



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2017 – 08:05 pm GMT

PDB ID : 1A0A
Title : PHOSPHATE SYSTEM POSITIVE REGULATORY PROTEIN PHO4/DNA COMPLEX
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Deposited on : 1997-11-27
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

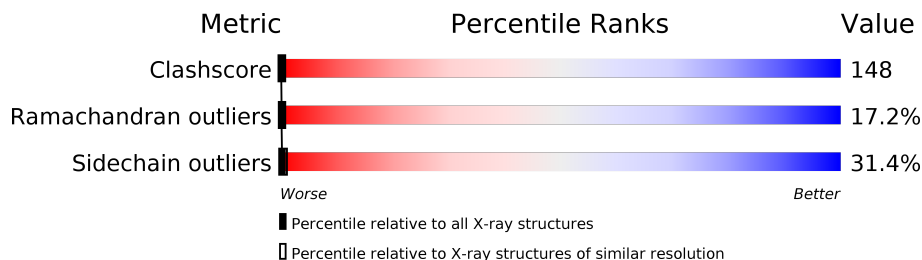
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

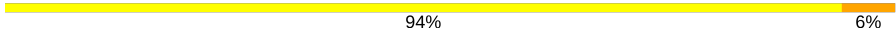



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 hydrogens and 0 are deuteriums.

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 the various outlier classes 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
M14
R15
L16
A17
V18
V19
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
M14
R15
L16
A17
V18
V19
L20
H21
E22
L23
A24
S25
L26
I27
P28
A29
E30
W31
K32
Q33
Q34
N35
Y36
S37
A38
A39
P40
S41
A42
A43
T44
T45
V46
E47
A48
A49
C50
R51
Y52
I53
R54
H55
L56
Q57
Q58
N59
G60
S61
T62

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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
3	B	498	0	503	153	0
4	A	23	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 148.

The worst 5 of 456 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 [i](#)

5.3.1 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 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	0
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

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Mol	Chain	Res	Type
3	A	32	LYS
3	A	39	ALA
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%)	0	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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.