Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 01:38 pm BST

PDB ID	:	4UZX
BMRB ID	:	25214
Title	:	High-resolution NMR structures of the domains of Saccharomyces cerevisiae Tho1
Authors	:	Jacobsen, J.O.B.; Allen, M.D.; Freund, S.M.V.; Bycroft, M.
Deposited on	:	2014-09-09

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

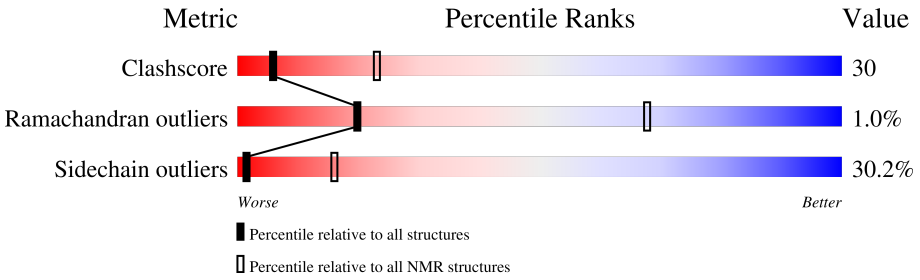
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 84%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	67	31% 49% 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:122-A:175 (54)	0.49	4

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1073 atoms, of which 546 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN THO1.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	67	1073	325	546	98	104	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP P40040
A	118	SER	-	expression tag	UNP P40040

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 THO1

Chain A:

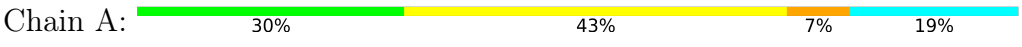
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PROTEIN THO1

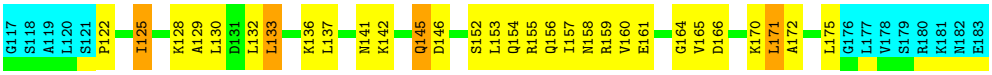
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN THO1

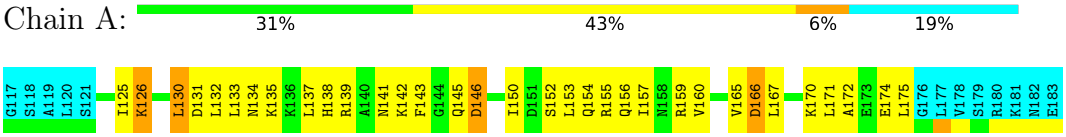
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN THO1

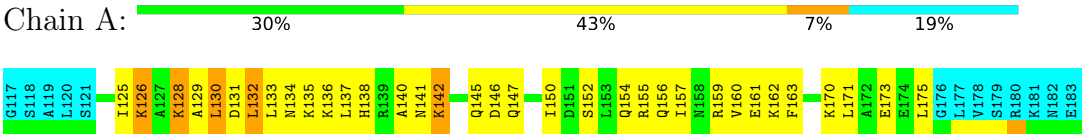
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: PROTEIN THO1

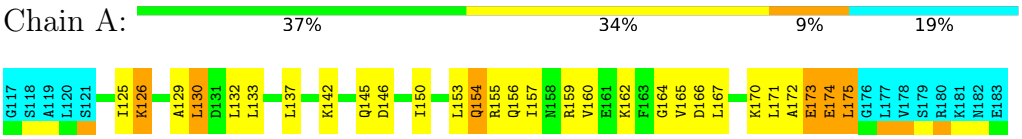
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: PROTEIN THO1

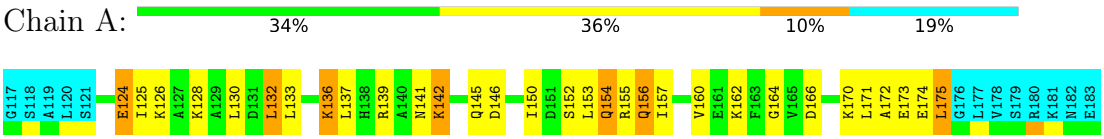
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: PROTEIN THO1

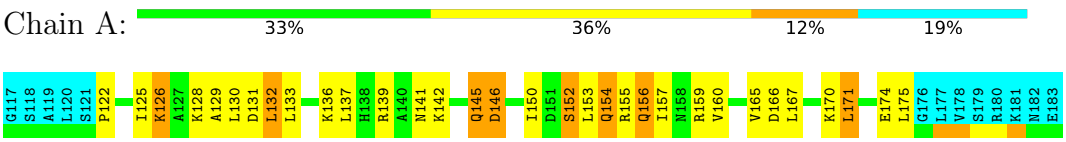
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: PROTEIN THO1

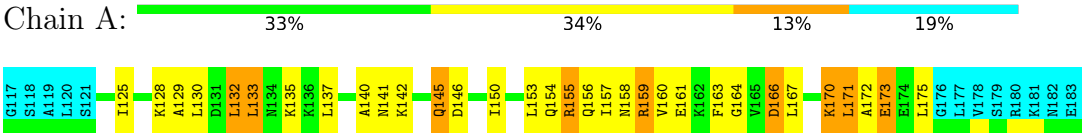
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: PROTEIN THO1

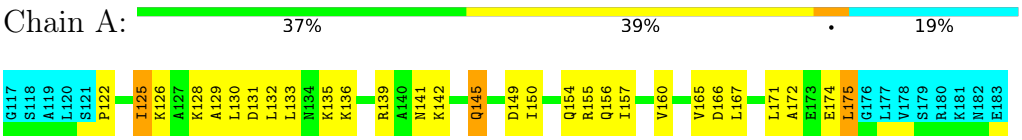
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: PROTEIN THO1

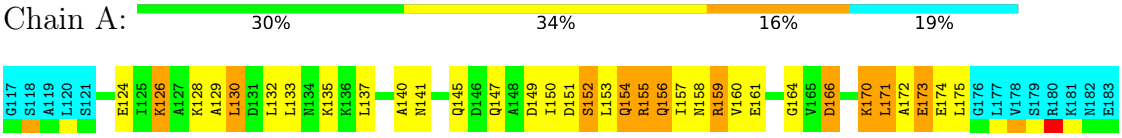
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: PROTEIN THO1

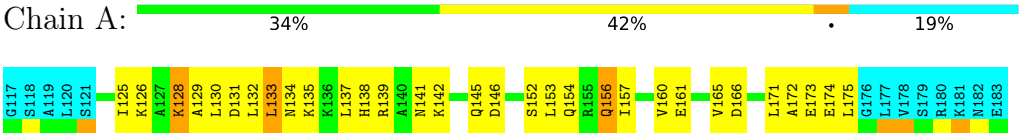
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: PROTEIN THO1

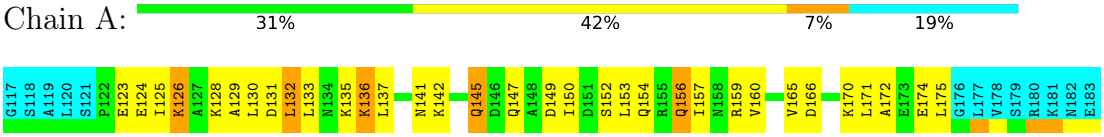
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: PROTEIN THO1

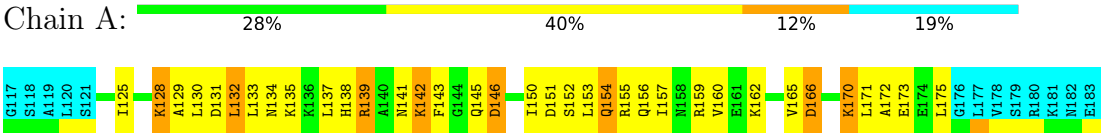
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: PROTEIN THO1

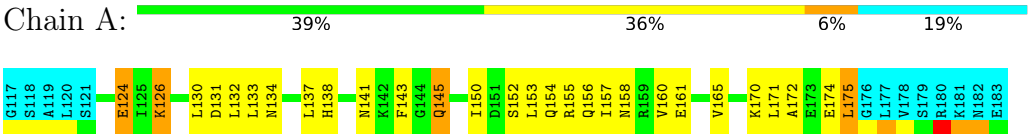
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN THO1

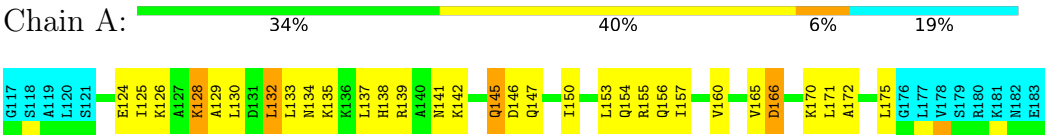
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN THO1

