



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:55 AM UTC

PDB ID : 5M30 / pdb_00005m30
Title : Structure of TssK from T6SS EAEC in complex with nanobody nb18
Authors : Nguyen, V.S.; Cambillau, C.; Spinelli, C.; Desmyter, A.; Legrand, P.; Cascales, E.
Deposited on : 2016-10-13
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

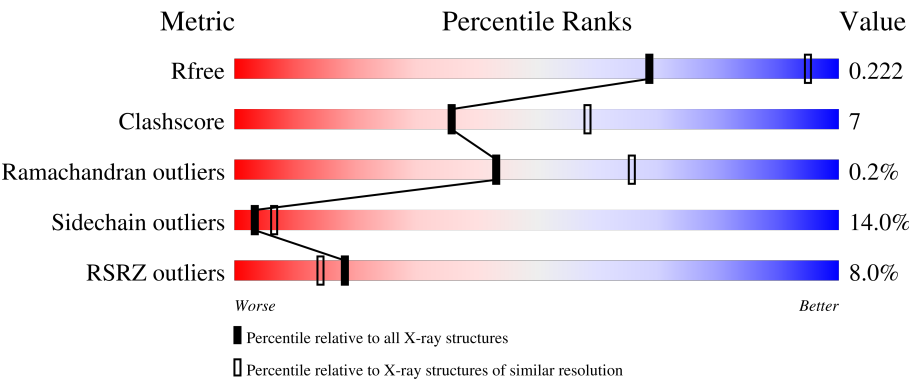
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	445	5% 46% 13% • • 36%
1	B	445	11% 66% 21% • • 9%
1	C	445	4% 47% 13% • • 37%
2	D	125	3% 82% 11% • 5%
2	E	125	6% 89% 10% •

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Mol	Chain	Length	Quality of chain
2	F	125	3% 82% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10331 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 Type VI secretion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2183	1389	391	395	8			
1	B	405	Total	C	N	O	S	0	0	0
			3096	1969	546	567	14			
1	C	282	Total	C	N	O	S	0	0	0
			2129	1357	371	392	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LEU	ALA	conflict	UNP A0A0P7QEP7
B	202	LEU	ALA	conflict	UNP A0A0P7QEP7
C	202	LEU	ALA	conflict	UNP A0A0P7QEP7

- Molecule 2 is a protein called Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	119	Total	C	N	O	S	0	0	0
			887	556	152	175	4			
2	E	123	Total	C	N	O	S	0	0	0
			912	571	158	179	4			
2	F	122	Total	C	N	O	S	0	0	0
			916	574	160	178	4			

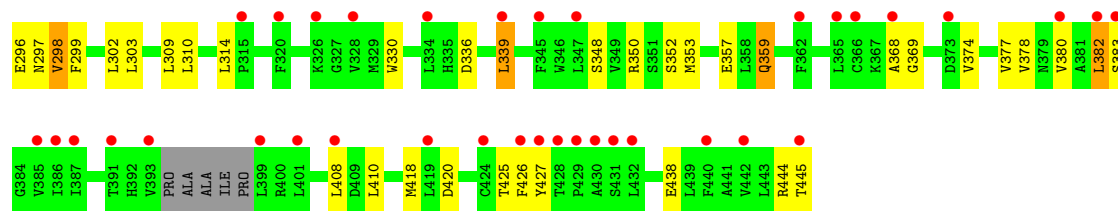
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	70	Total	O	0	0
			70	70		

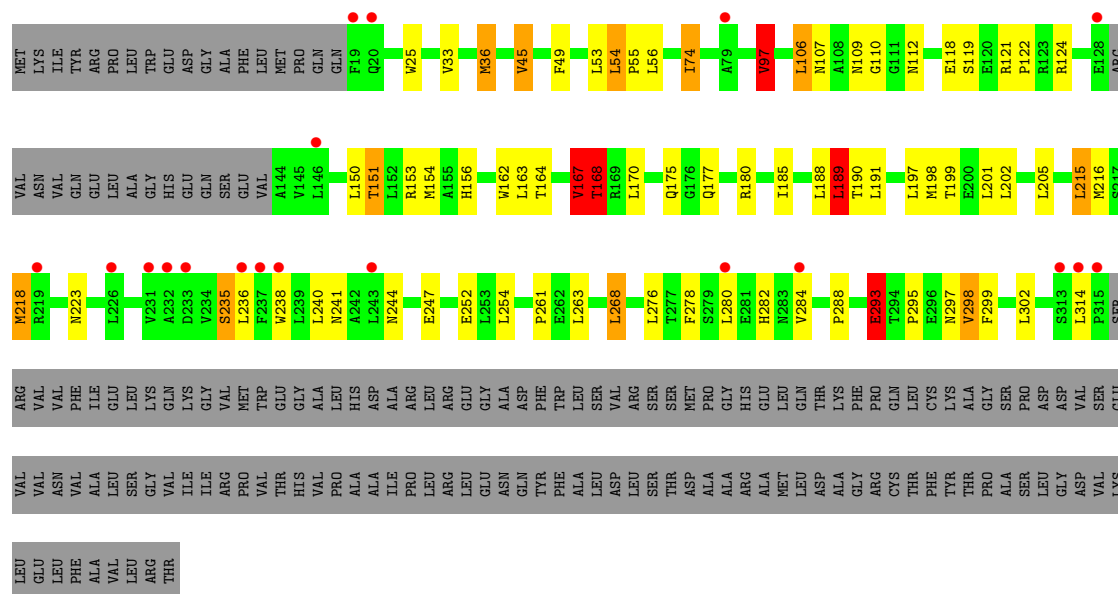
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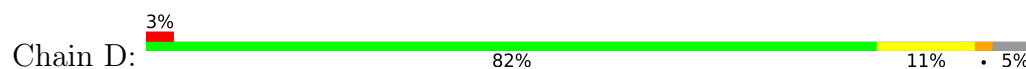
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	24	Total 24	O 24	0	0
3	E	18	Total 18	O 18	0	0
3	F	29	Total 29	O 29	0	0



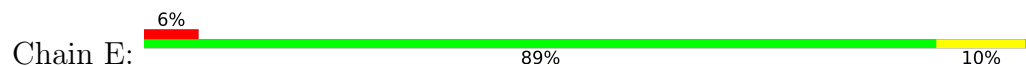
• Molecule 1: Type VI secretion protein



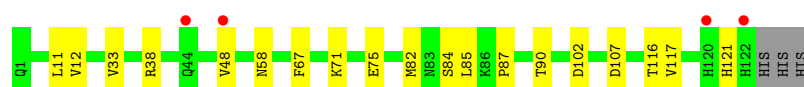
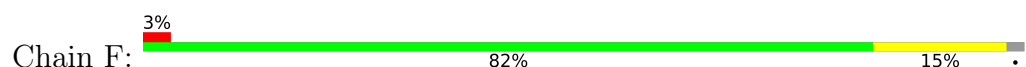
• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.24Å 153.67Å 154.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.60 48.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.5 (48.92-2.60) 85.3 (48.92-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.207 , 0.226 (Not available) , 0.222	Depositor DCC
R_{free} test set	2978 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

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	0.86	1/2233 (0.0%)	1.39	15/3056 (0.5%)
1	B	0.87	1/3164 (0.0%)	1.35	17/4320 (0.4%)
1	C	0.88	3/2177 (0.1%)	1.42	15/2985 (0.5%)
2	D	0.77	0/903	1.10	0/1224
2	E	0.77	0/930	1.12	1/1261 (0.1%)
2	F	0.75	0/934	1.15	1/1265 (0.1%)
All	All	0.84	5/10341 (0.0%)	1.32	49/14111 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	ILE	CA-C	6.08	1.57	1.52
1	A	36	MET	SD-CE	-5.93	1.64	1.79
1	B	185	ILE	CG1-CD1	-5.23	1.31	1.51
1	C	36	MET	SD-CE	-5.19	1.66	1.79
1	C	167	VAL	CA-C	5.04	1.59	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	VAL	CB-CA-C	8.02	118.17	110.63
1	C	167	VAL	CB-CA-C	7.58	117.75	110.63
1	A	45	VAL	N-CA-C	-7.11	106.14	111.90
1	B	19	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	189	LEU	N-CA-C	-6.88	105.04	113.50

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	2183	0	2129	37	0
1	B	3096	0	3030	65	0
1	C	2129	0	2067	41	0
2	D	887	0	849	6	0
2	E	912	0	857	2	0
2	F	916	0	876	5	0
3	A	35	0	0	0	0
3	B	70	0	0	0	0
3	C	32	0	0	0	0
3	D	24	0	0	0	0
3	E	18	0	0	0	0
3	F	29	0	0	0	0
All	All	10331	0	9808	145	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 7.

The worst 5 of 145 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:C:49:PHE:HZ	1:C:167:VAL:HG13	1.36	0.90
1:B:49:PHE:HZ	1:B:167:VAL:HG13	1.39	0.88
1:B:238:TRP:HB2	1:B:278:PHE:HZ	1.40	0.87
1:B:154:MET:H	1:B:157:GLN:HE21	1.24	0.85
1:A:185:ILE:HG12	1:A:296:GLU:HG3	1.59	0.81

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	245/445 (55%)	233 (95%)	11 (4%)	1 (0%)	30	51
1	B	350/445 (79%)	335 (96%)	15 (4%)	0	100	100
1	C	270/445 (61%)	262 (97%)	8 (3%)	0	100	100
2	D	117/125 (94%)	113 (97%)	3 (3%)	1 (1%)	14	30
2	E	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
2	F	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
All	All	1223/1710 (72%)	1180 (96%)	41 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	41	PRO
1	A	312	ALA

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	227/382 (59%)	184 (81%)	43 (19%)	1	2
1	B	325/382 (85%)	280 (86%)	45 (14%)	3	7
1	C	220/382 (58%)	185 (84%)	35 (16%)	2	4
2	D	90/101 (89%)	83 (92%)	7 (8%)	11	26
2	E	91/101 (90%)	84 (92%)	7 (8%)	12	27
2	F	93/101 (92%)	84 (90%)	9 (10%)	8	17
All	All	1046/1449 (72%)	900 (86%)	146 (14%)	3	6

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	263	LEU

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Mol	Chain	Res	Type
2	F	84	SER
1	C	282	HIS
2	E	27	SER
1	B	90	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	403	ASN
2	E	76	ASN
1	C	107	ASN
2	F	83	ASN
2	D	76	ASN

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 oligosaccharides 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 [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	284/445 (63%)	0.67	24 (8%) 16 13	38, 100, 172, 282	1 (0%)
1	B	405/445 (91%)	0.73	49 (12%) 8 6	57, 102, 224, 278	1 (0%)
1	C	282/445 (63%)	0.53	19 (6%) 24 19	63, 96, 198, 234	0
2	D	119/125 (95%)	0.25	4 (3%) 48 42	65, 85, 117, 128	0
2	E	123/125 (98%)	0.45	7 (5%) 29 24	65, 98, 134, 191	0
2	F	122/125 (97%)	0.16	4 (3%) 49 43	70, 87, 116, 216	0
All	All	1335/1710 (78%)	0.55	107 (8%) 18 14	38, 94, 199, 282	2 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	ALA	5.3
1	B	227	ALA	5.1
1	C	219	ARG	4.6
2	D	119	SER	4.6
1	B	228	ASP	4.3

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 oligosaccharides 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.