



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:36 AM UTC

PDB ID : 8V3W / pdb_00008v3w
EMDB ID : EMD-42956
Title : CryoEM Structure of Diffocin - precontracted - Baseplate - focused refinement on triplex region
Authors : Cai, X.Y.; He, Y.; Zhou, Z.H.
Deposited on : 2023-11-28
Resolution : 2.90 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

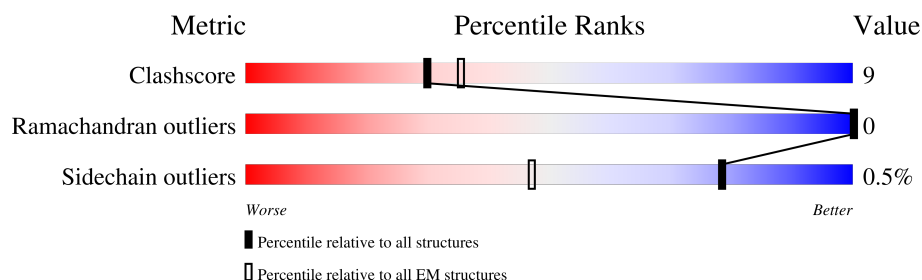
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



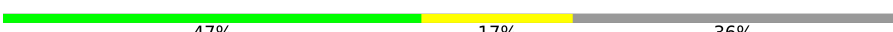
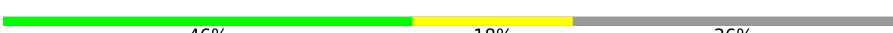
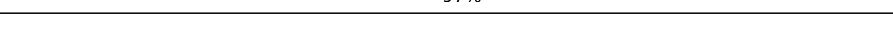
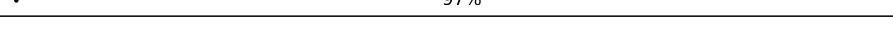
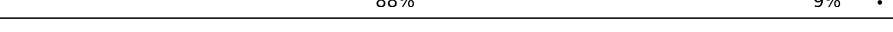
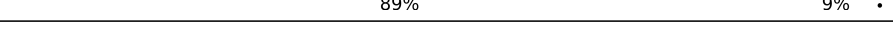
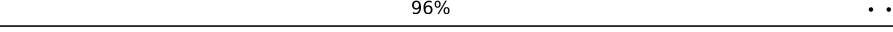
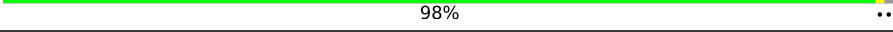
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	0	350	62% 36% ..
1	3	350	70% 29% .
1	A	350	63% 36% ..
1	E	350	63% 35% ..
1	J	350	60% 37% ..
1	M	350	69% 30% .
1	U	350	65% 34% .
1	Y	350	65% 33% ..
1	e	350	64% 33% ..

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Mol	Chain	Length	Quality of chain
1	h	350	
1	r	350	
1	v	350	
2	4	232	
2	6	232	
2	N	232	
2	Q	232	
2	i	232	
2	l	232	
3	C	108	
3	W	108	
3	t	108	
4	B	817	
4	V	817	
4	s	817	
5	G	140	
5	T	140	
5	Z	140	
5	o	140	
5	w	140	
5	y	140	
6	2	142	
6	F	142	
6	L	142	
6	O	142	

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Mol	Chain	Length	Quality of chain
6	g	142	 83% 11% 6%
6	j	142	 85% 9% 6%
7	1	354	 90% 9% .
7	8	354	 86% 13%
7	AA	354	 87% 13%
7	D	354	 87% 12% .
7	K	354	 87% 12% .
7	S	354	 86% 14%
7	X	354	 87% 12% .
7	c	354	 85% 14%
7	f	354	 88% 11% .
7	n	354	 87% 12% .
7	q	354	 86% 13%
7	u	354	 85% 14% .
8	5	142	 90% 8% .
8	7	142	 89% 9% .
8	9	142	 87% 11% .
8	I	142	 90% 8% .
8	P	142	 89% 9% .
8	R	142	 88% 11% .
8	a	142	 86% 13% .
8	d	142	 90% 8% .
8	k	142	 89% 9% .
8	m	142	 88% 11% .
8	p	142	 88% 11% .

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Mol	Chain	Length	Quality of chain
8	z	142	 92%7%
9	H	581	 81%19%
9	b	581	 82%18%
9	x	581	 82%18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 116790 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 TRI-2 (CD1371).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	A	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	J	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	M	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	v	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	r	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	0	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	3	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	Y	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	U	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	e	346	Total 2751	C 1736	N 452	O 555	S 8	0	0
1	h	346	Total 2751	C 1736	N 452	O 555	S 8	0	0

- Molecule 2 is a protein called TRI-1 (CD1372).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	148	Total 1214	C 774	N 192	O 240	S 8	0	0
2	Q	148	Total 1214	C 774	N 192	O 240	S 8	0	0
2	4	148	Total 1214	C 774	N 192	O 240	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	148	Total	C	N	O	S	0	0
			1214	774	192	240	8		
2	i	148	Total	C	N	O	S	0	0
			1214	774	192	240	8		
2	l	148	Total	C	N	O	S	0	0
			1214	774	192	240	8		

- Molecule 3 is a protein called Spike (CD1369).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	N	O	S	0	0
			879	564	144	168	3		
3	t	107	Total	C	N	O	S	0	0
			879	564	144	168	3		
3	W	107	Total	C	N	O	S	0	0
			879	564	144	168	3		

- Molecule 4 is a protein called Tape measure protein (CD1366).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	23	Total	C	N	O	0	0
			165	106	27	32		
4	s	23	Total	C	N	O	0	0
			165	106	27	32		
4	V	23	Total	C	N	O	0	0
			165	106	27	32		

- Molecule 5 is a protein called Tube tail (CD1367).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	136	Total	C	N	O	S	0	0
			1111	723	177	205	6		
5	w	136	Total	C	N	O	S	0	0
			1111	723	177	205	6		
5	T	138	Total	C	N	O	S	0	0
			1125	732	179	208	6		
5	y	138	Total	C	N	O	S	0	0
			1125	732	179	208	6		
5	Z	136	Total	C	N	O	S	0	0
			1111	723	177	205	6		
5	o	138	Total	C	N	O	S	0	0
			1125	732	179	208	6		

- Molecule 6 is a protein called Sheath initiator (CD1370).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		
6	2	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		
6	O	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		
6	g	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		
6	F	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		
6	j	134	Total	C	N	O	S	0	0
			1108	726	171	210	1		

- Molecule 7 is a protein called Sheath (CD1363).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	D	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
7	S	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	K	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
7	AA	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	u	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
7	8	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	1	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
7	q	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	X	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		
7	n	353	Total	C	N	O	S	0	0
			2743	1750	444	540	9		
7	f	352	Total	C	N	O	S	0	0
			2738	1747	443	539	9		

- Molecule 8 is a protein called Tube (CD1364).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	I	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	R	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	P	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	9	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	z	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	7	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	5	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	p	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	d	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	m	140	Total 1111	C 711	N 183	O 211	S 6	0	0
8	k	140	Total 1111	C 711	N 183	O 211	S 6	0	0

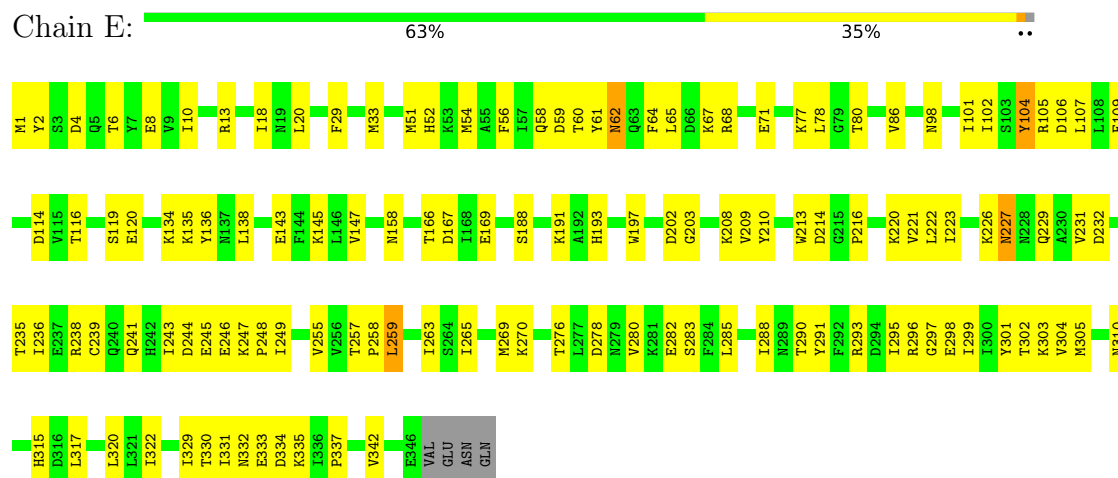
- Molecule 9 is a protein called Hub-Hydrolase (CD1368).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	581	Total 4596	C 2913	N 768	O 895	S 20	0	0
9	x	581	Total 4596	C 2913	N 768	O 895	S 20	0	0
9	b	581	Total 4596	C 2913	N 768	O 895	S 20	0	0

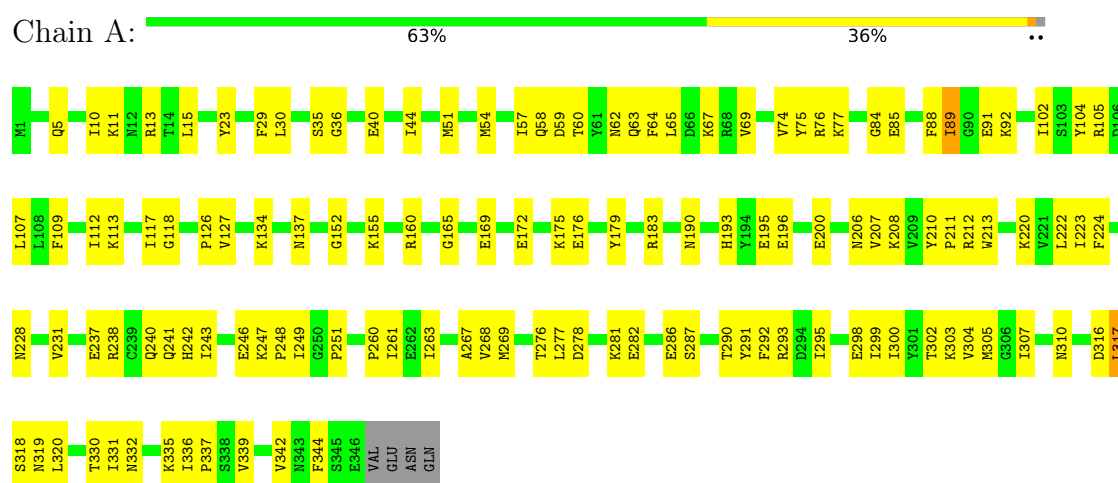
3 Residue-property plots

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.

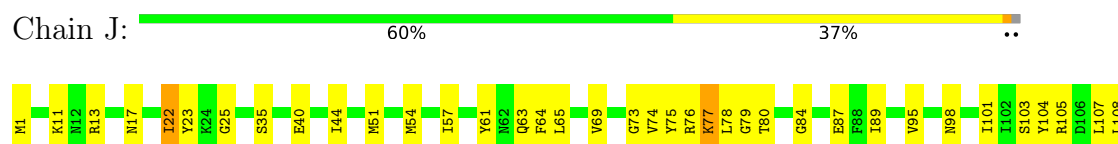
- Molecule 1: TRI-2 (CD1371)

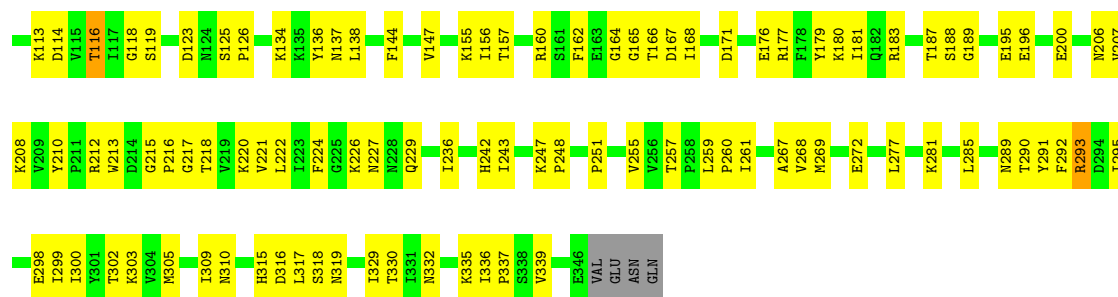


- Molecule 1: TRI-2 (CD1371)



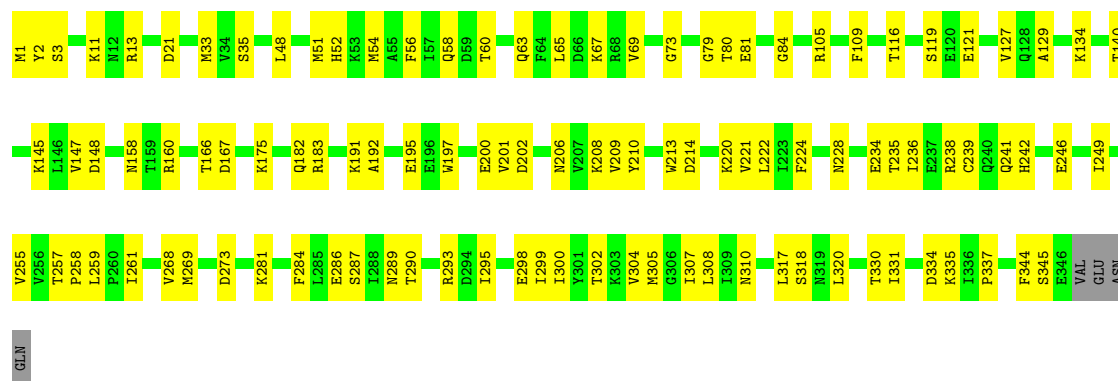
- Molecule 1: TRI-2 (CD1371)





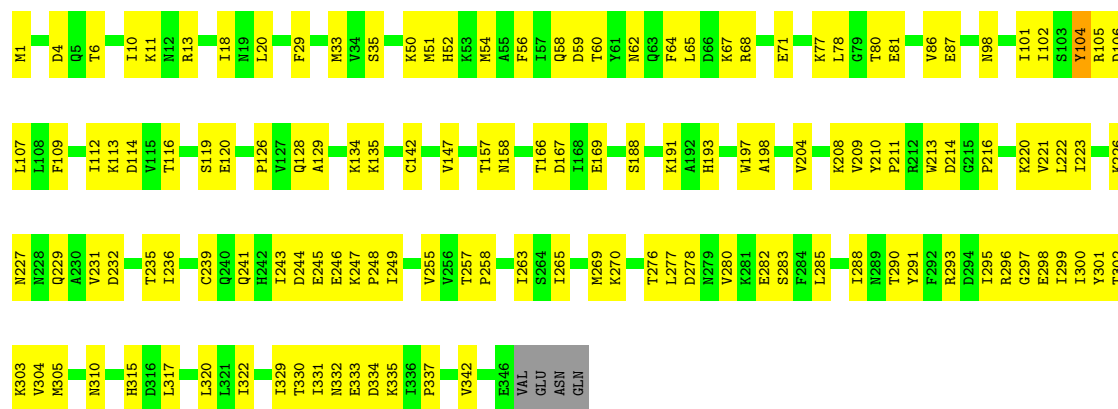
• Molecule 1: TRI-2 (CD1371)

Chain M: 69% 30%



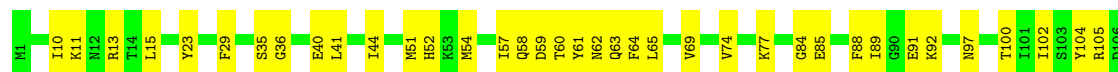
• Molecule 1: TRI-2 (CD1371)

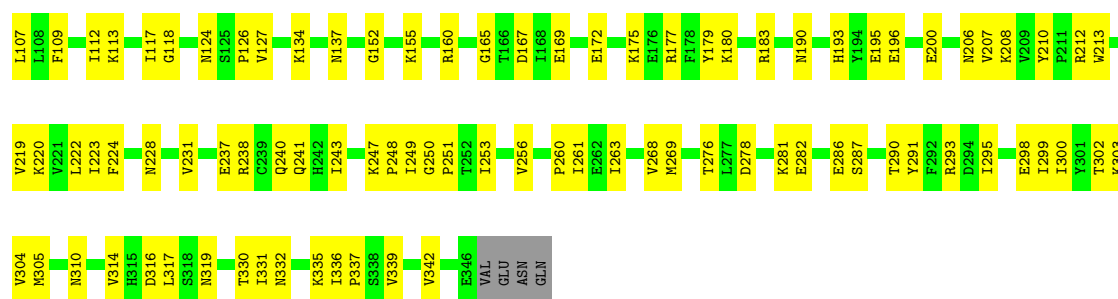
Chain v: 61% 38%



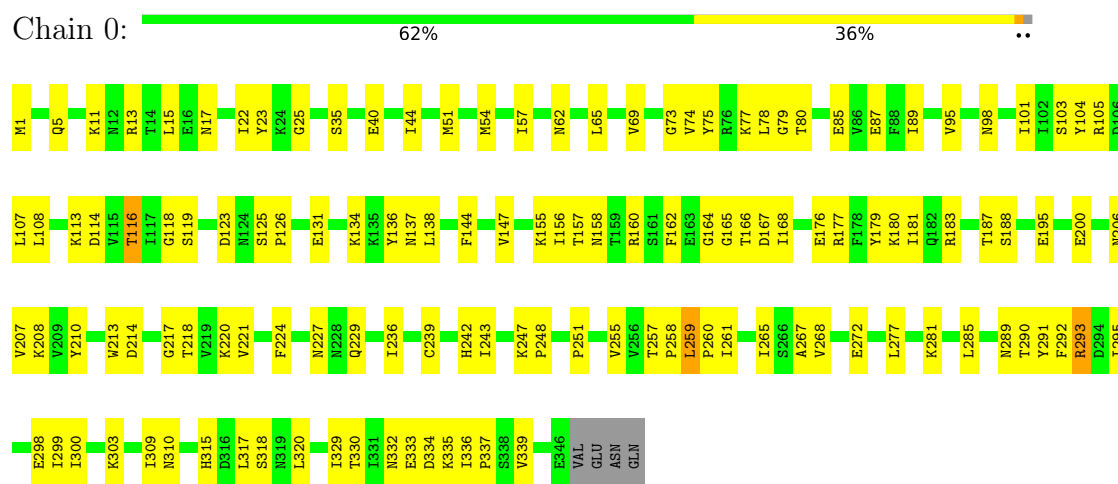
• Molecule 1: TRI-2 (CD1371)

Chain r: 63% 36%

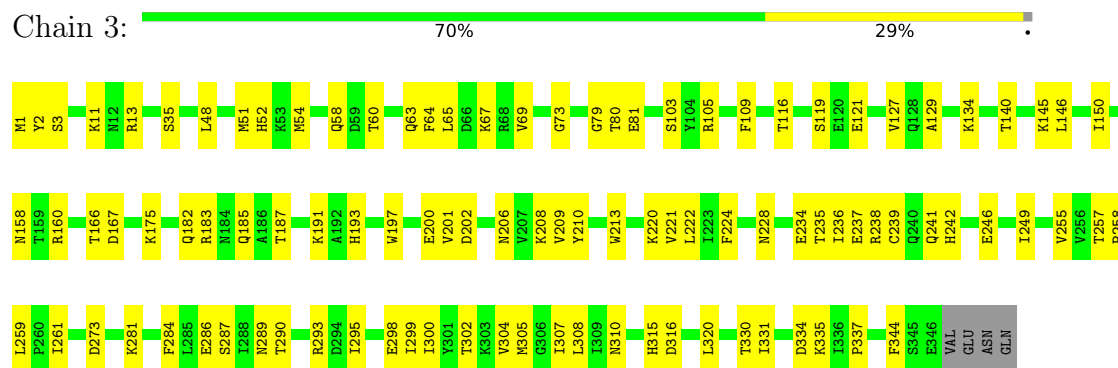




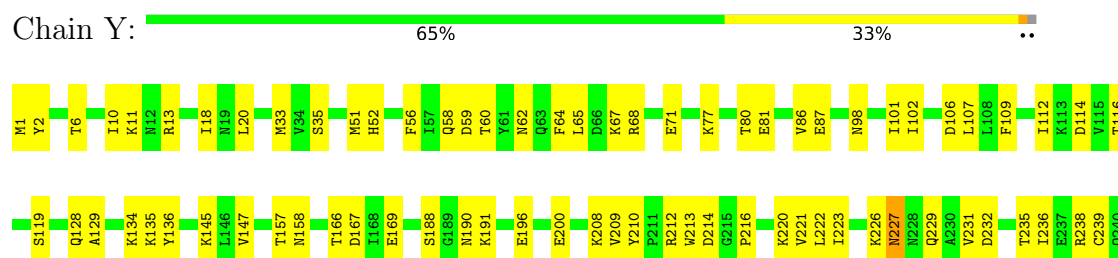
• Molecule 1: TRI-2 (CD1371)

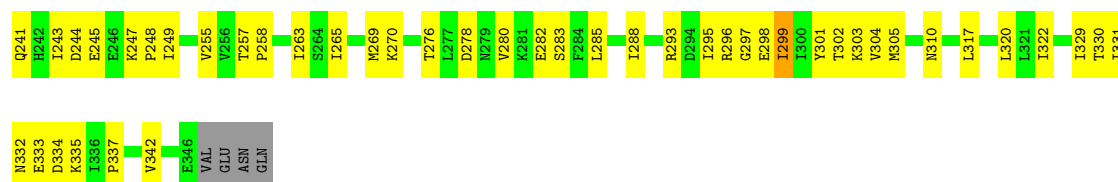


• Molecule 1: TRI-2 (CD1371)



• Molecule 1: TRI-2 (CD1371)





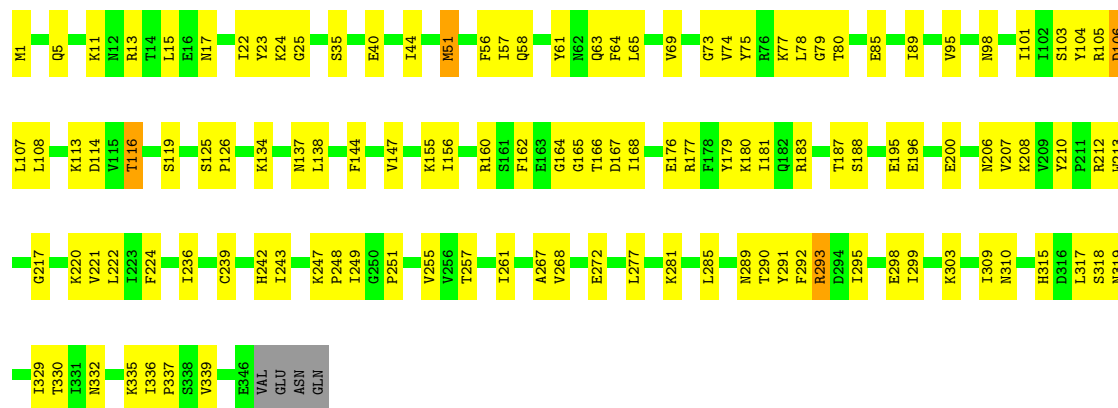
• Molecule 1: TRI-2 (CD1371)

Chain U: 65% 34%



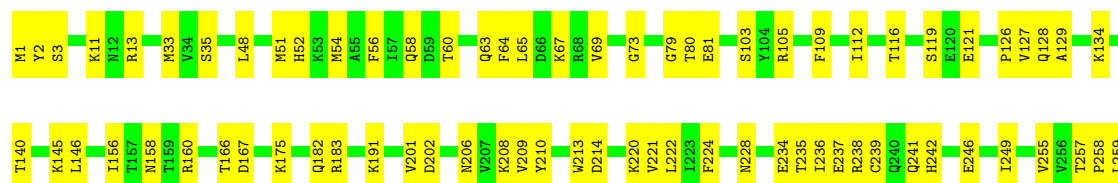
• Molecule 1: TRI-2 (CD1371)

Chain e: 64% 33%



• Molecule 1: TRI-2 (CD1371)

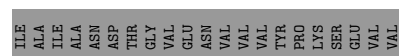
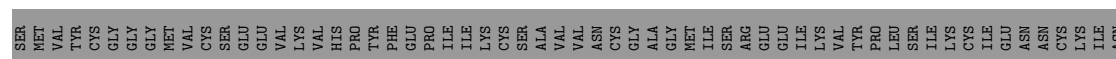
Chain h: 70% 29%





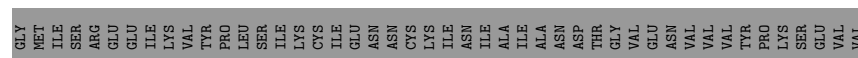
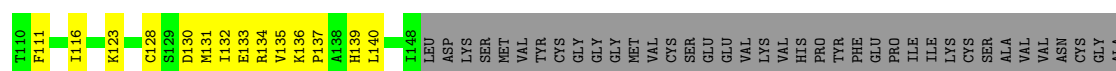
• Molecule 2: TRI-1 (CD1372)

Chain N: 49% 15% 36%



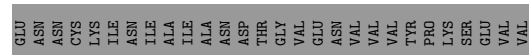
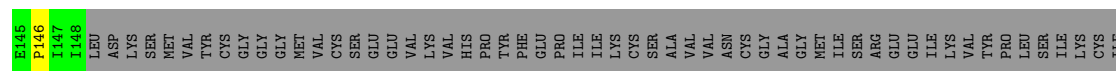
• Molecule 2: TRI-1 (CD1372)

Chain Q: 41% 22% 36%



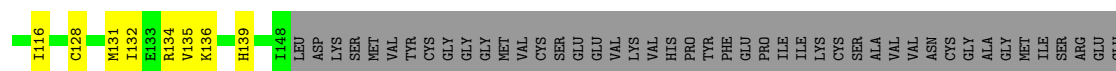
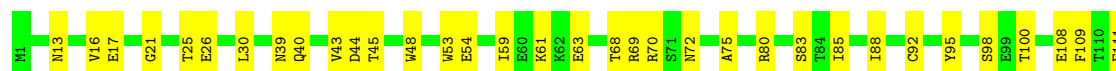
• Molecule 2: TRI-1 (CD1372)

Chain 4: 47% 17% 36%



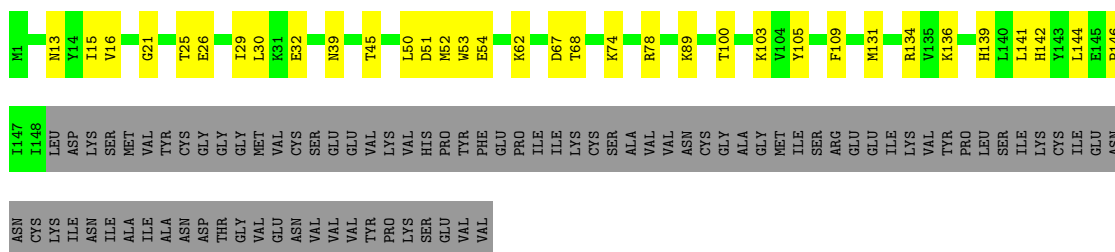
• Molecule 2: TRI-1 (CD1372)

Chain 6: 46% 18% 36%

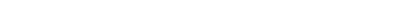


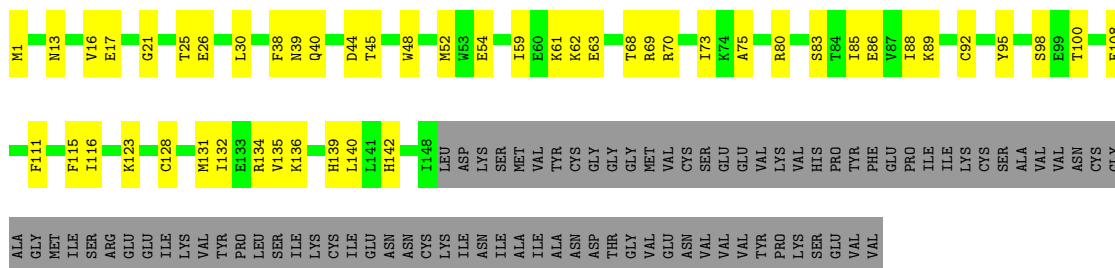
- Molecule 2: TRI-1 (CD1372)

Chain i:



- Molecule 2: TRI-1 (CD1372)

Chain 1:  43% 21% 36%



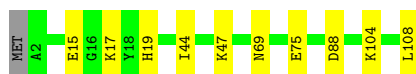
- Molecule 3: Spike (CD1369)

Chain C:  82% 17%



- Molecule 3: Spike (CD1369)

Chain t: 90% 9%



- Molecule 3: Spike (CD1369)

Chain W: 84% 15%



- Molecule 4: Tape measure protein (CD136)

97%

- Molecule 4: Tape measure protein (CD136)

97%

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

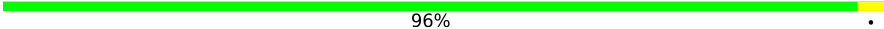
[illegible]

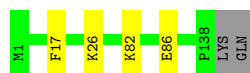
- Molecule 4: Tape measure protein (CD136)

Chain V: 97%

[illegible]



Chain o:  96%



• Molecule 6: Sheath initiator (CD1370)

Chain L:  82% 12% 6%



• Molecule 6: Sheath initiator (CD1370)

Chain 2:  80% 15% 6%



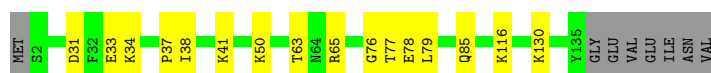
• Molecule 6: Sheath initiator (CD1370)

Chain O:  85% 9% 6%



• Molecule 6: Sheath initiator (CD1370)

Chain g:  83% 11% 6%



• Molecule 6: Sheath initiator (CD1370)

Chain F:  85% 9% 6%

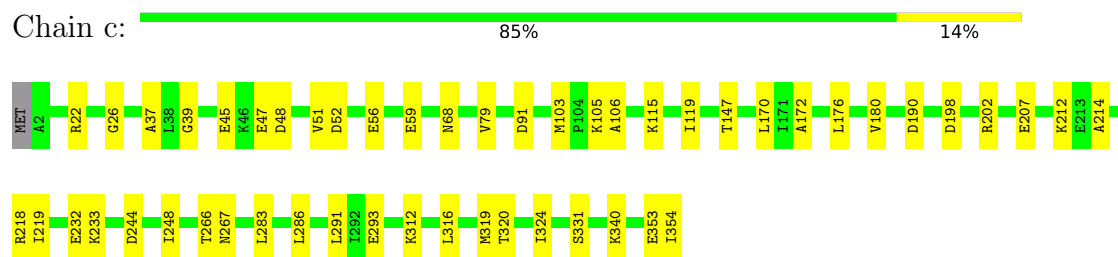


• Molecule 6: Sheath initiator (CD1370)

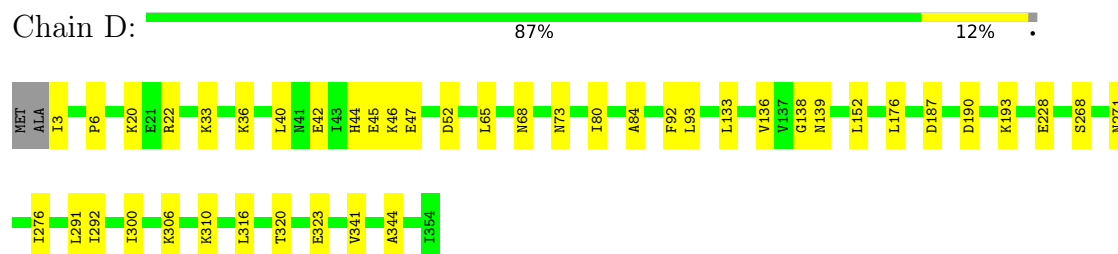
Chain j:  85% 9% 6%



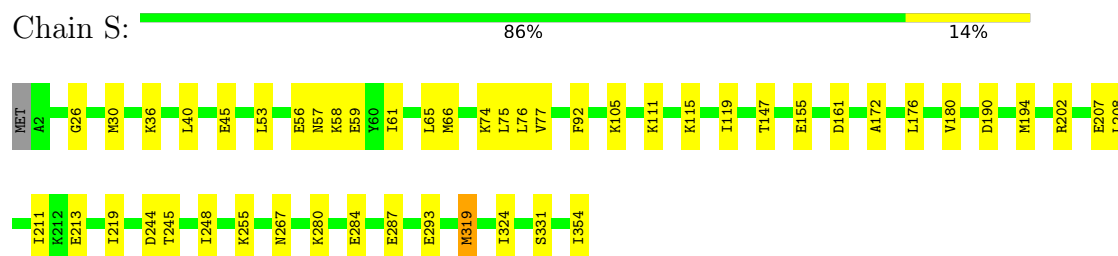
• Molecule 7: Sheath (CD1363)



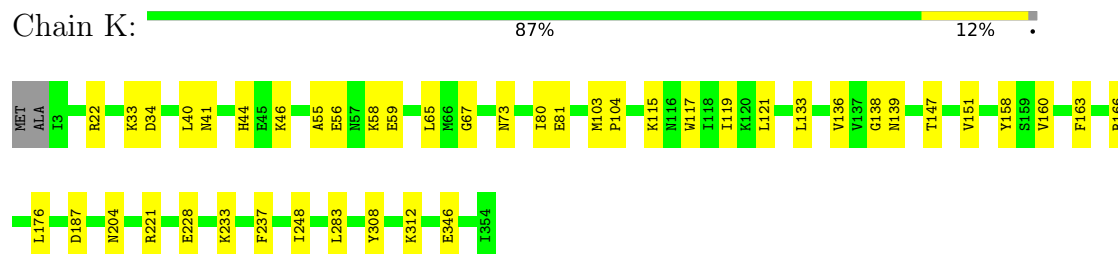
- Molecule 7: Sheath (CD1363)



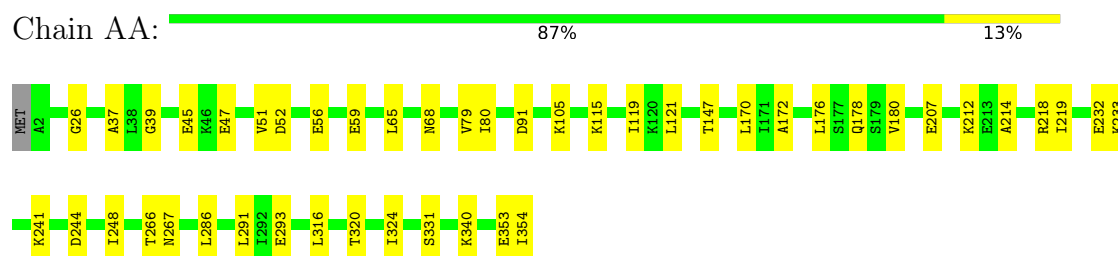
- Molecule 7: Sheath (CD1363)



- Molecule 7: Sheath (CD1363)

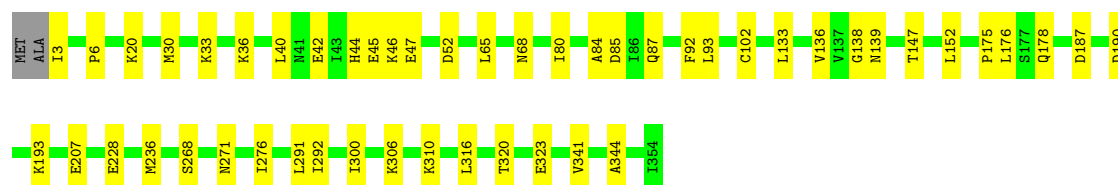


- Molecule 7: Sheath (CD1363)



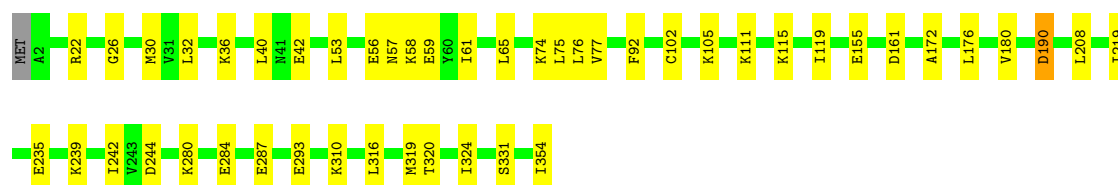
- Molecule 7: Sheath (CD1363)

Chain u:  85% 14%



• Molecule 7: Sheath (CD1363)

Chain 8:  86% 13%



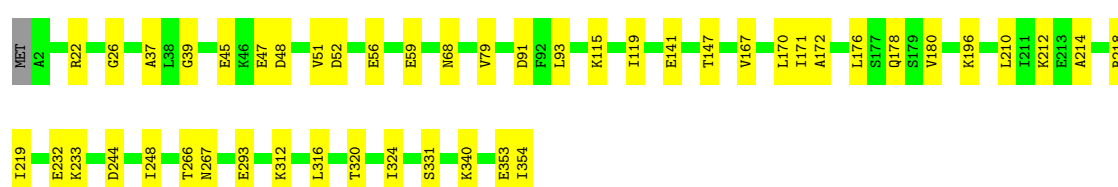
• Molecule 7: Sheath (CD1363)

Chain 1:  90% 9%



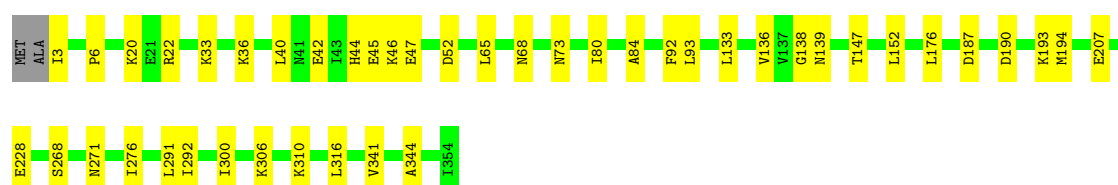
• Molecule 7: Sheath (CD1363)

Chain q:  86% 13%



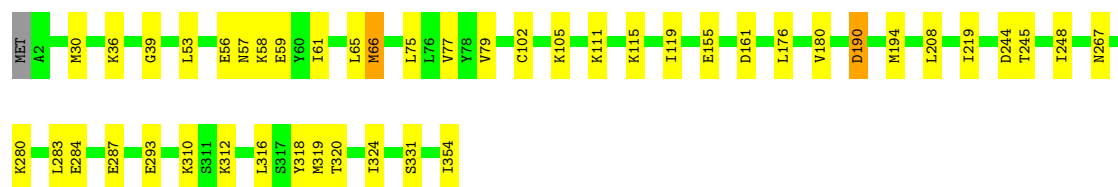
• Molecule 7: Sheath (CD1363)

Chain X:  87% 12%



• Molecule 7: Sheath (CD1363)

Chain n:  87% 12% .



- Molecule 7: Sheath (CD1363)

Chain f:  88% 11% .



- Molecule 8: Tube (CD1364)

Chain a:  86% 13% .



- Molecule 8: Tube (CD1364)

Chain I:  90% 8% .



- Molecule 8: Tube (CD1364)

Chain R:  88% 11% .



- Molecule 8: Tube (CD1364)

Chain P:  89% 9% .



- Molecule 8: Tube (CD1364)

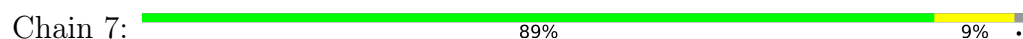
Chain 9:  87% 11% .



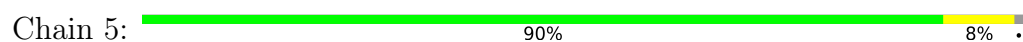
- Molecule 8: Tube (CD1364)



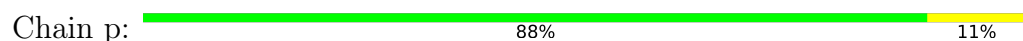
- Molecule 8: Tube (CD1364)



- Molecule 8: Tube (CD1364)



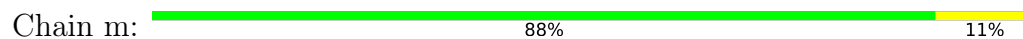
- Molecule 8: Tube (CD1364)



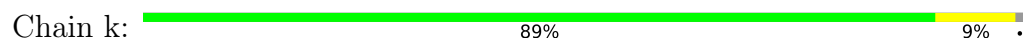
- Molecule 8: Tube (CD1364)



- Molecule 8: Tube (CD1364)



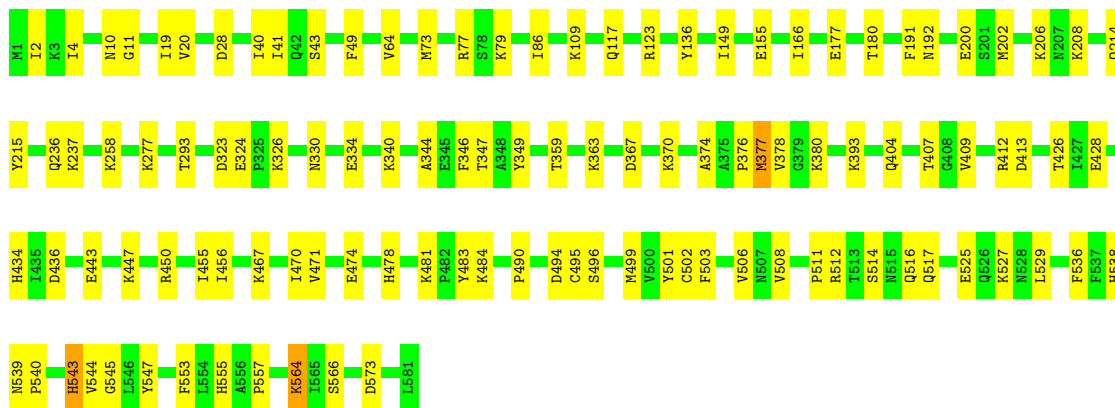
- Molecule 8: Tube (CD1364)





• Molecule 9: Hub-Hydrolase (CD1368)

Chain H: 81% 19%



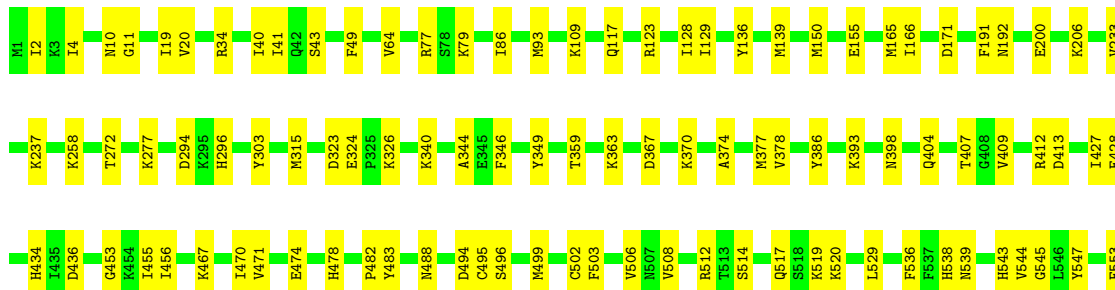
• Molecule 9: Hub-Hydrolase (CD1368)

Chain x: 82% 18%



• Molecule 9: Hub-Hydrolase (CD1368)

Chain b: 82% 18%



P557	D561	V562	V563	K564	I565	D573	L581
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116539	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	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	0	0.14	0/2795	0.35	0/3784
1	3	0.14	0/2795	0.34	0/3784
1	A	0.13	0/2795	0.32	0/3784
1	E	0.14	0/2795	0.36	1/3784 (0.0%)
1	J	0.13	0/2795	0.33	0/3784
1	M	0.14	0/2795	0.35	0/3784
1	U	0.13	0/2795	0.31	0/3784
1	Y	0.14	0/2795	0.34	0/3784
1	e	0.13	0/2795	0.33	0/3784
1	h	0.14	0/2795	0.34	0/3784
1	r	0.13	0/2795	0.34	0/3784
1	v	0.15	0/2795	0.39	1/3784 (0.0%)
2	4	0.14	0/1235	0.31	0/1668
2	6	0.14	0/1235	0.35	0/1668
2	N	0.13	0/1235	0.30	0/1668
2	Q	0.17	0/1235	0.40	1/1668 (0.1%)
2	i	0.13	0/1235	0.31	0/1668
2	l	0.14	0/1235	0.30	0/1668
3	C	0.19	0/896	0.41	0/1206
3	W	0.19	0/896	0.40	0/1206
3	t	0.19	0/896	0.40	0/1206
4	B	0.16	0/164	0.22	0/220
4	V	0.16	0/164	0.23	0/220
4	s	0.16	0/164	0.22	0/220
5	G	0.21	0/1139	0.35	0/1534
5	T	0.21	0/1154	0.34	0/1556
5	Z	0.21	0/1139	0.35	0/1534
5	o	0.21	0/1154	0.35	0/1556
5	w	0.21	0/1139	0.35	0/1534
5	y	0.21	0/1154	0.33	0/1556
6	2	0.18	0/1133	0.33	0/1532
6	F	0.19	0/1133	0.35	0/1532
6	L	0.18	0/1133	0.32	0/1532
6	O	0.19	0/1133	0.38	0/1532

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	g	0.18	0/1133	0.32	0/1532
6	j	0.19	0/1133	0.33	0/1532
7	1	0.14	0/2766	0.30	0/3729
7	8	0.17	0/2771	0.31	0/3736
7	AA	0.16	0/2771	0.29	0/3736
7	D	0.15	0/2766	0.31	0/3729
7	K	0.15	0/2766	0.32	0/3729
7	S	0.17	0/2771	0.31	0/3736
7	X	0.14	0/2766	0.30	0/3729
7	c	0.16	0/2771	0.29	0/3736
7	f	0.14	0/2766	0.30	0/3729
7	n	0.16	0/2771	0.30	0/3736
7	q	0.16	0/2771	0.29	0/3736
7	u	0.15	0/2766	0.31	0/3729
8	5	0.19	0/1133	0.30	0/1522
8	7	0.20	0/1133	0.34	0/1522
8	9	0.21	0/1133	0.40	0/1522
8	I	0.20	0/1133	0.30	0/1522
8	P	0.20	0/1133	0.32	0/1522
8	R	0.20	0/1133	0.34	0/1522
8	a	0.23	0/1133	0.42	0/1522
8	d	0.21	0/1133	0.31	0/1522
8	k	0.20	0/1133	0.30	0/1522
8	m	0.20	0/1133	0.34	0/1522
8	p	0.21	0/1133	0.37	0/1522
8	z	0.20	0/1133	0.31	0/1522
9	H	0.18	0/4678	0.35	0/6286
9	b	0.17	0/4678	0.34	0/6286
9	x	0.17	0/4678	0.34	0/6286
All	All	0.16	0/118659	0.33	3/160068 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	45	THR	N-CA-C	6.25	118.17	111.36
1	v	104	TYR	N-CA-C	-5.32	99.77	108.76
1	E	104	TYR	N-CA-C	-5.23	99.92	108.76

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	0	2751	0	2720	119	0
1	3	2751	0	2720	102	0
1	A	2751	0	2720	98	0
1	E	2751	0	2720	115	0
1	J	2751	0	2720	113	0
1	M	2751	0	2720	109	0
1	U	2751	0	2720	94	0
1	Y	2751	0	2720	104	0
1	e	2751	0	2720	104	0
1	h	2751	0	2720	104	0
1	r	2751	0	2720	96	0
1	v	2751	0	2720	116	0
2	4	1214	0	1203	32	0
2	6	1214	0	1203	36	0
2	N	1214	0	1203	27	0
2	Q	1214	0	1203	50	0
2	i	1214	0	1203	26	0
2	l	1214	0	1203	45	0
3	C	879	0	872	23	0
3	W	879	0	872	22	0
3	t	879	0	872	17	0
4	B	165	0	184	1	0
4	V	165	0	184	1	0
4	s	165	0	184	1	0
5	G	1111	0	1101	11	0
5	T	1125	0	1115	8	0
5	Z	1111	0	1101	10	0
5	o	1125	0	1115	3	0
5	w	1111	0	1101	12	0
5	y	1125	0	1115	1	0
6	2	1108	0	1119	15	0
6	F	1108	0	1119	10	0
6	L	1108	0	1119	14	0
6	O	1108	0	1119	11	0
6	g	1108	0	1119	13	0
6	j	1108	0	1119	10	0
7	1	2738	0	2864	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	8	2743	0	2869	32	0
7	AA	2743	0	2869	33	0
7	D	2738	0	2864	28	0
7	K	2738	0	2864	28	0
7	S	2743	0	2869	31	0
7	X	2738	0	2864	29	0
7	c	2743	0	2869	37	0
7	f	2738	0	2864	24	0
7	n	2743	0	2869	32	0
7	q	2743	0	2869	34	0
7	u	2738	0	2864	31	0
8	5	1111	0	1103	10	0
8	7	1111	0	1103	13	0
8	9	1111	0	1103	16	0
8	I	1111	0	1103	10	0
8	P	1111	0	1103	10	0
8	R	1111	0	1103	15	0
8	a	1111	0	1103	16	0
8	d	1111	0	1103	11	0
8	k	1111	0	1103	9	0
8	m	1111	0	1103	17	0
8	p	1111	0	1103	12	0
8	z	1111	0	1103	10	0
9	H	4596	0	4582	79	0
9	b	4596	0	4582	72	0
9	x	4596	0	4582	69	0
All	All	116790	0	117768	2132	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 2132 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:h:60:THR:CG2	1:h:65:LEU:HD13	1.66	1.24
1:3:60:THR:CG2	1:3:65:LEU:HD13	1.67	1.23
1:M:60:THR:CG2	1:M:65:LEU:HD13	1.72	1.19
1:r:219:VAL:HB	1:r:253:ILE:HD12	1.26	1.15
1:r:219:VAL:HB	1:r:253:ILE:CD1	1.80	1.12

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	0	344/350 (98%)	332 (96%)	12 (4%)	0	100	100
1	3	344/350 (98%)	331 (96%)	13 (4%)	0	100	100
1	A	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
1	E	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
1	J	344/350 (98%)	334 (97%)	10 (3%)	0	100	100
1	M	344/350 (98%)	330 (96%)	14 (4%)	0	100	100
1	U	344/350 (98%)	335 (97%)	9 (3%)	0	100	100
1	Y	344/350 (98%)	335 (97%)	9 (3%)	0	100	100
1	e	344/350 (98%)	333 (97%)	11 (3%)	0	100	100
1	h	344/350 (98%)	332 (96%)	12 (4%)	0	100	100
1	r	344/350 (98%)	338 (98%)	6 (2%)	0	100	100
1	v	344/350 (98%)	335 (97%)	9 (3%)	0	100	100
2	4	146/232 (63%)	145 (99%)	1 (1%)	0	100	100
2	6	146/232 (63%)	145 (99%)	1 (1%)	0	100	100
2	N	146/232 (63%)	145 (99%)	1 (1%)	0	100	100
2	Q	146/232 (63%)	145 (99%)	1 (1%)	0	100	100
2	i	146/232 (63%)	146 (100%)	0	0	100	100
2	l	146/232 (63%)	144 (99%)	2 (1%)	0	100	100
3	C	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
3	W	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
3	t	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
4	B	21/817 (3%)	21 (100%)	0	0	100	100
4	V	21/817 (3%)	21 (100%)	0	0	100	100
4	s	21/817 (3%)	21 (100%)	0	0	100	100
5	G	134/140 (96%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	T	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
5	Z	134/140 (96%)	130 (97%)	4 (3%)	0	100	100
5	o	136/140 (97%)	129 (95%)	7 (5%)	0	100	100
5	w	134/140 (96%)	130 (97%)	4 (3%)	0	100	100
5	y	136/140 (97%)	132 (97%)	4 (3%)	0	100	100
6	2	132/142 (93%)	129 (98%)	3 (2%)	0	100	100
6	F	132/142 (93%)	131 (99%)	1 (1%)	0	100	100
6	L	132/142 (93%)	130 (98%)	2 (2%)	0	100	100
6	O	132/142 (93%)	130 (98%)	2 (2%)	0	100	100
6	g	132/142 (93%)	129 (98%)	3 (2%)	0	100	100
6	j	132/142 (93%)	130 (98%)	2 (2%)	0	100	100
7	1	350/354 (99%)	334 (95%)	16 (5%)	0	100	100
7	8	351/354 (99%)	342 (97%)	9 (3%)	0	100	100
7	AA	351/354 (99%)	342 (97%)	9 (3%)	0	100	100
7	D	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
7	K	350/354 (99%)	332 (95%)	18 (5%)	0	100	100
7	S	351/354 (99%)	342 (97%)	9 (3%)	0	100	100
7	X	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
7	c	351/354 (99%)	340 (97%)	11 (3%)	0	100	100
7	f	350/354 (99%)	333 (95%)	17 (5%)	0	100	100
7	n	351/354 (99%)	342 (97%)	9 (3%)	0	100	100
7	q	351/354 (99%)	342 (97%)	9 (3%)	0	100	100
7	u	350/354 (99%)	337 (96%)	13 (4%)	0	100	100
8	5	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
8	7	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
8	9	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
8	I	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
8	P	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
8	R	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
8	a	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
8	d	138/142 (97%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	k	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
8	m	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
8	p	138/142 (97%)	131 (95%)	7 (5%)	0	100	100
8	z	138/142 (97%)	135 (98%)	3 (2%)	0	100	100
9	H	579/581 (100%)	553 (96%)	26 (4%)	0	100	100
9	b	579/581 (100%)	556 (96%)	23 (4%)	0	100	100
9	x	579/581 (100%)	559 (96%)	20 (4%)	0	100	100
All	All	14583/17754 (82%)	14150 (97%)	433 (3%)	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	0	313/317 (99%)	309 (99%)	4 (1%)	61	86
1	3	313/317 (99%)	313 (100%)	0	100	100
1	A	313/317 (99%)	311 (99%)	2 (1%)	78	93
1	E	313/317 (99%)	310 (99%)	3 (1%)	68	89
1	J	313/317 (99%)	309 (99%)	4 (1%)	61	86
1	M	313/317 (99%)	313 (100%)	0	100	100
1	U	313/317 (99%)	313 (100%)	0	100	100
1	Y	313/317 (99%)	310 (99%)	3 (1%)	68	89
1	e	313/317 (99%)	307 (98%)	6 (2%)	50	79
1	h	313/317 (99%)	313 (100%)	0	100	100
1	r	313/317 (99%)	313 (100%)	0	100	100
1	v	313/317 (99%)	313 (100%)	0	100	100
2	4	139/213 (65%)	139 (100%)	0	100	100
2	6	139/213 (65%)	138 (99%)	1 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	139/213 (65%)	139 (100%)	0	100	100
2	Q	139/213 (65%)	138 (99%)	1 (1%)	76	92
2	i	139/213 (65%)	139 (100%)	0	100	100
2	l	139/213 (65%)	139 (100%)	0	100	100
3	C	100/101 (99%)	99 (99%)	1 (1%)	68	89
3	W	100/101 (99%)	100 (100%)	0	100	100
3	t	100/101 (99%)	99 (99%)	1 (1%)	68	89
4	B	18/694 (3%)	18 (100%)	0	100	100
4	V	18/694 (3%)	18 (100%)	0	100	100
4	s	18/694 (3%)	18 (100%)	0	100	100
5	G	123/127 (97%)	122 (99%)	1 (1%)	73	90
5	T	125/127 (98%)	124 (99%)	1 (1%)	73	90
5	Z	123/127 (97%)	121 (98%)	2 (2%)	55	83
5	o	125/127 (98%)	125 (100%)	0	100	100
5	w	123/127 (97%)	122 (99%)	1 (1%)	73	90
5	y	125/127 (98%)	125 (100%)	0	100	100
6	2	123/130 (95%)	122 (99%)	1 (1%)	73	90
6	F	123/130 (95%)	123 (100%)	0	100	100
6	L	123/130 (95%)	122 (99%)	1 (1%)	73	90
6	O	123/130 (95%)	123 (100%)	0	100	100
6	g	123/130 (95%)	123 (100%)	0	100	100
6	j	123/130 (95%)	123 (100%)	0	100	100
7	1	308/309 (100%)	307 (100%)	1 (0%)	86	96
7	8	308/309 (100%)	307 (100%)	1 (0%)	86	96
7	AA	308/309 (100%)	306 (99%)	2 (1%)	78	93
7	D	308/309 (100%)	308 (100%)	0	100	100
7	K	308/309 (100%)	306 (99%)	2 (1%)	78	93
7	S	308/309 (100%)	306 (99%)	2 (1%)	78	93
7	X	308/309 (100%)	308 (100%)	0	100	100
7	c	308/309 (100%)	306 (99%)	2 (1%)	78	93
7	f	308/309 (100%)	306 (99%)	2 (1%)	78	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	n	308/309 (100%)	306 (99%)	2 (1%)	78	93
7	q	308/309 (100%)	307 (100%)	1 (0%)	86	96
7	u	308/309 (100%)	308 (100%)	0	100	100
8	5	117/118 (99%)	116 (99%)	1 (1%)	70	90
8	7	117/118 (99%)	117 (100%)	0	100	100
8	9	117/118 (99%)	117 (100%)	0	100	100
8	I	117/118 (99%)	117 (100%)	0	100	100
8	P	117/118 (99%)	116 (99%)	1 (1%)	70	90
8	R	117/118 (99%)	117 (100%)	0	100	100
8	a	117/118 (99%)	117 (100%)	0	100	100
8	d	117/118 (99%)	117 (100%)	0	100	100
8	k	117/118 (99%)	115 (98%)	2 (2%)	53	82
8	m	117/118 (99%)	115 (98%)	2 (2%)	53	82
8	p	117/118 (99%)	117 (100%)	0	100	100
8	z	117/118 (99%)	117 (100%)	0	100	100
9	H	513/513 (100%)	508 (99%)	5 (1%)	68	89
9	b	513/513 (100%)	512 (100%)	1 (0%)	87	96
9	x	513/513 (100%)	511 (100%)	2 (0%)	84	94
All	All	13065/15672 (83%)	13003 (100%)	62 (0%)	78	93

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	AA	80	ILE
7	f	163	PHE
5	T	96	GLU
7	f	160	VAL
1	e	106	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
7	8	238	GLN
1	e	319	ASN
1	0	319	ASN

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Mol	Chain	Res	Type
1	e	310	ASN
9	b	530	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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42956. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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.