



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:08 am BST

PDB ID : 2MZD
Title : Characterization of the p300 Taz2-p53 TAD2 Complex and Comparison with the p300 Taz2-p53 TAD1 Complex
Authors : Miller Jenkins, L.M.; Feng, H.; Durell, S.R.; Tagad, H.D.; Mazur, S.J.; Tropea, J.E.; Bai, Y.; Appella, E.
Deposited on : 2015-02-11

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 ⓘ 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

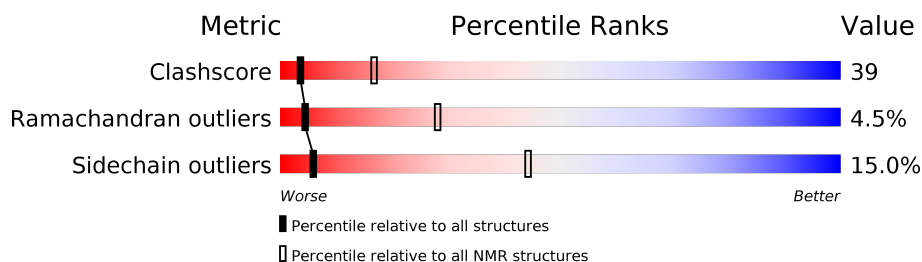
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	90	
2	B	25	

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 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:7-A:88, B:12-B:22 (93)	0.33	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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1791 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone acetyltransferase p300.

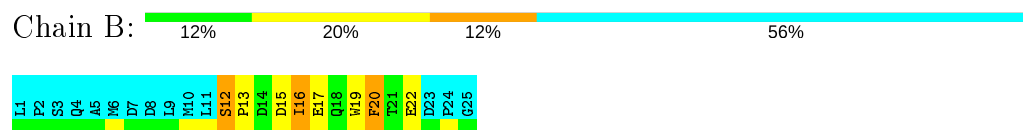
Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1415	420	726	140	119	10	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	CYS	ENGINEERED MUTATION	UNP Q09472
A	24	ALA	CYS	ENGINEERED MUTATION	UNP Q09472
A	67	ALA	CYS	ENGINEERED MUTATION	UNP Q09472
A	68	ALA	CYS	ENGINEERED MUTATION	UNP Q09472

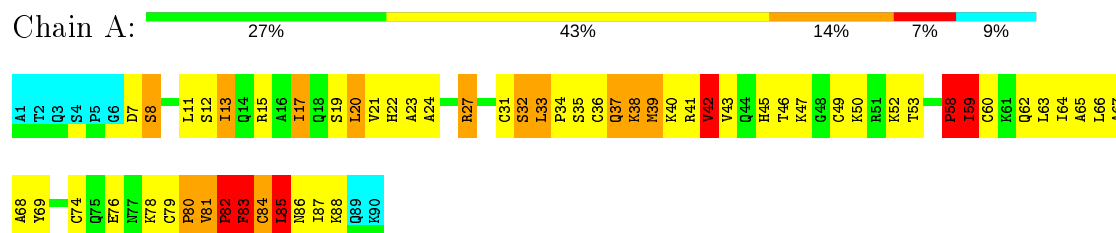
- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						Trace
2	B	25	Total	C	H	N	O	S	0
			376	124	177	28	45	2	

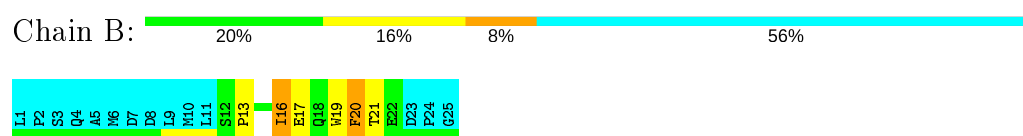


4.2.2 Score per residue for model 2

- Molecule 1: Histone acetyltransferase p300

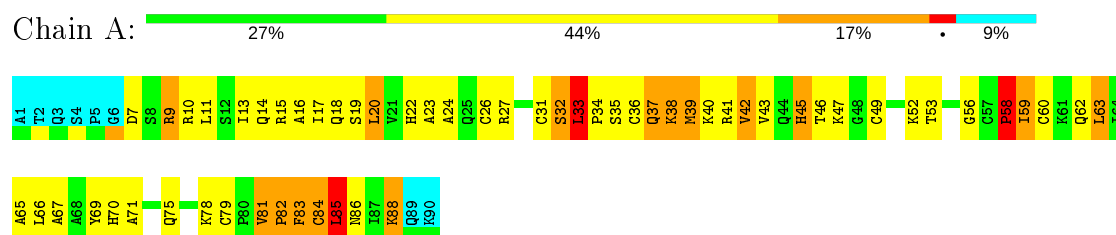


- Molecule 2: Cellular tumor antigen p53

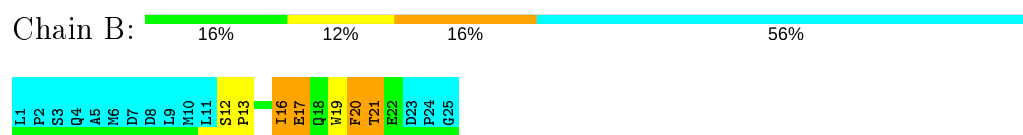


4.2.3 Score per residue for model 3

- Molecule 1: Histone acetyltransferase p300

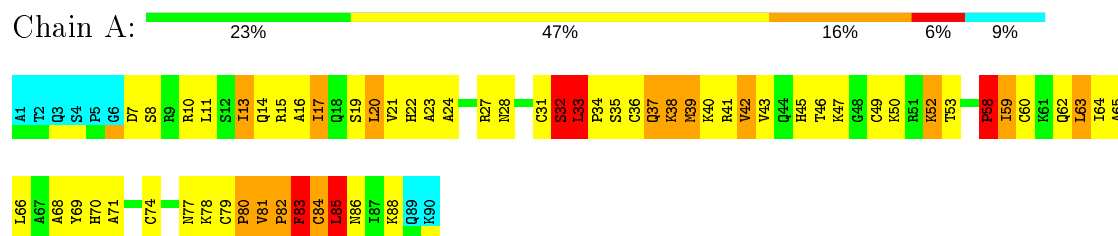


- Molecule 2: Cellular tumor antigen p53

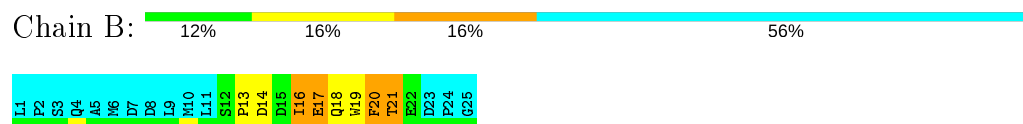


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Histone acetyltransferase p300

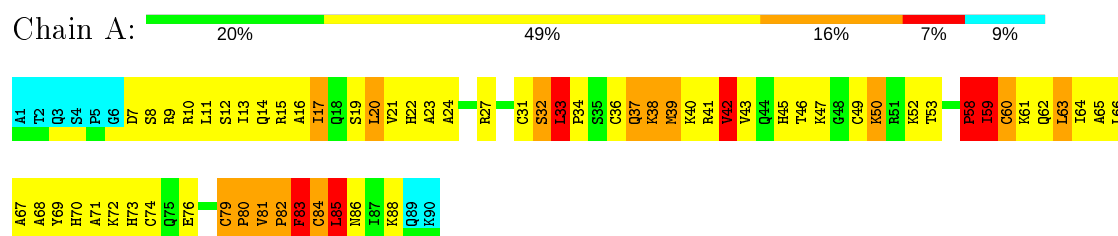


- Molecule 2: Cellular tumor antigen p53

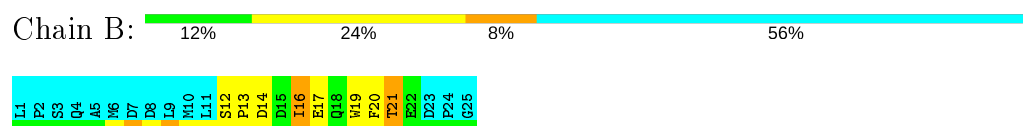


4.2.5 Score per residue for model 5

- Molecule 1: Histone acetyltransferase p300

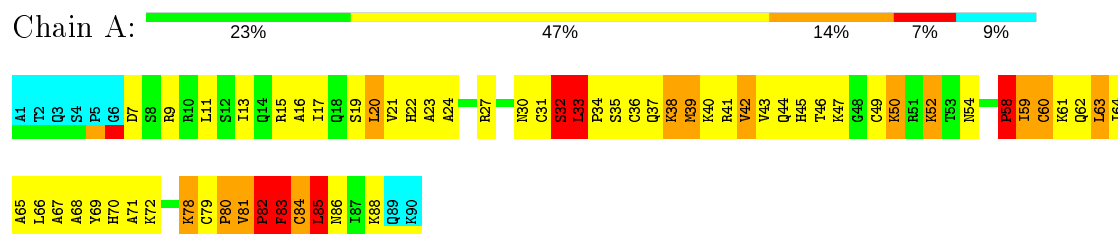


- Molecule 2: Cellular tumor antigen p53



4.2.6 Score per residue for model 6

- Molecule 1: Histone acetyltransferase p300



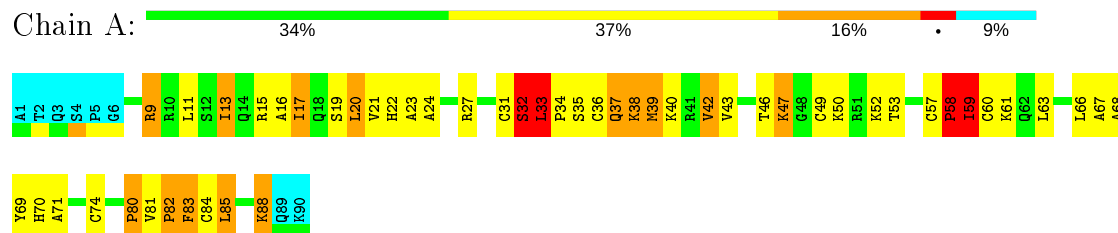
- Molecule 2: Cellular tumor antigen p53



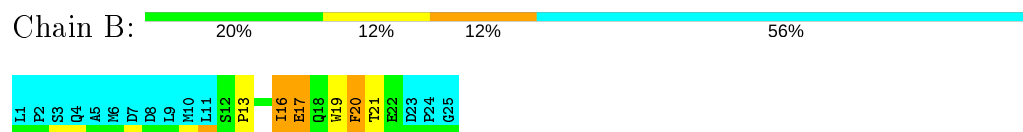


4.2.7 Score per residue for model 7

- Molecule 1: Histone acetyltransferase p300

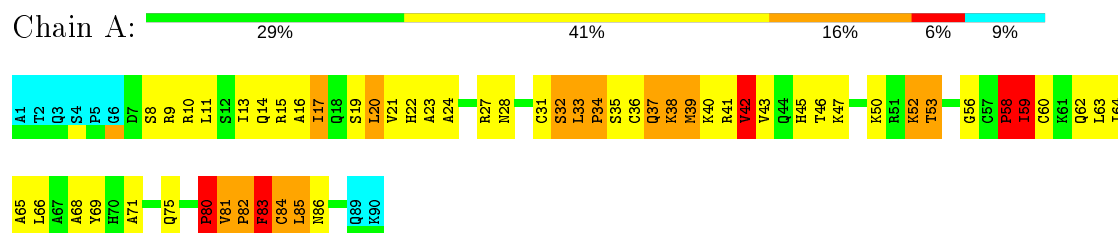


- Molecule 2: Cellular tumor antigen p53

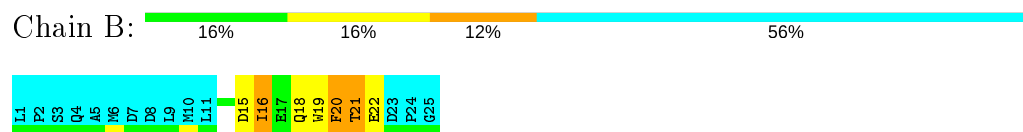


4.2.8 Score per residue for model 8

- Molecule 1: Histone acetyltransferase p300



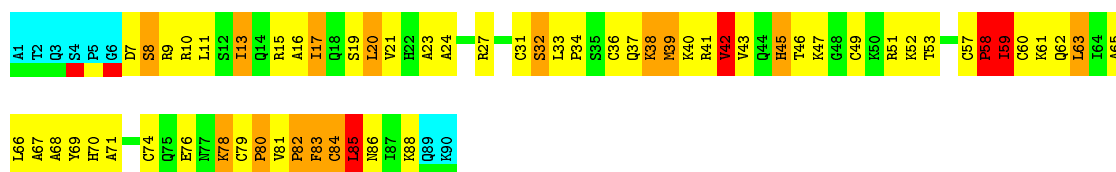
- Molecule 2: Cellular tumor antigen p53



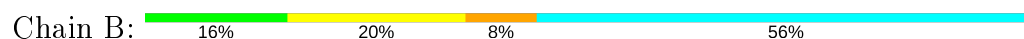
4.2.9 Score per residue for model 9

- Molecule 1: Histone acetyltransferase p300



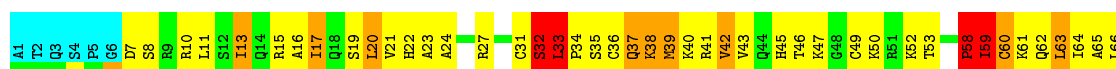


- Molecule 2: Cellular tumor antigen p53



4.2.10 Score per residue for model 10

- Molecule 1: Histone acetyltransferase p300

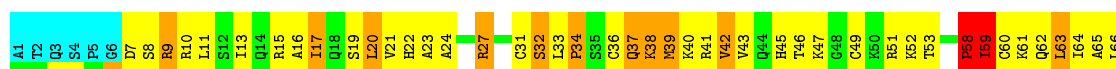


- Molecule 2: Cellular tumor antigen p53

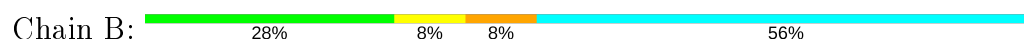


4.2.11 Score per residue for model 11

- Molecule 1: Histone acetyltransferase p300



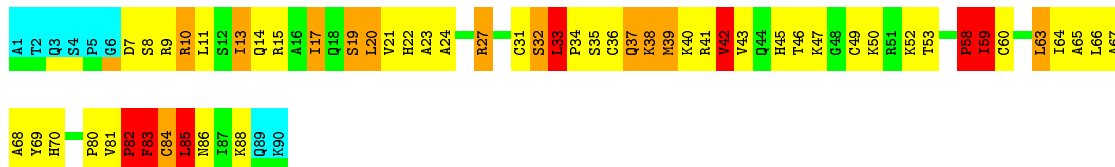
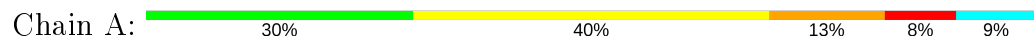
- Molecule 2: Cellular tumor antigen p53



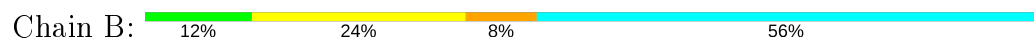


4.2.12 Score per residue for model 12

- Molecule 1: Histone acetyltransferase p300

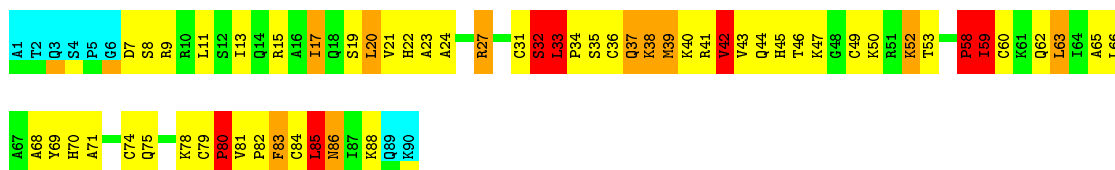
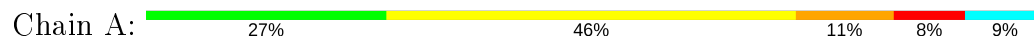


- Molecule 2: Cellular tumor antigen p53

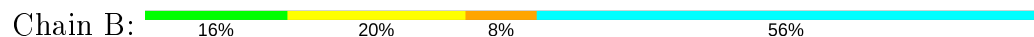


4.2.13 Score per residue for model 13

- Molecule 1: Histone acetyltransferase p300



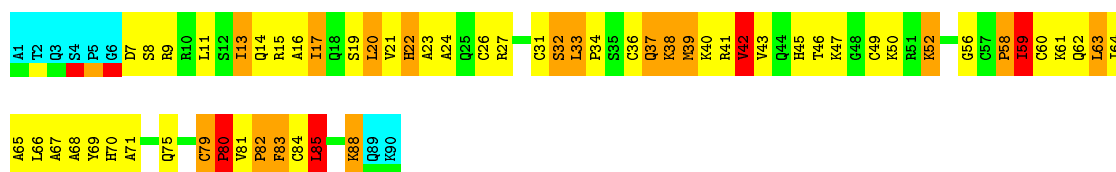
- Molecule 2: Cellular tumor antigen p53



4.2.14 Score per residue for model 14

- Molecule 1: Histone acetyltransferase p300



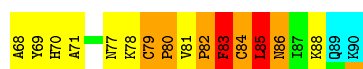
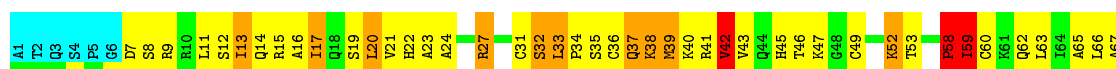


- Molecule 2: Cellular tumor antigen p53



4.2.15 Score per residue for model 15

- Molecule 1: Histone acetyltransferase p300



- Molecule 2: Cellular tumor antigen p53



5 Refinement protocol and experimental data overview

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

Of the 40000 calculated structures, 15 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
TALOS	structure solution	
CNS	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	1270
Number of shifts mapped to atoms	1270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	632	668	662	54±5
2	B	96	77	77	9±2
All	All	10920	11175	11088	862

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD22	2:B:16:ILE:HG13	0.84	1.49	13	7
1:A:42:VAL:HG13	1:A:59:ILE:HD11	0.81	1.53	14	6
1:A:49:CYS:O	1:A:52:LYS:HG3	0.80	1.77	10	11
1:A:79:CYS:HB2	1:A:84:CYS:SG	0.79	2.18	2	1
1:A:66:LEU:HA	1:A:69:TYR:CE1	0.76	2.15	11	1
1:A:52:LYS:HE2	1:A:60:CYS:SG	0.73	2.23	6	4
1:A:46:THR:HG23	1:A:60:CYS:SG	0.72	2.24	5	4
1:A:43:VAL:O	1:A:47:LYS:HG3	0.71	1.86	2	12
1:A:20:LEU:HD11	1:A:63:LEU:HD13	0.70	1.63	4	15
2:B:17:GLU:HA	2:B:20:PHE:CD2	0.69	2.23	5	1
1:A:38:LYS:HG2	2:B:19:TRP:O	0.69	1.86	10	14
1:A:42:VAL:HG21	1:A:59:ILE:HD13	0.68	1.65	9	2
1:A:52:LYS:HB3	1:A:60:CYS:CB	0.67	2.20	1	3
1:A:36:CYS:O	1:A:40:LYS:HB2	0.67	1.89	10	15
1:A:81:VAL:O	1:A:84:CYS:HB3	0.67	1.89	1	8
1:A:71:ALA:HB2	1:A:84:CYS:HA	0.67	1.67	13	11
1:A:59:ILE:O	1:A:63:LEU:HB3	0.66	1.91	7	7
1:A:79:CYS:HA	1:A:85:LEU:HD21	0.65	1.67	14	2
2:B:17:GLU:HA	2:B:20:PHE:CE1	0.65	2.27	10	1
1:A:11:LEU:O	1:A:15:ARG:HG3	0.64	1.91	2	15
1:A:52:LYS:HA	1:A:60:CYS:SG	0.64	2.33	11	8
1:A:66:LEU:HD22	2:B:16:ILE:CG1	0.63	2.23	13	7
1:A:43:VAL:O	1:A:46:THR:HG22	0.63	1.94	11	7
1:A:46:THR:O	1:A:52:LYS:HE3	0.62	1.94	6	8
1:A:43:VAL:HG13	1:A:82:PRO:HG3	0.62	1.72	1	7
2:B:16:ILE:HA	2:B:19:TRP:CE3	0.61	2.30	12	5
1:A:13:ILE:HB	1:A:69:TYR:OH	0.61	1.95	15	3
1:A:7:ASP:O	1:A:11:LEU:HD12	0.61	1.96	3	3
1:A:58:PRO:O	1:A:60:CYS:N	0.61	2.34	7	2
1:A:46:THR:HA	1:A:60:CYS:SG	0.61	2.36	8	7
1:A:23:ALA:HB1	1:A:40:LYS:CA	0.61	2.25	2	15
1:A:63:LEU:HA	1:A:66:LEU:HB3	0.60	1.73	11	15
1:A:85:LEU:HA	1:A:88:LYS:HB2	0.60	1.74	6	5
1:A:17:ILE:HG13	1:A:66:LEU:HD11	0.60	1.73	11	13
1:A:81:VAL:HG12	1:A:82:PRO:O	0.59	1.97	1	15
1:A:67:ALA:HB1	1:A:82:PRO:O	0.59	1.97	2	9
1:A:64:ILE:HG12	1:A:83:PHE:CD1	0.59	2.32	5	8
2:B:13:PRO:O	2:B:16:ILE:HG12	0.59	1.97	6	1
1:A:57:CYS:SG	1:A:58:PRO:HD2	0.59	2.38	7	2
1:A:71:ALA:O	1:A:88:LYS:HE3	0.58	1.99	14	3
2:B:17:GLU:HA	2:B:20:PHE:CE2	0.58	2.33	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:HIS:HA	1:A:73:HIS:CE1	0.58	2.34	1	1
1:A:71:ALA:O	1:A:88:LYS:HE2	0.58	1.98	3	2
1:A:17:ILE:HG13	1:A:66:LEU:CD1	0.58	2.29	3	14
1:A:9:ARG:O	1:A:13:ILE:HG13	0.58	1.99	5	4
1:A:49:CYS:O	1:A:52:LYS:HG2	0.57	2.00	6	2
2:B:16:ILE:HD13	2:B:16:ILE:H	0.57	1.59	13	4
1:A:46:THR:O	1:A:52:LYS:HG2	0.57	2.00	1	1
1:A:21:VAL:HA	1:A:81:VAL:CG2	0.57	2.30	15	14
2:B:16:ILE:H	2:B:16:ILE:HD13	0.57	1.60	3	7
1:A:70:HIS:CE1	1:A:74:CYS:HB2	0.56	2.35	11	3
2:B:15:ASP:HB3	2:B:19:TRP:CH2	0.56	2.35	12	3
1:A:19:SER:CB	2:B:20:PHE:HB2	0.56	2.30	5	3
1:A:35:SER:HB2	2:B:20:PHE:O	0.56	2.01	8	4
1:A:19:SER:HB3	1:A:39:MET:HG3	0.56	1.77	15	15
1:A:24:ALA:HB1	1:A:80:PRO:O	0.56	2.00	2	10
1:A:23:ALA:O	1:A:40:LYS:HG3	0.55	2.00	5	12
1:A:52:LYS:HB3	1:A:60:CYS:HB3	0.55	1.77	1	2
1:A:34:PRO:HA	1:A:37:GLN:HB2	0.55	1.79	12	13
1:A:11:LEU:HG	1:A:14:GLN:OE1	0.55	2.01	5	1
1:A:16:ALA:O	1:A:20:LEU:HB2	0.55	2.02	15	11
2:B:15:ASP:O	2:B:18:GLN:HG2	0.55	2.02	13	1
1:A:13:ILE:HG21	1:A:69:TYR:CE1	0.54	2.37	11	1
1:A:60:CYS:SG	1:A:64:ILE:HG13	0.54	2.42	10	3
1:A:35:SER:HB3	2:B:20:PHE:O	0.54	2.02	12	5
1:A:20:LEU:CD1	1:A:63:LEU:HD13	0.54	2.32	4	15
1:A:59:ILE:HA	2:B:19:TRP:CZ3	0.54	2.38	12	5
1:A:65:ALA:O	1:A:69:TYR:HB2	0.54	2.02	3	4
2:B:17:GLU:HA	2:B:20:PHE:CD1	0.54	2.38	6	2
1:A:43:VAL:O	1:A:46:THR:HB	0.54	2.02	8	7
1:A:13:ILE:HG12	2:B:13:PRO:HB3	0.54	1.80	5	4
1:A:23:ALA:HB1	1:A:40:LYS:N	0.54	2.18	6	15
1:A:42:VAL:HG22	1:A:59:ILE:HG13	0.54	1.80	2	8
1:A:13:ILE:HG22	2:B:13:PRO:HB2	0.54	1.80	6	1
1:A:36:CYS:SG	1:A:40:LYS:HE3	0.53	2.43	9	2
1:A:67:ALA:O	1:A:70:HIS:HB3	0.53	2.03	6	7
1:A:52:LYS:HB3	1:A:60:CYS:SG	0.53	2.43	1	3
1:A:38:LYS:HE3	2:B:19:TRP:O	0.53	2.03	13	2
1:A:41:ARG:O	1:A:45:HIS:HB2	0.53	2.04	11	14
1:A:68:ALA:O	1:A:71:ALA:HB3	0.53	2.04	13	9
1:A:42:VAL:CG1	1:A:59:ILE:HD11	0.53	2.30	14	1
1:A:78:LYS:O	1:A:85:LEU:HG	0.52	2.04	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:VAL:HG22	1:A:59:ILE:HD11	0.52	1.80	6	1
1:A:17:ILE:HG21	1:A:70:HIS:CG	0.52	2.38	13	2
1:A:46:THR:C	1:A:52:LYS:HE3	0.52	2.25	14	7
1:A:26:CYS:O	1:A:40:LYS:HE2	0.52	2.04	3	2
1:A:46:THR:OG1	1:A:63:LEU:HD23	0.52	2.04	8	5
1:A:40:LYS:O	1:A:43:VAL:HB	0.52	2.05	7	12
1:A:68:ALA:HA	1:A:83:PHE:O	0.52	2.05	1	4
1:A:84:CYS:O	1:A:86:ASN:N	0.52	2.43	10	12
1:A:59:ILE:HA	2:B:19:TRP:CH2	0.52	2.40	12	1
1:A:13:ILE:O	1:A:17:ILE:HG13	0.52	2.05	6	1
1:A:39:MET:HG2	2:B:19:TRP:O	0.51	2.05	10	3
1:A:79:CYS:SG	1:A:80:PRO:HD3	0.51	2.46	5	2
1:A:76:GLU:HG2	1:A:78:LYS:H	0.51	1.65	9	2
1:A:24:ALA:CB	1:A:81:VAL:HG22	0.51	2.36	9	13
1:A:17:ILE:N	1:A:66:LEU:HD11	0.50	2.21	5	5
1:A:27:ARG:O	1:A:27:ARG:HD3	0.50	2.07	2	2
1:A:27:ARG:HD3	1:A:27:ARG:O	0.50	2.05	13	3
1:A:59:ILE:HB	2:B:19:TRP:CH2	0.50	2.42	2	3
1:A:68:ALA:O	1:A:72:LYS:HB2	0.50	2.07	5	1
1:A:57:CYS:O	1:A:61:LYS:HB2	0.50	2.07	7	2
1:A:42:VAL:HG13	1:A:59:ILE:CD1	0.50	2.34	15	1
2:B:14:ASP:HA	2:B:17:GLU:OE1	0.49	2.07	5	1
1:A:9:ARG:HA	1:A:9:ARG:NE	0.49	2.23	7	2
1:A:62:GLN:O	1:A:65:ALA:HB3	0.49	2.08	15	12
1:A:79:CYS:HA	1:A:85:LEU:CD1	0.49	2.38	6	3
1:A:79:CYS:HA	1:A:85:LEU:HD11	0.49	1.84	13	4
2:B:17:GLU:O	2:B:20:PHE:HD2	0.49	1.90	7	4
1:A:42:VAL:CG2	1:A:59:ILE:HD11	0.49	2.38	3	3
1:A:39:MET:CG	2:B:20:PHE:HA	0.49	2.37	11	3
1:A:81:VAL:O	1:A:84:CYS:HB2	0.49	2.08	12	1
1:A:85:LEU:HA	1:A:88:LYS:CD	0.49	2.38	14	1
2:B:20:PHE:CE2	2:B:21:THR:HB	0.48	2.43	8	2
1:A:59:ILE:O	1:A:63:LEU:N	0.48	2.45	14	7
2:B:20:PHE:CE1	2:B:21:THR:HG22	0.48	2.43	2	1
1:A:8:SER:O	1:A:12:SER:HB2	0.48	2.08	5	3
1:A:83:PHE:CD1	1:A:86:ASN:HB3	0.48	2.44	2	1
1:A:79:CYS:H	1:A:85:LEU:HG	0.48	1.68	15	1
1:A:70:HIS:CD2	1:A:74:CYS:HB2	0.48	2.43	13	1
2:B:16:ILE:N	2:B:16:ILE:HD13	0.48	2.23	8	7
1:A:46:THR:HG1	1:A:60:CYS:CB	0.47	2.22	13	1
1:A:43:VAL:HG13	1:A:82:PRO:HD3	0.47	1.86	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:HD11	2:B:19:TRP:CE2	0.47	2.44	1	1
1:A:24:ALA:HB1	1:A:80:PRO:C	0.47	2.30	7	8
2:B:16:ILE:HD13	2:B:16:ILE:N	0.47	2.25	2	4
1:A:17:ILE:CG1	1:A:66:LEU:HD11	0.47	2.38	11	1
1:A:76:GLU:OE2	1:A:85:LEU:HD12	0.47	2.10	5	1
1:A:50:LYS:C	1:A:52:LYS:H	0.47	2.12	7	7
1:A:20:LEU:HD11	1:A:63:LEU:CD1	0.47	2.38	6	3
1:A:66:LEU:HD13	2:B:16:ILE:HG13	0.46	1.87	7	1
1:A:83:PHE:HB3	1:A:87:ILE:HD13	0.46	1.87	10	1
1:A:70:HIS:NE2	1:A:74:CYS:HB2	0.46	2.25	9	1
1:A:17:ILE:HG21	1:A:70:HIS:ND1	0.46	2.25	11	1
2:B:20:PHE:CE2	2:B:21:THR:HG22	0.46	2.45	15	1
2:B:16:ILE:H	2:B:16:ILE:CD1	0.46	2.21	1	4
1:A:10:ARG:HA	1:A:13:ILE:CD1	0.46	2.41	5	1
1:A:39:MET:HE3	2:B:19:TRP:HB2	0.46	1.88	11	1
1:A:77:ASN:HA	1:A:85:LEU:CB	0.46	2.41	15	1
1:A:21:VAL:HA	1:A:81:VAL:HG22	0.46	1.87	1	1
1:A:46:THR:HG23	1:A:52:LYS:HE2	0.46	1.87	6	2
1:A:60:CYS:HA	1:A:63:LEU:HB3	0.46	1.88	1	2
1:A:74:CYS:O	1:A:88:LYS:HE3	0.46	2.11	4	2
1:A:68:ALA:O	1:A:72:LYS:HD2	0.46	2.11	6	1
1:A:20:LEU:HD13	1:A:66:LEU:CD2	0.46	2.41	11	5
1:A:83:PHE:CD1	1:A:83:PHE:N	0.45	2.80	4	2
1:A:13:ILE:O	1:A:16:ALA:HB3	0.45	2.11	6	1
1:A:39:MET:CG	2:B:20:PHE:HB3	0.45	2.40	10	1
1:A:59:ILE:HA	1:A:62:GLN:HB2	0.45	1.88	9	1
1:A:66:LEU:HD22	2:B:16:ILE:CB	0.45	2.41	2	5
1:A:46:THR:HG1	1:A:60:CYS:HB3	0.45	1.72	13	1
1:A:33:LEU:HG	1:A:36:CYS:H	0.45	1.72	12	11
1:A:33:LEU:HD11	1:A:35:SER:HB2	0.45	1.89	6	1
1:A:52:LYS:HB2	1:A:60:CYS:SG	0.45	2.52	6	1
1:A:63:LEU:O	1:A:63:LEU:HD12	0.45	2.12	1	5
1:A:42:VAL:HG22	1:A:59:ILE:CD1	0.45	2.41	14	2
1:A:64:ILE:HG12	1:A:83:PHE:CE1	0.45	2.47	12	1
1:A:46:THR:OG1	1:A:52:LYS:HG2	0.45	2.11	3	1
1:A:47:LYS:HA	1:A:52:LYS:HE3	0.45	1.89	2	4
1:A:21:VAL:O	1:A:24:ALA:HB3	0.45	2.12	7	11
1:A:63:LEU:HD12	1:A:63:LEU:O	0.45	2.11	14	3
1:A:17:ILE:HG21	1:A:70:HIS:CD2	0.45	2.47	3	2
1:A:42:VAL:HG22	1:A:59:ILE:CG1	0.45	2.42	5	2
1:A:17:ILE:HG12	1:A:66:LEU:CD1	0.45	2.42	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HD11	1:A:69:TYR:CE2	0.45	2.46	10	1
1:A:46:THR:OG1	1:A:60:CYS:HB3	0.44	2.12	2	3
1:A:59:ILE:O	1:A:63:LEU:CB	0.44	2.65	9	1
1:A:34:PRO:HG3	1:A:37:GLN:HE21	0.44	1.72	5	1
1:A:10:ARG:O	1:A:14:GLN:HG3	0.44	2.13	8	1
1:A:50:LYS:O	1:A:54:ASN:HB3	0.43	2.13	6	1
1:A:20:LEU:HD13	1:A:66:LEU:HD23	0.43	1.90	11	3
1:A:32:SER:C	1:A:34:PRO:HD3	0.43	2.33	6	4
1:A:38:LYS:CE	2:B:19:TRP:HA	0.43	2.43	15	1
2:B:18:GLN:O	2:B:22:GLU:HG3	0.43	2.13	8	1
1:A:33:LEU:HG	1:A:36:CYS:N	0.43	2.28	12	5
2:B:17:GLU:O	2:B:20:PHE:HD1	0.43	1.97	2	3
1:A:38:LYS:HG3	2:B:19:TRP:CE3	0.43	2.48	9	1
1:A:46:THR:OG1	1:A:60:CYS:HA	0.43	2.13	15	1
1:A:46:THR:HG23	1:A:60:CYS:CB	0.43	2.43	6	1
1:A:33:LEU:HD11	1:A:35:SER:HB3	0.43	1.89	10	1
1:A:23:ALA:HB1	1:A:40:LYS:HA	0.43	1.91	2	1
1:A:40:LYS:O	1:A:44:GLN:HG2	0.43	2.13	6	1
1:A:33:LEU:HD11	1:A:35:SER:OG	0.43	2.13	8	1
1:A:46:THR:HG23	1:A:60:CYS:HB3	0.43	1.91	1	1
1:A:71:ALA:CB	1:A:84:CYS:HA	0.42	2.44	7	1
1:A:38:LYS:NZ	2:B:22:GLU:HG2	0.42	2.28	10	1
1:A:81:VAL:HB	1:A:84:CYS:CB	0.42	2.43	1	1
1:A:76:GLU:OE2	1:A:78:LYS:HE3	0.42	2.13	10	1
1:A:79:CYS:O	1:A:85:LEU:HD13	0.42	2.14	2	1
1:A:7:ASP:CA	1:A:11:LEU:HD13	0.42	2.45	2	1
2:B:14:ASP:O	2:B:18:GLN:HG2	0.42	2.14	4	1
1:A:60:CYS:O	1:A:64:ILE:HG13	0.42	2.14	2	1
1:A:39:MET:HG2	2:B:20:PHE:HA	0.42	1.92	6	1
1:A:46:THR:OG1	1:A:59:ILE:HD13	0.42	2.14	10	1
1:A:47:LYS:HA	1:A:52:LYS:CE	0.42	2.44	12	2
1:A:84:CYS:SG	1:A:85:LEU:N	0.42	2.92	3	2
2:B:17:GLU:O	2:B:20:PHE:CD2	0.42	2.72	4	2
1:A:13:ILE:HG23	2:B:13:PRO:HA	0.42	1.91	9	1
1:A:16:ALA:HB1	2:B:16:ILE:CG1	0.42	2.45	9	1
1:A:13:ILE:HA	2:B:13:PRO:HB3	0.42	1.90	14	1
1:A:13:ILE:CG2	1:A:69:TYR:CE1	0.42	3.02	11	1
1:A:17:ILE:HD13	1:A:70:HIS:ND1	0.42	2.29	12	1
1:A:46:THR:HG1	1:A:52:LYS:HG2	0.42	1.74	13	1
1:A:76:GLU:HG2	1:A:77:ASN:N	0.42	2.30	1	1
1:A:80:PRO:HB2	1:A:81:VAL:HG23	0.42	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ARG:HA	1:A:13:ILE:HD12	0.42	1.91	5	1
1:A:21:VAL:HG22	1:A:81:VAL:HG21	0.41	1.91	1	1
1:A:60:CYS:CA	1:A:63:LEU:HB3	0.41	2.45	3	1
1:A:50:LYS:C	1:A:52:LYS:N	0.41	2.73	7	2
1:A:34:PRO:HA	1:A:37:GLN:CG	0.41	2.46	6	1
1:A:17:ILE:HG13	1:A:66:LEU:HD12	0.41	1.92	5	1
1:A:17:ILE:CG1	1:A:66:LEU:CD1	0.41	2.98	13	1
1:A:88:LYS:HG3	1:A:88:LYS:O	0.41	2.15	15	1
1:A:13:ILE:HG23	2:B:13:PRO:HB3	0.41	1.92	12	1
2:B:17:GLU:HA	2:B:20:PHE:HB3	0.41	1.92	12	1
1:A:79:CYS:HA	1:A:85:LEU:CD2	0.41	2.44	15	1
1:A:39:MET:HE1	2:B:16:ILE:HG22	0.41	1.92	6	1
1:A:85:LEU:C	1:A:85:LEU:HD22	0.41	2.36	15	1
1:A:66:LEU:HD22	2:B:16:ILE:HB	0.41	1.92	2	1
1:A:88:LYS:O	1:A:88:LYS:HD3	0.41	2.15	7	1
1:A:7:ASP:O	1:A:11:LEU:HD13	0.41	2.15	15	2
1:A:13:ILE:HA	1:A:16:ALA:HB3	0.41	1.92	15	1
1:A:27:ARG:HD2	1:A:27:ARG:O	0.41	2.16	1	1
1:A:33:LEU:CD1	1:A:35:SER:HB2	0.41	2.46	6	1
1:A:38:LYS:CD	2:B:19:TRP:HA	0.41	2.46	12	1
2:B:13:PRO:O	2:B:17:GLU:HG3	0.40	2.16	1	1
1:A:33:LEU:O	1:A:36:CYS:HB2	0.40	2.16	3	1
1:A:9:ARG:O	2:B:13:PRO:HG3	0.40	2.16	3	1
1:A:7:ASP:CG	1:A:11:LEU:HD13	0.40	2.37	10	1
1:A:14:GLN:O	1:A:18:GLN:HG3	0.40	2.15	3	1
1:A:53:THR:HG21	1:A:64:ILE:HD12	0.40	1.93	8	1
1:A:34:PRO:HG3	1:A:37:GLN:OE1	0.40	2.16	2	1
1:A:17:ILE:HD11	1:A:69:TYR:CZ	0.40	2.52	2	1
1:A:34:PRO:HA	1:A:37:GLN:CB	0.40	2.46	12	1
1:A:22:HIS:O	1:A:26:CYS:CB	0.40	2.70	14	1
1:A:34:PRO:HG3	1:A:37:GLN:NE2	0.40	2.31	5	1
1:A:13:ILE:HA	1:A:16:ALA:CB	0.40	2.47	15	1

5.2 Torsion angles [i](#)

5.2.1 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	82/90 (91%)	71±2 (87±2%)	7±1 (8±2%)	4±1 (5±1%)	4	24
2	B	11/25 (44%)	10±1 (89±8%)	1±1 (11±8%)	0±0 (0±0%)	100	100
All	All	1395/1725 (81%)	1211 (87%)	121 (9%)	63 (5%)	4	28

All 10 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	83	PHE	15
1	A	85	LEU	15
1	A	80	PRO	11
1	A	79	CYS	7
1	A	78	LYS	4
1	A	56	GLY	3
1	A	58	PRO	2
1	A	59	ILE	2
1	A	52	LYS	2
1	A	82	PRO	2

5.2.2 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	71/77 (92%)	62±2 (87±2%)	9±2 (13±2%)	7	48
2	B	11/23 (48%)	8±1 (73±9%)	3±1 (27±9%)	2	21
All	All	1230/1500 (82%)	1046 (85%)	184 (15%)	6	44

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)
2	B	16	ILE	15
1	A	27	ARG	15
1	A	39	MET	15
1	A	85	LEU	15
1	A	58	PRO	14
2	B	20	PHE	12

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Mol	Chain	Res	Type	Models (Total)
1	A	33	LEU	10
1	A	42	VAL	9
1	A	13	ILE	9
1	A	59	ILE	9
2	B	17	GLU	7
1	A	88	LYS	6
2	B	12	SER	5
1	A	50	LYS	5
1	A	83	PHE	4
1	A	75	GLN	4
1	A	9	ARG	3
1	A	87	ILE	3
1	A	78	LYS	3
2	B	21	THR	2
1	A	86	ASN	2
2	B	15	ASP	2
1	A	52	LYS	2
1	A	34	PRO	2
1	A	69	TYR	2
2	B	22	GLU	2
1	A	30	ASN	1
1	A	10	ARG	1
1	A	32	SER	1
1	A	73	HIS	1
1	A	44	GLN	1
1	A	8	SER	1
1	A	77	ASN	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 81% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 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	990
Number of shifts mapped to atoms	990
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	-0.51 ± 0.08	Should be applied
$^{13}\text{C}_\beta$	83	0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	-0.85 ± 0.07	Should be applied
^{15}N	74	-0.75 ± 0.43	None needed (imprecise)

6.1.3 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 71%, i.e. 833 atoms were assigned a chemical shift out of a possible 1180. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	369/455 (81%)	150/181 (83%)	149/186 (80%)	70/88 (80%)
Sidechain	464/655 (71%)	293/391 (75%)	171/224 (76%)	0/40 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/70 (0%)	0/36 (0%)	0/25 (0%)	0/9 (0%)
Overall	833/1180 (71%)	443/608 (73%)	320/435 (74%)	70/137 (51%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 898 atoms were assigned a chemical shift out of a possible 1423. 10 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	396/559 (71%)	161/222 (73%)	161/230 (70%)	74/107 (69%)
Sidechain	502/794 (63%)	318/474 (67%)	184/276 (67%)	0/44 (0%)
Aromatic	0/70 (0%)	0/36 (0%)	0/25 (0%)	0/9 (0%)
Overall	898/1423 (63%)	479/732 (65%)	345/531 (65%)	74/160 (46%)

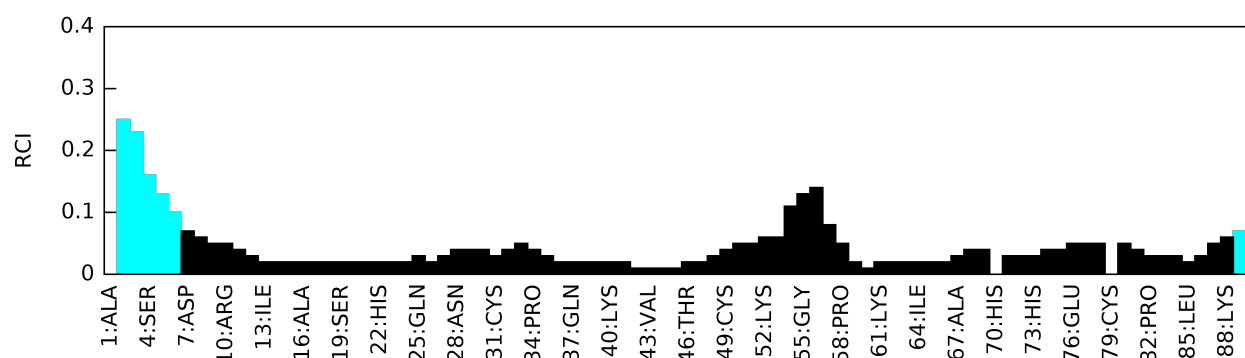
6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

6.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	280
Number of shifts mapped to atoms	280
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

6.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	25	-0.01 \pm 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	24	—	None (insufficient data)
$^{13}\text{C}'$	21	—	None (insufficient data)
^{15}N	22	—	None (insufficient data)

6.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 115 atoms were assigned a chemical shift out of a possible 1180. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	52/455 (11%)	21/181 (12%)	21/186 (11%)	10/88 (11%)
Sidechain	56/655 (9%)	36/391 (9%)	19/224 (8%)	1/40 (2%)
Aromatic	7/70 (10%)	6/36 (17%)	0/25 (0%)	1/9 (11%)
Overall	115/1180 (10%)	63/608 (10%)	40/435 (9%)	12/137 (9%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 256 atoms were assigned a chemical shift out of a possible 1423. 2 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	114/559 (20%)	46/222 (21%)	46/230 (20%)	22/107 (21%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	135/794 (17%)	86/474 (18%)	47/276 (17%)	2/44 (5%)
Aromatic	7/70 (10%)	6/36 (17%)	0/25 (0%)	1/9 (11%)
Overall	256/1423 (18%)	138/732 (19%)	93/531 (18%)	25/160 (16%)

6.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

