



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KLH / pdb_00002klh
Title : NMR Structure of RCL in complex with GMP
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Deposited on : 2009-07-02

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:9-A:47, A:61-A:153, B:9-B:47, B:61-B:153 (264)	0.69	8

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, 7, 10
2	1, 8, 9
Single-model clusters	6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4840 atoms, of which 2378 are hydrogens and 0 are deuteriums.

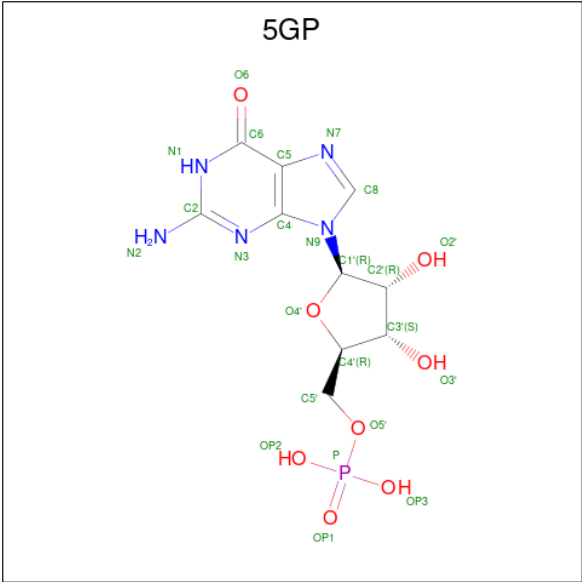
- Molecule 1 is a protein called c-Myc-responsive protein Rcl.

Mol	Chain	Residues	Atoms						Trace
1	A	152	Total	C	H	N	O	S	0
			2383	758	1176	223	221	5	
1	B	152	Total	C	H	N	O	S	0
			2383	758	1176	223	221	5	

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP O35820
A	9	ARG	-	expression tag	UNP O35820
A	10	ARG	-	expression tag	UNP O35820
A	69	ALA	ASP	engineered mutation	UNP O35820
A	152	VAL	-	expression tag	UNP O35820
A	153	GLU	-	expression tag	UNP O35820
A	154	HIS	-	expression tag	UNP O35820
A	155	HIS	-	expression tag	UNP O35820
A	156	HIS	-	expression tag	UNP O35820
A	157	HIS	-	expression tag	UNP O35820
A	158	HIS	-	expression tag	UNP O35820
A	159	HIS	-	expression tag	UNP O35820
B	8	MET	-	expression tag	UNP O35820
B	9	ARG	-	expression tag	UNP O35820
B	10	ARG	-	expression tag	UNP O35820
B	69	ALA	ASP	engineered mutation	UNP O35820
B	152	VAL	-	expression tag	UNP O35820
B	153	GLU	-	expression tag	UNP O35820
B	154	HIS	-	expression tag	UNP O35820
B	155	HIS	-	expression tag	UNP O35820
B	156	HIS	-	expression tag	UNP O35820
B	157	HIS	-	expression tag	UNP O35820
B	158	HIS	-	expression tag	UNP O35820
B	159	HIS	-	expression tag	UNP O35820

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



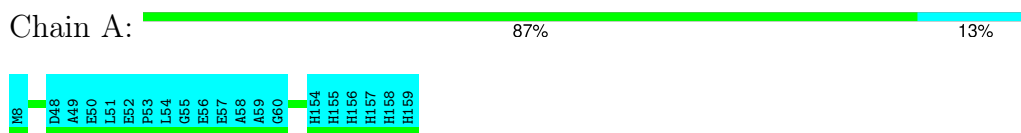
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	37	10	13	5	8	1
2	B	1	37	10	13	5	8	1

4 Residue-property plots [i](#)

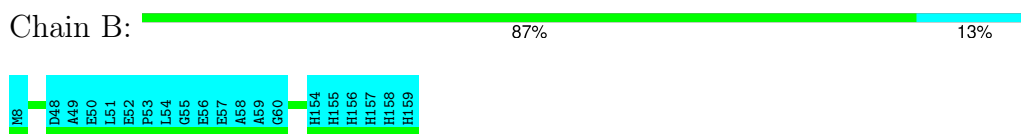
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: c-Myc-responsive protein Rcl



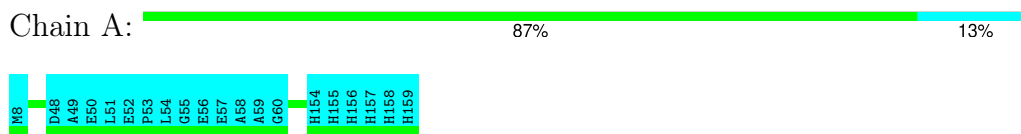
- Molecule 1: c-Myc-responsive protein Rcl



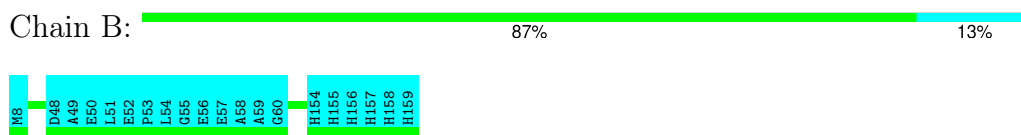
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: c-Myc-responsive protein Rcl



- Molecule 1: c-Myc-responsive protein Rcl



5 Refinement protocol and experimental data overview ⓘ

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CNS	refinement	1.2

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

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6.7 Other polymers [i](#)

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6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided