



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2025 – 07:32 PM JST

PDB ID : 9J1K / pdb_00009j1k
EMDB ID : EMD-61074
Title : Tip region of monocin
Authors : Wang, J.W.; Gu, Z.W.
Deposited on : 2024-08-05
Resolution : 2.88 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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

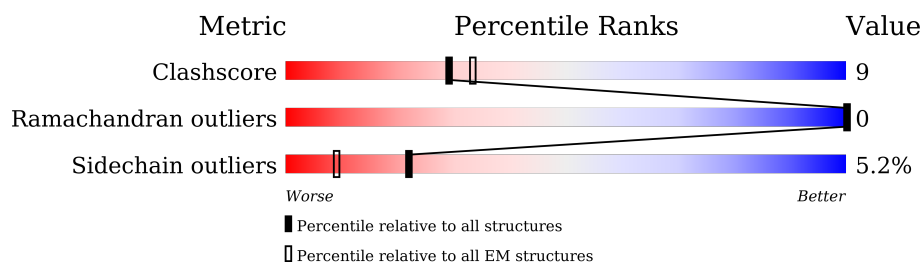
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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.















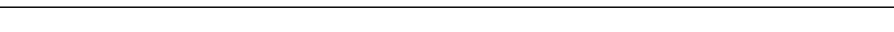

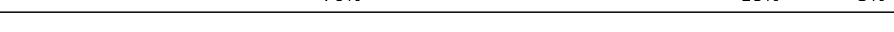

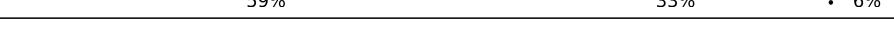








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	170	74% 19% • 5%
1	B	170	79% 14% • 5%
1	C	170	71% 22% • 5%
1	D	170	73% 21% • 5%
1	E	170	78% 15% • 5%
1	F	170	68% 25% • 5%
1	G	170	78% 15% • 5%
1	H	170	61% 30% • 6%
1	I	170	79% 15% • 5%












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Mol	Chain	Length	Quality of chain
1	N	170	
1	S	170	
1	T	170	
1	U	170	
1	V	170	
1	W	170	
1	Y	170	
1	Z	170	
1	a	170	
1	b	170	
1	c	170	
1	d	170	
1	e	170	
1	f	170	
1	g	170	
1	h	170	
1	n	170	
1	o	170	
1	p	170	
1	q	170	
1	r	170	
2	J	622	
2	O	622	
2	i	622	
3	K	272	

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Mol	Chain	Length	Quality of chain
3	P	272	 81% 18% .
3	X	272	 78% 21% .
3	j	272	 78% 21% .
3	k	272	 79% 19% .
3	s	272	 79% 19% .
4	L	378	 76% 23% .
4	Q	378	 81% 19%
4	l	378	 80% 19% .
5	M	99	 13% 14% 73%
5	R	99	 17% 10% 73%
5	m	99	 14% 13% 73%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60066 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 AA protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	E	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	F	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	G	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	H	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	a	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	b	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	c	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	d	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	g	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	A	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	B	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	C	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	I	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	N	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	S	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	T	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	V	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	W	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	Y	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	Z	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	e	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	f	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	h	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	n	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	o	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	p	161	Total	C	N	O	S	0	0
			1198	759	191	242	6		
1	q	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		
1	r	160	Total	C	N	O	S	0	0
			1194	757	190	241	6		

- Molecule 2 is a protein called FtbJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	50	Total	C	N	O	S	0	0
			396	247	70	77	2		
2	O	50	Total	C	N	O	S	0	0
			396	247	70	77	2		
2	i	50	Total	C	N	O	S	0	0
			396	247	70	77	2		

- Molecule 3 is a protein called FtbK.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		
3	P	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		
3	X	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		
3	j	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		
3	s	272	Total	C	N	O	S	0	0
			2210	1411	370	419	10		

- Molecule 4 is a protein called FtbL.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	378	Total	C	N	O	S	0	0
			3040	1930	499	600	11		
4	Q	378	Total	C	N	O	S	0	0
			3040	1930	499	600	11		
4	l	378	Total	C	N	O	S	0	0
			3040	1930	499	600	11		

- Molecule 5 is a protein called CCA-adding enzyme.

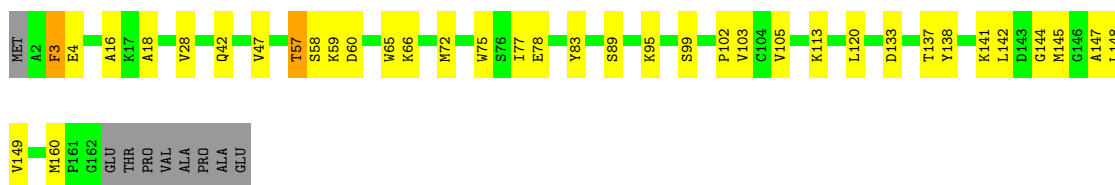
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	27	Total	C	N	O	0	0
			198	124	33	41		
5	R	27	Total	C	N	O	0	0
			198	124	33	41		
5	m	27	Total	C	N	O	0	0
			198	124	33	41		

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: AA protein

Chain D: 



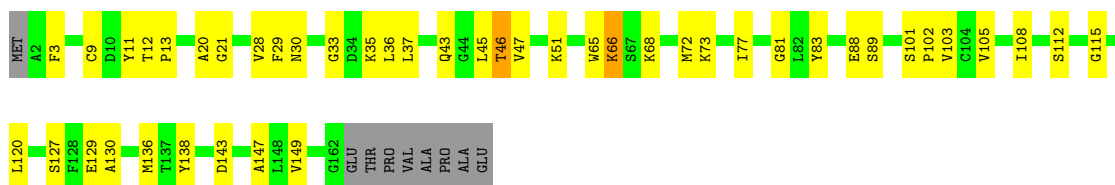
- Molecule 1: AA protein

Chain E: 




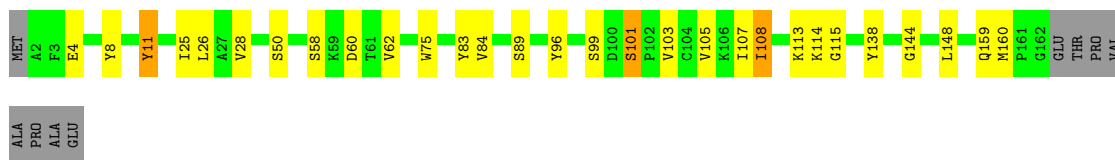
- Molecule 1: AA protein

Chain F: 



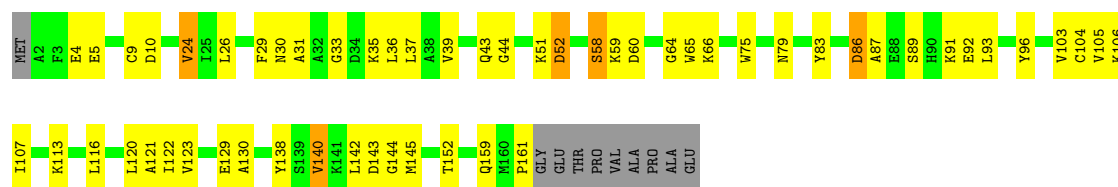
- Molecule 1: AA protein

Chain G: 




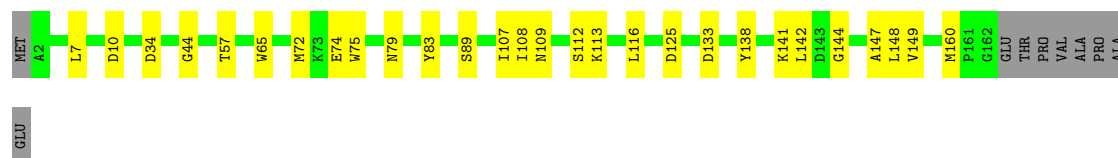
- Molecule 1: AA protein

Chain H:  61% 30% 6%



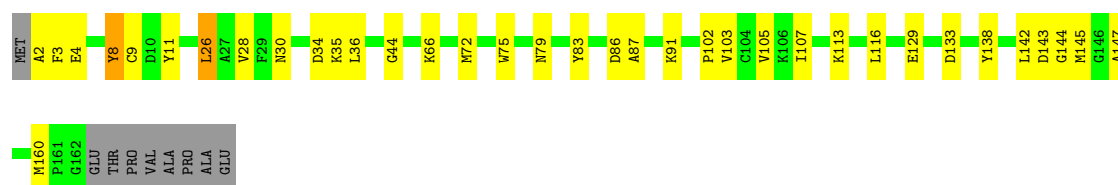
- Molecule 1: AA protein

Chain a:  78% 16% 5%



- Molecule 1: AA protein

Chain b:  74% 20% 5%



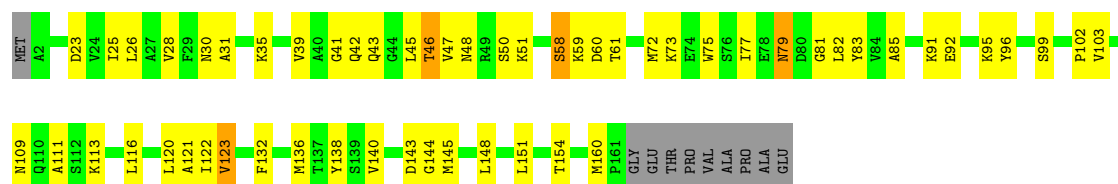
- Molecule 1: AA protein

Chain c:  72% 22% 5%




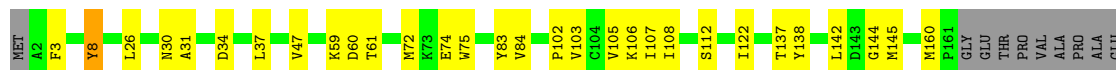
- Molecule 1: AA protein

Chain d:  61% 31% 6%



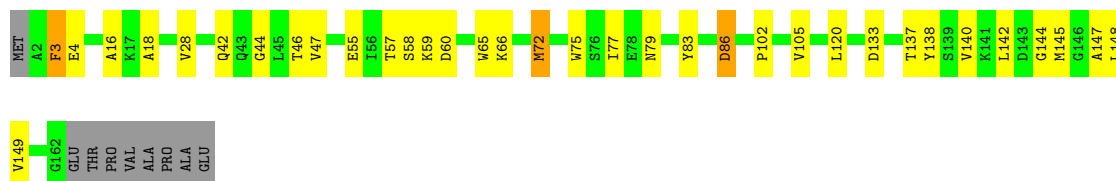
- Molecule 1: AA protein

Chain g:  76% 17% • 6%




• Molecule 1: AA protein

Chain A:  74% 19% • 5%



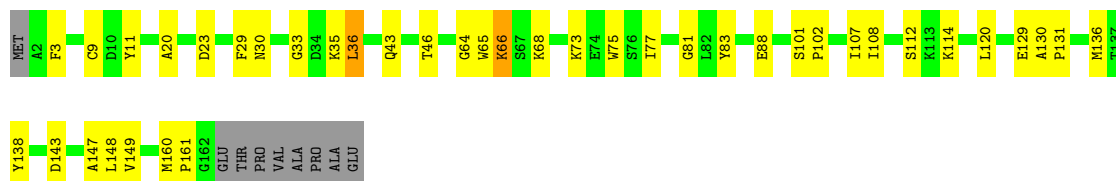
• Molecule 1: AA protein

Chain B:  79% 14% • 5%




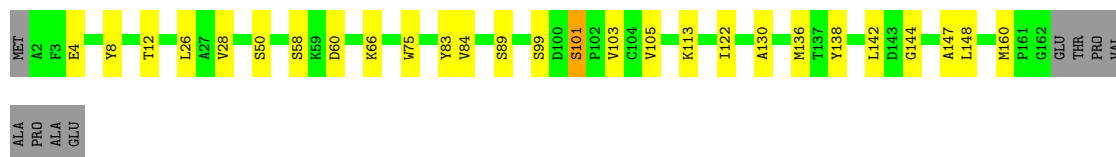
• Molecule 1: AA protein

Chain C:  71% 22% • 5%



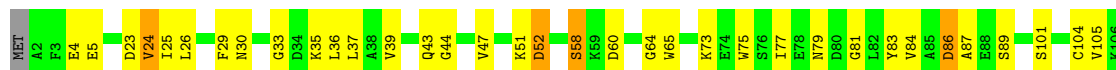
• Molecule 1: AA protein

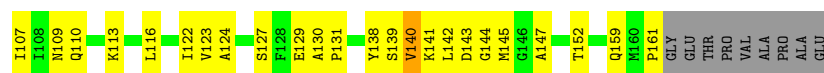
Chain I:  79% 15% • 5%



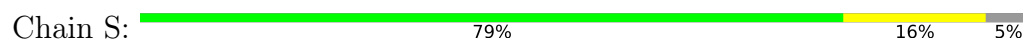
• Molecule 1: AA protein

Chain N:  59% 32% • 6%

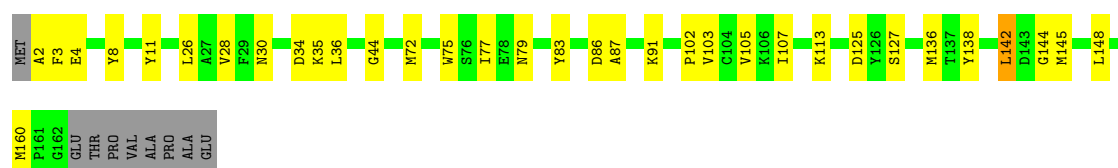
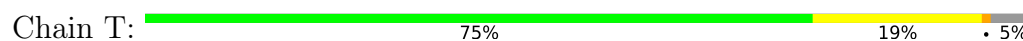




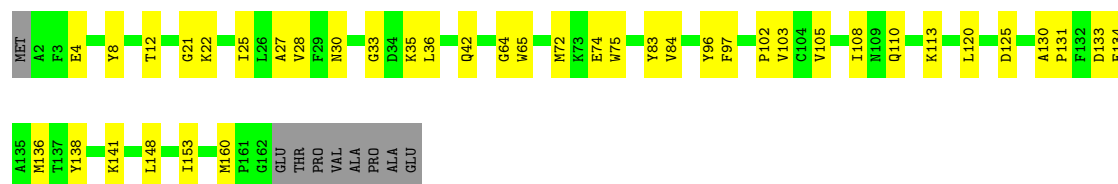
- Molecule 1: AA protein



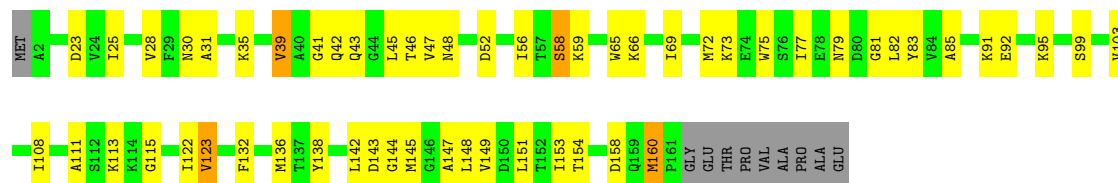
- Molecule 1: AA protein



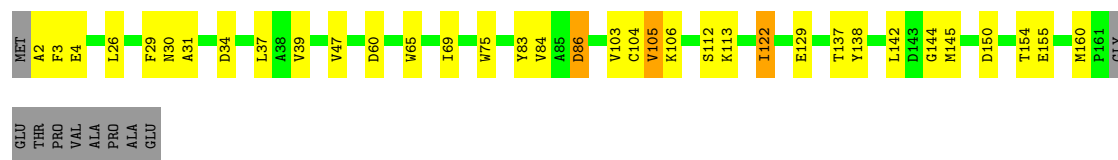
- Molecule 1: AA protein



- Molecule 1: AA protein

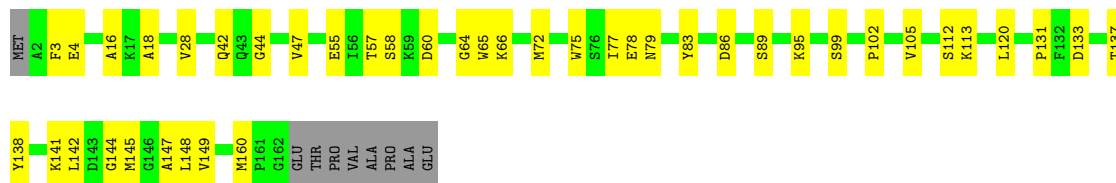


- Molecule 1: AA protein




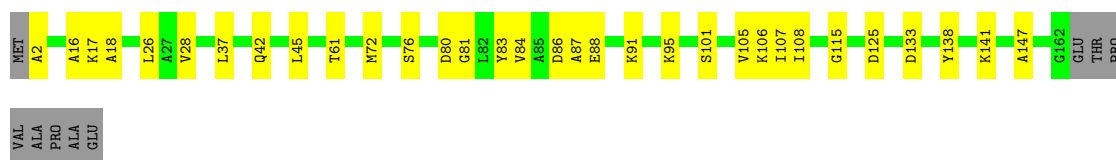
- Molecule 1: AA protein

Chain Y:  70% 25% 5%



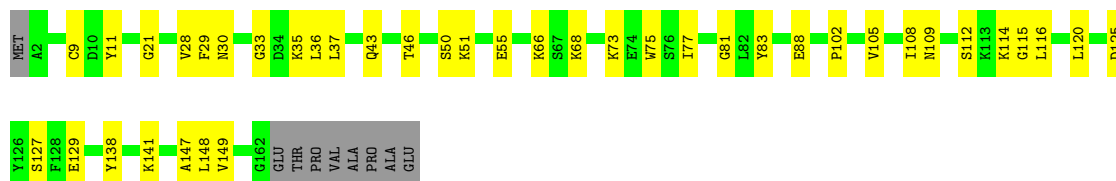
- Molecule 1: AA protein

Chain Z:  76% 19% 5%



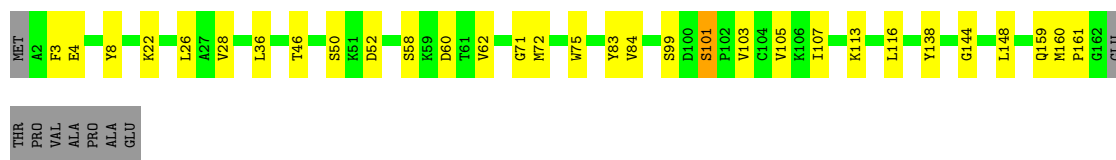
- Molecule 1: AA protein

Chain e:  71% 24% 5%



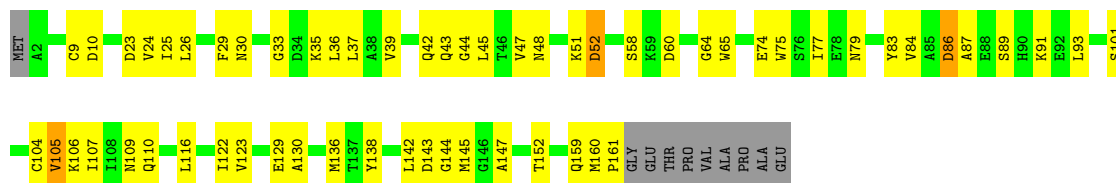
- Molecule 1: AA protein

Chain f:  76% 18% 5%



- Molecule 1: AA protein

Chain h:  59% 33% 6%



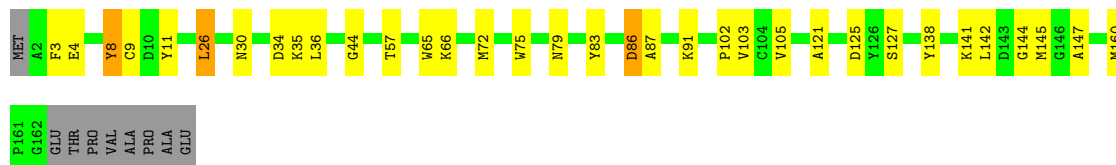
- Molecule 1: AA protein

Chain n:  75% 19% • 5%



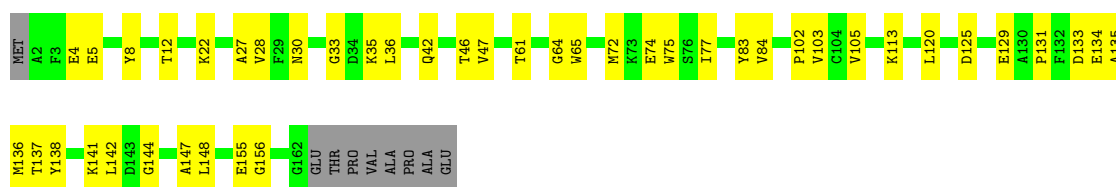
- Molecule 1: AA protein

Chain o:  75% 18% • 5%



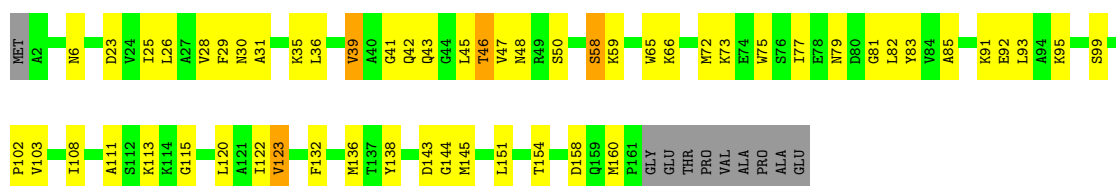
- Molecule 1: AA protein

Chain p:  69% 26% 5%



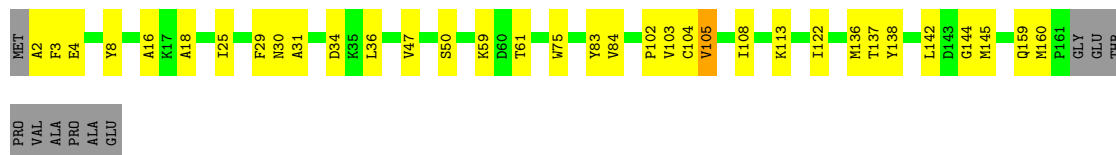
- Molecule 1: AA protein

Chain q:  61% 31% • 6%

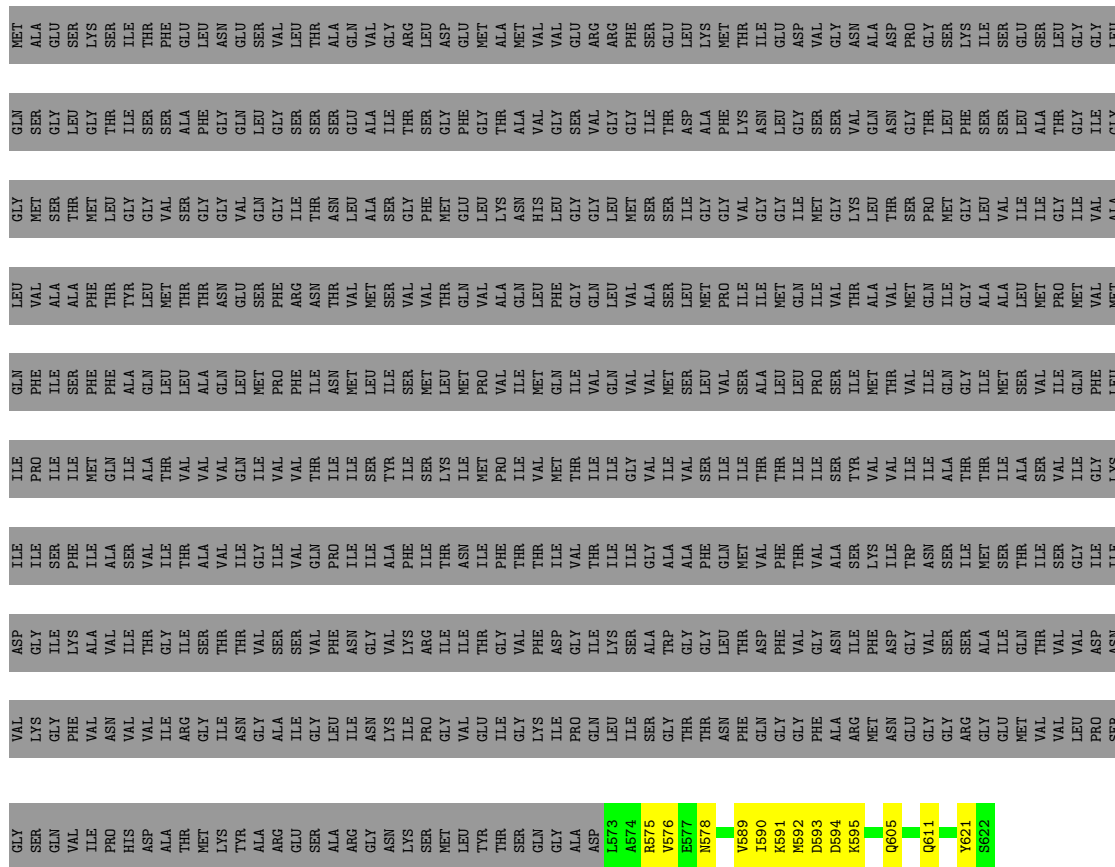


- Molecule 1: AA protein

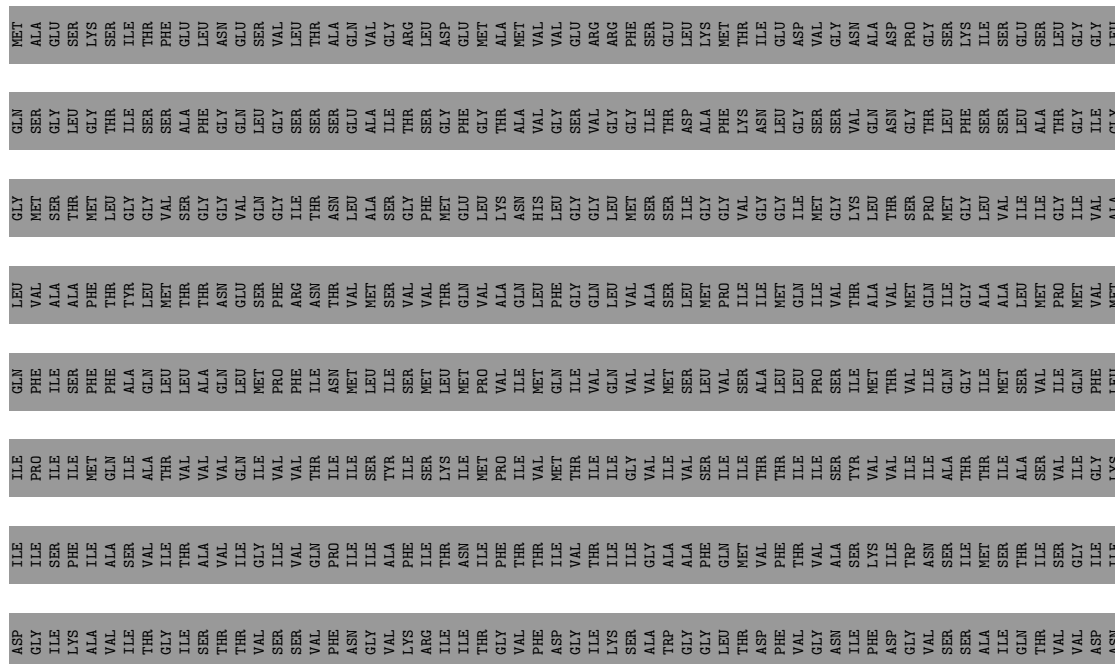
Chain r:  74% 19% • 6%



- Molecule 2: FtbJ

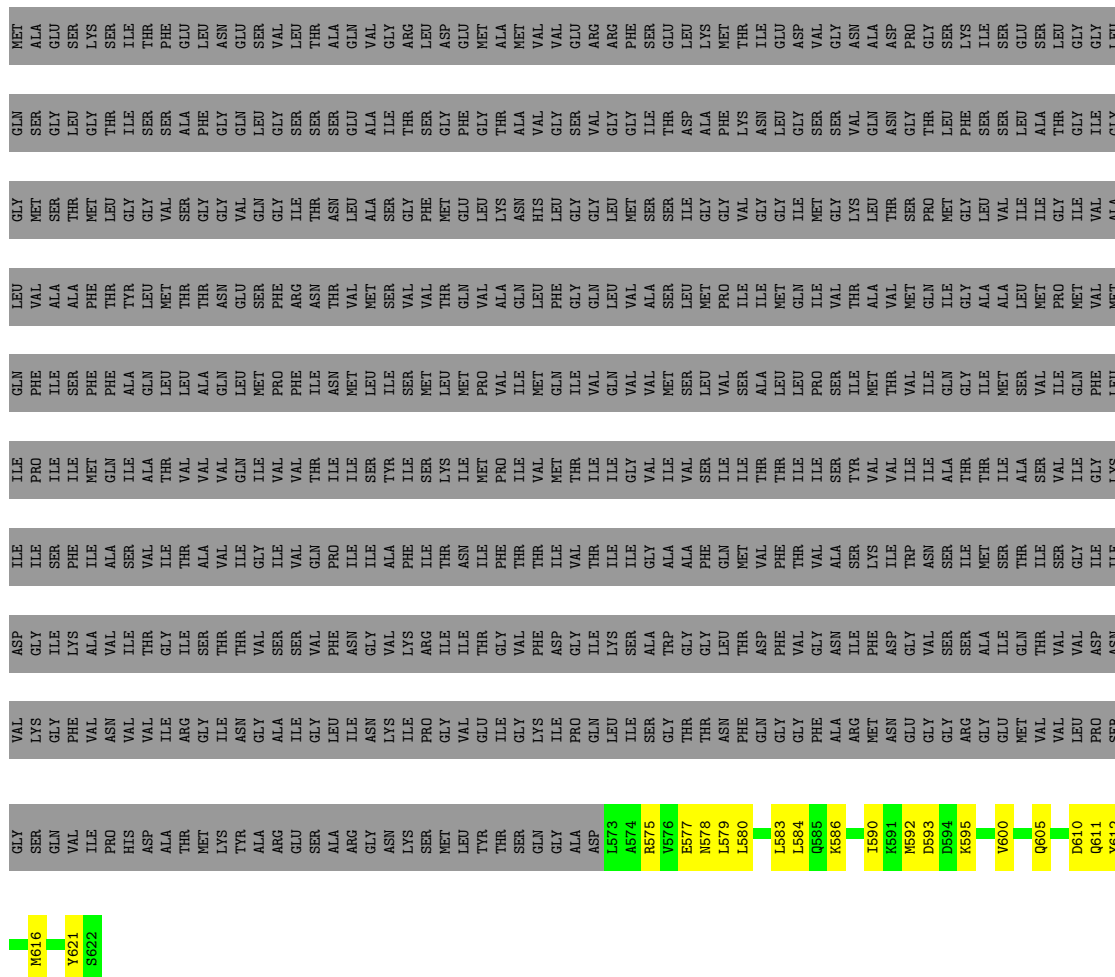


- Molecule 2: FtbJ



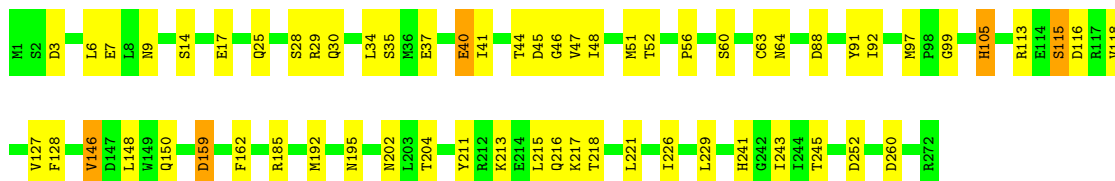
- Molecule 2: FtbJ

Chain i: 5% . 92%




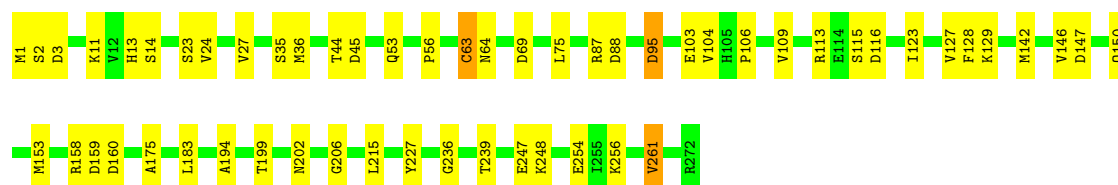
- Molecule 3: FtbK

Chain K: 77% 21% .




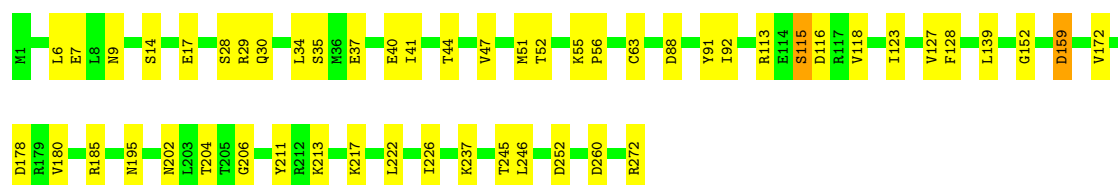
- Molecule 3: FtbK

Chain k:  79% 19%




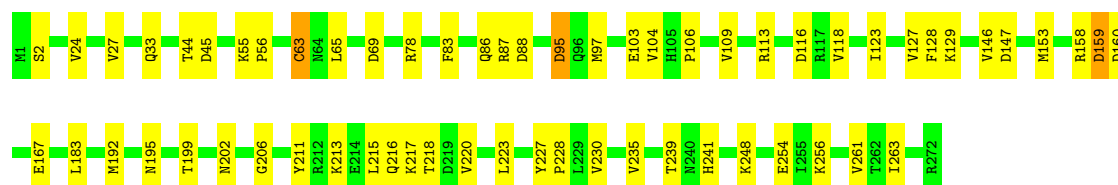
• Molecule 3: FtbK

Chain P:  81% 18%




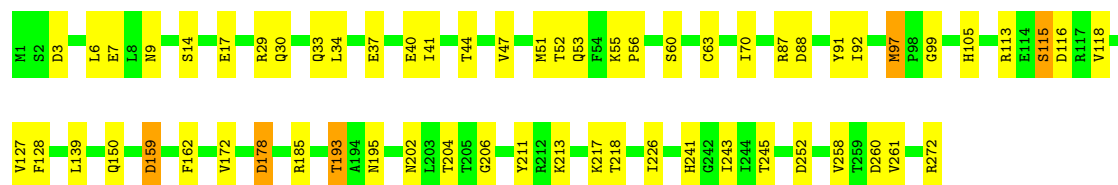
• Molecule 3: FtbK

Chain X:  78% 21%




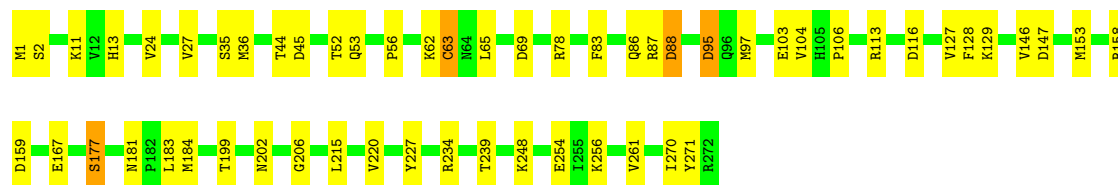
• Molecule 3: FtbK

Chain j:  78% 21%




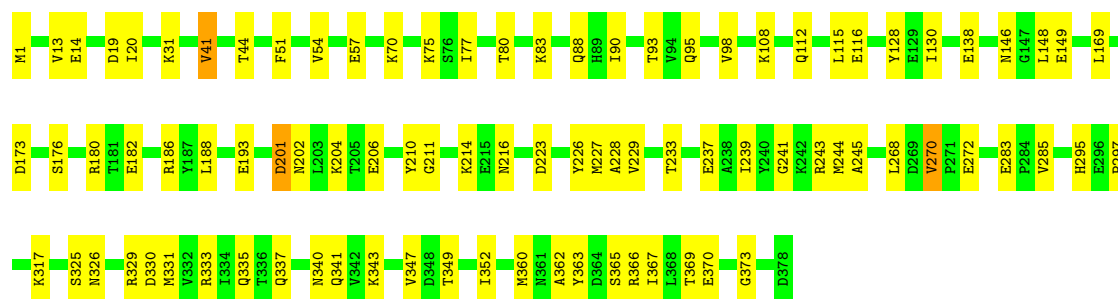
• Molecule 3: FtbK

Chain s:  79% 19%




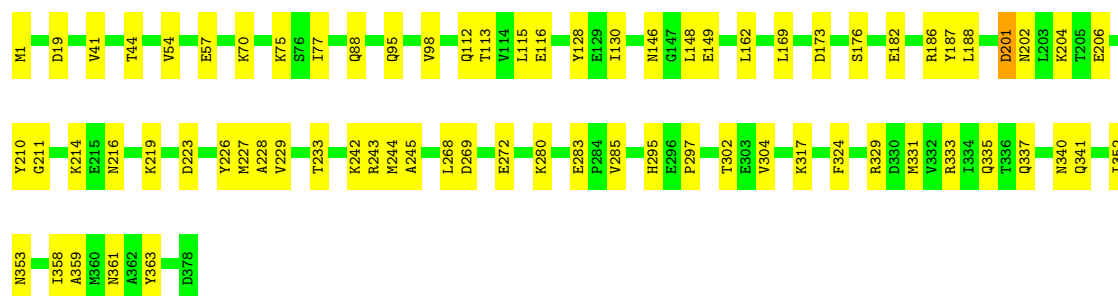
• Molecule 4: FtbL

Chain L:  76% 23% .




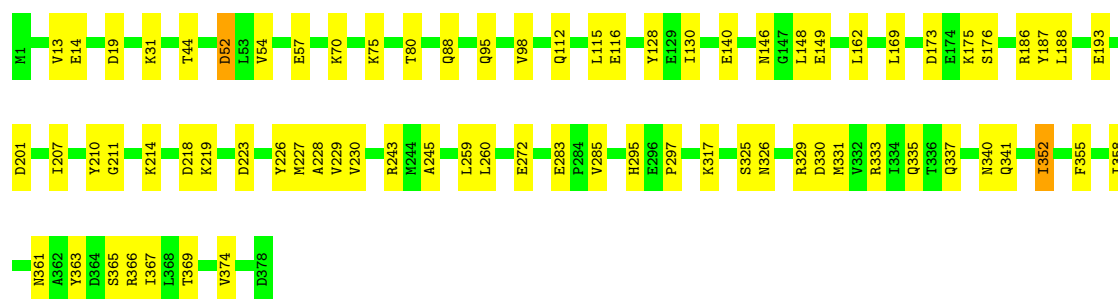
• Molecule 4: FtbL

Chain Q:  81% 19%



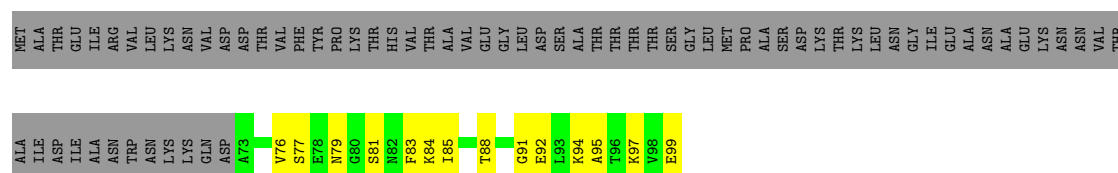
• Molecule 4: FtbL

Chain I:  80% 19% .

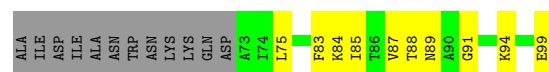


• Molecule 5: CCA-adding enzyme

Chain M:  13% 14% 73%



• Molecule 5: CCA-adding enzyme



- Molecule 5: CCA-adding enzyme



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	A	0.11	0/1218	0.29	0/1644
1	B	0.10	0/1218	0.28	0/1644
1	C	0.12	0/1218	0.32	0/1644
1	D	0.11	0/1218	0.32	0/1644
1	E	0.11	0/1218	0.32	0/1644
1	F	0.13	0/1218	0.35	0/1644
1	G	0.11	0/1218	0.28	0/1644
1	H	0.11	0/1214	0.38	0/1639
1	I	0.10	0/1218	0.27	0/1644
1	N	0.13	0/1214	0.42	0/1639
1	S	0.12	0/1218	0.34	0/1644
1	T	0.10	0/1218	0.30	0/1644
1	U	0.12	0/1218	0.31	0/1644
1	V	0.11	0/1214	0.35	0/1639
1	W	0.11	0/1214	0.29	0/1639
1	Y	0.10	0/1218	0.30	0/1644
1	Z	0.11	0/1218	0.32	0/1644
1	a	0.12	0/1218	0.37	0/1644
1	b	0.11	0/1218	0.32	0/1644
1	c	0.10	0/1218	0.30	0/1644
1	d	0.11	0/1214	0.35	0/1639
1	e	0.12	0/1218	0.34	0/1644
1	f	0.10	0/1218	0.27	0/1644
1	g	0.11	0/1214	0.29	0/1639
1	h	0.14	0/1214	0.44	0/1639
1	n	0.11	0/1218	0.35	0/1644
1	o	0.11	0/1218	0.31	0/1644
1	p	0.11	0/1218	0.32	0/1644
1	q	0.12	0/1214	0.35	0/1639
1	r	0.12	0/1214	0.30	0/1639
2	J	0.19	0/400	0.56	0/539
2	O	0.20	0/400	0.52	0/539
2	i	0.19	0/400	0.50	0/539
3	K	0.11	0/2264	0.29	0/3069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	P	0.12	0/2264	0.29	0/3069
3	X	0.11	0/2264	0.30	0/3069
3	j	0.11	0/2264	0.27	0/3069
3	k	0.12	0/2264	0.32	0/3069
3	s	0.11	0/2264	0.28	0/3069
4	L	0.09	0/3094	0.26	0/4176
4	Q	0.09	0/3094	0.26	0/4176
4	l	0.09	0/3094	0.27	0/4176
5	M	0.20	0/198	0.61	0/266
5	R	0.16	0/198	0.46	0/266
5	m	0.25	0/198	0.66	0/266
All	All	0.11	0/61164	0.32	0/82632

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	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	PHE	Peptide
1	D	3	PHE	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	1198	0	1173	22	0
1	B	1198	0	1173	13	0
1	C	1198	0	1173	28	0
1	D	1198	0	1173	23	0
1	E	1198	0	1173	16	0
1	F	1198	0	1173	32	0
1	G	1198	0	1174	15	0
1	H	1194	0	1171	43	0
1	I	1198	0	1174	14	0
1	N	1194	0	1171	47	0
1	S	1198	0	1173	19	0
1	T	1198	0	1173	21	0
1	U	1198	0	1173	30	0
1	V	1194	0	1171	41	0
1	W	1194	0	1171	20	0
1	Y	1198	0	1173	24	0
1	Z	1198	0	1173	17	0
1	a	1198	0	1173	18	0
1	b	1198	0	1173	23	0
1	c	1198	0	1173	27	0
1	d	1194	0	1171	41	0
1	e	1198	0	1173	28	0
1	f	1198	0	1174	17	0
1	g	1194	0	1171	17	0
1	h	1194	0	1171	51	0
1	n	1198	0	1173	21	0
1	o	1198	0	1173	20	0
1	p	1198	0	1173	32	0
1	q	1194	0	1171	41	0
1	r	1194	0	1171	23	0
2	J	396	0	395	11	0
2	O	396	0	395	17	0
2	i	396	0	395	20	0
3	K	2210	0	2142	40	0
3	P	2210	0	2142	29	0
3	X	2210	0	2142	40	0
3	j	2210	0	2142	41	0
3	k	2210	0	2142	40	0
3	s	2210	0	2142	40	0
4	L	3040	0	3009	64	0
4	Q	3040	0	3009	50	0
4	l	3040	0	3009	57	0
5	M	198	0	206	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	198	0	206	16	0
5	m	198	0	206	19	0
All	All	60066	0	58857	1087	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 9.

The worst 5 of 1087 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:r:108:ILE:HD11	1:r:160:MET:HE2	1.59	0.85
1:r:83:TYR:HB2	1:r:138:TYR:HB3	1.58	0.84
1:d:83:TYR:HB2	1:d:138:TYR:HB3	1.62	0.81
3:K:29:ARG:NH1	3:K:30:GLN:O	2.15	0.80
1:W:122:ILE:HG22	1:W:145:MET:HE2	1.64	0.78

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	159/170 (94%)	151 (95%)	8 (5%)	0	100	100
1	B	159/170 (94%)	153 (96%)	6 (4%)	0	100	100
1	C	159/170 (94%)	152 (96%)	7 (4%)	0	100	100
1	D	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	E	159/170 (94%)	152 (96%)	7 (4%)	0	100	100
1	F	159/170 (94%)	152 (96%)	7 (4%)	0	100	100
1	G	159/170 (94%)	146 (92%)	13 (8%)	0	100	100
1	H	158/170 (93%)	151 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	159/170 (94%)	148 (93%)	11 (7%)	0	100	100
1	N	158/170 (93%)	151 (96%)	7 (4%)	0	100	100
1	S	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	T	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	U	159/170 (94%)	149 (94%)	10 (6%)	0	100	100
1	V	158/170 (93%)	153 (97%)	5 (3%)	0	100	100
1	W	158/170 (93%)	152 (96%)	6 (4%)	0	100	100
1	Y	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	Z	159/170 (94%)	151 (95%)	8 (5%)	0	100	100
1	a	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	b	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	c	159/170 (94%)	149 (94%)	10 (6%)	0	100	100
1	d	158/170 (93%)	153 (97%)	5 (3%)	0	100	100
1	e	159/170 (94%)	153 (96%)	6 (4%)	0	100	100
1	f	159/170 (94%)	148 (93%)	11 (7%)	0	100	100
1	g	158/170 (93%)	152 (96%)	6 (4%)	0	100	100
1	h	158/170 (93%)	149 (94%)	9 (6%)	0	100	100
1	n	159/170 (94%)	149 (94%)	10 (6%)	0	100	100
1	o	159/170 (94%)	150 (94%)	9 (6%)	0	100	100
1	p	159/170 (94%)	149 (94%)	10 (6%)	0	100	100
1	q	158/170 (93%)	153 (97%)	5 (3%)	0	100	100
1	r	158/170 (93%)	152 (96%)	6 (4%)	0	100	100
2	J	48/622 (8%)	46 (96%)	2 (4%)	0	100	100
2	O	48/622 (8%)	46 (96%)	2 (4%)	0	100	100
2	i	48/622 (8%)	46 (96%)	2 (4%)	0	100	100
3	K	270/272 (99%)	265 (98%)	5 (2%)	0	100	100
3	P	270/272 (99%)	265 (98%)	5 (2%)	0	100	100
3	X	270/272 (99%)	263 (97%)	7 (3%)	0	100	100
3	j	270/272 (99%)	264 (98%)	6 (2%)	0	100	100
3	k	270/272 (99%)	261 (97%)	9 (3%)	0	100	100
3	s	270/272 (99%)	261 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	376/378 (100%)	363 (96%)	13 (4%)	0	100	100
4	Q	376/378 (100%)	363 (96%)	13 (4%)	0	100	100
4	l	376/378 (100%)	364 (97%)	12 (3%)	0	100	100
5	M	25/99 (25%)	20 (80%)	5 (20%)	0	100	100
5	R	25/99 (25%)	20 (80%)	5 (20%)	0	100	100
5	m	25/99 (25%)	21 (84%)	4 (16%)	0	100	100
All	All	7728/10029 (77%)	7386 (96%)	342 (4%)	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	A	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	B	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	C	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	D	124/131 (95%)	118 (95%)	6 (5%)	21	51
1	E	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	F	124/131 (95%)	115 (93%)	9 (7%)	11	32
1	G	124/131 (95%)	114 (92%)	10 (8%)	9	27
1	H	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	I	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	N	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	S	124/131 (95%)	119 (96%)	5 (4%)	27	58
1	T	124/131 (95%)	119 (96%)	5 (4%)	27	58
1	U	124/131 (95%)	121 (98%)	3 (2%)	44	74
1	V	124/131 (95%)	112 (90%)	12 (10%)	6	19
1	W	124/131 (95%)	114 (92%)	10 (8%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	Z	124/131 (95%)	118 (95%)	6 (5%)	21	51
1	a	124/131 (95%)	119 (96%)	5 (4%)	27	58
1	b	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	c	124/131 (95%)	118 (95%)	6 (5%)	21	51
1	d	124/131 (95%)	115 (93%)	9 (7%)	11	32
1	e	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	f	124/131 (95%)	116 (94%)	8 (6%)	14	37
1	g	124/131 (95%)	115 (93%)	9 (7%)	11	32
1	h	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	n	124/131 (95%)	117 (94%)	7 (6%)	17	44
1	o	124/131 (95%)	115 (93%)	9 (7%)	11	32
1	p	124/131 (95%)	118 (95%)	6 (5%)	21	51
1	q	124/131 (95%)	114 (92%)	10 (8%)	9	27
1	r	124/131 (95%)	118 (95%)	6 (5%)	21	51
2	J	43/510 (8%)	41 (95%)	2 (5%)	22	52
2	O	43/510 (8%)	42 (98%)	1 (2%)	45	75
2	i	43/510 (8%)	42 (98%)	1 (2%)	45	75
3	K	245/245 (100%)	229 (94%)	16 (6%)	14	37
3	P	245/245 (100%)	233 (95%)	12 (5%)	21	50
3	X	245/245 (100%)	235 (96%)	10 (4%)	26	57
3	j	245/245 (100%)	231 (94%)	14 (6%)	17	43
3	k	245/245 (100%)	239 (98%)	6 (2%)	44	74
3	s	245/245 (100%)	233 (95%)	12 (5%)	21	50
4	L	339/339 (100%)	329 (97%)	10 (3%)	37	69
4	Q	339/339 (100%)	327 (96%)	12 (4%)	31	63
4	l	339/339 (100%)	329 (97%)	10 (3%)	37	69
5	M	22/83 (26%)	21 (96%)	1 (4%)	23	53
5	R	22/83 (26%)	21 (96%)	1 (4%)	23	53
5	m	22/83 (26%)	22 (100%)	0	100	100
All	All	6402/8196 (78%)	6071 (95%)	331 (5%)	22	47

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	86	ASP
1	n	109	ASN
1	e	112	SER
3	j	97	MET
1	p	84	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	h	48	ASN
4	l	42	ASN
1	h	110	GLN
3	j	150	GLN
4	l	335	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 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 ⓘ

There are no chain breaks in this entry.