Full wwPDB NMR Structure Validation Report (i)

Mar 24, 2022 – 12:55 pm GMT

PDB ID	:	6FGP
Title	:	NMR solution structure of monomeric CCL5 in complex with a doubly-sulfated N-terminal segment of CCR5
Authors	:	Anglister, J.; Abayev, M.
Deposited on	:	2018-01-11

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

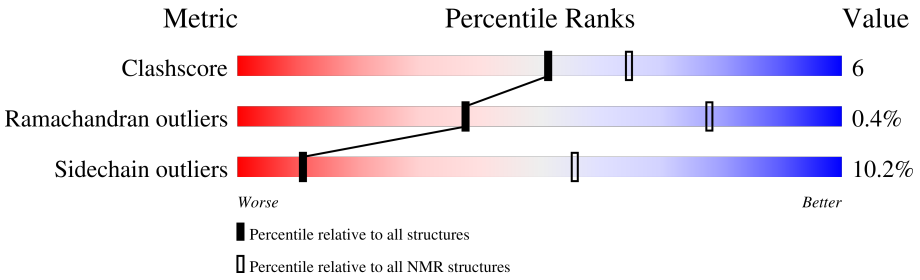
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 90%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	27	100%
2	B	69	55% 17% 25%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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	B:10-B:30, B:36-B:65 (51)	0.12	1

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1523 atoms, of which 745 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-C chemokine receptor type 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	27	443	143	211	34	52	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	CYS	conflict	UNP P51681

- Molecule 2 is a protein called C-C motif chemokine 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	68	1080	346	534	96	99	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P13501
B	9	SER	PRO	engineered mutation	UNP P13501
B	66	SER	GLU	engineered mutation	UNP P13501

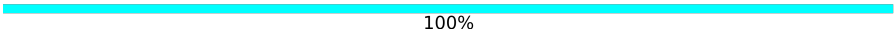
4 Residue-property plots (i)

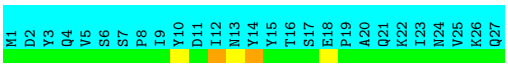
4.1 Average score per residue in the NMR ensemble

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: C-C chemokine receptor type 5

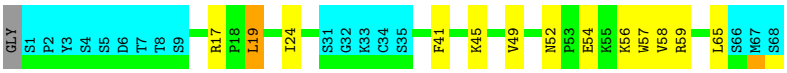
Chain A:





• Molecule 2: C-C motif chemokine 5

Chain B:



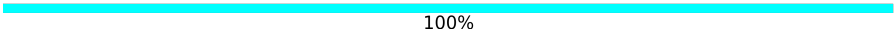
4.2 Scores per residue for each member of the ensemble

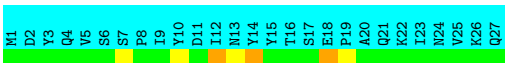
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: C-C chemokine receptor type 5

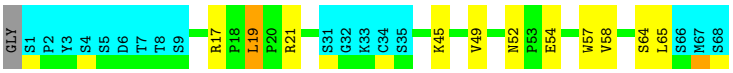
Chain A:





• Molecule 2: C-C motif chemokine 5

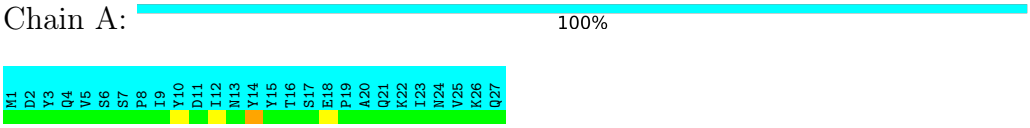
Chain B:



4.2.2 Score per residue for model 2

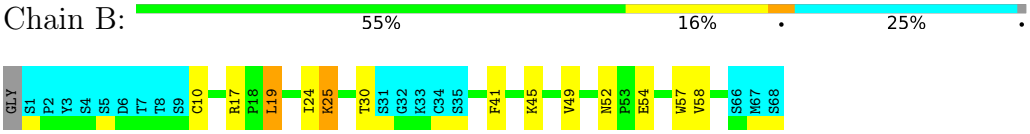
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

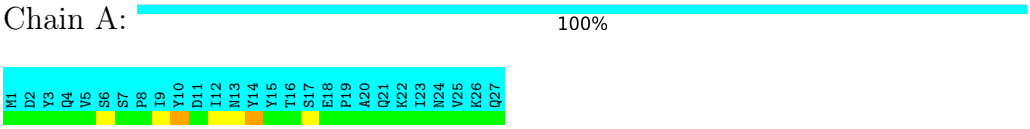
Chain B:



4.2.3 Score per residue for model 3

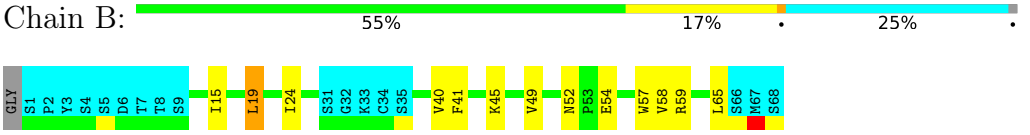
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

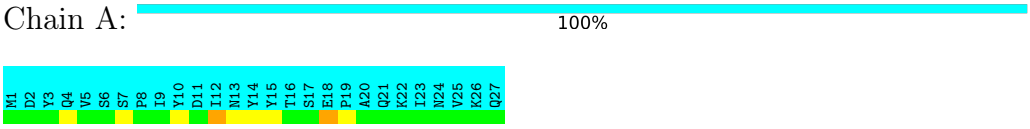
Chain B:



4.2.4 Score per residue for model 4

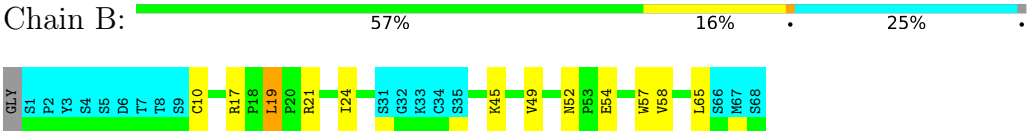
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

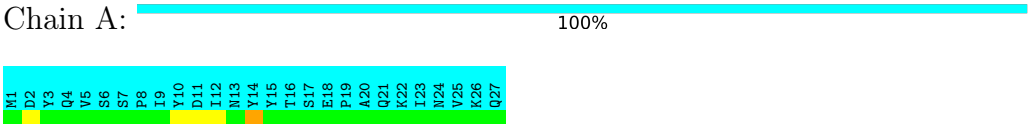
Chain B:



4.2.5 Score per residue for model 5

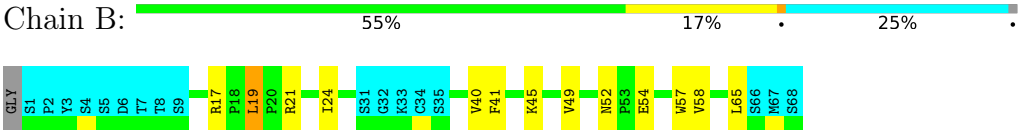
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

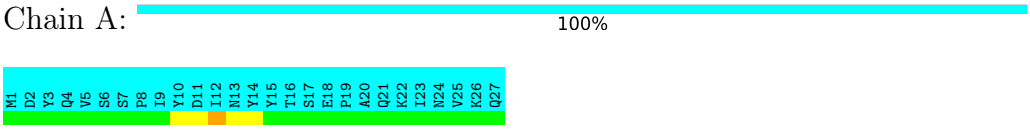
Chain B:



4.2.6 Score per residue for model 6

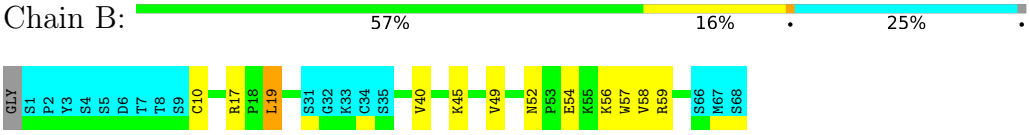
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

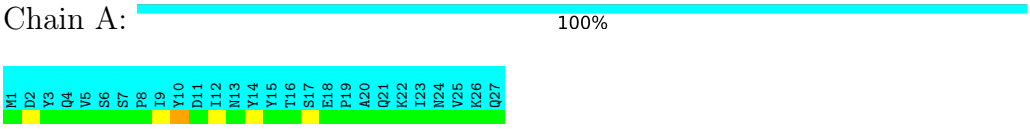
Chain B:



4.2.7 Score per residue for model 7

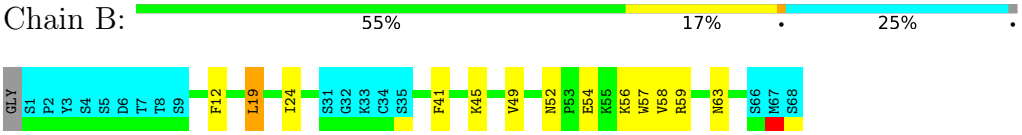
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

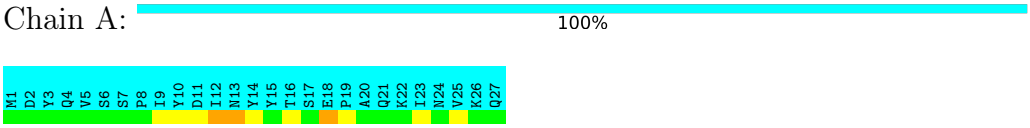
Chain B:



4.2.8 Score per residue for model 8

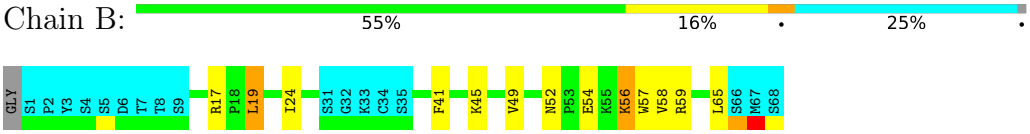
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

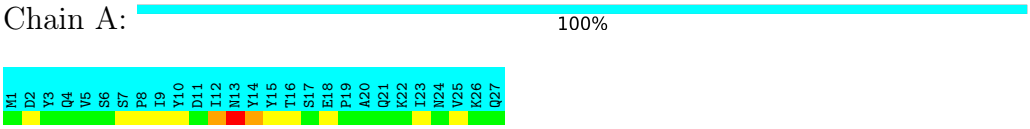
Chain B:



4.2.9 Score per residue for model 9

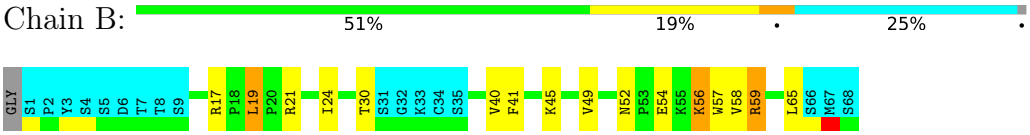
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

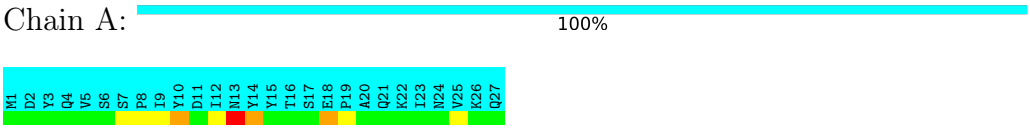
Chain B:



4.2.10 Score per residue for model 10

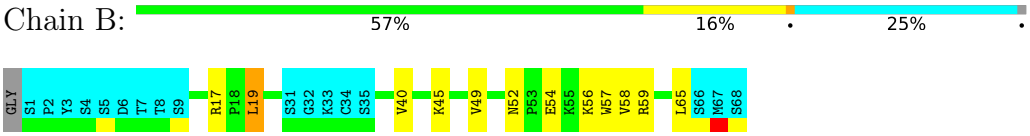
• Molecule 1: C-C chemokine receptor type 5

Chain A:



• Molecule 2: C-C motif chemokine 5

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 106 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
Xplor-NIH	structure calculation	
HADDOCK	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)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	991
Number of shifts mapped to atoms	991
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

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.

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

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	0	0	0	0±0
2	B	430	431	431	5±1
All	All	4300	4310	4310	50

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:LEU:HD22	2:B:49:VAL:HG21	0.61	1.72	6	9
2:B:52:ASN:OD1	2:B:54:GLU:HB2	0.51	2.06	6	10
2:B:56:LYS:O	2:B:59:ARG:HG2	0.50	2.07	7	5
2:B:24:ILE:HD12	2:B:41:PHE:HB3	0.49	1.85	3	6
2:B:57:TRP:CD1	2:B:58:VAL:HG23	0.48	2.44	4	10
2:B:40:VAL:HA	2:B:49:VAL:O	0.47	2.10	3	5
2:B:25:LYS:HA	2:B:25:LYS:NZ	0.45	2.27	2	1
2:B:19:LEU:HD13	2:B:49:VAL:CG2	0.43	2.44	2	1
2:B:19:LEU:HD13	2:B:49:VAL:HG22	0.41	1.90	2	1
2:B:24:ILE:CG2	2:B:65:LEU:HD21	0.41	2.46	4	1
2:B:40:VAL:HG13	2:B:49:VAL:O	0.40	2.17	6	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	0	-	-	-	-
2	B	51/69 (74%)	49±1 (96±2%)	2±1 (4±1%)	0±0 (0±1%)	38 78
All	All	510/960 (53%)	490 (96%)	18 (4%)	2 (0%)	38 78

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	30	THR	2

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	0	-	-	-
2	B	46/62 (74%)	41±1 (90±2%)	5±1 (10±2%)	11 56
All	All	460/860 (53%)	413 (90%)	47 (10%)	11 56

All 10 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)
2	B	19	LEU	10
2	B	45	LYS	10
2	B	17	ARG	8
2	B	65	LEU	6
2	B	21	ARG	4
2	B	10	CYS	3
2	B	59	ARG	2
2	B	56	LYS	2

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Mol	Chain	Res	Type	Models (Total)
2	B	25	LYS	1
2	B	12	PHE	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)

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
1	TYS	A	14	1	15,16,17	1.91±0.11	2±0 (10±3%)
1	TYS	A	10	1	15,16,17	1.95±0.07	2±0 (13±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
1	TYS	A	14	1	18,22,24	0.87±0.03	0±0 (2±2%)
1	TYS	A	10	1	18,22,24	0.64±0.03	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
1	TYS	A	14	1	-	0±0,10,11,13	0±0,1,1,1
1	TYS	A	10	1	-	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
1	A	10	TYS	OH-S	7.40	1.47	1.58	4	10
1	A	14	TYS	OH-S	7.28	1.47	1.58	9	10
1	A	10	TYS	OH-CZ	2.64	1.38	1.42	8	10
1	A	14	TYS	OH-CZ	2.46	1.38	1.42	9	5

All 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
1	A	14	TYS	O3-S-OH	2.31	111.40	105.83	10	3
1	A	14	TYS	CB-CA-C	2.10	107.53	111.47	7	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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *NtCCR5_CS.str*

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	134
Number of shifts mapped to atoms	134
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 694. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/247 (0%)	0/98 (0%)	0/102 (0%)	0/47 (0%)
Sidechain	0/369 (0%)	0/220 (0%)	0/125 (0%)	0/24 (0%)
Aromatic	0/78 (0%)	0/41 (0%)	0/35 (0%)	0/2 (0%)
Overall	0/694 (0%)	0/359 (0%)	0/262 (0%)	0/73 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 97 atoms were assigned a chemical shift out of a possible 1165. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/451 (0%)	0/179 (0%)	0/186 (0%)	0/86 (0%)
Sidechain	89/612 (15%)	89/366 (24%)	0/214 (0%)	0/32 (0%)
Aromatic	8/102 (8%)	8/53 (15%)	0/47 (0%)	0/2 (0%)
Overall	97/1165 (8%)	97/598 (16%)	0/447 (0%)	0/120 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (NtCCR5_CS.str). RCI is only applicable to proteins.

7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *RANTES_CS.str*

7.2.1 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	857
Number of shifts mapped to atoms	857
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	69	0.06 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	67	0.51 ± 0.15	Should be applied
$^{13}C'$	63	0.02 ± 0.27	None needed (< 0.5 ppm)
^{15}N	63	1.06 ± 0.36	Should be applied

7.2.3 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 90%, i.e. 626 atoms were assigned a chemical shift out of a possible 694. 7 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	243/247 (98%)	98/98 (100%)	98/102 (96%)	47/47 (100%)
Sidechain	308/369 (83%)	193/220 (88%)	110/125 (88%)	5/24 (21%)
Aromatic	75/78 (96%)	39/41 (95%)	35/35 (100%)	1/2 (50%)
Overall	626/694 (90%)	330/359 (92%)	243/262 (93%)	53/73 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 781 atoms were assigned a chemical shift out of a possible 1165. 7 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	324/451 (72%)	131/179 (73%)	130/186 (70%)	63/86 (73%)
Sidechain	374/612 (61%)	236/366 (64%)	133/214 (62%)	5/32 (16%)
Aromatic	83/102 (81%)	43/53 (81%)	39/47 (83%)	1/2 (50%)
Overall	781/1165 (67%)	410/598 (69%)	302/447 (68%)	69/120 (58%)

7.2.4 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
2	B	18	PRO	HA	1.97	6.05 – 2.75	-7.4
2	B	58	VAL	HG21	-0.80	2.20 – -0.60	-5.7
2	B	58	VAL	HG22	-0.80	2.20 – -0.60	-5.7
2	B	58	VAL	HG23	-0.80	2.20 – -0.60	-5.7
2	B	40	VAL	HB	0.25	3.59 – 0.39	-5.4

7.2.5 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 B: