



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2025 – 04:11 pm BST

PDB ID : 9RDC / pdb_00009rdc
Title : Crystal structure of Phytophthora infestans effector AVRcap1b in complex with the ENTH domain of Nicotiana benthamiana NbTOL9a protein
Authors : Contreras, M.P.; Madhuprakash, J.; Lawson, D.M.; Kamoun, S.
Deposited on : 2025-06-02
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

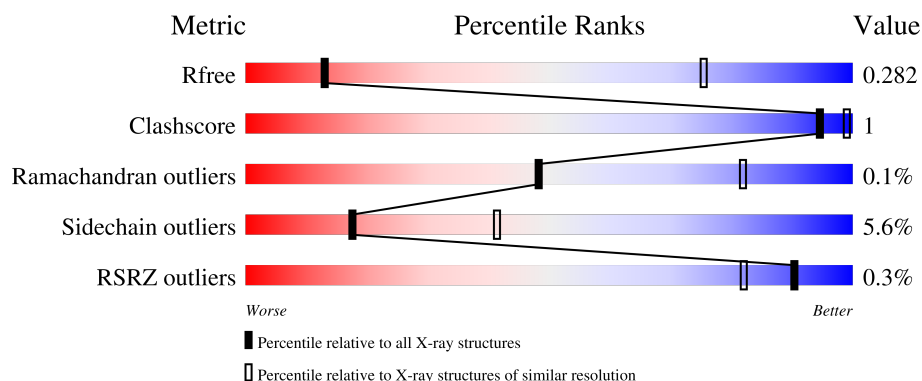
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

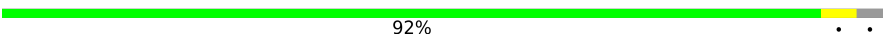



The reported resolution of this entry is 4.10 Å.

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1145 (4.40-3.80)
Clashscore	180529	1211 (4.40-3.80)
Ramachandran outliers	177936	1140 (4.40-3.80)
Sidechain outliers	177891	1127 (4.40-3.80)
RSRZ outliers	164620	1143 (4.40-3.80)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	619	 92% . .
1	B	619	 89% 6% . .
2	C	150	 83% 7% .. 8%
2	D	150	 82% 7% . 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11839 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 RxLR effector protein PITG_16705.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4832	3104	815	901	12			
1	B	598	Total	C	N	O	S	0	0	0
			4832	3104	815	901	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLY	-	expression tag	UNP D0NVF3
A	61	PRO	-	expression tag	UNP D0NVF3
B	60	GLY	-	expression tag	UNP D0NVF3
B	61	PRO	-	expression tag	UNP D0NVF3

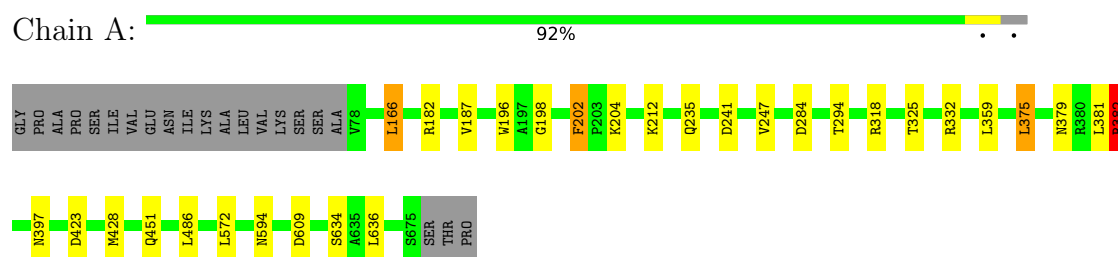
- Molecule 2 is a protein called Target of myb protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1095	701	192	193	9			
2	D	136	Total	C	N	O	S	0	0	0
			1080	691	190	191	8			

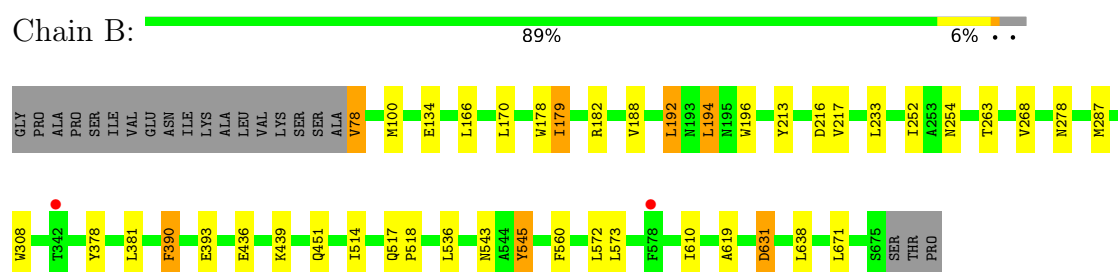
3 Residue-property plots [i](#)

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.

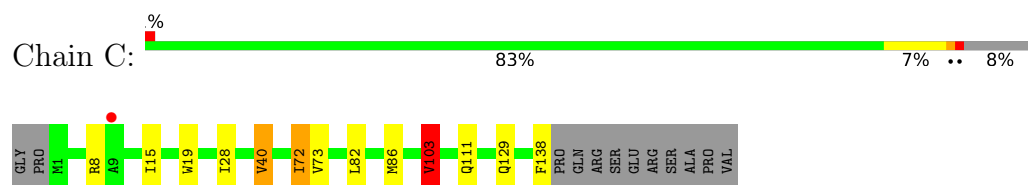
- Molecule 1: RxLR effector protein PITG_16705



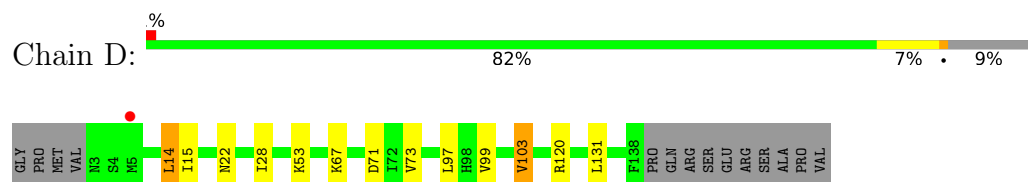
- Molecule 1: RxLR effector protein PITG_16705



- Molecule 2: Target of myb protein 1



- Molecule 2: Target of myb protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.87Å 136.91Å 195.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.57 – 4.10 79.57 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.57-4.10) 99.7 (79.57-4.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.248 , 0.286 0.248 , 0.282	Depositor DCC
R_{free} test set	939 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	238.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 311.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11839	wwPDB-VP
Average B, all atoms (Å ²)	276.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	A	0.52	0/4948	1.11	5/6702 (0.1%)
1	B	0.52	0/4948	1.10	4/6702 (0.1%)
2	C	0.54	0/1115	1.16	3/1504 (0.2%)
2	D	0.51	0/1100	1.15	4/1484 (0.3%)
All	All	0.52	0/12111	1.11	16/16392 (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 outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	103	VAL	N-CA-CB	7.76	119.63	110.55
1	A	202	PHE	CA-CB-CG	7.66	121.45	113.80
1	A	241	ASP	CA-CB-CG	7.14	119.74	112.60
1	B	631	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	382	ARG	CB-CA-C	-6.76	99.19	110.68
2	C	103	VAL	N-CA-CB	6.48	118.14	110.55
1	B	216	ASP	CA-CB-CG	5.94	118.54	112.60
2	C	40	VAL	N-CA-CB	5.86	118.51	110.54
2	D	99	VAL	N-CA-CB	5.63	117.13	110.55
1	B	560	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	166	LEU	N-CA-CB	5.60	118.19	110.07
1	A	284	ASP	CA-CB-CG	5.50	118.11	112.60
1	B	263	THR	CA-CB-OG1	-5.38	101.53	109.60
2	D	14	LEU	CB-CA-C	5.11	118.13	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	71	ASP	CA-CB-CG	5.07	117.67	112.60
2	C	72	ILE	CB-CA-C	-5.05	105.42	112.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain

5.2 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 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	4832	0	4826	9	1
1	B	4832	0	4826	18	1
2	C	1095	0	1140	1	0
2	D	1080	0	1119	0	0
All	All	11839	0	11911	28	1

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 (28) 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:B:179:ILE:CD1	1:B:213:TYR:CE1	2.22	1.23
1:A:379:ASN:OD1	1:A:382:ARG:NH2	1.78	1.14
1:B:179:ILE:HD11	1:B:213:TYR:CD1	1.88	1.07
1:B:179:ILE:HD12	1:B:213:TYR:CE1	1.95	0.98
1:B:179:ILE:CD1	1:B:213:TYR:CD1	2.47	0.97
1:A:379:ASN:HA	1:A:382:ARG:NH2	1.84	0.91
1:B:179:ILE:HD13	1:B:213:TYR:CE1	2.17	0.78
1:B:178:TRP:HB3	1:B:213:TYR:OH	1.84	0.76
1:B:188:VAL:HG21	1:B:213:TYR:CE2	2.28	0.68
1:A:379:ASN:CG	1:A:382:ARG:HH22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASN:HA	1:A:382:ARG:CZ	2.24	0.66
1:B:78:VAL:HG12	1:B:100:MET:HE1	1.81	0.62
1:B:179:ILE:CD1	1:B:213:TYR:HE1	2.07	0.60
2:C:86:MET:HE2	2:C:103:VAL:HG23	1.86	0.58
1:B:179:ILE:HD13	1:B:213:TYR:HE1	1.64	0.57
1:B:381:LEU:HD11	1:B:390:PHE:CD1	2.39	0.57
1:A:379:ASN:CA	1:A:382:ARG:NH2	2.67	0.53
1:A:379:ASN:OD1	1:A:382:ARG:CZ	2.55	0.50
1:B:517:GLN:HB3	1:B:518:PRO:HD2	1.94	0.50
1:B:192:LEU:HB3	1:B:194:LEU:HD13	1.95	0.48
1:A:375:LEU:HD23	1:A:375:LEU:H	1.80	0.47
1:B:179:ILE:HD12	1:B:213:TYR:CZ	2.46	0.46
1:B:252:ILE:HD11	1:B:268:VAL:HG12	1.99	0.45
1:B:287:MET:HA	1:B:308:TRP:CD1	2.53	0.43
1:A:451:GLN:CG	1:A:486:LEU:HD21	2.49	0.43
1:A:451:GLN:HG2	1:A:486:LEU:HD21	2.01	0.42
1:B:179:ILE:HA	1:B:217:VAL:HG22	2.02	0.41
1:B:573:LEU:HD12	1:B:619:ALA:CB	2.51	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ASN:ND2	1:B:278:ASN:O[3_644]	2.12	0.08

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
1	A	596/619 (96%)	579 (97%)	16 (3%)	1 (0%)	44 77
1	B	596/619 (96%)	584 (98%)	11 (2%)	1 (0%)	44 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	136/150 (91%)	136 (100%)	0	0	100	100
2	D	134/150 (89%)	134 (100%)	0	0	100	100
All	All	1462/1538 (95%)	1433 (98%)	27 (2%)	2 (0%)	48	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	TYR
1	A	198	GLY

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	
1	A	523/540 (97%)	500 (96%)	23 (4%)	24	47
1	B	523/540 (97%)	497 (95%)	26 (5%)	20	44
2	C	120/130 (92%)	108 (90%)	12 (10%)	6	23
2	D	118/130 (91%)	107 (91%)	11 (9%)	7	25
All	All	1284/1340 (96%)	1212 (94%)	72 (6%)	17	41

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	182	ARG
1	A	187	VAL
1	A	196	TRP
1	A	202	PHE
1	A	204	LYS
1	A	212	LYS
1	A	235	GLN
1	A	247	VAL
1	A	294	THR

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Mol	Chain	Res	Type
1	A	318	ARG
1	A	325	THR
1	A	332	ARG
1	A	359	LEU
1	A	375	LEU
1	A	381	LEU
1	A	397	ASN
1	A	423	ASP
1	A	428	MET
1	A	572	LEU
1	A	609	ASP
1	A	634	SER
1	A	636	LEU
1	B	78	VAL
1	B	134	GLU
1	B	166	LEU
1	B	170	LEU
1	B	179	ILE
1	B	182	ARG
1	B	192	LEU
1	B	194	LEU
1	B	196	TRP
1	B	233	LEU
1	B	254	ASN
1	B	378	TYR
1	B	390	PHE
1	B	393	GLU
1	B	436	GLU
1	B	439	LYS
1	B	451	GLN
1	B	514	ILE
1	B	536	LEU
1	B	543	ASN
1	B	545	TYR
1	B	572	LEU
1	B	610	ILE
1	B	631	ASP
1	B	638	LEU
1	B	671	LEU
2	C	8	ARG
2	C	15	ILE
2	C	19	TRP

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Mol	Chain	Res	Type
2	C	28	ILE
2	C	40	VAL
2	C	72	ILE
2	C	73	VAL
2	C	82	LEU
2	C	103	VAL
2	C	111	GLN
2	C	129	GLN
2	C	138	PHE
2	D	14	LEU
2	D	15	ILE
2	D	22	ASN
2	D	28	ILE
2	D	53	LYS
2	D	67	LYS
2	D	73	VAL
2	D	97	LEU
2	D	103	VAL
2	D	120	ARG
2	D	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	112	HIS
1	A	235	GLN
1	A	360	GLN
1	A	495	GLN
1	B	379	ASN
1	B	594	ASN
2	C	35	GLN
2	C	111	GLN
2	C	129	GLN
2	D	35	GLN
2	D	129	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 oligosaccharides 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 [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, 95th 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	598/619 (96%)	-0.69	0 100 100	171, 245, 347, 410	0
1	B	598/619 (96%)	-0.70	2 (0%) 90 82	192, 297, 398, 463	0
2	C	138/150 (92%)	-0.45	1 (0%) 84 71	166, 234, 300, 324	0
2	D	136/150 (90%)	-0.67	1 (0%) 84 71	227, 317, 387, 413	0
All	All	1470/1538 (95%)	-0.67	4 (0%) 90 82	166, 265, 380, 463	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.6
2	D	5	MET	2.6
1	B	578	PHE	2.4
2	C	9	ALA	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.