



wwPDB NMR Structure Validation Summary Report ⓘ

Oct 11, 2021 – 01:37 AM EDT

PDB ID : 2K03
Title : Structure of SDF1 in complex with the CXCR4 N-terminus containing a sulfotyrosine at position 21
Authors : Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C.
Deposited on : 2008-01-24

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

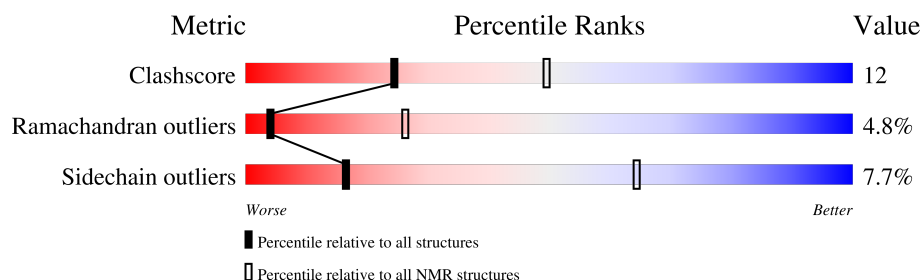
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	70	56% 24% 16% .
1	C	70	53% 29% 16% .
2	B	40	22% 10% 62% 5%
2	D	40	25% 12% 58% 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:114-B:120, B:122-B:127, C:208-C:243, C:247-C:267, D:312-D:320, D:322-D:327 (142)	0.59	11

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 and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3417 atoms, of which 1686 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 mutation	UNP P48061
A	65	CYS	ALA	engineered mutation	UNP P48061
C	199	GLY	-	expression tag	UNP P48061
C	200	MET	-	expression tag	UNP P48061
C	236	CYS	LEU	engineered mutation	UNP P48061
C	265	CYS	ALA	engineered mutation	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
			572	185	264	47	72	4	
2	D	38	Total	C	H	N	O	S	0
			573	185	264	47	73	4	

There are 6 discrepancies between the modelled and reference sequences:

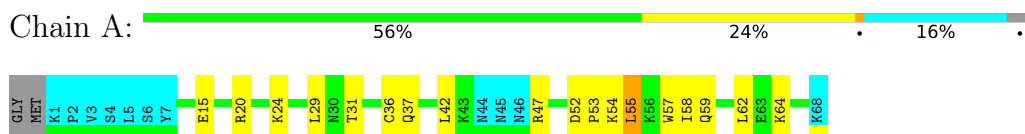
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	GLY	-	expression tag	UNP P61073
B	100	SER	-	expression tag	UNP P61073
B	128	ALA	CYS	engineered mutation	UNP P61073
D	299	GLY	-	expression tag	UNP P61073
D	300	SER	-	expression tag	UNP P61073
D	328	ALA	CYS	engineered mutation	UNP P61073

4 Residue-property plots

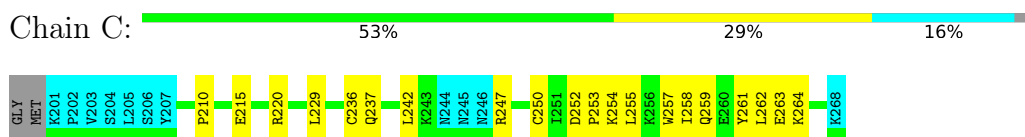
4.1 Average score per residue in the NMR ensemble

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.

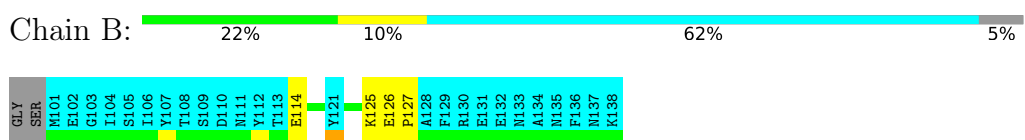
- Molecule 1: Stromal cell-derived factor 1



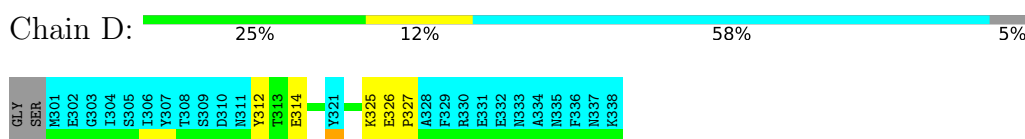
- Molecule 1: Stromal cell-derived factor 1



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



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

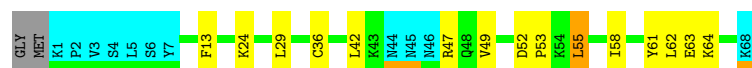


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

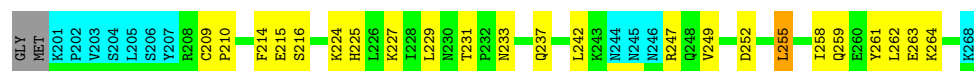
- Molecule 1: Stromal cell-derived factor 1

Chain A: 



- Molecule 1: Stromal cell-derived factor 1

Chain C: 



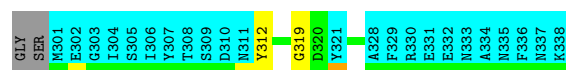
- Molecule 2: C-X-C chemokine receptor type 4

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
Xplor-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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	4956
Number of shifts mapped to atoms	2478
Number of unparsed shifts	2478
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality

6.1 Standard geometry

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

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	0.85±0.03	0±0/479 (0.0± 0.0%)	0.75±0.03	0±0/646 (0.0± 0.0%)
1	C	0.86±0.03	0±0/479 (0.0± 0.0%)	0.74±0.03	0±0/646 (0.0± 0.0%)
2	B	0.89±0.10	0±0/95 (0.0± 0.0%)	0.88±0.07	0±0/124 (0.0± 0.0%)
2	D	0.93±0.07	0±0/115 (0.0± 0.0%)	0.92±0.10	0±0/152 (0.0± 0.1%)
All	All	0.86	0/23360 (0.0%)	0.77	1/31360 (0.0%)

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	0.0±0.0	0.1±0.4
1	C	0.0±0.0	0.1±0.2
All	All	0	4

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	D	312	TYR	CB-CG-CD1	-5.57	117.66	121.00	2	1

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	A	47	ARG	Sidechain	2
1	A	20	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	C	220	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	12±3
1	C	469	489	487	14±3
2	B	95	80	80	2±1
2	D	114	96	96	4±2
All	All	22940	23080	23000	543

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.

5 of 230 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:254:LYS:O	2:D:327:PRO:HA	0.75	1.81	14	9
1:C:229:LEU:HG	2:D:312:TYR:CE2	0.72	2.19	16	7
1:C:220:ARG:HG2	1:C:257:TRP:CE3	0.65	2.25	6	3
1:C:215:GLU:HG2	1:C:250:CYS:O	0.65	1.91	3	4
1:A:10:PRO:HA	2:B:114:GLU:O	0.64	1.92	8	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	57/70 (81%)	51±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	9	45
1	C	57/70 (81%)	52±2 (90±3%)	4±2 (7±3%)	1±1 (2±1%)	9	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	13/40 (32%)	7±2 (55±15%)	4±2 (31±12%)	2±1 (14±7%)	1	5
2	D	15/40 (38%)	8±2 (55±10%)	5±1 (31±8%)	2±1 (15±7%)	0	4
All	All	2840/4400 (65%)	2367 (83%)	337 (12%)	136 (5%)	4	26

5 of 36 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	35	ALA	8
2	B	119	GLY	8
1	C	235	ALA	8
2	B	126	GLU	8
2	D	326	GLU	7

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	53/65 (82%)	48±1 (91±3%)	5±1 (9±3%)	13	60
1	C	53/65 (82%)	49±2 (92±3%)	4±2 (8±3%)	16	64
2	B	11/33 (33%)	10±1 (95±5%)	0±1 (5±5%)	31	80
2	D	13/33 (39%)	12±1 (95±5%)	1±1 (5±5%)	28	77
All	All	2600/3920 (66%)	2401 (92%)	199 (8%)	16	64

5 of 49 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	47	ARG	16
1	C	247	ARG	14
1	A	55	LEU	11
1	C	260	GLU	10
1	A	14	PHE	9

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	TYS	B	121	2	15,16,17	2.69±0.21	2±0 (10±3%)
2	TYS	D	321	2	15,16,17	2.69±0.19	2±1 (11±3%)

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	121	2	18,22,24	1.04±0.03	2±1 (9±3%)
2	TYS	D	321	2	18,22,24	1.03±0.04	1±1 (7±3%)

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	121	2	-	0±0,10,11,13	0±0,1,1,1
2	TYS	D	321	2	-	0±0,10,11,13	0±0,1,1,1

All 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	321	TYS	OH-S	11.03	1.41	1.58	4	20
2	B	121	TYS	OH-S	10.93	1.41	1.58	8	20
2	D	321	TYS	OH-CZ	2.81	1.38	1.42	4	12
2	B	121	TYS	OH-CZ	2.74	1.38	1.42	20	11
2	D	321	TYS	CB-CG	2.00	1.46	1.51	1	1

5 of 6 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(°)	Ideal(°)	Models	
								Worst	Total
2	D	321	TYS	OH-S-O2	3.08	116.68	107.71	14	19
2	B	121	TYS	OH-S-O2	2.87	116.07	107.71	4	20
2	B	121	TYS	O3-S-O2	2.21	100.82	108.49	4	11
2	D	321	TYS	O3-S-O2	2.12	101.12	108.49	10	8
2	D	321	TYS	OH-S-O1	2.06	113.72	107.71	6	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 84% 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 [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	4956
Number of shifts mapped to atoms	2478
Number of unparsed shifts	2478
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 2478) occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2479	A	1	LYS	H	8.402	0.020	1
2480	C	201	LYS	H	8.402	0.020	1
2481	A	1	LYS	N	124.577	0.1	1
2482	C	201	LYS	N	124.577	0.1	1
2483	A	2	PRO	HA	4.509	0.020	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
$^{13}\text{C}_\alpha$	202	-0.47 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	194	-0.42 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	188	-0.27 ± 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	194	-0.50 \pm 0.43	None needed (< 0.5 ppm)

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 87%, i.e. 1615 atoms were assigned a chemical shift out of a possible 1849. 18 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	672/694 (97%)	272/276 (99%)	266/284 (94%)	134/134 (100%)
Sidechain	861/1039 (83%)	547/618 (89%)	300/363 (83%)	14/58 (24%)
Aromatic	82/116 (71%)	48/60 (80%)	32/46 (70%)	2/10 (20%)
Overall	1615/1849 (87%)	867/954 (91%)	598/693 (86%)	150/202 (74%)

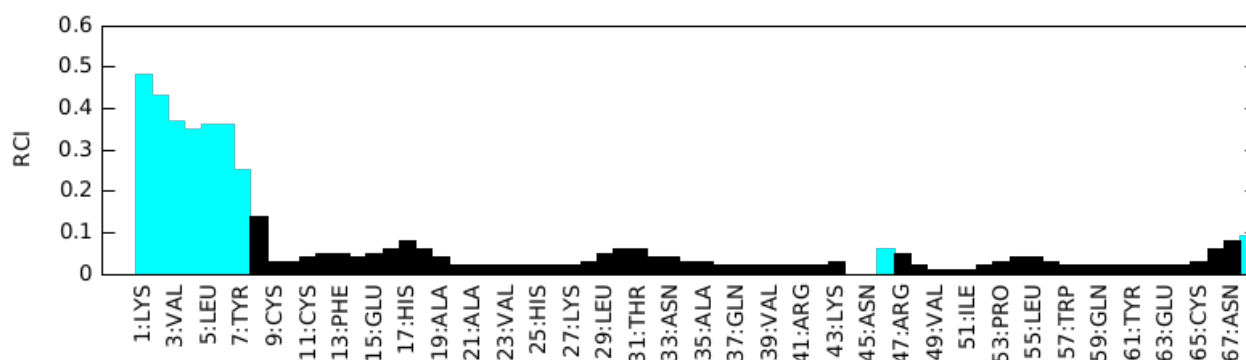
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

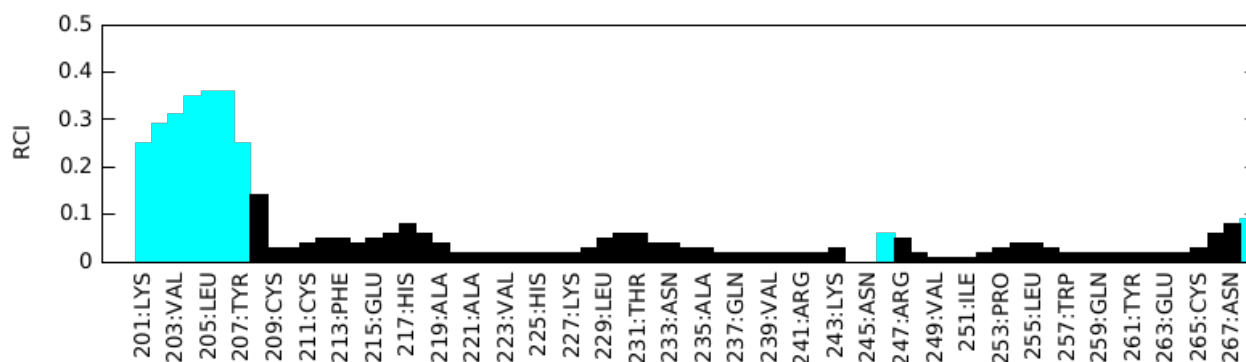
7.1.5 Random Coil Index (RCI) plots [i](#)

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.

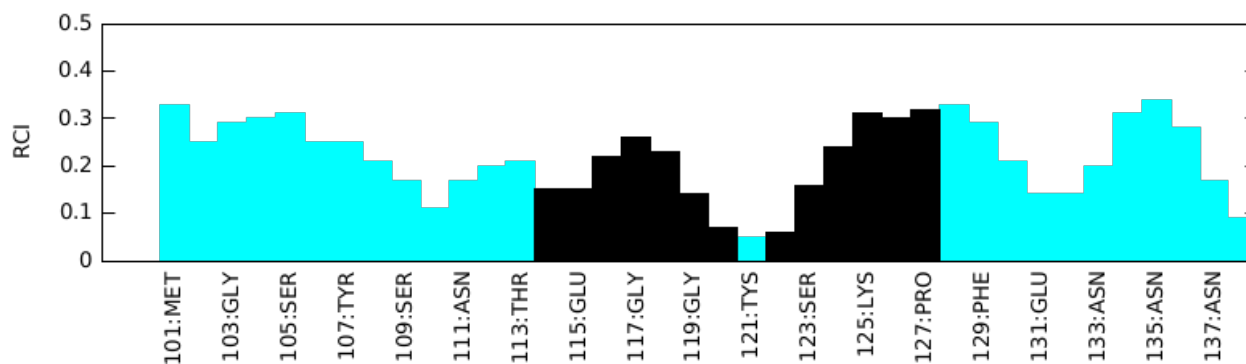
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain D:

