



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1KBE
Title : Solution structure of the cysteine-rich C1 domain of Kinase Suppressor of Ras
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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

<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
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

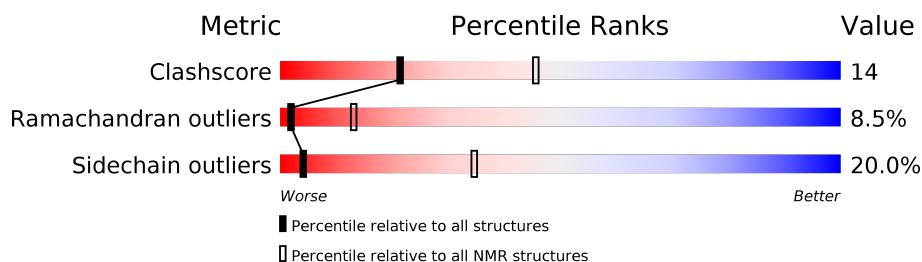
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	49	 65% 22% 10% .

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 778 atoms, of which 392 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kinase Suppressor of Ras.

Mol	Chain	Residues	Atoms						Trace
1	A	49	Total	C	H	N	O	S	0
			776	236	392	76	64	8	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLY	-	CLONING ARTIFACT	UNP Q61097

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

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: Kinase Suppressor of Ras

Chain A: 



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 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	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5203
Number of chemical shift lists	1
Total number of shifts	452
Number of shifts mapped to atoms	452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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

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	384	392	388	11
All	All	386	392	388	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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:357:VAL:HG22	1:A:366:CYS:O	0.69	1.87
1:A:336:PHE:CE1	1:A:357:VAL:HG23	0.58	2.33
1:A:334:HIS:N	1:A:334:HIS:CD2	0.51	2.79
1:A:360:LYS:C	1:A:362:CYS:H	0.45	2.15
1:A:357:VAL:N	1:A:366:CYS:O	0.45	2.50
1:A:360:LYS:O	1:A:362:CYS:N	0.44	2.51
1:A:336:PHE:CE1	1:A:359:CYS:HB3	0.43	2.48
1:A:342:LEU:O	1:A:354:ILE:HD11	0.43	2.13
1:A:355:PHE:CB	1:A:367:HIS:CD2	0.43	3.01
1:A:336:PHE:CD1	1:A:357:VAL:HB	0.43	2.49
1:A:366:CYS:O	1:A:367:HIS:O	0.40	2.40

6.3 Torsion angles

6.3.1 Protein backbone

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	47/49 (96%)	30 (64%)	13 (28%)	4 (9%)	2	13
All	All	47/49 (96%)	30 (64%)	13 (28%)	4 (9%)	2	13

All 4 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	350	GLN
1	A	341	TRP
1	A	367	HIS
1	A	342	LEU

6.3.2 Protein sidechains

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	45/45 (100%)	36 (80%)	9 (20%)	4	34
All	All	45/45 (100%)	36 (80%)	9 (20%)	4	34

All 9 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	359	CYS
1	A	377	CYS
1	A	353	MET
1	A	362	CYS
1	A	360	LYS
1	A	367	HIS

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Mol	Chain	Res	Type
1	A	336	PHE
1	A	337	SER
1	A	369	LYS

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5203

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	452
Number of shifts mapped to atoms	452
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	48	-0.33 ± 0.43	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	47	0.06 ± 0.33	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	44	1.01 ± 0.51	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 408 atoms were assigned a chemical shift out of a possible 619. 5 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	184/243 (76%)	92/97 (95%)	48/98 (49%)	44/48 (92%)
Sidechain	222/324 (69%)	135/195 (69%)	87/109 (80%)	0/20 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/52 (4%)	2/28 (7%)	0/19 (0%)	0/5 (0%)
Overall	408/619 (66%)	229/320 (72%)	135/226 (60%)	44/73 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 408 atoms were assigned a chemical shift out of a possible 619. 5 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	184/243 (76%)	92/97 (95%)	48/98 (49%)	44/48 (92%)
Sidechain	222/324 (69%)	135/195 (69%)	87/109 (80%)	0/20 (0%)
Aromatic	2/52 (4%)	2/28 (7%)	0/19 (0%)	0/5 (0%)
Overall	408/619 (66%)	229/320 (72%)	135/226 (60%)	44/73 (60%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	351	LYS	HD2	3.14	2.76 – 0.46	6.7

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

