Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2L4M
Title	:	Solution structure of the Zbeta domain of human DAI and its binding modes to B- and Z-DNA
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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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

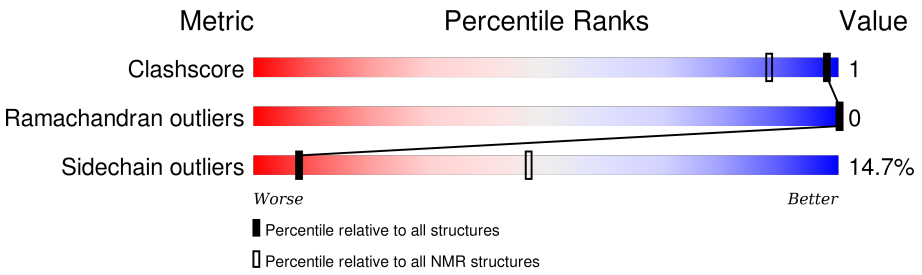
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	69	72% 12% 16%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:109-A:166 (58)	0.11	15

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1147 atoms, of which 571 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1147	356	571	110	106	4	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	SER	-	EXPRESSION TAG	UNP C9J523
A	99	HIS	-	EXPRESSION TAG	UNP C9J523
A	100	MET	-	EXPRESSION TAG	UNP C9J523
A	101	ALA	-	EXPRESSION TAG	UNP C9J523
A	102	SER	-	EXPRESSION TAG	UNP C9J523

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: Uncharacterized protein

Chain A:

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

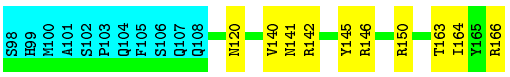
- Molecule 1: Uncharacterized protein

Chain A:

4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein

Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

Chain A: 70% 14% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 D112 N120 V140 N141 R142 Y145 R146 R150 T163 I164 Y165 R166

4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

Chain A: 67% 14% • 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 N120 A129 V140 N141 R142 Y145 R146 D156 T163 I164 Y165 R166

4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

Chain A: 70% 14% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 D112 R115 K118 D119 N120 V140 N141 Y145 R150 T163 I164 Y165 R166

4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

Chain A: 72% 12% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 D112 R115 N120 V140 N141 Y145 R150 I164 Y165 R166

4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein

Chain A: 68% 16% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 D112 N120 R124 V140 N141 Y145 R146 R150 D156 I164 Y165 R166

4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein

Chain A: 64% 20% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 N120 A125 I128 R135 V140 N141 R142 Y145 R146 R150 D156 T163 I164 Y165 R166

4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein

Chain A: 67% 16% • 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 D112 R115 N120 A129 V140 N141 R142 Y145 R150 S159 T163 I164 Y165 R166

4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein

Chain A: 68% 14% • 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 D112 N120 A129 V140 N141 Y145 R146 R150 T163 I164 Y165 R166

4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

Chain A: 70% 13% • 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 N120 V140 N141 Y145 R150 D156 T163 I164 Y165 R166

4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

Chain A: 68% 16% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 D112 R115 N120 V140 N141 R142 Y145 D156 T163 I164 Y165 R166

4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

Chain A: 70% 14% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 N120 R124 A125 I128 V140 N141 Y145 R150 D156 I164 Y165 R166

4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

Chain A: 71% 13% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 N120 V140 N141 R142 Y145 R146 R150 I164 Y165 R166

4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Uncharacterized protein

Chain A: 64% 20% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 D112 R115 N120 A125 I128 V140 N141 Y145 R150 S159 T163 I164 Y165 R166

4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

Chain A: 65% 19% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 R109 N120 A125 I128 V140 N141 R142 Y145 R146 R150 S159 T163 I164 Y165 R166

4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

Chain A: 74% 10% 16%

S98 H99 M100 A101 S102 P103 Q104 F105 S106 Q107 Q108 N120 V140 N141 R142 Y145 R150 I164 Y165 R166

4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

Chain A:

4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle 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
CNS	refinement	

No chemical shift data was provided. 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	0.73±0.00	0±0/497 (0.0±0.0%)	1.14±0.03	3±1/663 (0.4±0.1%)
All	All	0.73	0/9940 (0.0%)	1.14	54/13260 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	115	ARG	NE-CZ-NH1	9.60	125.10	120.30	1	7
1	A	146	ARG	NE-CZ-NH1	7.71	124.15	120.30	14	10
1	A	150	ARG	NE-CZ-NH1	7.03	123.81	120.30	5	15
1	A	115	ARG	NE-CZ-NH2	-6.43	117.08	120.30	20	1
1	A	115	ARG	CD-NE-CZ	6.21	132.29	123.60	1	1
1	A	109	ARG	NE-CZ-NH1	6.03	123.31	120.30	4	8
1	A	166	ARG	NE-CZ-NH1	5.84	123.22	120.30	15	5
1	A	146	ARG	NE-CZ-NH2	-5.67	117.46	120.30	1	1
1	A	150	ARG	NE-CZ-NH2	-5.58	117.51	120.30	9	1
1	A	124	ARG	NE-CZ-NH1	5.32	122.96	120.30	7	4
1	A	135	ARG	NE-CZ-NH1	5.03	122.82	120.30	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	109	ARG	Sidechain	1
1	A	150	ARG	Sidechain	1

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	490	493	493	1±0
All	All	9800	9860	9860	11

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ALA:HB2	1:A:140:VAL:CG2	0.47	2.40	1	7
1:A:125:ALA:HA	1:A:128:ILE:HG12	0.41	1.93	15	4

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	57/69 (83%)	55±1 (96±1%)	2±1 (4±1%)	0±0 (0±0%)	100	100
All	All	1140/1380 (83%)	1091 (96%)	49 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	51/61 (84%)	44±1 (85±2%)	8±1 (15±2%)	8 47
All	All	1020/1220 (84%)	870 (85%)	150 (15%)	8 47

All 13 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	140	VAL	20
1	A	145	TYR	20
1	A	141	ASN	20
1	A	164	ILE	20
1	A	120	ASN	20
1	A	163	THR	15
1	A	112	ASP	11
1	A	142	ARG	9
1	A	156	ASP	6
1	A	159	SER	4
1	A	166	ARG	3
1	A	118	LYS	1
1	A	111	GLU	1

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 (i)

No chemical shift data were provided