



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 03:58 pm BST

PDB ID : 3EE1
Title : Novel fold of VirA, a type III secretion system effector protein from *Shigella flexneri*
Authors : Davis, J.S.
Deposited on : 2008-09-03
Resolution : 3.01 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

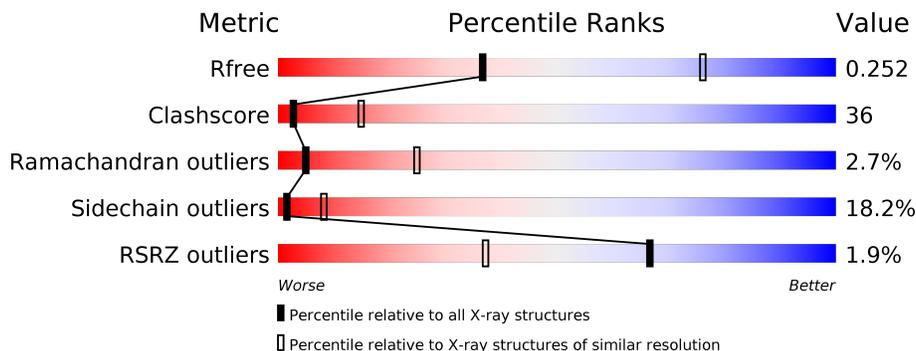
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 on 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	400	 2% 41% 36% 8% • 15%
1	B	400	 2% 40% 36% 9% • 15%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5244 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 Effector protein virA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	341	2622	1660	439	511	7	5	0	0	0
1	B	341	2622	1660	439	511	7	5	0	0	0

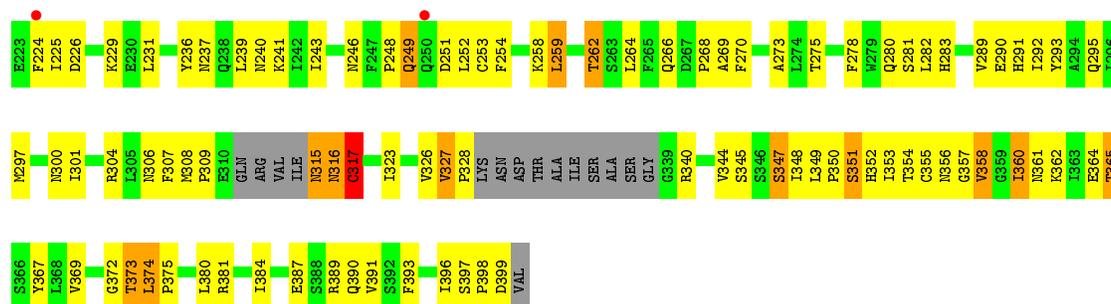
There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	EXPRESSION TAG	UNP Q7BU69
A	2	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	3	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	4	SER	-	EXPRESSION TAG	UNP Q7BU69
A	5	TYR	-	EXPRESSION TAG	UNP Q7BU69
A	6	CYS	-	EXPRESSION TAG	UNP Q7BU69
A	7	ASP	-	EXPRESSION TAG	UNP Q7BU69
A	8	ARG	-	EXPRESSION TAG	UNP Q7BU69
A	9	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	10	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	11	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	12	ALA	-	EXPRESSION TAG	UNP Q7BU69
A	13	VAL	-	EXPRESSION TAG	UNP Q7BU69
A	36	VAL	ILE	VARIANT	UNP Q7BU69
A	56	TYR	HIS	VARIANT	UNP Q7BU69
A	173	PRO	HIS	VARIANT	UNP Q7BU69
A	239	LEU	VAL	VARIANT	UNP Q7BU69
B	1	GLU	-	EXPRESSION TAG	UNP Q7BU69
B	2	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	3	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	4	SER	-	EXPRESSION TAG	UNP Q7BU69
B	5	TYR	-	EXPRESSION TAG	UNP Q7BU69
B	6	CYS	-	EXPRESSION TAG	UNP Q7BU69
B	7	ASP	-	EXPRESSION TAG	UNP Q7BU69
B	8	ARG	-	EXPRESSION TAG	UNP Q7BU69

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	10	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	11	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	12	ALA	-	EXPRESSION TAG	UNP Q7BU69
B	13	VAL	-	EXPRESSION TAG	UNP Q7BU69
B	36	VAL	ILE	VARIANT	UNP Q7BU69
B	56	TYR	HIS	VARIANT	UNP Q7BU69
B	173	PRO	HIS	VARIANT	UNP Q7BU69
B	239	LEU	VAL	VARIANT	UNP Q7BU69



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.25Å 170.91Å 46.16Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	28.63 – 3.01 28.63 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.2 (28.63-3.01) 96.3 (28.63-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.00Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.208 , 0.252	Depositor DCC
R_{free} test set	1097 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.032 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/2670	0.74	2/3618 (0.1%)
1	B	0.53	0/2670	0.72	2/3618 (0.1%)
All	All	0.54	0/5340	0.73	4/7236 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	N-CA-C	-6.59	96.63	113.10
1	B	104	GLY	N-CA-C	-6.23	97.52	113.10
1	A	102	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	102	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Peptide
1	B	103	ASP	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	2622	0	2537	190	0
1	B	2622	0	2537	187	0
All	All	5244	0	5074	369	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 36.

The worst 5 of 369 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:102:LEU:HA	1:A:108:GLN:HA	1.24	1.13
1:B:102:LEU:HA	1:B:108:GLN:HA	1.28	1.12
1:A:102:LEU:HD13	1:A:103:ASP:OD1	1.59	1.00
1:B:102:LEU:HD13	1:B:103:ASP:OD1	1.61	0.98
1:A:102:LEU:HB2	1:A:108:GLN:HG3	1.54	0.90

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	333/400 (83%)	283 (85%)	41 (12%)	9 (3%)	5	25
1	B	333/400 (83%)	285 (86%)	39 (12%)	9 (3%)	5	25
All	All	666/800 (83%)	568 (85%)	80 (12%)	18 (3%)	5	25

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	316	ASN
1	A	317	CYS
1	A	373	THR
1	B	4	SER

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	294/357 (82%)	242 (82%)	52 (18%)	2 9
1	B	294/357 (82%)	239 (81%)	55 (19%)	1 8
All	All	588/714 (82%)	481 (82%)	107 (18%)	1 8

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	THR
1	B	102	LEU
1	B	345	SER
1	A	374	LEU
1	B	75	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	B	119	ASN
1	B	306	ASN
1	A	352	HIS
1	B	111	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 carbohydrates 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	336/400 (84%)	-0.30	6 (1%) 68 39	68, 103, 171, 489	0
1	B	336/400 (84%)	-0.21	7 (2%) 63 34	71, 115, 212, 465	0
All	All	672/800 (84%)	-0.26	13 (1%) 66 37	68, 110, 192, 489	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	3.0
1	A	1	GLU	2.9
1	A	171	TYR	2.5
1	A	71	GLN	2.4
1	B	140	PRO	2.3

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 carbohydrates 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.