



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 09:56 PM BST

PDB ID : 2G46
Title : structure of vSET in complex with meK27 H3 Pept. and cofactor product SAH
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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 ⓘ 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 : 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

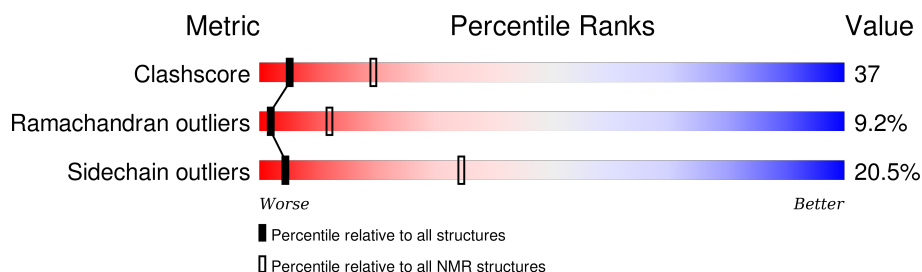
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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	119	 30% 51% 7% 11%
1	B	119	 29% 52% 8% 11%
2	C	21	 19% 81%
2	D	21	 19% 81%

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:2-A:11, A:15-A:110, C:214-C:214, C:216-C:218, B:2-B:11, B:15-B:110, D:214-D:214, D:216-D:218 (220)	0.59	20

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4540 atoms, of which 2278 are hydrogens and 0 are deuteriums.

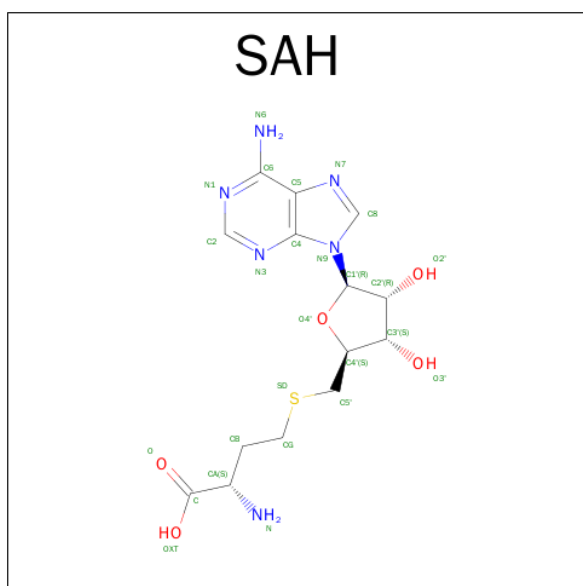
- Molecule 1 is a protein called PBCV-1 histone H3-Lys 27 methyltransferase.

Mol	Chain	Residues	Atoms						Trace
1	A	119	Total	C	H	N	O	S	0
			1907	608	951	169	173	6	
1	B	119	Total	C	H	N	O	S	0
			1907	608	951	169	173	6	

- Molecule 2 is a protein called meK27 H3 Peptide.

Mol	Chain	Residues	Atoms					Trace
2	C	21	Total	C	H	N	O	0
			318	91	169	32	26	
2	D	21	Total	C	H	N	O	0
			318	91	169	32	26	

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



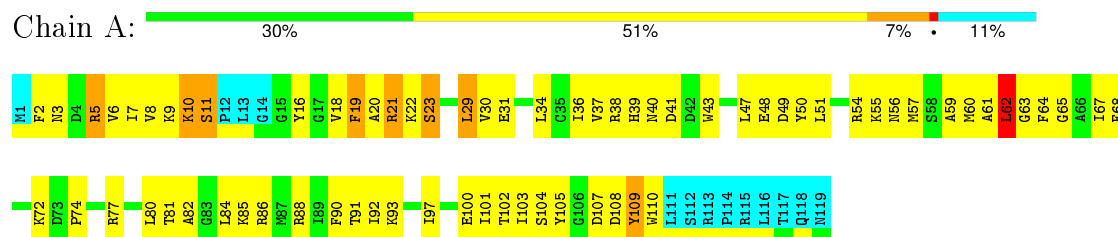
Mol	Chain	Residues	Atoms					
3	A	1	Total	C	H	N	O	S
			45	14	19	6	5	1
3	B	1	Total	C	H	N	O	S
			45	14	19	6	5	1

4 Residue-property plots [i](#)

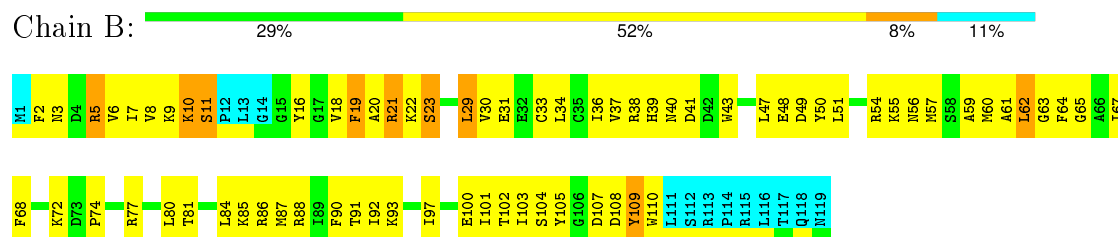
4.1 Average score per residue in the NMR ensemble

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: PBCV-1 histone H3-Lys 27 methyltransferase



- Molecule 1: PBCV-1 histone H3-Lys 27 methyltransferase



- Molecule 2: meK27 H3 Peptide



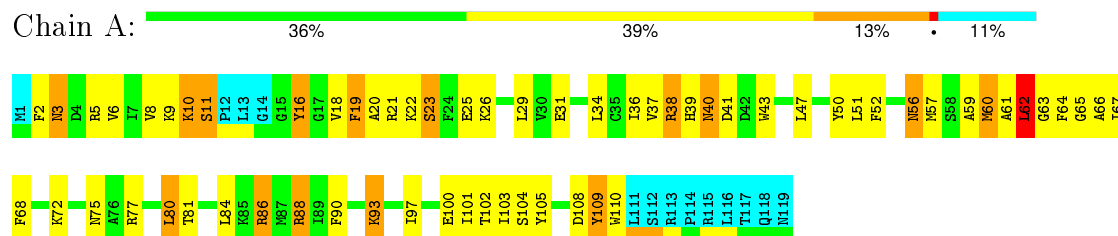
- Molecule 2: meK27 H3 Peptide



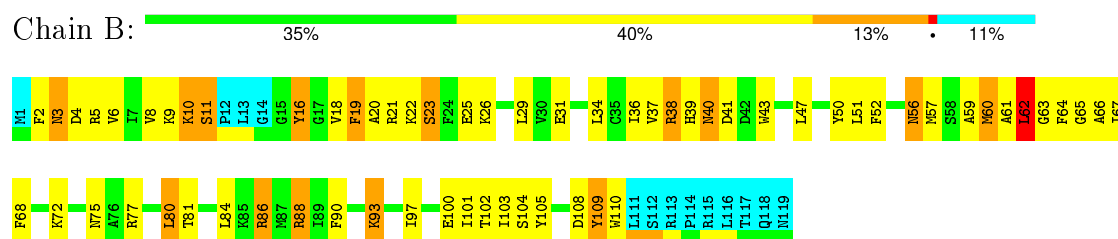
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 20. Colouring as in section 4.1 above.

- Molecule 1: PBCV-1 histone H3-Lys 27 methyltransferase



- Molecule 1: PBCV-1 histone H3-Lys 27 methyltransferase



- Molecule 2: meK27 H3 Peptide



- Molecule 2: meK27 H3 Peptide



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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	refinement	1.1
Aria	refinement	1.2

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 6997
Number of chemical shift lists	1
Total number of shifts	2595
Number of shifts mapped to atoms	2570
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

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

6 Model quality

6.1 Standard geometry

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

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

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	3.0±0.0	0.0±0.0
1	B	3.0±0.0	0.0±0.0
2	C	1.0±0.0	0.0±0.0
2	D	1.0±0.0	0.0±0.0
All	All	160	0

There are no bond-length outliers.

There are no bond-angle outliers.

5 of 8 unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	23	SER	CA	20
1	A	56	ASN	CA	20
1	A	62	LEU	CA	20
2	C	216	SER	CA	20
1	B	23	SER	CA	20

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	853	838	838	69±8

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	853	838	838	68±8
2	C	29	30	30	1±1
2	D	29	30	30	1±1
3	A	26	19	19	1±1
3	B	26	19	19	1±1
All	All	36320	35480	35480	2660

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 37.

5 of 1048 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:36:ILE:HD11	1:B:62:LEU:HD23	1.14	1.14	5	8
1:A:36:ILE:HD11	1:A:62:LEU:HD23	1.08	1.24	6	8
1:B:33:CYS:SG	1:B:87:MET:SD	1.07	2.52	10	1
1:A:33:CYS:SG	1:A:87:MET:SD	1.06	2.52	10	1
1:B:35:CYS:SG	1:B:87:MET:SD	1.03	2.55	7	6

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	106/119 (89%)	75±4 (71±4%)	22±4 (21±4%)	9±2 (8±2%)	2	14
1	B	106/119 (89%)	76±4 (71±4%)	22±4 (20±4%)	9±2 (8±2%)	2	14
2	C	4/21 (19%)	2±1 (44±21%)	1±1 (24±22%)	1±1 (32±18%)	0	0
2	D	4/21 (19%)	2±1 (44±21%)	1±1 (24±22%)	1±1 (32±18%)	0	0
All	All	4400/5600 (79%)	3086 (70%)	911 (21%)	403 (9%)	2	12

5 of 78 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	23	SER	20
1	A	56	ASN	20
1	A	23	SER	20
1	B	56	ASN	20
1	B	63	GLY	18

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/101 (88%)	71±3 (80±3%)	18±3 (20±3%)	4	35
1	B	89/101 (88%)	71±3 (79±3%)	18±3 (21±3%)	4	34
2	C	3/12 (25%)	2±1 (78±22%)	1±1 (22±22%)	4	32
2	D	3/12 (25%)	2±1 (78±22%)	1±1 (22±22%)	4	32
All	All	3680/4520 (81%)	2926 (80%)	754 (20%)	4	34

5 of 122 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	B	62	LEU	20
1	A	62	LEU	20
1	B	57	MET	18
1	A	57	MET	18
1	B	48	GLU	15

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	MLZ	C	215	2	7,9,10	0.52±0.02	0±0 (0±0%)
2	MLZ	D	215	2	7,9,10	0.54±0.02	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	MLZ	C	215	2	7,9,11	1.51±0.02	0±0 (0±0%)
2	MLZ	D	215	2	7,9,11	1.50±0.02	0±0 (0±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	MLZ	C	215	2	-	0±0,6,8,10	0±0,0,0,0
2	MLZ	D	215	2	-	0±0,6,8,10	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

2 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
3	SAH	A	301	-	22,28,28	0.99±0.01	0±0 (0±0%)
3	SAH	B	302	-	22,28,28	0.99±0.00	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
3	SAH	A	301	-	18,40,40	1.25±0.01	0±0 (0±0%)
3	SAH	B	302	-	18,40,40	1.25±0.01	0±0 (0±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
3	SAH	A	301	-	-	0±0,7,31,31	0±0,3,3,3
3	SAH	B	302	-	-	0±0,7,31,31	0±0,3,3,3

There are no bond-length outliers.

There are no bond-angle outliers.

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

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6997

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	2595
Number of shifts mapped to atoms	2570
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

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

- Residue not found in structure. First 5 (of 14) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
D	215	MEK	HB3	1.86	0.03	1
C	215	MEK	HB3	1.86	0.03	1
C	215	MEK	HM1	1.78	0.03	1
D	215	MEK	H	8.26	0.03	1
D	215	MEK	HB2	1.94	0.03	1

- Chain not found in structure. First 5 (of 11) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	SAH	H2''	4.92	0.03	1
UNMAPPED	1	SAH	HG2	2.76	0.03	1
UNMAPPED	1	SAH	HG1	3.1	0.03	1
UNMAPPED	1	SAH	H1'	6.13	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	SAH	H2	8.22	0.03	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	224	-0.20 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	200	-0.18 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	220	1.00 ± 0.40	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 72%, i.e. 1990 atoms were assigned a chemical shift out of a possible 2770. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	824/1088 (76%)	424/434 (98%)	198/440 (45%)	202/214 (94%)
Sidechain	952/1402 (68%)	586/826 (71%)	366/502 (73%)	0/74 (0%)
Aromatic	214/280 (76%)	112/150 (75%)	102/120 (85%)	0/10 (0%)
Overall	1990/2770 (72%)	1122/1410 (80%)	666/1062 (63%)	202/298 (68%)

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
2	B	68	PHE	HA	59.70	7.46 – 1.76	96.6
1	A	68	PHE	HA	59.70	7.46 – 1.76	96.6
1	C	220	THR	HB	1.29	5.82 – 2.52	-8.7
2	D	220	THR	HB	1.29	5.82 – 2.52	-8.7
1	A	46	ALA	HB3	0.04	2.61 – 0.11	-5.3
2	B	46	ALA	HB1	0.04	2.61 – 0.11	-5.3
1	A	46	ALA	HB2	0.04	2.61 – 0.11	-5.3
2	B	46	ALA	HB2	0.04	2.61 – 0.11	-5.3

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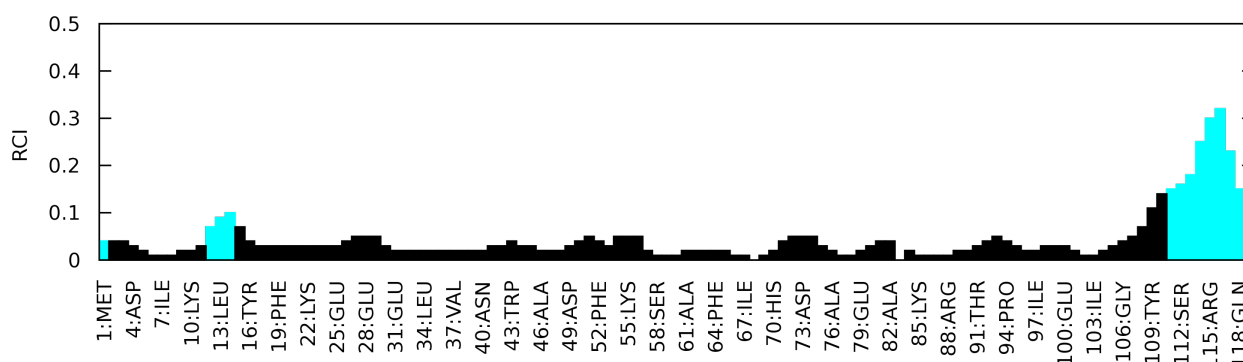
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	46	ALA	HB1	0.04	2.61 – 0.11	-5.3
2	B	46	ALA	HB3	0.04	2.61 – 0.11	-5.3
1	A	65	GLY	N	129.50	129.07 – 90.27	5.1
2	B	65	GLY	N	129.50	129.07 – 90.27	5.1

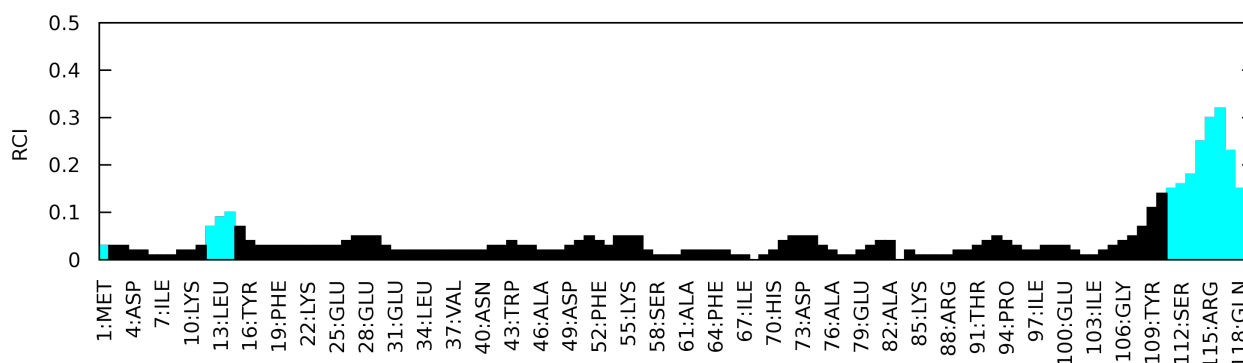
7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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.

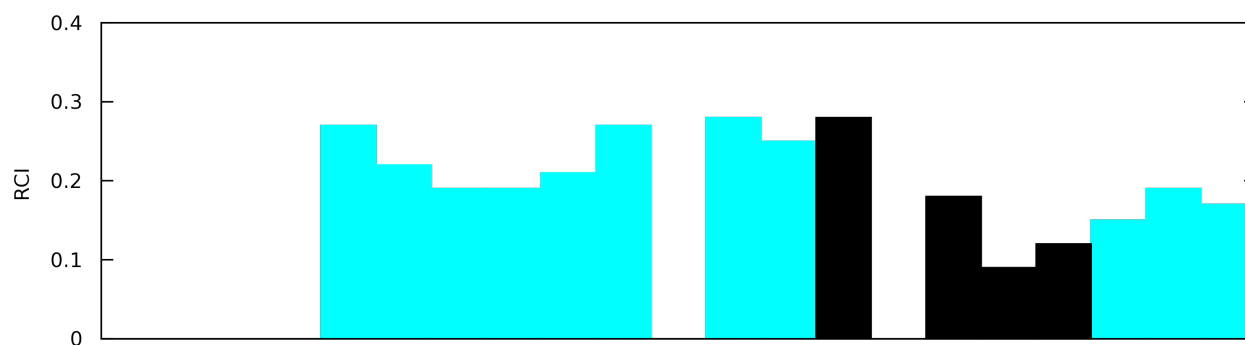
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:

