

Full wwPDB NMR Structure Validation Report (i)

Feb 10, 2022 – 11:34 AM EST

PDB ID	:	1F40
Title	:	SOLUTION STRUCTURE OF FKBP12 COMPLEXED WITH GPI-1046, A
		NEUROTROPHIC LIGAND
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Deposited on	:	2000-06-07

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

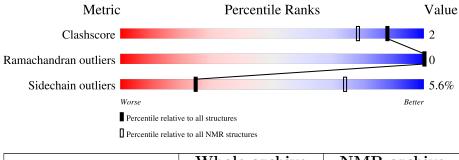
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	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.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} { m archive} \ (\#{ m Entries})$
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	107	87%	13%



2 Ensemble composition and analysis (i)

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

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 r						
1	A:1-A:107 (107)	0.00	10			

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: No clusters in NmrClust output



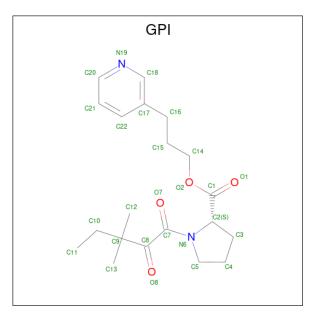
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1720 atoms, of which 862 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called FK506 BINDING PROTEIN (FKBP12).

Mol	Chain	Residues	Atoms						Trace
1	Δ	107	Total	С	Н	Ν	0	S	0
	A	107	1666	527	834	146	155	4	0

• Molecule 2 is (2S)-[3-PYRIDYL-1-PROPYL]-1-[3,3-DIMETHYL-1,2-DIOXOPENTYL]-2-P YRROLIDINECARBOXYLATE (three-letter code: GPI) (formula: $C_{20}H_{28}N_2O_4$).



[Mol	Chain	Residues	Atoms				
	0	۸	1	Total	С	Η	Ν	Ο
	2	А	1	54	20	28	2	4

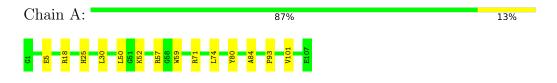


4 Residue-property plots (i)

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: FK506 BINDING PROTEIN (FKBP12)

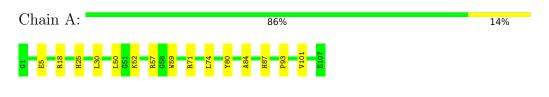


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

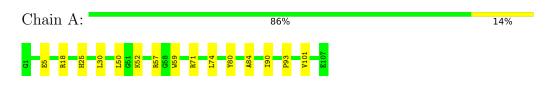
4.2.1 Score per residue for model 1

• Molecule 1: FK506 BINDING PROTEIN (FKBP12)



4.2.2 Score per residue for model 2

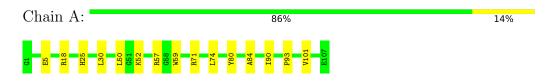
• Molecule 1: FK506 BINDING PROTEIN (FKBP12)



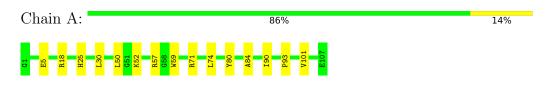


4.2.3 Score per residue for model 3

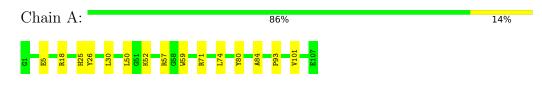
• Molecule 1: FK506 BINDING PROTEIN (FKBP12)



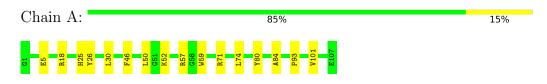
- 4.2.4 Score per residue for model 4
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)



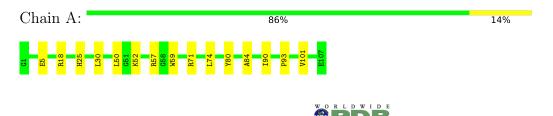
- 4.2.5 Score per residue for model 5
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)



- 4.2.6 Score per residue for model 6
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)

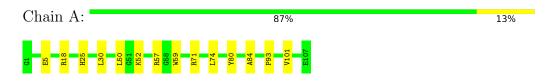


- 4.2.7 Score per residue for model 7
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)

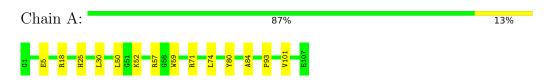


4.2.8 Score per residue for model 8

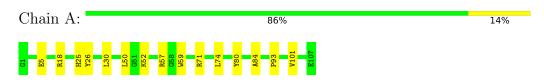
• Molecule 1: FK506 BINDING PROTEIN (FKBP12)



- 4.2.9 Score per residue for model 9
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)



- 4.2.10 Score per residue for model 10 (medoid)
- Molecule 1: FK506 BINDING PROTEIN (FKBP12)





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations.

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

Software name	Classification	Version
X-PLOR	refinement	3.851

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: GPI

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	E	Sond lengths	Bond angles		
		RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$0.85 {\pm} 0.00$	$0{\pm}0/851~(~0.0{\pm}~0.0\%)$	1.45 ± 0.00	$11{\pm}0/1146~(~1.0{\pm}~0.0\%)$	
All	All	0.85	0/8510 ($0.0%$)	1.45	109/11460~(~1.0%)	

There are no bond-length outliers.

All 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	rpe Atoms		Observed ⁽⁰⁾	Ideal(0)	Models	
	Ullalli	nes	туре	Atoms	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$		Worst	Total	
1	А	18	ARG	NE-CZ-NH2	-9.85	115.37	120.30	2	10
1	А	18	ARG	NE-CZ-NH1	7.58	124.09	120.30	8	10
1	А	57	ARG	NE-CZ-NH2	-7.43	116.58	120.30	5	10
1	А	59	TRP	CD1-CG-CD2	7.34	112.17	106.30	3	10
1	А	57	ARG	NE-CZ-NH1	7.12	123.86	120.30	5	10
1	А	59	TRP	CE2-CD2-CG	-6.67	101.97	107.30	2	10
1	А	80	TYR	CB-CG-CD2	-6.06	117.36	121.00	4	10
1	А	71	ARG	NE-CZ-NH2	-6.04	117.28	120.30	1	10
1	А	101	VAL	CG1-CB-CG2	-6.03	101.26	110.90	2	10
1	А	52	LYS	CB-CG-CD	-6.00	96.00	111.60	7	10
1	А	59	TRP	CG-CD1-NE1	-5.11	104.99	110.10	6	9

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	832	834	831	2 ± 1
2	А	26	28	28	2 ± 1
All	All	8580	8620	8590	32

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 2.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:87:HIS:CE1	2:A:108:GPI:H111	0.64	2.27	1	1
1:A:90:ILE:HD13	2:A:108:GPI:C11	0.61	2.25	2	3
1:A:26:TYR:CZ	2:A:108:GPI:C5	0.46	2.99	10	2
2:A:108:GPI:O7	2:A:108:GPI:C1	0.43	2.67	3	7
1:A:90:ILE:HD13	2:A:108:GPI:H111	0.43	1.91	7	1
2:A:108:GPI:C14	2:A:108:GPI:O7	0.42	2.67	1	1
2:A:108:GPI:O8	2:A:108:GPI:H113	0.42	2.15	10	1
1:A:84:ALA:O	1:A:93:PRO:HB3	0.41	2.16	8	10
1:A:90:ILE:HG21	2:A:108:GPI:C11	0.41	2.45	3	1
1:A:46:PHE:CZ	2:A:108:GPI:H41	0.41	2.50	6	1
2:A:108:GPI:H113	2:A:108:GPI:O8	0.41	2.15	5	1
1:A:26:TYR:CZ	2:A:108:GPI:H52	0.41	2.51	10	2
2:A:108:GPI:H151	2:A:108:GPI:H132	0.41	1.92	10	1

All unique clashes are listed below, sorted by their clash magnitude.

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	105/107~(98%)	$103 \pm 0 (98 \pm 0\%)$	$3\pm0 (98\pm0\%)$ 2±0 (2±0%)		100	100
All	All	1050/1070~(98%)	1030 (98%)	20 (2%)	0 (0%)	100	100

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	89/89~(100%)	84±0 (94±0%)	5±0 (6±0%)	25 74		
All	All	890/890~(100%)	840 (94%)	50 (6%)	25 74		

All 5 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	А	5	GLU	10
1	А	25	HIS	10
1	А	30	LEU	10
1	А	50	LEU	10
1	А	74	LEU	10

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is



considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mal	Turne	Chain	Dec	Tiple		Bond len	gths
IVIOI	туре	Unam	nes		Counts	RMSZ	#Z>2
2	GPI	А	108	-	27,27,27	$1.51{\pm}0.02$	4 ± 0 (14 $\pm0\%$)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Type	Chain	Dec	Tiple		Bond an	gles
	туре	Chain	nes	Link	Counts	RMSZ	#Z>2
2	GPI	А	108	-	35,37,37	$1.67{\pm}0.02$	8±1 (22±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GPI	А	108	-	-	$0\pm 0,28,38,38$	$0\pm0,2,2,2$

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

Mal	Chain	Dec	Turne	Atoma	Z	Observed(Å)	Ideal(Å)	Models	
10101	Unam	Res	Type	Atoms	L	Observed(A)	Ideal(A)	Worst	Total
2	А	108	GPI	C2-N6	3.72	1.54	1.47	8	10
2	А	108	GPI	C5-N6	3.71	1.54	1.47	8	10
2	А	108	GPI	C18-N19	3.40	1.41	1.34	8	10
2	А	108	GPI	C20-N19	2.69	1.41	1.33	1	10

All 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	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$	Moo Worst	dels Total
2	А	108	GPI	C5-N6-C2	4.95	104.15	112.00	7	10
2	А	108	GPI	O2-C1-C2	4.57	120.19	110.54	8	10

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Mol	Mol Chain		Turne	Atoma	Z	Observed(°)	$Ideal(^{o})$	Models	
	Unam	Res	Type	Atoms		Observed()	Ideal()	Worst	Total
2	А	108	GPI	C14-O2-C1	3.37	109.46	116.58	8	10
2	А	108	GPI	C3-C2-N6	2.44	106.64	103.03	8	2
2	А	108	GPI	O7-C7-C8	2.34	120.12	116.28	6	10
2	А	108	GPI	O2-C1-O1	2.22	119.93	124.13	8	7
2	А	108	GPI	C20-N19-C18	2.19	120.64	116.85	2	10
2	А	108	GPI	C4-C5-N6	2.15	107.03	103.25	8	3
2	А	108	GPI	O1-C1-C2	2.14	119.68	124.49	9	5
2	А	108	GPI	C17-C18-N19	2.07	119.67	123.72	9	10

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There are no chirality outliers.

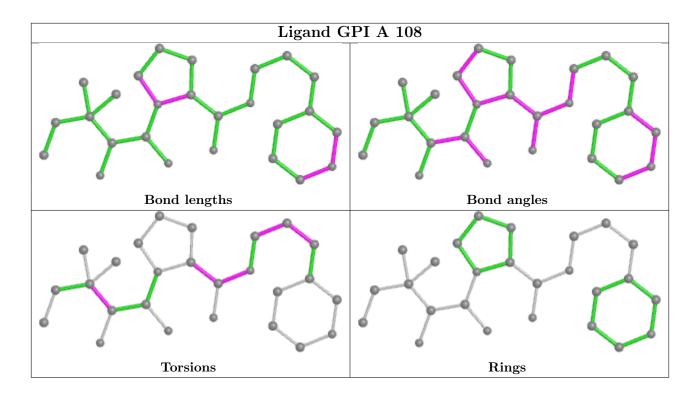
There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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

