



Full wwPDB NMR Structure Validation Report ⓘ

Dec 7, 2016 – 07:54 AM EST

PDB ID : 2MK0
Title : Structure of the PSCD4-domain of the cell wall protein pleuralin-1 from the diatom *Cylindrotheca fusiformis*
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Deposited on : 2014-01-22

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
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-20028442
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

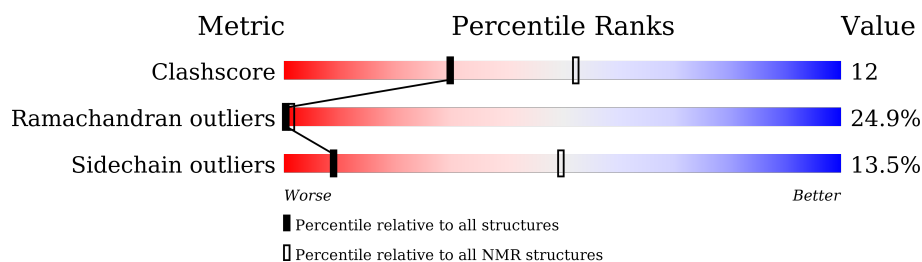
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	120	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:376-A:453 (78)	0.49	2

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 9, 10
2	4, 7, 8

3 Entry composition

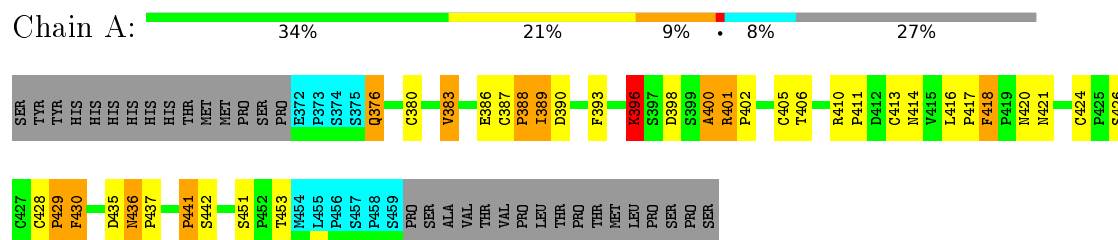
There is only 1 type of molecule in this entry. The entry contains 1204 atoms, of which 570 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEP200 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1204	388	570	101	133	12	

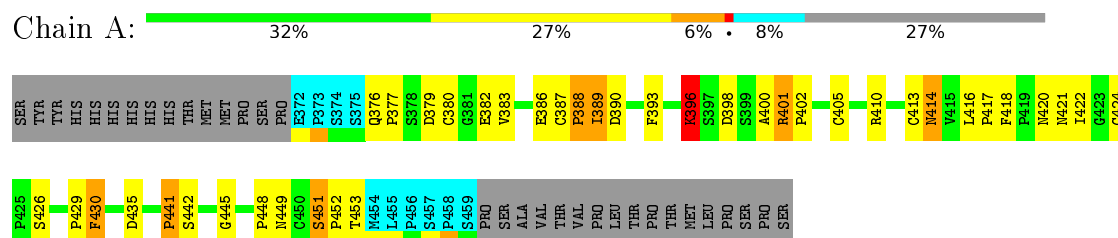
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	SER	-	EXPRESSION TAG	UNP O22015
A	358	TYR	-	EXPRESSION TAG	UNP O22015
A	359	TYR	-	EXPRESSION TAG	UNP O22015
A	360	HIS	-	EXPRESSION TAG	UNP O22015
A	361	HIS	-	EXPRESSION TAG	UNP O22015
A	362	HIS	-	EXPRESSION TAG	UNP O22015
A	363	HIS	-	EXPRESSION TAG	UNP O22015
A	364	HIS	-	EXPRESSION TAG	UNP O22015
A	365	HIS	-	EXPRESSION TAG	UNP O22015
A	470	THR	-	EXPRESSION TAG	UNP O22015
A	471	MET	-	EXPRESSION TAG	UNP O22015
A	472	LEU	-	EXPRESSION TAG	UNP O22015
A	473	PRO	-	EXPRESSION TAG	UNP O22015
A	474	SER	-	EXPRESSION TAG	UNP O22015
A	475	PRO	-	EXPRESSION TAG	UNP O22015
A	476	SER	-	EXPRESSION TAG	UNP O22015



