



Full wwPDB NMR Structure Validation Report ⓘ

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Title : Structure of the PSCD-region of the cell wall protein pleuralin-1
Authors : De Sanctis, S.; Wenzler, M.; Kroeger, N.; Malloni, W.M.; Sumper, M.; Rainer, D.; Zadavec, P.; Brunner, E.; Kremer, W.; Kalbitzer, H.R.
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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

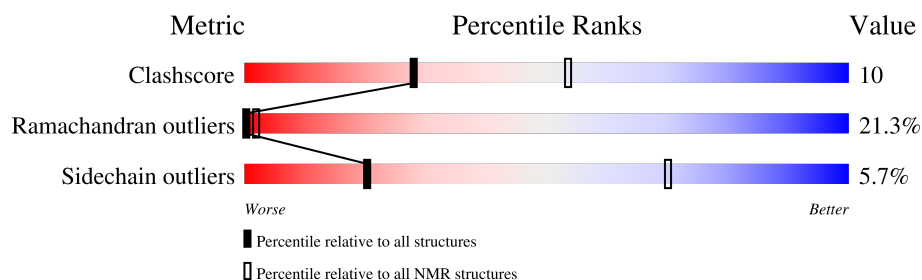
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 18%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	503	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6886 atoms, of which 3285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEP200 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	494	Total	C	H	N	O	S	0
			6886	2209	3285	576	754	62	

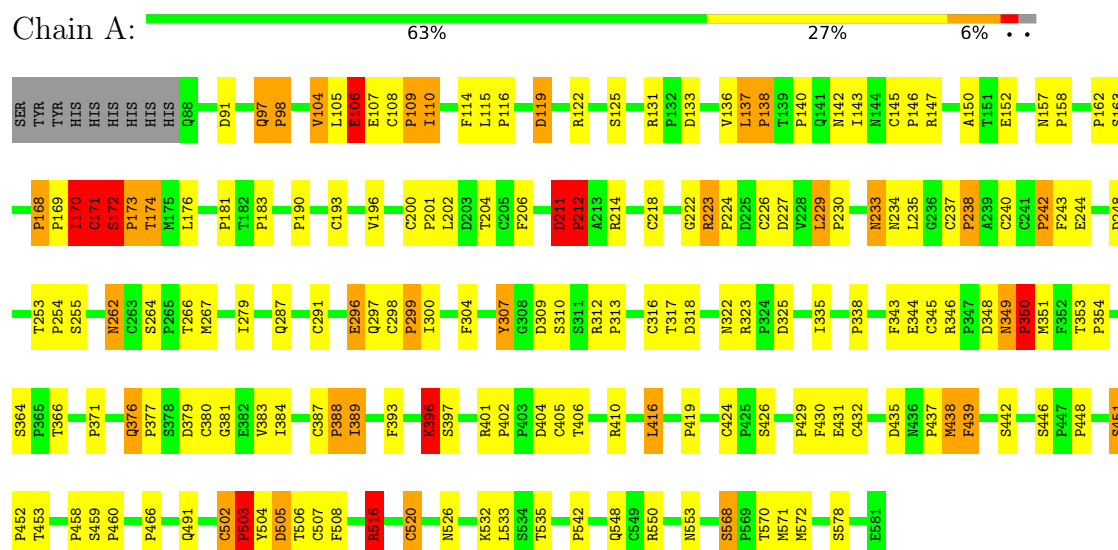
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O22015
A	2	TYR	-	expression tag	UNP O22015
A	3	TYR	-	expression tag	UNP O22015
A	4	HIS	-	expression tag	UNP O22015
A	5	HIS	-	expression tag	UNP O22015
A	6	HIS	-	expression tag	UNP O22015
A	7	HIS	-	expression tag	UNP O22015
A	8	HIS	-	expression tag	UNP O22015
A	9	HIS	-	expression tag	UNP O22015

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: HEP200 protein



5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.21
CNS	refinement	
AUREMOL	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1074
Number of shifts mapped to atoms	1046
Number of unparsed shifts	0
Number of shifts with mapping errors	28
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	18%

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	1.31	17/3735 (0.5%)	1.24	11/5181 (0.2%)
All	All	1.31	17/3735 (0.5%)	1.24	11/5181 (0.2%)

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	ILE	CA-C	13.35	1.69	1.52
1	A	106	GLU	C-O	-10.36	1.10	1.24
1	A	171	CYS	N-CA	10.03	1.59	1.46
1	A	170	ILE	C-N	6.84	1.43	1.33
1	A	229	LEU	C-N	6.29	1.41	1.33
1	A	211	ASP	CA-C	6.21	1.60	1.52
1	A	172	SER	CA-C	6.17	1.60	1.52
1	A	553	ASN	C-N	6.16	1.41	1.33
1	A	110	ILE	CA-C	6.11	1.60	1.52
1	A	505	ASP	N-CA	6.06	1.54	1.46
1	A	350	PRO	N-CD	-6.04	1.39	1.47
1	A	416	LEU	C-N	5.64	1.40	1.33
1	A	183	PRO	CA-C	5.60	1.57	1.52
1	A	350	PRO	CA-C	5.55	1.60	1.52
1	A	172	SER	C-O	-5.21	1.17	1.24
1	A	516	ARG	C-N	5.12	1.39	1.33
1	A	416	LEU	CA-C	5.02	1.57	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	CA-CB-CG	7.30	119.90	112.60
1	A	507	CYS	N-CA-C	-6.87	104.43	114.39
1	A	262	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	350	PRO	N-CA-CB	-6.81	96.10	103.25
1	A	168	PRO	N-CA-C	-6.21	103.12	110.70
1	A	133	ASP	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	N-CA-C	-5.46	106.61	113.28
1	A	516	ARG	CA-C-O	-5.24	116.42	121.08
1	A	503	PRO	N-CA-CB	-5.05	97.95	103.25
1	A	520	CYS	CA-C-N	5.01	127.26	120.44
1	A	520	CYS	C-N-CA	5.01	127.26	120.44

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	3601	3285	3284	66
All	All	3601	3285	3284	66

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:98:PRO:HA	1:A:104:VAL:HG11	0.78	1.54
1:A:107:GLU:HG2	1:A:109:PRO:CD	0.76	2.11
1:A:107:GLU:HG2	1:A:109:PRO:HD2	0.71	1.63
1:A:108:CYS:SG	1:A:109:PRO:HD3	0.67	2.29
1:A:107:GLU:CB	1:A:170:ILE:H	0.66	2.03
1:A:104:VAL:HA	1:A:170:ILE:C	0.66	2.16
1:A:106:GLU:HB3	1:A:174:THR:HB	0.65	1.68
1:A:106:GLU:CB	1:A:174:THR:HB	0.62	2.25
1:A:106:GLU:C	1:A:171:CYS:H	0.61	2.04
1:A:396:LYS:HD2	1:A:397:SER:N	0.60	2.12
1:A:104:VAL:HG12	1:A:170:ILE:HB	0.59	1.73
1:A:325:ASP:OD2	1:A:335:ILE:HB	0.59	1.98
1:A:104:VAL:HA	1:A:170:ILE:CA	0.57	2.29
1:A:349:ASN:OD1	1:A:350:PRO:HD3	0.55	2.01
1:A:387:CYS:SG	1:A:388:PRO:HD3	0.55	2.41

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:107:GLU:HB2	1:A:170:ILE:H	0.55	1.62
1:A:106:GLU:HG3	1:A:172:SER:N	0.54	2.17
1:A:107:GLU:H	1:A:169:PRO:C	0.53	2.11
1:A:404:ASP:OD2	1:A:437:PRO:HB3	0.53	2.04
1:A:107:GLU:C	1:A:109:PRO:HD2	0.53	2.29
1:A:211:ASP:HB3	1:A:212:PRO:HD3	0.53	1.79
1:A:503:PRO:HB2	1:A:568:SER:C	0.53	2.29
1:A:502:CYS:H	1:A:503:PRO:CD	0.52	2.17
1:A:532:LYS:HG2	1:A:548:GLN:OE1	0.51	2.06
1:A:107:GLU:H	1:A:170:ILE:N	0.51	2.04
1:A:446:SER:O	1:A:448:PRO:HD3	0.50	2.05
1:A:222:GLY:O	1:A:224:PRO:HD3	0.48	2.08
1:A:238:PRO:HD2	1:A:240:CYS:SG	0.48	2.49
1:A:379:ASP:HB3	1:A:383:VAL:HG22	0.48	1.86
1:A:108:CYS:HA	1:A:173:PRO:CD	0.47	2.39
1:A:323:ARG:NE	1:A:323:ARG:HA	0.47	2.24
1:A:226:CYS:O	1:A:242:PRO:HA	0.47	2.09
1:A:438:MET:O	1:A:439:PHE:HB2	0.47	2.09
1:A:119:ASP:O	1:A:162:PRO:HB2	0.46	2.09
1:A:451:SER:HB2	1:A:452:PRO:HD3	0.46	1.87
1:A:410:ARG:HA	1:A:410:ARG:NE	0.46	2.26
1:A:223:ARG:NE	1:A:223:ARG:HA	0.46	2.25
1:A:226:CYS:SG	1:A:237:CYS:N	0.45	2.90
1:A:503:PRO:HA	1:A:571:MET:HB3	0.45	1.89
1:A:317:THR:HB	1:A:343:PHE:CD2	0.43	2.47
1:A:296:GLU:O	1:A:299:PRO:HD2	0.43	2.14
1:A:406:THR:HB	1:A:430:PHE:CD1	0.43	2.48
1:A:200:CYS:SG	1:A:201:PRO:HD3	0.43	2.54
1:A:229:LEU:HB3	1:A:230:PRO:CD	0.43	2.43
1:A:508:PHE:O	1:A:516:ARG:HB2	0.43	2.14
1:A:383:VAL:HA	1:A:389:ILE:CD1	0.43	2.42
1:A:106:GLU:HG3	1:A:172:SER:H	0.43	1.71
1:A:107:GLU:N	1:A:170:ILE:N	0.42	2.67
1:A:105:LEU:N	1:A:170:ILE:HA	0.42	2.28
1:A:125:SER:CB	1:A:158:PRO:HA	0.42	2.45
1:A:106:GLU:HA	1:A:173:PRO:O	0.42	2.15
1:A:137:LEU:HB3	1:A:138:PRO:HD3	0.42	1.91
1:A:211:ASP:CB	1:A:212:PRO:HD3	0.42	2.45
1:A:131:ARG:NE	1:A:131:ARG:HA	0.42	2.30
1:A:346:ARG:HD2	1:A:346:ARG:N	0.42	2.29
1:A:297:GLN:CD	1:A:351:MET:HB3	0.41	2.40
1:A:379:ASP:CB	1:A:383:VAL:HG22	0.41	2.45

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:506:THR:O	1:A:572:MET:HG2	0.41	2.15
1:A:107:GLU:CB	1:A:170:ILE:N	0.41	2.80
1:A:104:VAL:HA	1:A:170:ILE:O	0.41	2.15
1:A:376:GLN:H	1:A:377:PRO:HD2	0.41	1.76
1:A:516:ARG:HE	1:A:516:ARG:C	0.41	2.24
1:A:502:CYS:O	1:A:571:MET:HB3	0.40	2.16
1:A:97:GLN:OE1	1:A:168:PRO:HB2	0.40	2.16
1:A:98:PRO:CA	1:A:104:VAL:HG21	0.40	2.47
1:A:152:GLU:O	1:A:157:ASN:HB3	0.40	2.15

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	492/503 (98%)	240 (49%)	147 (30%)	105 (21%)	0	2
All	All	492/503 (98%)	240 (49%)	147 (30%)	105 (21%)	0	2

All 105 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	91	ASP
1	A	97	GLN
1	A	98	PRO
1	A	104	VAL
1	A	106	GLU
1	A	109	PRO
1	A	110	ILE
1	A	114	PHE
1	A	115	LEU
1	A	116	PRO
1	A	119	ASP
1	A	137	LEU
1	A	138	PRO
1	A	140	PRO

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Mol	Chain	Res	Type
1	A	145	CYS
1	A	146	PRO
1	A	147	ARG
1	A	150	ALA
1	A	163	SER
1	A	171	CYS
1	A	172	SER
1	A	173	PRO
1	A	174	THR
1	A	181	PRO
1	A	190	PRO
1	A	193	CYS
1	A	202	LEU
1	A	206	PHE
1	A	211	ASP
1	A	212	PRO
1	A	218	CYS
1	A	235	LEU
1	A	238	PRO
1	A	242	PRO
1	A	244	GLU
1	A	248	ASP
1	A	253	THR
1	A	254	PRO
1	A	255	SER
1	A	264	SER
1	A	266	THR
1	A	279	ILE
1	A	287	GLN
1	A	291	CYS
1	A	296	GLU
1	A	298	CYS
1	A	299	PRO
1	A	300	ILE
1	A	304	PHE
1	A	307	TYR
1	A	309	ASP
1	A	310	SER
1	A	313	PRO
1	A	316	CYS
1	A	318	ASP
1	A	322	ASN

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Mol	Chain	Res	Type
1	A	338	PRO
1	A	344	GLU
1	A	345	CYS
1	A	348	ASP
1	A	350	PRO
1	A	353	THR
1	A	354	PRO
1	A	364	SER
1	A	366	THR
1	A	371	PRO
1	A	376	GLN
1	A	380	CYS
1	A	381	GLY
1	A	384	ILE
1	A	388	PRO
1	A	389	ILE
1	A	393	PHE
1	A	396	LYS
1	A	402	PRO
1	A	405	CYS
1	A	419	PRO
1	A	424	CYS
1	A	426	SER
1	A	429	PRO
1	A	431	GLU
1	A	432	CYS
1	A	435	ASP
1	A	438	MET
1	A	439	PHE
1	A	442	SER
1	A	451	SER
1	A	453	THR
1	A	458	PRO
1	A	459	SER
1	A	460	PRO
1	A	466	PRO
1	A	491	GLN
1	A	502	CYS
1	A	503	PRO
1	A	504	TYR
1	A	505	ASP
1	A	520	CYS

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Mol	Chain	Res	Type
1	A	526	ASN
1	A	535	THR
1	A	542	PRO
1	A	550	ARG
1	A	568	SER
1	A	570	THR
1	A	578	SER

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	460/469 (98%)	434 (94%)	26 (6%)	20	70
All	All	460/469 (98%)	434 (94%)	26 (6%)	20	70

All 26 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	122	ARG
1	A	136	VAL
1	A	142	ASN
1	A	143	ILE
1	A	170	ILE
1	A	171	CYS
1	A	176	LEU
1	A	196	VAL
1	A	204	THR
1	A	212	PRO
1	A	214	ARG
1	A	223	ARG
1	A	233	ASN
1	A	234	ASN
1	A	243	PHE
1	A	262	ASN
1	A	267	MET
1	A	307	TYR

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Mol	Chain	Res	Type
1	A	312	ARG
1	A	349	ASN
1	A	396	LYS
1	A	401	ARG
1	A	416	LEU
1	A	503	PRO
1	A	516	ARG
1	A	533	LEU

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 oligosaccharides 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 18% for the well-defined parts and 18% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	1074
Number of shifts mapped to atoms	1046
Number of unparsed shifts	0
Number of shifts with mapping errors	28
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 28 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	TYR	C	175.42	0.20	1
1	A	2	TYR	CA	57.75	0.20	1
1	A	2	TYR	CB	40.12	0.20	1
1	A	3	TYR	H	7.64	0.02	1
1	A	3	TYR	HA	4.77	0.05	1
1	A	3	TYR	C	176.1	0.20	1
1	A	3	TYR	CA	59.3	0.20	1
1	A	3	TYR	N	115.11	0.33	1
1	A	5	HIS	HA	3.97	0.05	1
1	A	5	HIS	HB2	3.11	0.05	2
1	A	5	HIS	HB3	3.2	0.05	2
1	A	5	HIS	C	176.39	0.20	1
1	A	5	HIS	CA	56.7	0.20	1
1	A	5	HIS	CB	30.07	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	HIS	HA	4.57	0.05	1
1	A	8	HIS	HB2	2.98	0.05	1
1	A	8	HIS	HB3	2.98	0.05	1
1	A	8	HIS	C	173.92	0.20	1
1	A	8	HIS	CA	55.82	0.20	1
1	A	8	HIS	CB	30.6	0.20	1
1	A	9	HIS	H	8.35	0.02	1
1	A	9	HIS	HA	4.65	0.05	1
1	A	9	HIS	HB2	3.08	0.05	1
1	A	9	HIS	HB3	3.08	0.05	1
1	A	9	HIS	C	175.59	0.20	1
1	A	9	HIS	CA	56.17	0.20	1
1	A	9	HIS	CB	30.74	0.20	1
1	A	9	HIS	N	120.44	0.33	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	0.34 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	0.28 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	91	-0.00 ± 0.17	None needed (< 0.5 ppm)
^{15}N	78	0.14 ± 0.58	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 18%, i.e. 1042 atoms were assigned a chemical shift out of a possible 5832. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	441/2256 (20%)	179/888 (20%)	186/988 (19%)	76/380 (20%)
Sidechain	589/3369 (17%)	390/2192 (18%)	191/1095 (17%)	8/82 (10%)
Aromatic	12/207 (6%)	12/102 (12%)	0/105 (0%)	0/0 (—%)
Overall	1042/5832 (18%)	581/3182 (18%)	377/2188 (17%)	84/462 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 1042 atoms were assigned a chemical shift out of a possible 5832. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	441/2256 (20%)	179/888 (20%)	186/988 (19%)	76/380 (20%)
Sidechain	589/3369 (17%)	390/2192 (18%)	191/1095 (17%)	8/82 (10%)
Aromatic	12/207 (6%)	12/102 (12%)	0/105 (0%)	0/0 (—%)
Overall	1042/5832 (18%)	581/3182 (18%)	377/2188 (17%)	84/462 (18%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	401	ARG	NE	127.48	76.53 – 92.65	26.6
1	A	410	ARG	NE	124.58	76.53 – 92.65	24.8

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

