



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 11:14 PM BST

PDB ID : 2K05  
Title : Structure of SDF1 in complex with the CXCR4 N-terminus containing sulfo-tyrosines at positions 7, 12 and 21  
Authors : Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C.  
Deposited on : 2008-01-24

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

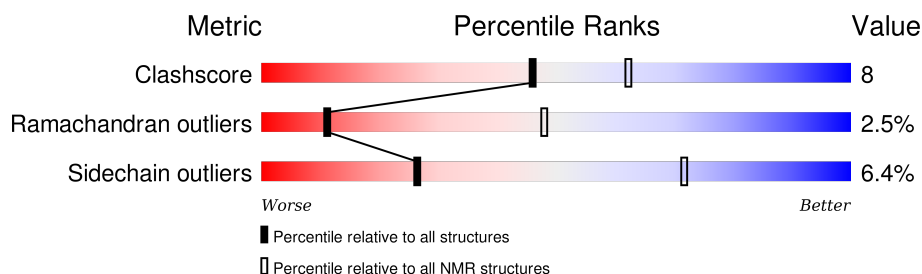
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 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  $\geq 3$ , 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	70	69% 13% 16% •
1	C	70	61% 19% 17% •
2	B	40	20% 75% 5%
2	D	40	20% 75% 5%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 13 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:8-A:43, A:47-A:67, B:119-B:120, B:122-B:127, C:209-C:243, C:247-C:267, D:319-D:320, D:322-D:327 (129)	0.54	13

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 4 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3429 atoms, of which 1682 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	
1	C	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P48061
A	0	MET	-	EXPRESSION TAG	UNP P48061
A	36	CYS	LEU	ENGINEERED	UNP P48061
A	65	CYS	ALA	ENGINEERED	UNP P48061
C	199	GLY	-	EXPRESSION TAG	UNP P48061
C	200	MET	-	EXPRESSION TAG	UNP P48061
C	236	CYS	LEU	ENGINEERED	UNP P48061
C	265	CYS	ALA	ENGINEERED	UNP P48061

- Molecule 2 is a protein called C-X-C chemokine receptor type 4.

Mol	Chain	Residues	Atoms						Trace
2	B	38	Total	C	H	N	O	S	0
			578	185	262	47	78	6	
2	D	38	Total	C	H	N	O	S	0
			579	185	262	47	79	6	

There are 6 discrepancies between the modelled and reference sequences:

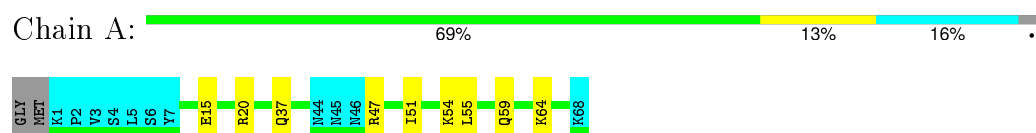
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	GLY	-	EXPRESSION TAG	UNP P61073
B	100	SER	-	EXPRESSION TAG	UNP P61073
B	128	ALA	CYS	ENGINEERED	UNP P61073
D	299	GLY	-	EXPRESSION TAG	UNP P61073
D	300	SER	-	EXPRESSION TAG	UNP P61073
D	328	ALA	CYS	ENGINEERED	UNP P61073

## 4 Residue-property plots [i](#)

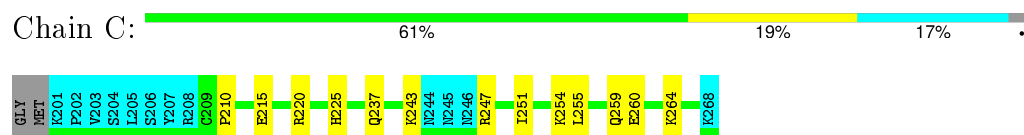
### 4.1 Average score per residue in the NMR ensemble

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.

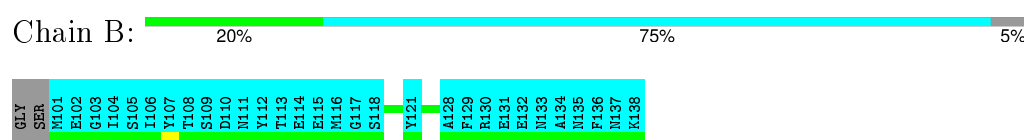
- Molecule 1: Stromal cell-derived factor 1



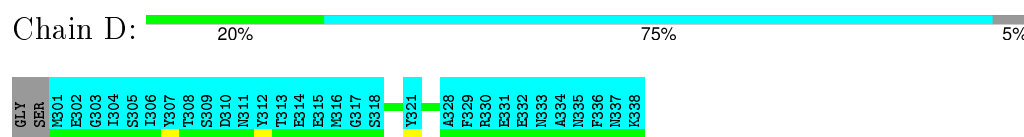
- Molecule 1: Stromal cell-derived factor 1



- Molecule 2: C-X-C chemokine receptor type 4




- Molecule 2: C-X-C chemokine receptor type 4



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

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Stromal cell-derived factor 1

Chain A: 



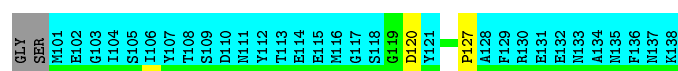
- Molecule 1: Stromal cell-derived factor 1

Chain C: 



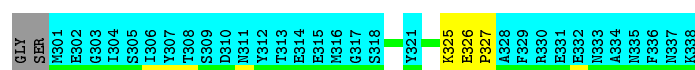
- Molecule 2: C-X-C chemokine receptor type 4

Chain B: 



- Molecule 2: C-X-C chemokine receptor type 4

Chain D: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT..*

Of the 100 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
CYANA	structure solution	2.1
X-PLOR NIH	refinement	2.9.3

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 15637
Number of chemical shift lists	1
Total number of shifts	4962
Number of shifts mapped to atoms	2494
Number of unparsed shifts	2468
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](#)

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

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	C	0.0±0.0	0.1±0.3
1	A	0.0±0.0	0.1±0.2
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

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	C	247	ARG	Sidechain	1
1	C	220	ARG	Sidechain	1
1	A	47	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	469	489	487	9±2
1	C	458	476	474	9±3
2	B	59	51	51	1±1
2	D	59	51	51	1±1
All	All	20900	21340	21260	338



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 8.

5 of 186 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:O	2:B:123:SER:HA	0.71	1.86	19	2
1:A:60:GLU:O	1:A:64:LYS:HG2	0.66	1.91	18	7
1:C:220:ARG:HB3	1:C:257:TRP:CE3	0.64	2.28	11	6
1:A:20:ARG:HB3	1:A:57:TRP:CE3	0.63	2.28	17	4
1:C:260:GLU:O	1:C:264:LYS:HG2	0.63	1.93	11	9

## 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	57/70 (81%)	51±3 (90±5%)	5±2 (9±4%)	1±1 (2±2%)	15	58
1	C	56/70 (80%)	51±2 (91±3%)	4±1 (7±2%)	1±1 (2±2%)	13	52
2	B	8/40 (20%)	5±1 (59±14%)	3±1 (38±13%)	0±1 (4±7%)	7	35
2	D	8/40 (20%)	5±1 (57±16%)	3±1 (35±14%)	1±1 (8±9%)	3	16
All	All	2580/4400 (59%)	2222 (86%)	294 (11%)	64 (2%)	11	48

5 of 25 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	210	PRO	10
1	A	10	PRO	6
1	A	35	ALA	4
1	A	43	LYS	3
2	D	324	MET	3

### 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	53/65 (82%)	50±2 (94±3%)	3±2 (6±3%)	27	72
1	C	52/65 (80%)	48±3 (93±5%)	4±3 (7±5%)	23	68
2	B	7/31 (23%)	7±1 (96±8%)	0±1 (4±8%)	40	83
2	D	7/31 (23%)	7±1 (96±8%)	0±1 (4±8%)	40	83
All	All	2380/3840 (62%)	2227 (94%)	153 (6%)	26	72

5 of 46 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	64	LYS	9
1	A	47	ARG	9
1	C	215	GLU	8
1	C	264	LYS	7
1	A	15	GLU	7

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	TYS	B	107	2	14,16,17	3.03±0.18	1±0 (7±0%)
2	TYS	B	112	2	14,16,17	2.95±0.14	1±0 (7±0%)
2	TYS	B	121	2	14,16,17	2.98±0.14	1±0 (7±0%)
2	TYS	D	307	2	14,16,17	3.06±0.24	1±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TYS	D	312	2	14,16,17	3.00±0.16	1±0 (7±0%)
2	TYS	D	321	2	14,16,17	2.98±0.14	1±0 (7±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	TYS	B	107	2	16,22,24	0.80±0.04	0±0 (0±0%)
2	TYS	B	112	2	16,22,24	0.80±0.06	0±0 (0±0%)
2	TYS	B	121	2	16,22,24	0.78±0.07	0±0 (0±0%)
2	TYS	D	307	2	16,22,24	0.83±0.06	0±0 (0±0%)
2	TYS	D	312	2	16,22,24	0.80±0.06	0±0 (0±0%)
2	TYS	D	321	2	16,22,24	0.79±0.06	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	TYS	B	107	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	B	112	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	B	121	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	D	307	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	D	312	2	-	0±0,9,11,13	0±0,1,1,1
2	TYS	D	321	2	-	0±0,9,11,13	0±0,1,1,1

5 of 6 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
2	D	307	TYS	OH-S	12.57	1.40	1.63	14	20
2	B	107	TYS	OH-S	11.89	1.41	1.63	14	20
2	B	121	TYS	OH-S	11.72	1.41	1.63	6	20
2	D	312	TYS	OH-S	11.58	1.42	1.63	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	112	TYS	OH-S	11.54	1.42	1.63	1	20

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 15637

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	4962
Number of shifts mapped to atoms	2494
Number of unparsed shifts	2468
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chemical shift has been reported more than once. First 5 (of 2468) occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2469	A	1	LYS	H	8.402	0.020	1
2470	C	201	LYS	H	8.402	0.020	1
2483	A	1	LYS	N	126.523	0.1	1
2484	C	201	LYS	N	126.523	0.1	1
2485	A	2	PRO	HA	4.510	0.004	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
$^{13}\text{C}_\alpha$	204	$-0.46 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	196	$-0.43 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	188	$-0.25 \pm 0.07$	None needed ( $< 0.5$ ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{15}\text{N}$	194	-0.51 $\pm$ 0.40	None needed (imprecise)

### 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 88%, i.e. 1490 atoms were assigned a chemical shift out of a possible 1701. 18 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	607/629 (97%)	246/250 (98%)	240/258 (93%)	121/121 (100%)
Sidechain	807/964 (84%)	510/573 (89%)	283/336 (84%)	14/55 (25%)
Aromatic	76/108 (70%)	44/56 (79%)	30/42 (71%)	2/10 (20%)
Overall	1490/1701 (88%)	800/879 (91%)	553/636 (87%)	137/186 (74%)

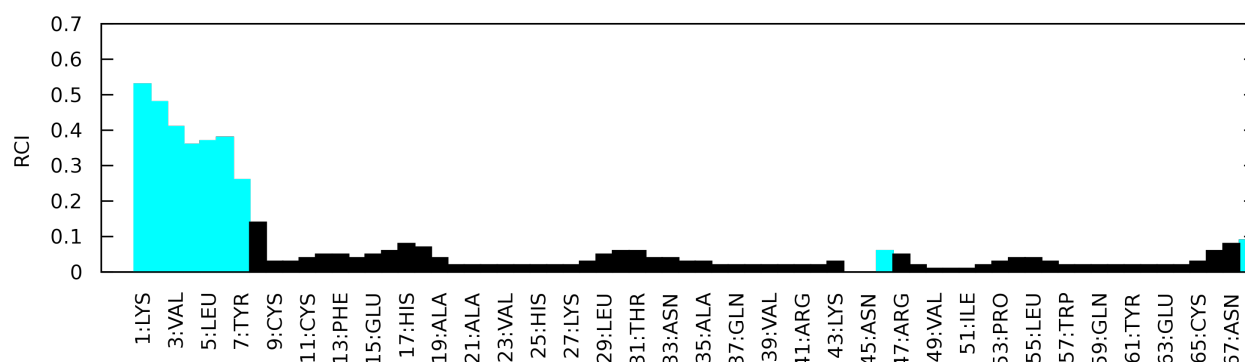
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

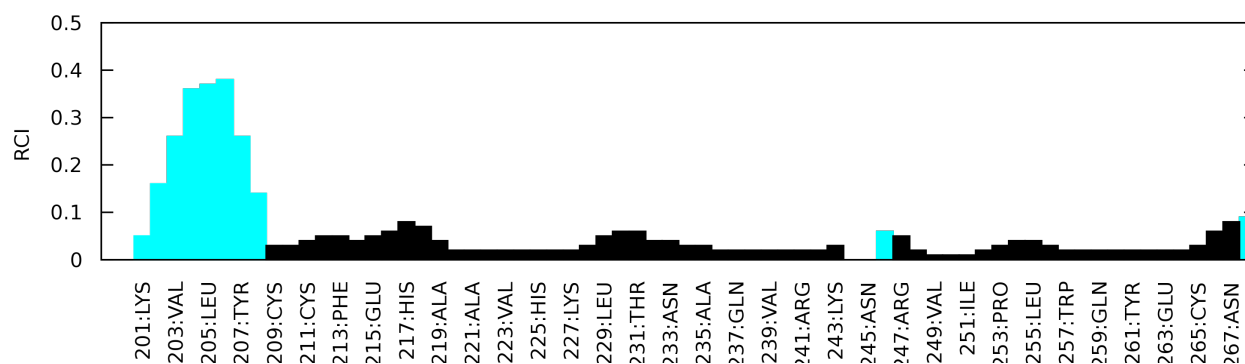
### 7.1.5 Random Coil Index (RCI) plots [i](#)

The 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.

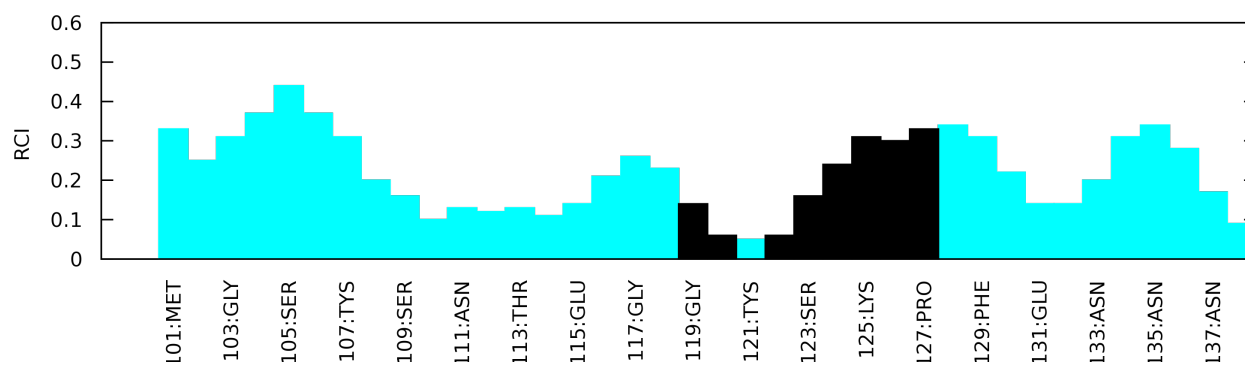
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain D:

