

Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:53 pm BST

PDB ID	:	2L1O
Title	:	Zinc to cadmium replacement in the A. thaliana SUPERMAN Cys2His2 zinc
		finger induces structural rearrangements of typical DNA base determinant po-
		sitions
Authors	:	Malgieri, G.; Zaccaro, L.; Leone, M.; Bucci, E.; Esposito, S.; Baglivo, I.; Del
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Deposited on	:	2010-07-31

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 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)
$\operatorname{NmrClust}$:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)
${ m ShiftChecker}$:	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 was not calculated.

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	Percentile Rank	ks Value
Clashscore		10
Ramachandran outliers		5.2%
Sidechain outliers		23.7%
Worse		Better
Percentile	e relative to all structures	
Percentile	e relative to all NMR structures	
Metric	Whole archive	NMR archive
wietric	(#Entring)	(#Entring)

Metric	(# Entries)	(#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	А	39	28%	28%	•	41%				



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

	Well-defined (core) protein residues									
Well-defined core	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model									
1	A:6-A:28 (23)	0.17	5							

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 4 clusters. No single-model clusters were found.

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



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 630 atoms, of which 313 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Transcriptional regulator SUPERMAN.

Mol	Chain	Residues		Atoms								
1	Λ	20	Total	С	Η	Ν	Ο	S	1			
	A	39	629	194	313	70	49	3				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP Q38895
A	38	NH2	-	AMIDATION	UNP Q38895

• Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms
2	А	1	Total Cd



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: Transcriptional regulator SUPERMAN



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

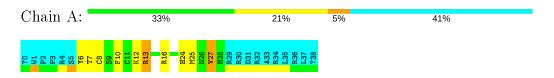
4.2.1 Score per residue for model 1

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.2 Score per residue for model 2

• Molecule 1: Transcriptional regulator SUPERMAN





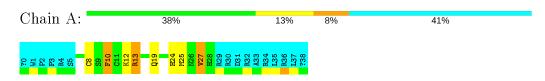
4.2.3 Score per residue for model 3

• Molecule 1: Transcriptional regulator SUPERMAN



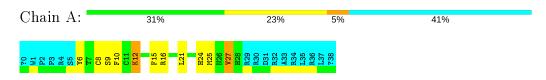
4.2.4 Score per residue for model 4

• Molecule 1: Transcriptional regulator SUPERMAN



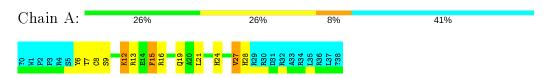
4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Transcriptional regulator SUPERMAN



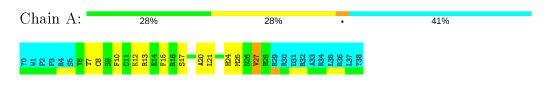
4.2.6 Score per residue for model 6

 \bullet Molecule 1: Transcriptional regulator SUPERMAN



4.2.7 Score per residue for model 7

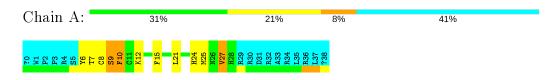
 \bullet Molecule 1: Transcriptional regulator SUPERMAN





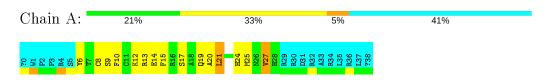
4.2.8 Score per residue for model 8

• Molecule 1: Transcriptional regulator SUPERMAN



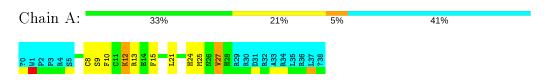
4.2.9 Score per residue for model 9

• Molecule 1: Transcriptional regulator SUPERMAN



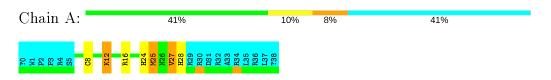
4.2.10 Score per residue for model 10

• Molecule 1: Transcriptional regulator SUPERMAN



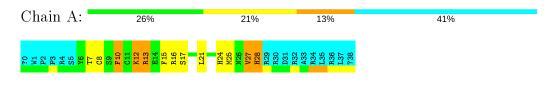
4.2.11 Score per residue for model 11

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.12 Score per residue for model 12

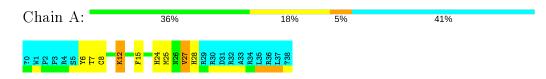
• Molecule 1: Transcriptional regulator SUPERMAN





