

wwPDB X-ray Structure Validation Summary Report (i)

Jan 23, 2024 – 12:32 pm GMT

PDB ID : 8PQ7

Title: The Potato Late Blight pathogen (Phytophthora infestans) effector protein

Pi04134 in complex with potato protein phosphatase type 1c (PP1c).

Authors: Bentham, A.R.; Banfield, M.J.

Deposited on : 2023-07-10

Resolution : 2.10 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

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)
oteins) : Engh & Huber (2001)

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

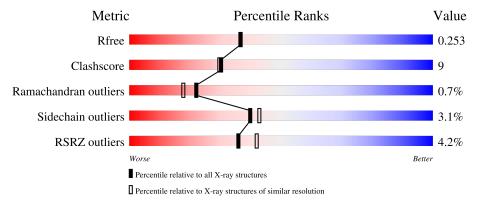
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% 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.

Mol	Chain	Length	Quality of chain					
1	A	295	79%	179	% ···			
1	С	295	76%	20%				
2	В	89	7% 67% 16%		15%			
2	D	89	79%	8%	13%			

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	303	-	-	X	X
4	EDO	С	303	-	-	X	-
4	EDO	С	304	-	-	X	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6116 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 protein called Serine/threonine-protein phosphatase.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	288	Total 2305	C 1477	N 385	O 426	S 17	0	0	0
1	С	289	Total 2312	C 1482	N 386	O 427	S 17	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP M1C5B8
A	2	PRO	-	expression tag	UNP M1C5B8
A	186	GLY	ASN	conflict	UNP M1C5B8
A	210	GLU	ASP	conflict	UNP M1C5B8
A	238	ASP	GLU	conflict	UNP M1C5B8
С	1	GLY	-	expression tag	UNP M1C5B8
С	2	PRO	-	expression tag	UNP M1C5B8
С	186	GLY	ASN	conflict	UNP M1C5B8
С	210	GLU	ASP	conflict	UNP M1C5B8
С	238	ASP	GLU	conflict	UNP M1C5B8

• Molecule 2 is a protein called RxLR effector protein PexRD24.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	76	Total	С	N	О	S	0	0	0
2	Ъ	70	632	411	109	110	2			
2	D	77	Total	С	N	О	S	0	0	0
2	ע	11	640	418	111	109	2	0	U	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	66	GLY	-	expression tag	UNP D0N0Z8
В	67	PRO	-	expression tag	UNP D0N0Z8

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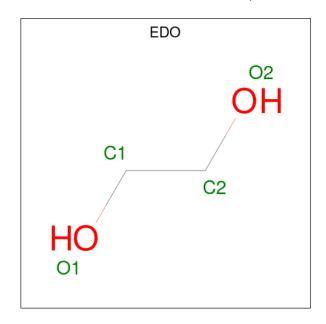
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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	GLY	-	expression tag	UNP D0N0Z8
D	67	PRO	-	expression tag	UNP D0N0Z8

• Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0
3	С	2	Total Mn 2 2	0	0

 \bullet Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0

 \bullet Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	75	Total O 75 75	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	26	Total O 26 26	0	0
5	С	79	Total O 79 79	0	0
5	D	31	Total O 31 31	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: Serine/threonine-protein phosphatase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	$55.49 { $	Donositon
a, b, c, α , β , γ	84.35° 86.49° 89.85°	Depositor
Resolution (Å)	58.62 - 2.10	Depositor
Resolution (A)	58.62 - 2.10	EDS
% Data completeness	97.4 (58.62-2.10)	Depositor
(in resolution range)	97.4 (58.62-2.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
D.D.	0.202 , 0.251	Depositor
R, R_{free}	0.212 , 0.253	DCC
R_{free} test set	1979 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 39.5	EDS
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6116	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	Chain Bond lengths Bo		Bo	ond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.48	0/2355	0.84	4/3185 (0.1%)	
1	С	0.49	0/2362	0.84	3/3195 (0.1%)	
2	В	0.53	0/645	0.84	1/861 (0.1%)	
2	D	0.46	0/653	0.75	0/871	
All	All	0.49	0/6015	0.84	8/8112 (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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	С	0	2
2	В	0	4
All	All	0	8

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	В	91	ARG	CG-CD-NE	-7.49	96.07	111.80
1	С	190	PRO	N-CA-C	-6.46	95.30	112.10
1	A	190	PRO	N-CA-C	-6.38	95.51	112.10
1	С	189	ARG	CA-CB-CG	-5.81	100.62	113.40
1	A	191	THR	CB-CA-C	-5.47	96.84	111.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	8	LEU	Peptide
2	В	104	ARG	Sidechain
2	В	126	GLY	Peptide
2	В	91	ARG	Sidechain

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	A	2305	0	2281	45	0
1	С	2312	0	2290	52	0
2	В	632	0	654	11	0
2	D	640	0	672	8	0
3	A	2	0	0	0	0
3	С	2	0	0	0	0
4	A	4	0	6	8	0
4	С	8	0	12	15	0
5	A	75	0	0	3	0
5	В	26	0	0	0	0
5	С	79	0	0	3	0
5	D	31	0	0	0	0
All	All	6116	0	5915	110	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 9.

The worst 5 of 110 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:A:189:ARG:O	1:A:191:THR:N	1.95	0.99
1:C:189:ARG:O	1:C:191:THR:N	1.95	0.99
1:C:273:GLU:OE2	5:C:401:HOH:O	1.86	0.93
1:A:189:ARG:O	1:A:190:PRO:C	2.09	0.88
1:C:189:ARG:O	1:C:190:PRO:C	2.09	0.88

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	Percent	tiles
1	A	$286/295 \ (97\%)$	268 (94%)	16 (6%)	2 (1%)	22	18
1	С	287/295 (97%)	267 (93%)	18 (6%)	2 (1%)	22	18
2	В	74/89 (83%)	70 (95%)	4 (5%)	0	100	100
2	D	75/89~(84%)	71 (95%)	3 (4%)	1 (1%)	12	7
All	All	$722/768 \; (94\%)$	676 (94%)	41 (6%)	5 (1%)	22	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
2	D	144	LYS
1	A	189	ARG
1	С	189	ARG
1	С	164	ASP

5.3.2 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 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
1	A	253/259 (98%)	246 (97%)	7 (3%)	43 47
1	\mathbf{C}	$254/259 \ (98\%)$	244 (96%)	10 (4%)	32 33
2	В	69/80 (86%)	67 (97%)	2 (3%)	42 46
2	D	70/80 (88%)	69 (99%)	1 (1%)	67 73
All	All	646/678 (95%)	626 (97%)	20 (3%)	40 43



5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	145	ARG
1	С	244	ARG
2	D	143	ASN
1	С	285	GLU
1	A	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	180	HIS
2	D	135	ASN
2	В	117	ASN
2	В	120	ASN
2	В	135	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Dec	Res Link	Bond lengths			Bond angles		
MIOI	туре	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	303	-	3,3,3	0.34	0	2,2,2	0.78	0
4	EDO	С	303	-	3,3,3	0.52	0	2,2,2	0.70	0
4	EDO	С	304	-	3,3,3	0.18	0	2,2,2	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	С	303	-	=	1/1/1/1	-
4	EDO	С	304	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	EDO	O1-C1-C2-O2
4	С	304	EDO	O1-C1-C2-O2
4	С	303	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	EDO	8	0
4	С	303	EDO	6	0
4	С	304	EDO	9	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	$288/295 \ (97\%)$	0.06	11 (3%) 40 46	16, 35, 74, 133	0
1	С	289/295~(97%)	0.05	7 (2%) 59 64	17, 35, 72, 145	0
2	В	76/89 (85%)	0.28	6 (7%) 12 16	22, 43, 76, 100	0
2	D	77/89 (86%)	0.31	7 (9%) 9 12	19, 40, 84, 113	0
All	All	730/768 (95%)	0.10	31 (4%) 36 42	16, 37, 76, 145	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	26	VAL	13.2
1	A	26	VAL	9.7
2	D	145	VAL	7.6
2	В	68	ASP	6.6
2	D	69	LEU	4.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	EDO	A	303	4/4	0.73	0.90	60,68,68,83	0
4	EDO	С	304	4/4	0.77	0.60	64,67,70,74	0
3	MN	A	301	1/1	0.83	0.10	103,103,103,103	0
3	MN	С	302	1/1	0.92	0.12	93,93,93,93	0
3	MN	A	302	1/1	0.93	0.11	83,83,83,83	0
4	EDO	С	303	4/4	0.96	0.36	27,31,31,39	0
3	MN	C	301	1/1	0.96	0.14	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.