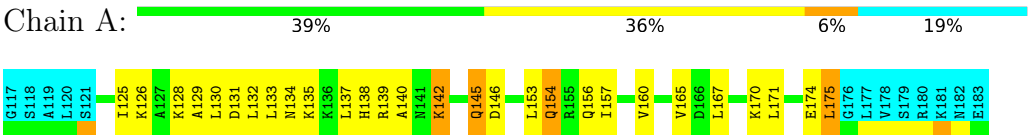
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN THO1

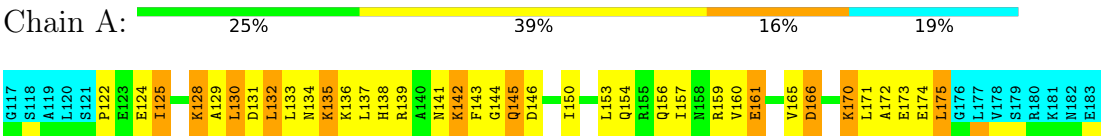
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN THO1

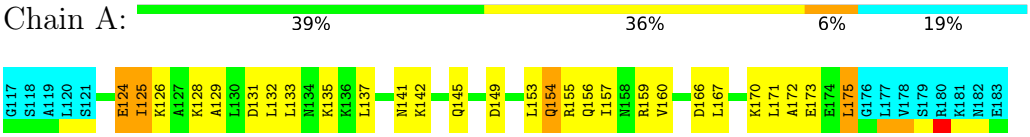
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN THO1

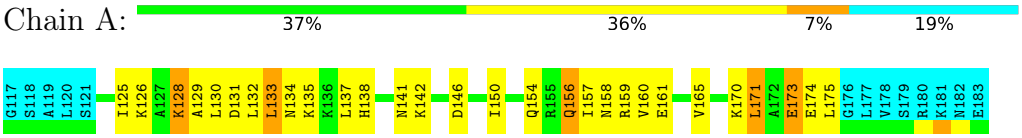
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN THO1

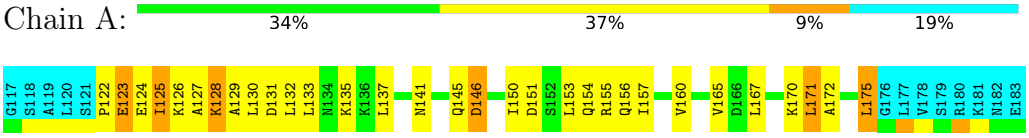
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN THO1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *NO VIOLATIONS*.

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

Software name	Classification	Version
CNS	refinement	
ANSIG	structure solution	
CNS	structure solution	

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	789
Number of shifts mapped to atoms	789
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	435	449	448	26±6
All	All	8700	8980	8960	527

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD21	1:A:171:LEU:HD13	1.15	1.18	4	7
1:A:156:GLN:O	1:A:160:VAL:HG23	0.91	1.65	3	20
1:A:133:LEU:HD11	1:A:171:LEU:HD11	0.87	1.43	17	9
1:A:133:LEU:HD11	1:A:171:LEU:HD21	0.87	1.47	8	5
1:A:133:LEU:HD11	1:A:171:LEU:HD22	0.85	1.46	15	4
1:A:132:LEU:CD2	1:A:175:LEU:HD21	0.84	2.01	18	6
1:A:137:LEU:HD22	1:A:157:ILE:CD1	0.83	2.03	6	18
1:A:171:LEU:CD1	1:A:175:LEU:HD12	0.82	2.05	7	4
1:A:133:LEU:HD11	1:A:171:LEU:HD13	0.81	1.52	7	4
1:A:137:LEU:HD22	1:A:157:ILE:HD13	0.79	1.52	10	13
1:A:133:LEU:HD22	1:A:156:GLN:OE1	0.79	1.78	6	4
1:A:133:LEU:HB3	1:A:157:ILE:HD12	0.78	1.52	3	1
1:A:125:ILE:HD11	1:A:165:VAL:HB	0.78	1.55	20	1
1:A:141:ASN:OD1	1:A:150:ILE:HG21	0.77	1.79	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LEU:HD22	1:A:132:LEU:O	0.77	1.79	4	3
1:A:128:LYS:CD	1:A:175:LEU:HD22	0.77	2.10	19	2
1:A:132:LEU:HD13	1:A:133:LEU:N	0.75	1.96	7	2
1:A:171:LEU:HD11	1:A:175:LEU:HD12	0.75	1.57	7	4
1:A:129:ALA:O	1:A:133:LEU:HD12	0.75	1.81	12	5
1:A:133:LEU:CD1	1:A:171:LEU:HD11	0.74	2.13	9	5
1:A:133:LEU:HD21	1:A:171:LEU:CD2	0.74	2.12	3	2
1:A:132:LEU:HD21	1:A:175:LEU:HD21	0.74	1.57	2	6
1:A:133:LEU:HD11	1:A:171:LEU:CD1	0.73	2.13	17	8
1:A:129:ALA:C	1:A:133:LEU:HD12	0.73	2.04	12	2
1:A:133:LEU:HD21	1:A:171:LEU:HD23	0.73	1.59	3	2
1:A:133:LEU:HD23	1:A:136:LYS:HE3	0.72	1.58	12	1
1:A:137:LEU:HD22	1:A:157:ILE:HD12	0.72	1.61	8	6
1:A:132:LEU:HD21	1:A:175:LEU:CD2	0.72	2.15	10	1
1:A:133:LEU:HD21	1:A:156:GLN:OE1	0.71	1.85	10	1
1:A:165:VAL:HG13	1:A:171:LEU:HD23	0.70	1.63	14	1
1:A:133:LEU:CD1	1:A:171:LEU:HD22	0.70	2.16	7	4
1:A:132:LEU:HD21	1:A:175:LEU:HD11	0.70	1.64	18	1
1:A:133:LEU:CD2	1:A:171:LEU:HD13	0.69	2.10	4	3
1:A:126:LYS:CE	1:A:130:LEU:HD11	0.69	2.17	11	1
1:A:133:LEU:HD11	1:A:171:LEU:CD2	0.69	2.18	16	11
1:A:129:ALA:HA	1:A:175:LEU:HD11	0.69	1.63	13	8
1:A:133:LEU:HD23	1:A:136:LYS:CE	0.69	2.17	12	1
1:A:132:LEU:C	1:A:132:LEU:HD12	0.69	2.07	6	1
1:A:165:VAL:HG13	1:A:171:LEU:HD12	0.68	1.64	3	3
1:A:132:LEU:HD22	1:A:175:LEU:HD21	0.67	1.65	18	3
1:A:133:LEU:HD11	1:A:171:LEU:CG	0.67	2.20	5	5
1:A:153:LEU:HD23	1:A:156:GLN:CD	0.66	2.09	3	3
1:A:133:LEU:HD21	1:A:171:LEU:CD1	0.66	2.20	16	5
1:A:165:VAL:HG12	1:A:172:ALA:HB2	0.66	1.67	2	2
1:A:133:LEU:HD23	1:A:153:LEU:HD22	0.66	1.67	10	5
1:A:133:LEU:HD23	1:A:153:LEU:CD2	0.65	2.21	16	9
1:A:137:LEU:HD21	1:A:154:GLN:OE1	0.65	1.92	14	1
1:A:129:ALA:O	1:A:132:LEU:HD23	0.64	1.93	8	1
1:A:165:VAL:HG13	1:A:171:LEU:CD2	0.64	2.22	9	2
1:A:153:LEU:O	1:A:156:GLN:HG2	0.63	1.92	3	2
1:A:133:LEU:HD11	1:A:156:GLN:OE1	0.63	1.94	10	1
1:A:132:LEU:HD12	1:A:133:LEU:N	0.63	2.09	2	3
1:A:126:LYS:HE2	1:A:130:LEU:HD11	0.62	1.72	11	1
1:A:153:LEU:O	1:A:157:ILE:HD12	0.61	1.96	10	5
1:A:128:LYS:HE3	1:A:175:LEU:HD22	0.61	1.72	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ALA:HB2	1:A:175:LEU:HD11	0.61	1.71	8	3
1:A:165:VAL:HG13	1:A:171:LEU:CD1	0.61	2.26	3	1
1:A:129:ALA:HB1	1:A:171:LEU:HD21	0.60	1.74	20	2
1:A:133:LEU:HD13	1:A:156:GLN:CG	0.60	2.27	1	2
1:A:132:LEU:HD13	1:A:175:LEU:HD21	0.60	1.74	13	2
1:A:156:GLN:OE1	1:A:171:LEU:HD22	0.59	1.97	18	1
1:A:133:LEU:HD13	1:A:156:GLN:OE1	0.59	1.96	1	2
1:A:156:GLN:OE1	1:A:171:LEU:HD13	0.59	1.98	18	1
1:A:153:LEU:HD23	1:A:156:GLN:OE1	0.59	1.98	15	3
1:A:137:LEU:HD21	1:A:154:GLN:NE2	0.59	2.12	15	4
1:A:132:LEU:HD13	1:A:132:LEU:C	0.58	2.19	7	4
1:A:128:LYS:HD3	1:A:175:LEU:HD22	0.58	1.74	19	1
1:A:156:GLN:NE2	1:A:171:LEU:HD23	0.58	2.14	8	1
1:A:141:ASN:CG	1:A:150:ILE:HG21	0.58	2.19	7	4
1:A:133:LEU:CD1	1:A:171:LEU:HD13	0.57	2.27	7	2
1:A:137:LEU:HD12	1:A:150:ILE:HG22	0.57	1.76	1	1
1:A:140:ALA:HB1	1:A:145:GLN:CB	0.57	2.29	10	2
1:A:132:LEU:HD23	1:A:133:LEU:N	0.57	2.15	8	1
1:A:132:LEU:HD12	1:A:136:LYS:HD3	0.57	1.77	12	1
1:A:156:GLN:NE2	1:A:171:LEU:HD13	0.57	2.14	16	1
1:A:133:LEU:HD21	1:A:156:GLN:CD	0.56	2.20	10	1
1:A:133:LEU:HD13	1:A:156:GLN:CD	0.56	2.21	1	2
1:A:133:LEU:CD1	1:A:160:VAL:HG21	0.56	2.30	3	1
1:A:166:ASP:O	1:A:172:ALA:HB2	0.56	2.01	8	8
1:A:125:ILE:C	1:A:125:ILE:HD13	0.55	2.22	20	2
1:A:125:ILE:HG22	1:A:165:VAL:CG2	0.55	2.31	19	1
1:A:130:LEU:HD21	1:A:161:GLU:CG	0.55	2.31	10	2
1:A:133:LEU:CD1	1:A:171:LEU:HD21	0.55	2.27	16	2
1:A:137:LEU:CD1	1:A:150:ILE:HG22	0.54	2.32	1	4
1:A:165:VAL:CG1	1:A:172:ALA:HB2	0.54	2.32	9	2
1:A:137:LEU:HD13	1:A:153:LEU:CB	0.54	2.31	6	1
1:A:153:LEU:O	1:A:157:ILE:HG12	0.54	2.03	3	1
1:A:133:LEU:CG	1:A:171:LEU:HD13	0.54	2.33	20	1
1:A:133:LEU:HD11	1:A:171:LEU:HG	0.53	1.80	11	3
1:A:165:VAL:HG13	1:A:171:LEU:HD22	0.53	1.80	9	1
1:A:141:ASN:OD1	1:A:150:ILE:HD13	0.53	2.03	12	4
1:A:154:GLN:HA	1:A:157:ILE:HD12	0.53	1.80	16	4
1:A:171:LEU:HD22	1:A:175:LEU:CD1	0.53	2.33	10	1
1:A:130:LEU:HD21	1:A:161:GLU:HG3	0.53	1.81	1	2
1:A:122:PRO:O	1:A:125:ILE:HG22	0.53	2.03	7	2
1:A:155:ARG:HA	1:A:158:ASN:ND2	0.53	2.19	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:CG	1:A:171:LEU:HD11	0.53	2.34	16	2
1:A:173:GLU:HG3	1:A:174:GLU:N	0.53	2.17	19	2
1:A:129:ALA:CA	1:A:175:LEU:HD11	0.53	2.33	13	2
1:A:157:ILE:N	1:A:157:ILE:HD13	0.52	2.19	3	2
1:A:134:ASN:O	1:A:138:HIS:CD2	0.51	2.63	15	10
1:A:132:LEU:HD22	1:A:132:LEU:C	0.51	2.25	7	2
1:A:129:ALA:CB	1:A:175:LEU:HD11	0.51	2.34	11	5
1:A:129:ALA:HA	1:A:132:LEU:HD22	0.51	1.83	8	1
1:A:133:LEU:HD22	1:A:157:ILE:HG12	0.51	1.82	11	1
1:A:129:ALA:HB2	1:A:165:VAL:HG21	0.50	1.82	20	7
1:A:146:ASP:OD2	1:A:146:ASP:N	0.50	2.43	2	1
1:A:139:ARG:HA	1:A:142:LYS:HG2	0.50	1.82	6	2
