

Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:24 PM EDT

PDB ID	:	5OTA
Title	:	Structure of the periplasmic binding protein (PBP) NocT from Agrobacterium
		tumefaciens C58 in complex with octopinic acid
Authors	:	Vigouroux, A.; Morera, S.
Deposited on	:	2017-08-21
Resolution	:	2.10 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 (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:

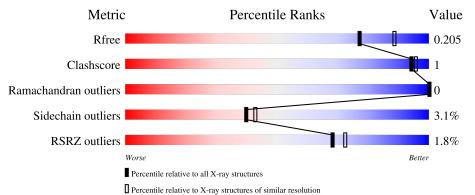
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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	А	265	91%	5% •				
1	В	265	3% 	6% •				



50TA

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4161 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	254	Total	С	Ν	0	\mathbf{S}	0	1	0
		204	1954	1252	318	371	13	0	1	0
1	Р	254	Total	С	Ν	0	S	0	0	0
	I B	204	1949	1248	318	371	12	0	U	U

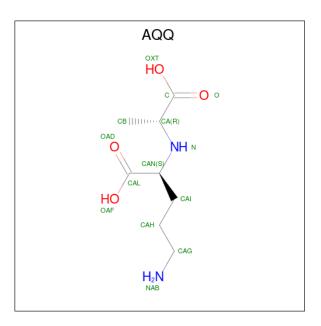
• Molecule 1 is a protein called Nopaline-binding periplasmic protein.

		Actual	$\operatorname{Comment}$	Reference
25	MET	-	initiating methionine	UNP P35120
284	HIS	-	expression tag	UNP P35120
285	HIS	-	expression tag	UNP P35120
286	HIS	-	expression tag	UNP P35120
287	HIS	-	expression tag	UNP P35120
288	HIS	-	expression tag	UNP P35120
289	HIS	-	expression tag	UNP P35120
25	MET	-	initiating methionine	UNP P35120
284	HIS	-	expression tag	UNP P35120
285	HIS	-	expression tag	UNP P35120
286	HIS	-	expression tag	UNP P35120
287	HIS	-	expression tag	UNP P35120
288	HIS	-	expression tag	UNP P35120
289	HIS	-	expression tag	UNP P35120
	284 285 286 287 288 289 25 284 285 286 286 287 288	284 HIS 285 HIS 286 HIS 287 HIS 288 HIS 289 HIS 25 MET 284 HIS 285 HIS 286 HIS 286 HIS 286 HIS 287 HIS 288 HIS	284 HIS - 285 HIS - 286 HIS - 287 HIS - 288 HIS - 289 HIS - 25 MET - 284 HIS - 284 HIS - 285 HIS - 286 HIS - 286 HIS - 287 HIS - 288 HIS -	284HIS-expression tag285HIS-expression tag286HIS-expression tag287HIS-expression tag288HIS-expression tag289HIS-expression tag25MET-initiating methionine284HIS-expression tag285HIS-expression tag286HIS-expression tag287HIS-expression tag288HIS-expression tag

There are 14 discrepancies between the modelled and reference sequences:

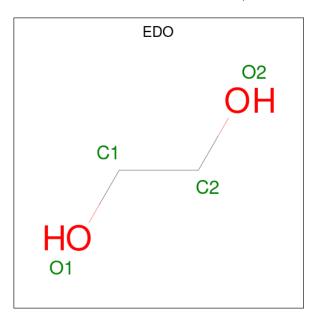
• Molecule 2 is (2 {S})-5-azanyl-2-[[(2 {R})-1-oxidanyl-1-oxidanylidene-propan-2-yl]amino]pe ntanoic acid (three-letter code: AQQ) (formula: $C_8H_{16}N_2O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 14			0 4	0	0
2	В	1	Total 14	C 8	N 2	0 4	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0



• Molecule 4 is water.

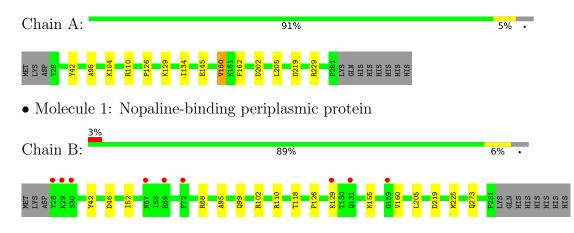
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	151	Total O 151 151	0	0
4	В	71	Total O 71 71	0	0



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: Nopaline-binding periplasmic protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	115.23Å 115.23Å 37.84Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.17 - 2.10	Depositor
Resolution (A)	37.72 - 2.10	EDS
% Data completeness	100.0 (19.17-2.10)	Depositor
(in resolution range)	99.7(37.72-2.10)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 2.10 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
D D	0.177 , 0.205	Depositor
R, R_{free}	0.178 , 0.205	DCC
R_{free} test set	1643 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	34.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 42.2	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
	0.025 for -h,-k,l	
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
	0.016 for -k,-h,-l	
F_o, F_c correlation	0.96	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: EDO, AQQ

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.51	0/1995	0.64	0/2693	
1	В	0.47	0/1987	0.63	0/2683	
All	All	0.49	0/3982	0.63	0/5376	

There are no bond length outliers.

There are no bond angle outliers.

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	А	1954	0	1975	5	0
1	В	1949	0	1966	5	0
2	А	14	0	0	0	0
2	В	14	0	0	0	0
3	А	8	0	12	1	0
4	А	151	0	0	0	0
4	В	71	0	0	0	0
All	All	4161	0	3953	10	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 1.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG21	1:B:225:MET:HE3	1.79	0.65
1:A:104:LYS:HD2	3:A:303:EDO:H12	1.90	0.53
1:A:134:ILE:HD11	1:A:145:GLU:HG2	1.96	0.47
1:B:126:PRO:O	1:B:129:LYS:HG2	2.16	0.46
1:A:126:PRO:O	1:A:129:LYS:HG2	2.17	0.45
1:B:99:GLN:HE21	1:B:102:ARG:CZ	2.32	0.42
1:A:42:TYR:CG	1:A:95:ALA:HB2	2.55	0.41
1:B:46:ASP:HB3	1:B:52:ILE:HD13	2.03	0.41
1:A:160:VAL:HG13	1:A:202:ASP:HB2	2.04	0.41
1:B:42:TYR:CG	1:B:95:ALA:HB2	2.56	0.40

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Perce	\mathbf{ntiles}
1	А	253/265~(96%)	249~(98%)	4(2%)	0	100	100
1	В	252/265~(95%)	246~(98%)	6(2%)	0	100	100
All	All	505/530~(95%)	495 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	209/219~(95%)	203~(97%)	6 (3%)	42 46		
1	В	208/219~(95%)	201 (97%)	7 (3%)	37 39		
All	All	417/438~(95%)	404 (97%)	13 (3%)	40 43		

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	110	ARG
1	А	160	VAL
1	А	162	PHE
1	А	205	LEU
1	А	219	ASP
1	А	229	ARG
1	В	88	ARG
1	В	110	ARG
1	В	155	LYS
1	В	160	VAL
1	В	205	LEU
1	В	219	ASP
1	В	273	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	99	GLN

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)

4 ligands are modelled in this entry.

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).

Mal	Mol Type Chain	Chain	Res	Tink	Link Bond lengths				Bond angles		
NIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	AQQ	А	301	-	$13,\!13,\!13$	0.96	1 (7%)	$14,\!16,\!16$	1.42	4 (28%)	
3	EDO	А	302	-	3,3,3	0.61	0	2,2,2	0.21	0	
3	EDO	А	303	-	3,3,3	0.70	0	2,2,2	0.37	0	
2	AQQ	В	301	-	$13,\!13,\!13$	0.91	0	$14,\!16,\!16$	1.13	2 (14%)	

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
2	AQQ	А	301	-	-	1/16/16/16	-
3	EDO	А	302	-	-	1/1/1/1	-
3	EDO	А	303	-	-	1/1/1/1	-
2	AQQ	В	301	-	-	3/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	301	AQQ	CA-C	2.13	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	301	AQQ	OAF-CAL-CAN	2.55	121.86	113.40
2	А	301	AQQ	OAF-CAL-OAD	-2.50	118.41	124.09
2	А	301	AQQ	OXT-C-O	-2.32	118.81	124.09
2	В	301	AQQ	OAF-CAL-OAD	-2.27	118.94	124.09
2	В	301	AQQ	OAF-CAL-CAN	2.20	120.73	113.40
2	А	301	AQQ	OXT-C-CA	2.15	121.51	114.13



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	301	AQQ	CAL-CAN-N-CA
2	В	301	AQQ	CAL-CAN-N-CA
3	А	303	EDO	O1-C1-C2-O2
3	А	302	EDO	O1-C1-C2-O2
2	В	301	AQQ	CAH-CAI-CAN-CAL
2	В	301	AQQ	CAH-CAI-CAN-N

All (6) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	303	EDO	1	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	А	254/265~(95%)	-0.18	0 100 100	23, 32, 50, 70	0
1	В	254/265~(95%)	-0.01	9 (3%) 44 50	30, 43, 66, 92	0
All	All	508/530~(95%)	-0.09	9 (1%) 68 72	23, 38, 61, 92	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	159	GLY	3.4	
1	В	67	ASN	2.6	
1	В	28	TYR	2.5	
1	В	30	SER	2.4	
1	В	129	LYS	2.4	
1	В	69	GLU	2.2	
1	В	29	LYS	2.2	
1	В	131	GLN	2.1	
1	В	72	PHE	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 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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
3	EDO	А	303	4/4	0.72	0.28	$50,\!53,\!54,\!54$	0
3	EDO	А	302	4/4	0.91	0.22	56, 56, 57, 57	0
2	AQQ	А	301	14/14	0.97	0.12	22,26,28,29	0
2	AQQ	В	301	14/14	0.97	0.10	29,34,38,39	0

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.

6.5 Other polymers (i)

There are no such residues in this entry.

