

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 2OZW

Title : Solution structure of human phosphohistidine phosphatase 1 with phosphate

ligand

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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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 : 2.27

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

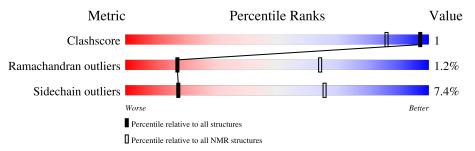
Validation Pipeline (wwPDB-VP) : 2.27

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	NMR archive
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries})$
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 <=5%

Mol	Chain	Length	Quality of chain					
1	A	125	64%	6%	• 29%			



2 Ensemble composition and analysis (i)

This entry contains 21 models. Model 1 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 mod								
1	A:4-A:14, A:20-A:31, A:39-	0.19	1					
	A:79, A:89-A:110, A:118-							
	A:120 (89)							

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 4 clusters and 3 single-model clusters were found.

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



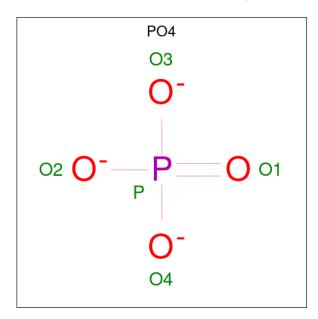
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1908 atoms, of which 931 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called 14 kDa phosphohistidine phosphatase.

Mol	Chain	Residues		Atoms					Trace
1	Λ	195	Total	С	Н	N	О	S	0
1	A	125	1903	613	931	165	188	6	U

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		
9	Λ	1	Total	О	Р
	A	1	5	4	1

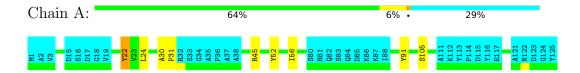


4 Residue-property plots (i)

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: 14 kDa phosphohistidine phosphatase



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

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

• Molecule 1: 14 kDa phosphohistidine phosphatase





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: torsion angle dynamics simulated annealing.

Of the 100 calculated structures, 21 were deposited, based on the following criterion: structures with favorable non-bond energy.

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

Software name	Classification	Version
DYANA	structure solution	cyana2.0
Amber	refinement	7.0

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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).

Mal	Chain	В	Sond lengths	Bond angles		
MIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.66 ± 0.00	$0\pm0/722$ ($0.0\pm~0.0\%$)	1.02 ± 0.18	$1\pm1/978~(~0.1\pm~0.1\%)$	
All	All	0.66	0/15162 (0.0%)	1.04	21/20538 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0 ± 0.0	1.6 ± 0.7
All	All	0	34

There are no bond-length outliers.

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	Iol Chain Res Typ		Type	Atoms	\mathbf{z}	$Observed(^o)$	$Ideal(^{o})$	Models	
MIOI	Chain	nes	Туре	Atoms	L	Observed(')	Ideal(*)	Worst	Total
1	A	39	GLU	OE1-CD-OE2	-38.15	77.52	123.30	1	1
1	A	39	GLU	CG-CD-OE2	22.17	162.65	118.30	1	1
1	A	39	GLU	CG-CD-OE1	-16.58	85.14	118.30	1	1
1	A	26	ARG	NE-CZ-NH2	-6.75	116.92	120.30	7	10
1	A	91	TYR	CB-CG-CD2	-5.78	117.53	121.00	15	4

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	22	TYR	Sidechain	19

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	ARG	Sidechain	11
1	A	91	TYR	Sidechain	3
1	A	93	TYR	Sidechain	1

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	Non-H H(model)		Clashes	
1	A	703	684	684	1±1	
All	All	14868	14364	14364	19	

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 9	Clash(Å)	Distance (Å)	${f Models}$	
Atom-1	Atom-2	Clash(A)	$\operatorname{Distance}(\check{\mathbf{A}})$	Worst	Total
1:A:30:ALA:N	1:A:31:PRO:CD	0.43	2.81	10	14
1:A:47:TYR:CD2	1:A:49:TRP:CZ2	0.42	3.08	20	1
1:A:47:TYR:CD1	1:A:49:TRP:CZ2	0.41	3.08	5	4

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	Perce	entiles
1	A	89/125 (71%)	86±1 (96±2%)	6±1 (96±2%) 2±1 (3±1%)		17	64
All	All	1869/2625 (71%)	1798 (96%)	48 (3%)	23 (1%)	17	64

All 3 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	30	ALA	17
1	A	29	SER	3
1	A	102	HIS	3

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	nin Analysed Rotameric		Outliers	Percentiles		
1	A	73/100 (73%)	68±1 (93±2%)	5±1 (7±2%)	17 65		
All	All	1533/2100 (73%)	1419 (93%)	114 (7%)	17 65		

5 of 13 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	22	TYR	21
1	A	52	TYR	21
1	A	56	ILE	21
1	A	24	LEU	19
1	A	105	SER	17

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)

1 ligand is modelled in this entry.



In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Peg	Link		Bond ler	ngths
			nes	LIIIK	Counts	RMSZ	#Z>2
2	PO4	A	126	-	4,4,4	2.01 ± 0.03	$3\pm0 (66\pm11\%)$

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Type	Chain	Pos	Link		Bond ang	gles
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
2	PO4	A	126	-	6,6,6	0.66 ± 0.04	0±0 (0±0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Chain Res	Tuno	e Atoms	\mathbf{Z}	Observed(Å)	$\operatorname{Ideal}(\mathring{\mathbf{A}})$	Models	
MIOI	Cham		Type			Observed(A)	Ideal(A)	Worst	Total
2	A	126	PO4	P-O4	2.37	1.47	1.54	9	21
2	A	126	PO4	P-O3	2.34	1.47	1.54	13	21
2	A	126	PO4	P-O2	2.14	1.48	1.54	13	14

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

No chemical shift data were provided

