wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 07:59 AM EDT

PDB ID	:	5VQM
Title	:	Clostridium difficile TcdB-GTD bound to PA41 Fab
Authors	:	Kroh, H.K.; Spiller, B.W.; Lacy, D.B.
Deposited on	:	2017-05-09
Resolution	:	2.79 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 (i)) were used in the production of this report:

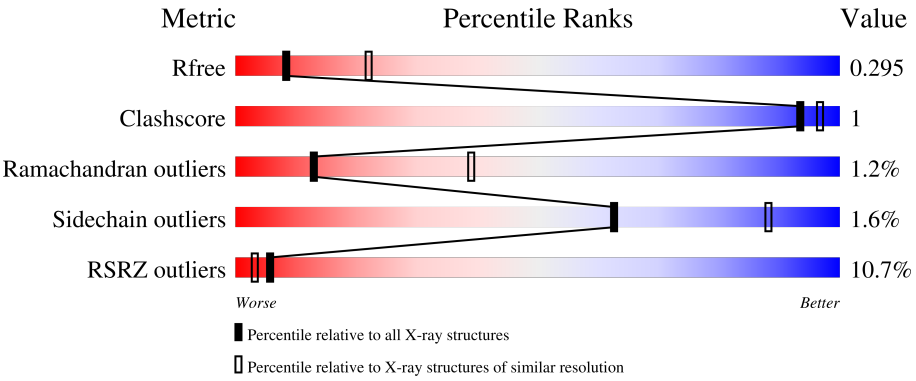
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	557	5% 92% · 5%
1	B	557	5% 90% · 5%
2	C	214	17% 91% 9%
2	L	214	14% 96% · ·
3	D	222	18% 86% 11% ·

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Mol	Chain	Length	Quality of chain
3	H	222	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30126 atoms, of which 14828 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 Toxin B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	528	Total	C	H	N	O	S	0	0	0
			8494	2726	4197	697	859	15			
1	B	528	Total	C	H	N	O	S	0	0	0
			8494	2726	4197	697	859	15			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	HIS	-	expression tag	UNP C9YJ35
A	546	ALA	-	expression tag	UNP C9YJ35
A	547	GLY	-	expression tag	UNP C9YJ35
A	548	LEU	-	expression tag	UNP C9YJ35
A	549	ARG	-	expression tag	UNP C9YJ35
A	550	GLY	-	expression tag	UNP C9YJ35
A	551	SER	-	expression tag	UNP C9YJ35
A	552	HIS	-	expression tag	UNP C9YJ35
A	553	HIS	-	expression tag	UNP C9YJ35
A	554	HIS	-	expression tag	UNP C9YJ35
A	555	HIS	-	expression tag	UNP C9YJ35
A	556	HIS	-	expression tag	UNP C9YJ35
A	557	HIS	-	expression tag	UNP C9YJ35
B	545	HIS	-	expression tag	UNP C9YJ35
B	546	ALA	-	expression tag	UNP C9YJ35
B	547	GLY	-	expression tag	UNP C9YJ35
B	548	LEU	-	expression tag	UNP C9YJ35
B	549	ARG	-	expression tag	UNP C9YJ35
B	550	GLY	-	expression tag	UNP C9YJ35
B	551	SER	-	expression tag	UNP C9YJ35
B	552	HIS	-	expression tag	UNP C9YJ35
B	553	HIS	-	expression tag	UNP C9YJ35
B	554	HIS	-	expression tag	UNP C9YJ35
B	555	HIS	-	expression tag	UNP C9YJ35
B	556	HIS	-	expression tag	UNP C9YJ35

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Chain	Residue	Modelled	Actual	Comment	Reference
B	557	HIS	-	expression tag	UNP C9YJ35

- Molecule 2 is a protein called PA41 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	214	Total	C	H	N	O	S	0	0	0
			3250	1033	1605	277	330	5			
2	C	214	Total	C	H	N	O	S	0	0	0
			3241	1033	1596	277	330	5			

- Molecule 3 is a protein called PA41 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	216	Total	C	H	N	O	S	0	0	0
			3250	1035	1616	275	317	7			
3	D	216	Total	C	H	N	O	S	0	0	0
			3251	1035	1617	275	317	7			

- Molecule 4 is water.

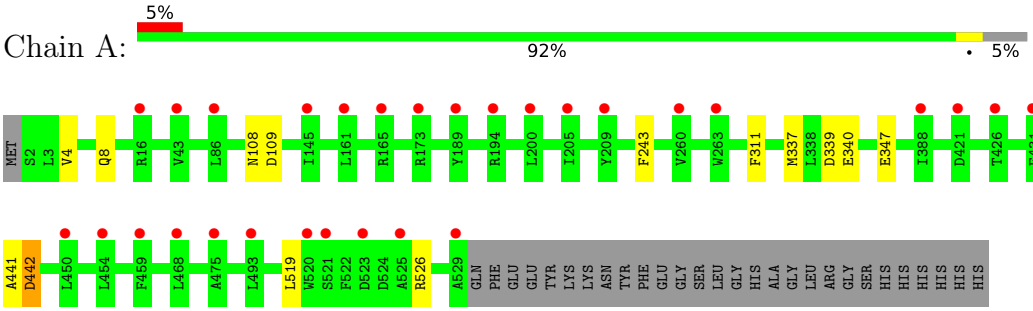
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	L	14	Total	O	0	0
			14	14		
4	H	14	Total	O	0	0
			14	14		
4	B	57	Total	O	0	0
			57	57		
4	C	11	Total	O	0	0
			11	11		
4	D	9	Total	O	0	0
			9	9		

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.

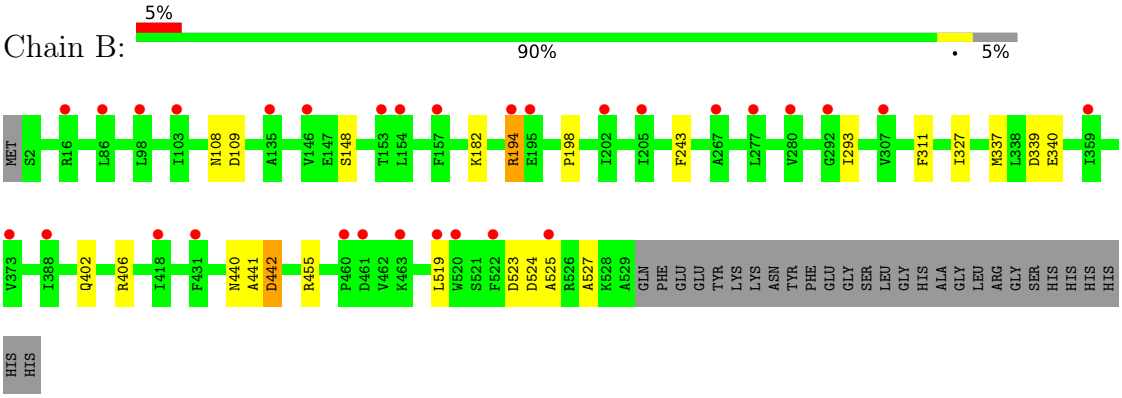
• Molecule 1: Toxin B

Chain A:



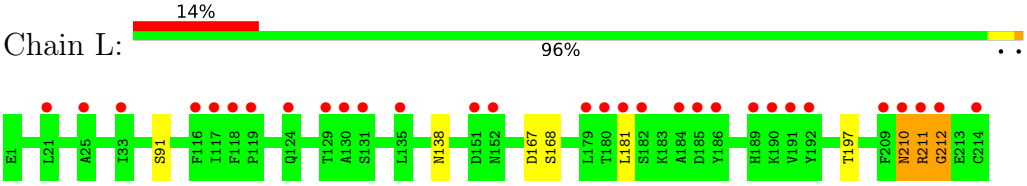
• Molecule 1: Toxin B

Chain B:



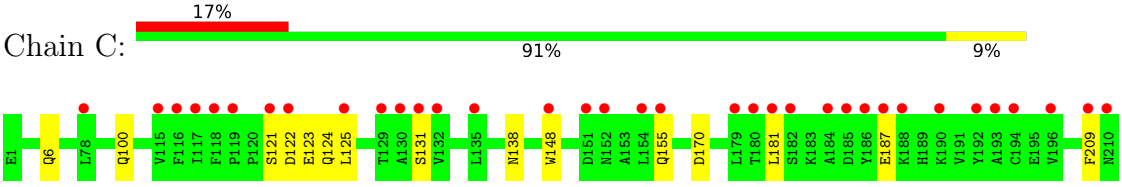
• Molecule 2: PA41 FAB LIGHT CHAIN

Chain L:



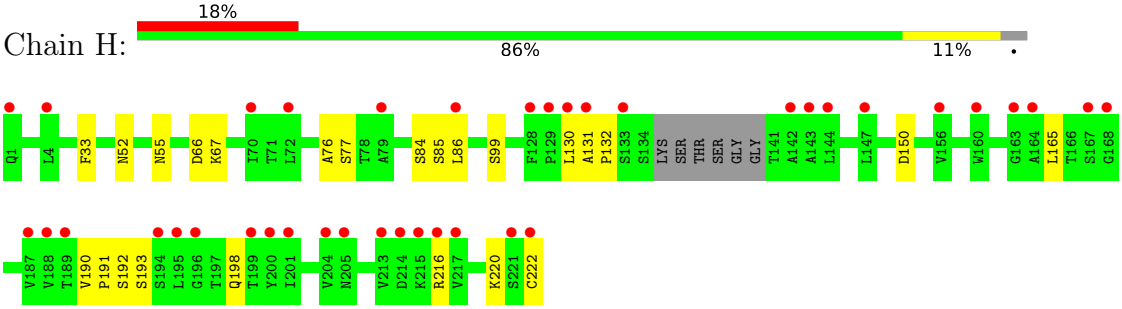
• Molecule 2: PA41 FAB LIGHT CHAIN

Chain C:



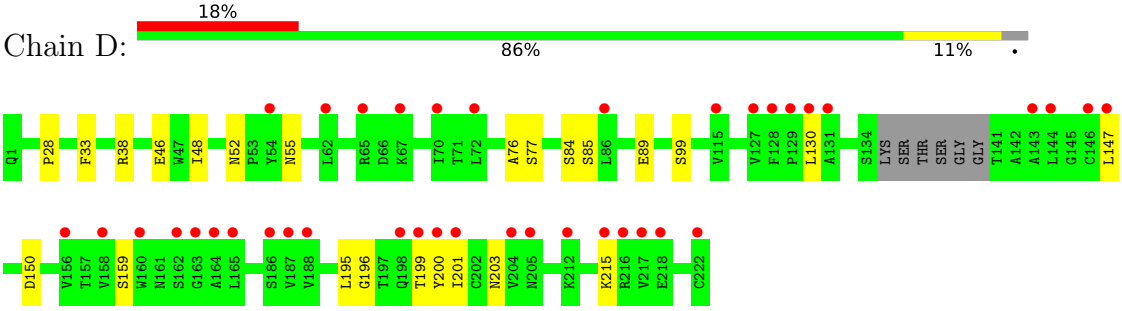
• Molecule 3: PA41 FAB HEAVY CHAIN

Chain H:



• Molecule 3: PA41 FAB HEAVY CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.13Å 251.74Å 224.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.85 – 2.79 60.85 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.85-2.79) 99.9 (60.85-2.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.240 , 0.292 0.240 , 0.295	Depositor DCC
R_{free} test set	2503 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30126	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0281e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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	0.24	0/4374	0.38	0/5905
1	B	0.24	0/4374	0.38	0/5905
2	C	0.26	0/1682	0.44	0/2283
2	L	0.25	0/1682	0.45	0/2283
3	D	0.25	0/1674	0.44	0/2283
3	H	0.25	0/1674	0.45	0/2283
All	All	0.25	0/15460	0.41	0/20942

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

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	4297	4197	4197	8	0
1	B	4297	4197	4197	12	0
2	C	1645	1596	1605	8	0
2	L	1645	1605	1605	3	0
3	D	1634	1617	1617	6	0
3	H	1634	1616	1617	8	0
4	A	41	0	0	0	0
4	B	57	0	0	1	0
4	C	11	0	0	0	0
4	D	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	14	0	0	0	0
4	L	14	0	0	0	0
All	All	15298	14828	14838	41	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.

The worst 5 of 41 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:523:ASP:O	1:B:525:ALA:N	2.25	0.70
2:L:210:ASN:O	2:L:212:GLY:N	2.29	0.65
2:C:121:SER:O	2:C:125:LEU:HG	1.97	0.64
3:H:66:ASP:OD2	1:B:455:ARG:NH1	2.32	0.61
1:B:402:GLN:OE1	1:B:406:ARG:NH1	2.34	0.59

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
1	A	526/557 (94%)	498 (95%)	26 (5%)	2 (0%)	34 66
1	B	526/557 (94%)	499 (95%)	23 (4%)	4 (1%)	19 49
2	C	212/214 (99%)	200 (94%)	10 (5%)	2 (1%)	17 46
2	L	212/214 (99%)	198 (93%)	11 (5%)	3 (1%)	11 34
3	D	212/222 (96%)	188 (89%)	17 (8%)	7 (3%)	4 13
3	H	212/222 (96%)	178 (84%)	30 (14%)	4 (2%)	8 26
All	All	1900/1986 (96%)	1761 (93%)	117 (6%)	22 (1%)	13 39

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	211	ARG
3	H	85	SER
3	H	130	LEU
1	B	524	ASP
1	A	441	ALA

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	481/505 (95%)	478 (99%)	3 (1%)	86	96
1	B	481/505 (95%)	477 (99%)	4 (1%)	81	94
2	C	187/187 (100%)	183 (98%)	4 (2%)	53	84
2	L	187/187 (100%)	183 (98%)	4 (2%)	53	84
3	D	186/190 (98%)	181 (97%)	5 (3%)	44	78
3	H	186/190 (98%)	179 (96%)	7 (4%)	33	67
All	All	1708/1764 (97%)	1681 (98%)	27 (2%)	62	88

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	194	ARG
1	B	519	LEU
3	D	147	LEU
1	B	327	ILE
2	C	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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

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	528/557 (94%)	0.68	30 (5%) 23 15	43, 80, 126, 155	0
1	B	528/557 (94%)	0.68	30 (5%) 23 15	50, 81, 138, 195	0
2	C	214/214 (100%)	1.09	37 (17%) 1 1	50, 79, 144, 177	0
2	L	214/214 (100%)	0.87	30 (14%) 2 1	46, 77, 135, 161	0
3	D	216/222 (97%)	1.15	39 (18%) 1 1	59, 107, 163, 192	0
3	H	216/222 (97%)	1.17	39 (18%) 1 1	45, 90, 153, 190	0
All	All	1916/1986 (96%)	0.85	205 (10%) 6 3	43, 83, 142, 195	0

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	181	LEU	7.5
3	H	188	VAL	6.6
3	H	164	ALA	6.4
2	C	130	ALA	6.4
3	H	200	TYR	6.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.