wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2RR7
Title	:	Microtubule Binding Domain of DYNEIN-C
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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
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:

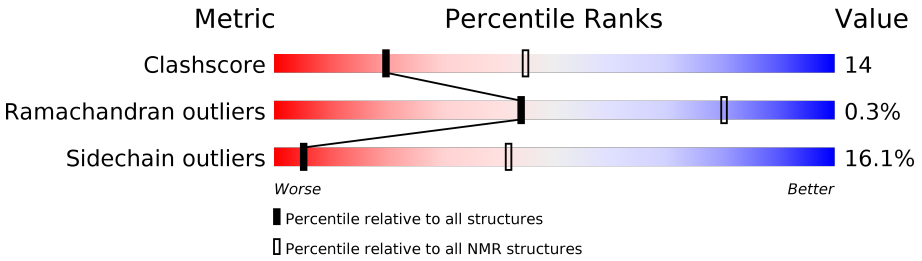
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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 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	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	155	56% 24% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:2-A:55, A:72-A:146 (129)	0.47	1

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2489 atoms, of which 1273 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dynein heavy chain 9.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	155	2489	779	1273	207	222	8	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q4AC22
A	2	SER	-	EXPRESSION TAG	UNP Q4AC22
A	3	GLN	-	EXPRESSION TAG	UNP Q4AC22

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: Dynein heavy chain 9

Chain A: 56% 24% • 17%

G1 L6 L10 P11 A16 L17 K18 A19 L20 L23 I28 K32 V41 V44 L45 I48 M51 K52 P56 A57 R58 V59 K60 D61 T62 A63 S64 G65 R66 M67 V68 D69 D70 Y71 K76 L79 L85 L88 K93 P97 V100

I104 R105 P106 Q109 D110 P111 E112 F113 V117 K120 V123 A124 C125 A126 G127 L128 W131 V132 I133 A134 L135 D139 K140 V141 I142 V145 E146 P147 K148 R149 Q150 K151 L152 R153 E154 A155

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Dynein heavy chain 9

Chain A: 54% 26% • 17%

G1 S2 Q3 L6 L10 P11 A16 L17 K18 A19 L20 L23 I28 K32 S36 V41 L45 E46 A47 I48 M51 P56 A57 R58 V59 K60 D61 T62 A63 S64 G65 R66 M67 V68 D69 D70 Y71 K76 L79 L85 L88 R89 K93

P97 V100 K103 I104 R105 P106 Q109 D110 P111 E112 F113 V117 I118 E119 S122 V123 A124 C125 L128 W131 V132 I133 A134 L135 D139 K140 V141 I142 V145 E146 P147 K148 R149 Q150 K151 L152 R153 E154 A155

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure solution	

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.

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 (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	1011	1062	1062	29±3
All	All	20220	21240	21240	571

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 14.

5 of 133 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD21	1:A:85:LEU:HD13	0.81	1.50	20	1
1:A:28:ILE:HD11	1:A:85:LEU:HD11	0.80	1.53	10	8
1:A:20:LEU:HD11	1:A:88:LEU:HD11	0.77	1.54	15	15
1:A:41:VAL:HG12	1:A:45:LEU:HD23	0.76	1.56	9	14
1:A:20:LEU:HD21	1:A:88:LEU:HD21	0.74	1.59	14	1

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	129/155 (83%)	124±2 (96±1%)	5±1 (4±1%)	0±1 (0±0%)	44 80
All	All	2580/3100 (83%)	2470 (96%)	103 (4%)	7 (0%)	44 80

All 3 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	23	LEU	4
1	A	95	HIS	2
1	A	35	LYS	1

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	111/132 (84%)	93±3 (84±3%)	18±3 (16±3%)	5 42
All	All	2220/2640 (84%)	1862 (84%)	358 (16%)	5 42

5 of 58 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	18	LYS	20
1	A	109	GLN	20
1	A	93	LYS	20
1	A	76	LYS	18
1	A	32	LYS	18

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