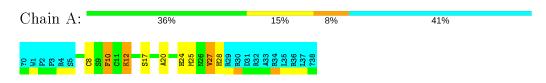
4.2.13 Score per residue for model 13

• Molecule 1: Transcriptional regulator SUPERMAN



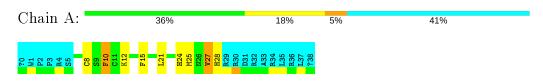
4.2.14 Score per residue for model 14

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.15 Score per residue for model 15

• Molecule 1: Transcriptional regulator SUPERMAN



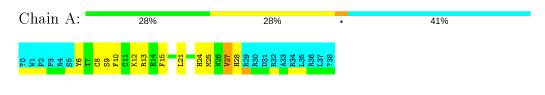
4.2.16 Score per residue for model 16

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.17 Score per residue for model 17

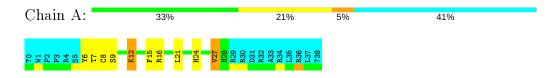
 \bullet Molecule 1: Transcriptional regulator SUPERMAN





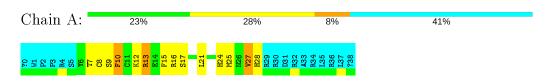
4.2.18 Score per residue for model 18

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.19 Score per residue for model 19

• Molecule 1: Transcriptional regulator SUPERMAN



4.2.20 Score per residue for model 20

• Molecule 1: Transcriptional regulator SUPERMAN

Chain A:					4	419	6									13%	5%			41%)		
70 11 12 12 12 13 13 14 13 15	C8	K12 R13	H24	N26	V27 1100	H28 R20	R30	Śά	ന	A33	R34	L35	R36	L37	738								



5 Refinement protocol and experimental data overview (i)

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

Of the 200 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	${ m refinement}$	

No chemical shift data was provided. 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	А	183	170	170	3 ± 1
All	All	3680	3400	3400	69

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 10.

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

Atom-1	Atom-2	$Clash(\lambda)$	Distance (Å)	Models		
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total	
1:A:15:PHE:HB2	1:A:21:LEU:HD12	0.71	1.60	6	5	
1:A:15:PHE:HB2	1:A:21:LEU:HD11	0.55	1.77	1	6	
1:A:24:HIS:O	1:A:27:VAL:HG12	0.53	2.03	5	20	
1:A:17:SER:O	1:A:21:LEU:HB2	0.51	2.05	9	2	
1:A:7:THR:HA	1:A:13:ARG:O	0.49	2.07	19	4	
1:A:25:MET:HA	1:A:28:HIS:CD2	0.48	2.43	15	10	
1:A:15:PHE:CG	1:A:21:LEU:HD23	0.47	2.44	10	1	
1:A:24:HIS:C	1:A:24:HIS:CD2	0.46	2.89	8	8	
1:A:7:THR:HG22	1:A:9:SER:H	0.45	1.71	8	3	
1:A:24:HIS:CD2	1:A:24:HIS:C	0.45	2.90	3	5	
1:A:17:SER:OG	1:A:20:ALA:HB3	0.44	2.13	14	3	

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:17:SER:O	1:A:21:LEU:HD13	0.43	2.14	19	2	

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	l Allowed Outliers		Percentiles		
1	А	23/39~(59%)	$19\pm1 (82\pm3\%)$	$3\pm1~(13\pm3\%)$	$1\pm0~(5\pm2\%)$		4	24
All	All	460/780~(59%)	375~(82%)	61~(13%)	24~(5%)		4	24

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	12	LYS	20
1	А	28	HIS	4

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	ain Analysed Rotan		Outliers	P	erc	entiles
1	А	19/32~(59%)	$15\pm1~(76\pm7\%)$	$5\pm1~(24\pm7\%)$		2	27
All	All	380/640~(59%)	290~(76%)	90 (24%)		2	27

All 11 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	А	27	VAL	20
1	А	8	CYS	20

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Mol	Chain	Res	Type	Models (Total)
1	А	10	PHE	15
1	А	25	MET	9
1	А	12	LYS	8
1	А	13	ARG	6
1	А	16	ARG	5
1	А	19	GLN	4
1	А	21	LEU	1
1	А	7	THR	1
1	А	14	GLU	1

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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.

5.5 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

No chemical shift data were provided

