.47	2.25	3	2
1:A:15:VAL:HG11	1:A:23:LEU:HG	0.47	1.87	2	1
1:A:164:MET:O	1:A:167:LEU:HG	0.47	2.10	5	1
1:A:24:SER:O	1:A:33:ILE:HB	0.47	2.09	7	1
1:A:78:THR:O	1:A:82:GLN:HB2	0.47	2.10	8	1
1:A:58:ALA:HB1	1:A:59:PRO:HD2	0.46	1.87	6	1
1:A:85:PHE:O	1:A:89:MET:HG3	0.46	2.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:ASP:OD1	1:A:251:VAL:HB	0.46	2.10	3	1
1:A:85:PHE:CZ	1:A:103:PHE:CE1	0.46	3.03	3	1
1:A:251:VAL:HG22	1:A:256:PHE:HB2	0.46	1.86	5	2
1:A:187:LYS:HB3	1:A:220:TRP:CD1	0.46	2.46	3	1
1:A:37:VAL:HG23	1:A:43:MET:O	0.46	2.10	2	1
1:A:132:PHE:CB	1:A:135:TRP:HB2	0.46	2.41	4	1
1:A:39:GLN:O	1:A:40:HIS:HB2	0.46	2.11	6	1
1:A:138:SER:HB2	1:A:250:ALA:HB2	0.46	1.87	7	2
1:A:90:ASP:HA	1:A:93:PHE:HB2	0.46	1.88	10	1
1:A:187:LYS:HA	1:A:194:THR:HG22	0.46	1.88	5	3
1:A:19:TYR:HB2	1:A:22:LEU:HB3	0.45	1.88	2	1
1:A:126:ASP:O	1:A:147:THR:HG21	0.45	2.11	8	2
1:A:87:GLU:O	1:A:90:ASP:HB3	0.45	2.11	7	1
1:A:132:PHE:HB3	1:A:135:TRP:HB2	0.45	1.88	4	1
1:A:39:GLN:HB3	1:A:41:GLU:OE1	0.45	2.11	6	1
1:A:140:PRO:O	1:A:141:ILE:HG12	0.45	2.11	10	2
1:A:177:ALA:HA	1:A:229:TRP:NE1	0.45	2.26	5	1
1:A:50:PRO:C	1:A:52:HIS:N	0.45	2.69	9	1
1:A:173:LYS:O	1:A:176:LYS:HG3	0.45	2.10	10	1
1:A:48:SER:O	1:A:60:ASN:HB2	0.45	2.11	5	1
1:A:219:VAL:CG2	1:A:256:PHE:HA	0.45	2.42	6	1
1:A:99:CYS:SG	1:A:100:LEU:N	0.45	2.90	2	1
1:A:45:LEU:HD12	1:A:64:VAL:HG12	0.45	1.88	2	1
1:A:236:GLY:O	1:A:239:ARG:HB2	0.45	2.11	6	1
1:A:148:PHE:O	1:A:148:PHE:HD1	0.44	1.94	2	1
1:A:61:VAL:CG1	1:A:85:PHE:CD1	0.44	3.00	2	1
1:A:142:THR:HB	1:A:240:PHE:HB3	0.44	1.89	5	1
1:A:101:PHE:O	1:A:104:LEU:HG	0.44	2.13	3	4
1:A:81:LEU:HA	1:A:84:LEU:HD21	0.44	1.90	3	2
1:A:127:ILE:HD11	1:A:235:ILE:HD13	0.44	1.89	4	1
1:A:241:LYS:C	1:A:241:LYS:HD3	0.44	2.32	3	1
1:A:139:ASP:O	1:A:149:MET:HA	0.44	2.13	1	1
1:A:77:ASP:OD1	1:A:79:LYS:HG3	0.44	2.13	4	1
1:A:89:MET:HA	1:A:92:VAL:HG12	0.43	1.89	7	1
1:A:100:LEU:HD23	1:A:100:LEU:H	0.43	1.73	9	1
1:A:161:ALA:O	1:A:165:LEU:HB3	0.43	2.13	2	3
1:A:77:ASP:OD2	1:A:79:LYS:HE3	0.43	2.13	3	1
1:A:141:ILE:HB	1:A:148:PHE:HB2	0.43	1.90	9	1
1:A:188:GLN:HB3	1:A:191:SER:HB2	0.43	1.90	4	2
1:A:172:SER:HA	1:A:175:ARG:HB2	0.43	1.90	10	3
1:A:100:LEU:H	1:A:100:LEU:CD2	0.43	2.24	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:GLU:OE1	1:A:100:LEU:HD22	0.43	2.13	3	1
1:A:187:LYS:CG	1:A:220:TRP:CD1	0.43	3.01	6	1
1:A:140:PRO:HB2	1:A:239:ARG:NH2	0.43	2.28	1	1
1:A:248:ARG:HH11	1:A:252:VAL:CG2	0.42	2.27	3	1
1:A:141:ILE:N	1:A:148:PHE:O	0.42	2.52	5	2