1:A:140:ALA:HB1	1:A:145:GLN:CD	0.50	2.26	16	1
1:A:153:LEU:O	1:A:157:ILE:HG13	0.50	2.06	11	1
1:A:137:LEU:HD21	1:A:154:GLN:HE22	0.50	1.65	12	1
1:A:158:ASN:OD1	1:A:159:ARG:N	0.50	2.45	8	2
1:A:128:LYS:O	1:A:132:LEU:HD12	0.50	2.07	13	3
1:A:153:LEU:HA	1:A:156:GLN:CG	0.50	2.37	20	1
1:A:133:LEU:HD22	1:A:157:ILE:HG13	0.49	1.84	10	1
1:A:137:LEU:HD22	1:A:157:ILE:HG13	0.49	1.82	3	1
1:A:133:LEU:HD23	1:A:153:LEU:HD23	0.49	1.83	17	4
1:A:122:PRO:HA	1:A:125:ILE:HG22	0.49	1.84	17	3
1:A:146:ASP:N	1:A:146:ASP:OD1	0.49	2.45	3	1
1:A:146:ASP:O	1:A:150:ILE:HG13	0.49	2.08	13	10
1:A:141:ASN:OD1	1:A:142:LYS:N	0.49	2.46	2	8
1:A:171:LEU:HD13	1:A:171:LEU:C	0.49	2.28	13	2
1:A:126:LYS:HG2	1:A:160:VAL:HG12	0.49	1.85	1	3
1:A:145:GLN:HB3	1:A:150:ILE:HD11	0.48	1.85	4	1
1:A:129:ALA:O	1:A:133:LEU:HB2	0.48	2.08	10	1
1:A:133:LEU:HD13	1:A:156:GLN:HG2	0.48	1.84	1	1
1:A:129:ALA:CB	1:A:165:VAL:HG21	0.48	2.38	20	2
1:A:125:ILE:HD12	1:A:128:LYS:HD3	0.48	1.84	4	1
1:A:125:ILE:HD13	1:A:125:ILE:O	0.48	2.08	17	1
1:A:165:VAL:HG13	1:A:171:LEU:HD21	0.48	1.86	7	1
1:A:167:LEU:H	1:A:167:LEU:HD23	0.48	1.68	18	1
1:A:156:GLN:HG3	1:A:157:ILE:HD13	0.48	1.84	3	1
1:A:137:LEU:HD11	1:A:154:GLN:HG2	0.48	1.85	6	2
1:A:135:LYS:HG3	1:A:136:LYS:N	0.48	2.23	17	1
1:A:156:GLN:OE1	1:A:171:LEU:HD12	0.48	2.08	9	1
1:A:133:LEU:HD22	1:A:156:GLN:CD	0.47	2.29	7	3
1:A:126:LYS:HG3	1:A:127:ALA:N	0.47	2.23	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HG	1:A:171:LEU:HD13	0.47	1.86	20	1
1:A:170:LYS:O	1:A:173:GLU:HG3	0.47	2.09	8	2
1:A:137:LEU:CD2	1:A:157:ILE:HD13	0.47	2.32	10	1
1:A:133:LEU:HD22	1:A:153:LEU:CD2	0.47	2.39	20	1
1:A:128:LYS:CE	1:A:175:LEU:HD22	0.47	2.39	11	2
1:A:140:ALA:HB1	1:A:145:GLN:CG	0.47	2.40	16	1
1:A:137:LEU:HD12	1:A:150:ILE:CG2	0.47	2.39	1	2
1:A:132:LEU:C	1:A:132:LEU:CD1	0.47	2.80	6	1
1:A:139:ARG:O	1:A:143:PHE:CG	0.46	2.68	13	1
1:A:141:ASN:HA	1:A:150:ILE:HD13	0.46	1.87	6	1
1:A:132:LEU:O	1:A:135:LYS:HG2	0.46	2.11	8	1
1:A:137:LEU:CD2	1:A:157:ILE:HD12	0.46	2.39	11	1
1:A:125:ILE:O	1:A:128:LYS:HG2	0.46	2.11	2	2
1:A:137:LEU:HD13	1:A:153:LEU:HB3	0.46	1.85	6	1
1:A:137:LEU:HD21	1:A:154:GLN:HG2	0.46	1.86	10	1
1:A:128:LYS:HD2	1:A:175:LEU:HD22	0.46	1.88	11	2
1:A:142:LYS:CG	1:A:143:PHE:CD1	0.46	2.98	13	1
1:A:129:ALA:HB2	1:A:165:VAL:CG2	0.46	2.41	19	1
1:A:166:ASP:O	1:A:172:ALA:CB	0.46	2.64	8	2
1:A:132:LEU:HD12	1:A:132:LEU:C	0.45	2.32	2	1
1:A:156:GLN:CG	1:A:157:ILE:HD13	0.45	2.41	3	1
1:A:171:LEU:HG	1:A:175:LEU:HD12	0.45	1.88	6	2
1:A:171:LEU:C	1:A:171:LEU:HD23	0.45	2.31	9	1
1:A:133:LEU:CD1	1:A:171:LEU:CD2	0.45	2.95	13	1
1:A:140:ALA:O	1:A:145:GLN:HB2	0.45	2.11	8	1
1:A:133:LEU:CD2	1:A:153:LEU:CD2	0.45	2.95	10	1
1:A:133:LEU:CD2	1:A:156:GLN:OE1	0.45	2.64	15	1
1:A:133:LEU:HD22	1:A:157:ILE:CD1	0.44	2.41	3	1
1:A:160:VAL:O	1:A:164:GLY:HA2	0.44	2.12	6	3
1:A:129:ALA:O	1:A:133:LEU:CD1	0.44	2.60	12	1
1:A:150:ILE:N	1:A:150:ILE:HD13	0.44	2.28	7	1
1:A:133:LEU:HA	1:A:136:LYS:CE	0.44	2.42	12	1
1:A:129:ALA:HB2	1:A:175:LEU:CD1	0.44	2.40	8	2
1:A:160:VAL:HA	1:A:164:GLY:CA	0.44	2.42	5	2
1:A:145:GLN:O	1:A:150:ILE:HD11	0.44	2.13	7	1
1:A:153:LEU:HA	1:A:156:GLN:CD	0.44	2.33	20	1
1:A:130:LEU:HD11	1:A:161:GLU:HG2	0.43	1.90	4	1
1:A:143:PHE:CD1	1:A:143:PHE:N	0.43	2.86	1	4
1:A:155:ARG:HG3	1:A:156:GLN:N	0.43	2.28	4	3
1:A:125:ILE:CG1	1:A:126:LYS:N	0.43	2.81	5	1
1:A:129:ALA:CB	1:A:165:VAL:CG2	0.43	2.97	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:LEU:HD23	1:A:172:ALA:N	0.43	2.29	9	1
1:A:128:LYS:HG3	1:A:129:ALA:N	0.43	2.28	10	1
1:A:156:GLN:OE1	1:A:171:LEU:HD11	0.43	2.12	10	1
1:A:144:GLY:O	1:A:145:GLN:O	0.43	2.36	17	1
1:A:125:ILE:CG2	1:A:126:LYS:N	0.43	2.81	12	4
1:A:132:LEU:HD12	1:A:136:LYS:HD2	0.43	1.91	6	1
1:A:158:ASN:O	1:A:161:GLU:HG2	0.42	2.14	14	4
1:A:139:ARG:O	1:A:143:PHE:CD2	0.42	2.72	13	1
1:A:153:LEU:CD2	1:A:156:GLN:OE1	0.42	2.67	6	1
1:A:133:LEU:HB3	1:A:157:ILE:CG1	0.42	2.43	10	2
1:A:153:LEU:HA	1:A:156:GLN:HG2	0.42	1.91	15	1
1:A:170:LYS:O	1:A:173:GLU:CG	0.42	2.67	17	1
1:A:125:ILE:HG23	1:A:126:LYS:N	0.42	2.29	7	1
1:A:146:ASP:O	1:A:150:ILE:HG12	0.42	2.15	7	1
1:A:152:SER:O	1:A:155:ARG:HG2	0.42	2.15	7	1
1:A:142:LYS:HG3	1:A:143:PHE:CD1	0.42	2.50	13	1
1:A:125:ILE:HD13	1:A:126:LYS:N	0.42	2.30	20	1
1:A:165:VAL:HG13	1:A:171:LEU:HG	0.42	1.91	1	2
1:A:145:GLN:HG3	1:A:146:ASP:N	0.41	2.30	4	1
1:A:152:SER:O	1:A:155:ARG:HG3	0.41	2.16	10	2
1:A:126:LYS:CD	1:A:130:LEU:CD1	0.41	2.98	10	1
1:A:170:LYS:O	1:A:173:GLU:HG2	0.41	2.14	13	1
1:A:162:LYS:HG3	1:A:163:PHE:CD2	0.41	2.51	4	1
1:A:128:LYS:O	1:A:132:LEU:HD23	0.41	2.16	18	1
1:A:171:LEU:HD12	1:A:175:LEU:HD12	0.41	1.86	7	1
1:A:156:GLN:OE1	1:A:171:LEU:CD1	0.41	2.69	10	1
1:A:128:LYS:CD	1:A:175:LEU:CD2	0.41	2.98	11	1
1:A:142:LYS:CG	1:A:143:PHE:CE1	0.41	3.04	13	1
1:A:165:VAL:HG22	1:A:171:LEU:HD21	0.41	1.91	20	1
1:A:171:LEU:HD13	1:A:175:LEU:HD12	0.41	1.93	19	1
1:A:133:LEU:HA	1:A:136:LYS:HD2	0.41	1.93	6	1
1:A:133:LEU:HD21	1:A:171:LEU:HD11	0.40	1.91	16	1
1:A:150:ILE:O	1:A:154:GLN:HB2	0.40	2.17	10	1
1:A:122:PRO:HA	1:A:125:ILE:CG2	0.40	2.47	20	1
1:A:123:GLU:O	1:A:127:ALA:CB	0.40	2.70	20	1
1:A:125:ILE:HG22	1:A:165:VAL:HG23	0.40	1.92	19	1
1:A:130:LEU:O	1:A:134:ASN:ND2	0.40	2.54	3	1
1:A:130:LEU:HD23	1:A:157:ILE:HG23	0.40	1.94	5	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	54/67 (81%)	52±1 (97±2%)	1±0 (2±1%)	1±0 (1±1%)	20 68
All	All	1080/1340 (81%)	1044 (97%)	25 (2%)	11 (1%)	20 68

All 2 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	145	GLN	10
1	A	146	ASP	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/57 (82%)	33±3 (70±5%)	14±3 (30±5%)	1 16
All	All	940/1140 (82%)	656 (70%)	284 (30%)	1 16

All 33 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	130	LEU	18
1	A	170	LYS	18
1	A	154	GLN	17
1	A	131	ASP	14
1	A	135	LYS	14
1	A	145	GLN	13
1	A	159	ARG	13
1	A	166	ASP	13

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Mol	Chain	Res	Type	Models (Total)
1	A	128	LYS	13
1	A	132	LEU	12
1	A	126	LYS	11
1	A	142	LYS	11
1	A	174	GLU	11
1	A	152	SER	10
1	A	155	ARG	10
1	A	139	ARG	8
1	A	173	GLU	8
1	A	175	LEU	8
1	A	156	GLN	7
1	A	124	GLU	7
1	A	125	ILE	6
1	A	136	LYS	6
1	A	171	LEU	6
1	A	147	GLN	5
1	A	146	ASP	5
1	A	133	LEU	4
1	A	149	ASP	4
1	A	162	LYS	3
1	A	151	ASP	3
1	A	161	GLU	2
1	A	123	GLU	2
1	A	150	ILE	1
1	A	163	PHE	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

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 84% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *tho1.dep.data.csh*

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	789
Number of shifts mapped to atoms	789
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	67	-0.81 ± 0.12	Should be applied
$^{13}C_{\beta}$	63	-0.62 ± 0.17	Should be applied
$^{13}C'$	67	-0.97 ± 0.10	Should be applied
^{15}N	66	0.06 ± 0.43	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 84%, i.e. 646 atoms were assigned a chemical shift out of a possible 773. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	270/270 (100%)	109/109 (100%)	108/108 (100%)	53/53 (100%)
Sidechain	364/475 (77%)	290/303 (96%)	74/148 (50%)	0/24 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	12/28 (43%)	12/14 (86%)	0/12 (0%)	0/2 (0%)
Overall	646/773 (84%)	411/426 (96%)	182/268 (68%)	53/79 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 786 atoms were assigned a chemical shift out of a possible 934. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	336/337 (100%)	136/137 (99%)	134/134 (100%)	66/66 (100%)
Sidechain	438/569 (77%)	347/364 (95%)	91/176 (52%)	0/29 (0%)
Aromatic	12/28 (43%)	12/14 (86%)	0/12 (0%)	0/2 (0%)
Overall	786/934 (84%)	495/515 (96%)	225/322 (70%)	66/97 (68%)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: