



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:16 pm GMT

PDB ID : 1OO9
Title : Orientation in Solution of MMP-3 Catalytic Domain and N-TIMP-1 from
Residual Dipolar Couplings
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Deposited on : 2003-03-03

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

<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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

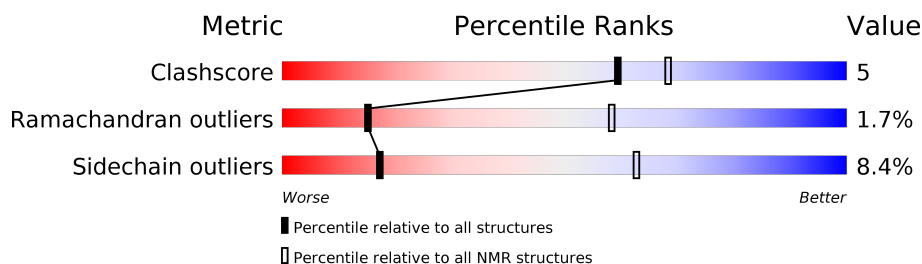
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 33%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	168	 83% 16% .
2	B	126	 74% 22% . .

2 Ensemble composition and analysis ⓘ

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4526 atoms, of which 2189 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromelysin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	168	Total	C	H	N	O	S	0
			2577	861	1239	223	252	2	


- Molecule 2 is a protein called Metalloproteinase inhibitor 1.

Mol	Chain	Residues	Atoms						Trace
2	B	126	Total	C	H	N	O	S	0
			1949	635	950	172	183	9	

4 Residue-property plots

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: Stromelysin-1

Chain A: 



- Molecule 2: Metalloproteinase inhibitor 1

Chain B: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *RIGID BODY MINIMIZATION FOLLOWED BY RESTRAINED SIMULATED ANNEALING*.

Of the 25 calculated structures, 1 were deposited, based on the following criterion: *lowest energy structure*.

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

Software name	Classification	Version
XPLOR	refinement	NIH

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 5785
Number of chemical shift lists	1
Total number of shifts	1362
Number of shifts mapped to atoms	1316
Number of unparsed shifts	0
Number of shifts with mapping errors	46
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	0.79	3/1382 (0.2%)	1.03	5/1888 (0.3%)
2	B	0.79	2/1024 (0.2%)	1.20	9/1387 (0.6%)
All	All	0.79	5/2406 (0.2%)	1.10	14/3275 (0.4%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	TRP	CG-CD2	6.27	1.54	1.43
1	A	124	TRP	CG-CD2	6.09	1.54	1.43
1	A	92	TRP	CG-CD2	5.63	1.53	1.43
2	B	353	GLY	N-CA	5.44	1.54	1.46
1	A	186	TRP	CG-CD2	5.11	1.52	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	A	100	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	413	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	A	93	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	84	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	B	359	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	402	VAL	CA-CB-CG2	-5.93	102.00	110.90
1	A	92	TRP	CE2-CD2-CG	-5.88	102.60	107.30
2	B	405	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	A	124	TRP	CE2-CD2-CG	-5.60	102.82	107.30
2	B	352	LEU	C-N-CA	-5.44	110.89	122.30
2	B	414	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	B	379	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	330	ASN	CA-CB-CG	-5.04	102.31	113.40

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	1338	1239	1266	7
2	B	999	950	969	20
All	All	2337	2189	2235	25

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:330:ASN:ND2	2:B:337:ARG:CZ	0.85	2.39
2:B:330:ASN:ND2	2:B:337:ARG:NH1	0.79	2.31
2:B:330:ASN:HB2	2:B:337:ARG:HD3	0.76	1.56
2:B:330:ASN:HD22	2:B:337:ARG:CZ	0.73	1.94
2:B:330:ASN:OD1	2:B:331:GLN:N	0.68	2.27
1:A:180:PHE:CE2	1:A:202:GLU:OE2	0.58	2.56
1:A:119:LYS:HG3	1:A:196:PHE:CE1	0.57	2.34
2:B:330:ASN:CG	2:B:337:ARG:NH1	0.56	2.58
2:B:353:GLY:O	2:B:355:ALA:N	0.53	2.42
2:B:410:LEU:H	2:B:410:LEU:HD12	0.53	1.64
2:B:332:THR:HG22	2:B:334:LEU:H	0.52	1.64
1:A:211:HIS:CE1	2:B:301:CYS:O	0.51	2.64
2:B:396:ILE:HD11	2:B:402:VAL:HG21	0.49	1.85
2:B:377:HIS:H	2:B:377:HIS:CD2	0.49	2.26
2:B:330:ASN:ND2	2:B:337:ARG:NH2	0.48	2.60
2:B:304:VAL:HG13	2:B:304:VAL:O	0.48	2.08
2:B:330:ASN:CG	2:B:331:GLN:N	0.46	2.66
1:A:215:THR:HG22	1:A:220:TYR:CZ	0.43	2.49
1:A:222:LEU:HA	2:B:303:CYS:O	0.43	2.13
2:B:369:VAL:O	2:B:369:VAL:HG13	0.43	2.13
2:B:329:VAL:HG13	2:B:332:THR:O	0.42	2.14
2:B:330:ASN:HB2	2:B:337:ARG:CD	0.42	2.35
2:B:304:VAL:O	2:B:304:VAL:CG1	0.41	2.67
1:A:159:GLY:HA2	1:A:183:ASP:OD2	0.41	2.16
1:A:120:ALA:HA	1:A:196:PHE:CE1	0.40	2.51

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	166/168 (99%)	147 (89%)	17 (10%)	2 (1%)	20	66
2	B	124/126 (98%)	108 (87%)	13 (10%)	3 (2%)	11	48
All	All	290/294 (99%)	255 (88%)	30 (10%)	5 (2%)	15	58

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

Mol	Chain	Res	Type
2	B	356	ALA
2	B	354	ASP
2	B	330	ASN
1	A	227	THR
1	A	225	SER

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	142/142 (100%)	132 (93%)	10 (7%)	22	68
2	B	109/109 (100%)	98 (90%)	11 (10%)	13	57
All	All	251/251 (100%)	230 (92%)	21 (8%)	17	63

All 21 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	95	THR
1	A	216	GLU

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Mol	Chain	Res	Type
2	B	369	VAL
2	B	375	ARG
1	A	233	ARG
2	B	310	THR
2	B	408	LEU
1	A	229	LEU
2	B	319	ILE
1	A	226	LEU
1	A	118	GLU
2	B	426	GLU
1	A	98	THR
2	B	350	GLN
2	B	326	THR
1	A	84	ARG
1	A	86	PHE
2	B	377	HIS
2	B	344	LYS
2	B	328	GLU
1	A	164	LEU

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 33% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5785

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	1362
Number of shifts mapped to atoms	1316
Number of unparsed shifts	0
Number of shifts with mapping errors	46
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 46 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	170	SER	H	8.04	0.02	1
A	169	ASP	CB	41.0	0.12	1
A	171	PRO	C	176.93	0.12	1
A	172	GLU	C	176.09	0.12	1
A	169	ASP	HB3	2.49	0.02	2
A	172	GLU	HG2	2.18	0.02	2
A	172	GLU	H	8.34	0.02	1
A	171	PRO	HB2	2.15	0.02	2
A	173	THR	HG21	1.04	0.02	1
A	172	GLU	HB2	1.97	0.02	2
A	169	ASP	HB2	2.55	0.02	2
A	172	GLU	HA	4.2	0.02	1
A	169	ASP	H	8.22	0.02	1
A	172	GLU	N	121.71	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	GLN	C	178.94	0.12	1
A	171	PRO	HG2	1.89	0.02	2
A	173	THR	HB	4.12	0.02	1
A	169	ASP	N	120.62	0.1	1
A	170	SER	HB3	3.74	0.02	2
A	170	SER	HB2	3.69	0.02	2
A	173	THR	HG22	1.04	0.02	1
A	173	THR	CB	70.53	0.12	1
A	172	GLU	CB	29.94	0.12	1
A	171	PRO	HA	4.34	0.02	1
A	173	THR	CG2	21.63	0.12	1
A	171	PRO	HD2	3.67	0.02	2
A	173	THR	HG23	1.04	0.02	1
A	173	THR	H	7.63	0.02	1
A	169	ASP	C	176.05	0.12	1
A	170	SER	HA	4.64	0.02	1
A	170	SER	N	117.28	0.1	1
A	171	PRO	HB3	1.82	0.02	2
A	120	GLN	CA	58.53	0.12	1
A	171	PRO	CD	50.45	0.12	1
A	171	PRO	CG	26.83	0.02	1
A	170	SER	CA	56.07	0.12	1
A	172	GLU	CA	56.59	0.12	1
A	172	GLU	CG	36.04	0.12	1
A	170	SER	C	172.79	0.12	1
A	169	ASP	CA	54.07	0.12	1
A	173	THR	N	120.53	0.1	1
A	171	PRO	CB	31.59	0.02	1
A	169	ASP	HA	4.43	0.02	1
A	173	THR	CA	62.88	0.12	1
A	170	SER	CB	63.35	0.12	1
A	172	GLU	HB3	1.82	0.02	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	137	0.32 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	0.47 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	140	0.08 ± 0.12	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	138	0.38 ± 0.49	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 33%, i.e. 1175 atoms were assigned a chemical shift out of a possible 3578. 17 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	650/1432 (45%)	249/569 (44%)	267/588 (45%)	134/275 (49%)
Sidechain	525/1752 (30%)	326/1031 (32%)	199/648 (31%)	0/73 (0%)
Aromatic	0/394 (0%)	0/218 (0%)	0/172 (0%)	0/4 (0%)
Overall	1175/3578 (33%)	575/1818 (32%)	466/1408 (33%)	134/352 (38%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 1175 atoms were assigned a chemical shift out of a possible 3578. 17 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	650/1432 (45%)	249/569 (44%)	267/588 (45%)	134/275 (49%)
Sidechain	525/1752 (30%)	326/1031 (32%)	199/648 (31%)	0/73 (0%)
Aromatic	0/394 (0%)	0/218 (0%)	0/172 (0%)	0/4 (0%)
Overall	1175/3578 (33%)	575/1818 (32%)	466/1408 (33%)	134/352 (38%)

7.1.4 Statistically unusual chemical shifts [i](#)

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
1	A	215	THR	HA	1.88	6.86 – 2.06	-5.4
1	A	121	LEU	HD21	-0.68	2.14 – -0.66	-5.1
1	A	121	LEU	HD23	-0.68	2.14 – -0.66	-5.1
1	A	121	LEU	HD22	-0.68	2.14 – -0.66	-5.1

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:

