wwPDB NMR Structure Validation Summary Report (i)

Apr 27, 2016 – 12:34 AM BST

PDB ID	:	2KMY
Title	:	NMR Solution structures of fully oxidised cytochrome c3 from Desulfovibrio desulfuricans ATCC 27774
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Deposited on	:	2009-08-05

This is a wwPDB NMR Structure Validation Summary 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 (i) symbol.

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

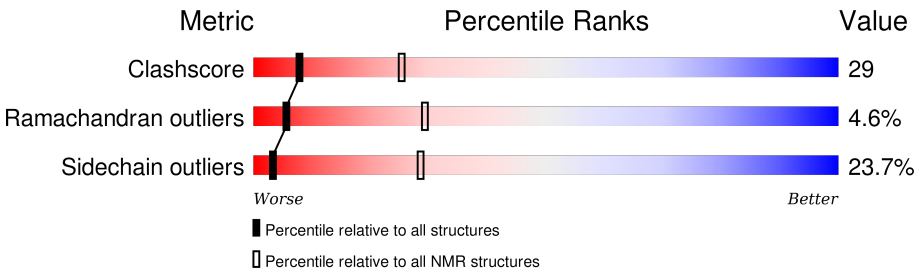
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	107	45% 48% 7% •

2 Ensemble composition and analysis (i)

This entry contains 20 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:1-A:107 (107)	0.24	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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 8, 9, 11, 14, 16, 18
2	4, 5, 7, 13, 15, 19, 20
3	12, 17
Single-model clusters	10

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1774 atoms, of which 796 are hydrogens and 0 are deuteriums.

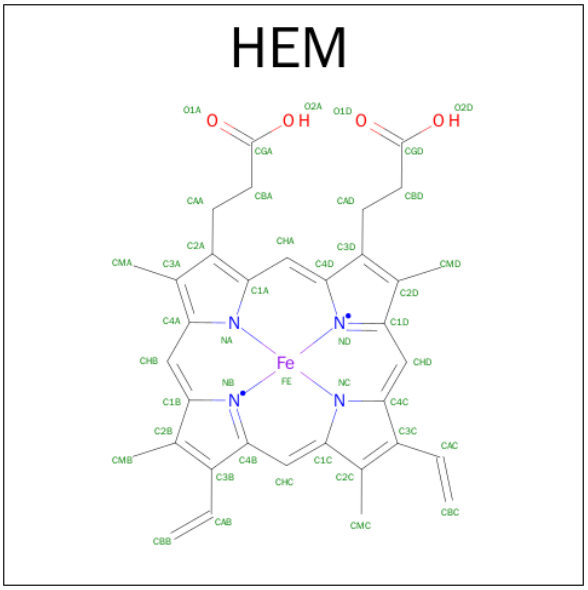
- Molecule 1 is a protein called Cytochrome c3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1602	503	796	144	150	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	ARG	LYS	SEE REMARK 999	UNP Q9L915

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				
			Total	C	Fe	N	O
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4

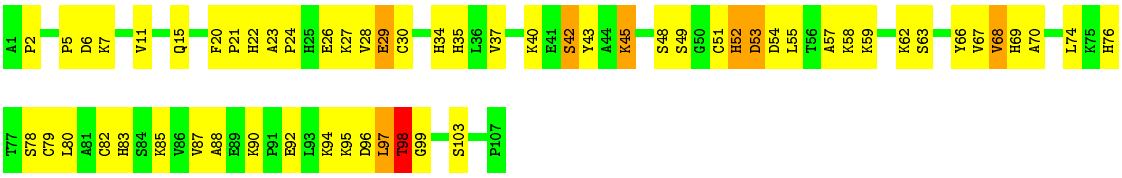
4 Residue-property plots (i)

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: Cytochrome c3

Chain A: 45% 48% 7% •

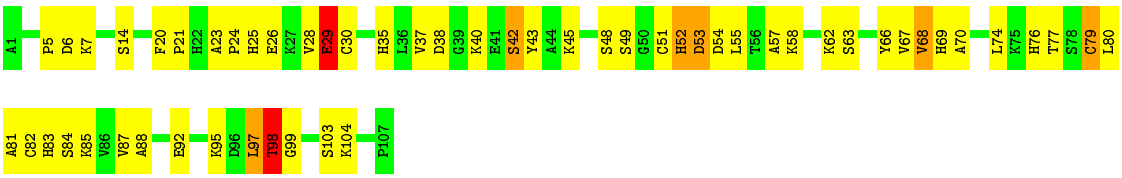


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Cytochrome c3

Chain A: 49% 44% 6% •



5 Refinement protocol and experimental data overview (i)

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

Of the 600 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
Paradyana	structure solution	
Paradyana	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)	BMRB entry 16443
Number of chemical shift lists	1
Total number of shifts	725
Number of shifts mapped to atoms	647
Number of unparsed shifts	58
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (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	806	796	798	49±5
2	A	172	0	120	16±4
All	All	19560	15920	18360	1107

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 29.

5 of 276 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD11	2:A:282:HEM:CHA	0.96	1.91	4	15
1:A:23:ALA:HB3	1:A:24:PRO:HD3	0.94	1.39	12	20
1:A:9:VAL:HG11	2:A:233:HEM:CGA	0.93	1.93	10	5
1:A:83:HIS:CE1	1:A:97:LEU:HD13	0.92	1.99	15	4
1:A:68:VAL:O	1:A:80:LEU:HD23	0.90	1.66	16	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	105/107 (98%)	75±2 (72±2%)	25±3 (24±2%)	5±1 (5±1%)	5 29
All	All	2100/2140 (98%)	1505 (72%)	499 (24%)	96 (5%)	5 29

5 of 15 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	52	HIS	20
1	A	98	THR	18
1	A	68	VAL	17
1	A	29	GLU	14
1	A	2	PRO	7

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	91/91 (100%)	69±2 (76±2%)	22±2 (24±2%)	3 28
All	All	1820/1820 (100%)	1388 (76%)	432 (24%)	3 28

5 of 51 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	6	ASP	20
1	A	42	SER	20
1	A	63	SER	19
1	A	53	ASP	18
1	A	98	THR	18

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEM	A	233	1	24,50,50	1.70±0.00	0±0 (0±0%)
2	HEM	A	251	1	24,50,50	1.70±0.00	0±0 (0±0%)
2	HEM	A	282	1	24,50,50	1.70±0.00	0±0 (0±0%)
2	HEM	A	305	1	24,50,50	1.70±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEM	A	233	1	16,82,82	2.45±0.00	2±0 (12±0%)
2	HEM	A	251	1	16,82,82	2.45±0.00	2±0 (12±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEM	A	282	1	16,82,82	2.45±0.00	2±0 (12±0%)
2	HEM	A	305	1	16,82,82	2.45±0.00	2±0 (12±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	233	1	-	0±0,6,54,54	0±0,0,8,8
2	HEM	A	251	1	-	0±0,6,54,54	0±0,0,8,8
2	HEM	A	282	1	-	0±0,6,54,54	0±0,0,8,8
2	HEM	A	305	1	-	0±0,6,54,54	0±0,0,8,8

There are no bond-length outliers.

5 of 8 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	282	HEM	C3C-CAC-CBC	6.20	113.93	126.40	9	20
2	A	233	HEM	C3C-CAC-CBC	6.20	113.94	126.40	15	20
2	A	305	HEM	C3C-CAC-CBC	6.20	113.94	126.40	11	20
2	A	251	HEM	C3C-CAC-CBC	6.19	113.95	126.40	5	20
2	A	233	HEM	C3B-CAB-CBB	6.19	113.95	126.40	2	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 46% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16443

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	725
Number of shifts mapped to atoms	647
Number of unparsed shifts	58
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	104

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 58) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
668	UNMAPPED	1	HEM_ox	1HAD	2.082	0.001	1
669	UNMAPPED	1	HEM_ox	2HAD	0.649	0.008	1
670	UNMAPPED	1	HEM_ox	1HAA	14.558	0.005	1
671	UNMAPPED	1	HEM_ox	2HAA	4.106	0.005	1
672	UNMAPPED	1	HEM_ox	HHC	2.817	0.005	1

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

- Chain not found in structure. First 5 (of 20) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEM_ox	2HBA	4.9	0.019	1
UNMAPPED	1	HEM_ox	HAB	3.09	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	HEM_ox	HHB	-3.323	0.0	1
UNMAPPED	1	HEM_ox	1HBD	1.59	0.013	1
UNMAPPED	1	HEM_ox	HAC	-4.154	0.0	1

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 46%, i.e. 578 atoms were assigned a chemical shift out of a possible 1254. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	206/521 (40%)	206/207 (100%)	0/214 (0%)	0/100 (0%)
Sidechain	356/637 (56%)	356/379 (94%)	0/238 (0%)	0/20 (0%)
Aromatic	16/96 (17%)	16/53 (30%)	0/34 (0%)	0/9 (0%)
Overall	578/1254 (46%)	578/639 (90%)	0/486 (0%)	0/129 (0%)

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.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	106	HIS	HB3	19.06	5.00 – 1.10	41.1
1	A	34	HIS	HB3	15.34	5.00 – 1.10	31.5
1	A	52	HIS	HB3	14.81	5.00 – 1.10	30.2
1	A	35	HIS	HB2	11.82	4.91 – 1.31	24.2
1	A	69	HIS	HB2	10.03	4.91 – 1.31	19.2
1	A	22	HIS	HB3	10.06	5.00 – 1.10	18.0
1	A	52	HIS	HD2	14.44	9.28 – 4.78	16.5
1	A	35	HIS	HB3	9.31	5.00 – 1.10	16.1
1	A	52	HIS	HB2	8.68	4.91 – 1.31	15.5
1	A	83	HIS	HB2	8.32	4.91 – 1.31	14.5
1	A	22	HIS	HB2	8.30	4.91 – 1.31	14.4
1	A	97	LEU	HD21	-2.92	2.14 – -0.66	-13.1

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	97	LEU	HD22	-2.92	2.14 – -0.66	-13.1
1	A	97	LEU	HD23	-2.92	2.14 – -0.66	-13.1
1	A	52	HIS	HA	10.32	6.81 – 2.41	13.0
1	A	25	HIS	HB2	7.77	4.91 – 1.31	12.9
1	A	33	CYS	HB3	-3.16	5.25 – 0.55	-12.9
1	A	34	HIS	HB2	7.72	4.91 – 1.31	12.8
1	A	68	VAL	HG13	-2.49	2.13 – -0.47	-12.8
1	A	68	VAL	HG12	-2.49	2.13 – -0.47	-12.8
1	A	68	VAL	HG11	-2.49	2.13 – -0.47	-12.8
1	A	106	HIS	HB2	7.48	4.91 – 1.31	12.1
1	A	83	HIS	HA	9.57	6.81 – 2.41	11.3
1	A	18	VAL	HG12	-2.08	2.13 – -0.47	-11.2
1	A	18	VAL	HG13	-2.08	2.13 – -0.47	-11.2
1	A	18	VAL	HG11	-2.08	2.13 – -0.47	-11.2
1	A	22	HIS	HA	9.49	6.81 – 2.41	11.1
1	A	79	CYS	HA	-1.45	7.47 – 1.87	-10.9
1	A	18	VAL	HB	-1.42	3.59 – 0.39	-10.6
1	A	5	PRO	HG3	-1.52	3.56 – 0.26	-10.4
1	A	82	CYS	HB3	-1.87	5.25 – 0.55	-10.2
1	A	106	HIS	HA	8.99	6.81 – 2.41	9.9
1	A	4	VAL	HA	-1.51	7.09 – 1.29	-9.8
1	A	35	HIS	HA	8.89	6.81 – 2.41	9.7
1	A	46	CYS	HB3	-1.46	5.25 – 0.55	-9.3
1	A	58	LYS	HE2	4.63	3.87 – 1.97	9.0
1	A	20	PHE	HD2	4.42	8.56 – 5.56	-8.8
1	A	2	PRO	HG3	-0.94	3.56 – 0.26	-8.6
1	A	46	CYS	HA	-0.11	7.47 – 1.87	-8.5
1	A	77	THR	HG23	-0.79	2.29 – -0.01	-8.4
1	A	77	THR	HG22	-0.79	2.29 – -0.01	-8.4
1	A	77	THR	HG21	-0.79	2.29 – -0.01	-8.4
1	A	62	LYS	HD3	3.46	2.75 – 0.45	8.1
1	A	63	SER	HB2	5.89	5.18 – 2.58	7.7
1	A	105	CYS	HB3	-0.64	5.25 – 0.55	-7.5
1	A	16	LYS	HD2	3.32	2.76 – 0.46	7.5
1	A	62	LYS	HD2	3.31	2.76 – 0.46	7.4
1	A	62	LYS	HA	7.45	6.46 – 2.06	7.3
1	A	25	HIS	HA	7.80	6.81 – 2.41	7.3
1	A	104	LYS	HB2	-0.03	3.03 – 0.53	-7.2
1	A	45	LYS	HD3	-0.05	2.75 – 0.45	-7.2
1	A	20	PHE	HB2	0.37	4.85 – 1.15	-7.1
1	A	11	VAL	HG12	-1.02	2.13 – -0.47	-7.1
1	A	11	VAL	HG11	-1.02	2.13 – -0.47	-7.1

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	11	VAL	HG13	-1.02	2.13 – -0.47	-7.1
1	A	2	PRO	HB2	-0.42	3.82 – 0.32	-7.1
1	A	18	VAL	HG23	-1.18	2.20 – -0.60	-7.1
1	A	18	VAL	HG22	-1.18	2.20 – -0.60	-7.1
1	A	18	VAL	HG21	-1.18	2.20 – -0.60	-7.1
1	A	78	SER	HB2	5.71	5.18 – 2.58	7.1
1	A	21	PRO	HD2	1.14	5.45 – 1.85	-7.0
1	A	2	PRO	HD3	0.97	5.52 – 1.72	-7.0
1	A	62	LYS	HB2	3.49	3.03 – 0.53	6.8
1	A	34	HIS	HA	7.55	6.81 – 2.41	6.7
1	A	33	CYS	HB2	-0.06	5.20 – 0.70	-6.7
1	A	11	VAL	HG21	-1.07	2.20 – -0.60	-6.7
1	A	11	VAL	HG22	-1.07	2.20 – -0.60	-6.7
1	A	11	VAL	HG23	-1.07	2.20 – -0.60	-6.7
1	A	65	TYR	HD2	8.88	8.44 – 5.44	6.5
1	A	65	TYR	HD1	8.88	8.44 – 5.44	6.5
1	A	65	TYR	HB2	5.26	4.76 – 1.06	6.4
1	A	104	LYS	HB3	0.09	3.10 – 0.40	-6.2
1	A	100	CYS	HB3	0.03	5.25 – 0.55	-6.1
1	A	35	HIS	H	12.38	11.68 – 4.78	6.0
1	A	52	HIS	H	12.35	11.68 – 4.78	6.0
1	A	68	VAL	HG22	-0.81	2.20 – -0.60	-5.7
1	A	68	VAL	HG23	-0.81	2.20 – -0.60	-5.7
1	A	68	VAL	HG21	-0.81	2.20 – -0.60	-5.7
1	A	82	CYS	HB2	0.38	5.20 – 0.70	-5.7
1	A	46	CYS	HB2	0.39	5.20 – 0.70	-5.7
1	A	67	VAL	HG11	2.28	2.13 – -0.47	5.6
1	A	67	VAL	HG12	2.28	2.13 – -0.47	5.6
1	A	67	VAL	HG13	2.28	2.13 – -0.47	5.6
1	A	36	LEU	H	11.83	11.47 – 4.97	5.6
1	A	31	VAL	HG21	2.35	2.20 – -0.60	5.5
1	A	31	VAL	HG22	2.35	2.20 – -0.60	5.5
1	A	31	VAL	HG23	2.35	2.20 – -0.60	5.5
1	A	64	LEU	HB3	3.51	3.34 – -0.26	5.5
1	A	2	PRO	HG2	0.24	3.48 – 0.38	-5.4
1	A	66	TYR	HB2	4.91	4.76 – 1.06	5.4
1	A	45	LYS	HD2	2.85	2.76 – 0.46	5.4
1	A	63	SER	HA	6.67	6.53 – 2.43	5.3
1	A	36	LEU	HB3	3.45	3.34 – -0.26	5.3
1	A	11	VAL	HB	0.30	3.59 – 0.39	-5.3
1	A	97	LEU	HG	-0.22	3.16 – -0.14	-5.3
1	A	32	THR	HG21	-0.06	2.29 – -0.01	-5.2

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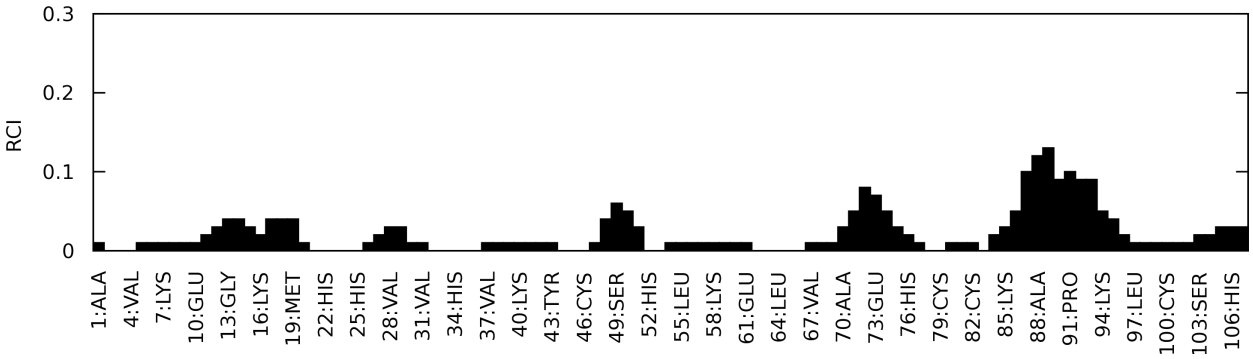
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	32	THR	HG22	-0.06	2.29 – -0.01	-5.2
1	A	32	THR	HG23	-0.06	2.29 – -0.01	-5.2
1	A	80	LEU	HG	3.21	3.16 – -0.14	5.2
1	A	36	LEU	HG	3.21	3.16 – -0.14	5.2
1	A	26	GLU	HB2	3.11	3.08 – 0.98	5.1
1	A	21	PRO	HG2	0.34	3.48 – 0.38	-5.1
1	A	104	LYS	HE3	1.95	3.86 – 1.96	-5.1
1	A	22	HIS	H	11.71	11.68 – 4.78	5.0

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: