



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LNL
Title : Structure of human CXCR1 in phospholipid bilayers
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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 : unknown
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

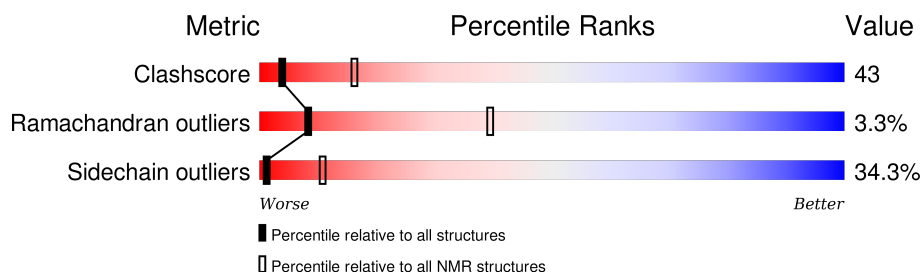
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 28%.

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	309	

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	A:29-A:312 (284)	0.80	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 and 2 single-model clusters were found.

Cluster number	Models
1	3, 5, 6
2	4, 8, 10
3	1, 9
Single-model clusters	2; 7

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4857 atoms, of which 2485 are hydrogens and 0 are deuteriums.

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

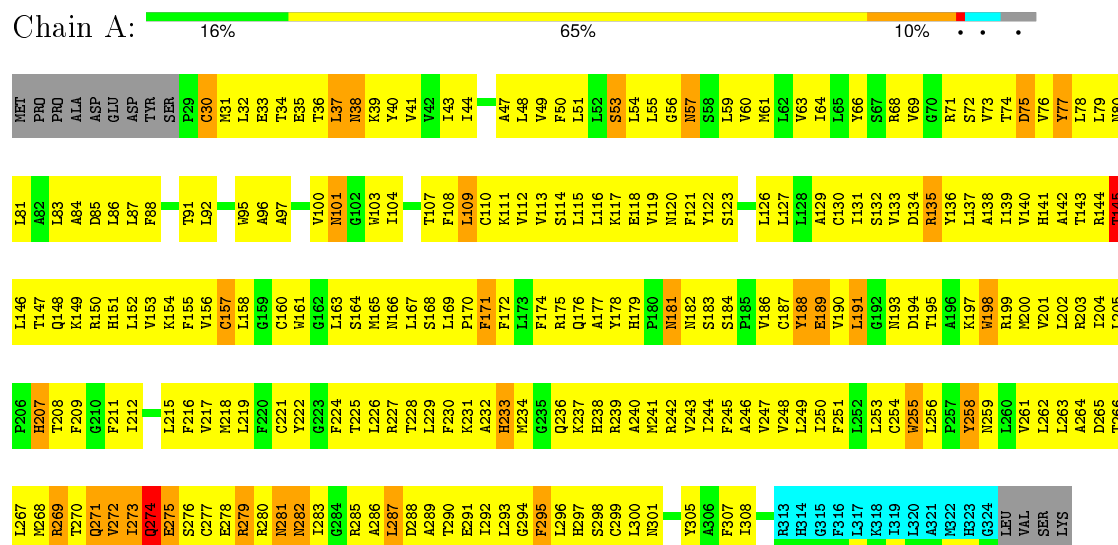
Mol	Chain	Residues	Atoms						Trace
1	A	296	Total	C	H	N	O	S	0
			4857	1574	2485	397	382	19	

4 Residue-property plots

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.

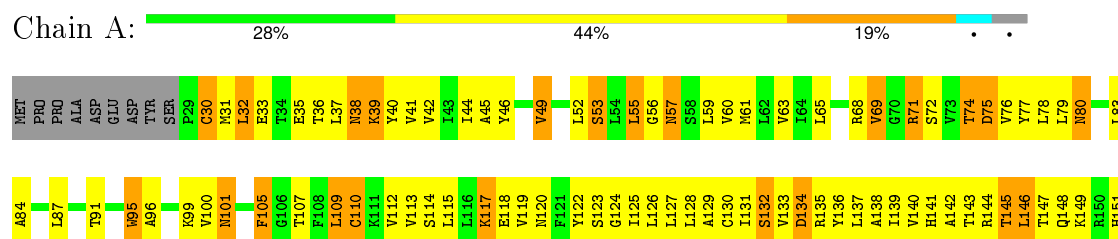
- Molecule 1: C-X-C chemokine receptor type 1



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: C-X-C chemokine receptor type 1



R285	A286	L287	D288	L292	F295	L296	H297	S298	G299	L300	T304	Y305	A306	F307	I308	G309	Q310	R313	H314	G315	F316	L317	K318	I319	L320	A321	H322	H323	G324	LEU	VAL	SER	LYS																					
M218	C221	Y222	G223	F224	R227	T228	K231	A232	H233	M234	G235	Q236	K237	H238	R239	A240	M241	R242	V243	I244	F245	A246	V247	F251	G254	M255	L256	P257	Y258	M259	L260	V261	A264	D265	T266	L267	M268	R269	T270	Q271	V272	I273	Q274	E275	S276	C277	E278	R279	R280	M281	M282	I283	G284	
L152	V153	K154	F155	V156	C157	C160	M161	S164	M165	M166	L167	S168	L169	P170	F171	F174	R175	Q176	A177	M181	M182	S183	S184	P185	V186	C187	Y188	E189	V190	L191	G192	M193	D194	T195	A196	K197	M198	R199	M200	V201	L202	R203	I204	L205	P206	H207	T208	F209	G210	F211	I212	V213	P214	V217

5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	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)	2lnl_cs.str
Number of chemical shift lists	1
Total number of shifts	1120
Number of shifts mapped to atoms	1120
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	28%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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](#)

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	0.66±0.01	0±0/2333 (0.0±0.0%)	0.98±0.01	0±0/3174 (0.0±0.0%)
All	All	0.66	0/23330 (0.0%)	0.98	1/31740 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	136	TYR	CB-CG-CD2	-5.33	117.80	121.00	7	1

There are no chirality outliers.

There are no planarity outliers.

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	2276	2381	2374	202±12
All	All	22760	23810	23740	2017

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 43.

5 of 1240 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:H	1:A:78:LEU:HD13	0.93	1.24	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:287:LEU:HD13	1:A:288:ASP:N	0.90	1.82	8	1
1:A:191:LEU:HD13	1:A:192:GLY:N	0.89	1.82	3	1
1:A:293:LEU:HD13	1:A:294:GLY:N	0.89	1.82	5	1
1:A:293:LEU:HD23	1:A:294:GLY:N	0.89	1.82	3	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	283/309 (92%)	249±2 (88±1%)	25±1 (9±0%)	9±1 (3±0%)	8	39
All	All	2830/3090 (92%)	2488 (88%)	249 (9%)	93 (3%)	8	39

5 of 15 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	33	GLU	10
1	A	274	GLN	10
1	A	269	ARG	10
1	A	145	THR	10
1	A	272	VAL	10

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	251/272 (92%)	165±5 (66±2%)	86±5 (34±2%)	1	11
All	All	2510/2720 (92%)	1650 (66%)	860 (34%)	1	11

5 of 222 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	109	LEU	10
1	A	49	VAL	10
1	A	38	ASN	10
1	A	195	THR	10
1	A	145	THR	10

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 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 28% for the well-defined parts and 28% for the entire structure.

7.1 Chemical shift list 1

File name: 2lnl_cs.str

Chemical shift list name: *assigned_chem_shift_list_2*

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	1120
Number of shifts mapped to atoms	1120
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	299	-0.42 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	234	1.66 ± 0.16	Should be applied
$^{13}\text{C}'$	289	0.40 ± 0.12	None needed (< 0.5 ppm)
^{15}N	298	-0.68 ± 0.15	Should be applied

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 28%, i.e. 1033 atoms were assigned a chemical shift out of a possible 3625. 0 out of 77 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	815/1402 (58%)	0/559 (0%)	543/568 (96%)	272/275 (99%)
Sidechain	218/1839 (12%)	0/1069 (0%)	218/696 (31%)	0/74 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/384 (0%)	0/202 (0%)	0/163 (0%)	0/19 (0%)
Overall	1033/3625 (28%)	0/1830 (0%)	761/1427 (53%)	272/368 (74%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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.

Random coil index (RCI) for chain A:

