



Full wwPDB NMR Structure Validation Report ⓘ

Oct 10, 2021 – 07:38 PM EDT

PDB ID : 2K3G
Title : NMR structure analysis of a BMP receptor
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Deposited on : 2008-05-07

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 ⓘ symbol.

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

MolProbity : 4.02b-467
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 : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

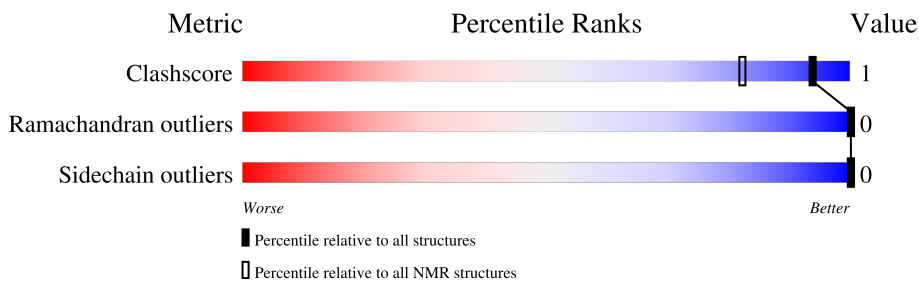
1 Overall quality at a glance i

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	Whole archive (#Entries)	NMR archive (#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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	102	

2 Ensemble composition and analysis

This entry contains 21 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:34-A:79, A:97-A:115 (65)	0.19	3

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1515 atoms, of which 732 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bone morphogenetic protein receptor type-1A.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	102	1515	483	732	132	157	11	0

There is a discrepancy between the modelled and reference sequences:

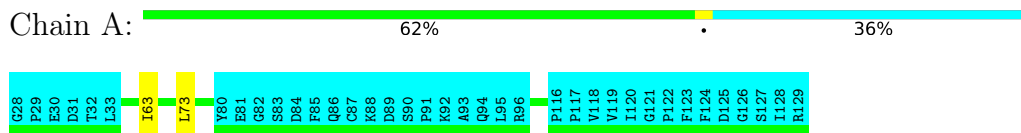
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	ALA	engineered mutation	UNP P36894

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: Bone morphogenetic protein receptor type-1A

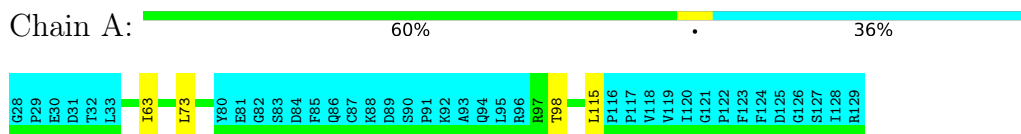


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

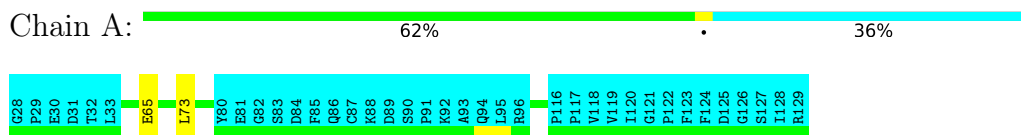
4.2.1 Score per residue for model 1

- Molecule 1: Bone morphogenetic protein receptor type-1A



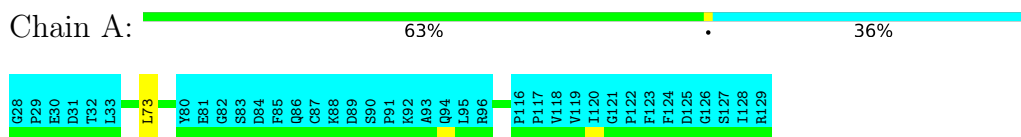
4.2.2 Score per residue for model 2

- Molecule 1: Bone morphogenetic protein receptor type-1A



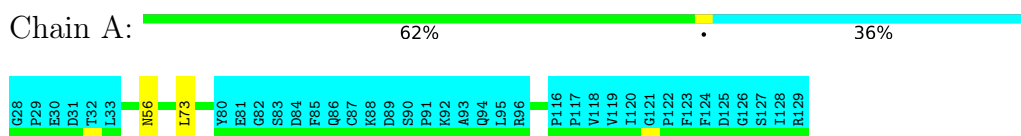
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Bone morphogenetic protein receptor type-1A



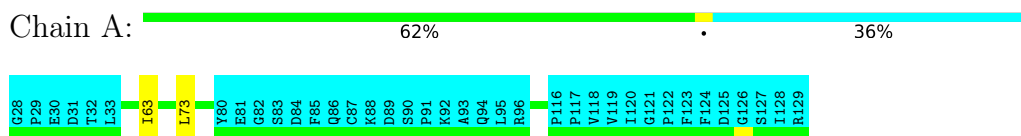
4.2.4 Score per residue for model 4

- Molecule 1: Bone morphogenetic protein receptor type-1A



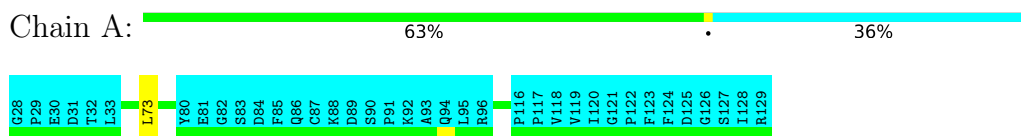
4.2.5 Score per residue for model 5

- Molecule 1: Bone morphogenetic protein receptor type-1A



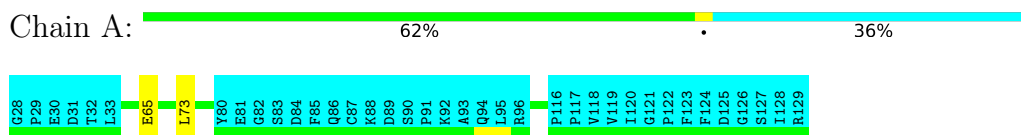
4.2.6 Score per residue for model 6

- Molecule 1: Bone morphogenetic protein receptor type-1A



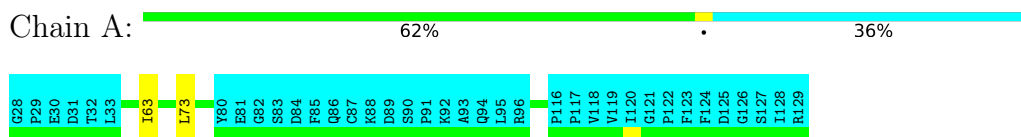
4.2.7 Score per residue for model 7

- Molecule 1: Bone morphogenetic protein receptor type-1A



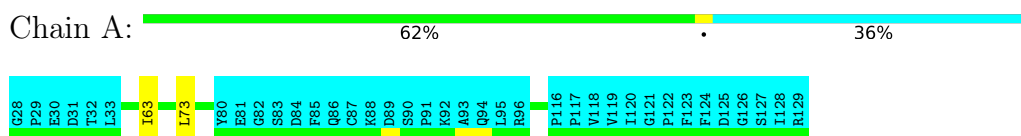
4.2.8 Score per residue for model 8

- Molecule 1: Bone morphogenetic protein receptor type-1A



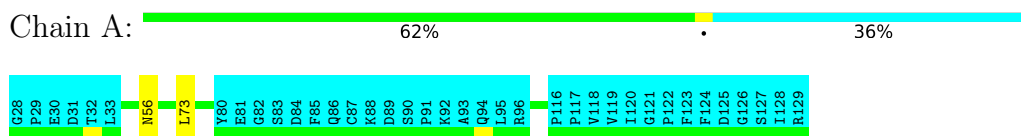
4.2.9 Score per residue for model 9

- Molecule 1: Bone morphogenetic protein receptor type-1A



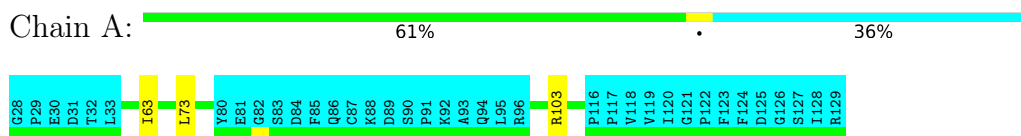
4.2.10 Score per residue for model 10

- Molecule 1: Bone morphogenetic protein receptor type-1A



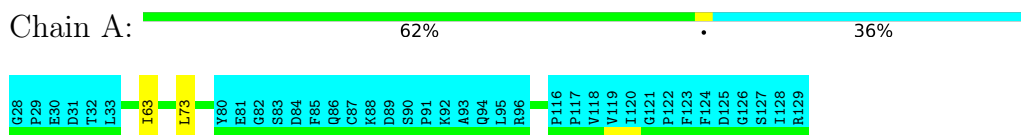
4.2.11 Score per residue for model 11

- Molecule 1: Bone morphogenetic protein receptor type-1A



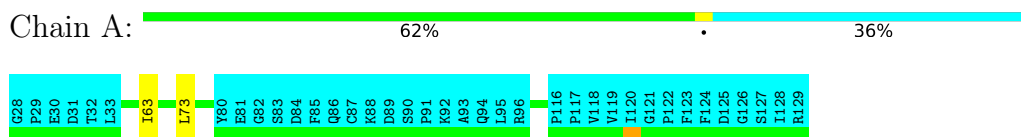
4.2.12 Score per residue for model 12

- Molecule 1: Bone morphogenetic protein receptor type-1A



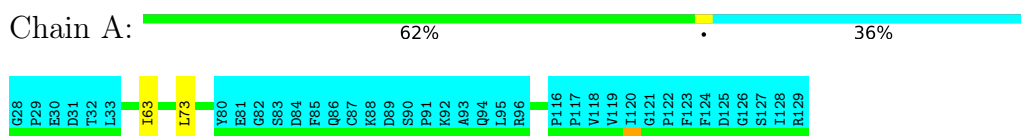
4.2.13 Score per residue for model 13

- Molecule 1: Bone morphogenetic protein receptor type-1A



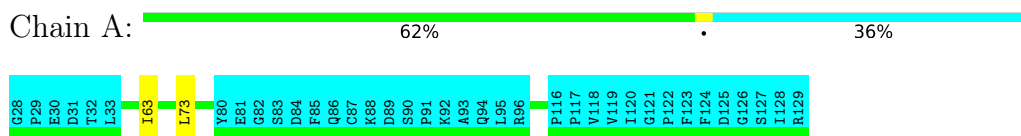
4.2.14 Score per residue for model 14

- Molecule 1: Bone morphogenetic protein receptor type-1A



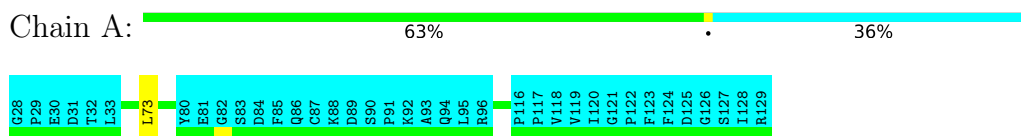
4.2.15 Score per residue for model 15

- Molecule 1: Bone morphogenetic protein receptor type-1A



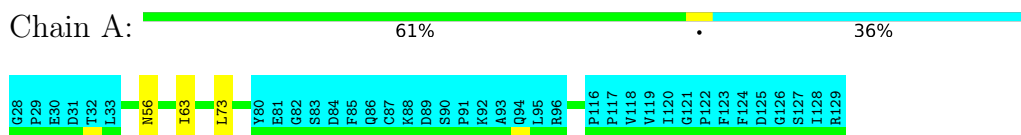
4.2.16 Score per residue for model 16

- Molecule 1: Bone morphogenetic protein receptor type-1A



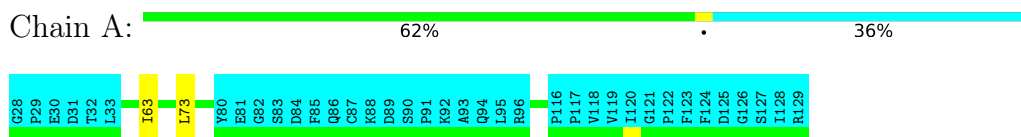
4.2.17 Score per residue for model 17

- Molecule 1: Bone morphogenetic protein receptor type-1A



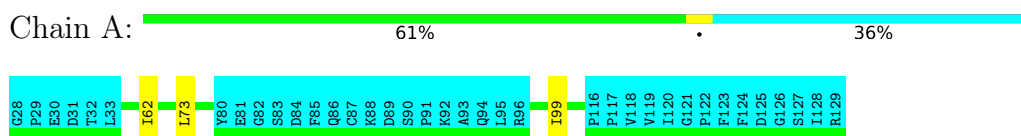
4.2.18 Score per residue for model 18

- Molecule 1: Bone morphogenetic protein receptor type-1A



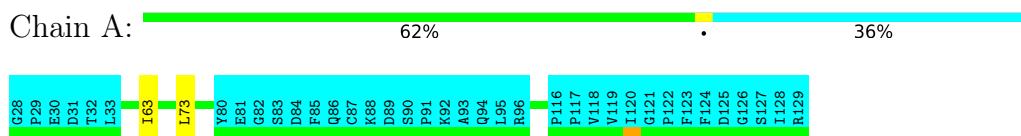
4.2.19 Score per residue for model 19

- Molecule 1: Bone morphogenetic protein receptor type-1A



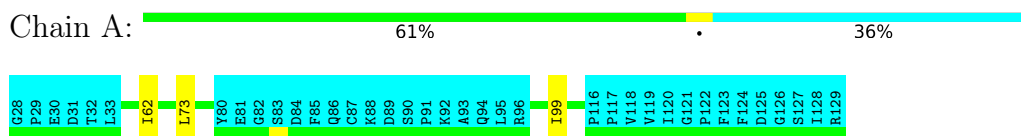
4.2.20 Score per residue for model 20

- Molecule 1: Bone morphogenetic protein receptor type-1A



4.2.21 Score per residue for model 21

- Molecule 1: Bone morphogenetic protein receptor type-1A



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.9.4a
ProcheckNMR	geometry optimization	
AQUA	geometry optimization	
WHAT IF	geometry optimization	
X-PLOR NIH	refinement	2.9.4a

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.21±0.00	0±0/505 (0.0± 0.0%)	1.11±0.01	0±0/686 (0.0± 0.0%)
All	All	1.21	0/10605 (0.0%)	1.11	1/14406 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	103	ARG	NE-CZ-NH1	5.44	123.02	120.30	11	1

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	A	496	458	458	1±0
All	All	10416	9618	9618	25

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ILE:HD12	1:A:73:LEU:HD21	0.67	1.65	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ILE:HD12	1:A:73:LEU:HD11	0.61	1.72	1	2
1:A:62:ILE:HD12	1:A:99:ILE:HD12	0.50	1.84	19	2
1:A:73:LEU:HD12	1:A:73:LEU:N	0.48	2.24	16	9
1:A:63:ILE:HD12	1:A:73:LEU:CD2	0.44	2.39	13	1
1:A:98:THR:OG1	1:A:115:LEU:HD23	0.40	2.17	1	1

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	65/102 (64%)	61±1 (93±1%)	4±1 (7±1%)	0±0 (0±0%)	100	100
All	All	1365/2142 (64%)	1273 (93%)	92 (7%)	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	A	58/90 (64%)	58±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1218/1890 (64%)	1218 (100%)	0 (0%)	100	100

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

No chemical shift data were provided