



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 19, 2026 – 09:58 PM UTC

PDB ID : 3EZB / pdb_00003ezb
Title : COMPLEX OF THE AMINO TERMINAL DOMAIN OF ENZYME I AND
THE HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN HPR
FROM ESCHERICHIA COLI
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Deposited on : 1998-11-03

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	:	4-5-2 with Phenix2.0
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

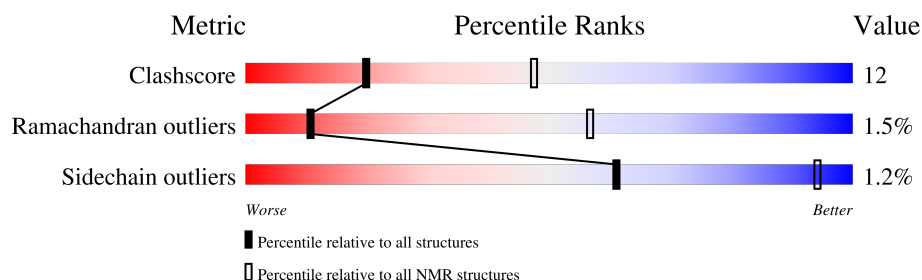
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	259	
2	B	85	

2 Ensemble composition and analysis

This entry contains 40 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. No representative model was identified.

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:1-A:236, B:301-B:385 (321)	Not calculated	Not calculated

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: Inconsistent models in file

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5319 atoms, of which 2691 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I).

Mol	Chain	Residues	Atoms						Trace
1	A	259	Total	C	H	N	O	S	0
			4026	1243	2038	337	403	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	ARG	LEU	conflict	UNP P08839

- Molecule 2 is a protein called PROTEIN (PHOSPHOCARRIER PROTEIN HPR).

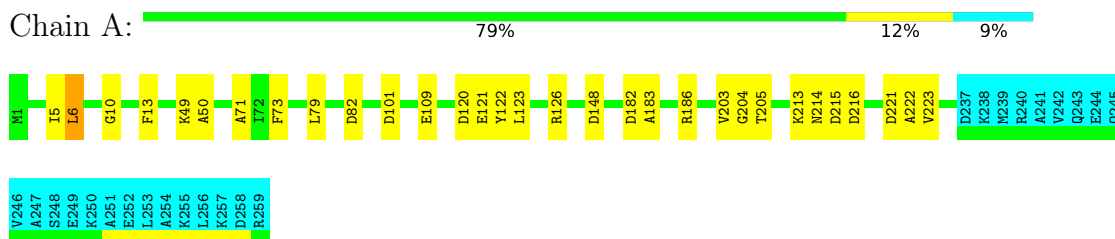
Mol	Chain	Residues	Atoms						Trace
2	B	85	Total	C	H	N	O	S	0
			1293	401	653	107	130	2	

4 Residue-property plots

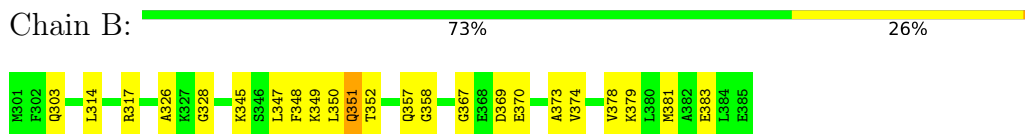
4.1 Average score per residue in the NMR ensemble

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: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



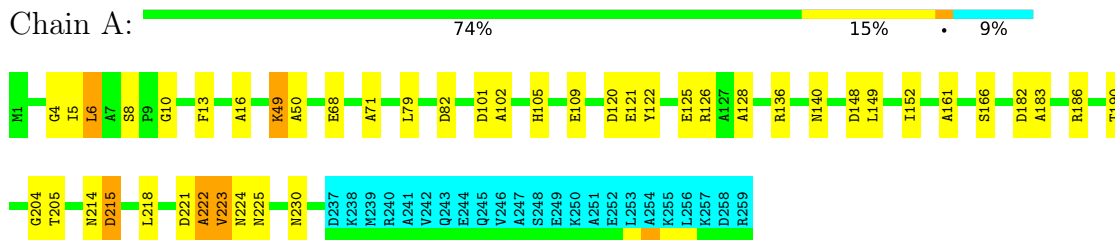
- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



4.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 4.1 above.

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



K301	Y306	L314	R317	A326	K327	G328	A342	L347	F348	K349	L350	Q351	T352	L353	Q357	G358	T359	G367	E368	D369	E370	A373	V374	V378	K379	E383	L384	E385
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5 Refinement protocol and experimental data overview ⓘ

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

Of the 40 calculated structures, 40 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURE*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

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	1.53±0.01	1±1/1820 (0.0± 0.0%)	1.16±0.01	1±1/2457 (0.0± 0.0%)
2	B	1.53±0.01	0±0/647 (0.0± 0.1%)	1.21±0.01	1±0/871 (0.1± 0.0%)
All	All	1.53	29/98719 (0.0%)	1.17	77/133198 (0.1%)

All unique bond 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	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	203	VAL	N-CA	5.58	1.51	1.46	15	16
1	A	4	GLY	N-CA	5.52	1.50	1.44	19	1
2	B	317	ARG	N-CA	5.44	1.50	1.46	37	6
1	A	230	ASN	N-CA	5.34	1.50	1.46	18	5
1	A	178	GLY	N-CA	5.13	1.50	1.45	33	1

5 of 8 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	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	PHE	CA-CB-CG	-7.11	106.69	113.80	4	20
1	A	223	VAL	N-CA-C	-6.54	106.63	112.12	19	5
2	B	345	LYS	N-CA-C	-6.33	105.84	112.93	38	35
1	A	43	PHE	CA-CB-CG	-5.78	108.02	113.80	29	5
2	B	376	HIS	CA-CB-CG	-5.57	108.23	113.80	29	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	1805	1847	1847	43±6
2	B	640	653	650	26±5
All	All	97799	99997	99876	2443

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 12.

5 of 540 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD22	2:B:347:LEU:HD23	0.93	1.40	24	38
1:A:10:GLY:O	1:A:222:ALA:HB3	0.81	1.76	28	40
1:A:123:LEU:HD22	2:B:351:GLN:O	0.80	1.76	7	14
1:A:79:LEU:HD11	2:B:348:PHE:CE2	0.78	2.14	22	39
1:A:79:LEU:HD11	2:B:348:PHE:CZ	0.73	2.18	3	24

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	235/259 (91%)	218±2 (93±1%)	14±2 (6±1%)	3±1 (1±0%)	11	58
2	B	83/85 (98%)	75±2 (91±2%)	6±1 (8±2%)	2±1 (2±1%)	8	51
All	All	12720/13760 (92%)	11730 (92%)	795 (6%)	195 (2%)	11	57

5 of 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	6	LEU	40

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Mol	Chain	Res	Type	Models (Total)
1	A	183	ALA	39
2	B	351	GLN	35
1	A	148	ASP	33
2	B	373	ALA	17

6.3.2 Protein sidechains ⓘ

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	195/214 (91%)	193±1 (99±1%)	2±1 (1±1%)	65	95
2	B	70/70 (100%)	69±1 (98±1%)	1±1 (2±1%)	52	92
All	All	10599/11360 (93%)	10475 (99%)	124 (1%)	61	94

5 of 39 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)
2	B	351	GLN	13
1	A	190	THR	10
1	A	215	ASP	10
2	B	370	GLU	8
1	A	213	LYS	7

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides 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