



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 03:38 PM BST

PDB ID : 1MSH
Title : SOLUTION STRUCTURE OF GRO(SLASH)MELANOMA GROWTH
STIMULATORY ACTIVITY DETERMINED BY 1H NMR SPEC-
TROSCOPY
Authors : Kim, K.-S.; Clark-Lewis, I.; Sykes, B.D.
Deposited on : 1995-01-25

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 ⓘ symbol.

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

Cyrange	:	NOT EXECUTED
NmrClust	:	NOT EXECUTED
MolProbity	:	NOT EXECUTED
Mogul	:	unknown
Percentile statistics	:	NOT EXECUTED
RCI	:	NOT EXECUTED
PANAV	:	NOT EXECUTED
ShiftChecker	:	NOT EXECUTED
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 ⓘ

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 percentiles available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2222 atoms, of which 1144 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY.

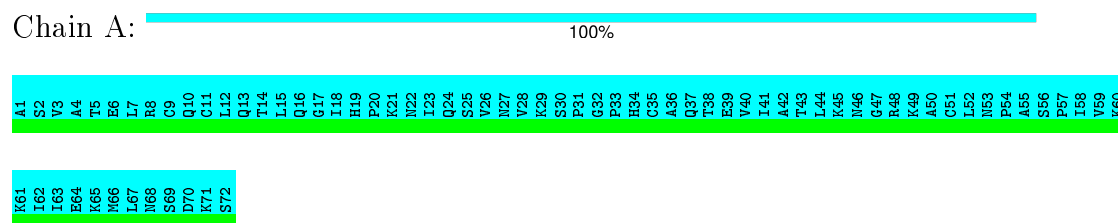
Mol	Chain	Residues	Atoms						Trace
1	A	72	Total	C	H	N	O	S	0
			1111	333	572	100	101	5	
1	B	72	Total	C	H	N	O	S	0
			1111	333	572	100	101	5	

4 Residue-property plots

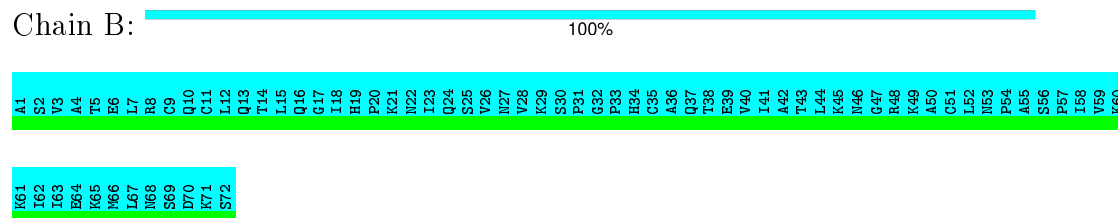
4.1 Average score per residue in the NMR ensemble

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: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY



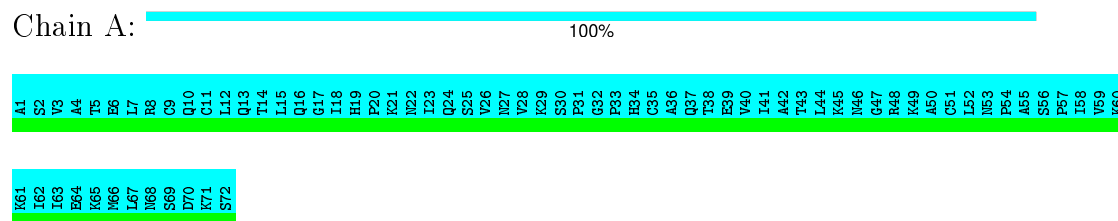
- Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY



4.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 4.1 above.

- Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY



- Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY



A1	S2	V3	A4	T5	E6	L7	R8	C9	Q10	C11	L12	Q13	T14	L15	Q16	G17	I18	H19	P20	K21	N22	I23	Q24	S25	V26	N27	V28	K29	S30	F31	G32	P33	H34	C35	A36	Q37	T38	E39	V40	A41	I42	L43	L44	K45	N46	G47	R48	K49	A50	C51	L52	S53	N54	P55	A56	S57	P58	V59	W60
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K61	I62	I63	E64	K65	M66	L67	N68	S69	D70	K71	S72
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5 Refinement protocol and experimental data overview

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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](#)

MolProbity was not executed - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity was not executed - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity was not executed - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity was not executed - this section will have to be empty.

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

MolProbity was not executed - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity was not executed - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity was not executed - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity was not executed - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided