wwPDB NMR Structure Validation Summary Report (i)

May 29, 2020 – 03:08 am BST

PDB ID	:	2M0Z
Title	:	cis form of a photoswitchable PDZ domain crosslinked with an azobenzene derivative
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Deposited on	:	2012-11-09

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
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:

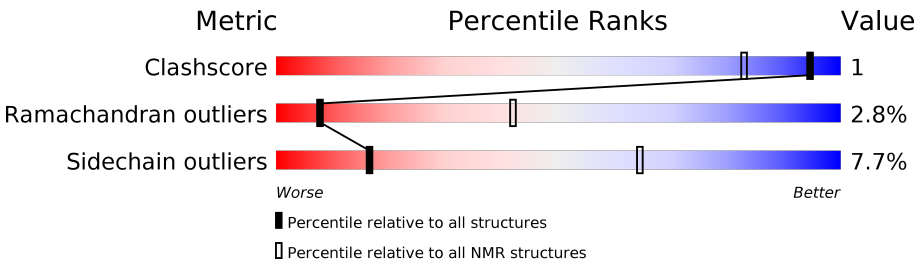
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	97	77% 5% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:14, A:20-A:91 (80)	0.35	18

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 6, 11, 12, 13, 15, 17
2	1, 2, 5, 14
3	16, 18, 20
4	8, 9, 19
5	7, 10
Single-model clusters	4

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1468 atoms, of which 733 are hydrogens and 0 are deuteriums.

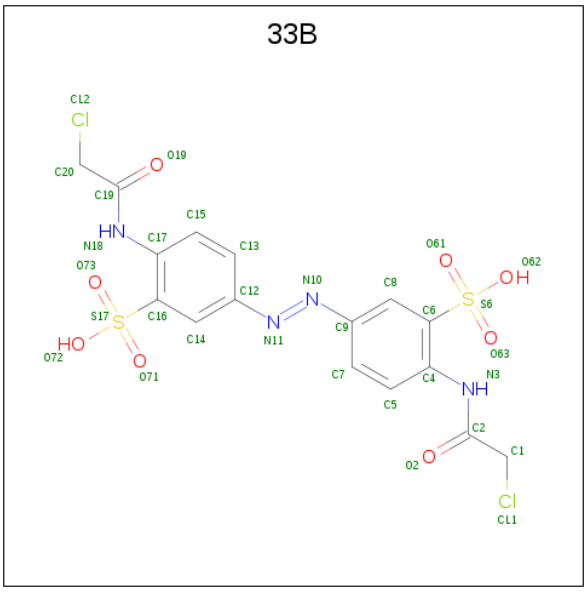
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 13.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1426	435	721	132	136	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q12923
A	22	CYS	SER	ENGINEERED MUTATION	UNP Q12923
A	77	CYS	GLU	ENGINEERED MUTATION	UNP Q12923

- Molecule 2 is 3,3'-(E)-diazene-1,2-diylbis{6-[(chloroacetyl)amino]benzenesulfonic acid} (three-letter code: 33B) (formula: $C_{16}H_{14}Cl_2N_4O_8S_2$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	42	16	12	4	8	2

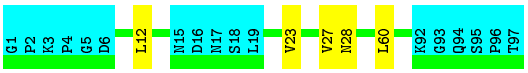
4 Residue-property plots (i)

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: Tyrosine-protein phosphatase non-receptor type 13

Chain A:

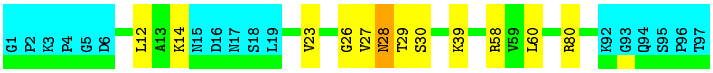


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 18. Colouring as in section 4.1 above.

- Molecule 1: Tyrosine-protein phosphatase non-receptor type 13

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, molecular dynamics.*

Of the 100 calculated structures, 20 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
CYANA	structure solution	3.0
X-PLOR NIH	refinement	2.32

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1123
Number of shifts mapped to atoms	1123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	586	607	603	1±1
2	A	30	12	8	0±0
All	All	12320	12380	12220	28

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 1.

5 of 9 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:THR:HG22	1:A:30:SER:H	0.56	1.60	6	7
1:A:20:GLY:HA3	1:A:42:ILE:HG12	0.50	1.83	12	4
1:A:20:GLY:CA	1:A:42:ILE:HG12	0.48	2.38	12	8
1:A:51:GLY:O	1:A:54:HIS:CE1	0.46	2.69	2	4
1:A:20:GLY:HA2	1:A:42:ILE:HD12	0.43	1.89	9	1

5.2 Torsion angles (i)

5.2.1 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	80/97 (82%)	74±1 (93±2%)	4±1 (5±2%)	2±0 (3±0%)	8	42
All	All	1600/1940 (82%)	1481 (93%)	75 (5%)	44 (3%)	8	42

All 4 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	28	ASN	20
1	A	27	VAL	20
1	A	26	GLY	3
1	A	67	LEU	1

5.2.2 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	62/76 (82%)	57±2 (92±3%)	5±2 (8±3%)	16	64
All	All	1240/1520 (82%)	1145 (92%)	95 (8%)	16	64

5 of 19 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	60	LEU	20
1	A	12	LEU	18
1	A	23	VAL	15
1	A	14	LYS	7
1	A	55	LYS	5

5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

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

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

5.5 Other polymers (i)

There are no such molecules in this entry.

5.6 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 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	1123
Number of shifts mapped to atoms	1123
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

6.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	97	-0.22 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	83	0.10 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	87	-0.08 ± 0.09	None needed (< 0.5 ppm)
^{15}N	90	0.25 ± 0.42	None needed (< 0.5 ppm)

6.1.3 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 88%, i.e. 815 atoms were assigned a chemical shift out of a possible 921. 19 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	392/398 (98%)	158/159 (99%)	156/160 (98%)	78/79 (99%)
Sidechain	393/474 (83%)	234/271 (86%)	159/181 (88%)	0/22 (0%)

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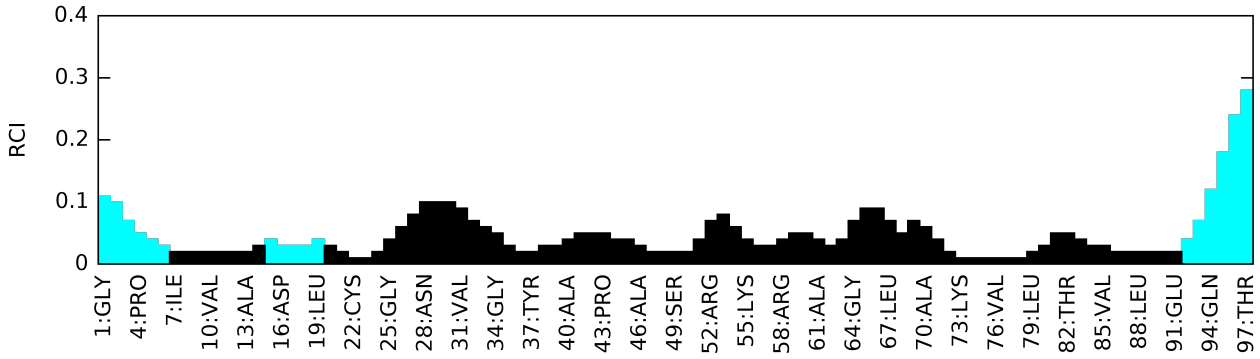
	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/49 (61%)	16/25 (64%)	14/16 (88%)	0/8 (0%)
Overall	815/921 (88%)	408/455 (90%)	329/357 (92%)	78/109 (72%)

6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 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: