W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:06 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

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

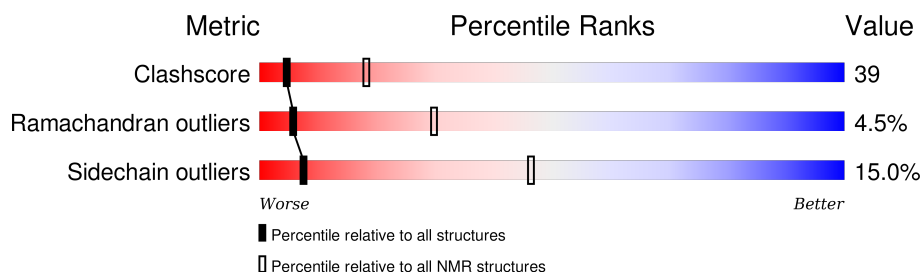|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	Percentile Ranks	Value
Clashscore		39
Ramachandran outliers		4.5%
Sidechain outliers		15.0%

Worse　　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	90	24% 　 48% 　 14% · 9%
2	B	25	16% 20% 8% 56%

2 Ensemble composition and analysis (i)

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 (i)

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
			Total	C	H	N	O	S	
1	A	90	1415	420	726	140	119	10	0

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
			Total	C	H	N	O	S	
2	B	25	376	124	177	28	45	2	0

4 Residue-property plots (i)

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: Histone acetyltransferase p300
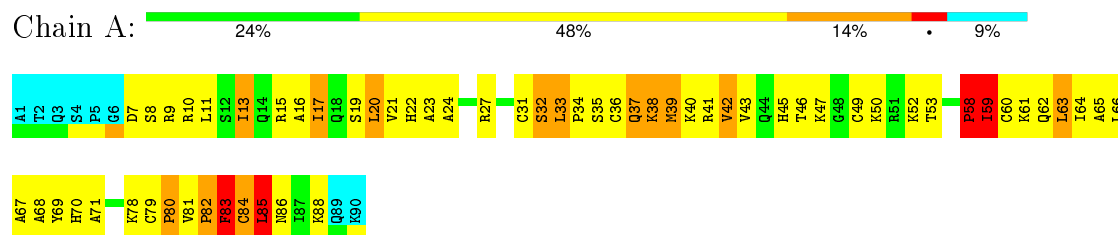
- Molecule 2: Cellular tumor antigen p53
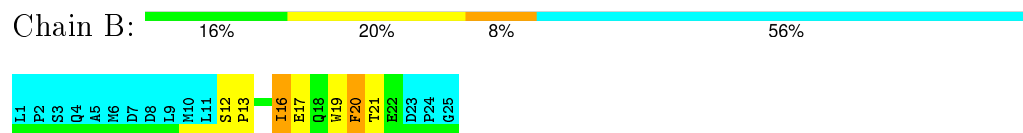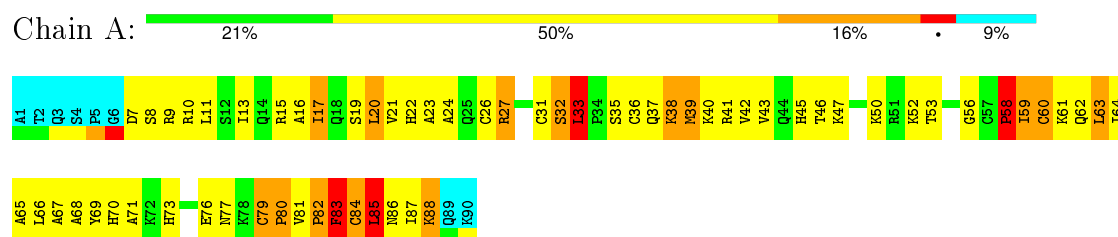

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Histone acetyltransferase p300

- Molecule 2: Cellular tumor antigen p53

Chain B: 12% 20% 12% 56%
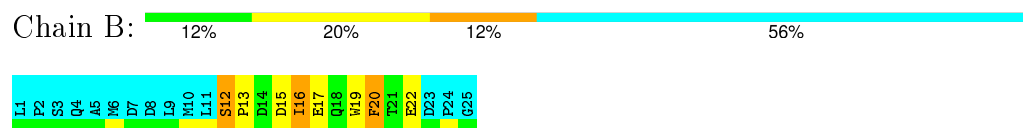
4.2.2 Score per residue for model 2

• Molecule 1: Histone acetyltransferase p300

Chain A: 27% 43% 14% 7% 9%

• Molecule 2: Cellular tumor antigen p53

Chain B: 20% 16% 8% 56%

4.2.3 Score per residue for model 3

• Molecule 1: Histone acetyltransferase p300

Chain A: 27% 44% 17% • 9%

• Molecule 2: Cellular tumor antigen p53

Chain B: 16% 12% 16% 56%

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Histone acetyltransferase p300

Chain A:

- Molecule 2: Cellular tumor antigen p53

Chain B:

4.2.5 Score per residue for model 5

- Molecule 1: Histone acetyltransferase p300

Chain A:

- Molecule 2: Cellular tumor antigen p53
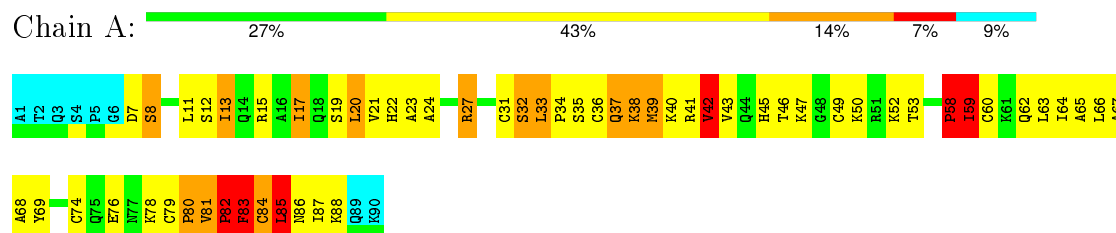
Chain B:

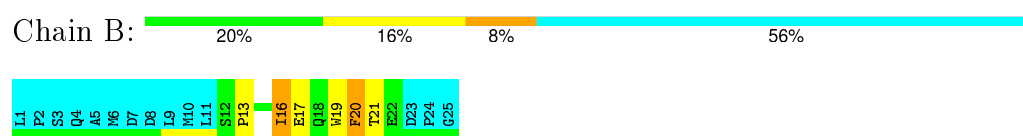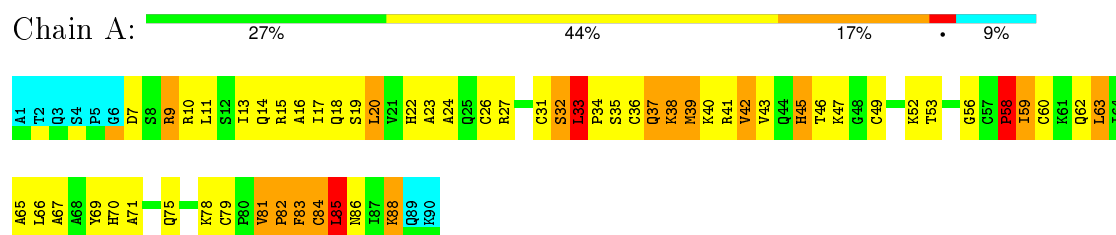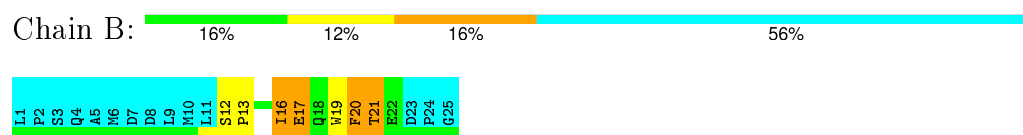### 4.2.6 Score per residue for model 6

- Molecule 1: Histone acetyltransferase p300

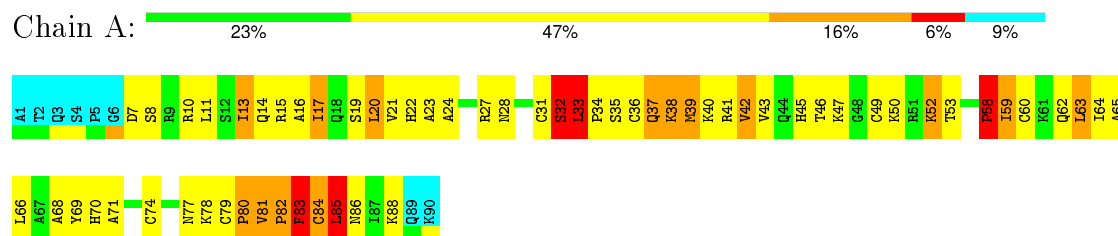Chain A:

- Molecule 2: Cellular tumor antigen p53

Chain B:

L1 P2 S3 Q4 A5 M6 D7 D8 L9 M10 L11 S12 P13 I16 E17 Q18 W19 F20 T21 E22 D23 P24 G25

4.2.7 Score per residue for model 7

• Molecule 1: Histone acetyltransferase p300

Chain A: 34% 37% 16% • 9%

A1 T2 Q3 S4 P5 G6 R9 R10 L11 S12 I13 Q14 R15 A16 I17 Q18 S19 L20 V21 H22 A23 A24 R27 C31 S32 L33 P34 S35 C36 Q37 K38 M39 K40 R41 V42 V43 T46 K47 G48 C49 K50 R51 K52 T53 C57 P58 I59 C60 K61 Q62 L63 L66 A67 A68

Y69 H70 A71 C74 P80 V81 P82 F83 C84 L85 K88 Q89 K90

• Molecule 2: Cellular tumor antigen p53

Chain B: 20% 12% 12% 56%

L1 P2 S3 Q4 A5 M6 D7 D8 L9 M10 L11 S12 P13 I16 E17 Q18 W19 F20 T21 E22 D23 P24 G25

4.2.8 Score per residue for model 8

• Molecule 1: Histone acetyltransferase p300

Chain A: 29% 41% 16% 6% 9%

A1 T2 Q3 S4 P5 G6 D7 S8 R9 R10 L11 S12 I13 Q14 R15 A16 I17 Q18 S19 L20 V21 H22 A23 A24 R27 N28 C31 S32 L33 P34 S35 C36 Q37 K38 M39 K40 R41 V42 V43 Q44 H45 T46 K47 K50 R51 K52 T53 G56 C57 P58 I59 C60 K61 Q62 L63 I64

A65 L66 A67 A68 Y69 H70 A71 Q75 P80 V81 P82 F83 C84 L85 N86 Q89 K90

• Molecule 2: Cellular tumor antigen p53

Chain B: 16% 16% 12% 56%

L1 P2 S3 Q4 A5 M6 D7 D8 L9 M10 L11 D15 I16 E17 Q18 W19 F20 T21 E22 D23 P24 G25

4.2.9 Score per residue for model 9

• Molecule 1: Histone acetyltransferase p300

Chain A: 24% 47% 16% • 9%

A1 T2 Q3 S4 P5 G6 D7 S8 R9 R10 L11 S12 I13 Q14 R15 A16 I17 Q18 S19 L20 V21 H22 A23 A24 R27 C31 S32 L33 P34 S35 C36 Q37 K38 M39 K40 R41 V42 V43 Q44 H45 T46 K47 G48 C49 K50 R51 K52 T53 C57 P58 I59 C60 K61 Q62 L63 I64 A65

L66 A67 A68 Y69 H70 A71 C74 Q75 E76 N77 K78 C79 P80 V81 P82 F83 C84 L85 N86 I87 K88 Q89 K90

• Molecule 2: Cellular tumor antigen p53

Chain B: 16% 20% 8% 56%

L1 P2 S3 Q4 A5 M6 D7 D8 L9 M10 L11 S12 P13 I16 E17 Q18 W19 F20 T21 E22 D23 P24 G25

4.2.10 Score per residue for model 10

• Molecule 1: Histone acetyltransferase p300

Chain A: 24% 43% 17% 7% 9%

A1 T2 Q3 S4 P5 G6 D7 S8 R9 R10 L11 S12 I13 Q14 R15 A16 I17 Q18 S19 L20 V21 H22 A23 A24 R27 C31 S32 L33 P34 S35 C36 Q37 K38 M39 K40 R41 V42 V43 Q44 H45 T46 K47 G48 C49 K50 R51 K52 T53 P58 I59 C60 K61 Q62 L63 I64 A65 L66

A67 A68 Y69 H70 A71 E76 N77 K78 C79 P80 V81 P82 F83 C84 L85 N86 I87 K88 Q89 K90

• Molecule 2: Cellular tumor antigen p53

Chain B: 16% 12% 12% • 56%

L1 P2 S3 Q4 A5 M6 D7 D8 L9 M10 L11 D15 I16 E17 Q18 W19 F20 T21 E22 D23 P24 G25

4.2.11 Score per residue for model 11

• Molecule 1: Histone acetyltransferase p300

Chain A: 26% 43% 17% 6% 9%

A1 T2 Q3 S4 P5 G6 D7 S8 R9 R10 L11 S12 I13 Q14 R15 A16 I17 Q18 S19 L20 V21 H22 A23 A24 R27 C31 S32 L33 P34 S35 C36 Q37 K38 M39 K40 R41 V42 V43 Q44 H45 T46 K47 G48 C49 K50 R51 K52 T53 P58 I59 C60 K61 Q62 L63 I64 A65 L66

A67 A68 Y69 H70 A71 C74 K78 C79 P80 V81 P82 F83 C84 L85 N86 I87 K88 Q89 K90

• Molecule 2: Cellular tumor antigen p53

Chain B: 28% 8% 8% 56%

4.2.12 Score per residue for model 12

- Molecule 1: Histone acetyltransferase p300
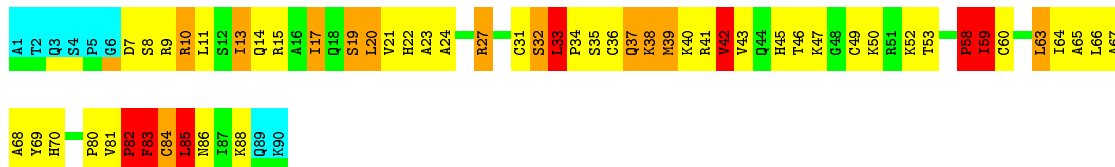
- Molecule 2: Cellular tumor antigen p53
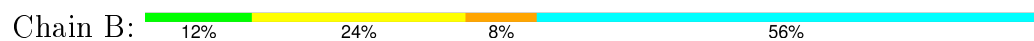
4.2.13 Score per residue for model 13

- Molecule 1: Histone acetyltransferase p300
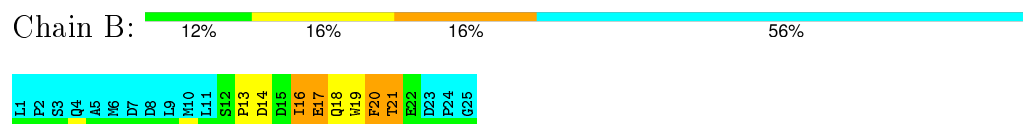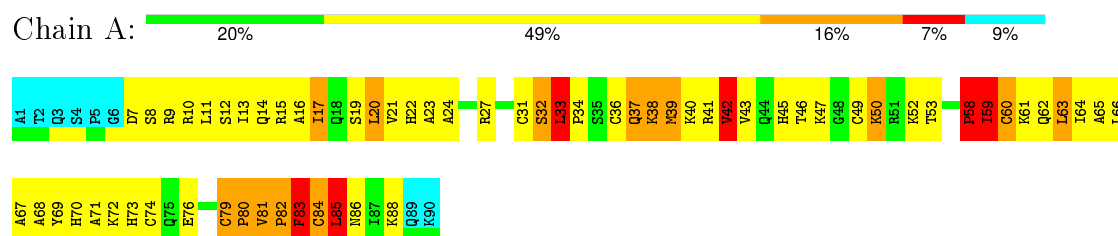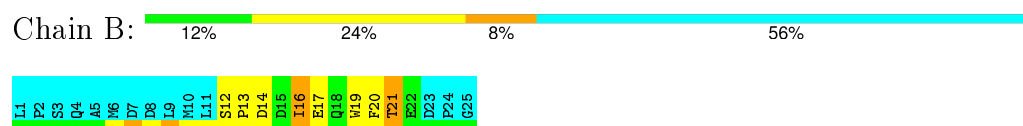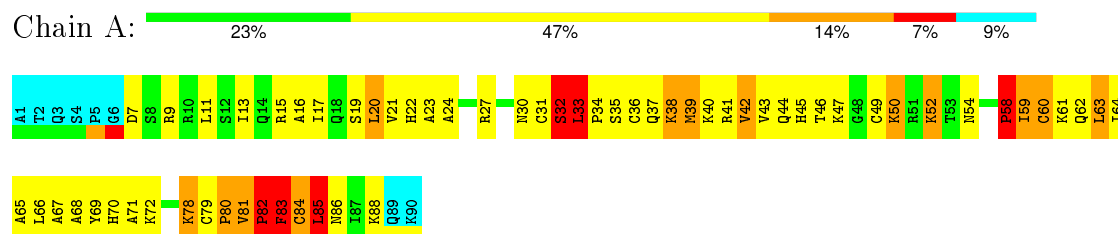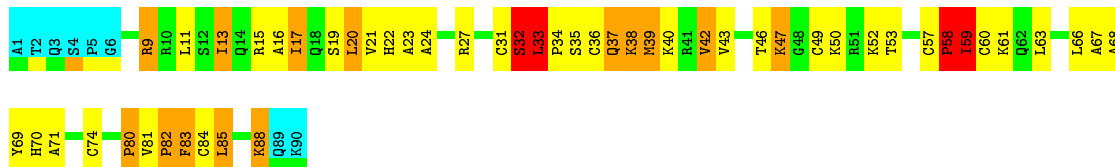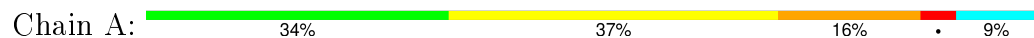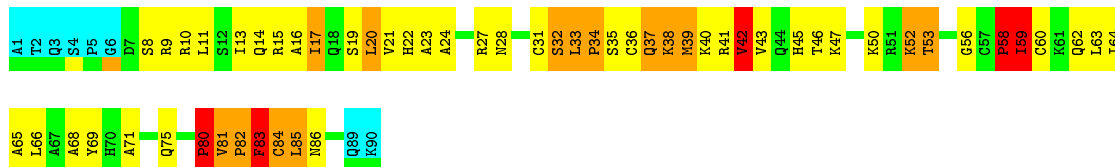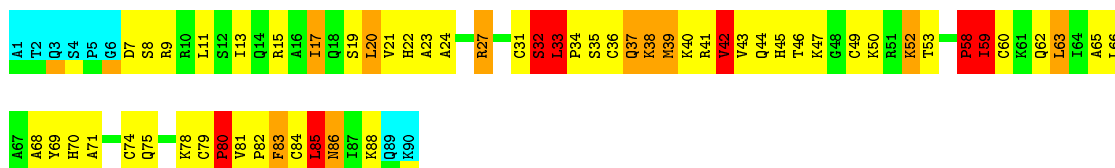

- Molecule 2: Cellular tumor antigen p53
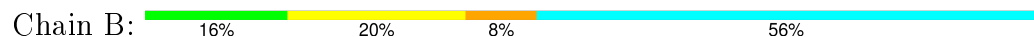
4.2.14 Score per residue for model 14

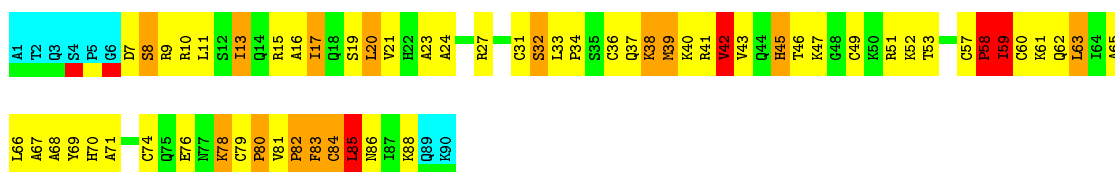- Molecule 1: Histone acetyltransferase p300
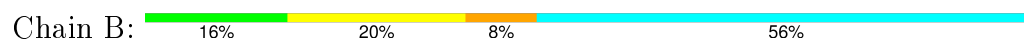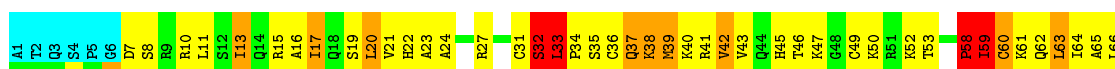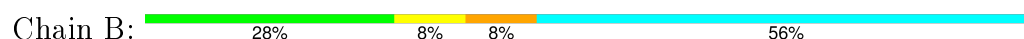
• Molecule 2: Cellular tumor antigen p53

Chain B:
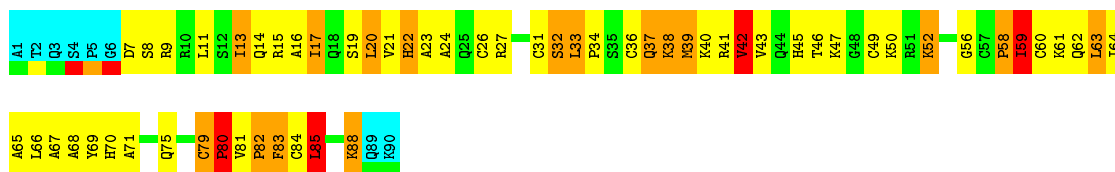
4.2.15 Score per residue for model 15

• Molecule 1: Histone acetyltransferase p300

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:
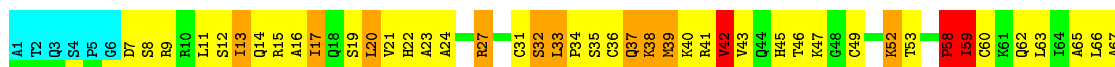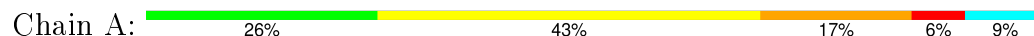
5 Refinement protocol and experimental data overview (i)

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 7 of this report.

Chemical shift file(s)	2mzd_cs.str
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.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.04±0.04	17±2/642 (2.6±0.4%)	1.46±0.03	7±1/861 (0.9±0.2%)
2	B	1.39±0.13	1±1/100 (0.9±0.6%)	1.15±0.08	0±0/138 (0.0±0.2%)
All	All	1.96	268/11130 (2.4%)	1.42	111/14985 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.0±0.7
2	B	0.0±0.0	0.1±0.3
All	All	0	47

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	A	33	LEU	N-CA	-9.80	1.26	1.46	6	15
1	A	59	ILE	N-CA	-8.51	1.29	1.46	15	13
1	A	32	SER	N-CA	-8.50	1.29	1.46	14	15
1	A	53	THR	N-CA	-8.12	1.30	1.46	11	13
2	B	21	THR	N-CA	-7.64	1.31	1.46	5	10
1	A	22	HIS	C-O	-7.37	1.09	1.23	14	14
2	B	20	PHE	N-CA	-7.18	1.31	1.46	10	2
1	A	59	ILE	C-O	-7.17	1.09	1.23	12	12
1	A	42	VAL	N-CA	-7.01	1.32	1.46	9	11
1	A	38	LYS	N-CA	-7.01	1.32	1.46	15	15
1	A	81	VAL	C-O	6.94	1.36	1.23	6	7
1	A	58	PRO	C-O	-6.92	1.09	1.23	7	2
1	A	38	LYS	CA-CB	-6.78	1.39	1.53	1	15
1	A	58	PRO	CA-CB	-6.71	1.40	1.53	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	A	85	LEU	N-CA	6.64	1.59	1.46	12	4
1	A	20	LEU	CB-CG	-6.54	1.33	1.52	6	15
1	A	81	VAL	C-N	6.45	1.46	1.34	4	6
1	A	61	LYS	CA-CB	-6.30	1.40	1.53	14	6
1	A	63	LEU	C-O	-6.20	1.11	1.23	11	11
1	A	59	ILE	CA-C	-6.13	1.37	1.52	12	6
1	A	58	PRO	C-N	-5.82	1.20	1.34	4	9
1	A	37	GLN	C-N	-5.74	1.20	1.34	1	11
1	A	8	SER	N-CA	-5.74	1.34	1.46	4	8
1	A	17	ILE	C-O	-5.66	1.12	1.23	8	13
1	A	19	SER	CA-CB	-5.59	1.44	1.52	12	1
1	A	51	ARG	N-CA	-5.51	1.35	1.46	9	2
1	A	56	GLY	N-CA	-5.47	1.37	1.46	14	1
1	A	52	LYS	CD-CE	-5.47	1.37	1.51	15	2
1	A	37	GLN	CA-C	-5.47	1.38	1.52	15	5
1	A	47	LYS	CA-CB	-5.43	1.42	1.53	3	2
1	A	80	PRO	N-CA	-5.26	1.38	1.47	10	5
1	A	28	ASN	N-CA	-5.22	1.35	1.46	4	2
1	A	61	LYS	N-CA	-5.21	1.35	1.46	14	1
1	A	42	VAL	CB-CG2	-5.20	1.42	1.52	4	1
1	A	60	CYS	C-O	-5.14	1.13	1.23	5	2
1	A	45	HIS	CA-C	-5.09	1.39	1.52	9	2
2	B	16	ILE	C-N	-5.08	1.22	1.34	15	1
1	A	22	HIS	C-N	-5.06	1.22	1.34	14	1
1	A	82	PRO	C-N	-5.05	1.22	1.34	6	2
1	A	34	PRO	N-CD	-5.04	1.40	1.47	8	1
1	A	58	PRO	N-CD	5.04	1.54	1.47	9	1
1	A	84	CYS	N-CA	-5.04	1.36	1.46	2	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Total
1	A	58	PRO	N-CA-CB	-10.19	91.07	103.30	2	13
1	A	83	PHE	C-N-CA	9.18	144.65	121.70	9	15
1	A	58	PRO	CA-N-CD	-7.33	101.25	111.50	7	2
1	A	84	CYS	N-CA-C	-7.07	91.90	111.00	9	12
1	A	59	ILE	CB-CA-C	6.74	125.07	111.60	6	9
1	A	83	PHE	CA-C-N	-6.63	102.62	117.20	2	12
1	A	60	CYS	CB-CA-C	-6.35	97.70	110.40	6	2
1	A	31	CYS	C-N-CA	-6.21	106.18	121.70	10	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Models Total
1	A	58	PRO	CB-CA-C	-6.17	96.57	112.00	3	13
1	A	42	VAL	CA-CB-CG2	-6.04	101.84	110.90	1	9
1	A	69	TYR	CB-CG-CD2	-5.83	117.50	121.00	11	1
1	A	42	VAL	CB-CA-C	5.39	121.65	111.40	9	2
1	A	69	TYR	CB-CG-CD1	5.30	124.18	121.00	11	1
2	B	22	GLU	N-CA-C	-5.28	96.73	111.00	10	1
1	A	13	ILE	CB-CA-C	-5.17	101.26	111.60	14	2
1	A	69	TYR	CA-CB-CG	5.10	123.09	113.40	11	1
1	A	59	ILE	C-N-CA	5.03	134.28	121.70	1	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	SER	Peptide	15
1	A	82	PRO	Peptide	14
1	A	58	PRO	Mainchain,Peptide	13
2	B	21	THR	Peptide	2
1	A	9	ARG	Sidechain	1
1	A	10	ARG	Sidechain	1

6.2 Too-close contacts (i)

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:36:CYS:O	1:A:40:LYS:HB2	0.67	1.89	10	15
1:A:52:LYS:HB3	1:A:60:CYS:CB	0.67	2.20	1	3
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:43:VAL:O	1:A:46:THR:HG22	0.63	1.94	11	7
1:A:66:LEU:HD22	2:B:16:ILE:CG1	0.63	2.23	13	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:58:PRO:O	1:A:60:CYS:N	0.61	2.34	7	2
1:A:7:ASP:O	1:A:11:LEU:HD12	0.61	1.96	3	3
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:17:ILE:HG13	1:A:66:LEU:HD11	0.60	1.73	11	13
1:A:85:LEU:HA	1:A:88:LYS:HB2	0.60	1.74	6	5
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
1:A:70:HIS:HA	1:A:73:HIS:CE1	0.58	2.34	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:21:VAL:HA	1:A:81:VAL:CG2	0.57	2.30	15	14
1:A:46:THR:O	1:A:52:LYS:HG2	0.57	2.00	1	1
2:B:16:ILE:H	2:B:16:ILE:HD13	0.57	1.60	3	7
2:B:15:ASP:HB3	2:B:19:TRP:CH2	0.56	2.35	12	3
1:A:70:HIS:CE1	1:A:74:CYS:HB2	0.56	2.35	11	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:34:PRO:HA	1:A:37:GLN:HB2	0.55	1.79	12	13
1:A:52:LYS:HB3	1:A:60:CYS:HB3	0.55	1.77	1	2
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: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:35:SER:HB3	2:B:20:PHE:O	0.54	2.02	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
1:A:42:VAL:HG22	1:A:59:ILE:HD11	0.52	1.80	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HG21	1:A:70:HIS:CG	0.52	2.38	13	2
1:A:40:LYS:O	1:A:43:VAL:HB	0.52	2.05	7	12
1:A:46:THR:C	1:A:52:LYS:HE3	0.52	2.25	14	7
1:A:46:THR:OG1	1:A:63:LEU:HD23	0.52	2.04	8	5
1:A:26:CYS:O	1:A:40:LYS:HE2	0.52	2.04	3	2
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:27:ARG:HD3	1:A:27:ARG:O	0.50	2.05	13	3
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:59:ILE:HB	2:B:19:TRP:CH2	0.50	2.42	2	3
1:A:42:VAL:HG13	1:A:59:ILE:CD1	0.50	2.34	15	1
1:A:57:CYS:O	1:A:61:LYS:HB2	0.50	2.07	7	2
1:A:68:ALA:O	1:A:72:LYS:HB2	0.50	2.07	5	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:8:SER:O	1:A:12:SER:HB2	0.48	2.08	5	3
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: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	6
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
1:A:59:ILE:HD11	2:B:19:TRP:CE2	0.47	2.44	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:24:ALA:HB1	1:A:80:PRO:C	0.47	2.30	7	8
1:A:17:ILE:CG1	1:A:66:LEU:HD11	0.47	2.38	11	1
2:B:16:ILE:HD13	2:B:16:ILE:N	0.47	2.25	2	5
1:A:76:GLU:OE2	1:A:85:LEU:HD12	0.47	2.10	5	1
1:A:20:LEU:HD11	1:A:63:LEU:CD1	0.47	2.38	6	3
1:A:50:LYS:C	1:A:52:LYS:H	0.47	2.12	7	7
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:17:ILE:HG21	1:A:70:HIS:ND1	0.46	2.25	11	1
1:A:70:HIS:NE2	1:A:74:CYS:HB2	0.46	2.25	9	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:77:ASN:HA	1:A:85:LEU:CB	0.46	2.41	15	1
1:A:39:MET:HE3	2:B:19:TRP:HB2	0.46	1.88	11	1
1:A:10:ARG:HA	1:A:13:ILE:CD1	0.46	2.41	5	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:20:LEU:HD13	1:A:66:LEU:CD2	0.46	2.41	11	5
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: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:64:ILE:HG12	1:A:83:PHE:CE1	0.45	2.47	12	1
1:A:63:LEU:O	1:A:63:LEU:HD12	0.45	2.12	1	4
1:A:42:VAL:HG22	1:A:59:ILE:CD1	0.45	2.41	14	2
1:A:46:THR:OG1	1:A:52:LYS:HG2	0.45	2.11	3	1
1:A:63:LEU:HD12	1:A:63:LEU:O	0.45	2.11	14	4
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: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
1:A:17:ILE:HD11	1:A:69:TYR:CE2	0.45	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
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:38:LYS:CE	2:B:19:TRP:HA	0.43	2.43	15	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
2:B:18:GLN:O	2:B:22:GLU:HG3	0.43	2.13	8	1
1:A:46:THR:OG1	1:A:60:CYS:HA	0.43	2.13	15	1
2:B:17:GLU:O	2:B:20:PHE:HD1	0.43	1.97	2	3
1:A:33:LEU:HG	1:A:36:CYS:N	0.43	2.28	12	5
1:A:38:LYS:HG3	2:B:19:TRP:CE3	0.43	2.48	9	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:33:LEU:HD11	1:A:35:SER:OG	0.43	2.13	8	1
1:A:40:LYS:O	1:A:44:GLN:HG2	0.43	2.13	6	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:13:ILE:HA	2:B:13:PRO:HB3	0.42	1.90	14	1
1:A:16:ALA:HB1	2:B:16:ILE:CG1	0.42	2.45	9	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:80:PRO:HB2	1:A:81:VAL:HG23	0.42	1.91	1	1
1:A:76:GLU:HG2	1:A:77:ASN:N	0.42	2.30	1	1
1:A:10:ARG:HA	1:A:13:ILE:HD12	0.42	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:88:LYS:HG3	1:A:88:LYS:O	0.41	2.15	15	1
1:A:17:ILE:CG1	1:A:66:LEU:CD1	0.41	2.98	13	1
1:A:17:ILE:HG13	1:A:66:LEU:HD12	0.41	1.92	5	1
1:A:79:CYS:HA	1:A:85:LEU:CD2	0.41	2.44	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:85:LEU:C	1:A:85:LEU:HD22	0.41	2.36	15	1
1:A:39:MET:HE1	2:B:16:ILE:HG22	0.41	1.92	6	1
1:A:13:ILE:HA	1:A:16:ALA:HB3	0.41	1.92	15	1
1:A:7:ASP:O	1:A:11:LEU:HD13	0.41	2.15	15	2
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: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:HA	1:A:37:GLN:CB	0.40	2.46	12	1
1:A:17:ILE:HD11	1:A:69:TYR:CZ	0.40	2.52	2	1
1:A:34:PRO:HG3	1:A:37:GLN:OE1	0.40	2.16	2	1
1:A:22:HIS:O	1:A:26:CYS:CB	0.40	2.70	14	1
1:A:13:ILE:HA	1:A:16:ALA:CB	0.40	2.47	15	1
1:A:34:PRO:HG3	1:A:37:GLN:NE2	0.40	2.31	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	82/90 (91%)	71±2 (87±2%)	7±1 (8±2%)	4±1 (5±1%)	5	26
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%)	6	30

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

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	71/77 (92%)	62±2 (87±2%)	9±2 (13±2%)	9	50
2	B	11/23 (48%)	8±1 (73±9%)	3±1 (27±9%)	2	22
All	All	1230/1500 (82%)	1046 (85%)	184 (15%)	7	46

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

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 (i)

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

7.1 Chemical shift list 1

File name: 2mzd_cs.str

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 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	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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	87	-0.52 ± 0.19	Should be applied
$^{13}C_{\beta}$	83	0.25 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	74	-0.85 ± 0.10	Should be applied
^{15}N	74	-0.76 ± 0.30	Should be applied

7.1.3 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 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	^{1}H	^{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	**¹H**	**¹³C**	**¹⁵N**
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**	**¹H**	**¹³C**	**¹⁵N**
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%)

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.

Random coil index (RCI) for chain A:
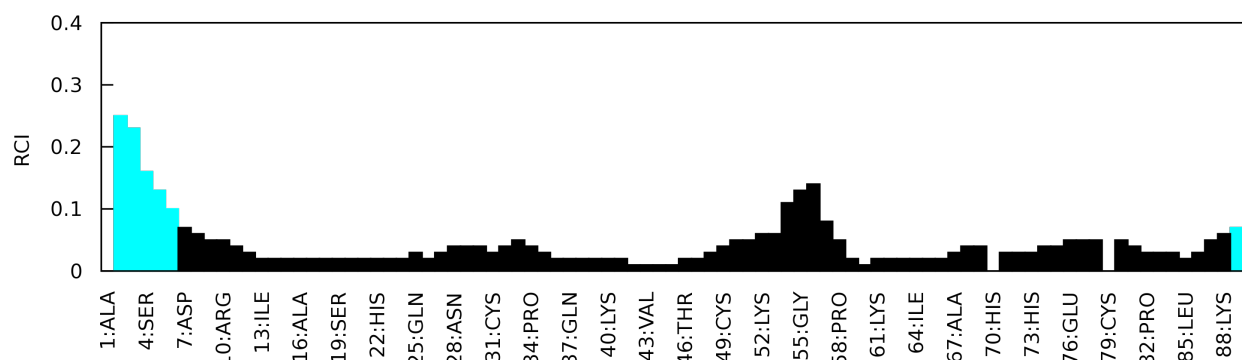
7.2 Chemical shift list 2

File name: 2mzd_cs.str

Chemical shift list name: *assigned_ chem_ shift_ list_ 2*

7.2.1 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

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, *ppm*	Suggested action
$^{13}C_\alpha$	25	-0.01 $\pm$ 0.23	None needed ($<$ 0.5 ppm)
$^{13}C_\beta$	24	0.47 $\pm$ 0.29	None needed ($<$ 0.5 ppm)
$^{13}C'$	21	-0.22 $\pm$ 0.15	None needed ($<$ 0.5 ppm)
^{15}N	22	0.24 $\pm$ 0.81	None needed ($<$ 0.5 ppm)

7.2.3 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	^{1}H	^{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	^{1}H	^{13}C	^{15}N
Backbone	114/559 (20%)	46/222 (21%)	46/230 (20%)	22/107 (21%)

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	Total	^{1}H	^{13}C	^{15}N
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%)

7.2.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.2.5 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 B: