wwPDB NMR Structure Validation Summary Report

Feb 16, 2022 – 12:57 PM EST

PDB ID	:	1MSH
Title	:	SOLUTION STRUCTURE OF GRO(SLASH)MELANOMA GROWTH STIMULATORY ACTIVITY DETERMINED BY 1H NMR SPECTROSCOPY
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
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:

MolProbity	:	4.02b-467
Percentile statistics	:	FAILED
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

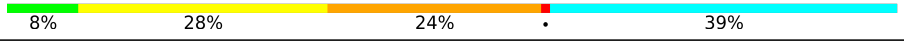
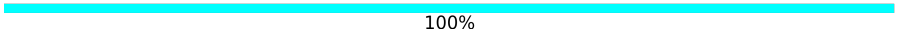
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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

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	72	
1	B	72	

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. Model 30 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:13-A:28, A:39-A:66 (44)	0.07	30

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

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	

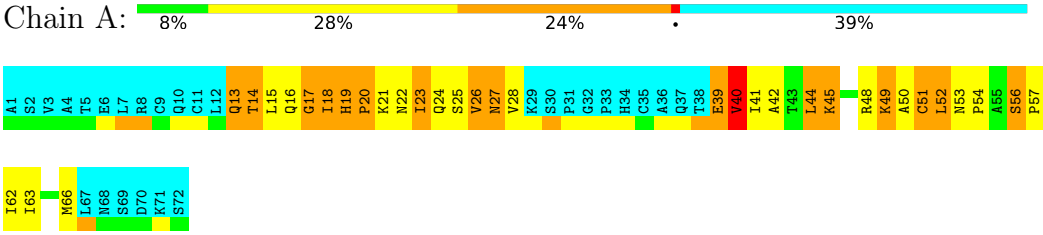
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

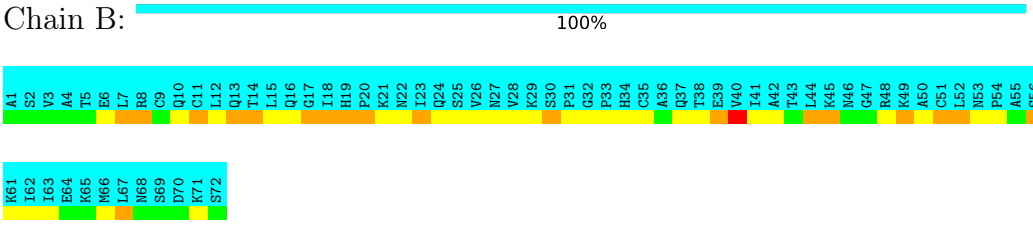
• Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY

Chain A:



• Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY

Chain B:

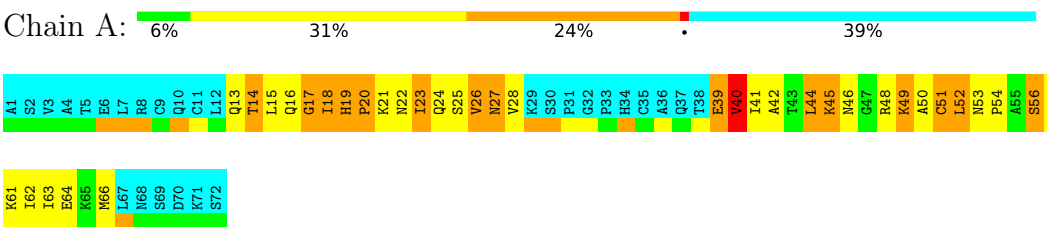


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 30. Colouring as in section 4.1 above.

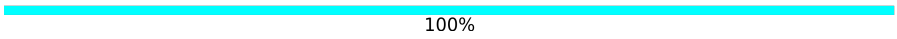
• Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY

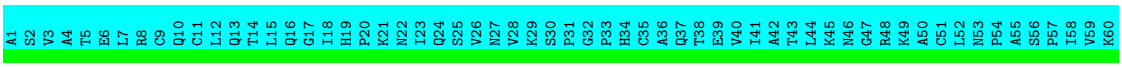
Chain A:



• Molecule 1: HUMAN MELANOMA GROWTH STIMULATORY ACTIVITY

Chain B:


100%


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
P31
G32
P33
H34
C35
A36
Q37
T38
E39
V40
I41
A42
T43
L44
K45
N46
G47
R48
K49
A50
C51
L52
N53
P54
A55
S56
P57
I58
V59
K60


K61
I62
I63
E64
K65
M66
L67
N68
S69
D70
K71
S72

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.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	30

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	ARG	Sidechain	30

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	336	372	372	50±3
1	B	0	0	0	0±0
All	All	10080	11160	11160	1485

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 70.

5 of 104 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ILE:HD13	1:A:49:LYS:HG3	0.93	1.40	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:VAL:HG11	1:A:54:PRO:HG3	0.90	1.43	21	30
1:A:26:VAL:HG12	1:A:66:MET:HE1	0.90	1.41	3	7
1:A:52:LEU:N	1:A:52:LEU:HD13	0.84	1.88	6	29
1:A:51:CYS:C	1:A:52:LEU:HD13	0.82	1.94	29	30

PROTEIN-BACKBONE INFOmissingINFO

PROTEIN-SIDECHAINS INFOmissingINFO

6.2.1 RNA

There are no RNA molecules in this entry.

6.3 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.4 Carbohydrates

There are no monosaccharides in this entry.

6.5 Ligand geometry

There are no ligands in this entry.

6.6 Other polymers

There are no such molecules in this entry.

6.7 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided