



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 5, 2017 – 01:39 PM EDT

PDB ID : 5URX
EMDB ID: : EMD-8602
Title : Structure of the contracted type VI secretion system sheath in Myxococcus xanthus
Authors : Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on : unknown
Resolution : 28.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

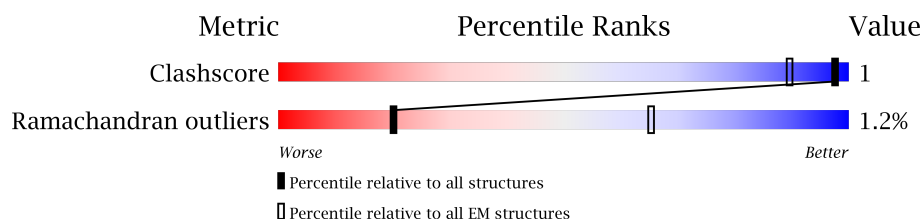
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 28.00 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	125131	1336
Ramachandran outliers	121729	1120

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	1A	164	80% 18%
1	1C	164	80% 18%
1	1E	164	80% 18%
1	1G	164	80% 18%
1	1I	164	81% 18%
1	1K	164	81% 18%
1	2A	164	80% 18%
1	2C	164	81% 18%
1	2E	164	80% 18%
1	2G	164	80% 18%
1	2I	164	80% 18%

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Mol	Chain	Length	Quality of chain
1	2K	164	 80% 18%
1	3A	164	 80% 18%
1	3C	164	 80% 18%
1	3E	164	 81% 18%
1	3G	164	 81% 18%
1	3I	164	 80% 18%
1	3K	164	 80% 18%
2	1B	494	 85% 13%
2	1D	494	 85% 13%
2	1F	494	 85% 13%
2	1H	494	 85% 13%
2	1J	494	 86% 13%
2	1L	494	 86% 13%
2	2B	494	 85% 13%
2	2D	494	 86% 13%
2	2F	494	 85% 13%
2	2H	494	 85% 13%
2	2J	494	 85% 13%
2	2L	494	 85% 13%
2	3B	494	 85% 13%
2	3D	494	 85% 13%
2	3F	494	 86% 13%
2	3H	494	 86% 13%
2	3J	494	 85% 13%
2	3L	494	 85% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40752 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 TssB.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1A	135	Total 540	C 270	N 135	O 135	0	0
1	1C	135	Total 540	C 270	N 135	O 135	0	0
1	1E	135	Total 540	C 270	N 135	O 135	0	0
1	1G	135	Total 540	C 270	N 135	O 135	0	0
1	1I	135	Total 540	C 270	N 135	O 135	0	0
1	1K	135	Total 540	C 270	N 135	O 135	0	0
1	2A	135	Total 540	C 270	N 135	O 135	0	0
1	2C	135	Total 540	C 270	N 135	O 135	0	0
1	2E	135	Total 540	C 270	N 135	O 135	0	0
1	2G	135	Total 540	C 270	N 135	O 135	0	0
1	2I	135	Total 540	C 270	N 135	O 135	0	0
1	2K	135	Total 540	C 270	N 135	O 135	0	0
1	3A	135	Total 540	C 270	N 135	O 135	0	0
1	3C	135	Total 540	C 270	N 135	O 135	0	0
1	3E	135	Total 540	C 270	N 135	O 135	0	0
1	3G	135	Total 540	C 270	N 135	O 135	0	0
1	3I	135	Total 540	C 270	N 135	O 135	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	3K	135	Total	C	N	O	0	0
			540	270	135	135		

- Molecule 2 is a protein called TssC.

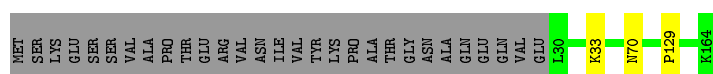
Mol	Chain	Residues	Atoms				AltConf	Trace
2	1B	431	Total	C	N	O	0	0
			1724	862	431	431		
2	1D	431	Total	C	N	O	0	0
			1724	862	431	431		
2	1F	431	Total	C	N	O	0	0
			1724	862	431	431		
2	1H	431	Total	C	N	O	0	0
			1724	862	431	431		
2	1J	431	Total	C	N	O	0	0
			1724	862	431	431		
2	1L	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2B	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2D	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2F	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2H	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2J	431	Total	C	N	O	0	0
			1724	862	431	431		
2	2L	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3B	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3D	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3F	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3H	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3J	431	Total	C	N	O	0	0
			1724	862	431	431		
2	3L	431	Total	C	N	O	0	0
			1724	862	431	431		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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. 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. 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.

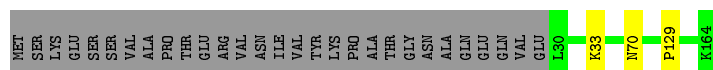
- Molecule 1: TssB

Chain 1A: 



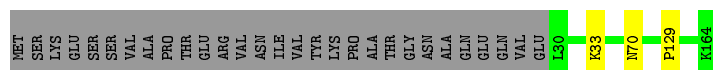
- Molecule 1: TssB

Chain 1C: 




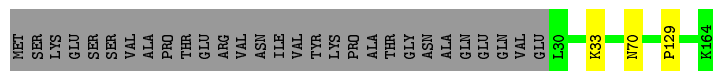
- Molecule 1: TssB

Chain 1E: 




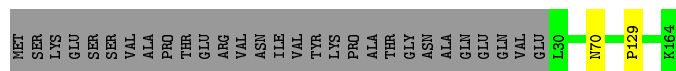
- Molecule 1: TssB

Chain 1G: 




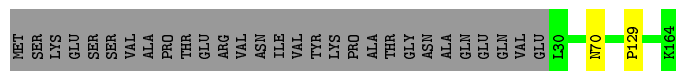
- Molecule 1: TssB

Chain 1I: 


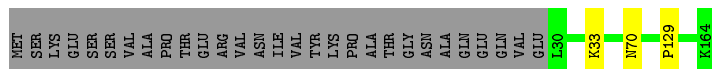


- Molecule 1: TssB


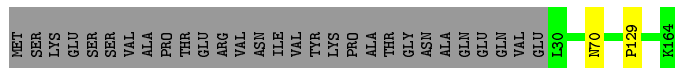
Chain 1K: 




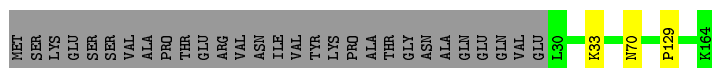
● Molecule 1: TssB

Chain 2A:  80% 18%


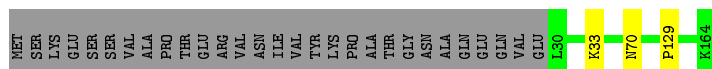
● Molecule 1: TssB

Chain 2C:  81% 18%

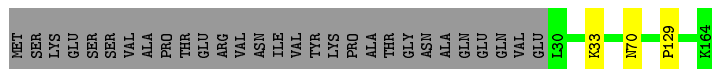
● Molecule 1: TssB

Chain 2E:  80% 18%


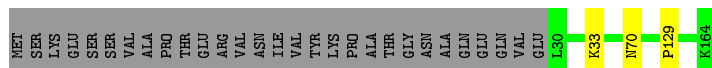
● Molecule 1: TssB

Chain 2G:  80% 18%


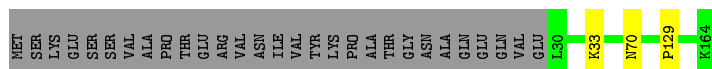
● Molecule 1: TssB

Chain 2I:  80% 18%


● Molecule 1: TssB

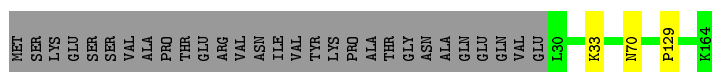
Chain 2K:  80% 18%

● Molecule 1: TssB

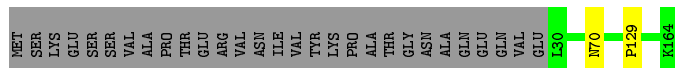
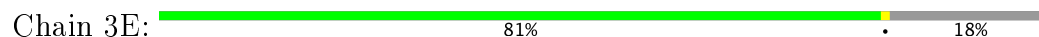
Chain 3A:  80% 18%

● Molecule 1: TssB

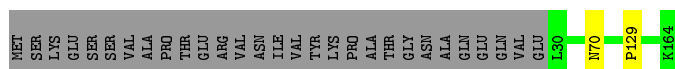
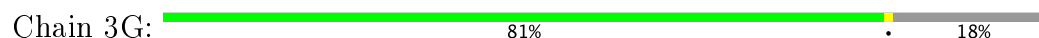
Chain 3C:  80% 18%



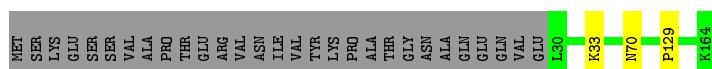
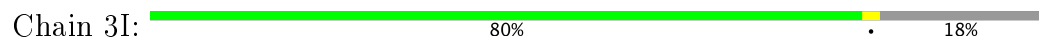
- Molecule 1: TssB



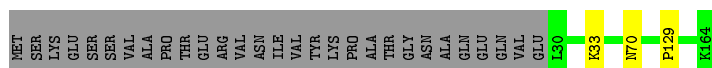
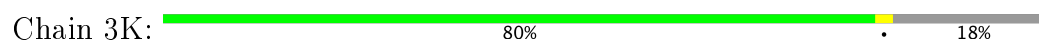
- Molecule 1: TssB



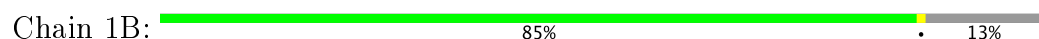
- Molecule 1: TssB



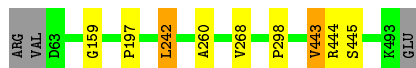
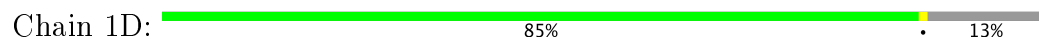
- Molecule 1: TssB




- Molecule 2: TssC



- Molecule 2: TssC



- Molecule 2: TssC

Chain 1F:  85% 13%

MET ALA ASN GLU THR GLN THR LYS SER THR GLY VAL ALA ASN ASP ALA SER LEU SER LEU LEU ASP ASP GLU ILE LEU SER SER GLU ALA VAL LYS LEU LYS PRO LYS ASP ASP GLU GLY TYR ASP VAL LYS ARG GLY VAL GLN PHE ILE THR GLU MET LEU ALA PRO ASN ARG SER GLU

ARG VAL D63 G159 P197 L242 A260 V268 P298 V443 R444 S445 K493 GLU

• Molecule 2: TssC

Chain 1H:  85% 13%

MET ALA ASN GLU THR GLN THR LYS SER THR GLY VAL ALA ASN ASP ALA SER LEU SER LEU LEU ASP ASP GLU ILE LEU SER SER GLU ALA VAL LYS LEU LYS PRO LYS ASP ASP GLU GLY TYR ASP VAL LYS ARG GLY VAL GLN PHE ILE THR GLU MET LEU ALA PRO ASN ARG SER GLU

ARG VAL D63 G159 P197 L242 A260 V268 P298 V443 R444 S445 K493 GLU

• Molecule 2: TssC

Chain 1J:  86% 13%

MET ALA ASN GLU THR GLN THR LYS SER THR GLY VAL ALA ASN ASP ALA SER LEU SER LEU LEU ASP ASP GLU ILE LEU SER SER GLU ALA VAL LYS LEU LYS PRO LYS ASP ASP GLU GLY TYR ASP VAL LYS ARG GLY VAL GLN PHE ILE THR GLU MET LEU ALA PRO ASN ARG SER GLU

ARG VAL D63 P197 L242 A260 V268 P298 V443 R444 S445 K493 GLU

• Molecule 2: TssC

Chain 1L:  86% 13%

MET ALA ASN GLU THR GLN THR LYS SER THR GLY VAL ALA ASN ASP ALA SER LEU SER LEU LEU ASP ASP GLU ILE LEU SER SER GLU ALA VAL LYS LEU LYS PRO LYS ASP ASP GLU GLY TYR ASP VAL LYS ARG GLY VAL GLN PHE ILE THR GLU MET LEU ALA PRO ASN ARG SER GLU

ARG VAL D63 P197 L242 A260 V268 P298 V443 R444 S445 K493 GLU

• Molecule 2: TssC

Chain 2B:  85% 13%

MET ALA ASN GLU THR GLN THR LYS SER THR GLY VAL ALA ASN ASP ALA SER LEU SER LEU LEU ASP ASP GLU ILE LEU SER SER GLU ALA VAL LYS LEU LYS PRO LYS ASP ASP GLU GLY TYR ASP VAL LYS ARG GLY VAL GLN PHE ILE THR GLU MET LEU ALA PRO ASN ARG SER GLU

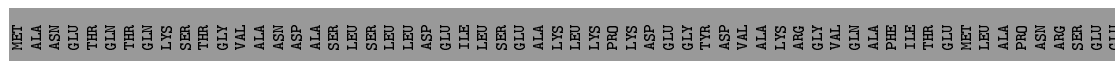
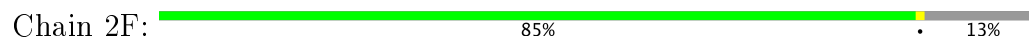
ARG VAL D63 G159 P197 L242 A260 V268 P298 V443 R444 S445 K493 GLU

• Molecule 2: TssC

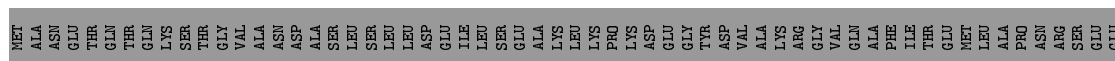
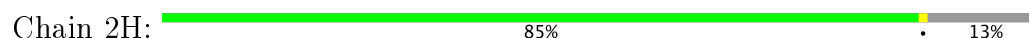
Chain 2D:  86% 13%



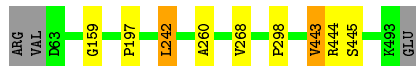
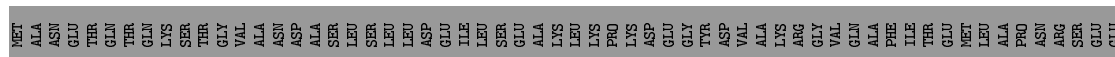
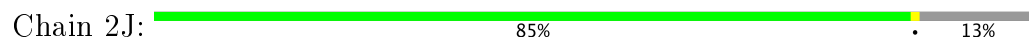
- Molecule 2: TssC



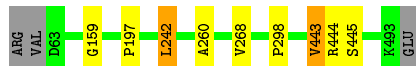
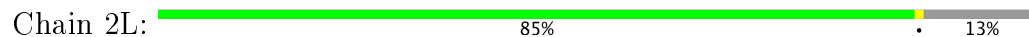
- Molecule 2: TssC



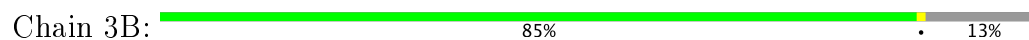
- Molecule 2: TssC



- Molecule 2: TssC



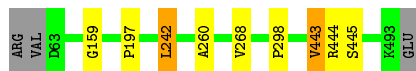
- Molecule 2: TssC





- Molecule 2: TssC

Chain 3D: 85% • 13%



- Molecule 2: TssC

Chain 3F: 86% : 13%



- Molecule 2: TssC

Chain 3H: 86% • 13%

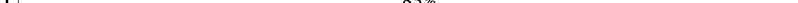


- Molecule 2: TssC

Chain 3.J: 85% • 13%



- Molecule 2: TssC

Chain 3L:  85% : 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of subtomograms used	407	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1A	0.60	0/539	0.66	0/672
1	1C	0.60	0/539	0.66	0/672
1	1E	0.60	0/539	0.66	0/672
1	1G	0.60	0/539	0.66	0/672
1	1I	0.60	0/539	0.66	0/672
1	1K	0.60	0/539	0.66	0/672
1	2A	0.60	0/539	0.66	0/672
1	2C	0.60	0/539	0.66	0/672
1	2E	0.60	0/539	0.66	0/672
1	2G	0.60	0/539	0.66	0/672
1	2I	0.60	0/539	0.66	0/672
1	2K	0.60	0/539	0.66	0/672
1	3A	0.60	0/539	0.66	0/672
1	3C	0.60	0/539	0.66	0/672
1	3E	0.60	0/539	0.66	0/672
1	3G	0.60	0/539	0.66	0/672
1	3I	0.60	0/539	0.66	0/672
1	3K	0.60	0/539	0.66	0/672
2	1B	0.68	3/1723 (0.2%)	0.72	0/2152
2	1D	0.68	3/1723 (0.2%)	0.72	0/2152
2	1F	0.68	3/1723 (0.2%)	0.72	0/2152
2	1H	0.68	3/1723 (0.2%)	0.72	0/2152
2	1J	0.68	3/1723 (0.2%)	0.72	0/2152
2	1L	0.68	3/1723 (0.2%)	0.72	0/2152
2	2B	0.68	3/1723 (0.2%)	0.72	0/2152
2	2D	0.68	3/1723 (0.2%)	0.72	0/2152
2	2F	0.68	3/1723 (0.2%)	0.72	0/2152
2	2H	0.68	3/1723 (0.2%)	0.72	0/2152
2	2J	0.68	3/1723 (0.2%)	0.72	0/2152
2	2L	0.68	3/1723 (0.2%)	0.72	0/2152
2	3B	0.68	3/1723 (0.2%)	0.72	0/2152
2	3D	0.68	3/1723 (0.2%)	0.72	0/2152
2	3F	0.68	3/1723 (0.2%)	0.72	0/2152
2	3H	0.68	3/1723 (0.2%)	0.72	0/2152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	3J	0.68	3/1723 (0.2%)	0.72	0/2152
2	3L	0.68	3/1723 (0.2%)	0.72	0/2152
All	All	0.66	54/40716 (0.1%)	0.70	0/50832

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
2	1B	0	1
2	1D	0	1
2	1F	0	1
2	1H	0	1
2	1J	0	1
2	1L	0	1
2	2B	0	1
2	2D	0	1
2	2F	0	1
2	2H	0	1
2	2J	0	1
2	2L	0	1
2	3B	0	1
2	3D	0	1
2	3F	0	1
2	3H	0	1
2	3J	0	1
2	3L	0	1
All	All	0	18

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2L	242	LEU	C-N	7.51	1.48	1.34
2	1F	242	LEU	C-N	7.49	1.48	1.34
2	3B	242	LEU	C-N	7.49	1.48	1.34
2	3H	242	LEU	C-N	7.48	1.48	1.34
2	1B	242	LEU	C-N	7.48	1.48	1.34
2	2H	242	LEU	C-N	7.47	1.48	1.34
2	3F	242	LEU	C-N	7.47	1.48	1.34
2	1L	242	LEU	C-N	7.46	1.48	1.34
2	2D	242	LEU	C-N	7.45	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	242	LEU	C-N	7.45	1.48	1.34
2	2J	242	LEU	C-N	7.44	1.48	1.34
2	1J	242	LEU	C-N	7.44	1.48	1.34
2	1H	242	LEU	C-N	7.43	1.48	1.34
2	3J	242	LEU	C-N	7.43	1.48	1.34
2	1D	242	LEU	C-N	7.42	1.48	1.34
2	3D	242	LEU	C-N	7.41	1.48	1.34
2	3L	242	LEU	C-N	7.41	1.48	1.34
2	2F	242	LEU	C-N	7.40	1.48	1.34
2	2B	242	LEU	C-O	-7.04	1.09	1.23
2	3F	242	LEU	C-O	-7.03	1.09	1.23
2	1J	242	LEU	C-O	-7.02	1.10	1.23
2	2H	242	LEU	C-O	-7.02	1.10	1.23
2	3H	242	LEU	C-O	-7.01	1.10	1.23
2	3L	242	LEU	C-O	-7.00	1.10	1.23
2	2J	242	LEU	C-O	-6.99	1.10	1.23
2	3B	242	LEU	C-O	-6.99	1.10	1.23
2	1F	242	LEU	C-O	-6.98	1.10	1.23
2	2D	242	LEU	C-O	-6.96	1.10	1.23
2	2L	242	LEU	C-O	-6.96	1.10	1.23
2	1B	242	LEU	C-O	-6.96	1.10	1.23
2	1L	242	LEU	C-O	-6.95	1.10	1.23
2	3J	242	LEU	C-O	-6.95	1.10	1.23
2	1D	242	LEU	C-O	-6.94	1.10	1.23
2	1H	242	LEU	C-O	-6.92	1.10	1.23
2	3D	242	LEU	C-O	-6.90	1.10	1.23
2	2F	242	LEU	C-O	-6.87	1.10	1.23
2	1F	197	PRO	C-O	-5.56	1.12	1.23
2	1L	197	PRO	C-O	-5.56	1.12	1.23
2	3B	197	PRO	C-O	-5.55	1.12	1.23
2	3L	197	PRO	C-O	-5.53	1.12	1.23
2	2F	197	PRO	C-O	-5.52	1.12	1.23
2	1H	197	PRO	C-O	-5.50	1.12	1.23
2	3H	197	PRO	C-O	-5.50	1.12	1.23
2	1B	197	PRO	C-O	-5.50	1.12	1.23
2	3J	197	PRO	C-O	-5.50	1.12	1.23
2	2L	197	PRO	C-O	-5.49	1.12	1.23
2	1J	197	PRO	C-O	-5.49	1.12	1.23
2	2H	197	PRO	C-O	-5.48	1.12	1.23
2	3F	197	PRO	C-O	-5.47	1.12	1.23
2	2D	197	PRO	C-O	-5.46	1.12	1.23
2	1D	197	PRO	C-O	-5.45	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2J	197	PRO	C-O	-5.45	1.12	1.23
2	2B	197	PRO	C-O	-5.44	1.12	1.23
2	3D	197	PRO	C-O	-5.43	1.12	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	443	VAL	Peptide
2	1D	443	VAL	Peptide
2	1F	443	VAL	Peptide
2	1H	443	VAL	Peptide
2	1J	443	VAL	Peptide
2	1L	443	VAL	Peptide
2	2B	443	VAL	Peptide
2	2D	443	VAL	Peptide
2	2F	443	VAL	Peptide
2	2H	443	VAL	Peptide
2	2J	443	VAL	Peptide
2	2L	443	VAL	Peptide
2	3B	443	VAL	Peptide
2	3D	443	VAL	Peptide
2	3F	443	VAL	Peptide
2	3H	443	VAL	Peptide
2	3J	443	VAL	Peptide
2	3L	443	VAL	Peptide

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	1A	540	0	138	1	0
1	1C	540	0	138	1	0
1	1E	540	0	138	1	0
1	1G	540	0	138	1	0
1	1I	540	0	138	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1K	540	0	138	0	0
1	2A	540	0	138	1	0
1	2C	540	0	138	0	0
1	2E	540	0	138	1	0
1	2G	540	0	138	1	0
1	2I	540	0	138	1	0
1	2K	540	0	138	1	0
1	3A	540	0	138	1	0
1	3C	540	0	138	1	0
1	3E	540	0	138	0	0
1	3G	540	0	138	0	0
1	3I	540	0	138	1	0
1	3K	540	0	138	1	0
2	1B	1724	0	462	2	0
2	1D	1724	0	462	2	0
2	1F	1724	0	462	2	0
2	1H	1724	0	462	2	0
2	1J	1724	0	462	1	0
2	1L	1724	0	462	1	0
2	2B	1724	0	462	2	0
2	2D	1724	0	462	1	0
2	2F	1724	0	462	2	0
2	2H	1724	0	462	2	0
2	2J	1724	0	462	2	0
2	2L	1724	0	462	2	0
2	3B	1724	0	462	2	0
2	3D	1724	0	462	2	0
2	3F	1724	0	462	1	0
2	3H	1724	0	462	1	0
2	3J	1724	0	462	2	0
2	3L	1724	0	462	2	0
All	All	40752	0	10800	31	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.

All (31) 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)
2:2H:443:VAL:C	2:2H:445:SER:N	2.71	0.44
2:1B:443:VAL:C	2:1B:445:SER:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1F:443:VAL:C	2:1F:445:SER:N	2.72	0.44
1:1G:33:LYS:O	2:1H:159:GLY:N	2.48	0.44
2:3D:443:VAL:C	2:3D:445:SER:N	2.72	0.44
2:1H:443:VAL:C	2:1H:445:SER:N	2.72	0.43
2:3L:443:VAL:C	2:3L:445:SER:N	2.72	0.43
2:2F:443:VAL:C	2:2F:445:SER:N	2.72	0.43
2:2L:443:VAL:C	2:2L:445:SER:N	2.71	0.43
2:3B:443:VAL:C	2:3B:445:SER:N	2.72	0.43
2:3F:443:VAL:C	2:3F:445:SER:N	2.71	0.43
2:2B:443:VAL:C	2:2B:445:SER:N	2.72	0.43
1:2A:33:LYS:O	2:2B:159:GLY:N	2.48	0.43
2:2J:443:VAL:C	2:2J:445:SER:N	2.71	0.43
1:3A:33:LYS:O	2:3B:159:GLY:N	2.48	0.43
2:2D:443:VAL:C	2:2D:445:SER:N	2.71	0.43
2:3J:443:VAL:C	2:3J:445:SER:N	2.72	0.43
1:3K:33:LYS:O	2:3L:159:GLY:N	2.48	0.43
2:1L:443:VAL:C	2:1L:445:SER:N	2.72	0.43
1:1C:33:LYS:O	2:1D:159:GLY:N	2.48	0.43
2:3H:443:VAL:C	2:3H:445:SER:N	2.72	0.42
1:1A:33:LYS:O	2:1B:159:GLY:N	2.48	0.42
2:1J:443:VAL:C	2:1J:445:SER:N	2.71	0.42
2:1D:443:VAL:C	2:1D:445:SER:N	2.71	0.42
1:2E:33:LYS:O	2:2F:159:GLY:N	2.48	0.41
1:2I:33:LYS:O	2:2J:159:GLY:N	2.48	0.41
1:2G:33:LYS:O	2:2H:159:GLY:N	2.48	0.41
1:2K:33:LYS:O	2:2L:159:GLY:N	2.48	0.41
1:3I:33:LYS:O	2:3J:159:GLY:N	2.48	0.41
1:3C:33:LYS:O	2:3D:159:GLY:N	2.48	0.41
1:1E:33:LYS:O	2:1F:159:GLY:N	2.48	0.40

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 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	1A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	1C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	1E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	1G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	1I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	1K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	2K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
1	3K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	12	53
2	1B	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	1D	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	1F	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	1H	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	1J	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	1L	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	2B	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	2D	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	2F	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	2H	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	2J	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	2L	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	3B	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	3D	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3F	429/494 (87%)	404 (94%)	20 (5%)	5 (1%)	15	57
2	3H	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	15	57
2	3J	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
2	3L	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	15	57
All	All	10116/11844 (85%)	9548 (94%)	442 (4%)	126 (1%)	20	57

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	129	PRO
2	1B	242	LEU
2	1B	444	ARG
1	1C	129	PRO
2	1D	242	LEU
2	1D	444	ARG
1	1E	129	PRO
2	1F	242	LEU
2	1F	444	ARG
1	1G	129	PRO
2	1H	242	LEU
2	1H	444	ARG
1	1I	129	PRO
2	1J	242	LEU
2	1J	444	ARG
1	1K	129	PRO
2	1L	242	LEU
2	1L	444	ARG
1	2A	129	PRO
2	2B	242	LEU
2	2B	444	ARG
1	2C	129	PRO
2	2D	242	LEU
2	2D	444	ARG
1	2E	129	PRO
2	2F	242	LEU
2	2F	444	ARG
1	2G	129	PRO
2	2H	242	LEU
2	2H	444	ARG
1	2I	129	PRO
2	2J	242	LEU

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Mol	Chain	Res	Type
2	2J	444	ARG
1	2K	129	PRO
2	2L	242	LEU
2	2L	444	ARG
1	3A	129	PRO
2	3B	242	LEU
2	3B	444	ARG
1	3C	129	PRO
2	3D	242	LEU
2	3D	444	ARG
1	3E	129	PRO
2	3F	242	LEU
2	3F	444	ARG
1	3G	129	PRO
2	3H	242	LEU
2	3H	444	ARG
1	3I	129	PRO
2	3J	242	LEU
2	3J	444	ARG
1	3K	129	PRO
2	3L	242	LEU
2	3L	444	ARG
2	1B	260	ALA
2	1B	268	VAL
2	1D	260	ALA
2	1D	268	VAL
2	1F	260	ALA
2	1F	268	VAL
2	1H	260	ALA
2	1H	268	VAL
2	1J	260	ALA
2	1J	268	VAL
2	1L	260	ALA
2	1L	268	VAL
2	2B	260	ALA
2	2B	268	VAL
2	2D	260	ALA
2	2D	268	VAL
2	2F	260	ALA
2	2F	268	VAL
2	2H	260	ALA
2	2H	268	VAL

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Mol	Chain	Res	Type
2	2J	260	ALA
2	2J	268	VAL
2	2L	260	ALA
2	2L	268	VAL
2	3B	260	ALA
2	3B	268	VAL
2	3D	260	ALA
2	3D	268	VAL
2	3F	260	ALA
2	3F	268	VAL
2	3H	260	ALA
2	3H	268	VAL
2	3J	260	ALA
2	3J	268	VAL
2	3L	260	ALA
2	3L	268	VAL
1	1A	70	ASN
1	1C	70	ASN
1	1E	70	ASN
1	1G	70	ASN
1	1I	70	ASN
1	1K	70	ASN
1	2A	70	ASN
1	2C	70	ASN
1	2E	70	ASN
1	2G	70	ASN
1	2I	70	ASN
1	2K	70	ASN
1	3A	70	ASN
1	3C	70	ASN
1	3E	70	ASN
1	3G	70	ASN
1	3I	70	ASN
1	3K	70	ASN
2	1B	298	PRO
2	1D	298	PRO
2	1F	298	PRO
2	1H	298	PRO
2	1J	298	PRO
2	1L	298	PRO
2	2B	298	PRO
2	2D	298	PRO

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Mol	Chain	Res	Type
2	2F	298	PRO
2	2H	298	PRO
2	2J	298	PRO
2	2L	298	PRO
2	3B	298	PRO
2	3D	298	PRO
2	3F	298	PRO
2	3H	298	PRO
2	3J	298	PRO
2	3L	298	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.