W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 12:27 pm GMT

PDB ID	:	5L6L
Title	:	Structure of Caulobacter crescentus VapBC1 bound to operator DNA
Authors	:	Bendtsen, K.L.; Xu, K.; Luckmann, M.; Brodersen, D.E.
Deposited on	:	2016-05-30
Resolution	:	2.70 Å(reported)

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

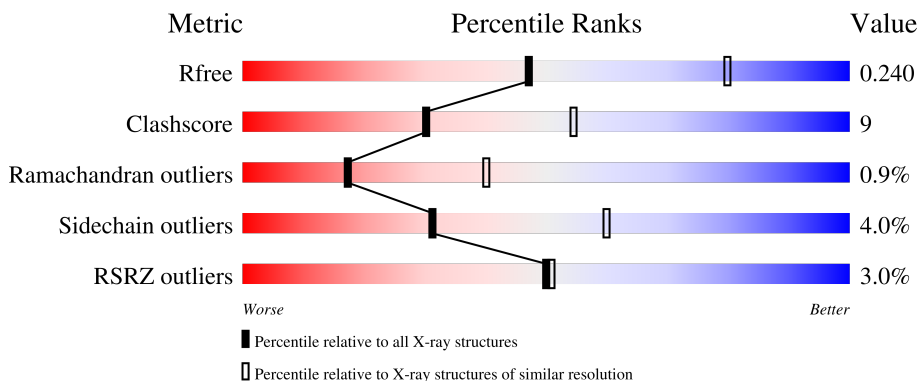|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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.
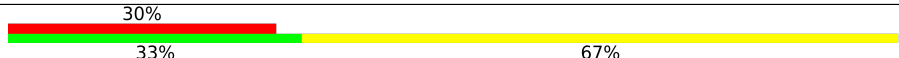
Metric	Percentile Ranks	Value
Rfree		0.240
Clashscore		9
Ramachandran outliers		0.9%
Sidechain outliers		4.0%
RSRZ outliers		3.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
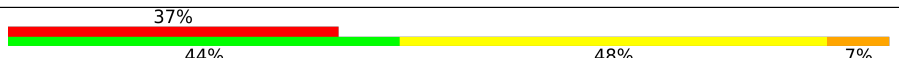
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	85	2% · 68% · 8% · 24%
1	D	85	2% · 80% · 15% · · ·
1	E	85	62% · 12% · · 25%
1	H	85	4% · 71% · 16% · 7% · 5%
2	B	128	76% · 23% · ·

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Mol	Chain	Length	Quality of chain
2	C	128	88% 10%
2	F	128	77% 20%
2	G	128	86% 13%
3	M	27	30% / 33% 67%
4	N	27	37% / 44% 48% 7%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7441 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 VapB family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	Se	0	0	0
			491	304	92	94	1			
1	D	84	Total	C	N	O	Se	0	0	0
			656	407	125	123	1			
1	E	64	Total	C	N	O	Se	0	0	0
			485	301	91	92	1			
1	H	81	Total	C	N	O	Se	0	0	0
			628	389	118	120	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MSE	-	initiating methionine	UNP Q9AC34
A	-4	HIS	-	expression tag	UNP Q9AC34
A	-3	HIS	-	expression tag	UNP Q9AC34
A	-2	HIS	-	expression tag	UNP Q9AC34
A	-1	HIS	-	expression tag	UNP Q9AC34
A	0	HIS	-	expression tag	UNP Q9AC34
A	1	HIS	-	expression tag	UNP Q9AC34
D	-5	MSE	-	initiating methionine	UNP Q9AC34
D	-4	HIS	-	expression tag	UNP Q9AC34
D	-3	HIS	-	expression tag	UNP Q9AC34
D	-2	HIS	-	expression tag	UNP Q9AC34
D	-1	HIS	-	expression tag	UNP Q9AC34
D	0	HIS	-	expression tag	UNP Q9AC34
D	1	HIS	-	expression tag	UNP Q9AC34
E	-5	MSE	-	initiating methionine	UNP Q9AC34
E	-4	HIS	-	expression tag	UNP Q9AC34
E	-3	HIS	-	expression tag	UNP Q9AC34
E	-2	HIS	-	expression tag	UNP Q9AC34
E	-1	HIS	-	expression tag	UNP Q9AC34
E	0	HIS	-	expression tag	UNP Q9AC34
E	1	HIS	-	expression tag	UNP Q9AC34

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MSE	-	initiating methionine	UNP Q9AC34
H	-4	HIS	-	expression tag	UNP Q9AC34
H	-3	HIS	-	expression tag	UNP Q9AC34
H	-2	HIS	-	expression tag	UNP Q9AC34
H	-1	HIS	-	expression tag	UNP Q9AC34
H	0	HIS	-	expression tag	UNP Q9AC34
H	1	HIS	-	expression tag	UNP Q9AC34

- Molecule 2 is a protein called Ribonuclease VapC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total 986	C 621	N 181	O 182	Se 2	0	0	0
2	C	127	Total 986	C 621	N 181	O 182	Se 2	0	0	0
2	F	127	Total 986	C 621	N 181	O 182	Se 2	0	0	0
2	G	127	Total 986	C 621	N 181	O 182	Se 2	0	0	0

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	27	Total 541	C 261	N 92	O 162	P 26	0	0	0

- Molecule 4 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	27	Total 556	C 265	N 109	O 156	P 26	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	32	Total 32	O 32	0	0
5	C	26	Total 26	O 26	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	12	Total 12	O 12	0	0
5	E	3	Total 3	O 3	0	0
5	F	15	Total 15	O 15	0	0
5	G	25	Total 25	O 25	0	0
5	H	13	Total 13	O 13	0	0
5	M	1	Total 1	O 1	0	0
5	N	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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: VapB family protein

- Molecule 1: VapB family protein
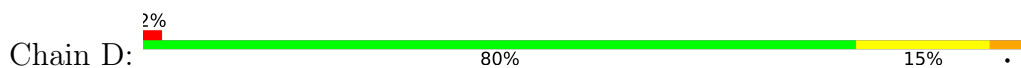
- Molecule 1: VapB family protein

- Molecule 1: VapB family protein

- Molecule 2: Ribonuclease VapC

- Molecule 2: Ribonuclease VapC

Chain C:

• Molecule 2: Ribonuclease VapC

Chain F:

• Molecule 2: Ribonuclease VapC

Chain G:
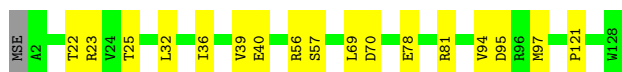
• Molecule 3: DNA (27-MER)

Chain M:
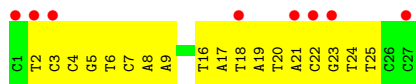
• Molecule 4: DNA (27-MER)

Chain N:

4 Data and refinement statistics ⓘ
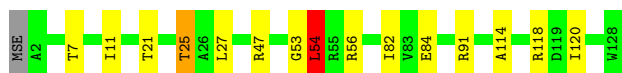
Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.18Å 144.16Å 160.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.80 – 2.70 45.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.80-2.70) 93.7 (45.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.178 , 0.240 0.179 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (5.64%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.2	EDS
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7441	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.39	0/498	0.62	0/673
1	D	0.49	0/670	0.66	0/907
1	E	0.42	0/492	0.65	0/665
1	H	0.57	0/640	0.79	3/866 (0.3%)
2	B	0.54	0/998	0.69	0/1350
2	C	0.46	0/998	0.69	1/1350 (0.1%)
2	F	0.43	0/998	0.62	0/1350
2	G	0.49	0/998	0.67	0/1350
3	M	0.80	0/604	1.15	0/929
4	N	0.68	0/626	0.99	2/966 (0.2%)
All	All	0.53	0/7522	0.76	6/10406 (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	H	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	52	LEU	CA-CB-CG	-6.47	100.41	115.30
1	H	52	LEU	CB-CG-CD1	-6.18	100.49	111.00
1	H	12	GLY	N-CA-C	-5.88	98.39	113.10
4	N	10	DA	O5'-P-OP1	5.61	117.44	110.70
4	N	12	DA	O4'-C4'-C3'	-5.30	102.38	104.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

W O R L D W I D E
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PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	H	48	SER	Peptide
1	H	53	VAL	Peptide

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	491	0	497	6	0
1	D	656	0	645	18	0
1	E	485	0	492	10	0
1	H	628	0	620	23	0
2	B	986	0	1001	23	0
2	C	986	0	1001	10	0
2	F	986	0	1001	23	0
2	G	986	0	1001	17	0
3	M	541	0	304	18	0
4	N	556	0	301	16	0
5	A	11	0	0	2	0
5	B	32	0	0	2	0
5	C	26	0	0	1	0
5	D	12	0	0	3	0
5	E	3	0	0	1	0
5	F	15	0	0	3	0
5	G	25	0	0	2	0
5	H	13	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
All	All	7441	0	6863	130	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 130 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:H:49:ILE:HD12	1:H:50:ALA:H	1.06	1.10
1:A:59:MSE:HE1	2:B:57:SER:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:VAL:O	5:F:201:HOH:O	1.88	0.89
2:C:21:THR:HB	1:H:52:LEU:HD11	1.56	0.87
4:N:8:DA:H2"	4:N:9:DT:H5"	1.56	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	63/85 (74%)	56 (89%)	6 (10%)	1 (2%)	9	24
1	D	82/85 (96%)	81 (99%)	0	1 (1%)	13	32
1	E	62/85 (73%)	57 (92%)	5 (8%)	0	100	100
1	H	79/85 (93%)	71 (90%)	5 (6%)	3 (4%)	3	7
2	B	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
2	C	125/128 (98%)	122 (98%)	2 (2%)	1 (1%)	19	43
2	F	125/128 (98%)	121 (97%)	3 (2%)	1 (1%)	19	43
2	G	125/128 (98%)	124 (99%)	1 (1%)	0	100	100
All	All	786/852 (92%)	755 (96%)	24 (3%)	7 (1%)	17	40

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	50	ALA
1	H	48	SER
1	H	49	ILE
1	A	12	GLY
2	C	54	LEU

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	53/70 (76%)	53 (100%)	0	100	100
1	D	71/70 (101%)	64 (90%)	7 (10%)	8	18
1	E	52/70 (74%)	50 (96%)	2 (4%)	33	62
1	H	68/70 (97%)	63 (93%)	5 (7%)	13	32
2	B	101/99 (102%)	96 (95%)	5 (5%)	24	51
2	C	101/99 (102%)	98 (97%)	3 (3%)	41	70
2	F	101/99 (102%)	99 (98%)	2 (2%)	55	81
2	G	101/99 (102%)	99 (98%)	2 (2%)	55	81
All	All	648/676 (96%)	622 (96%)	26 (4%)	31	60

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	79	LEU
2	F	56	ARG
1	H	56	LEU
1	E	11	SER
2	F	67	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	0	HIS
1	H	1	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	64/85 (75%)	-0.04	2 (3%)	49	49	32, 49, 77, 87	0
1	D	83/85 (97%)	-0.07	2 (2%)	59	60	30, 54, 77, 95	0
1	E	63/85 (74%)	-0.02	0	100	100	39, 61, 85, 97	0
1	H	80/85 (94%)	-0.04	3 (3%)	40	39	31, 59, 81, 92	0
2	B	125/128 (97%)	-0.40	0	100	100	24, 32, 48, 73	0
2	C	125/128 (97%)	-0.29	0	100	100	28, 43, 64, 75	0
2	F	125/128 (97%)	-0.27	0	100	100	26, 46, 89, 97	0
2	G	125/128 (97%)	-0.44	0	100	100	23, 39, 61, 82	0
3	M	27/27 (100%)	1.62	8 (29%)	0	0	64, 107, 152, 182	0
4	N	27/27 (100%)	1.69	10 (37%)	0	0	68, 108, 183, 188	0
All	All	844/906 (93%)	-0.12	25 (2%)	50	51	23, 46, 95, 188	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	27	DG	5.3
4	N	1	DG	5.1
3	M	1	DC	4.3
4	N	26	DA	4.3
3	M	2	DT	4.2

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 ⓘ

There are no such residues in this entry.