

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	3GBQ
Title	:	SOLUTION NMR STRUCTURE OF THE GRB2 N-TERMINAL SH3 DO-
		MAIN COMPLEXED WITH A TEN-RESIDUE PEPTIDE DERIVED FROM
		SOS DIRECT REFINEMENT AGAINST NOES, J-COUPLINGS, AND 1H
		AND 13C CHEMICAL SHIFTS, MINIMIZED AVERAGE STRUCTURE
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Deposited on	:	1996-12-23

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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.29
PANAV ShiftChecker Ideal geometry (proteins)	: : :	Wang et al. (2010) 2.29 Engh & Huber (2001) Parkinson et al. (1996)

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	А	74	77%	23%		
2	В	12	100%			



2 Ensemble composition and analysis (i)

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



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1102 atoms, of which 550 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called GRB2.

Mol	Chain	Residues	Atoms					Trace	
1	٨	57	Total	С	Η	Ν	0	S	0
	A	57	919	298	453	74	91	3	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	GLU	TRP	conflict	UNP Q60631

• Molecule 2 is a protein called SOS-1.

Mol	Chain	Residues	Atoms				Trace	
2	В	12	Total	C	H 07	N	0	1
			183	55	97	20	11	



4 Residue-property plots (i)

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.

Chain A:	77%	23%
GLY SER ARG ARG ARG ARG ARG SER VAL VAL CAL GE A1 A3 SER A3 SER A3 SER A3 SER A3 SER A1 A SER ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	79 79 71 711 711 711 711 711 712 719 719 719 722 723 723 723 723 723 723 723 723 723	E31 C32 C32 C32 C32 C32 C32 C32 C34 C43 C44 C41 C41 C43 C44 C43 C44 C43 C44 C43 C44 C43 C44 C43 C43
Y52 153 153 155 153 155 155 155 155 155 155		
• Molecule 2: SOS-1		
Chain B:	100%	
ACE0 V1 P2 P3 P4 V5 V5 P7 P6 P7 R8 R8 R10 NH211		

• Molecule 1: GRB2



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: DG, SA.

Of the 200 calculated structures, 1 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	
X-PLOR	structure solution	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE $\,$

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 (i)

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	А	0	0	0	0
2	В	0	0	0	0
All	All	0	0	0	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is -.

There are no clashes.

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	А	0	-	-	-	-
2	В	0	-	-	-	-

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	0	-	-	-	-

There are no Ramachandran outliers.

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	А	0	-	-	-
2	В	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

No chemical shift data were provided

