



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1AIY / pdb_00001aiy
Title : R6 HUMAN INSULIN HEXAMER (SYMMETRIC), NMR, 10 STRUCTURES
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Deposited on : 1997-04-30

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

<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 10 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 9 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:2-A:21, B:1-B:30, C:1-C:21, D:1-D:28, E:2-E:21, F:1-F:30, G:1-G:21, H:1-H:30, I:1-I:21, J:1-J:30, K:1-K:21, L:1-L:30 (302)	1.26	9

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 1 clusters and 7 single-model clusters were found.

Cluster number	Models
1	5, 8, 9
Single-model clusters	1; 2; 3; 4; 6; 7; 10

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4802 atoms, of which 2326 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called R6 INSULIN HEXAMER.

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 R6 INSULIN HEXAMER.

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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1
3	D	1	Total	Zn
			1	1

- Molecule 4 is PHENOL (CCD ID: HOH) (formula: H₂O).

Mol	Chain	Residues	Atoms			
4	B	1	Total	C	H	O
			13	6	6	1
4	D	1	Total	C	H	O
			13	6	6	1
4	F	1	Total	C	H	O
			13	6	6	1
4	H	1	Total	C	H	O
			13	6	6	1
4	J	1	Total	C	H	O
			13	6	6	1
4	L	1	Total	C	H	O
			13	6	6	1

- Molecule 5 is water.

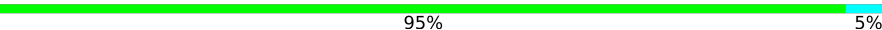
Mol	Chain	Residues	Atoms		
5	F	1	Total	H	O
			3	2	1
5	H	1	Total	H	O
			3	2	1

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: R6 INSULIN HEXAMER

Chain A:  95% 5%



- Molecule 1: R6 INSULIN HEXAMER

Chain C:  100%

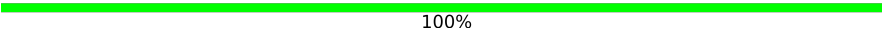
There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain E:  95% 5%

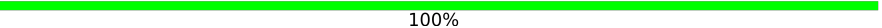


- Molecule 1: R6 INSULIN HEXAMER

Chain G:  100%

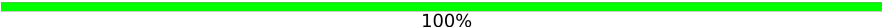
There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain I:  100%

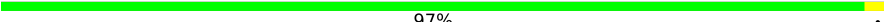
There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain K:  100%

There are no outlier residues in this chain.

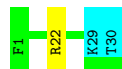
- Molecule 2: R6 INSULIN HEXAMER

Chain B:  97% .

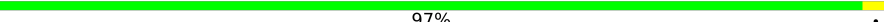


- Molecule 2: R6 INSULIN HEXAMER

Chain D:  90% . 7%

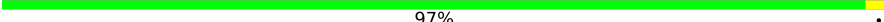


- Molecule 2: R6 INSULIN HEXAMER

Chain F:  97% .

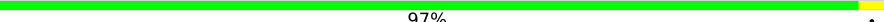


- Molecule 2: R6 INSULIN HEXAMER

Chain H:  97% .

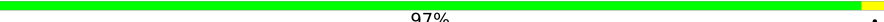


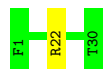
- Molecule 2: R6 INSULIN HEXAMER

Chain J:  97% .



- Molecule 2: R6 INSULIN HEXAMER

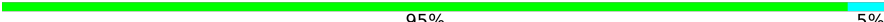
Chain L:  97% .



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

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: R6 INSULIN HEXAMER

Chain A:  95% 5%



- Molecule 1: R6 INSULIN HEXAMER

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain E:  95% 5%



- Molecule 1: R6 INSULIN HEXAMER

Chain G:  100%

There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain I:  100%

There are no outlier residues in this chain.

- Molecule 1: R6 INSULIN HEXAMER

Chain K:  100%

There are no outlier residues in this chain.

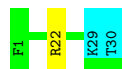
- Molecule 2: R6 INSULIN HEXAMER

Chain B:  97% .



- Molecule 2: R6 INSULIN HEXAMER

Chain D:  90% . 7%

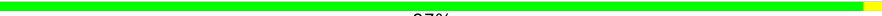


- Molecule 2: R6 INSULIN HEXAMER

Chain F:  97% .



- Molecule 2: R6 INSULIN HEXAMER

Chain H:  97% .



- Molecule 2: R6 INSULIN HEXAMER

Chain J:  97% .



- Molecule 2: R6 INSULIN HEXAMER

Chain L:  97% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING AND ENERGY MINIMIZATION*.

Of the 30 calculated structures, 10 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