



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:59 PM BST

PDB ID : 3J9O
EMDB ID: : EMD-6266
Title : CryoEM structure of a type VI secretion system
Authors : Clemens, D.L.; Ge, P.; Lee, B.-Y.; Horwitz, M.A.; Zhou, Z.H.
Deposited on : 2015-02-11
Resolution : 3.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

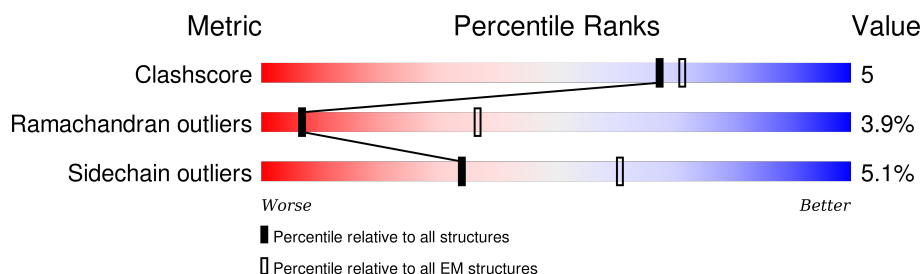
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	184	
1	C	184	
1	E	184	
1	G	184	
1	I	184	
1	K	184	
2	B	506	
2	D	506	
2	F	506	

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Mol	Chain	Length	Quality of chain
2	H	506	<div><div></div><div>69%</div><div>15%</div><div>•</div><div>16%</div></div>
2	J	506	<div><div></div><div>67%</div><div>16%</div><div>•</div><div>16%</div></div>
2	L	506	<div><div></div><div>69%</div><div>15%</div><div>•</div><div>16%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27264 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Intracellular growth locus protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	C	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	E	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	G	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	I	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		
1	K	134	Total	C	N	O	S	0	0
			1081	680	195	203	3		

- Molecule 2 is a protein called Intracellular growth locus protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	D	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	F	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	H	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	J	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		
2	L	427	Total	C	N	O	S	0	0
			3463	2228	556	662	17		

- Molecule 1: Intracellular growth locus protein A



SER	ASP	SER	ASN	GLU	LEU	GLU	SER	LEU	LYS	SER	LYS	ILE	PRO	ALA	LEU	THR	ASN	TYR	THR	ILE	LYS	ASP	SER	CYS	ASP	ALA	ALA	GLU	SER	GLN	ASP	LEU	SER	ASN	GLN	GLN	VAL	ASP	ASP	LYS
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| LYS | THR | ILE | ASP | MET | ILE | PHE | SER | ASP | SER | ASN | GLU | LEU | GLU | SER | SER | LYS | LYS | ILE | PRO | ALA | ALA | LEU | THR | ASN | TYR | THR | ILE | LYS | ASP | SER | CYS | ASP | ALA | ALA | GLU | SER | GLN | ASP | SER | ASN | GLN | GLN | VAL | ASP | ASP | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

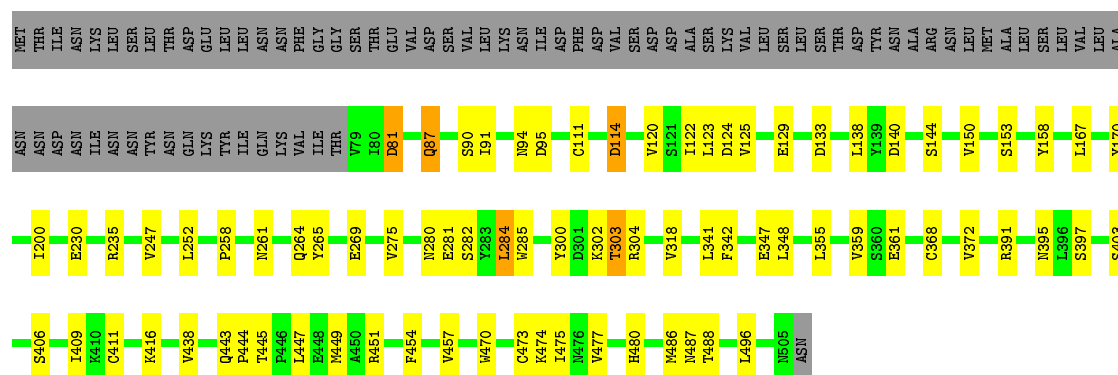
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| MET | THR | ILE | ASN | LYS | LEU | SER | LEU | THR | ASP | GLU | LEU | LEU | ASN | ASN | PHE | GLY | GLY | SER | THR | GLU | VAL | ASP | SER | SER | VAL | LEU | LYS | ASN | ILE | ASP | PHE | ASP | ASP | SER | SER | LYS | VAL | VAL | SER | SER | THR | LEU | SER | LEU | THR | ASP | TYR | ASN | ALA | ALA | ARG | ASN | ASN | LEU | MET | MET | ALA | ALA | LEU | SER | SER | LEU | VAL | VAL | LEU | LEU | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

I402	S403	S406	I409	K410	C411	K416	V438	Q443	P444	T445	P446	L447	E448	M449	A450	R451	F454	V457	M470	C473	K474	I475	M476	V477	H480	M486	M487	T488	L496	N505	ASN
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| NET | THR | ILE | ASN | LYS | LEU | SER | THR | ASP | GLU | LEU | LEU | ASN | ASN | PHE | GLY | GLY | SER | THR | GLU | VAL | ASP | SER | VAL | ASP | ASP | LYS | LYS | ASN | ILE | ASP | PHE | ASP | ASP | SER | SER | TYR | ASN | ALA | ARG | ASN | LEU | MET | MET | ALA | SER | SER | LEU | VAL | LEU | LEU | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

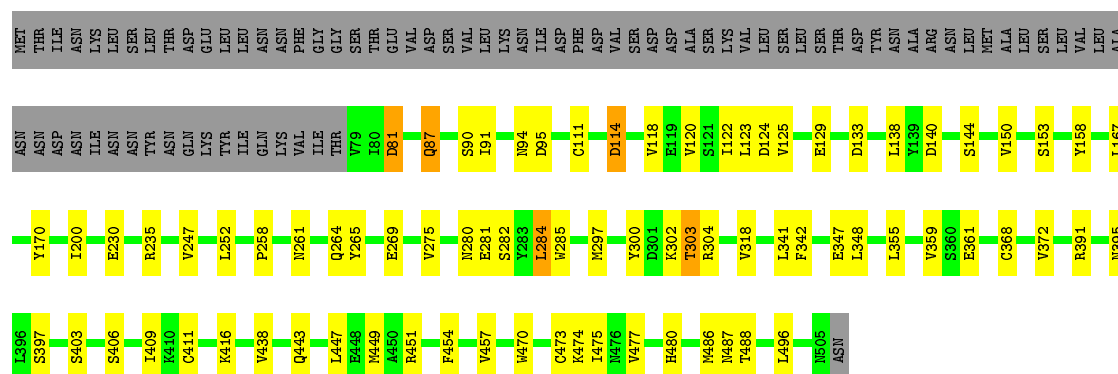
S397
S403
S406
I409
K410
C411
K416
V438
Q443
P444
T445
P446
L447
E449
M449
A450
R451
F454
V457
W470
C473
K474
I475
N476
V477
H480
M486
N487
T488
L496
N505
ASN

Chain F: 



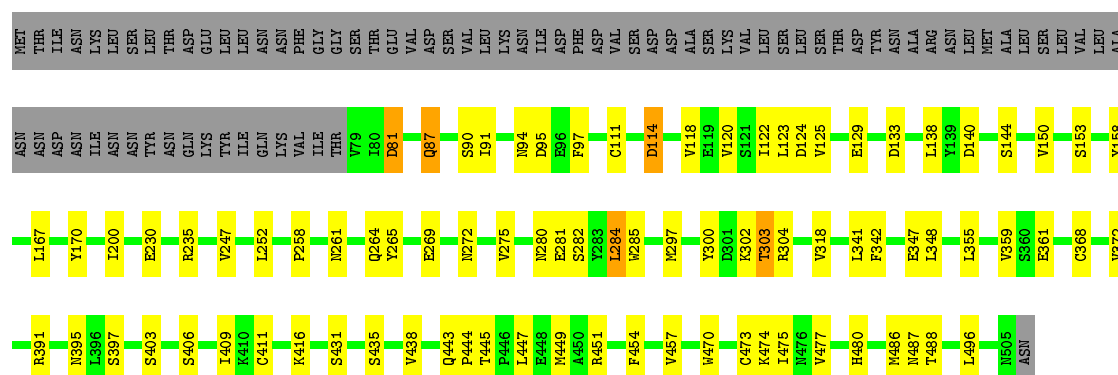
• Molecule 2: Intracellular growth locus protein B

Chain H: 



• Molecule 2: Intracellular growth locus protein B

Chain J: 



• Molecule 2: Intracellular growth locus protein B

Chain L: 



S406	I200	ASN
I409	E230	ASN
K410	R235	ASP
C411	V247	ILE
K416	L252	ASN
V438	P258	TYR
Q443	N261	ASN
P444	Q264	GLN
T445	Y265	LYS
P446	E269	TVR
L447	N272	ILE
E448	V275	GLN
N449	N280	VAL
A450	E281	ILE
R451	S282	THR
F454	Y283	V79
V457	L284	I80
V470	W285	D81
C473	Y300	Q87
K474	D801	S90
I475	K302	I91
N476	T303	N94
V477	R304	D95
H480	V318	C111
N486	L341	D114
N487	F342	V120
T488	E347	S121
L496	L348	I122
N505	L355	L123
ASN	V359	D124
	E361	V125
	C368	E129
	V372	D133
	R391	L138
	I402	Y139
	S403	D140
		S144
		Y150
		S153
		Y158
		L167
		Y170

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	A	0.23	0/1095	0.39	0/1470
1	C	0.23	0/1095	0.38	0/1470
1	E	0.23	0/1095	0.39	0/1470
1	G	0.23	0/1095	0.38	0/1470
1	I	0.23	0/1095	0.38	0/1470
1	K	0.23	0/1095	0.38	0/1470
2	B	0.26	0/3546	0.39	0/4806
2	D	0.26	0/3546	0.39	0/4806
2	F	0.26	0/3546	0.39	0/4806
2	H	0.26	0/3546	0.39	0/4806
2	J	0.26	0/3546	0.39	0/4806
2	L	0.26	0/3546	0.39	0/4806
All	All	0.25	0/27846	0.39	0/37656

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	A	1081	0	1114	11	0
1	C	1081	0	1114	12	0
1	E	1081	0	1114	12	0
1	G	1081	0	1114	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1081	0	1114	11	0
1	K	1081	0	1114	14	0
2	B	3463	0	3372	35	0
2	D	3463	0	3372	34	0
2	F	3463	0	3372	34	0
2	H	3463	0	3372	34	0
2	J	3463	0	3372	38	0
2	L	3463	0	3372	35	0
All	All	27264	0	26916	258	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 5.

The worst 5 of 258 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)
2:L:347:GLU:HG2	2:L:359:VAL:HG11	1.73	0.70
2:H:347:GLU:HG2	2:H:359:VAL:HG11	1.73	0.69
2:F:347:GLU:HG2	2:F:359:VAL:HG11	1.73	0.68
2:F:473:CYS:SG	2:F:474:LYS:N	2.68	0.67
2:J:473:CYS:SG	2:J:474:LYS:N	2.68	0.67

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 PDB entries followed by that with respect to all EM entries.

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	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	C	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26
1	E	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	I	132/184 (72%)	111 (84%)	13 (10%)	8 (6%)	2	26
1	K	132/184 (72%)	112 (85%)	12 (9%)	8 (6%)	2	26
2	B	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	D	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	F	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	H	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	J	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
2	L	425/506 (84%)	345 (81%)	66 (16%)	14 (3%)	5	44
All	All	3342/4140 (81%)	2739 (82%)	471 (14%)	132 (4%)	7	38

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	103	ASP
2	B	150	VAL
2	B	153	SER
2	B	411	CYS

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 PDB entries followed by that with respect to all EM entries.

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	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	C	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	E	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	G	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	I	121/168 (72%)	115 (95%)	6 (5%)	30	71
1	K	121/168 (72%)	115 (95%)	6 (5%)	30	71
2	B	387/460 (84%)	367 (95%)	20 (5%)	29	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	F	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	H	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	J	387/460 (84%)	367 (95%)	20 (5%)	29	70
2	L	387/460 (84%)	367 (95%)	20 (5%)	29	70
All	All	3048/3768 (81%)	2892 (95%)	156 (5%)	34	70

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	416	LYS
2	H	138	LEU
2	L	348	LEU
2	F	449	MET
1	G	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	291	HIS
2	L	291	HIS
2	H	291	HIS
2	D	291	HIS
2	J	291	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 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.