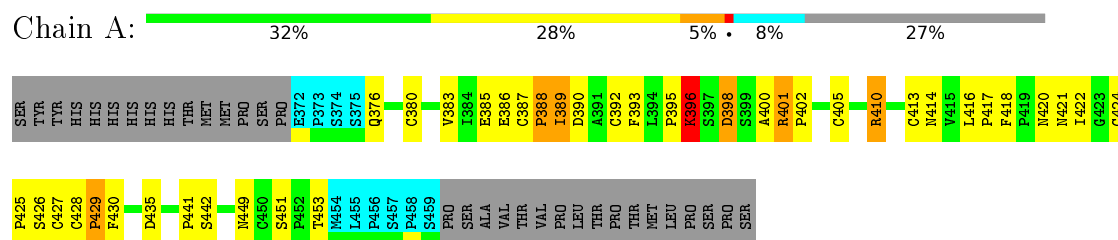
4.2.7 Score per residue for model 7

- Molecule 1: HEP200 protein



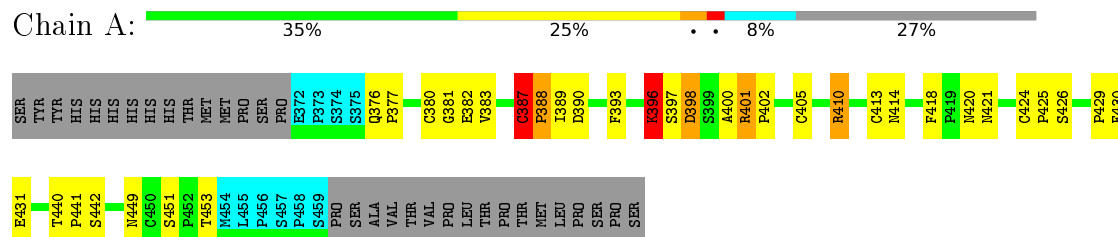
4.2.8 Score per residue for model 8

- Molecule 1: HEP200 protein



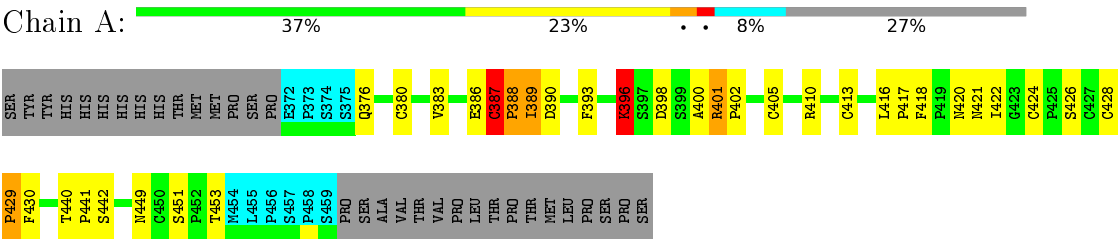
4.2.9 Score per residue for model 9

- Molecule 1: HEP200 protein



4.2.10 Score per residue for model 10

● Molecule 1: HEP200 protein



5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 10 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	

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)	2mk0_cs.cif
Number of chemical shift lists	1
Total number of shifts	1074
Number of shifts mapped to atoms	1074
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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	0.95±0.02	0±0/585 (0.0±0.1%)	0.92±0.01	0±0/809 (0.0±0.0%)
All	All	0.95	2/5850 (0.0%)	0.92	0/8090 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	387	CYS	C-N	5.45	1.44	1.34	9	2

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	564	503	503	13±3
All	All	5640	5030	5030	128

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:CYS:SG	1:A:429:PRO:HD2	0.63	2.33	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:CYS:N	1:A:388:PRO:HD2	0.60	2.12	5	8
1:A:387:CYS:SG	1:A:388:PRO:HD3	0.60	2.36	7	2
1:A:396:LYS:HA	1:A:401:ARG:CG	0.59	2.28	1	10
1:A:386:GLU:C	1:A:388:PRO:HD2	0.56	2.20	6	5
1:A:395:PRO:O	1:A:396:LYS:HE2	0.55	2.00	8	1
1:A:396:LYS:HA	1:A:401:ARG:HG2	0.55	1.77	1	10
1:A:410:ARG:NE	1:A:410:ARG:HA	0.55	2.15	2	4
1:A:413:CYS:SG	1:A:424:CYS:N	0.54	2.81	3	10
1:A:386:GLU:HG3	1:A:388:PRO:HD2	0.53	1.80	1	2
1:A:376:GLN:HB3	1:A:377:PRO:HD3	0.53	1.79	3	1
1:A:410:ARG:HA	1:A:410:ARG:NE	0.53	2.18	5	1
1:A:396:LYS:HE3	1:A:397:SER:H	0.52	1.64	2	3
1:A:388:PRO:HD3	1:A:432:CYS:SG	0.51	2.45	3	1
1:A:389:ILE:HG22	1:A:390:ASP:H	0.50	1.67	8	7
1:A:441:PRO:O	1:A:445:GLY:HA3	0.50	2.07	2	3
1:A:386:GLU:HG3	1:A:388:PRO:CG	0.49	2.37	2	3
1:A:416:LEU:HB3	1:A:417:PRO:HD3	0.48	1.86	3	3
1:A:386:GLU:HG3	1:A:388:PRO:CD	0.47	2.39	1	4
1:A:410:ARG:HG3	1:A:425:PRO:HD3	0.47	1.86	1	4
1:A:387:CYS:SG	1:A:416:LEU:HD21	0.46	2.51	4	2
1:A:425:PRO:HD2	1:A:427:CYS:SG	0.46	2.51	8	2
1:A:376:GLN:O	1:A:383:VAL:HB	0.46	2.09	6	2
1:A:389:ILE:HG22	1:A:390:ASP:N	0.46	2.26	8	7
1:A:401:ARG:HB2	1:A:402:PRO:HD2	0.45	1.89	1	3
1:A:416:LEU:HB3	1:A:417:PRO:CD	0.45	2.41	6	6
1:A:388:PRO:HA	1:A:392:CYS:HB2	0.45	1.89	8	1
1:A:386:GLU:HG2	1:A:388:PRO:HD2	0.44	1.88	3	2
1:A:400:ALA:HB2	1:A:441:PRO:HG3	0.44	1.88	6	1
1:A:414:ASN:HA	1:A:430:PHE:HB2	0.43	1.91	7	2
1:A:406:THR:OG1	1:A:411:PRO:HA	0.42	2.14	6	1
1:A:409:GLY:O	1:A:411:PRO:HD3	0.42	2.14	4	1
1:A:448:PRO:HD2	1:A:452:PRO:O	0.42	2.15	7	1
1:A:387:CYS:N	1:A:388:PRO:CD	0.42	2.83	4	1
1:A:449:ASN:O	1:A:452:PRO:HD2	0.42	2.15	4	1
1:A:410:ARG:CG	1:A:425:PRO:HD3	0.41	2.46	1	1
1:A:436:ASN:N	1:A:437:PRO:HD3	0.41	2.30	6	1
1:A:382:GLU:HA	1:A:386:GLU:OE2	0.41	2.15	7	1
1:A:418:PHE:CE1	1:A:429:PRO:HD3	0.41	2.51	6	1
1:A:393:PHE:O	1:A:394:LEU:HB2	0.41	2.16	5	1
1:A:405:CYS:O	1:A:408:VAL:HG22	0.40	2.16	2	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/120 (65%)	32±2 (41±2%)	27±2 (34±2%)	19±2 (25±2%)	0	1
All	All	780/1200 (65%)	321 (41%)	265 (34%)	194 (25%)	0	1

All 30 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	429	PRO	10
1	A	405	CYS	10
1	A	396	LYS	10
1	A	442	SER	10
1	A	402	PRO	10
1	A	388	PRO	10
1	A	376	GLN	10
1	A	441	PRO	10
1	A	451	SER	10
1	A	426	SER	10
1	A	393	PHE	10
1	A	398	ASP	10
1	A	453	THR	10
1	A	389	ILE	10
1	A	380	CYS	10
1	A	400	ALA	8
1	A	422	ILE	5
1	A	440	THR	5
1	A	414	ASN	5
1	A	377	PRO	4
1	A	435	ASP	4
1	A	431	GLU	3
1	A	395	PRO	2
1	A	379	ASP	2
1	A	384	ILE	1
1	A	436	ASN	1
1	A	449	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	437	PRO	1
1	A	424	CYS	1
1	A	381	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	71/112 (63%)	61±1 (86±2%)	10±1 (14±2%)	9	50
All	All	710/1120 (63%)	614 (86%)	96 (14%)	9	50

All 17 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	430	PHE	10
1	A	421	ASN	10
1	A	420	ASN	10
1	A	396	LYS	10
1	A	418	PHE	10
1	A	383	VAL	10
1	A	401	ARG	10
1	A	410	ARG	9
1	A	449	ASN	5
1	A	387	CYS	3
1	A	398	ASP	3
1	A	390	ASP	1
1	A	393	PHE	1
1	A	425	PRO	1
1	A	382	GLU	1
1	A	385	GLU	1
1	A	402	PRO	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: 2mk0_cs.cif

Chemical shift list name: *shift_set_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	1074
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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	0.40 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	0.28 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	91	-0.05 ± 0.25	None needed (< 0.5 ppm)
^{15}N	78	0.50 ± 0.62	None needed (imprecise)

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 88%, i.e. 747 atoms were assigned a chemical shift out of a possible 850. 5 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	336/356 (94%)	133/139 (96%)	145/156 (93%)	58/61 (95%)
Sidechain	399/458 (87%)	247/280 (88%)	144/165 (87%)	8/13 (62%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	12/36 (33%)	12/20 (60%)	0/16 (0%)	0/0 (—%)
Overall	747/850 (88%)	392/439 (89%)	289/337 (86%)	66/74 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 847 atoms were assigned a chemical shift out of a possible 957. 6 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	376/400 (94%)	150/156 (96%)	161/176 (91%)	65/68 (96%)
Sidechain	459/521 (88%)	286/320 (89%)	165/188 (88%)	8/13 (62%)
Aromatic	12/36 (33%)	12/20 (60%)	0/16 (0%)	0/0 (—%)
Overall	847/957 (89%)	448/496 (90%)	326/380 (86%)	73/81 (90%)

7.1.4 Statistically unusual chemical shifts ⓘ

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	401	ARG	NE	127.48	92.63 – 76.73	26.9
1	A	410	ARG	NE	124.58	92.63 – 76.73	25.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