1:A:188:GLN:CB	1:A:191:SER:HB2	0.42	2.45	10	1
1:A:156:THR:O	1:A:186:ILE:HD12	0.42	2.14	5	1
1:A:107:LEU:O	1:A:111:LEU:HB2	0.42	2.15	8	1
1:A:77:ASP:OD2	1:A:79:LYS:HG3	0.42	2.14	1	1
1:A:53:TYR:HB3	1:A:54:PRO:HD2	0.42	1.92	3	1
1:A:98:VAL:O	1:A:99:CYS:HB2	0.42	2.14	3	1
1:A:54:PRO:HA	1:A:58:ALA:HA	0.42	1.91	3	1
1:A:84:LEU:HA	1:A:87:GLU:HG2	0.42	1.92	3	1
1:A:181:MET:HA	1:A:200:ASP:O	0.42	2.15	5	1
1:A:142:THR:OG1	1:A:239:ARG:HB3	0.42	2.14	7	1
1:A:188:GLN:HG3	1:A:193:ALA:HB3	0.42	1.92	7	2
1:A:6:GLU:O	1:A:9:VAL:HG12	0.42	2.14	5	1
1:A:210:MET:HA	1:A:213:LEU:HB3	0.42	1.91	5	1
1:A:27:GLN:HB3	1:A:31:SER:OG	0.42	2.15	7	1
1:A:92:VAL:HG22	1:A:92:VAL:O	0.41	2.15	7	1
1:A:169:LYS:HZ3	1:A:169:LYS:HB3	0.41	1.75	9	1
1:A:37:VAL:CG1	1:A:41:GLU:HG2	0.41	2.45	6	1
1:A:127:ILE:HD11	1:A:235:ILE:HG12	0.41	1.92	7	1
1:A:92:VAL:HB	1:A:102:ASP:OD1	0.41	2.15	9	1
1:A:61:VAL:HG13	1:A:85:PHE:CD1	0.41	2.50	2	1
1:A:53:TYR:HB2	1:A:55:SER:OG	0.41	2.14	8	1
1:A:158:GLU:HA	1:A:186:ILE:CD1	0.41	2.45	10	1
1:A:77:ASP:H	1:A:80:TYR:HB2	0.41	1.76	7	1
1:A:187:LYS:HD2	1:A:194:THR:CG2	0.41	2.46	10	1
1:A:6:GLU:O	1:A:10:GLU:HG3	0.41	2.15	1	2
1:A:251:VAL:HG13	1:A:252:VAL:N	0.41	2.31	3	2
1:A:151:PHE:CD2	1:A:168:LEU:HD11	0.41	2.51	5	1
1:A:185:ARG:HG2	1:A:220:TRP:HA	0.41	1.92	5	1
1:A:148:PHE:HD1	1:A:148:PHE:O	0.41	1.97	10	1
1:A:5:HIS:O	1:A:9:VAL:HG22	0.41	2.16	10	1
1:A:85:PHE:CZ	1:A:103:PHE:HE1	0.41	2.34	6	1
1:A:15:VAL:HG23	1:A:19:TYR:CE1	0.41	2.50	6	1
1:A:23:LEU:HD13	1:A:24:SER:N	0.41	2.30	4	1
1:A:46:GLN:HA	1:A:46:GLN:HE21	0.41	1.76	9	1
1:A:92:VAL:CB	1:A:99:CYS:HA	0.41	2.46	10	1
1:A:140:PRO:HG2	1:A:243:ILE:HD11	0.41	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:GLN:CG	1:A:193:ALA:HB3	0.41	2.46	4	1
1:A:105:THR:O	1:A:108:ASP:HB3	0.40	2.16	8	1
1:A:146:SER:HA	1:A:229:TRP:O	0.40	2.16	7	1
1:A:214:ILE:O	1:A:219:VAL:HG12	0.40	2.16	9	1
1:A:100:LEU:N	1:A:100:LEU:HD23	0.40	2.31	5	1
1:A:200:ASP:CB	1:A:204:THR:HA	0.40	2.46	5	1
1:A:167:LEU:O	1:A:171:ASP:HB2	0.40	2.16	7	1
1:A:140:PRO:HA	1:A:148:PHE:O	0.40	2.16	10	1
1:A:187:LYS:HB3	1:A:221:ASN:OD1	0.40	2.16	10	1
1:A:92:VAL:CG1	1:A:102:ASP:HB3	0.40	2.47	10	1
1:A:139:ASP:OD2	1:A:247:ALA:HB1	0.40	2.17	4	2
1:A:50:PRO:CD	1:A:59:PRO:HA	0.40	2.46	5	1
1:A:53:TYR:HB2	1:A:54:PRO:HD2	0.40	1.94	6	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	231/258 (90%)	193±3 (84±1%)	30±3 (13±1%)	8±2 (4±1%)	6	34
All	All	2310/2580 (90%)	1931 (84%)	296 (13%)	83 (4%)	6	34

All 26 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	138	SER	10
1	A	99	CYS	10
1	A	20	PRO	7
1	A	54	PRO	6
1	A	53	TYR	6
1	A	31	SER	5
1	A	201	ASP	5
1	A	41	GLU	4
1	A	92	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	40	HIS	3
1	A	42	TYR	3
1	A	257	ASP	2
1	A	235	ILE	2
1	A	158	GLU	2
1	A	230	PHE	2
1	A	68	THR	2
1	A	254	ALA	2
1	A	58	ALA	1
1	A	177	ALA	1
1	A	202	GLY	1
1	A	51	THR	1
1	A	134	GLY	1
1	A	200	ASP	1
1	A	156	THR	1
1	A	256	PHE	1
1	A	112	TYR	1

### 6.3.2 Protein sidechains ⓘ

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	200/224 (89%)	180±3 (90±2%)	20±3 (10±2%)	11	57
All	All	2000/2240 (89%)	1802 (90%)	198 (10%)	11	57

All 69 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	98	VAL	10
1	A	154	HIS	10
1	A	84	LEU	10
1	A	79	LYS	8
1	A	211	LEU	8
1	A	81	LEU	7
1	A	19	TYR	7
1	A	168	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	229	TRP	7
1	A	174	MET	7
1	A	45	LEU	7
1	A	103	PHE	6
1	A	213	LEU	5
1	A	93	PHE	5
1	A	217	MET	5
1	A	60	ASN	4
1	A	53	TYR	4
1	A	85	PHE	4
1	A	239	ARG	3
1	A	27	GLN	3
1	A	173	LYS	3
1	A	105	THR	3
1	A	234	HIS	3
1	A	244	ASN	3
1	A	248	ARG	2
1	A	39	GLN	2
1	A	82	GLN	2
1	A	203	GLU	2
1	A	148	PHE	2
1	A	181	MET	2
1	A	162	PHE	2
1	A	23	LEU	2
1	A	149	MET	2
1	A	139	ASP	2
1	A	46	GLN	2
1	A	140	PRO	2
1	A	169	LYS	2
1	A	175	ARG	2
1	A	16	GLU	1
1	A	144	ARG	1
1	A	253	ARG	1
1	A	48	SER	1
1	A	11	GLU	1
1	A	187	LYS	1
1	A	5	HIS	1
1	A	56	GLU	1
1	A	33	ILE	1
1	A	129	THR	1
1	A	209	ARG	1
1	A	110	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	28	GLU	1
1	A	63	GLU	1
1	A	176	LYS	1
1	A	230	PHE	1
1	A	165	LEU	1
1	A	133	GLU	1
1	A	90	ASP	1
1	A	22	LEU	1
1	A	228	ARG	1
1	A	40	HIS	1
1	A	243	ILE	1
1	A	107	LEU	1
1	A	235	ILE	1
1	A	242	HIS	1
1	A	68	THR	1
1	A	196	GLN	1
1	A	4	ASP	1
1	A	86	GLN	1
1	A	201	ASP	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 monosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 76% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *yih.str.txt*

#### 7.1.1 Bookkeeping

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	2682
Number of shifts mapped to atoms	2682
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	249	$2.60 \pm 0.17$	Should be applied
$^{13}\text{C}_\beta$	237	$2.92 \pm 0.08$	Should be applied
$^{13}\text{C}'$	164	$2.91 \pm 0.22$	Should be applied
$^{15}\text{N}$	238	$0.17 \pm 0.26$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 2149 atoms were assigned a chemical shift out of a possible 2790. 33 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	1032/1142 (90%)	439/455 (96%)	377/464 (81%)	216/223 (97%)
Sidechain	1023/1364 (75%)	605/792 (76%)	414/526 (79%)	4/46 (9%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	94/284 (33%)	56/148 (38%)	36/114 (32%)	2/22 (9%)
Overall	2149/2790 (77%)	1100/1395 (79%)	827/1104 (75%)	222/291 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 2357 atoms were assigned a chemical shift out of a possible 3111. 34 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	1134/1268 (89%)	483/505 (96%)	413/516 (80%)	238/247 (96%)
Sidechain	1127/1551 (73%)	668/902 (74%)	455/594 (77%)	4/55 (7%)
Aromatic	96/292 (33%)	57/152 (38%)	37/116 (32%)	2/24 (8%)
Overall	2357/3111 (76%)	1208/1559 (77%)	905/1226 (74%)	244/326 (75%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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	234	HIS	CE1	115.05	149.70 – 125.30	-9.2
1	A	168	LEU	HD11	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD13	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD12	-1.26	2.16 – -0.64	-7.2
1	A	168	LEU	HD21	-0.91	2.14 – -0.66	-5.9
1	A	168	LEU	HD22	-0.91	2.14 – -0.66	-5.9
1	A	168	LEU	HD23	-0.91	2.14 – -0.66	-5.9
1	A	54	PRO	CG	20.90	32.66 – 21.76	-5.8
1	A	253	ARG	CD	38.49	47.57 – 38.77	-5.3
1	A	145	GLY	N	129.71	129.07 – 90.27	5.2
1	A	109	GLY	N	129.54	129.07 – 90.27	5.1

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

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:

