



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 10:11 PM GMT

PDB ID : 1A0A  
Title : PHOSPHATE SYSTEM POSITIVE REGULATORY PROTEIN PHO4/DNA  
COMPLEX  
Authors : Shimizu, T.; Toumoto, A.; Ihara, K.; Shimizu, M.; Kyogoku, Y.; Ogawa, N.;  
Oshima, Y.; Hakoshima, T.  
Deposited on : 1997-11-27  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

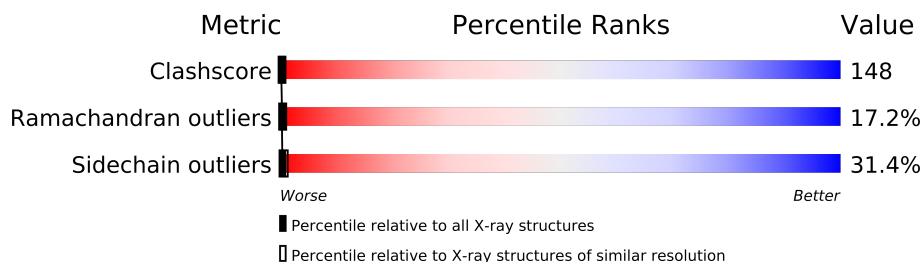
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	17	
2	D	17	
3	A	63	
3	B	63	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1767 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*TP\*CP\*AP\*CP\*AP\*CP\*GP\*TP\*GP\*GP\*GP\*AP\*CP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*TP\*AP\*GP\*TP\*CP\*CP\*CP\*AP\*CP\*GP\*TP\*GP\*TP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			

- Molecule 3 is a protein called PROTEIN (PHOSPHATE SYSTEM POSITIVE REGULATORY PROTEIN PHO4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	63	Total	C	N	O	S	0	0	0
			498	303	102	91	2			
3	B	63	Total	C	N	O	S	0	0	0
			498	303	102	91	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	ASP	CONFLICT	UNP P07270
A	19	ALA	PRO	CONFLICT	UNP P07270
B	0	MET	ASP	CONFLICT	UNP P07270
B	19	ALA	PRO	CONFLICT	UNP P07270

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	16	Total 16	O 16	0	0
4	C	18	Total 18	O 18	0	0
4	D	23	Total 23	O 23	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(\*CP\*TP\*CP\*AP\*CP\*AP\*CP\*GP\*TP\*GP\*GP\*GP\*AP\*CP\*TP\*AP\*G)-3')

Chain C: 

C1	T2	C3	A4	C5	A6	C7	G8	T9	G10	G11	G12	A13	C14	T15	A16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: DNA (5'-D(\*CP\*TP\*AP\*GP\*TP\*CP\*CP\*CP\*AP\*CP\*GP\*TP\*GP\*TP\*GP\*AP\*G)-3')

Chain D: 

C1	T2	A3	G4	T5	C6	C7	C8	A9	C10	G11	T12	G13	T14	G15	A16	G17
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: PROTEIN (PHOSPHATE SYSTEM POSITIVE REGULATORY PROTEIN PHO4)

Chain A: 

M0	K1	R2	E3	S4	H5	K6	H7	A8	E9	Q10	A11	R12	R13	N14	R15	L16	A17	V18	A19	L20	H21	E22	L23	A24	S25	L26	I27	P28	W31	K32	Q33	Q34	N35	A39	P40	S41	K42	A43	T44	T45	V46	E47	A48	A49	C50	R51	Y52	I53	R54	H55	L56	Q57	Q58	N59	G60	S61	T62
----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: PROTEIN (PHOSPHATE SYSTEM POSITIVE REGULATORY PROTEIN PHO4)

Chain B: 

M0	K1	R2	E3	S4	H5	K6	H7	A8	E9	Q10	A11	R12	R13	N14	R15	L16	A17	V18	A19	L20	H21	E22	L23	A24	S25	L26	I27	P28	A29	E30	W31	K32	Q33	Q34	N35	V36	S37	A38	A39	P40	S41	K42	A43	T44	T45	V46	E47	A48	A49	C50	R51	Y52	I53	R54	H55	L56	Q57	N59
----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

G60	S61	T62
-----	-----	-----

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.51Å 68.30Å 108.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	77.3 (8.00-2.80)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.230 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality i

### 5.1 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 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	C	0.73	0/388	0.92	1/597 (0.2%)
2	D	0.77	0/386	1.13	2/594 (0.3%)
3	A	0.69	0/506	0.94	0/680
3	B	0.63	0/506	1.06	1/680 (0.1%)
All	All	0.70	0/1786	1.02	4/2551 (0.2%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	DT	N1-C1'-C2'	-10.04	93.53	112.60
2	D	4	DG	N9-C1'-C2'	-8.94	95.61	112.60
3	B	27	ILE	N-CA-C	-5.38	96.49	111.00
1	C	12	DG	C3'-C2'-C1'	-5.10	96.38	102.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	346	0	192	134	0
2	D	345	0	193	129	0
3	A	498	0	503	111	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	498	0	503	153	0
4	A	23	0	0	4	0
4	B	16	0	0	2	0
4	C	18	0	0	2	0
4	D	23	0	0	2	0
All	All	1767	0	1391	456	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 148.

The worst 5 of 456 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:4:DA:C5'	3:B:39:ALA:HB2	1.75	1.15
1:C:8:DG:H3'	3:B:6:LYS:NZ	1.61	1.15
3:A:28:PRO:HG2	3:A:31:TRP:HB2	1.29	1.14
3:A:31:TRP:CZ3	3:A:34:GLN:HB2	1.89	1.07
1:C:4:DA:H5''	3:B:39:ALA:HB2	1.09	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	A	61/63 (97%)	40 (66%)	12 (20%)	9 (15%)	0	1
3	B	61/63 (97%)	27 (44%)	22 (36%)	12 (20%)	0	0
All	All	122/126 (97%)	67 (55%)	34 (28%)	21 (17%)	0	0

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	6	LYS
3	A	32	LYS
3	A	39	ALA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	A	56	LEU
3	B	1	LYS

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	A	51/51 (100%)	38 (74%)	13 (26%)	1	2
3	B	51/51 (100%)	32 (63%)	19 (37%)	0	0
All	All	102/102 (100%)	70 (69%)	32 (31%)	0	1

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	5	HIS
3	B	13	ARG
3	B	45	THR
3	B	12	ARG
3	B	14	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	55	HIS
3	B	55	HIS
3	A	59	ASN
3	A	34	GLN
3	A	57	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.