



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:53 AM UTC

PDB ID : 4AIY / pdb_00004aiy
Title : R6 HUMAN INSULIN HEXAMER (SYMMETRIC), NMR, 'GREEN' SUB-
STATE, AVERAGE STRUCTURE
Authors : O'Donoghue, S.I.; Chang, X.; Abseher, R.; Nilges, M.; Led, J.J.
Deposited on : 1998-12-29

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 was not calculated.

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

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4794 atoms, of which 2322 are hydrogens and 0 are deuteriums.

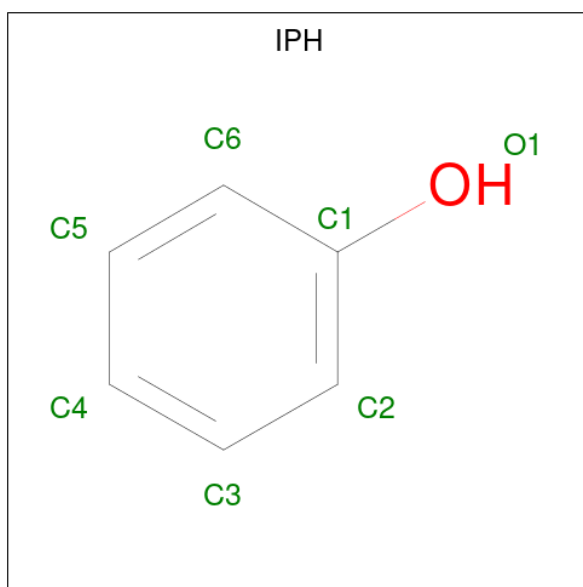
- Molecule 1 is a protein called PROTEIN (INSULIN).

Mol	Chain	Residues	Atoms						Trace
1	A	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	
1	C	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	
1	E	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	
1	G	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	
1	I	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	
1	K	21	Total	C	H	N	O	S	0
			312	99	149	25	35	4	

- Molecule 2 is a protein called PROTEIN (INSULIN).

Mol	Chain	Residues	Atoms						Trace
2	B	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	
2	D	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	
2	F	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	
2	H	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	
2	J	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	
2	L	30	Total	C	H	N	O	S	0
			474	158	232	40	42	2	

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			
3	A	1	Total	C	H	O
			13	6	6	1
3	C	1	Total	C	H	O
			13	6	6	1
3	E	1	Total	C	H	O
			13	6	6	1
3	G	1	Total	C	H	O
			13	6	6	1
3	I	1	Total	C	H	O
			13	6	6	1
3	K	1	Total	C	H	O
			13	6	6	1

4 Residue-property plots

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: PROTEIN (INSULIN)

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: PROTEIN (INSULIN)

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: PROTEIN (INSULIN)

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: PROTEIN (INSULIN)

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: PROTEIN (INSULIN)

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: PROTEIN (INSULIN)

Chain K:  100%

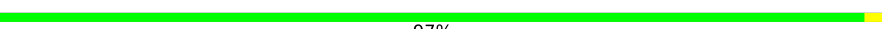
There are no outlier residues in this chain.

- Molecule 2: PROTEIN (INSULIN)

Chain B:  97%



- Molecule 2: PROTEIN (INSULIN)

Chain D:  97% .

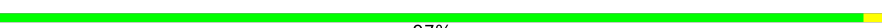


- Molecule 2: PROTEIN (INSULIN)

Chain F:  97% .

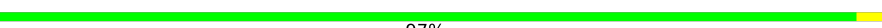


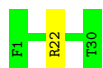
- Molecule 2: PROTEIN (INSULIN)

Chain H:  97% .

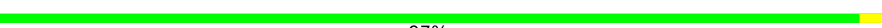


- Molecule 2: PROTEIN (INSULIN)

Chain J:  97% .



- Molecule 2: PROTEIN (INSULIN)

Chain L:  97% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SYMMETRY-ADR METHOD: SIMULATED ANNEALING, WATER-SHELL REFINEMENT, AND ENERGY MINIMIZATION*.

Of the 40 calculated structures, 1 were deposited, based on the following criterion: *LOWEST TOTAL ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided