



# wwPDB NMR Structure Validation Summary Report ⓘ

Nov 17, 2024 – 10:12 AM EST

PDB ID : 2L9H  
BMRB ID : 17453  
Title : Oligomeric Structure of the Chemokine CCL5/RANTES from NMR, MS, and SAXS Data  
Authors : Wang, X.; Watson, C.M.; Sharp, J.S.; Handel, T.M.; Prestegard, J.H.  
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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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

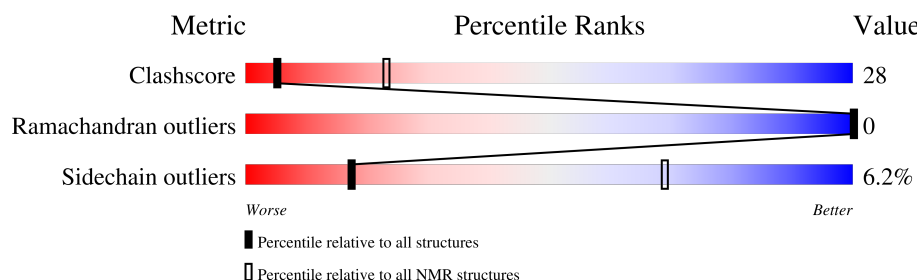
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR, SOLUTION SCATTERING*

The overall completeness of chemical shifts assignment is 3%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	68	62% 22% 10% . .
1	B	68	72% 21% . .
1	C	68	66% 21% 10% ..
1	D	68	68% 24% . .

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4248 atoms, of which 2110 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-C motif chemokine 5.

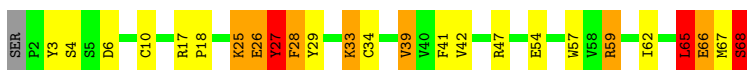
Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1080	347	536	95	97	5	
1	B	65	Total	C	H	N	O	S	0
			1044	333	519	93	94	5	
1	C	67	Total	C	H	N	O	S	0
			1080	347	536	95	97	5	
1	D	65	Total	C	H	N	O	S	0
			1044	333	519	93	94	5	

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

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 motif chemokine 5

Chain A: 



- Molecule 1: C-C motif chemokine 5

Chain B: 



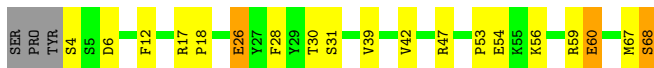
- Molecule 1: C-C motif chemokine 5

Chain C: 



- Molecule 1: C-C motif chemokine 5

Chain D: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics, SAXS-potential guided scoring within grid search*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *target function based on SAXS & knowledge-based potential*.

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

Software name	Classification	Version
NAMD	refinement	
VMD	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	1
Total number of shifts	117
Number of shifts mapped to atoms	117
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	0.95	1/560 ( 0.2%)	1.23	9/759 ( 1.2%)
1	B	0.92	0/539 ( 0.0%)	1.16	7/730 ( 1.0%)
1	C	0.87	0/560 ( 0.0%)	1.25	7/759 ( 0.9%)
1	D	0.89	1/539 ( 0.2%)	1.15	5/730 ( 0.7%)
All	All	0.91	2/2198 ( 0.1%)	1.20	28/2978 ( 0.9%)

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	1	2
1	B	0	1
1	C	0	2
All	All	1	5

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLU	CA-C	-5.20	1.39	1.52
1	D	60	GLU	CD-OE1	5.14	1.31	1.25

5 of 28 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	LEU	CB-CA-C	8.54	126.42	110.20
1	C	28	PHE	CB-CA-C	8.44	127.28	110.40
1	C	42	VAL	CB-CA-C	6.59	123.91	111.40
1	B	27	TYR	CB-CG-CD1	5.99	124.59	121.00
1	C	66	GLU	CA-CB-CG	-5.95	100.32	113.40

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	65	LEU	CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	41	PHE	Sidechain
1	A	59	ARG	Sidechain
1	B	59	ARG	Sidechain
1	C	3	TYR	Sidechain
1	C	27	TYR	Sidechain

## 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	544	536	534	74
1	B	525	519	517	14
1	C	544	536	534	73
1	D	525	519	517	14
All	All	2138	2110	2102	119

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 28.

5 of 119 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:66:GLU:CA	1:C:28:PHE:HB2	1.08	1.77
1:A:65:LEU:HB3	1:C:28:PHE:CE2	1.02	1.90
1:A:28:PHE:HB3	1:C:66:GLU:CB	1.00	1.86
1:A:66:GLU:HA	1:C:28:PHE:HB2	0.95	1.32
1:A:28:PHE:CD1	1:C:66:GLU:HB3	0.91	2.00



## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	65/68 (96%)	65 (100%)	0 (0%)	0 (0%)	100	100
1	B	63/68 (93%)	63 (100%)	0 (0%)	0 (0%)	100	100
1	C	65/68 (96%)	65 (100%)	0 (0%)	0 (0%)	100	100
1	D	63/68 (93%)	63 (100%)	0 (0%)	0 (0%)	100	100
All	All	256/272 (94%)	256 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	61/62 (98%)	54 (89%)	7 (11%)	7	50
1	B	59/62 (95%)	57 (97%)	2 (3%)	34	85
1	C	61/62 (98%)	57 (93%)	4 (7%)	16	67
1	D	59/62 (95%)	57 (97%)	2 (3%)	34	85
All	All	240/248 (97%)	225 (94%)	15 (6%)	17	69

5 of 15 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	4	SER
1	A	26	GLU
1	A	27	TYR
1	A	28	PHE
1	A	33	LYS

### 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 oligosaccharides 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 3% for the well-defined parts and 3% 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	117
Number of shifts mapped to atoms	117
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	59	$1.23 \pm 0.32$	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 3%, i.e. 117 atoms were assigned a chemical shift out of a possible 3650. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	117/1280 (9%)	58/510 (11%)	0/528 (0%)	59/242 (24%)
Sidechain	0/2008 (0%)	0/1300 (0%)	0/608 (0%)	0/100 (0%)

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	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	0/362 (0%)	0/172 (0%)	0/178 (0%)	0/12 (0%)
Overall	117/3650 (3%)	58/1982 (3%)	0/1314 (0%)	59/354 (17%)

#### 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 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

