



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1JBA
Title : UNMYRISTOYLATED GCAP-2 WITH THREE CALCIUM IONS BOUND
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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	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

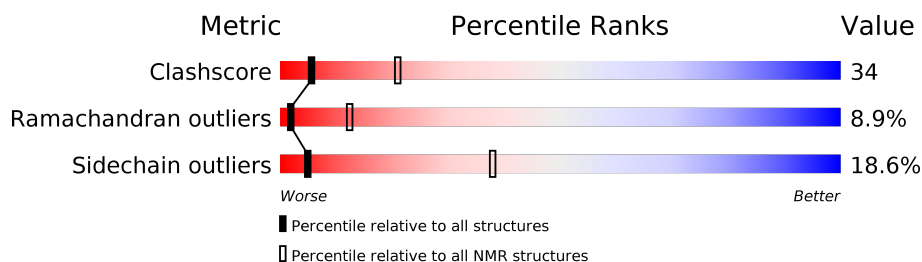
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	204	

2 Ensemble composition and analysis

This entry contains 22 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 19 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:19-A:131, A:144-A:186 (156)	0.85	19

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 7, 13, 16, 17, 18, 19, 21, 22
2	9, 14, 20
3	3, 12
4	1, 15
5	8, 10
Single-model clusters	2; 11

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3033 atoms, of which 1489 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (GUANYLATE CYCLASE ACTIVATING PROTEIN 2).

Mol	Chain	Residues	Atoms						Trace
1	A	189	Total	C	H	N	O	S	0
			3030	980	1489	254	299	8	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

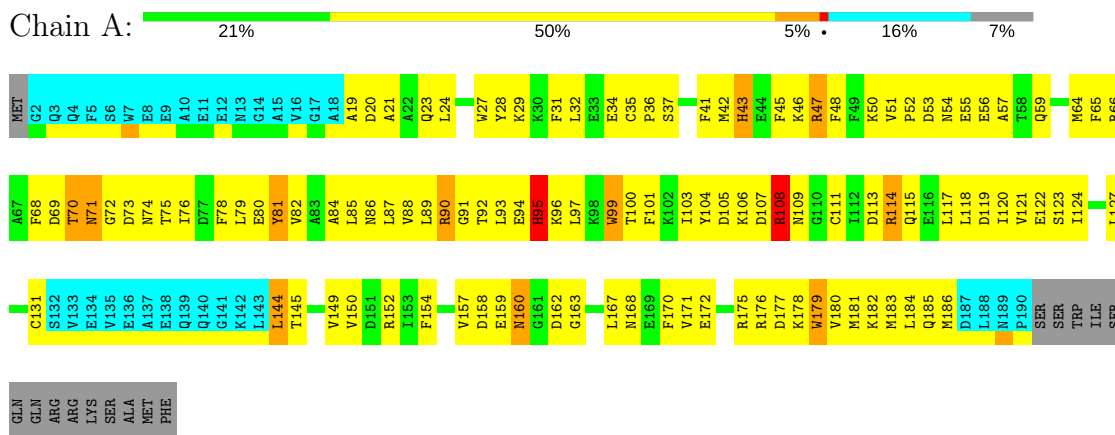
Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

4 Residue-property plots [i](#)

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: PROTEIN (GUANYLATE CYCLASE ACTIVATING PROTEIN 2)



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

The representative model is number 19. Colouring as in section 4.1 above.

- Molecule 1: PROTEIN (GUANYLATE CYCLASE ACTIVATING PROTEIN 2)



P190	SER
	SER
	TRP
	ILE
	SER
	GLN
	GLN
	ARG
	LYS
	SER
	ALA
	MET
	PHE

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY*.

Of the 50 calculated structures, 22 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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 4492
Number of chemical shift lists	1
Total number of shifts	1418
Number of shifts mapped to atoms	1418
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

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: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.08±0.01	5±0/1319 (0.4±0.0%)	1.32±0.01	18±1/1777 (1.0±0.0%)
All	All	1.08	111/29018 (0.4%)	1.32	402/39094 (1.0%)

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	7.4±0.9
All	All	0	162

5 of 6 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	27	TRP	CG-CD2	-7.80	1.30	1.43	15	22
1	A	99	TRP	CG-CD2	-7.53	1.30	1.43	12	22
1	A	179	TRP	CG-CD2	-7.20	1.31	1.43	14	22
1	A	95	HIS	CG-ND1	-6.37	1.24	1.38	21	22
1	A	43	HIS	CG-ND1	-6.20	1.25	1.38	7	22

5 of 21 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	TRP	NE1-CE2-CZ2	10.10	141.51	130.40	22	22
1	A	99	TRP	NE1-CE2-CZ2	9.19	140.51	130.40	12	22
1	A	179	TRP	NE1-CE2-CZ2	8.99	140.29	130.40	14	22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	TRP	NE1-CE2-CD2	-8.04	99.25	107.30	22	22
1	A	99	TRP	NE1-CE2-CD2	-7.62	99.68	107.30	20	22

There are no chirality outliers.

5 of 8 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	175	ARG	Sidechain	22
1	A	108	ARG	Sidechain	21
1	A	176	ARG	Sidechain	21
1	A	114	ARG	Sidechain	21
1	A	66	ARG	Sidechain	20

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	1292	1269	1269	88±12
All	All	28489	27918	27917	1925

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 34.

5 of 939 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD13	1:A:118:LEU:N	1.06	1.65	12	1
1:A:93:LEU:HD23	1:A:93:LEU:H	0.97	1.19	12	2
1:A:89:LEU:HD12	1:A:90:ARG:N	0.95	1.74	3	3
1:A:79:LEU:H	1:A:79:LEU:HD22	0.92	1.19	9	5
1:A:68:PHE:CZ	1:A:84:ALA:HB2	0.90	2.01	9	9

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	156/204 (76%)	107±5 (69±3%)	35±5 (22±3%)	14±3 (9±2%)	2	12
All	All	3432/4488 (76%)	2360 (69%)	766 (22%)	306 (9%)	2	12

5 of 65 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	95	HIS	18
1	A	20	ASP	16
1	A	108	ARG	16
1	A	90	ARG	12
1	A	186	MET	12

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	139/178 (78%)	113±4 (81±3%)	26±4 (19±3%)	5	38
All	All	3058/3916 (78%)	2489 (81%)	569 (19%)	5	38

5 of 111 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)
1	A	160	ASN	21
1	A	103	ILE	19
1	A	87	LEU	18
1	A	71	ASN	18
1	A	144	LEU	16

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 54% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4492

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	1418
Number of shifts mapped to atoms	1418
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	196	-0.54 ± 0.07	Should be applied
$^{13}\text{C}_\beta$	183	-0.04 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	179	-0.29 ± 0.06	None needed (< 0.5 ppm)
^{15}N	185	0.03 ± 0.22	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 1079 atoms were assigned a chemical shift out of a possible 2021. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	732/774 (95%)	294/309 (95%)	293/312 (94%)	145/153 (95%)
Sidechain	347/1058 (33%)	203/617 (33%)	144/391 (37%)	0/50 (0%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	0/189 (0%)	0/101 (0%)	0/83 (0%)	0/5 (0%)
Overall	1079/2021 (53%)	497/1027 (48%)	437/786 (56%)	145/208 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

