



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:35 AM UTC

PDB ID : 6U5B / pdb_00006u5b
EMDB ID : EMD-20643
Title : CryoEM Structure of Pyocin R2 - precontracted - baseplate
Authors : Ge, P.; Avaylon, J.; Scholl, D.; Shneider, M.M.; Browning, C.; Buth, S.A.; Plattner, M.; Ding, K.; Leiman, P.G.; Miller, J.F.; Zhou, Z.H.
Deposited on : 2019-08-27
Resolution : 3.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

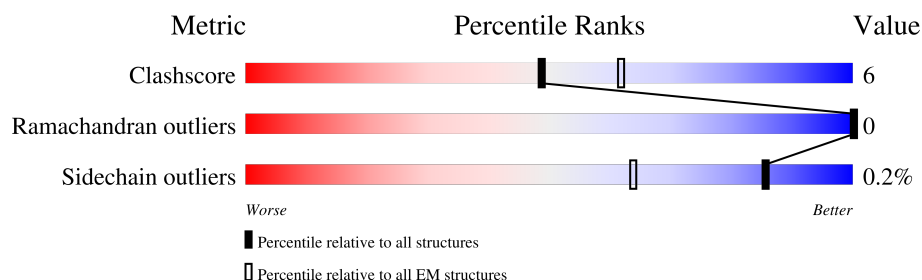
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



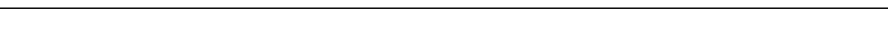
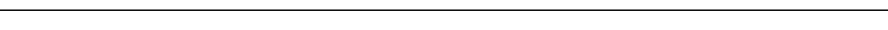
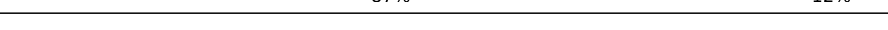
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	m	295	82% 16% .
1	n	295	81% 17% .
1	o	295	82% 17% .
1	p	295	82% 17% .
1	q	295	81% 17% .
1	r	295	82% 16% .
1	s	295	80% 18% .
1	t	295	82% 17% .
1	u	295	81% 17% .

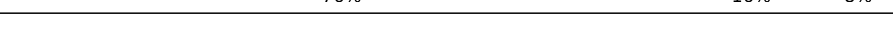
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Mol	Chain	Length	Quality of chain
1	v	295	 79% 19% .
1	w	295	 80% 19% .
1	x	295	 82% 17% .
2	A	386	 89% 10% .
2	B	386	 89% 10% .
2	C	386	 89% 10% .
2	D	386	 90% 9% .
2	E	386	 90% 9% .
2	F	386	 90% 9% .
2	M	386	 86% 13% .
2	N	386	 85% 13% .
2	O	386	 86% 13% .
2	P	386	 87% 12% .
2	Q	386	 87% 12% .
2	R	386	 85% 14% .
3	G	167	 84% 16% .
3	H	167	 84% 15% .
3	I	167	 86% 14% .
3	J	167	 83% 16% .
3	K	167	 84% 15% .
3	L	167	 84% 15% .
3	S	167	 81% 18% .
3	T	167	 82% 17% .
3	U	167	 80% 19% .
3	V	167	 81% 17% .

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Mol	Chain	Length	Quality of chain
3	W	167	 81% 17% .
3	X	167	 82% 17% .
4	0	177	 69% 16% 15%
4	1	177	 73% 12% 15%
4	2	177	 71% 14% 15%
4	3	177	 72% 14% 15%
4	4	177	 72% 13% 15%
4	5	177	 72% 13% 15%
5	a	108	 75% 17% 8%
5	b	108	 74% 18% 8%
5	c	108	 79% 13% 8%
5	d	108	 78% 14% 8%
5	e	108	 77% 15% 8%
5	f	108	 76% 16% 8%
6	6	68	 68% 13% 19%
6	7	68	 72% 9% 19%
6	8	68	 72% 9% 19%
6	9	68	 72% 9% 19%
6	Y	68	 72% 9% 19%
6	Z	68	 72% 9% 19%
7	g	290	 82% 16% .
7	h	290	 83% 16% .
7	i	290	 85% 13% .
7	j	290	 84% 14% .
7	k	290	 84% 14% .

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Mol	Chain	Length	Quality of chain
7	1	290	 82% 16% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 103392 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 Tri1a PA0618.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	n	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	q	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	r	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	o	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	p	291	Total	C	N	O	S	0	0
			2218	1394	392	428	4		
1	s	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		
1	t	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		
1	w	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		
1	x	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		
1	u	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		
1	v	292	Total	C	N	O	S	0	0
			2223	1397	393	429	4		

- Molecule 2 is a protein called Sheath PA0622.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	N	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	Q	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	O	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	P	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	A	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	B	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	E	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	F	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	C	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		
2	D	382	Total	C	N	O	S	0	0
			2876	1813	503	552	8		

- Molecule 3 is a protein called Tube PA0623.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	T	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	W	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	X	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	U	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	V	165	Total	C	N	O	S	0	0
			1250	792	213	240	5		
3	G	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
3	H	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
3	K	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
3	L	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		
3	J	166	Total	C	N	O	S	0	0
			1255	795	214	242	4		

- Molecule 4 is a protein called Tri2 PA0619.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		
4	1	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		
4	4	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		
4	5	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		
4	2	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		
4	3	151	Total	C	N	O	S	0	0
			1202	754	220	227	1		

- Molecule 5 is a protein called Sheath Initiator PA0617.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	99	Total	C	N	O	S	0	0
			759	474	144	136	5		
5	b	99	Total	C	N	O	S	0	0
			759	474	144	136	5		
5	e	99	Total	C	N	O	S	0	0
			759	474	144	136	5		
5	f	99	Total	C	N	O	S	0	0
			759	474	144	136	5		
5	c	99	Total	C	N	O	S	0	0
			759	474	144	136	5		
5	d	99	Total	C	N	O	S	0	0
			759	474	144	136	5		

- Molecule 6 is a protein called Glue PA0627.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	55	Total	C	N	O	S	0	0
			413	258	68	82	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	55	Total 413	C 258	N 68	O 82	S 5	0	0
6	Y	55	Total 413	C 258	N 68	O 82	S 5	0	0
6	Z	55	Total 413	C 258	N 68	O 82	S 5	0	0
6	8	55	Total 413	C 258	N 68	O 82	S 5	0	0
6	9	55	Total 413	C 258	N 68	O 82	S 5	0	0

- Molecule 7 is a protein called Ripcord PA0626.

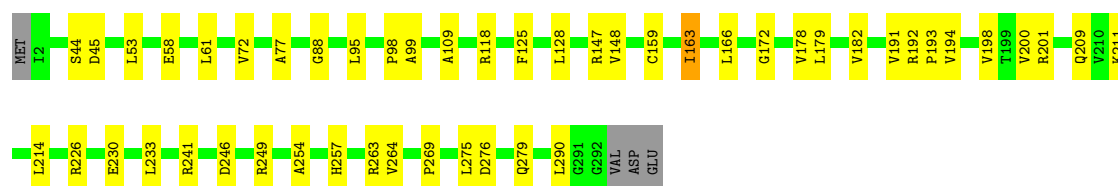
Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	285	Total 2160	C 1352	N 401	O 402	S 5	0	0
7	g	285	Total 2160	C 1352	N 401	O 402	S 5	0	0
7	l	285	Total 2160	C 1352	N 401	O 402	S 5	0	0
7	k	285	Total 2160	C 1352	N 401	O 402	S 5	0	0
7	j	285	Total 2160	C 1352	N 401	O 402	S 5	0	0
7	i	285	Total 2160	C 1352	N 401	O 402	S 5	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. 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.

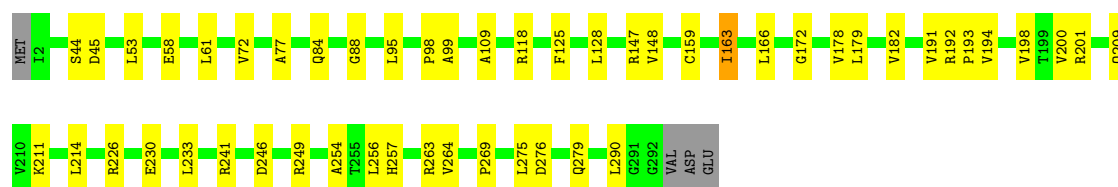
- Molecule 1: Tri1a PA0618

Chain m: 



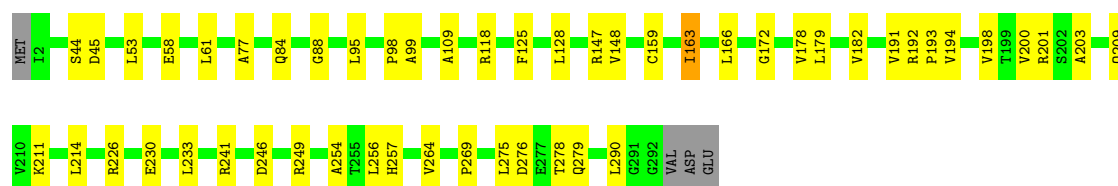
- Molecule 1: Tri1a PA0618

Chain n: 



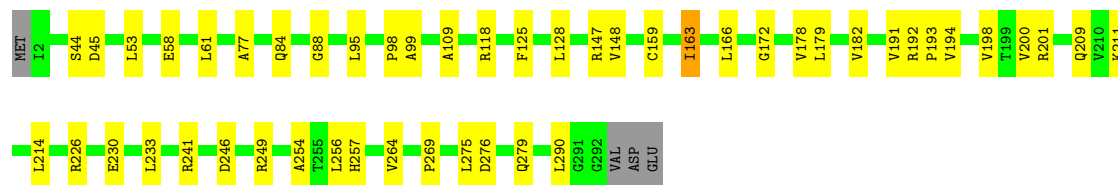
- Molecule 1: Tri1a PA0618

Chain q: 



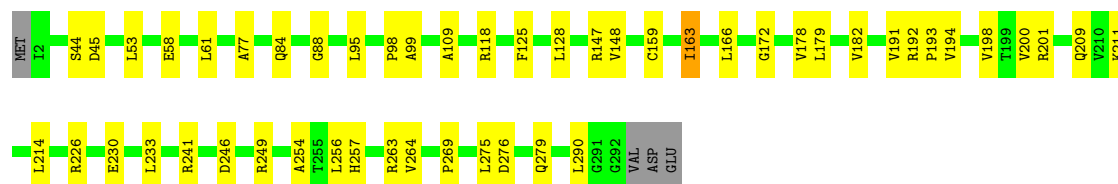
- Molecule 1: Tri1a PA0618

Chain r: 



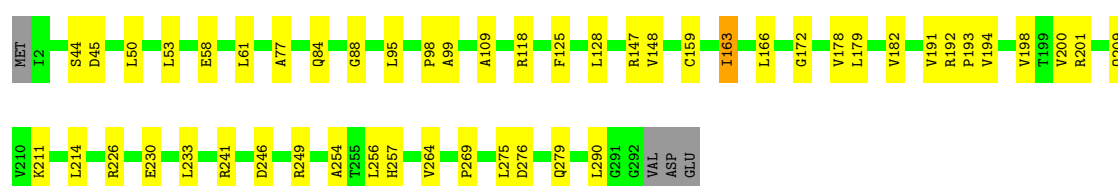
- Molecule 1: Tri1a PA0618

Chain o:  82% 17%



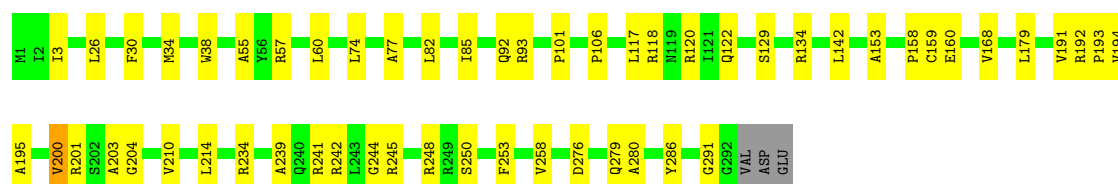
- Molecule 1: Tri1a PA0618

Chain p:  82% 17%



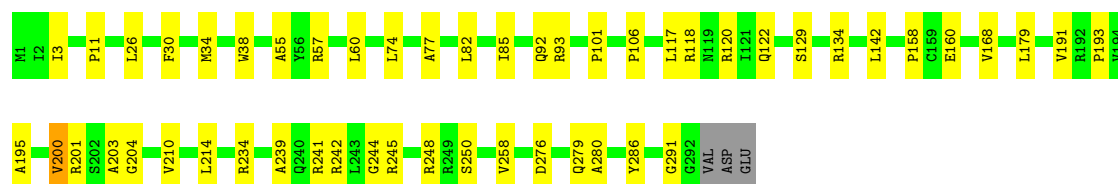
- Molecule 1: Tri1a PA0618

Chain s:  80% 18%



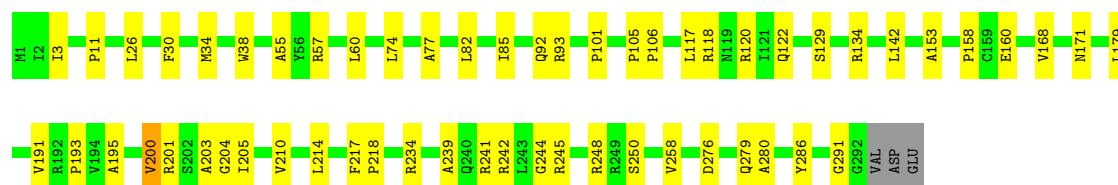
- Molecule 1: Tri1a PA0618

Chain t:  82% 17%

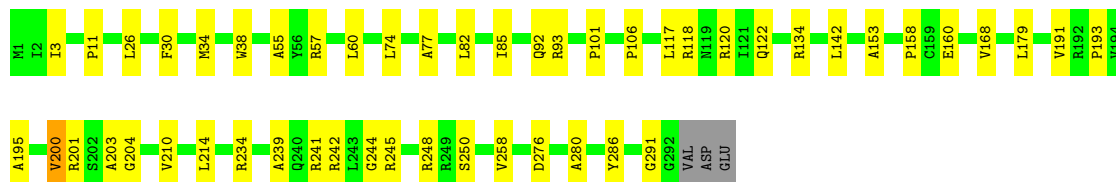


- Molecule 1: Tri1a PA0618

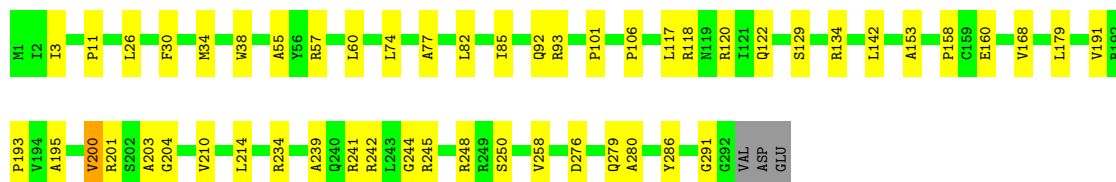
Chain w:  80% 19%



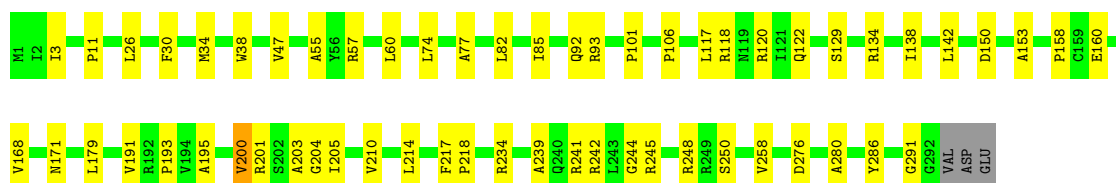
• Molecule 1: Tri1a PA0618

Chain x:  82% 17%

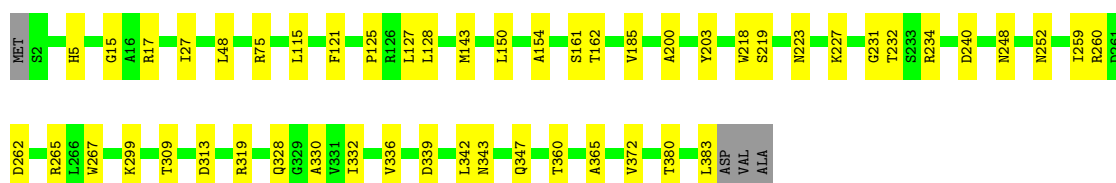
• Molecule 1: Tri1a PA0618

Chain u:  81% 17%

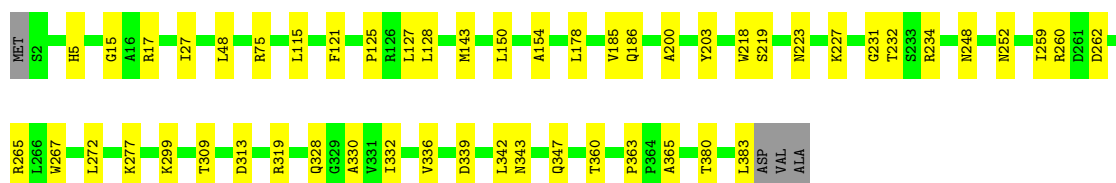
• Molecule 1: Tri1a PA0618

Chain v:  79% 19%

• Molecule 2: Sheath PA0622

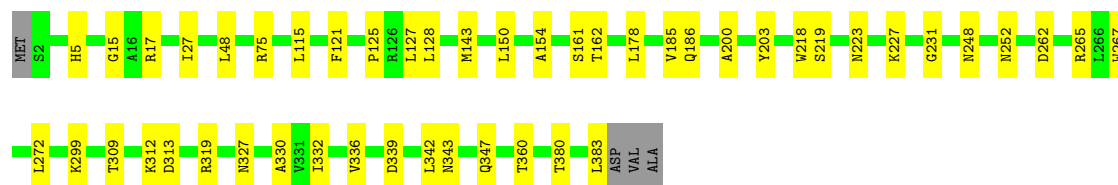
Chain M:  86% 13%

• Molecule 2: Sheath PA0622

Chain N:  85% 13%

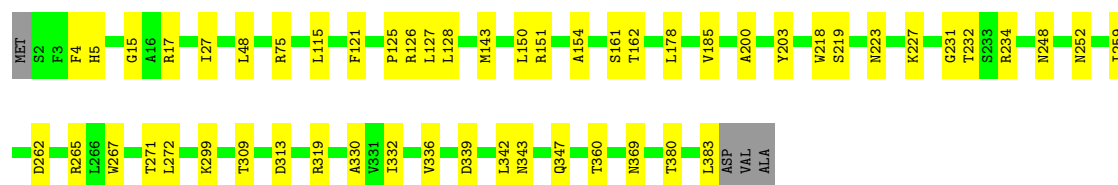
- Molecule 2: Sheath PA0622

Chain Q:  87% 12%



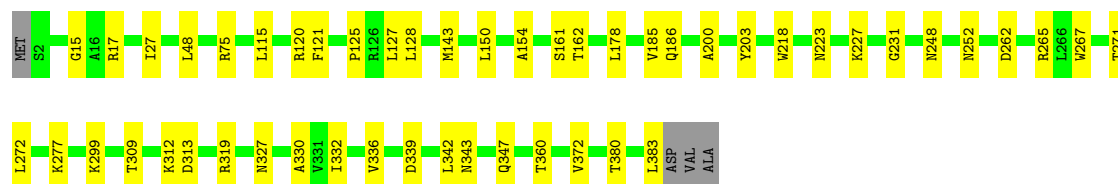
- Molecule 2: Sheath PA0622

Chain R:  85% 14%



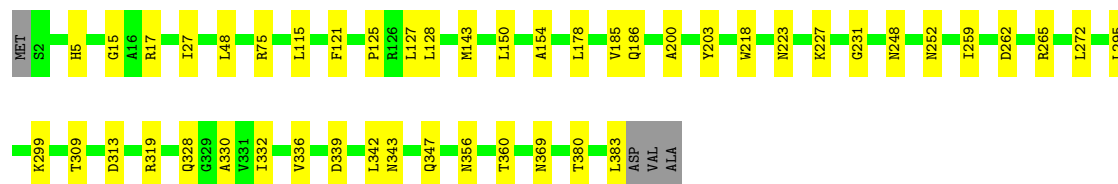
- Molecule 2: Sheath PA0622

Chain O:  86% 13%



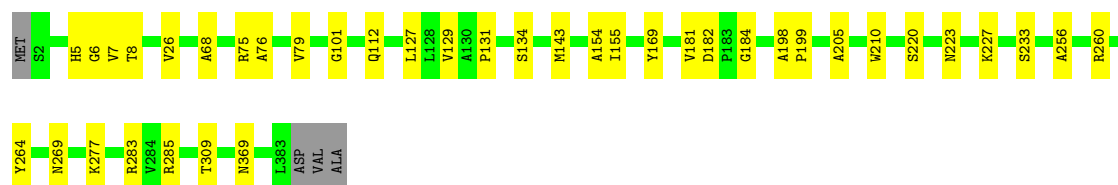
- Molecule 2: Sheath PA0622

Chain P:  87% 12%

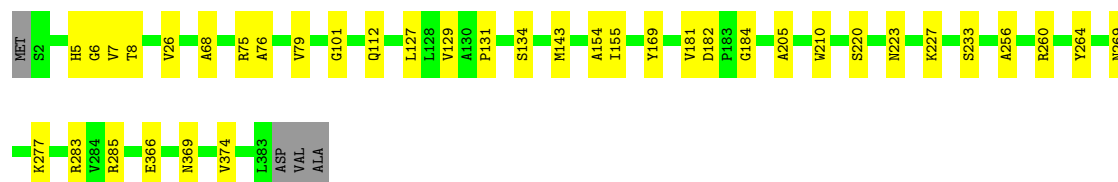


- Molecule 2: Sheath PA0622

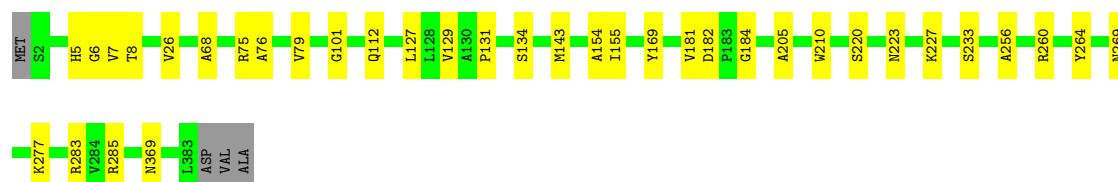
Chain A:  89% 10%



• Molecule 2: Sheath PA0622

Chain B:  89% 10%

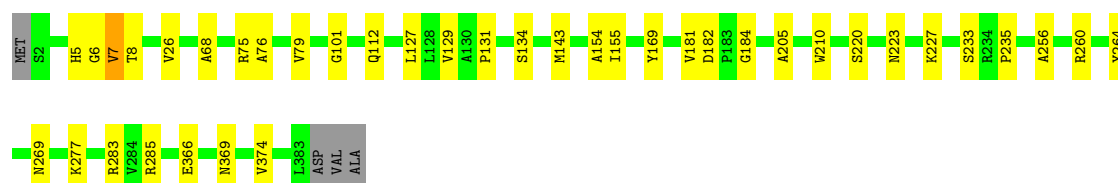
• Molecule 2: Sheath PA0622

Chain E:  90% 9%

• Molecule 2: Sheath PA0622

Chain F:  90% 9%

• Molecule 2: Sheath PA0622

Chain C:  89% 10%

• Molecule 2: Sheath PA0622

Chain D:  90% 9%

● Molecule 3: Tube PA0623

Chain S:  81% 18%

● Molecule 3: Tube PA0623

Chain T:  82% 17%

● Molecule 3: Tube PA0623

Chain W:  81% 17%

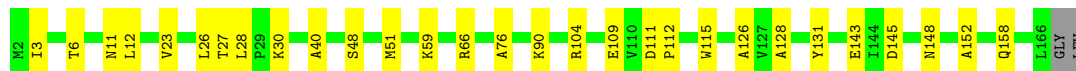
● Molecule 3: Tube PA0623

Chain X:  82% 17%

● Molecule 3: Tube PA0623

Chain U:  80% 19%

● Molecule 3: Tube PA0623

Chain V:  81% 17%

● Molecule 3: Tube PA0623

Chain G:  84% 16%

● Molecule 3: Tube PA0623

Chain H:  84% 15%



- Molecule 3: Tube PA0623

Chain K:  84% 15%



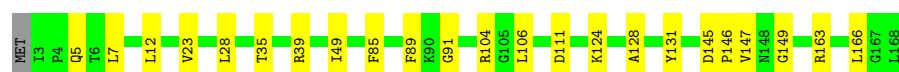
- Molecule 3: Tube PA0623

Chain L:  84% 15%



- Molecule 3: Tube PA0623

Chain I:  86% 14%



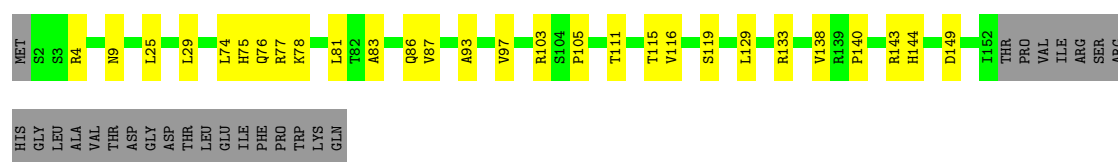
- Molecule 3: Tube PA0623

Chain J:  83% 16%



- Molecule 4: Tri2 PA0619

Chain 0:  69% 16% 15%



- Molecule 4: Tri2 PA0619

Chain 1:  73% 12% 15%



LEU
GLU
ILE
PHE
PRO
TRP
LYS
GLN

● Molecule 4: Tri2 PA0619

Chain 4:  72% 13% 15%

MET S2 S3 R4 N9 L25 L74 H75 Q76 Q77 K78 L81 T82 A83 Q86 V87 A93 V97 T115 V116 S119 L129 R133 V138 R139 P140 R143 H144 D149 I152 THR PRO VAL ILE ARG SER ARG HIS GLY LEU ALA VAL THR ASP GLY

ASP
THR
LEU
GLU
ILE
PHE
PRO
TRP
LYS
GLN

● Molecule 4: Tri2 PA0619

Chain 5:  72% 13% 15%

MET S2 S3 R4 N9 L74 H75 K78 L81 T82 A83 Q86 V87 A93 V97 R103 S104 P105 T115 V116 S119 L129 R133 V138 R139 P140 R143 H144 D149 I152 THR PRO VAL ILE ARG SER ARG HIS GLY LEU ALA VAL THR ASP

GLY
ASP
THR
LEU
GLU
ILE
PHE
PRO
TRP
LYS
GLN

● Molecule 4: Tri2 PA0619

Chain 2:  71% 14% 15%

MET S2 S3 R4 N9 L25 L74 H75 Q76 Q77 K78 L81 T82 A83 Q86 V87 A93 V97 R103 S104 P105 T115 V116 S119 L129 R133 V138 R139 P140 R143 H144 D149 I152 THR PRO VAL ILE ARG SER ARG HIS GLY LEU ALA

VAL
THR
ASP
GLY
ASP
THR
LEU
GLU
ILE
PHE
PRO
TRP
LYS
GLN

● Molecule 4: Tri2 PA0619

Chain 3:  72% 14% 15%

MET S2 S3 R4 N9 L74 H75 Q76 Q77 K78 L81 T82 A83 Q86 V87 A93 V97 R103 S104 P105 T115 V116 S119 L129 R133 V138 R139 P140 R143 H144 D149 I152 THR PRO VAL ILE ARG SER ARG HIS GLY LEU ALA THR

ASP
GLY
ASP
THR
LEU
GLU
ILE
PHE
PRO
TRP
LYS
GLN

● Molecule 5: Sheath Initiator PA0617

Chain a:  75% 17% 8%

H1 N4 G9 L10 P11 L18 T27 T28 P29 S32 R33 R34 P37 R45 P50 V51 Q60 R65 R69 I74 V79 L93 G99 GLU ASN ILE ASN MET GLU VAL SER ALA

● Molecule 5: Sheath Initiator PA0617

Chain b:  74% 18% 8%



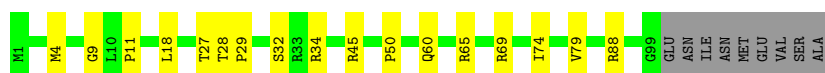
- Molecule 5: Sheath Initiator PA0617

Chain e: 77% 15% 8%



- Molecule 5: Sheath Initiator PA0617

Chain f: 76% 16% 8%



- Molecule 5: Sheath Initiator PA0617

Chain c: 79% 13% 8%



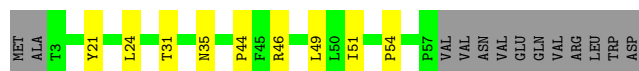
- Molecule 5: Sheath Initiator PA0617

Chain d: 78% 14% 8%



- Molecule 6: Glue PA0627

Chain 6: 68% 13% 19%



- Molecule 6: Glue PA0627

Chain 7: 72% 9% 19%



- Molecule 6: Glue PA0627

Chain Y: 72% 9% 19%



- Molecule 6: Glue PA0627

Chain Z: 72% 9% 19%



- Molecule 6: Glue PA0627

Chain 8: 72% 9% 19%



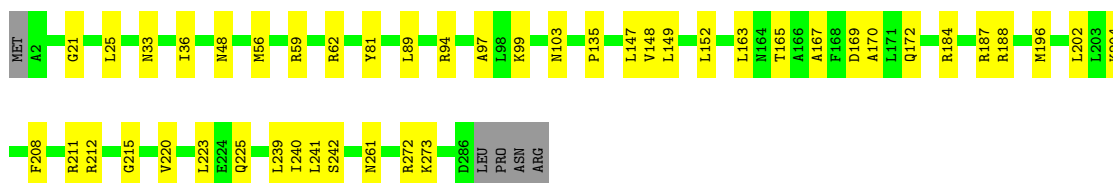
- Molecule 6: Glue PA0627

Chain 9: 72% 9% 19%



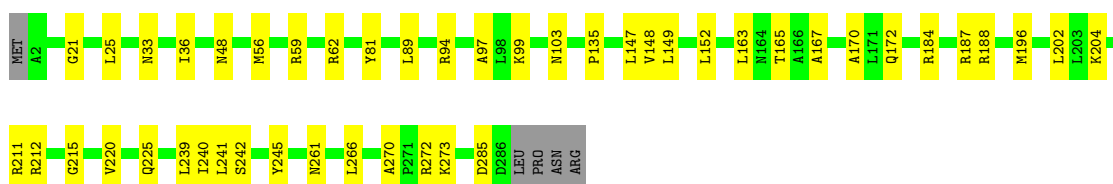
- Molecule 7: Ripcord PA0626

Chain h: 83% 16% .



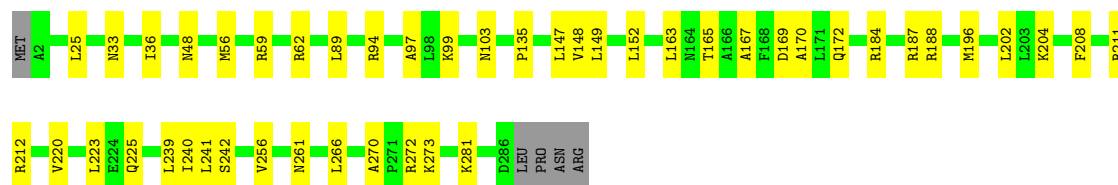
- Molecule 7: Ripcord PA0626

Chain g: 82% 16% .



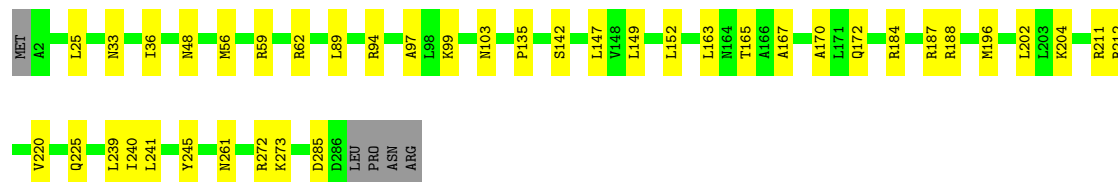
- Molecule 7: Ripcord PA0626

Chain l: 82% 16% .



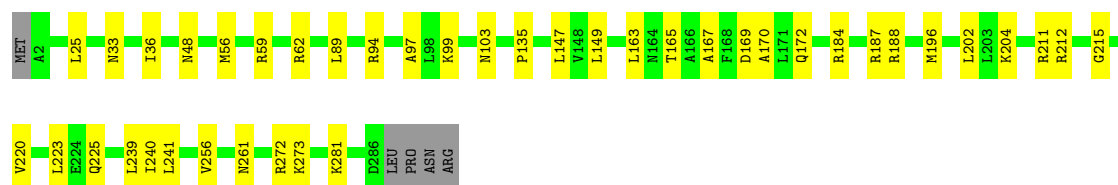
• Molecule 7: Ripcord PA0626

Chain k: 84% 14% .



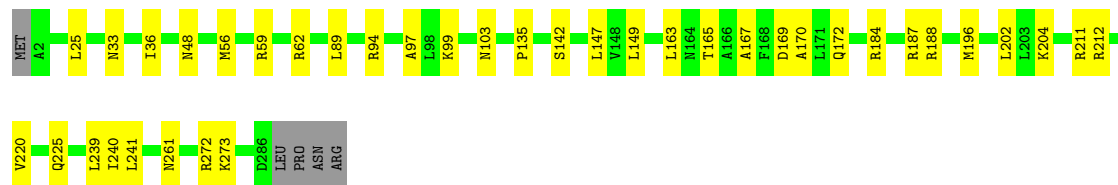
• Molecule 7: Ripcord PA0626

Chain j: 84% 14% .



• Molecule 7: Ripcord PA0626

Chain i: 85% 13% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	22001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	m	0.22	0/2253	0.56	0/3069
1	n	0.22	0/2253	0.56	0/3069
1	o	0.22	0/2253	0.56	0/3069
1	p	0.22	0/2253	0.56	0/3069
1	q	0.22	0/2253	0.56	0/3069
1	r	0.22	0/2253	0.56	0/3069
1	s	0.23	0/2258	0.55	1/3076 (0.0%)
1	t	0.23	0/2258	0.55	1/3076 (0.0%)
1	u	0.23	0/2258	0.55	1/3076 (0.0%)
1	v	0.23	0/2258	0.55	1/3076 (0.0%)
1	w	0.23	0/2258	0.55	1/3076 (0.0%)
1	x	0.23	0/2258	0.55	1/3076 (0.0%)
2	A	0.21	0/2934	0.54	1/3999 (0.0%)
2	B	0.21	0/2934	0.54	1/3999 (0.0%)
2	C	0.21	0/2934	0.54	1/3999 (0.0%)
2	D	0.21	0/2934	0.54	1/3999 (0.0%)
2	E	0.21	0/2934	0.54	1/3999 (0.0%)
2	F	0.21	0/2934	0.54	0/3999
2	M	0.23	0/2934	0.53	0/3999
2	N	0.23	0/2934	0.53	0/3999
2	O	0.23	0/2934	0.53	0/3999
2	P	0.23	0/2934	0.53	0/3999
2	Q	0.23	0/2934	0.53	0/3999
2	R	0.23	0/2934	0.53	0/3999
3	G	0.28	0/1277	0.60	2/1724 (0.1%)
3	H	0.28	0/1277	0.60	2/1724 (0.1%)
3	I	0.28	0/1277	0.60	2/1724 (0.1%)
3	J	0.28	0/1277	0.60	2/1724 (0.1%)
3	K	0.28	0/1277	0.60	2/1724 (0.1%)
3	L	0.28	0/1277	0.60	2/1724 (0.1%)
3	S	0.26	0/1272	0.53	0/1718
3	T	0.27	0/1272	0.53	0/1718
3	U	0.26	0/1272	0.53	0/1718
3	V	0.26	0/1272	0.53	0/1718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	W	0.27	0/1272	0.53	0/1718
3	X	0.27	0/1272	0.53	0/1718
4	0	0.24	0/1229	0.61	0/1680
4	1	0.24	0/1229	0.61	0/1680
4	2	0.24	0/1229	0.61	0/1680
4	3	0.24	0/1229	0.61	0/1680
4	4	0.24	0/1229	0.61	0/1680
4	5	0.24	0/1229	0.61	0/1680
5	a	0.24	0/770	0.53	0/1036
5	b	0.24	0/770	0.53	0/1036
5	c	0.24	0/770	0.53	0/1036
5	d	0.24	0/770	0.53	0/1036
5	e	0.24	0/770	0.53	0/1036
5	f	0.24	0/770	0.53	0/1036
6	6	0.22	0/422	0.51	0/575
6	7	0.22	0/422	0.51	0/575
6	8	0.22	0/422	0.51	0/575
6	9	0.22	0/422	0.51	0/575
6	Y	0.22	0/422	0.51	0/575
6	Z	0.22	0/422	0.51	0/575
7	g	0.25	0/2194	0.57	0/2970
7	h	0.25	0/2194	0.57	0/2970
7	i	0.25	0/2194	0.57	0/2970
7	j	0.25	0/2194	0.58	0/2970
7	k	0.25	0/2194	0.57	0/2970
7	l	0.25	0/2194	0.57	0/2970
All	All	0.24	0/105258	0.55	23/143076 (0.0%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	147	VAL	CA-C-N	5.64	132.31	121.54
3	K	147	VAL	C-N-CA	5.64	132.31	121.54
3	H	147	VAL	CA-C-N	5.63	132.30	121.54
3	H	147	VAL	C-N-CA	5.63	132.30	121.54
3	L	147	VAL	CA-C-N	5.63	132.30	121.54

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	m	2218	0	2222	33	0
1	n	2218	0	2222	33	0
1	o	2218	0	2222	32	0
1	p	2218	0	2222	31	0
1	q	2218	0	2222	32	0
1	r	2218	0	2222	30	0
1	s	2223	0	2227	43	0
1	t	2223	0	2227	35	0
1	u	2223	0	2227	34	0
1	v	2223	0	2227	39	0
1	w	2223	0	2227	39	0
1	x	2223	0	2227	34	0
2	A	2876	0	2837	23	0
2	B	2876	0	2837	24	0
2	C	2876	0	2837	27	0
2	D	2876	0	2837	22	0
2	E	2876	0	2837	21	0
2	F	2876	0	2837	21	0
2	M	2876	0	2837	32	0
2	N	2876	0	2837	34	0
2	O	2876	0	2837	33	0
2	P	2876	0	2837	33	0
2	Q	2876	0	2837	31	0
2	R	2876	0	2837	33	0
3	G	1255	0	1246	16	0
3	H	1255	0	1246	16	0
3	I	1255	0	1246	14	0
3	J	1255	0	1246	18	0
3	K	1255	0	1246	17	0
3	L	1255	0	1246	16	0
3	S	1250	0	1241	29	0
3	T	1250	0	1241	26	0
3	U	1250	0	1241	29	0
3	V	1250	0	1241	30	0
3	W	1250	0	1241	29	0
3	X	1250	0	1241	26	0
4	0	1202	0	1202	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1	1202	0	1202	18	0
4	2	1202	0	1202	18	0
4	3	1202	0	1202	17	0
4	4	1202	0	1202	18	0
4	5	1202	0	1202	17	0
5	a	759	0	794	16	0
5	b	759	0	794	18	0
5	c	759	0	794	11	0
5	d	759	0	794	12	0
5	e	759	0	794	13	0
5	f	759	0	794	13	0
6	6	413	0	389	6	0
6	7	413	0	389	5	0
6	8	413	0	389	4	0
6	9	413	0	389	5	0
6	Y	413	0	389	4	0
6	Z	413	0	389	4	0
7	g	2160	0	2202	34	0
7	h	2160	0	2202	34	0
7	i	2160	0	2202	28	0
7	j	2160	0	2202	30	0
7	k	2160	0	2202	30	0
7	l	2160	0	2202	36	0
All	All	103392	0	103182	1157	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 6.

The worst 5 of 1157 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)
3:W:26:LEU:HB2	3:V:115:TRP:HB2	1.70	0.74
2:E:8:THR:OG1	2:F:369:ASN:ND2	2.22	0.72
3:S:115:TRP:HB2	3:T:26:LEU:HB2	1.71	0.70
1:p:53:LEU:HD11	1:v:30:PHE:HB2	1.75	0.69
3:T:115:TRP:HB2	3:U:26:LEU:HB2	1.74	0.69

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	m	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	n	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	o	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	p	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	q	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	r	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	s	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	t	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	u	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	v	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	w	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	x	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
2	A	380/386 (98%)	345 (91%)	35 (9%)	0	100	100
2	B	380/386 (98%)	345 (91%)	35 (9%)	0	100	100
2	C	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	D	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	E	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	F	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	M	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	N	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	O	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	P	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	Q	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	R	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
3	G	164/167 (98%)	144 (88%)	20 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	I	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	J	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	K	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	L	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	S	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	T	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	U	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	V	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	W	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	X	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
4	0	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	1	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	2	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	3	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	4	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	5	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
5	a	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	b	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	c	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	d	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	e	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	f	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
6	6	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	7	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	8	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	9	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	Y	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	Z	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
7	g	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	h	283/290 (98%)	259 (92%)	24 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	i	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	j	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	k	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	l	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
All	All	13488/14034 (96%)	12292 (91%)	1196 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	m	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	n	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	o	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	p	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	q	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	r	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	s	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	t	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	u	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	v	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	w	226/230 (98%)	225 (100%)	1 (0%)	84	81
1	x	226/230 (98%)	225 (100%)	1 (0%)	84	81
2	A	295/298 (99%)	294 (100%)	1 (0%)	86	83
2	B	295/298 (99%)	294 (100%)	1 (0%)	86	83
2	C	295/298 (99%)	294 (100%)	1 (0%)	86	83
2	D	295/298 (99%)	294 (100%)	1 (0%)	86	83
2	E	295/298 (99%)	294 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	295/298 (99%)	294 (100%)	1 (0%)	86	83
2	M	295/298 (99%)	295 (100%)	0	100	100
2	N	295/298 (99%)	295 (100%)	0	100	100
2	O	295/298 (99%)	295 (100%)	0	100	100
2	P	295/298 (99%)	295 (100%)	0	100	100
2	Q	295/298 (99%)	295 (100%)	0	100	100
2	R	295/298 (99%)	295 (100%)	0	100	100
3	G	129/130 (99%)	129 (100%)	0	100	100
3	H	129/130 (99%)	129 (100%)	0	100	100
3	I	129/130 (99%)	129 (100%)	0	100	100
3	J	129/130 (99%)	129 (100%)	0	100	100
3	K	129/130 (99%)	129 (100%)	0	100	100
3	L	129/130 (99%)	129 (100%)	0	100	100
3	S	129/130 (99%)	129 (100%)	0	100	100
3	T	129/130 (99%)	129 (100%)	0	100	100
3	U	129/130 (99%)	129 (100%)	0	100	100
3	V	129/130 (99%)	129 (100%)	0	100	100
3	W	129/130 (99%)	129 (100%)	0	100	100
3	X	129/130 (99%)	129 (100%)	0	100	100
4	0	134/157 (85%)	134 (100%)	0	100	100
4	1	134/157 (85%)	134 (100%)	0	100	100
4	2	134/157 (85%)	134 (100%)	0	100	100
4	3	134/157 (85%)	134 (100%)	0	100	100
4	4	134/157 (85%)	134 (100%)	0	100	100
4	5	134/157 (85%)	134 (100%)	0	100	100
5	a	82/90 (91%)	82 (100%)	0	100	100
5	b	82/90 (91%)	82 (100%)	0	100	100
5	c	82/90 (91%)	82 (100%)	0	100	100
5	d	82/90 (91%)	82 (100%)	0	100	100
5	e	82/90 (91%)	82 (100%)	0	100	100
5	f	82/90 (91%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	45/57 (79%)	45 (100%)	0	100	100
6	7	45/57 (79%)	45 (100%)	0	100	100
6	8	45/57 (79%)	45 (100%)	0	100	100
6	9	45/57 (79%)	45 (100%)	0	100	100
6	Y	45/57 (79%)	45 (100%)	0	100	100
6	Z	45/57 (79%)	45 (100%)	0	100	100
7	g	221/226 (98%)	221 (100%)	0	100	100
7	h	221/226 (98%)	221 (100%)	0	100	100
7	i	221/226 (98%)	221 (100%)	0	100	100
7	j	221/226 (98%)	221 (100%)	0	100	100
7	k	221/226 (98%)	221 (100%)	0	100	100
7	l	221/226 (98%)	221 (100%)	0	100	100
All	All	10692/11076 (96%)	10674 (100%)	18 (0%)	85	85

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	w	200	VAL
1	v	200	VAL
1	u	200	VAL
2	B	7	VAL
1	t	200	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	252	ASN
3	H	148	ASN
1	u	127	GLN
3	X	164	ASN
3	X	158	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-20643. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.