



wwPDB NMR Structure Validation Summary Report ⓘ

May 29, 2020 – 05:12 am BST

PDB ID : 1E0A
Title : Cdc42 complexed with the GTPase binding domain of p21 activated kinase
Authors : Morreale, A.; Venkatesan, M.; Mott, H.R.; Owen, D.; Nietlispach, D.; Lowe, P.N.; Laue, E.D.
Deposited on : 2000-03-16

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

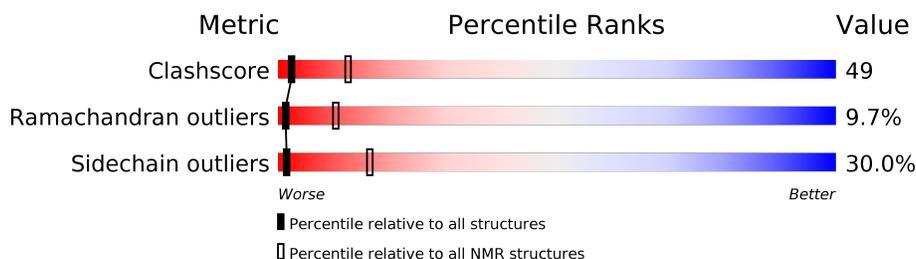
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	184	 24% 59% 13% . .
2	B	46	 22% 43% 20% . 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:1-A:178, B:73-B:112 (218)	0.77	7

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3655 atoms, of which 1825 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	184	2899	926	1463	228	275	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	LEU	GLN	engineered mutation	UNP P60953

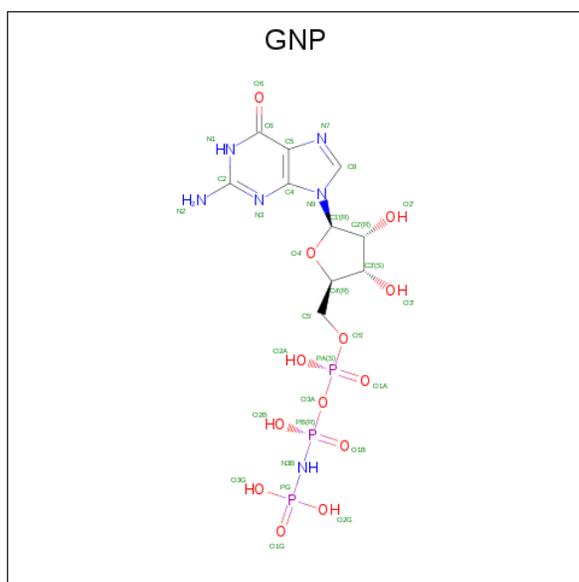
- Molecule 2 is a protein called Serine/threonine-protein kinase PAK 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	46	704	225	345	60	73	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	GLY	-	expression tag	UNP P35465
B	74	SER	-	expression tag	UNP P35465

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	A	1	45	10	13	6	13	3

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
4	A	1	1	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		
			Total	H	O
5	A	2	6	4	2



- Molecule 2: Serine/threonine-protein kinase PAK 1

Chain B: 33% 37% 15% • 13%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY OF A SUB-STRUCTURE FOLLOWED BY CARTESIAN DYNAMICS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *NO VIOLATIONS*.

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

Software name	Classification	Version
CNS	refinement	1.0
Azara	structure solution	
ANSIG	structure solution	
CNS	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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG

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	1387	1410	1408	152±13
2	B	309	293	288	37±7
3	A	32	13	13	8±4
5	A	2	4	0	0±1
All	All	34620	34400	34180	3377

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 49.

5 of 1724 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:THR:HG21	1:A:35:THR:HG21	1.04	1.04	3	2
1:A:149:LEU:HD11	1:A:151:ALA:HB2	1.03	1.13	11	1
1:A:55:LEU:HD21	1:A:79:LEU:HD21	1.02	1.31	14	1
1:A:55:LEU:HD11	1:A:79:LEU:HD23	1.02	1.32	1	2
1:A:20:LEU:HD21	1:A:55:LEU:HD13	0.99	1.34	15	3

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	177/184 (96%)	123±3 (70±2%)	38±4 (21±2%)	16±3 (9±2%)	1	12
2	B	39/46 (85%)	25±2 (64±6%)	9±2 (24±5%)	5±1 (13±3%)	1	6
All	All	4320/4600 (94%)	2957 (68%)	944 (22%)	419 (10%)	1	10

5 of 72 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	34	PRO	20
1	A	35	THR	19
1	A	159	ALA	19
2	B	108	GLN	18
1	A	72	TYR	16

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	158/164 (96%)	113±5 (71±3%)	45±5 (29±3%)	2	18
2	B	34/40 (85%)	22±2 (64±6%)	12±2 (36±6%)	1	8
All	All	3840/4080 (94%)	2689 (70%)	1151 (30%)	1	16

5 of 151 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)
2	B	77	LEU	20
2	B	106	LEU	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	107	LEU	20
1	A	28	PHE	19
2	B	112	ILE	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.

LIGAND-GEOMETRY INFOmissingINFO

6.6 Other polymers [i](#)

There are no such molecules in this entry.

6.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided