wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 01:58 PM BST

PDB ID	:	1C9F
Title	:	NMR STRUCTURE OF THE CAD DOMAIN OF CASPASE-ACTIVATED DNASE
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Deposited on	:	1999-08-02

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 (i) symbol.

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

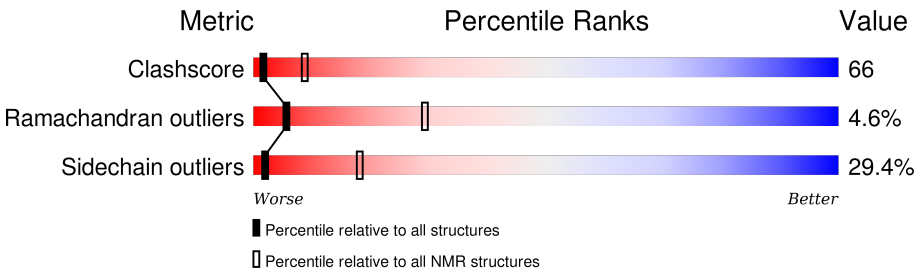
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	90	17% 49% 17% • 13% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 6 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	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:43, A:47-A:84 (75)	0.24	3

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 and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1336 atoms, of which 668 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CASPASE-ACTIVATED DNASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1336	419	668	118	122	9	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	VAL	-	insertion	UNP O54788
A	-1	PRO	-	insertion	UNP O54788
A	0	HIS	-	insertion	UNP O54788

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: CASPASE-ACTIVATED DNASE

Chain A: 17% 49% 17% • 13% •

VAL PRO HIS M1 C2 A3 V4 L5 R6 Q7 P8 K9 C10 V11 K12 L13 R14 A15 L16 H17 S18 A19 C20 K21 F22 G23 Y24 A25 A26 R27 S28 C29 Q30 E31 L32 L33 R34 V38 R39 F40 Q41 L42 P43 M44 P45 G46 S47 R48 L49 C50 L51 Y52 E53 D54 G55 T56 E57 V58 T59

D60 D61 C62 F63 P64 G65 L66 P67 N68 D69 A70 E71 L72 L73 L74 L75 T76 E79 T80 W81 H82 G83 Y84 V85 S86 D87

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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: CASPASE-ACTIVATED DNASE

Chain A: 27% 41% 13% • 13% •

VAL PRO HIS M1 C2 A3 V4 L5 R6 Q7 P8 K9 C10 V11 K12 L13 R14 A15 L16 H17 C20 K21 F22 G23 Y24 A25 A26 R27 S28 C29 Q30 E31 L32 L33 R34 C37 V38 R39 F40 Q41 L42 P43 M44 P45 G46 S47 R48 L49 C50 L51 D54 G55 T56 E57 V58 T59 D60

D61 C62 F63 P64 G65 L66 P67 N68 D69 A70 E71 L72 L73 L74 L75 T76 T80 V85 S86 D87

5 Refinement protocol and experimental data overview (i)

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

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
X-PLOR	structure solution	3.841
X-PLOR	refinement	3.841

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)

There are no covalent bond-length or bond-angle outliers.

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	4.7±0.5
All	All	0	94

There are no bond-length outliers.

There are no bond-angle outliers.

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	27	ARG	Sidechain	20
1	A	48	ARG	Sidechain	19
1	A	39	ARG	Sidechain	19
1	A	14	ARG	Sidechain	18
1	A	34	ARG	Sidechain	18

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	582	579	579	77±8
All	All	11640	11580	11580	1535

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 66.

5 of 361 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD12	1:A:73:LEU:HD21	1.09	1.24	4	17
1:A:63:PHE:CE1	1:A:66:LEU:HD21	1.05	1.84	2	5
1:A:63:PHE:CE2	1:A:72:LEU:HD21	1.04	1.85	5	6
1:A:63:PHE:CD1	1:A:66:LEU:HD11	1.03	1.89	6	13
1:A:24:VAL:HG13	1:A:32:LEU:HD22	0.98	1.28	17	12

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	75/90 (83%)	54±3 (72±4%)	18±3 (23±4%)	3±1 (5±2%)	5	29
All	All	1500/1800 (83%)	1080 (72%)	351 (23%)	69 (5%)	5	29

5 of 17 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	64	PRO	18
1	A	7	GLN	11
1	A	20	CYS	7
1	A	70	ALA	6
1	A	23	GLY	6

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	63/76 (83%)	44±2 (71±4%)	19±2 (29±4%)	2	18
All	All	1260/1520 (83%)	889 (71%)	371 (29%)	2	18

5 of 39 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	56	THR	20
1	A	42	LEU	20
1	A	51	LEU	20
1	A	80	THR	20
1	A	21	LYS	19

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