



Full wwPDB NMR Structure Validation Report ⓘ

Aug 14, 2017 – 12:14 PM EDT

PDB ID : 2NDH
Title : NMR solution structure of MAL/TIRAP TIR domain (C116A)
Authors : Lavrencic, P.; Mobli, M.
Deposited on : unknown

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20029824
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

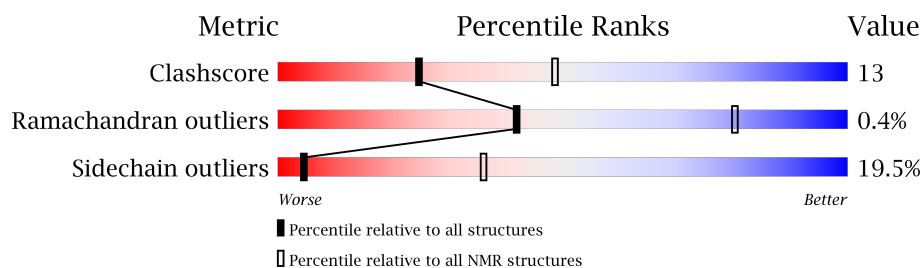
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	143	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 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:84-A:122, A:134-A:192, A:197-A:221 (123)	0.96	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2179 atoms, of which 1079 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Toll/interleukin-1 receptor domain-containing adapter protein.

Mol	Chain	Residues	Atoms						Trace
1	A	143	Total	C	H	N	O	S	0
			2179	694	1079	187	210	9	

There is a discrepancy between the modelled and reference sequences:

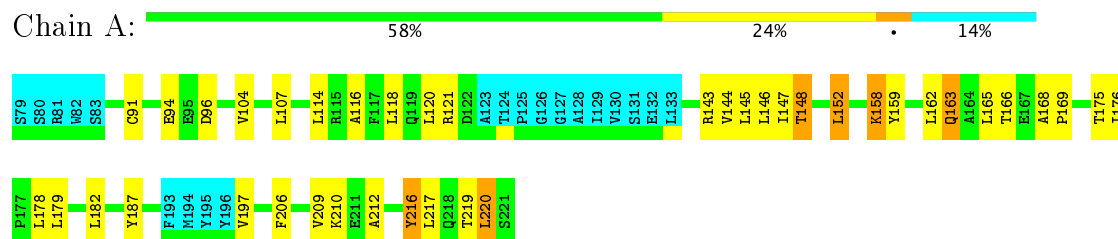
Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	CYS	ENGINEERED MUTATION	UNP P58753

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: Toll/interleukin-1 receptor domain-containing adapter protein

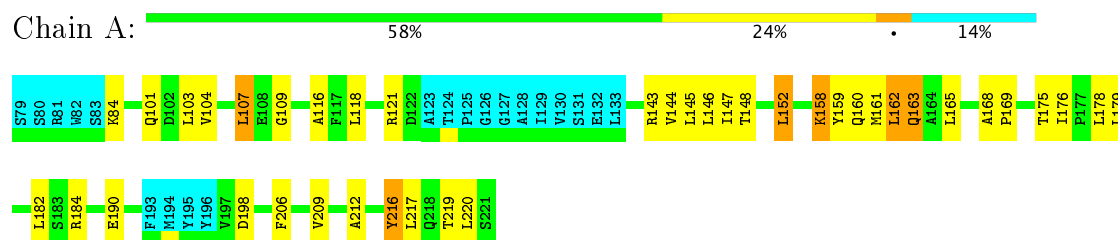


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

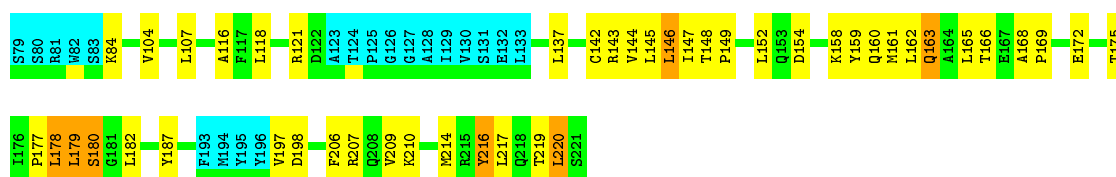
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.2 Score per residue for model 2

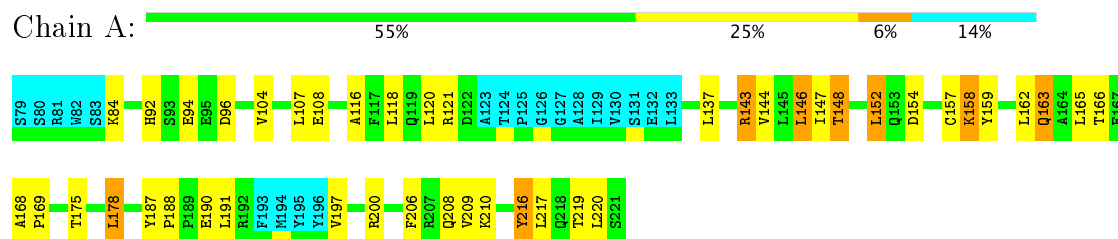
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein





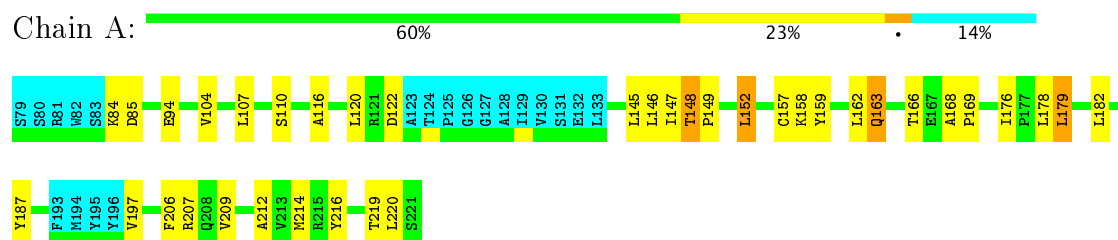
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



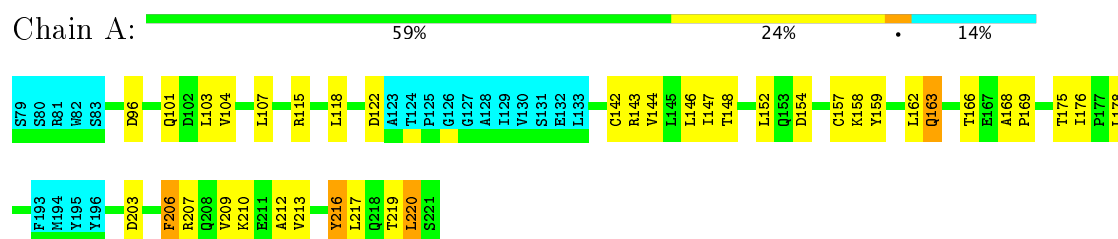
4.2.4 Score per residue for model 4

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



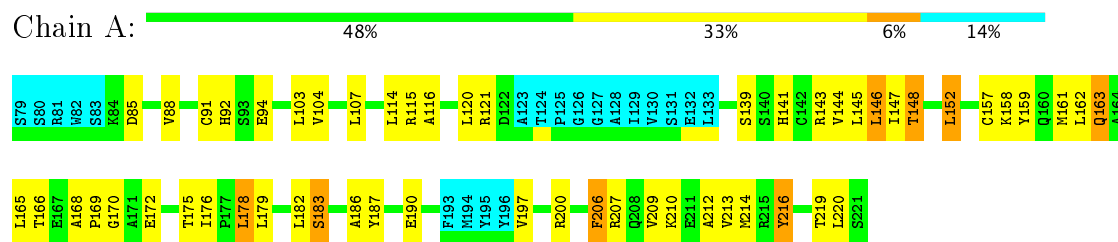
4.2.5 Score per residue for model 5

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



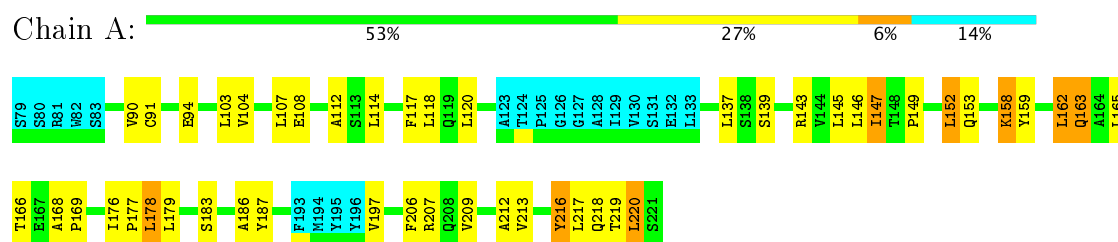
4.2.6 Score per residue for model 6

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



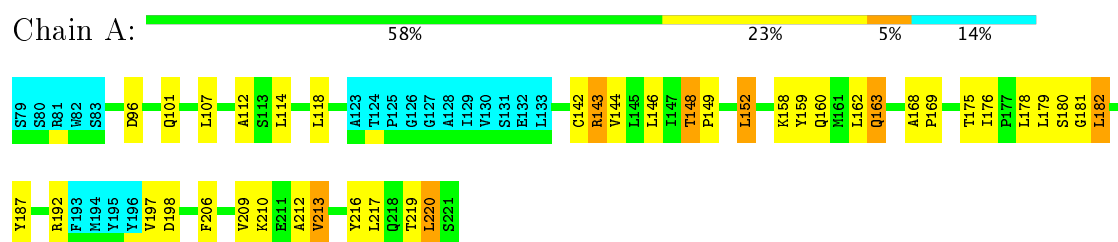
4.2.7 Score per residue for model 7

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



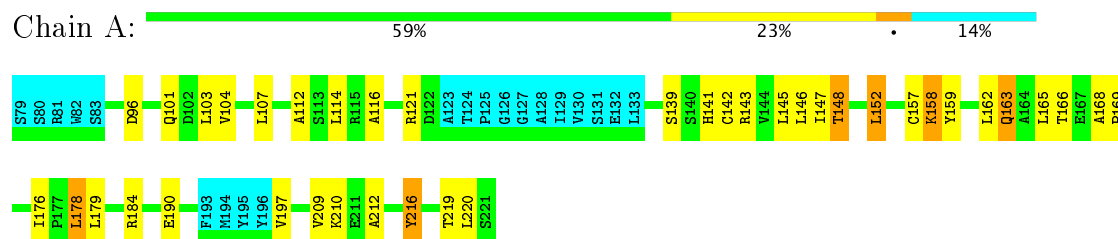
4.2.8 Score per residue for model 8

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



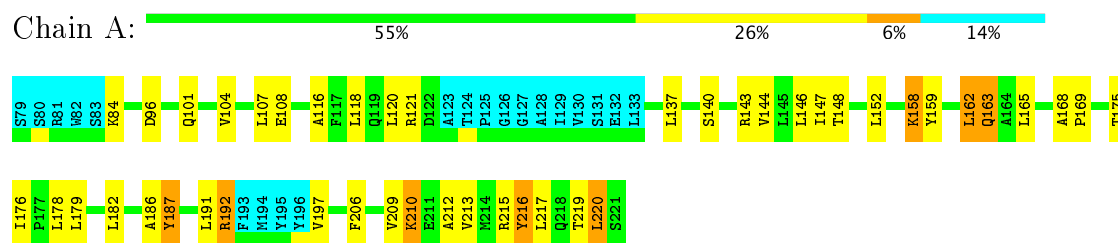
4.2.9 Score per residue for model 9

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



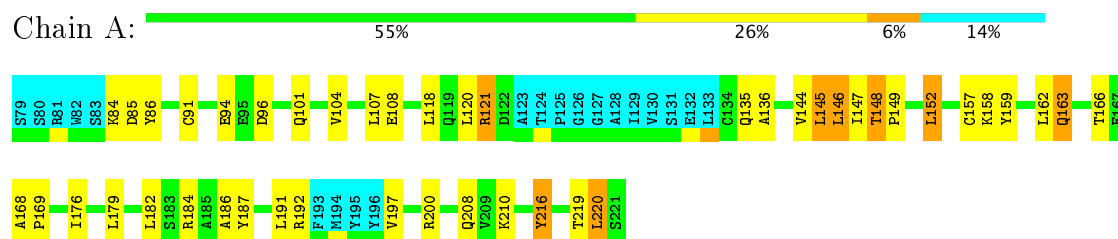
4.2.10 Score per residue for model 10

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.11 Score per residue for model 11

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



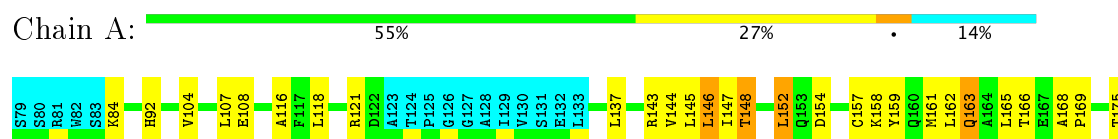
4.2.12 Score per residue for model 12

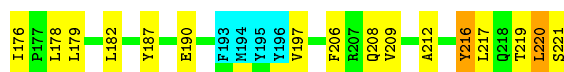
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.13 Score per residue for model 13

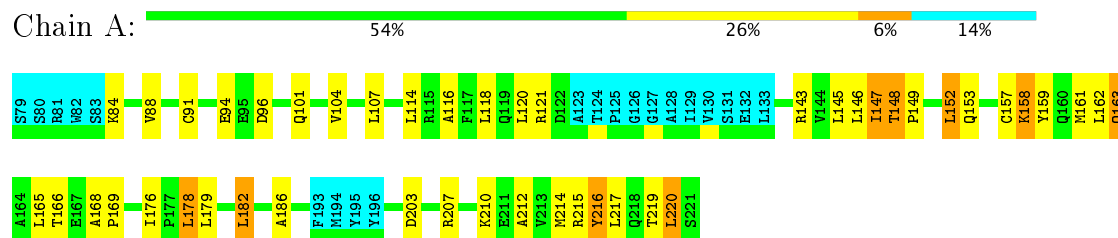
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein





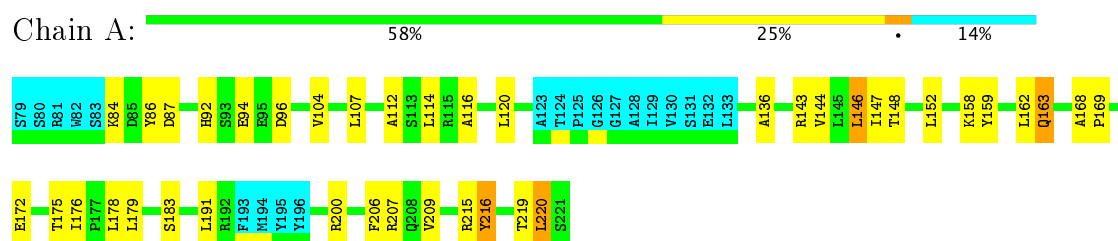
4.2.14 Score per residue for model 14

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



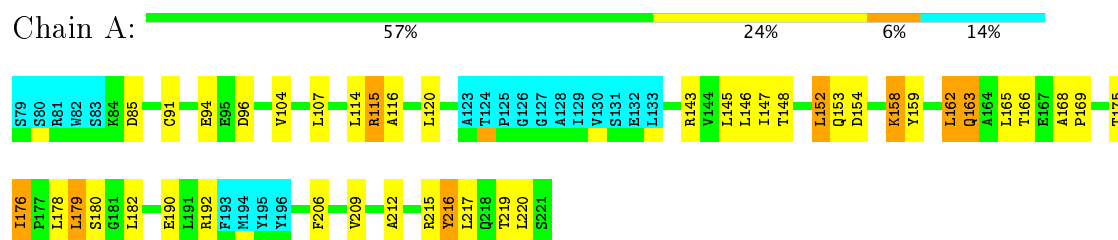
4.2.15 Score per residue for model 15

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.16 Score per residue for model 16

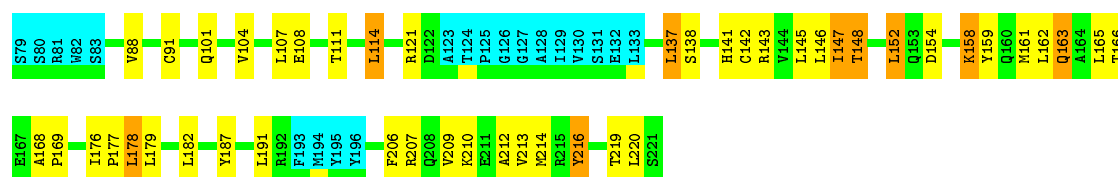
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.17 Score per residue for model 17

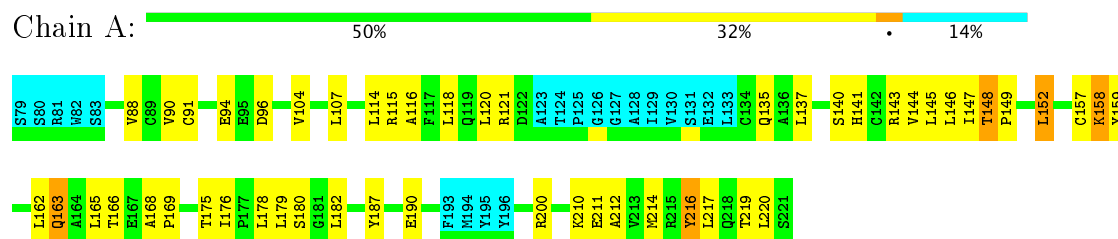
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein





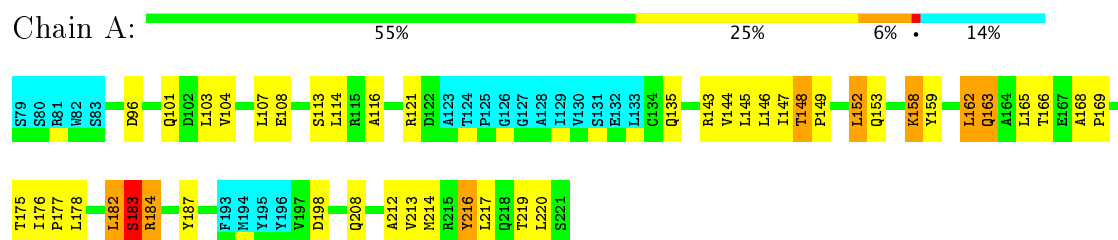
4.2.18 Score per residue for model 18

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



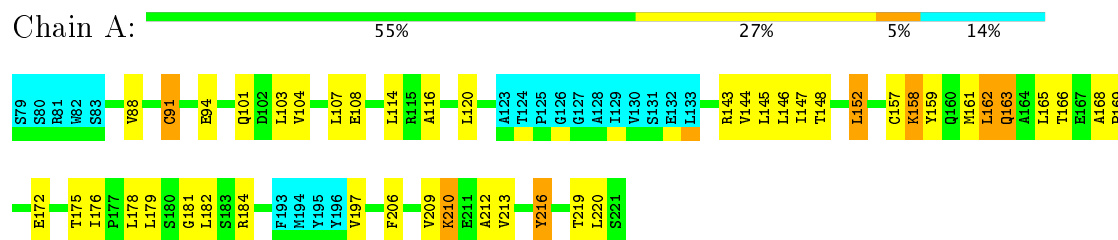
4.2.19 Score per residue for model 19

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.20 Score per residue for model 20

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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)	2ndh_cs.cif
Number of chemical shift lists	1
Total number of shifts	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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	944	933	933	25±5
All	All	18880	18660	18660	501

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:104:VAL:HG23	1:A:116:ALA:HB3	0.86	1.47	15	11
1:A:112:ALA:HB1	1:A:114:LEU:HD13	0.83	1.49	7	3
1:A:179:LEU:HD12	1:A:182:LEU:HD12	0.80	1.53	12	1
1:A:176:ILE:HD13	1:A:212:ALA:HB3	0.79	1.55	8	9
1:A:144:VAL:HG13	1:A:176:ILE:HD11	0.78	1.54	10	9
1:A:162:LEU:C	1:A:162:LEU:HD22	0.77	1.99	20	1
1:A:145:LEU:HD21	1:A:147:ILE:HD11	0.76	1.56	7	3
1:A:137:LEU:HD22	1:A:137:LEU:C	0.75	2.01	17	1
1:A:219:THR:HG23	1:A:220:LEU:HD23	0.71	1.63	15	5
1:A:182:LEU:HD12	1:A:187:TYR:CE1	0.67	2.25	8	2
1:A:216:TYR:O	1:A:219:THR:HG22	0.66	1.90	14	20
1:A:182:LEU:HD13	1:A:187:TYR:CZ	0.66	2.25	19	1
1:A:94:GLU:O	1:A:97:LEU:HD23	0.65	1.92	12	1
1:A:137:LEU:HD12	1:A:143:ARG:HD3	0.65	1.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ILE:HD13	1:A:212:ALA:HB1	0.64	1.68	12	6
1:A:176:ILE:HD13	1:A:212:ALA:CB	0.64	2.22	18	4
1:A:179:LEU:HD12	1:A:182:LEU:HD13	0.64	1.69	17	1
1:A:94:GLU:CB	1:A:120:LEU:HD21	0.63	2.23	15	7
1:A:88:VAL:CG2	1:A:114:LEU:HD21	0.63	2.24	18	3
1:A:159:TYR:O	1:A:162:LEU:HD22	0.62	1.95	7	15
1:A:88:VAL:CG2	1:A:114:LEU:HD11	0.62	2.25	20	2
1:A:162:LEU:HD13	1:A:163:GLN:N	0.62	2.09	20	1
1:A:187:TYR:CE2	1:A:197:VAL:HG21	0.61	2.30	4	3
1:A:143:ARG:HB2	1:A:175:THR:HG22	0.61	1.73	19	12
1:A:191:LEU:HD23	1:A:197:VAL:CG1	0.61	2.26	11	1
1:A:178:LEU:O	1:A:179:LEU:HD23	0.61	1.95	8	1
1:A:165:LEU:HD13	1:A:190:GLU:CB	0.61	2.26	3	2
1:A:86:TYR:CZ	1:A:136:ALA:HB1	0.61	2.31	15	2
1:A:159:TYR:O	1:A:162:LEU:HD23	0.60	1.96	4	4
1:A:143:ARG:CB	1:A:175:THR:HG22	0.59	2.27	16	7
1:A:104:VAL:HG22	1:A:108:GLU:HG3	0.59	1.75	17	6
1:A:149:PRO:O	1:A:186:ALA:HB1	0.59	1.98	11	1
1:A:182:LEU:HD21	1:A:186:ALA:HB3	0.59	1.74	14	1
1:A:187:TYR:HB2	1:A:191:LEU:HD21	0.59	1.75	12	1
1:A:145:LEU:HD12	1:A:175:THR:CB	0.59	2.28	19	1
1:A:88:VAL:HG23	1:A:114:LEU:HD11	0.59	1.74	20	1
1:A:179:LEU:HB3	1:A:182:LEU:HD11	0.59	1.75	8	1
1:A:182:LEU:HD22	1:A:187:TYR:CE1	0.58	2.33	19	4
1:A:187:TYR:CZ	1:A:197:VAL:HG21	0.58	2.32	7	2
1:A:176:ILE:CD1	1:A:212:ALA:HB1	0.58	2.29	12	6
1:A:91:CYS:O	1:A:145:LEU:HD23	0.57	1.99	18	3
1:A:182:LEU:HD21	1:A:186:ALA:CB	0.57	2.29	14	1
1:A:145:LEU:HD12	1:A:175:THR:OG1	0.57	1.99	18	2
1:A:159:TYR:O	1:A:162:LEU:HD12	0.57	2.00	20	1
1:A:165:LEU:HD13	1:A:190:GLU:HG2	0.57	1.77	18	1
1:A:165:LEU:HD13	1:A:190:GLU:HB3	0.57	1.77	9	4
1:A:147:ILE:HD12	1:A:152:LEU:CB	0.56	2.30	20	3
1:A:149:PRO:HB3	1:A:179:LEU:HD21	0.56	1.77	4	1
1:A:137:LEU:C	1:A:137:LEU:CD2	0.56	2.74	17	1
1:A:149:PRO:HA	1:A:152:LEU:HD22	0.56	1.77	7	1
1:A:181:GLY:O	1:A:182:LEU:HD22	0.56	2.00	20	1
1:A:91:CYS:O	1:A:145:LEU:HD22	0.56	2.00	11	1
1:A:91:CYS:O	1:A:145:LEU:HD12	0.56	2.01	7	3
1:A:182:LEU:HD12	1:A:187:TYR:CD1	0.56	2.35	11	2
1:A:112:ALA:HB1	1:A:114:LEU:CD1	0.56	2.31	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG21	1:A:114:LEU:HD21	0.56	1.78	18	2
1:A:148:THR:O	1:A:152:LEU:HD23	0.56	2.01	17	3
1:A:178:LEU:HD23	1:A:212:ALA:HB2	0.55	1.78	9	1
1:A:216:TYR:CD2	1:A:217:LEU:HD22	0.55	2.36	19	2
1:A:181:GLY:C	1:A:182:LEU:HD23	0.55	2.22	8	1
1:A:114:LEU:HD23	1:A:115:ARG:N	0.55	2.16	6	3
1:A:179:LEU:HD23	1:A:182:LEU:HG	0.55	1.77	20	1
1:A:104:VAL:CG2	1:A:116:ALA:HB3	0.54	2.32	12	6
1:A:216:TYR:CE1	1:A:217:LEU:HD23	0.54	2.36	5	4
1:A:178:LEU:HD11	1:A:208:GLN:OE1	0.54	2.01	3	1
1:A:182:LEU:O	1:A:182:LEU:HD12	0.54	2.01	6	1
1:A:148:THR:O	1:A:152:LEU:HD22	0.54	2.02	14	8
1:A:192:ARG:HB3	1:A:197:VAL:HG13	0.54	1.79	10	1
1:A:86:TYR:CE2	1:A:136:ALA:HB1	0.54	2.36	11	2
1:A:94:GLU:HB3	1:A:120:LEU:HD21	0.54	1.78	15	1
1:A:179:LEU:HD13	1:A:180:SER:N	0.54	2.18	2	1
1:A:162:LEU:C	1:A:162:LEU:HD12	0.54	2.24	4	2
1:A:178:LEU:HD23	1:A:209:VAL:HG23	0.54	1.79	6	1
1:A:94:GLU:HB2	1:A:120:LEU:HD21	0.54	1.80	11	1
1:A:179:LEU:HD22	1:A:197:VAL:HG11	0.54	1.80	20	1
1:A:179:LEU:HD21	1:A:182:LEU:O	0.54	2.03	14	1
1:A:149:PRO:CB	1:A:182:LEU:HD12	0.54	2.33	19	1
1:A:149:PRO:HB3	1:A:179:LEU:HD11	0.53	1.79	2	1
1:A:158:LYS:HE3	1:A:165:LEU:HD12	0.53	1.79	7	12
1:A:182:LEU:HD23	1:A:187:TYR:CE1	0.53	2.39	2	1
1:A:177:PRO:O	1:A:178:LEU:HD22	0.53	2.04	19	1
1:A:162:LEU:HD12	1:A:162:LEU:C	0.53	2.24	5	2
1:A:179:LEU:HD11	1:A:200:ARG:HA	0.53	1.81	6	1
1:A:94:GLU:CG	1:A:120:LEU:HD21	0.53	2.34	3	4
1:A:137:LEU:HD11	1:A:143:ARG:NE	0.53	2.19	12	1
1:A:178:LEU:C	1:A:179:LEU:HD23	0.53	2.24	8	1
1:A:191:LEU:HD23	1:A:197:VAL:HG11	0.52	1.81	11	1
1:A:179:LEU:HD12	1:A:182:LEU:HB2	0.52	1.80	10	1
1:A:103:LEU:HD22	1:A:210:LYS:HB2	0.52	1.79	12	1
1:A:152:LEU:O	1:A:152:LEU:HD12	0.52	2.05	11	2
1:A:179:LEU:HB2	1:A:182:LEU:HD13	0.52	1.81	16	2
1:A:91:CYS:O	1:A:145:LEU:HD13	0.52	2.05	20	2
1:A:144:VAL:HG12	1:A:146:LEU:CD2	0.52	2.35	15	6
1:A:143:ARG:O	1:A:176:ILE:HG22	0.52	2.05	17	5
1:A:152:LEU:HD23	1:A:153:GLN:N	0.51	2.20	7	1
1:A:103:LEU:HD11	1:A:213:VAL:HG11	0.51	1.83	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:CB	1:A:182:LEU:HD13	0.51	2.35	16	1
1:A:162:LEU:C	1:A:162:LEU:CD2	0.51	2.73	20	1
1:A:178:LEU:O	1:A:179:LEU:HD22	0.51	2.06	9	3
1:A:137:LEU:HD12	1:A:143:ARG:NE	0.51	2.20	18	1
1:A:145:LEU:CD2	1:A:147:ILE:HD11	0.50	2.36	14	1
1:A:206:PHE:O	1:A:209:VAL:HG22	0.50	2.07	3	7
1:A:162:LEU:HD23	1:A:163:GLN:N	0.50	2.22	12	15
1:A:104:VAL:HG22	1:A:108:GLU:CG	0.49	2.36	7	1
1:A:145:LEU:HD23	1:A:177:PRO:HB3	0.49	1.84	2	1
1:A:152:LEU:HD12	1:A:152:LEU:O	0.49	2.07	16	2
1:A:103:LEU:HD13	1:A:209:VAL:CG1	0.49	2.37	9	1
1:A:188:PRO:HG2	1:A:191:LEU:HD13	0.49	1.85	3	1
1:A:219:THR:CG2	1:A:220:LEU:HD23	0.49	2.37	10	5
1:A:181:GLY:C	1:A:182:LEU:HD22	0.49	2.28	20	1
1:A:149:PRO:HD3	1:A:179:LEU:HD12	0.49	1.83	18	1
1:A:161:MET:HE2	1:A:165:LEU:HD11	0.49	1.83	1	4
1:A:182:LEU:HD23	1:A:187:TYR:CD1	0.49	2.43	2	1
1:A:162:LEU:HD12	1:A:163:GLN:N	0.49	2.23	5	4
1:A:162:LEU:HD13	1:A:163:GLN:H	0.49	1.65	20	1
1:A:178:LEU:HD22	1:A:198:ASP:HB3	0.48	1.84	12	1
1:A:217:LEU:HD13	1:A:220:LEU:HD23	0.48	1.83	19	2
1:A:178:LEU:C	1:A:179:LEU:HD22	0.48	2.28	7	3
1:A:217:LEU:HD12	1:A:218:GLN:N	0.48	2.24	7	1
1:A:178:LEU:CD2	1:A:212:ALA:HB2	0.48	2.39	9	1
1:A:187:TYR:CE2	1:A:197:VAL:HG11	0.47	2.44	6	1
1:A:118:LEU:HD12	1:A:120:LEU:HD13	0.47	1.85	12	1
1:A:103:LEU:HD12	1:A:104:VAL:N	0.47	2.24	1	2
1:A:137:LEU:HD13	1:A:143:ARG:NH1	0.47	2.25	7	1
1:A:145:LEU:HD12	1:A:175:THR:HB	0.47	1.85	19	2
1:A:143:ARG:HB3	1:A:175:THR:HG22	0.47	1.86	18	2
1:A:176:ILE:O	1:A:176:ILE:HG23	0.47	2.10	12	2
1:A:114:LEU:HD22	1:A:216:TYR:OH	0.47	2.09	19	1
1:A:219:THR:CG2	1:A:220:LEU:HD22	0.46	2.40	19	15
1:A:176:ILE:HG23	1:A:176:ILE:O	0.46	2.10	9	4
1:A:210:LYS:O	1:A:213:VAL:HG12	0.46	2.10	8	5
1:A:137:LEU:HD22	1:A:138:SER:N	0.46	2.24	17	1
1:A:103:LEU:HD13	1:A:209:VAL:HG11	0.46	1.87	9	1
1:A:152:LEU:CD2	1:A:179:LEU:HD11	0.46	2.41	11	1
1:A:177:PRO:HG2	1:A:197:VAL:HG12	0.46	1.88	7	1
1:A:179:LEU:HD23	1:A:197:VAL:HB	0.46	1.87	12	1
1:A:177:PRO:HG3	1:A:191:LEU:HD22	0.46	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ILE:HD12	1:A:152:LEU:HB2	0.46	1.88	20	2
1:A:187:TYR:CD2	1:A:191:LEU:HD12	0.46	2.45	17	1
1:A:182:LEU:HD22	1:A:187:TYR:CD2	0.45	2.46	10	1
1:A:213:VAL:O	1:A:217:LEU:HD12	0.45	2.11	10	1
1:A:103:LEU:O	1:A:103:LEU:HD13	0.45	2.11	6	1
1:A:187:TYR:OH	1:A:197:VAL:HG21	0.45	2.12	3	1
1:A:206:PHE:O	1:A:209:VAL:HG12	0.45	2.12	10	8
1:A:192:ARG:HG3	1:A:197:VAL:HG22	0.45	1.88	8	1
1:A:178:LEU:HD13	1:A:179:LEU:N	0.45	2.26	14	2
1:A:90:VAL:HG12	1:A:117:PHE:O	0.45	2.11	7	2
1:A:183:SER:OG	1:A:186:ALA:HB2	0.45	2.12	7	1
1:A:178:LEU:HD13	1:A:198:ASP:HB2	0.45	1.88	19	1
1:A:182:LEU:HD11	1:A:186:ALA:HB3	0.45	1.89	14	1
1:A:103:LEU:HD21	1:A:213:VAL:HG11	0.45	1.88	19	1
1:A:137:LEU:HD12	1:A:143:ARG:CD	0.44	2.41	10	1
1:A:161:MET:HE3	1:A:165:LEU:HD11	0.44	1.88	13	1
1:A:149:PRO:CB	1:A:182:LEU:HD23	0.44	2.41	14	1
1:A:179:LEU:HD23	1:A:197:VAL:CG1	0.44	2.43	12	1
1:A:182:LEU:HD13	1:A:187:TYR:OH	0.44	2.12	19	1
1:A:219:THR:HG23	1:A:220:LEU:HD22	0.43	1.90	11	15
1:A:168:ALA:HB1	1:A:169:PRO:HD2	0.43	1.90	17	19
1:A:182:LEU:HD23	1:A:186:ALA:HB1	0.43	1.90	10	1
1:A:94:GLU:HG3	1:A:120:LEU:HD21	0.43	1.90	20	3
1:A:161:MET:HE3	1:A:165:LEU:HD21	0.43	1.91	20	2
1:A:179:LEU:HD12	1:A:182:LEU:CD1	0.43	2.42	17	1
1:A:149:PRO:HB3	1:A:182:LEU:HD12	0.43	1.91	19	1
1:A:162:LEU:HD22	1:A:163:GLN:N	0.43	2.28	20	1
1:A:178:LEU:C	1:A:178:LEU:HD13	0.43	2.34	20	4
1:A:183:SER:CB	1:A:186:ALA:HB2	0.43	2.44	6	1
1:A:179:LEU:CD2	1:A:182:LEU:HD13	0.43	2.44	4	1
1:A:86:TYR:OH	1:A:136:ALA:HB1	0.43	2.14	15	1
1:A:179:LEU:HD12	1:A:182:LEU:HG	0.42	1.91	1	1
1:A:137:LEU:HD21	1:A:143:ARG:NH1	0.42	2.29	2	1
1:A:90:VAL:HG21	1:A:100:ALA:HB1	0.42	1.91	12	1
1:A:182:LEU:HD13	1:A:187:TYR:CE1	0.42	2.50	6	1
1:A:179:LEU:HB3	1:A:182:LEU:HD23	0.42	1.91	20	1
1:A:178:LEU:HD22	1:A:198:ASP:O	0.42	2.14	2	1
1:A:210:LYS:HG2	1:A:211:GLU:N	0.42	2.29	18	1
1:A:104:VAL:HG22	1:A:108:GLU:HG2	0.42	1.90	7	1
1:A:178:LEU:HD13	1:A:178:LEU:C	0.42	2.35	8	2
1:A:149:PRO:HB3	1:A:182:LEU:HD22	0.42	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:VAL:HG12	1:A:146:LEU:HD22	0.41	1.91	2	1
1:A:162:LEU:HD23	1:A:163:GLN:H	0.41	1.75	6	9
1:A:182:LEU:HD23	1:A:183:SER:H	0.41	1.76	19	1
1:A:162:LEU:O	1:A:162:LEU:HD22	0.41	2.13	20	1
1:A:179:LEU:HD23	1:A:197:VAL:CB	0.41	2.45	12	1
1:A:178:LEU:HG	1:A:209:VAL:HG12	0.41	1.92	8	1
1:A:118:LEU:HD13	1:A:120:LEU:HD13	0.41	1.91	10	1
1:A:176:ILE:HD12	1:A:212:ALA:HB1	0.41	1.91	16	1
1:A:178:LEU:HD21	1:A:208:GLN:OE1	0.41	2.16	19	1
1:A:144:VAL:HG12	1:A:146:LEU:HD23	0.41	1.92	11	1
1:A:216:TYR:CD1	1:A:217:LEU:HD23	0.41	2.51	14	1
1:A:165:LEU:HD13	1:A:190:GLU:CG	0.41	2.44	18	1
1:A:103:LEU:O	1:A:107:LEU:HD22	0.41	2.16	1	1
1:A:112:ALA:O	1:A:114:LEU:HD12	0.40	2.15	9	1
1:A:118:LEU:HD12	1:A:118:LEU:O	0.40	2.16	14	1
1:A:217:LEU:H	1:A:217:LEU:HD22	0.40	1.76	8	1
1:A:176:ILE:CG1	1:A:176:ILE:O	0.40	2.70	13	1
1:A:90:VAL:HG23	1:A:144:VAL:O	0.40	2.16	18	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	122/143 (85%)	106±2 (87±2%)	15±2 (13±2%)	1±1 (0±1%)	42	80
All	All	2440/2860 (85%)	2121 (87%)	309 (13%)	10 (0%)	42	80

All 8 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	184	ARG	2
1	A	206	PHE	2
1	A	109	GLY	1
1	A	183	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	121	ARG	1
1	A	192	ARG	1
1	A	170	GLY	1
1	A	197	VAL	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	103/119 (87%)	83±3 (80±3%)	20±3 (20±3%)	4	36
All	All	2060/2380 (87%)	1658 (80%)	402 (20%)	4	36

All 65 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	163	GLN	20
1	A	146	LEU	20
1	A	152	LEU	20
1	A	107	LEU	20
1	A	158	LYS	20
1	A	148	THR	19
1	A	216	TYR	18
1	A	166	THR	16
1	A	147	ILE	16
1	A	121	ARG	13
1	A	178	LEU	12
1	A	96	ASP	11
1	A	157	CYS	10
1	A	101	GLN	10
1	A	84	LYS	10
1	A	220	LEU	10
1	A	118	LEU	10
1	A	207	ARG	9
1	A	210	LYS	8
1	A	162	LEU	7
1	A	214	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	154	ASP	7
1	A	92	HIS	5
1	A	200	ARG	5
1	A	142	CYS	5
1	A	141	HIS	5
1	A	145	LEU	5
1	A	215	ARG	4
1	A	139	SER	4
1	A	180	SER	4
1	A	172	GLU	4
1	A	184	ARG	4
1	A	85	ASP	4
1	A	135	GLN	3
1	A	183	SER	3
1	A	182	LEU	3
1	A	192	ARG	3
1	A	153	GLN	3
1	A	191	LEU	3
1	A	160	GLN	3
1	A	143	ARG	3
1	A	208	GLN	3
1	A	179	LEU	3
1	A	217	LEU	2
1	A	203	ASP	2
1	A	176	ILE	2
1	A	190	GLU	2
1	A	115	ARG	2
1	A	137	LEU	2
1	A	198	ASP	2
1	A	140	SER	2
1	A	110	SER	1
1	A	114	LEU	1
1	A	221	SER	1
1	A	120	LEU	1
1	A	187	TYR	1
1	A	94	GLU	1
1	A	87	ASP	1
1	A	91	CYS	1
1	A	113	SER	1
1	A	122	ASP	1
1	A	103	LEU	1
1	A	108	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	111	THR	1
1	A	213	VAL	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

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: 2ndh_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1185
Number of shifts mapped to atoms	1185
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	-0.31 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	109	0.42 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.01 ± 0.09	None needed (< 0.5 ppm)
^{15}N	100	0.18 ± 0.29	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 67%, i.e. 978 atoms were assigned a chemical shift out of a possible 1468. 11 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	499/601 (83%)	195/239 (82%)	209/246 (85%)	95/116 (82%)
Sidechain	442/774 (57%)	272/455 (60%)	167/284 (59%)	3/35 (9%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	37/93 (40%)	23/49 (47%)	13/41 (32%)	1/3 (33%)
Overall	978/1468 (67%)	490/743 (66%)	389/571 (68%)	99/154 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1701. 11 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	530/699 (76%)	207/278 (74%)	223/286 (78%)	100/135 (74%)
Sidechain	467/872 (54%)	286/514 (56%)	178/320 (56%)	3/38 (8%)
Aromatic	37/130 (28%)	23/68 (34%)	13/58 (22%)	1/4 (25%)
Overall	1034/1701 (61%)	516/860 (60%)	414/664 (62%)	104/177 (59%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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:

