



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 26, 2026 – 01:49 AM UTC

PDB ID : 2KX9 / pdb_00002kx9
Title : Solution Structure of the Enzyme I dimer Using Residual Dipolar Couplings and Small Angle X-Ray Scattering
Authors : Schwieters, C.D.; Suh, J.; Grishaev, A.; Takayama, Y.; Guirlando, R.; Clore, G.
Deposited on : 2010-04-29

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

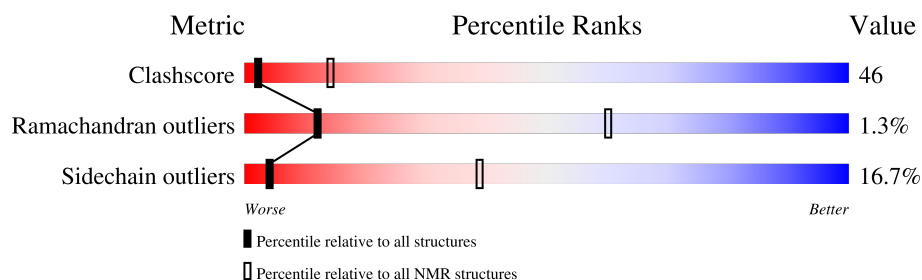
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

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	573	52% 35% 13% .
1	B	573	52% 34% 13% .

2 Ensemble composition and analysis ⓘ

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17912 atoms, of which 9028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Phosphoenolpyruvate-protein phosphotransferase.

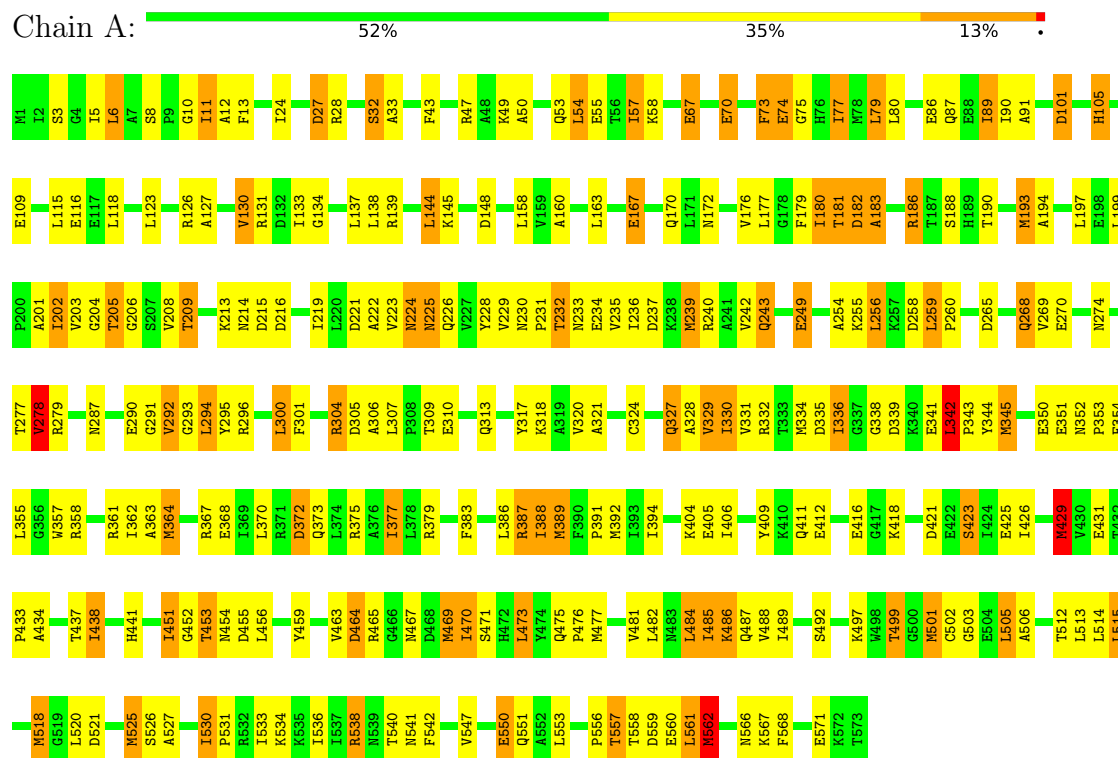
Mol	Chain	Residues	Atoms						Trace
1	A	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	
1	B	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	

4 Residue-property plots

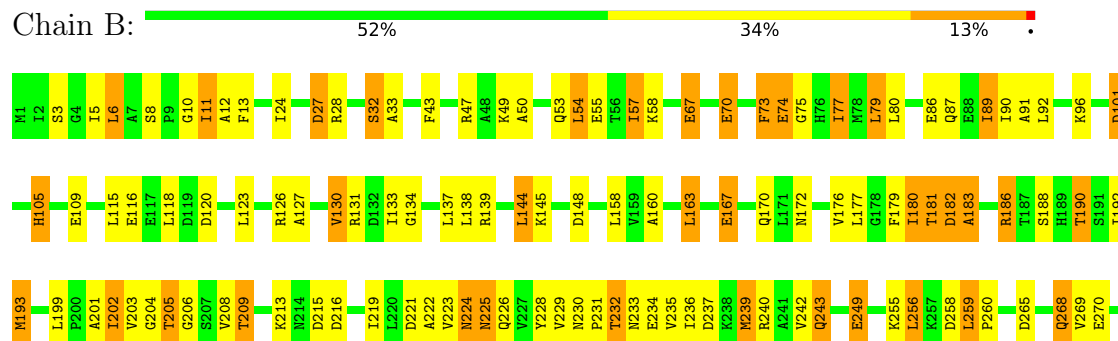
4.1 Average score per residue in the NMR ensemble

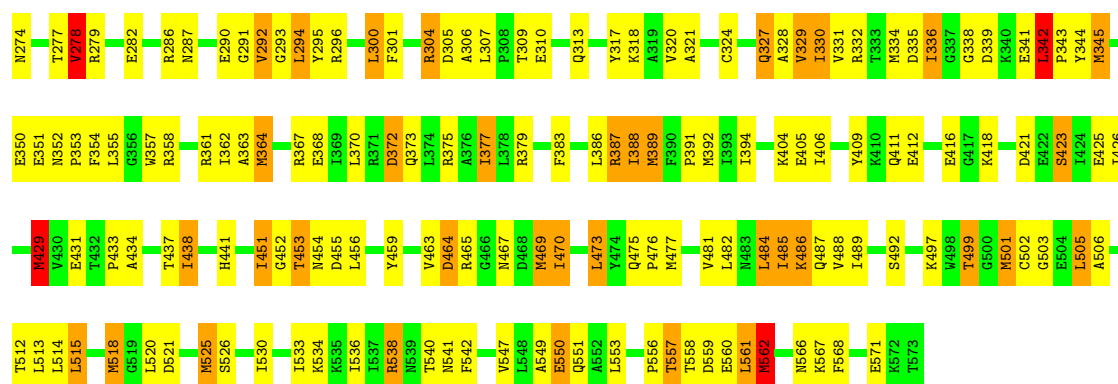
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

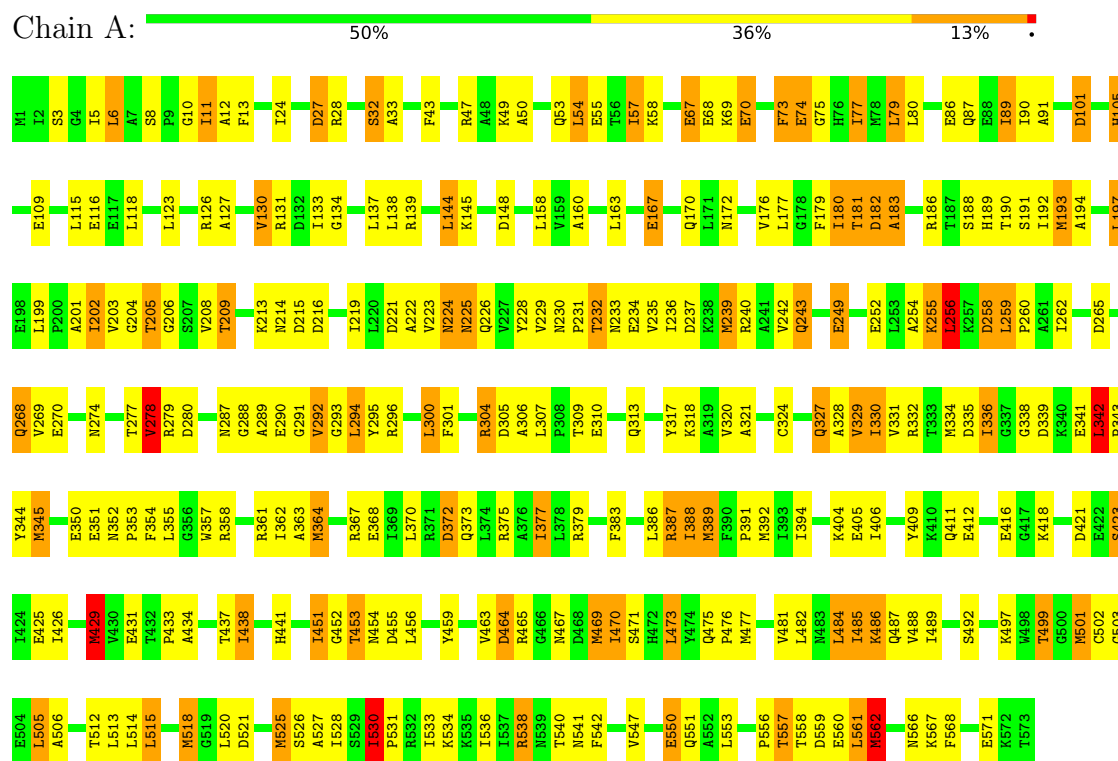




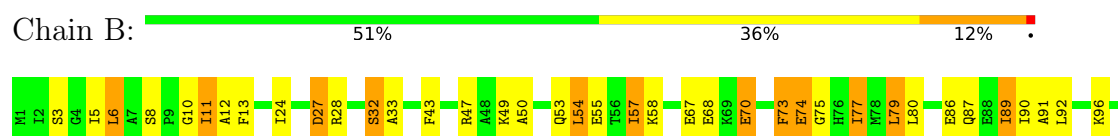
4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



M501	C502	G503	E504	L505	A506	T512	L513	L514	L515	M518	G519	L520	D521	M525	S526	A527	I528	I533	K534	K535	I536	I537	R538	N539	T540	N541	F542	V547	L548	A549	E550	Q551	A552	L553	P556	T557	T558	D559	E560	L561	M562	N566	K567	F568	E571	K572	T573								
D421	E422	S423	L424	E425	L426	M429	V430	E431	T432	P433	A434	T437	L438	H441	T451	G452	T453	N454	D455	L456	Y459	V463	D464	R465	G466	D467	N469	L470	L473	T474	Q475	P476	M477	V481	L482	N483	L484	T485	K486	Q487	V488	L489	S492	K497	W498	T499	G500								
K340	E341	L342	P343	Y344	M345	E350	E351	N352	P353	F354	L355	G356	W357	R358	R361	I362	A363	M364	R367	E368	I369	L370	R371	D372	Q373	L374	R375	A376	I377	L378	R379	F383	L386	R387	I388	M389	F390	P391	M392	I393	I394	K404	E405	I406	Y409	K410	Q411	E412	E416	G417	K418				
D265	Q268	V269	E270	N274	T277	T278	R279	E282	R286	N287	E290	G291	V292	G293	L294	Y295	R296	L300	F301	R304	D305	A306	P308	T309	E310	Q313	Y317	K318	A319	V320	A321	C324	Q327	A328	V329	I330	V331	R332	T333	M334	D335	I336	G337	D338	D339										
S191	I192	M193	A194	R195	S196	L199	P200	A201	I202	V203	G204	T205	G206	S207	V208	T209	K213	N214	D215	D216	I219	L220	D221	A222	V223	N224	N225	Q226	V227	Y228	V229	N230	P231	T232	N233	E234	V235	I236	D237	K238	M239	R240	A241	V242	Q243	E249	K255	D256	K257	D258	L259	P260	A261	H189	I262
D101	H105	E109	L115	E116	E117	L118	D119	D120	L123	R126	A127	V130	R131	D132	I133	G134	L137	L138	R139	L144	K145	D148	L158	V159	A160	L163	E167	T168	A169	Q170	L171	N172	V176	L177	G178	F179	I180	D182	T181	A183	R186	T187	S188	H189	T190										

5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 2 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Xplor-NIH	structure solution	2.25
Xplor-NIH	refinement	2.25

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	1.37±0.00	21±0/4495 (0.5± 0.0%)	1.17±0.00	10±0/6061 (0.2± 0.0%)
1	B	1.37±0.00	22±0/4495 (0.5± 0.0%)	1.17±0.00	9±0/6061 (0.1± 0.0%)
All	All	1.37	86/17980 (0.5%)	1.17	37/24244 (0.2%)

5 of 43 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	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	B	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	B	469	MET	SD-CE	13.78	2.14	1.79	1	2
1	A	469	MET	SD-CE	13.78	2.13	1.79	1	2
1	A	364	MET	SD-CE	10.61	2.06	1.79	1	2

5 of 19 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	530	ILE	N-CA-CB	8.43	117.03	110.45	1	1
1	A	561	LEU	CA-CB-CG	6.63	139.50	116.30	1	2
1	B	561	LEU	CA-CB-CG	6.63	139.49	116.30	1	2
1	A	278	VAL	CB-CA-C	-6.25	101.05	111.29	1	2
1	B	278	VAL	CB-CA-C	-6.24	101.06	111.29	1	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	4442	4514	4506	420±0
1	B	4442	4514	4506	416±5
All	All	17768	18056	18024	1635

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 46.

5 of 858 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:562:MET:SD	1:B:562:MET:CE	1.48	2.01	1	2
1:B:364:MET:SD	1:B:364:MET:CE	1.43	2.06	1	2
1:A:364:MET:SD	1:A:364:MET:CE	1.42	2.06	1	2
1:A:469:MET:SD	1:A:469:MET:CE	1.36	2.14	1	2
1:B:469:MET:CE	1:B:469:MET:SD	1.36	2.14	1	2

6.3 Torsion angles

6.3.1 Protein backbone

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	571/573 (100%)	536±0 (94±0%)	28±0 (5±0%)	7±0 (1±0%)	13	61
1	B	571/573 (100%)	536±0 (94±0%)	27±1 (5±0%)	8±0 (1±0%)	12	60
All	All	2284/2292 (100%)	2146 (94%)	109 (5%)	29 (1%)	12	60

5 of 19 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	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	148	ASP	2
1	A	183	ALA	2
1	A	232	THR	2
1	A	278	VAL	2

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	474/474 (100%)	394±2 (83±0%)	80±2 (17±0%)	4	38
1	B	474/474 (100%)	395±0 (83±0%)	79±0 (17±0%)	4	39
All	All	1896/1896 (100%)	1579 (83%)	317 (17%)	4	39

5 of 165 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	A	11	ILE	2
1	A	27	ASP	2
1	A	28	ARG	2
1	A	32	SER	2
1	A	54	LEU	2

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