



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1M3G
Title : SOLUTION STRUCTURE OF THE CATALYTIC DOMAIN OF MAPK PHOSPHATASE PAC-1: INSIGHTS INTO SUBSTRATE-INDUCED ENZY-MATIC ACTIVATION
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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

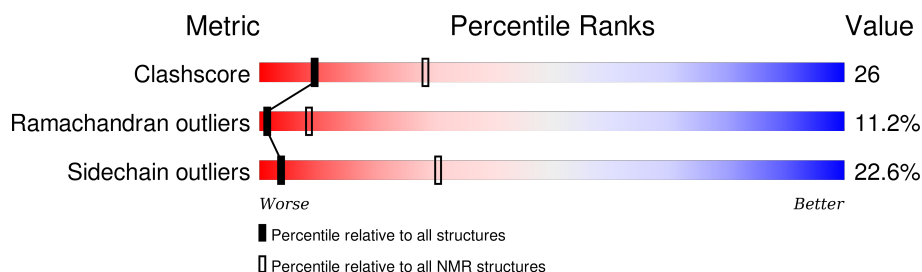
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 56%.

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	145	<div> <div>43%</div> <div>48%</div> <div>8% .</div> </div>

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 is only 1 type of molecule in this entry. The entry contains 2248 atoms, of which 1115 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DUAL SPECIFICITY PROTEIN PHOSPHATASE 2.

Mol	Chain	Residues	Atoms						Trace
1	A	145	Total	C	H	N	O	S	0
			2248	720	1115	198	207	8	

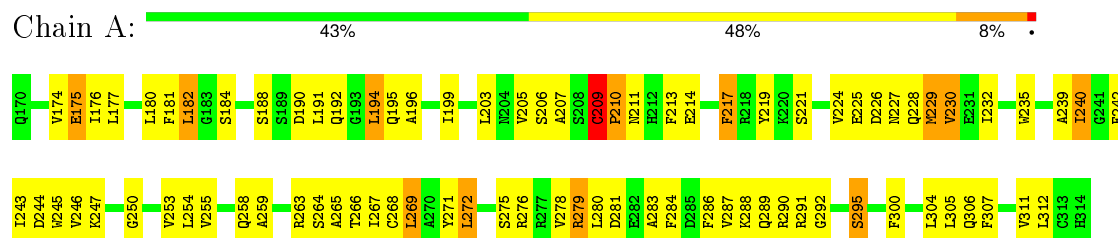
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	SER	CYS	ENGINEERED	UNP Q05923

4 Residue-property plots [i](#)

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: DUAL SPECIFICITY PROTEIN PHOSPHATASE 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 200 calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
XPLOR/ARIA	structure solution	
XPLOR/ARIA	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)	BMRB entry 5552
Number of chemical shift lists	1
Total number of shifts	1124
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

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

6 Model quality

6.1 Standard geometry

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	1133	1115	1112	59
All	All	1133	1115	1112	59

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 26.

5 of 59 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:176:ILE:HD11	1:A:287:VAL:HG13	1.09	1.24
1:A:243:ILE:HD13	1:A:253:VAL:HG21	0.76	1.54
1:A:240:ILE:HG22	1:A:271:TYR:HA	0.76	1.56
1:A:311:VAL:HG13	1:A:312:LEU:HD12	0.72	1.61
1:A:278:VAL:HG23	1:A:283:ALA:HB2	0.70	1.62

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	143/145 (99%)	100 (70%)	27 (19%)	16 (11%)	1	8
All	All	143/145 (99%)	100 (70%)	27 (19%)	16 (11%)	1	8

5 of 16 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	279	ARG
1	A	177	LEU
1	A	230	VAL
1	A	228	GLN
1	A	209	CYS

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	124/124 (100%)	96 (77%)	28 (23%)	4	30
All	All	124/124 (100%)	96 (77%)	28 (23%)	4	30

5 of 28 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	279	ARG
1	A	272	LEU
1	A	269	LEU
1	A	304	LEU
1	A	206	SER

6.3.3 RNA ⓘ

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 56% for the well-defined parts and 56% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5552

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	1124
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	-0.10 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	0.57 ± 0.12	Should be applied
$^{13}\text{C}'$	0	—	—
^{15}N	122	-0.27 ± 0.43	None needed (< 0.5 ppm)

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 56%, i.e. 994 atoms were assigned a chemical shift out of a possible 1773. 14 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	504/715 (70%)	246/285 (86%)	136/290 (47%)	122/140 (87%)
Sidechain	451/892 (51%)	256/525 (49%)	195/324 (60%)	0/43 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	39/166 (23%)	37/90 (41%)	0/70 (0%)	2/6 (33%)
Overall	994/1773 (56%)	539/900 (60%)	331/684 (48%)	124/189 (66%)

7.1.4 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
1	A	204	ASN	HD22	3.08	9.59 – 4.69	-8.3
1	A	264	SER	HB2	2.15	5.18 – 2.58	-6.7
1	A	263	ARG	H	12.22	11.29 – 5.19	6.5
1	A	232	ILE	CG1	39.05	36.54 – 18.94	6.4
1	A	241	GLY	N	131.97	129.07 – 90.27	5.7
1	A	264	SER	HB3	2.33	5.25 – 2.45	-5.4

7.1.5 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 A:

