



wwPDB EM Validation Summary Report ⓘ

Aug 19, 2024 – 07:45 PM EDT

PDB ID : 8V3W
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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

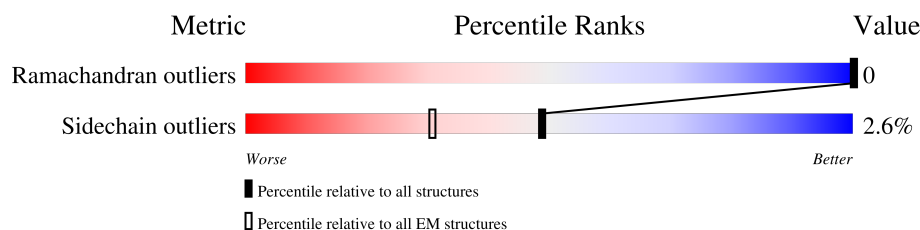
1 Overall quality at a glance

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	350	<div> <div>81%</div> <div>96%</div> <div>..</div> </div>
1	3	350	<div> <div>78%</div> <div>95%</div> <div>..</div> </div>
1	A	350	<div> <div>82%</div> <div>95%</div> <div>..</div> </div>
1	E	350	<div> <div>78%</div> <div>96%</div> <div>..</div> </div>
1	J	350	<div> <div>82%</div> <div>96%</div> <div>..</div> </div>
1	M	350	<div> <div>79%</div> <div>96%</div> <div>..</div> </div>
1	U	350	<div> <div>82%</div> <div>95%</div> <div>..</div> </div>
1	Y	350	<div> <div>75%</div> <div>96%</div> <div>..</div> </div>
1	e	350	<div> <div>82%</div> <div>96%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	h	350	78% 95% ..
1	r	350	81% 95% ..
1	v	350	78% 95% ..
2	4	232	42% 60% 36%
2	6	232	42% 59% 5% 36%
2	N	232	41% 61% 36%
2	Q	232	42% 59% 36%
2	i	232	39% 60% 36%
2	l	232	41% 60% 36%
3	C	108	99% .
3	W	108	99% .
3	t	108	99% .
4	B	817	97% .
4	V	817	97% .
4	s	817	97% .
5	G	140	95% ..
5	T	140	99% .
5	Z	140	96% ..
5	o	140	99% .
5	w	140	96% ..
5	y	140	99% .
6	2	142	5% 92% 6%
6	F	142	6% 93% 6%
6	L	142	6% 92% 6%
6	O	142	5% 93% 6%

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Mol	Chain	Length	Quality of chain
6	g	142	
6	j	142	
7	1	354	
7	8	354	
7	AA	354	
7	D	354	
7	K	354	
7	S	354	
7	X	354	
7	c	354	
7	f	354	
7	n	354	
7	q	354	
7	u	354	
8	5	142	
8	7	142	
8	9	142	
8	I	142	
8	P	142	
8	R	142	
8	a	142	
8	d	142	
8	k	142	
8	m	142	
8	p	142	

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Mol	Chain	Length	Quality of chain
8	z	142	<div><div></div><div>99%</div><div>.</div></div>
9	H	581	<div><div>46%</div><div>99%</div><div>.</div></div>
9	b	581	<div><div>46%</div><div>98%</div><div>.</div></div>
9	x	581	<div><div>46%</div><div>98%</div><div>.</div></div>

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	C	N	O	S	0	0
			2751	1736	452	555	8		
1	A	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	J	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	M	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	v	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	r	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	0	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	3	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	Y	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	U	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	e	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		
1	h	346	Total	C	N	O	S	0	0
			2751	1736	452	555	8		

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

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

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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

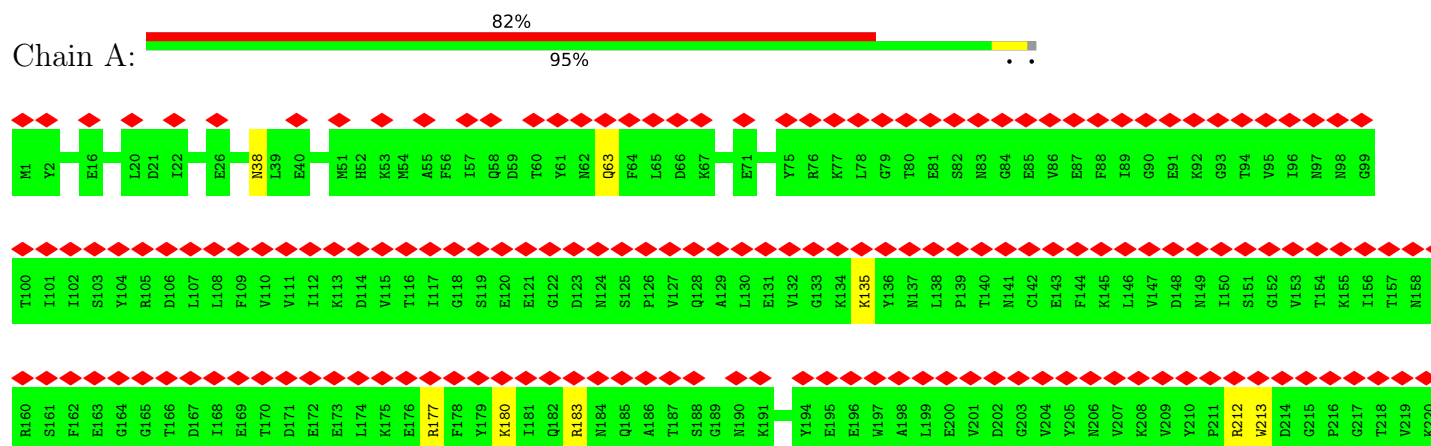
3 Residue-property plots

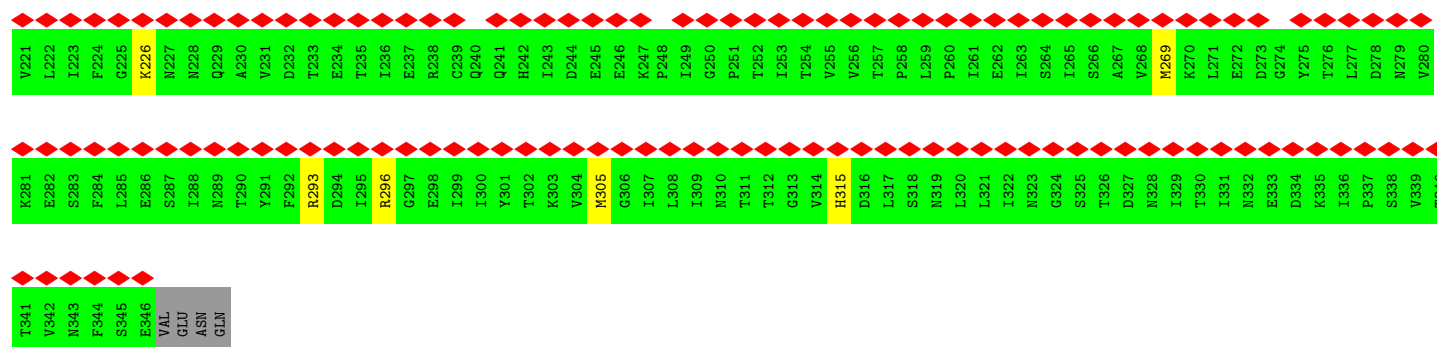
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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)



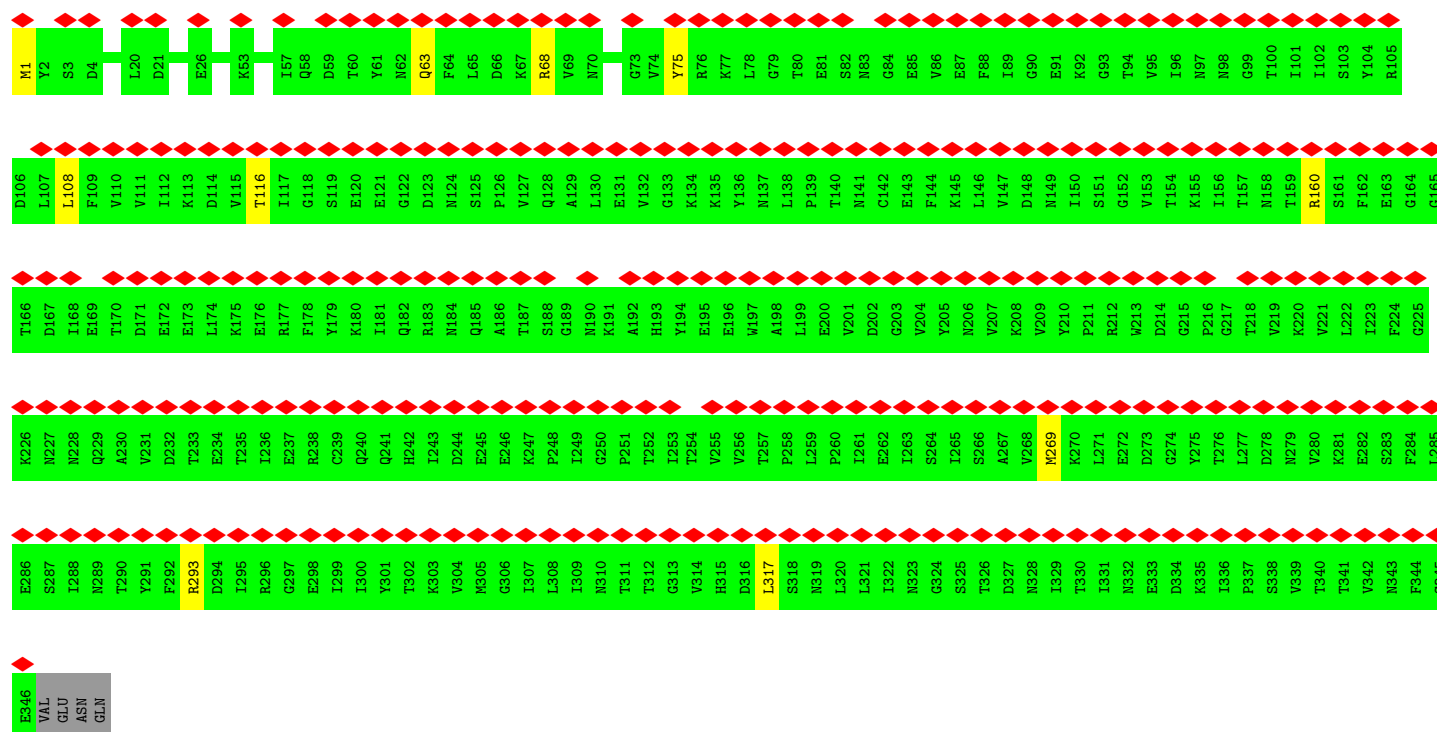
• Molecule 1: TRI-2 (CD1371)





• Molecule 1: TRI-2 (CD1371)

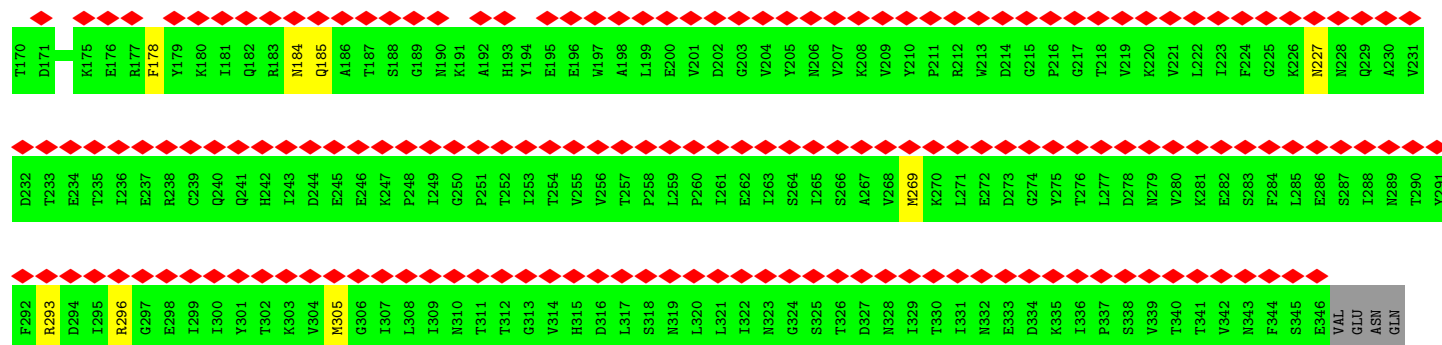
Chain J: 82% 96%



• Molecule 1: TRI-2 (CD1371)

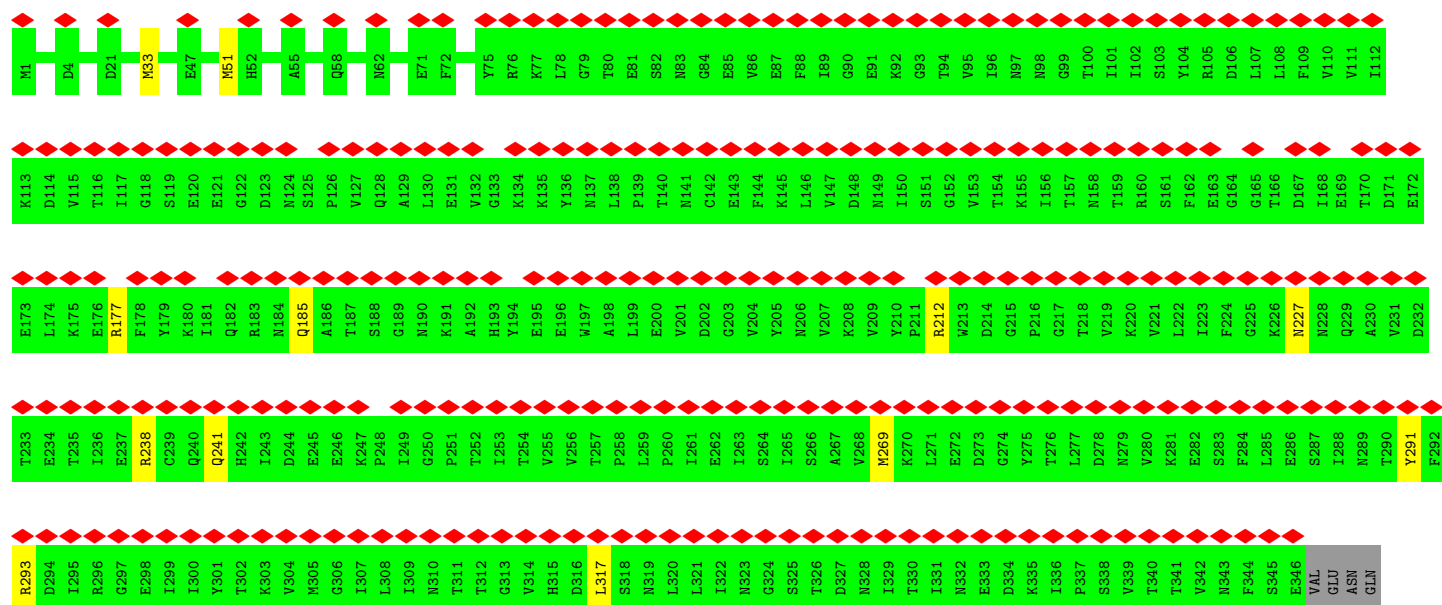
Chain M: 79% 96%





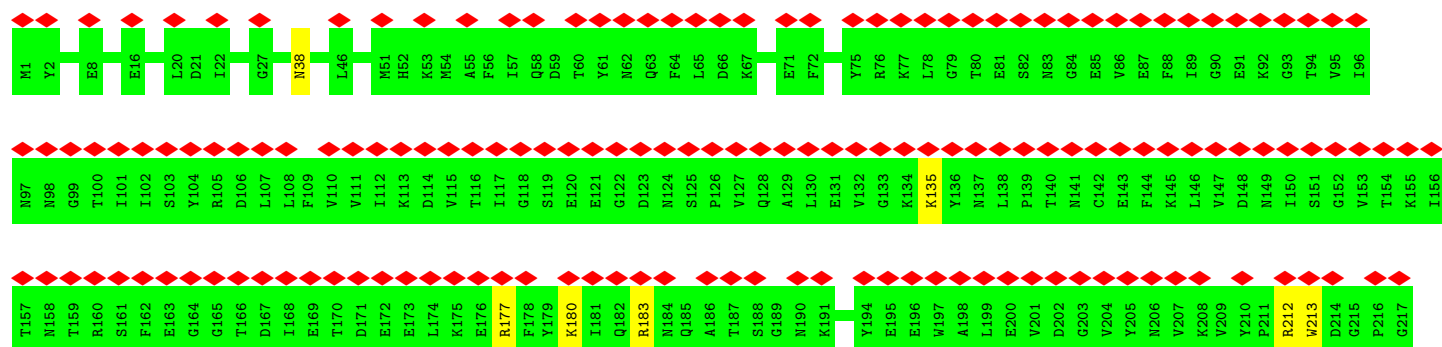
• Molecule 1: TRI-2 (CD1371)

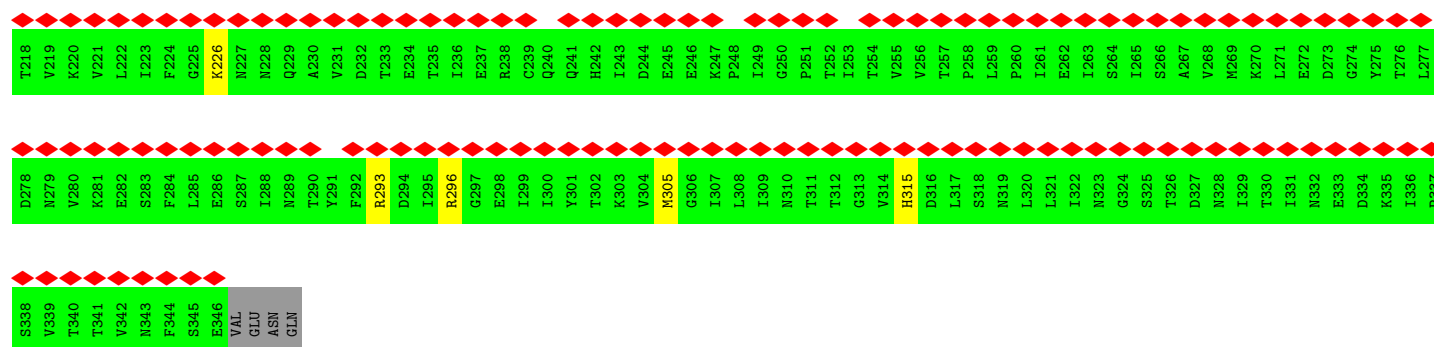
Chain v: 78% 95%



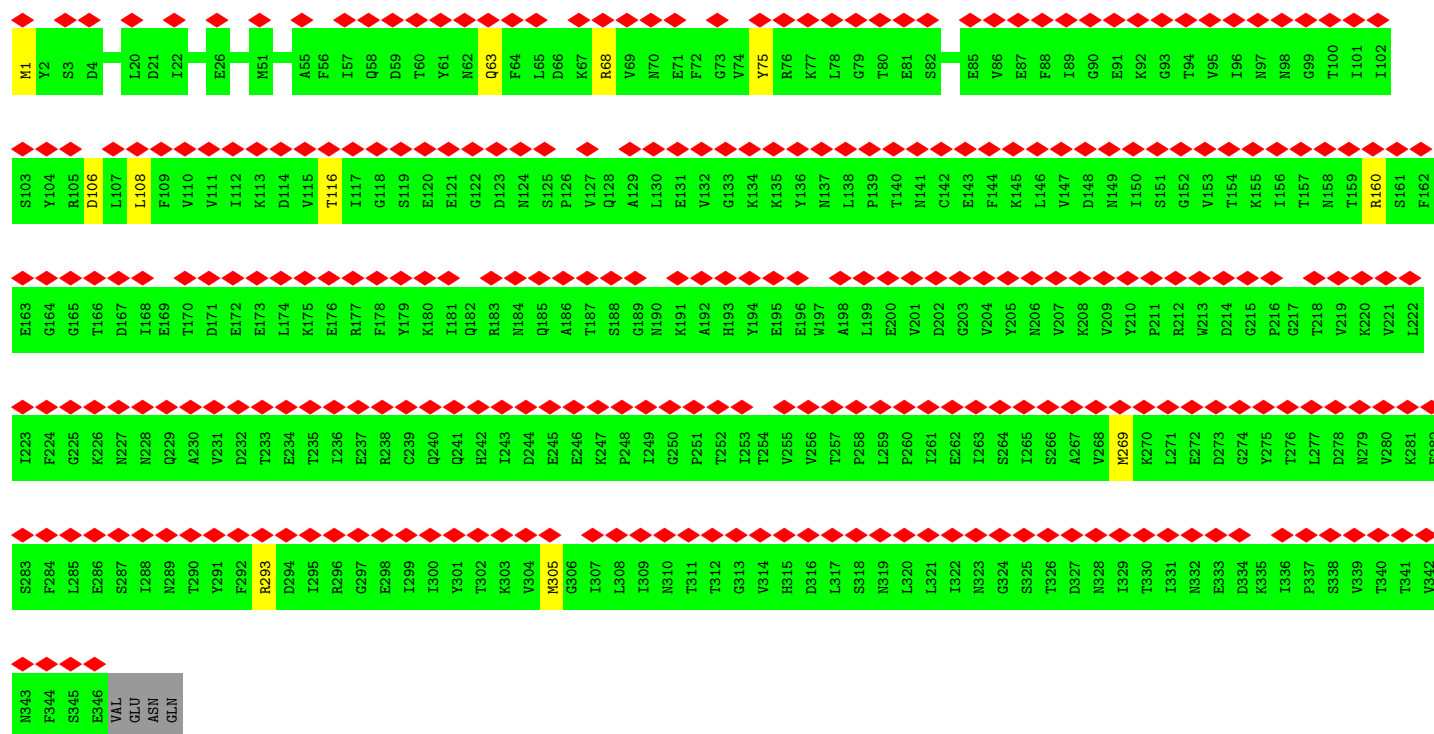
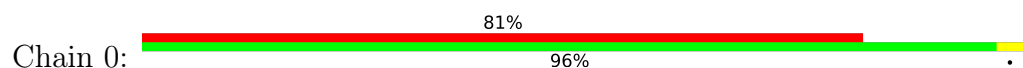
• Molecule 1: TRI-2 (CD1371)

Chain r: 81% 95%

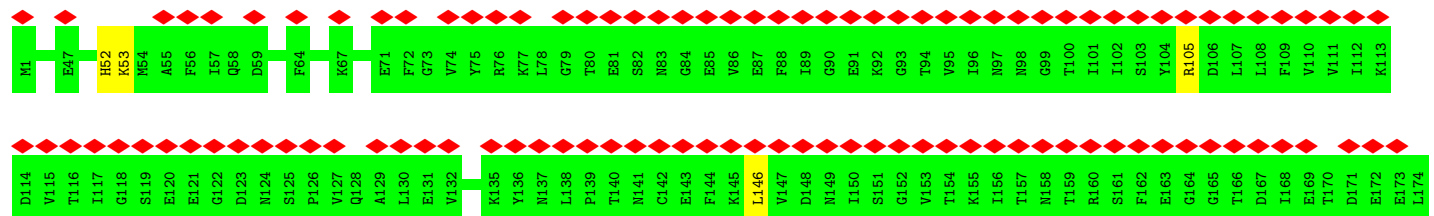
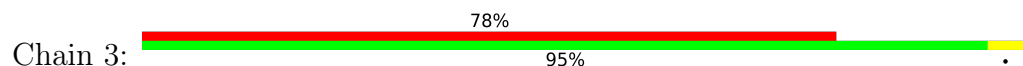


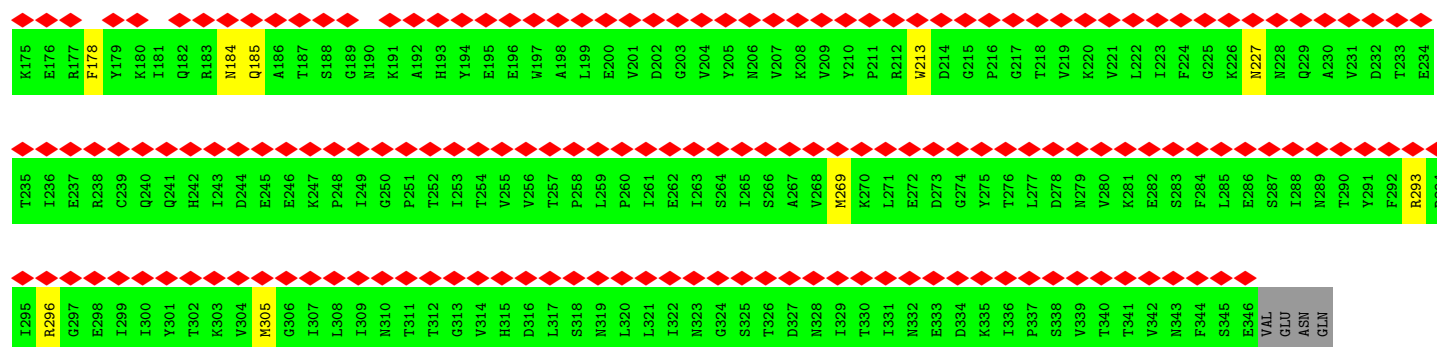


• Molecule 1: TRI-2 (CD1371)

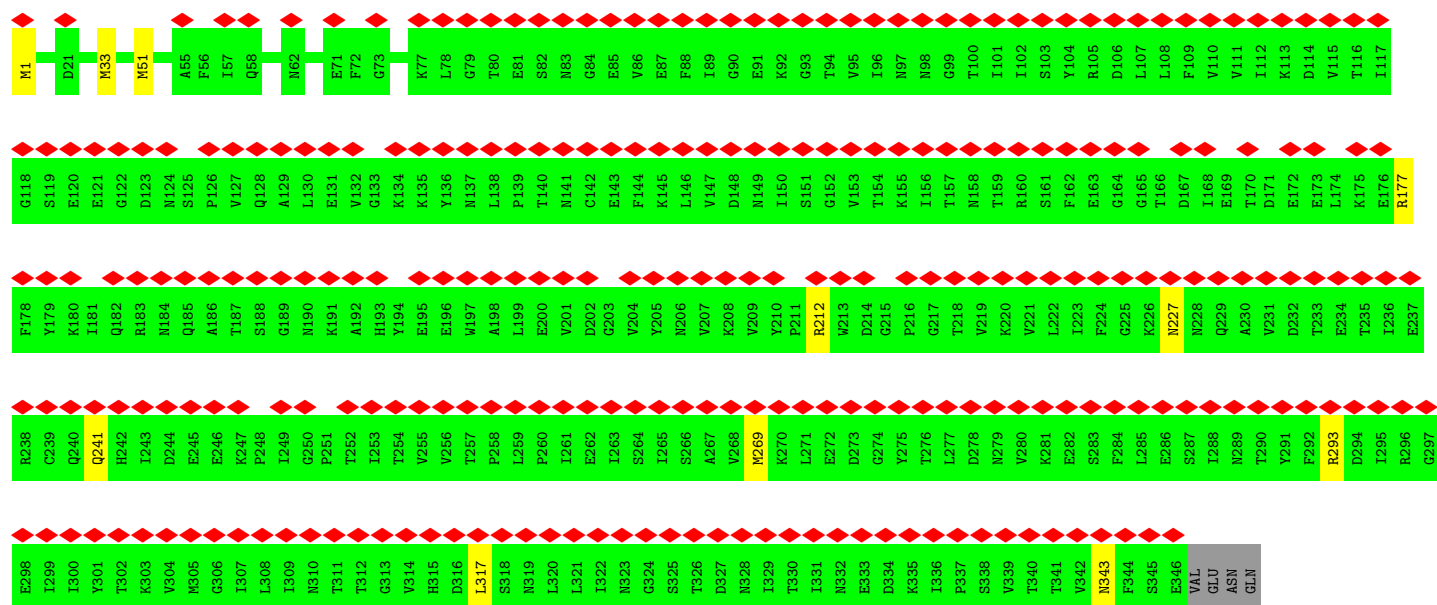
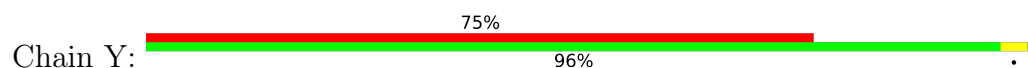


• Molecule 1: TRI-2 (CD1371)

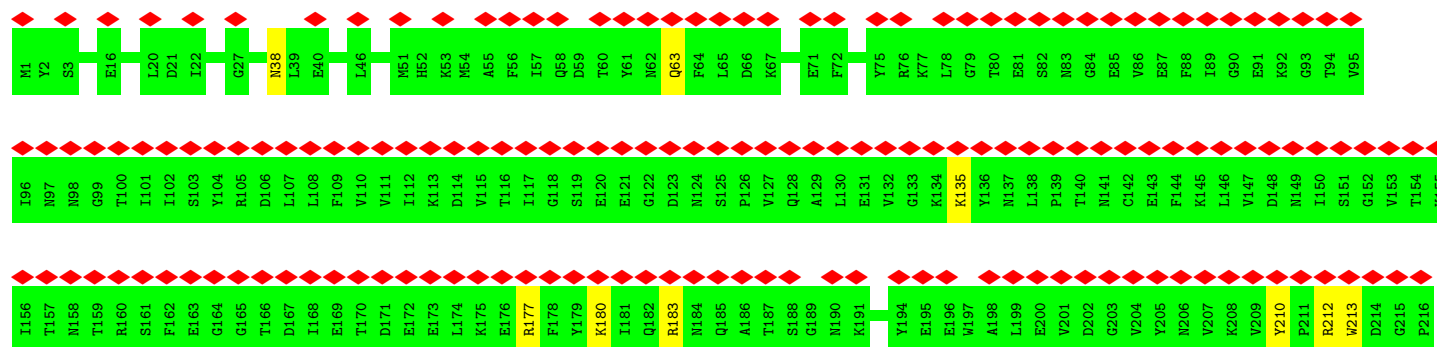
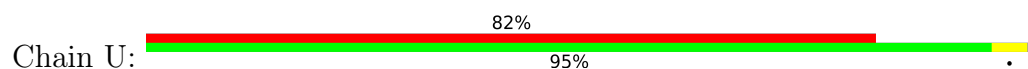




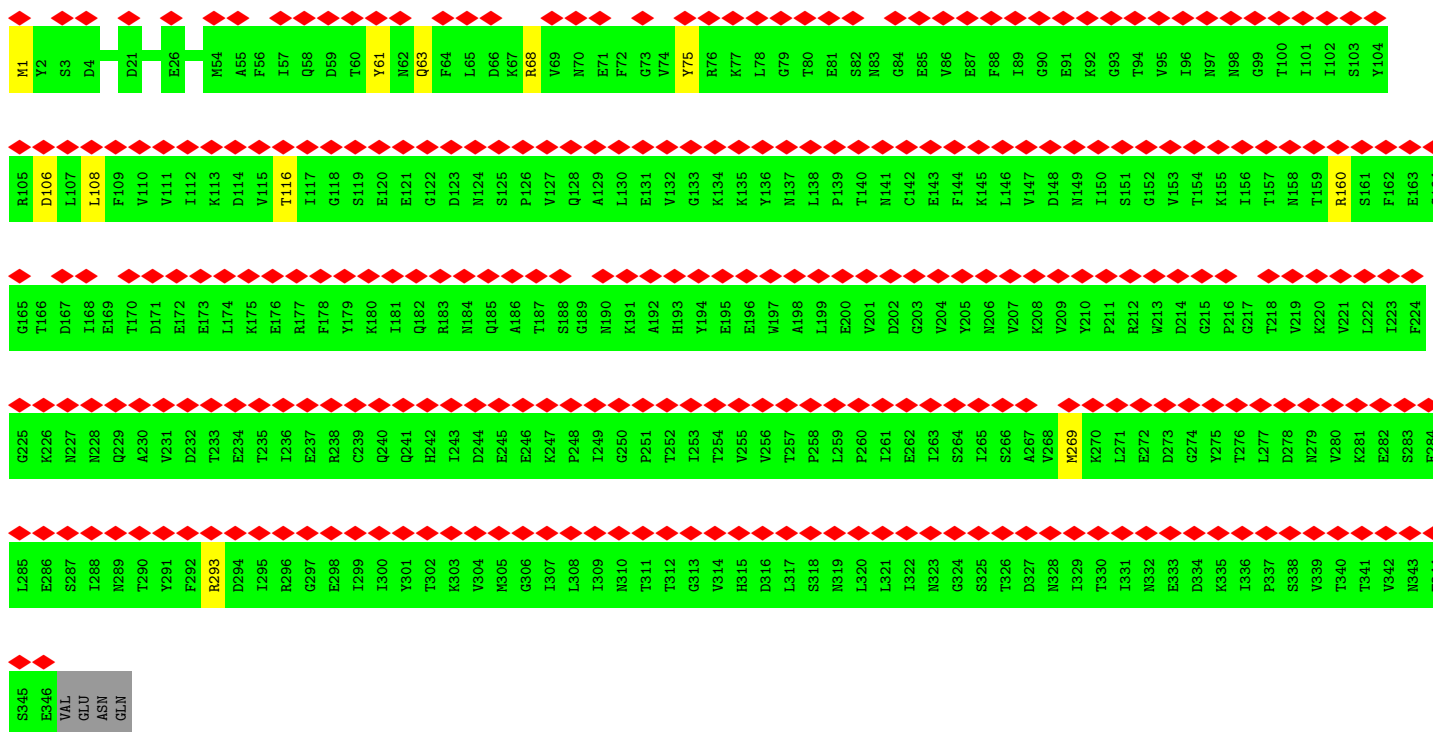
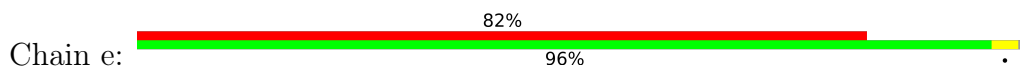
• Molecule 1: TRI-2 (CD1371)



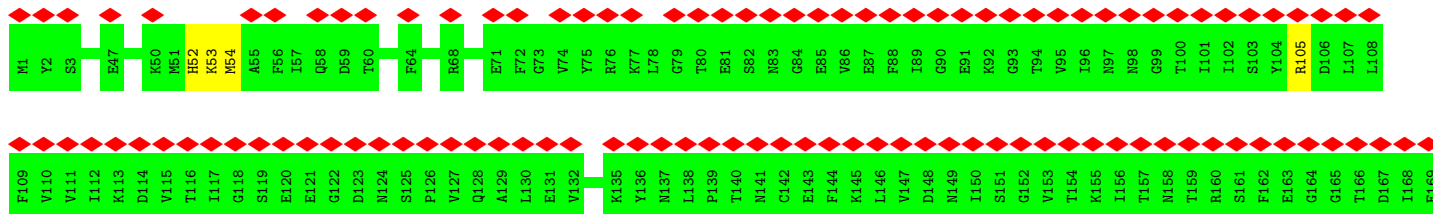
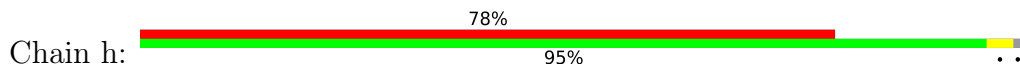
• Molecule 1: TRI-2 (CD1371)

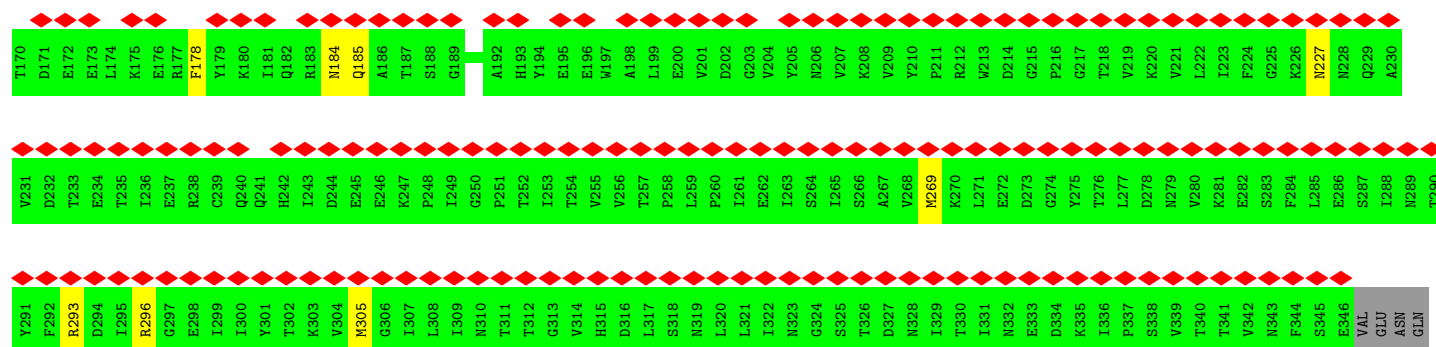


- Molecule 1: TRI-2 (CD1371)

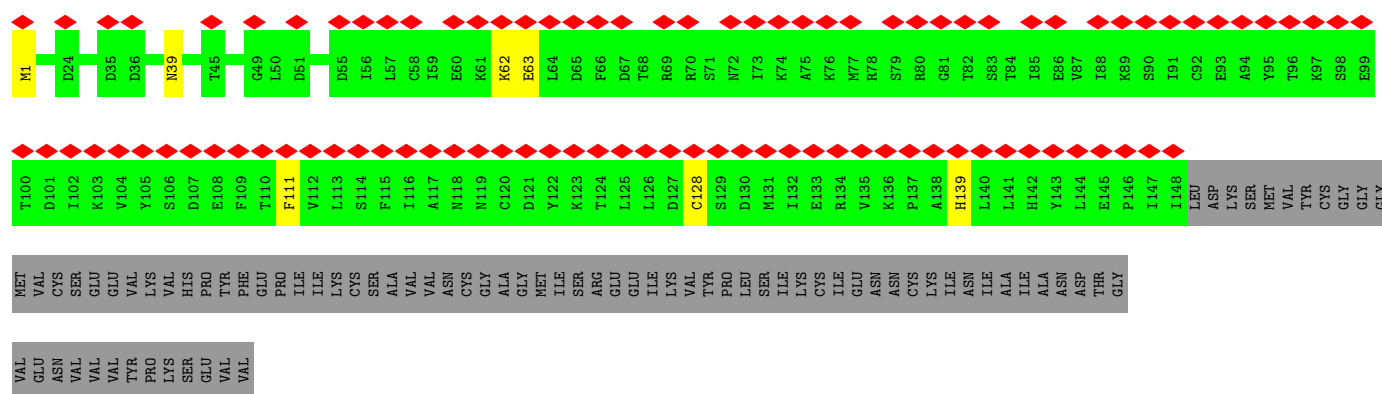
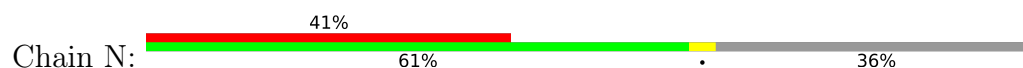


- Molecule 1: TRI-2 (CD1371)

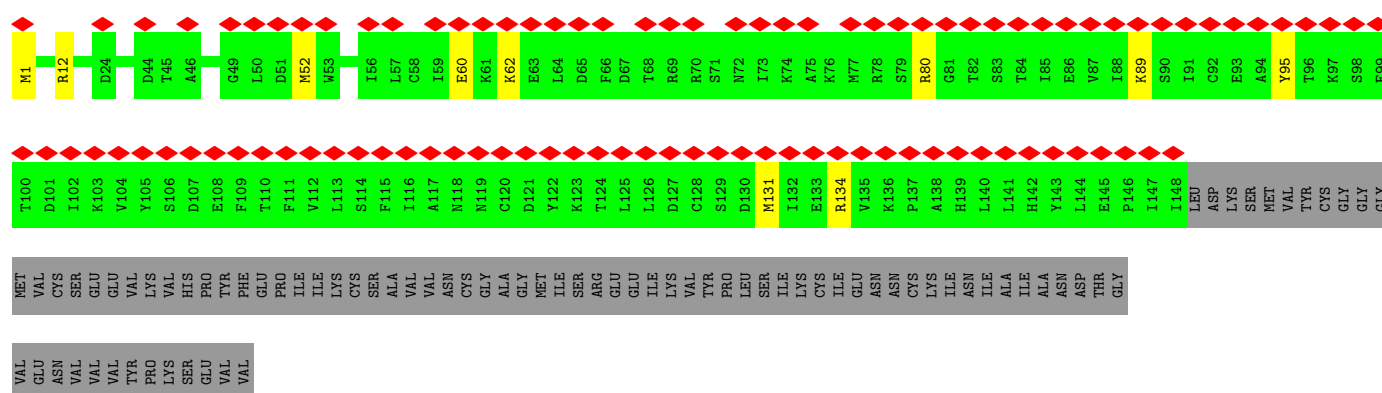
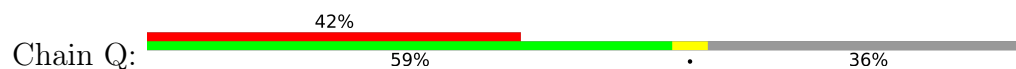




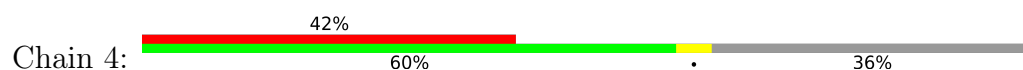
• Molecule 2: TRI-1 (CD1372)



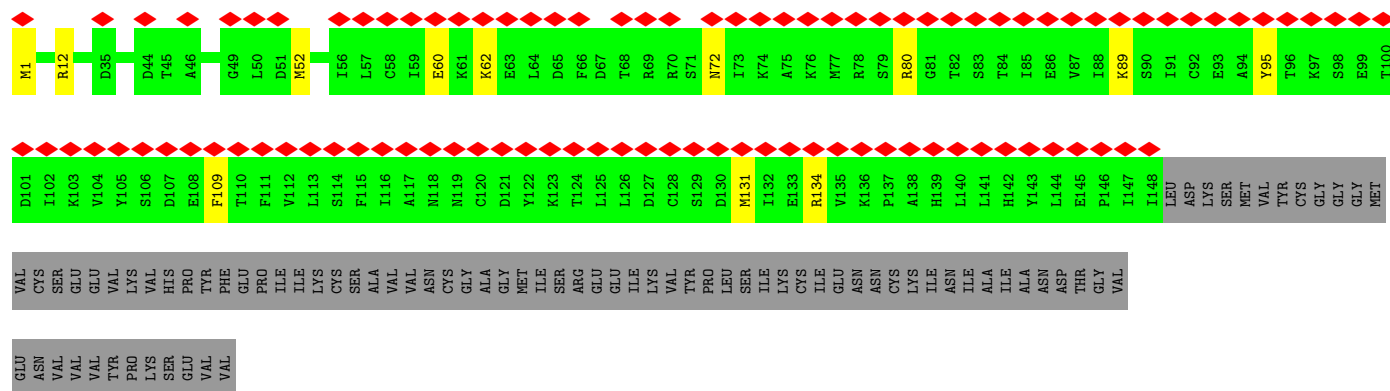
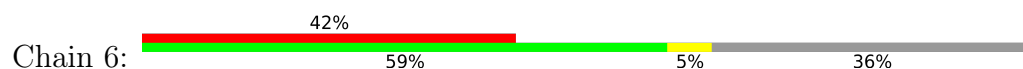
• Molecule 2: TRI-1 (CD1372)



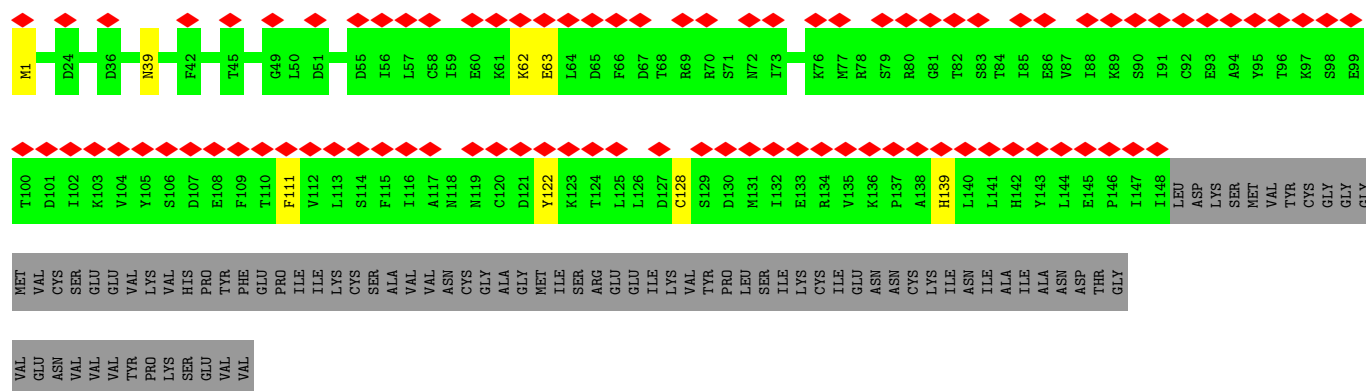
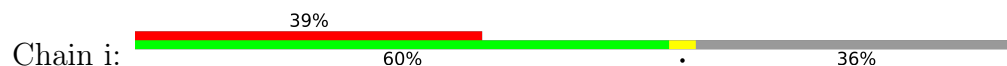
• Molecule 2: TRI-1 (CD1372)



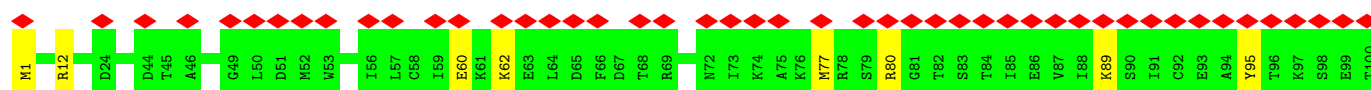
- Molecule 2: TRI-1 (CD1372)



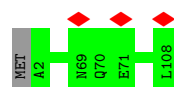
- Molecule 2: TRI-1 (CD1372)



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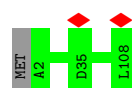
- Molecule 3: Spike (CD1369)



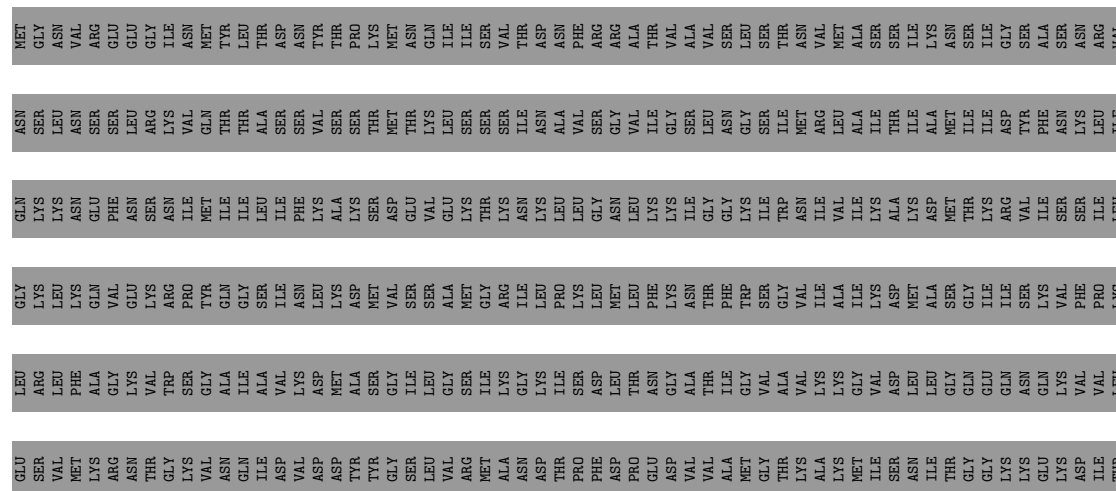
- Molecule 3: Spike (CD1369)



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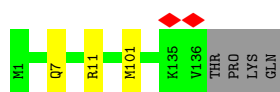
- Molecule 4: Tape measure protein (CD1366)





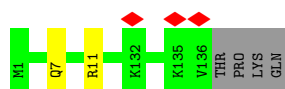
• Molecule 5: Tube tail (CD1367)

Chain G:  95% ..



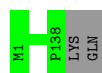
• Molecule 5: Tube tail (CD1367)

Chain w:  96% ..



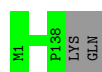
• Molecule 5: Tube tail (CD1367)

Chain T:  99% .



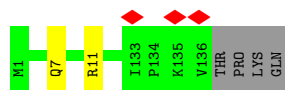
• Molecule 5: Tube tail (CD1367)

Chain y:  99% .



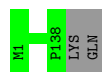
• Molecule 5: Tube tail (CD1367)

Chain Z:  96% ..




• Molecule 5: Tube tail (CD1367)

Chain o:  99% .

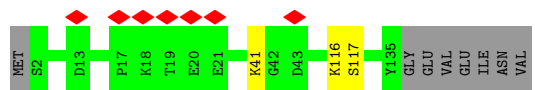
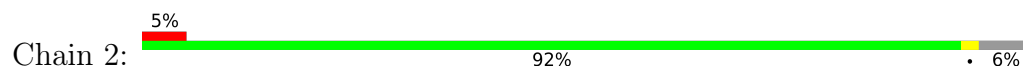


• Molecule 6: Sheath initiator (CD1370)

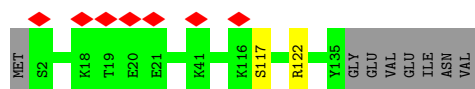
Chain L:  92% . 6%



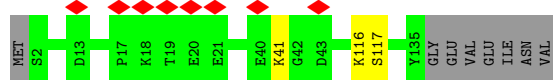
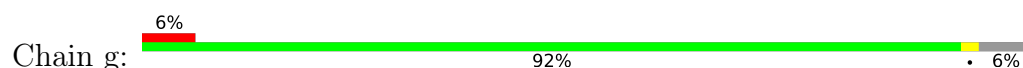
- Molecule 6: Sheath initiator (CD1370)



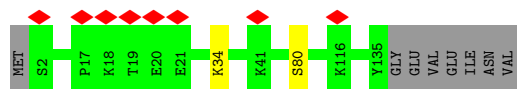
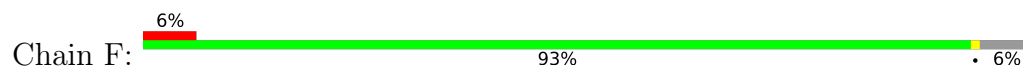
- Molecule 6: Sheath initiator (CD1370)



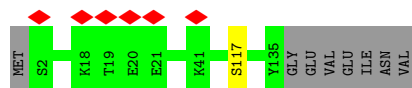
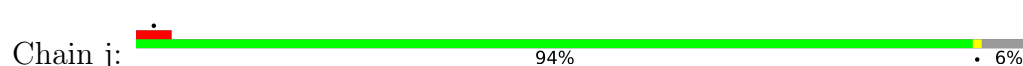
- Molecule 6: Sheath initiator (CD1370)



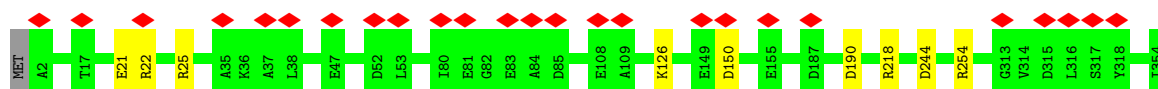
- Molecule 6: Sheath initiator (CD1370)



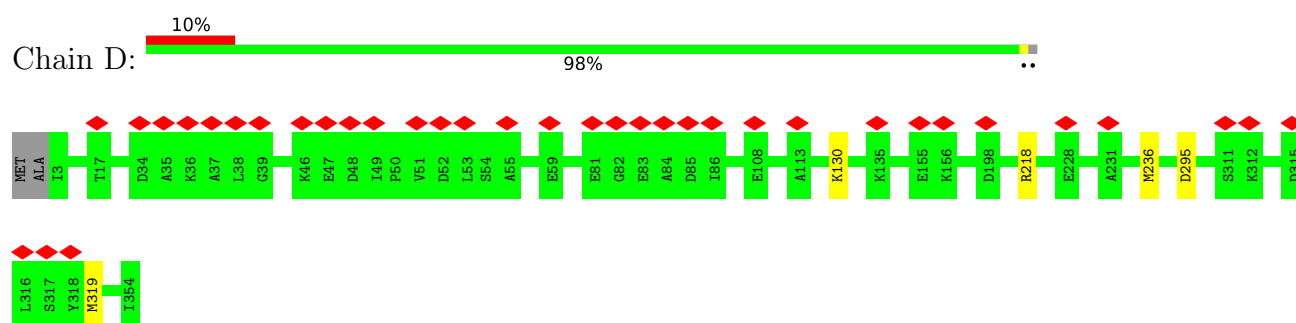
- Molecule 6: Sheath initiator (CD1370)



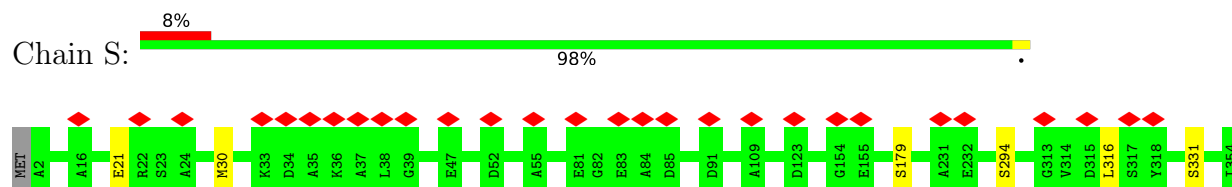
- Molecule 7: Sheath (CD1363)



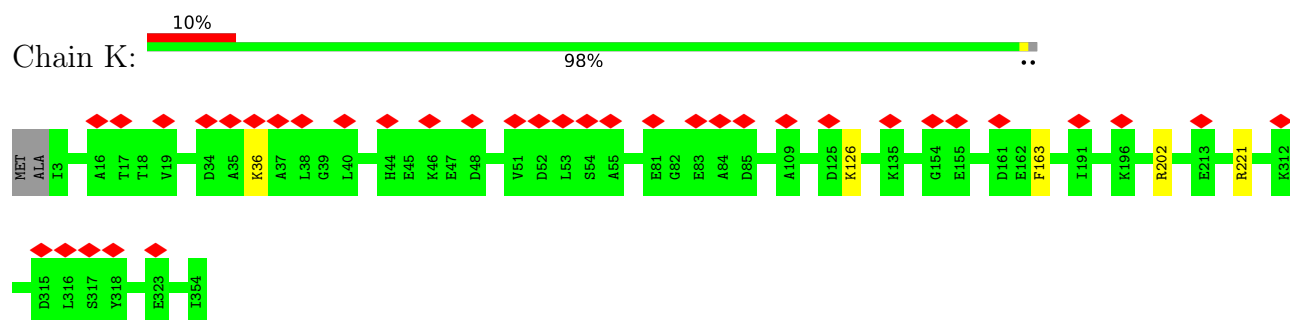
- Molecule 7: Sheath (CD1363)



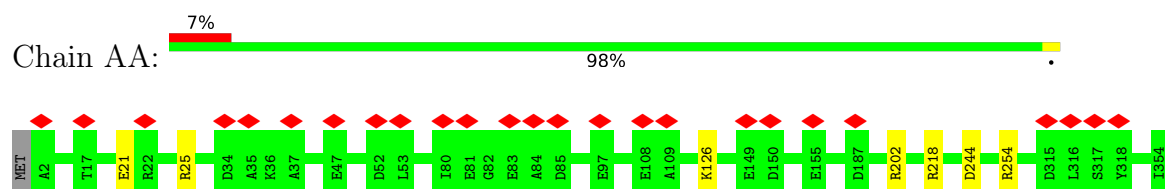
- Molecule 7: Sheath (CD1363)



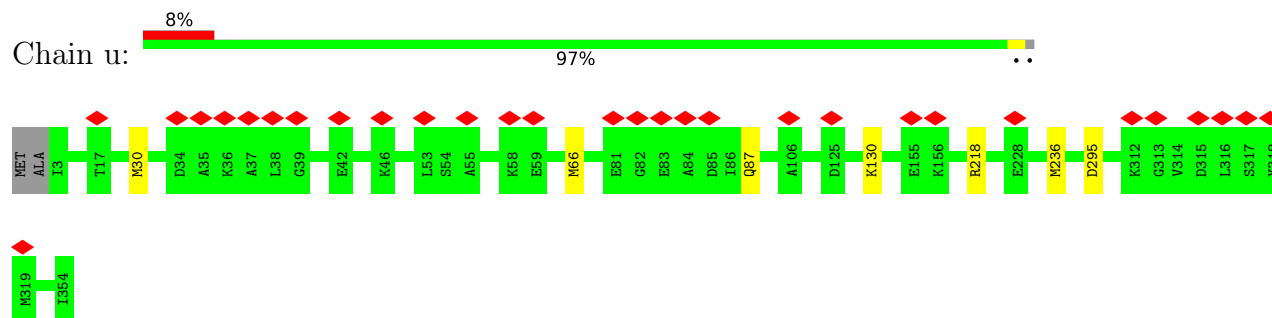
- Molecule 7: Sheath (CD1363)



- Molecule 7: Sheath (CD1363)

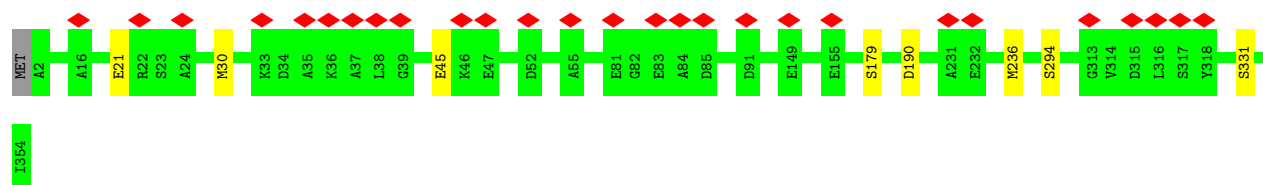


- Molecule 7: Sheath (CD1363)



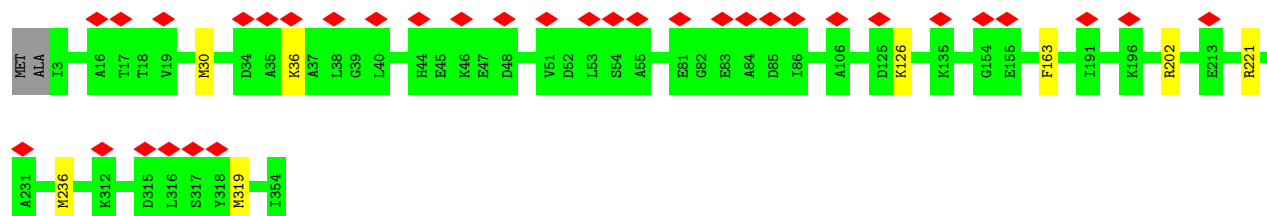
- Molecule 7: Sheath (CD1363)





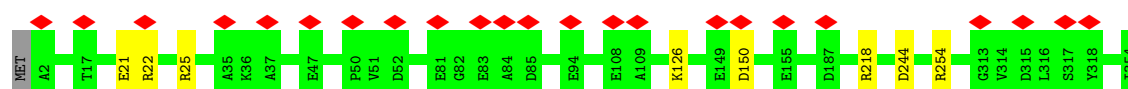
- Molecule 7: Sheath (CD1363)

Chain 1: 10% 97%



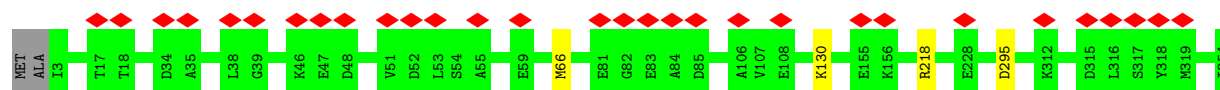
- Molecule 7: Sheath (CD1363)

Chain q: 6% 97%



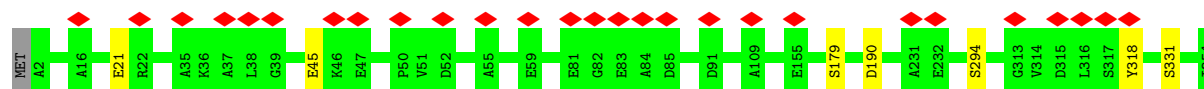
- Molecule 7: Sheath (CD1363)

Chain X: 8% 98%



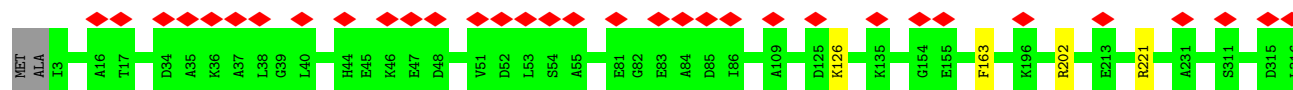
- Molecule 7: Sheath (CD1363)

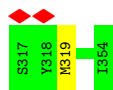
Chain n: 8% 98%



- Molecule 7: Sheath (CD1363)

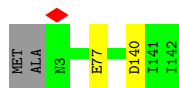
Chain f: 10% 98%





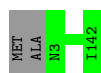
- Molecule 8: Tube (CD1364)

Chain a:  97%



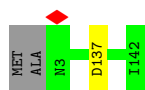
- Molecule 8: Tube (CD1364)

Chain I:  99%



- Molecule 8: Tube (CD1364)

Chain R:  98%



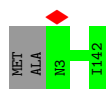
- Molecule 8: Tube (CD1364)

Chain P:  97%



- Molecule 8: Tube (CD1364)

Chain 9:  99%



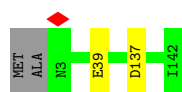
- Molecule 8: Tube (CD1364)

Chain z:  99%



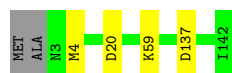
- Molecule 8: Tube (CD1364)

Chain 7:  97%



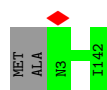
- Molecule 8: Tube (CD1364)

Chain 5:  96%



- Molecule 8: Tube (CD1364)

Chain p:  99%



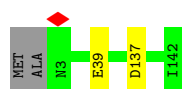
- Molecule 8: Tube (CD1364)

Chain d:  99%



- Molecule 8: Tube (CD1364)

Chain m:  97%



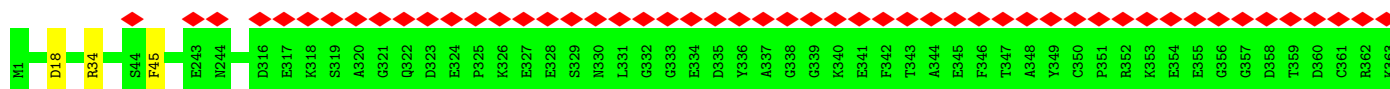
- Molecule 8: Tube (CD1364)

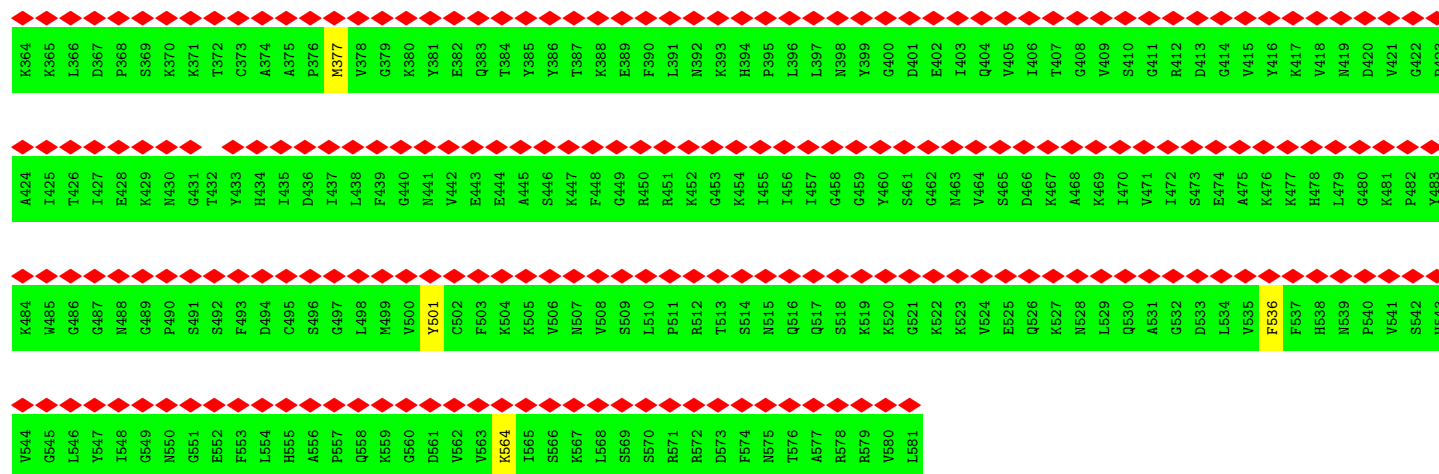
Chain k:  96%



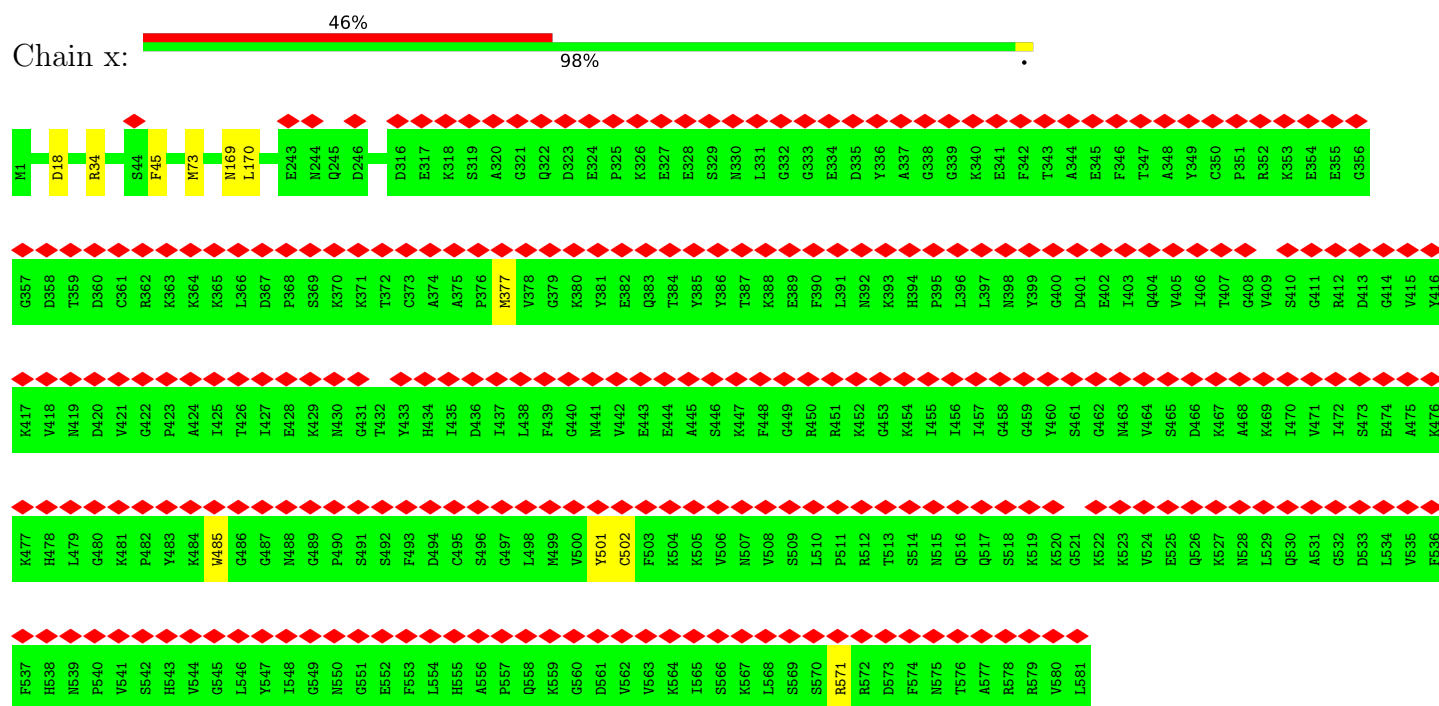
- Molecule 9: Hub-Hydrolase (CD1368)

Chain H:  46%

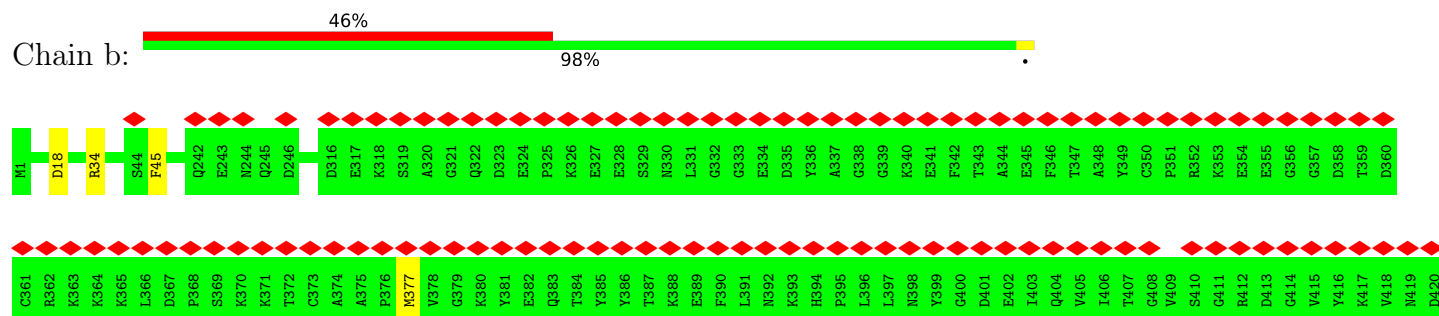




• Molecule 9: Hub-Hydrolase (CD1368)



• Molecule 9: Hub-Hydrolase (CD1368)



V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V663	V664	V665	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681																			
V421	V422	V423	V424	V425	V426	V427	V428	V429	V430	V431	V432	V433	V434	V435	V436	V437	V438	V439	V440	V441	V442	V443	V444	V445	V446	V447	V448	V449	V450	V451	V452	V453	V454	V455	V456	V457	V458	V459	V460	V461	V462	V463	V464	V465	V466	V467	V468	V469	V470	V471	V472	V473	V474	V475	V476	V477	V478	V479	V480
V481	V482	V483	V484	V485	V486	V487	V488	V489	V490	V491	V492	V493	V494	V495	V496	V497	V498	V499	V500	V501	V502	V503	V504	V505	V506	V507	V508	V509	V510	V511	V512	V513	V514	V515	V516	V517	V518	V519	V520	V521	V522	V523	V524	V525	V526	V527	V528	V529	V530	V531	V532	V533	V534	V535	V536	V537	V538	V539	V540

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
Maximum map value	0.195	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	0.26	0/2795	0.50	0/3784
1	3	0.27	0/2795	0.50	0/3784
1	A	0.26	0/2795	0.50	0/3784
1	E	0.27	0/2795	0.51	0/3784
1	J	0.26	0/2795	0.50	0/3784
1	M	0.27	0/2795	0.50	0/3784
1	U	0.26	0/2795	0.50	0/3784
1	Y	0.27	0/2795	0.50	0/3784
1	e	0.26	0/2795	0.50	0/3784
1	h	0.27	0/2795	0.50	0/3784
1	r	0.26	0/2795	0.50	0/3784
1	v	0.27	0/2795	0.51	0/3784
2	4	0.25	0/1235	0.47	0/1668
2	6	0.27	0/1235	0.49	0/1668
2	N	0.25	0/1235	0.46	0/1668
2	Q	0.28	0/1235	0.49	0/1668
2	i	0.25	0/1235	0.47	0/1668
2	l	0.26	0/1235	0.47	0/1668
3	C	0.27	0/896	0.49	0/1206
3	W	0.27	0/896	0.49	0/1206
3	t	0.28	0/896	0.49	0/1206
4	B	0.26	0/164	0.41	0/220
4	V	0.26	0/164	0.41	0/220
4	s	0.26	0/164	0.41	0/220
5	G	0.32	0/1139	0.53	0/1534
5	T	0.32	0/1154	0.52	0/1556
5	Z	0.32	0/1139	0.53	0/1534
5	o	0.32	0/1154	0.52	0/1556
5	w	0.33	0/1139	0.52	0/1534
5	y	0.32	0/1154	0.51	0/1556
6	2	0.30	0/1133	0.48	0/1532
6	F	0.29	0/1133	0.46	0/1532
6	L	0.30	0/1133	0.47	0/1532
6	O	0.30	0/1133	0.45	0/1532

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	g	0.30	0/1133	0.47	0/1532
6	j	0.29	0/1133	0.45	0/1532
7	1	0.26	0/2766	0.48	0/3729
7	8	0.28	0/2771	0.48	0/3736
7	AA	0.28	0/2771	0.47	0/3736
7	D	0.26	0/2766	0.47	0/3729
7	K	0.26	0/2766	0.47	0/3729
7	S	0.28	0/2771	0.48	0/3736
7	X	0.26	0/2766	0.47	0/3729
7	c	0.28	0/2771	0.47	0/3736
7	f	0.26	0/2766	0.47	0/3729
7	n	0.28	0/2771	0.47	0/3736
7	q	0.27	0/2771	0.46	0/3736
7	u	0.26	0/2766	0.47	0/3729
8	5	0.30	0/1133	0.50	0/1522
8	7	0.30	0/1133	0.50	0/1522
8	9	0.30	0/1133	0.52	0/1522
8	I	0.30	0/1133	0.49	0/1522
8	P	0.30	0/1133	0.50	0/1522
8	R	0.30	0/1133	0.50	0/1522
8	a	0.32	0/1133	0.52	0/1522
8	d	0.30	0/1133	0.49	0/1522
8	k	0.30	0/1133	0.50	0/1522
8	m	0.30	0/1133	0.50	0/1522
8	p	0.30	0/1133	0.52	0/1522
8	z	0.30	0/1133	0.49	0/1522
9	H	0.29	0/4678	0.48	0/6286
9	b	0.28	0/4678	0.48	0/6286
9	x	0.29	0/4678	0.48	0/6286
All	All	0.28	0/118659	0.49	0/160068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	302 (96%)	11 (4%)	36	70
1	3	313/317 (99%)	300 (96%)	13 (4%)	30	63
1	A	313/317 (99%)	299 (96%)	14 (4%)	27	61
1	E	313/317 (99%)	303 (97%)	10 (3%)	39	73
1	J	313/317 (99%)	303 (97%)	10 (3%)	39	73
1	M	313/317 (99%)	302 (96%)	11 (4%)	36	70
1	U	313/317 (99%)	299 (96%)	14 (4%)	27	61
1	Y	313/317 (99%)	302 (96%)	11 (4%)	36	70
1	e	313/317 (99%)	302 (96%)	11 (4%)	36	70
1	h	313/317 (99%)	301 (96%)	12 (4%)	33	67
1	r	313/317 (99%)	301 (96%)	12 (4%)	33	67
1	v	313/317 (99%)	301 (96%)	12 (4%)	33	67
2	4	139/213 (65%)	130 (94%)	9 (6%)	17	45
2	6	139/213 (65%)	127 (91%)	12 (9%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	139/213 (65%)	132 (95%)	7 (5%)	24	57
2	Q	139/213 (65%)	129 (93%)	10 (7%)	14	39
2	i	139/213 (65%)	131 (94%)	8 (6%)	20	50
2	l	139/213 (65%)	130 (94%)	9 (6%)	17	45
3	C	100/101 (99%)	100 (100%)	0	100	100
3	W	100/101 (99%)	100 (100%)	0	100	100
3	t	100/101 (99%)	100 (100%)	0	100	100
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%)	120 (98%)	3 (2%)	49	79
5	T	125/127 (98%)	125 (100%)	0	100	100
5	Z	123/127 (97%)	121 (98%)	2 (2%)	62	86
5	o	125/127 (98%)	125 (100%)	0	100	100
5	w	123/127 (97%)	121 (98%)	2 (2%)	62	86
5	y	125/127 (98%)	125 (100%)	0	100	100
6	2	123/130 (95%)	120 (98%)	3 (2%)	49	79
6	F	123/130 (95%)	121 (98%)	2 (2%)	62	86
6	L	123/130 (95%)	120 (98%)	3 (2%)	49	79
6	O	123/130 (95%)	121 (98%)	2 (2%)	62	86
6	g	123/130 (95%)	120 (98%)	3 (2%)	49	79
6	j	123/130 (95%)	122 (99%)	1 (1%)	81	94
7	1	308/309 (100%)	300 (97%)	8 (3%)	46	77
7	8	308/309 (100%)	300 (97%)	8 (3%)	46	77
7	AA	308/309 (100%)	301 (98%)	7 (2%)	50	80
7	D	308/309 (100%)	303 (98%)	5 (2%)	62	86
7	K	308/309 (100%)	303 (98%)	5 (2%)	62	86
7	S	308/309 (100%)	302 (98%)	6 (2%)	57	84
7	X	308/309 (100%)	304 (99%)	4 (1%)	69	90
7	c	308/309 (100%)	299 (97%)	9 (3%)	42	76
7	f	308/309 (100%)	303 (98%)	5 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	n	308/309 (100%)	301 (98%)	7 (2%)	50	80
7	q	308/309 (100%)	300 (97%)	8 (3%)	46	77
7	u	308/309 (100%)	301 (98%)	7 (2%)	50	80
8	5	117/118 (99%)	113 (97%)	4 (3%)	37	71
8	7	117/118 (99%)	115 (98%)	2 (2%)	60	86
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%)	115 (98%)	2 (2%)	60	86
8	R	117/118 (99%)	116 (99%)	1 (1%)	78	93
8	a	117/118 (99%)	115 (98%)	2 (2%)	60	86
8	d	117/118 (99%)	117 (100%)	0	100	100
8	k	117/118 (99%)	114 (97%)	3 (3%)	46	77
8	m	117/118 (99%)	115 (98%)	2 (2%)	60	86
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%)	506 (99%)	7 (1%)	67	89
9	b	513/513 (100%)	503 (98%)	10 (2%)	57	84
9	x	513/513 (100%)	502 (98%)	11 (2%)	53	81
All	All	13065/15672 (83%)	12725 (97%)	340 (3%)	49	77

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	177	ARG
9	b	501	TYR
1	Y	343	ASN
2	i	139	HIS
8	k	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	6	72	ASN
7	f	204	ASN
1	Y	229	GLN

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Mol	Chain	Res	Type
8	p	8	ASN
1	e	227	ASN

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 monosaccharides 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.

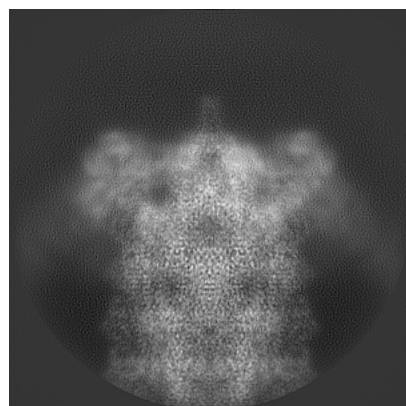
6 Map visualisation [i](#)

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.

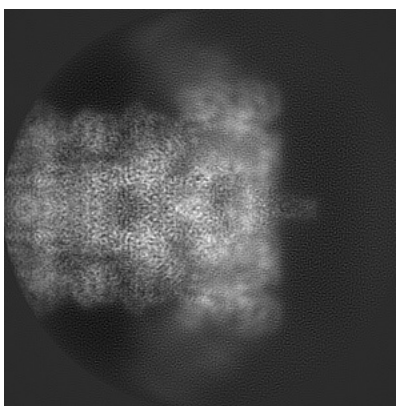
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

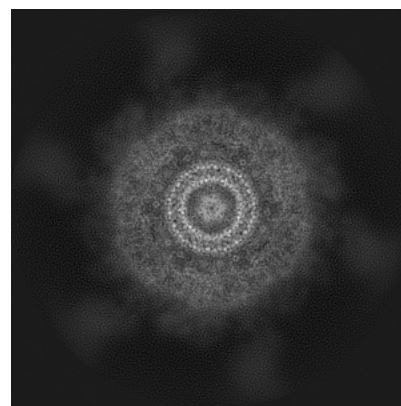
6.1.1 Primary map



X

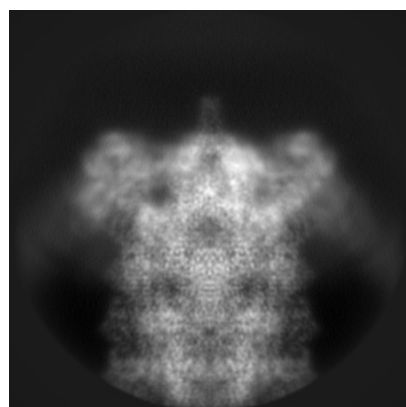


Y

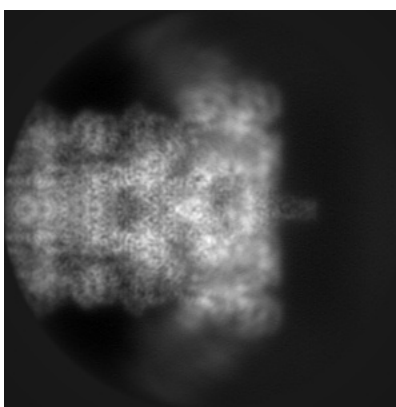


Z

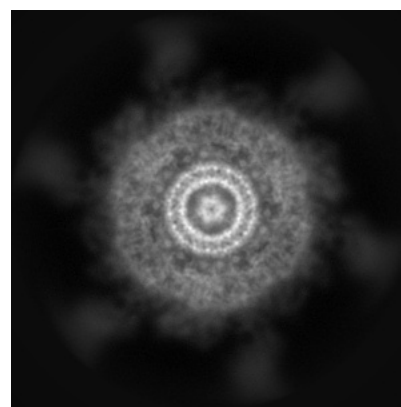
6.1.2 Raw map



X



Y

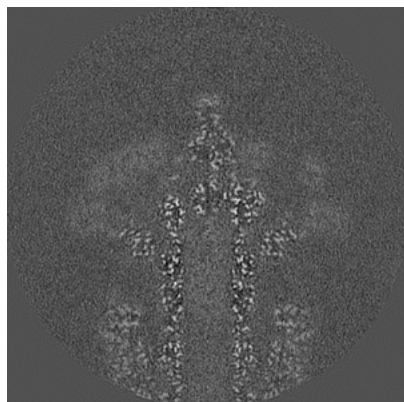


Z

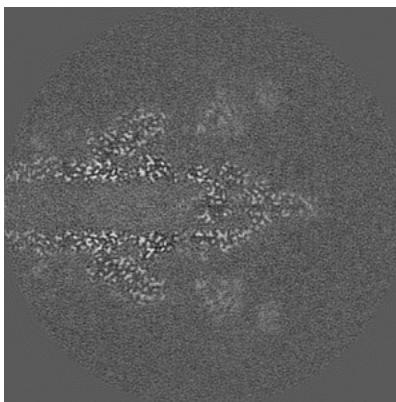
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

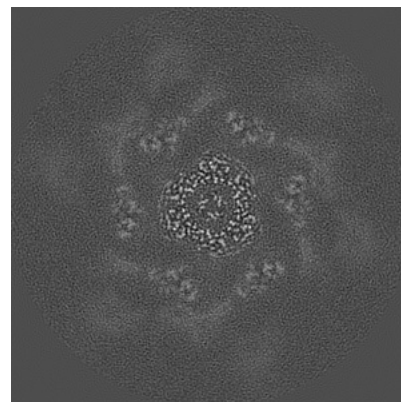
6.2.1 Primary map



X Index: 150

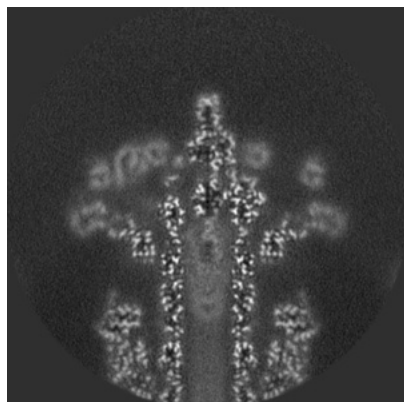


Y Index: 150

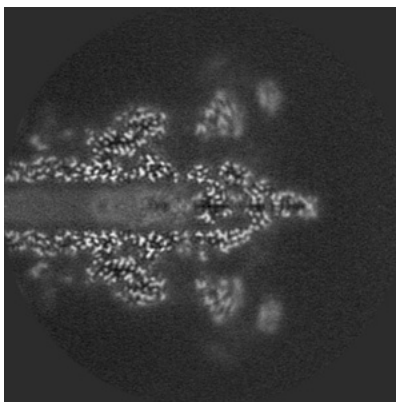


Z Index: 150

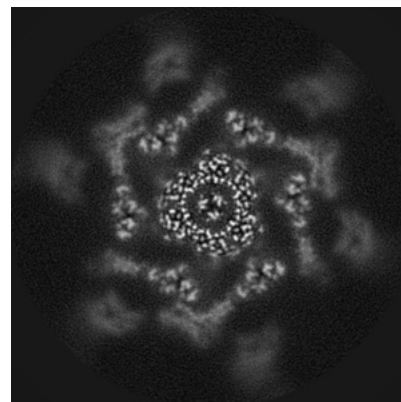
6.2.2 Raw map



X Index: 150



Y Index: 150

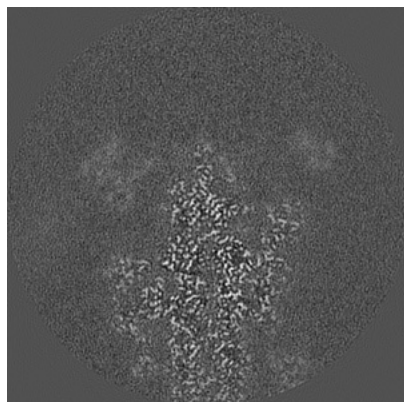


Z Index: 150

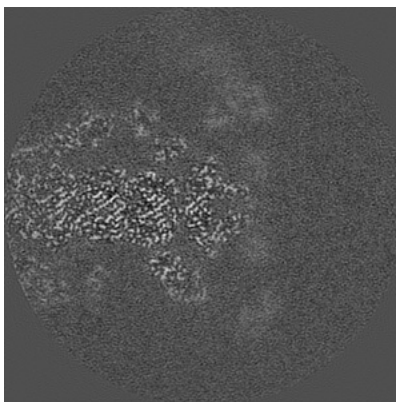
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

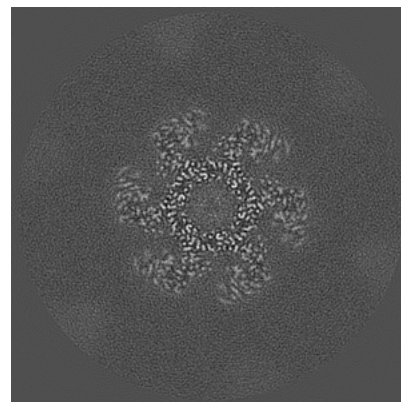
6.3.1 Primary map



X Index: 169

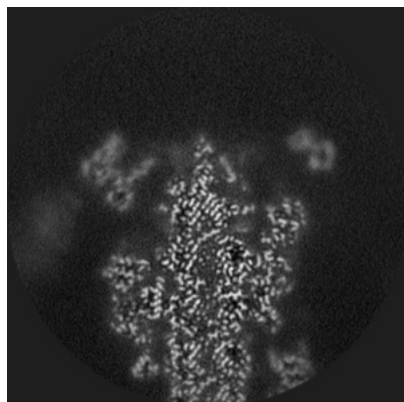


Y Index: 129

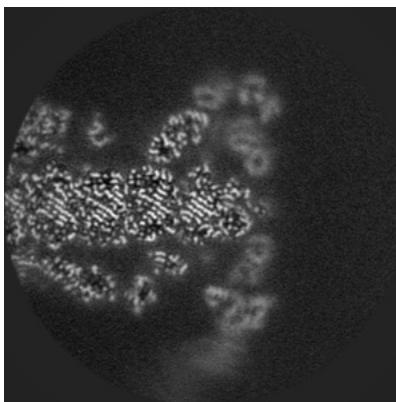


Z Index: 108

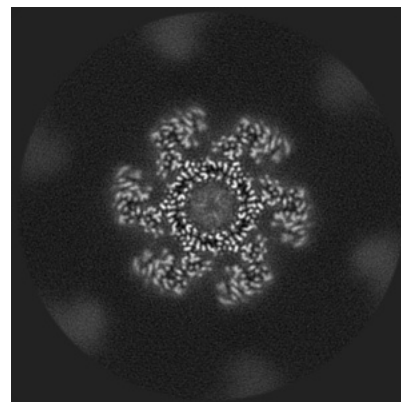
6.3.2 Raw map



X Index: 169



Y Index: 171

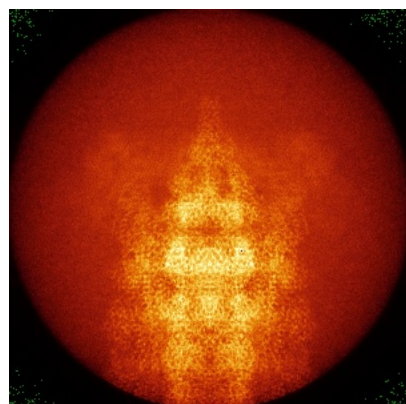


Z Index: 108

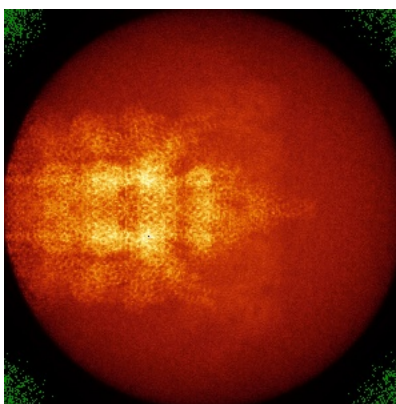
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

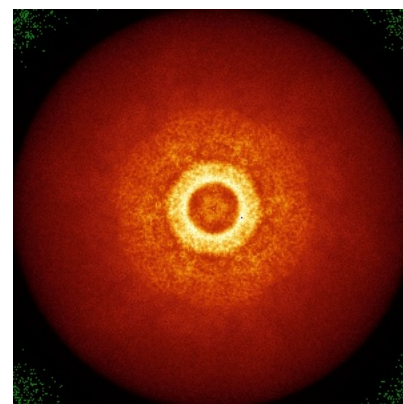
6.4.1 Primary map



X

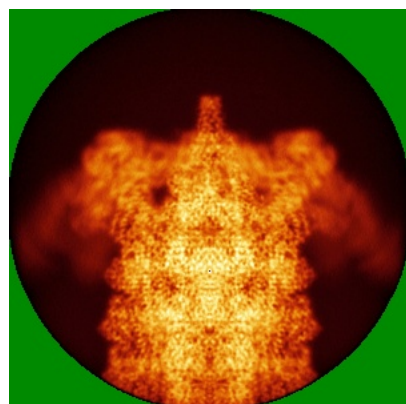


Y

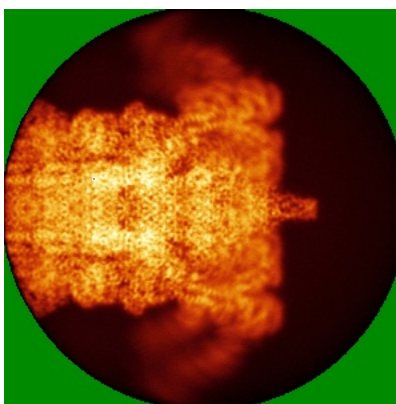


Z

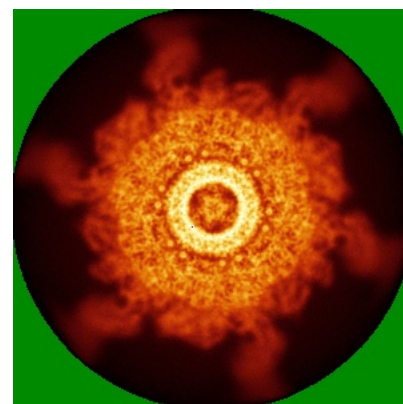
6.4.2 Raw map



X



Y

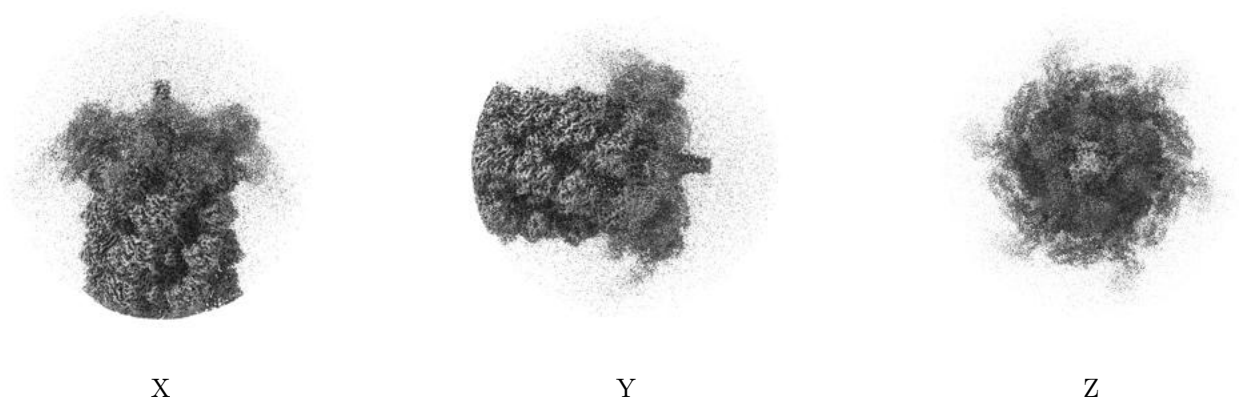


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

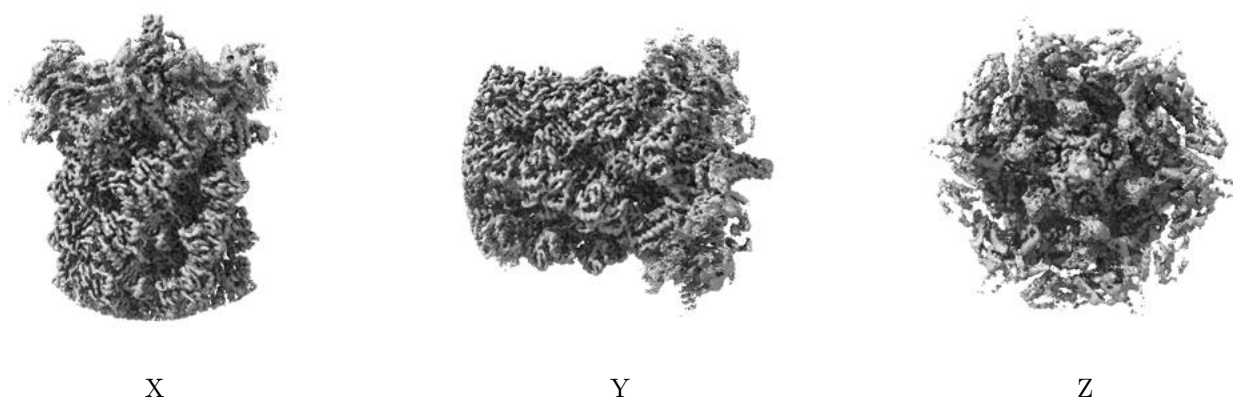
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

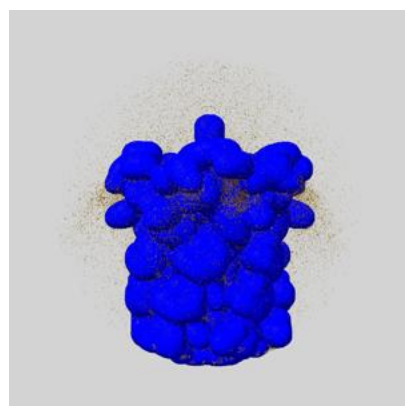
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

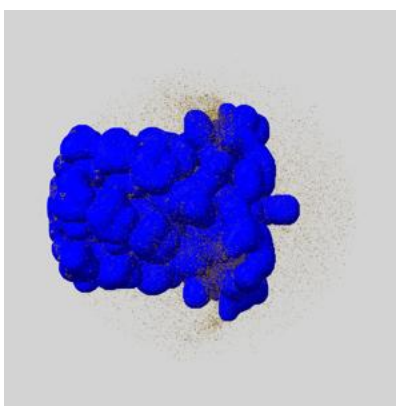
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

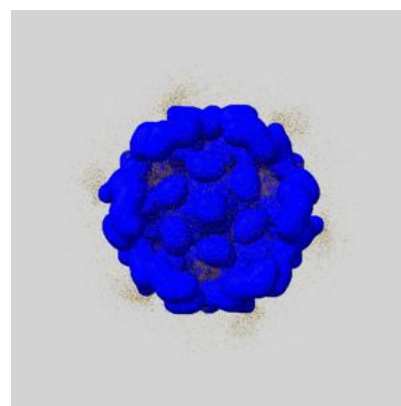
6.6.1 emd_42956_msk_1.map [i](#)



X



Y

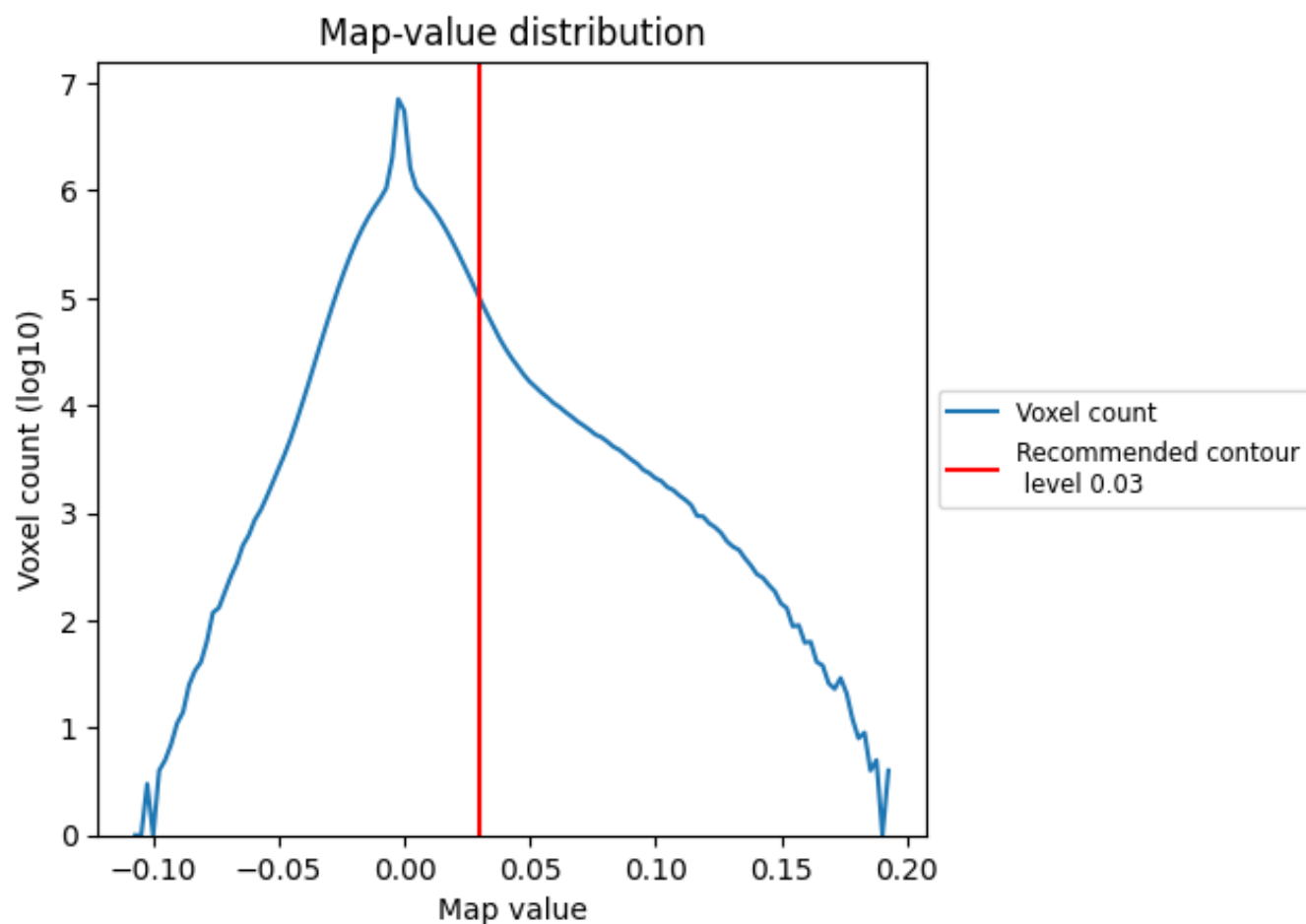


Z

7 Map analysis [i](#)

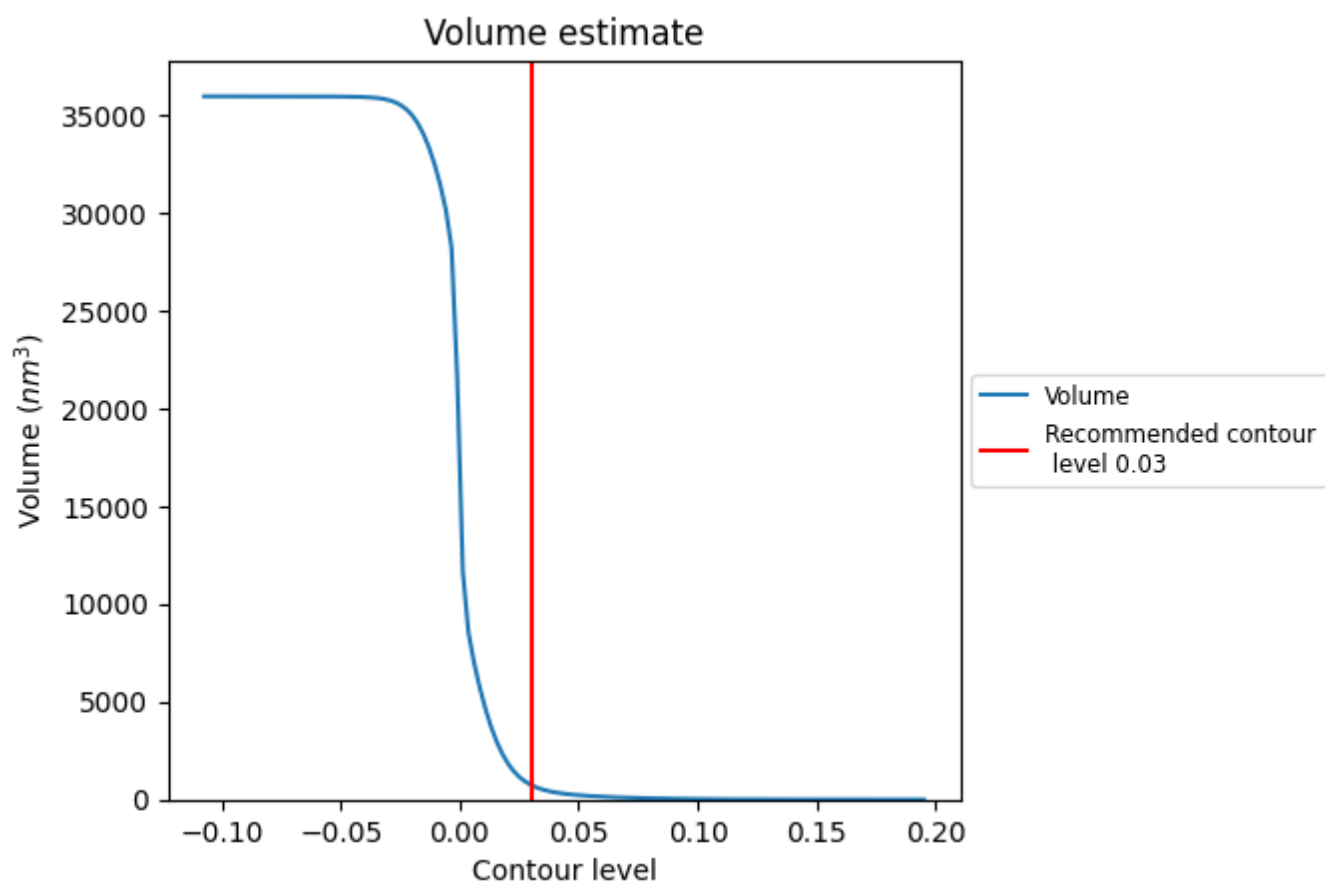
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

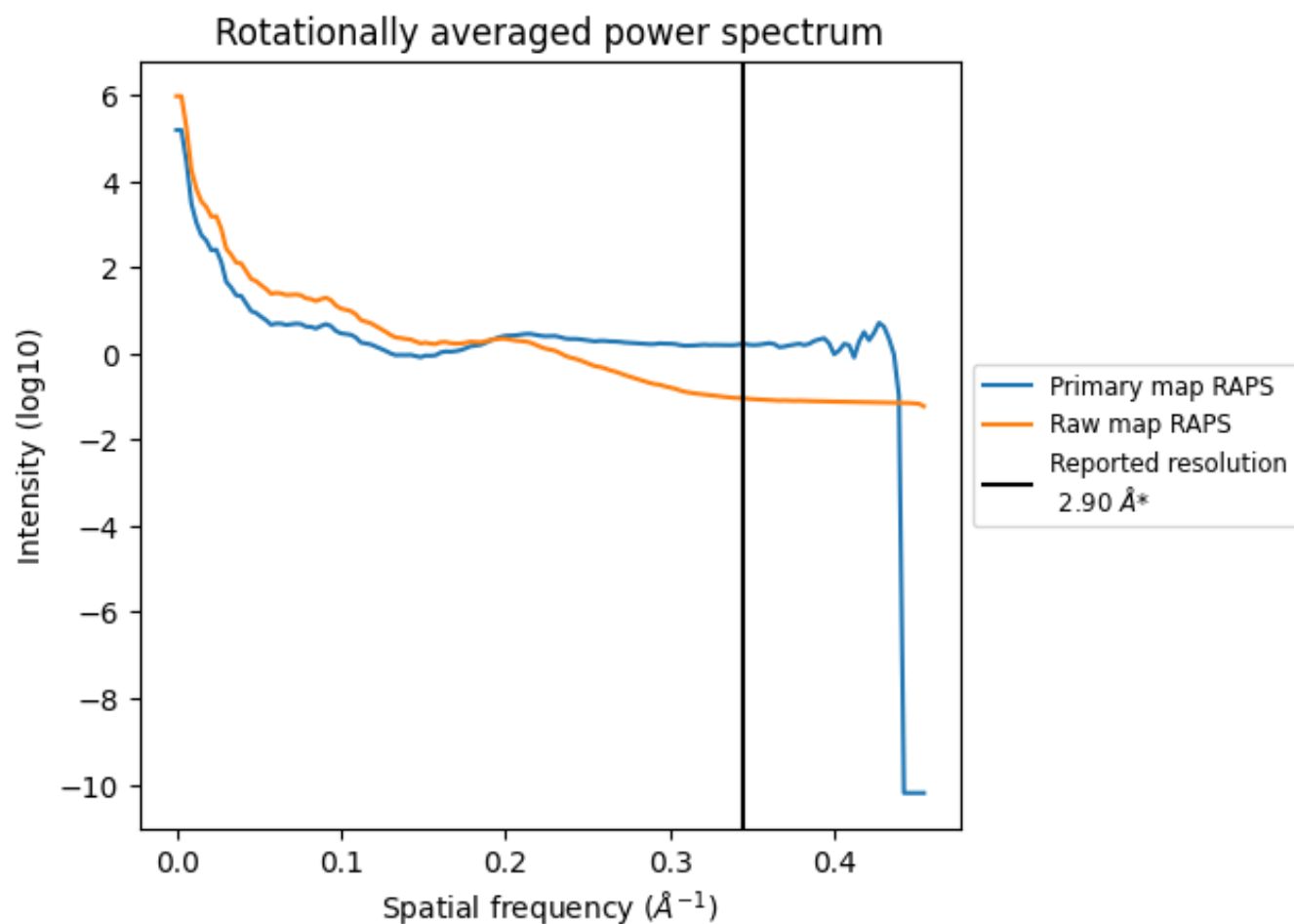
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 748 nm³; this corresponds to an approximate mass of 676 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

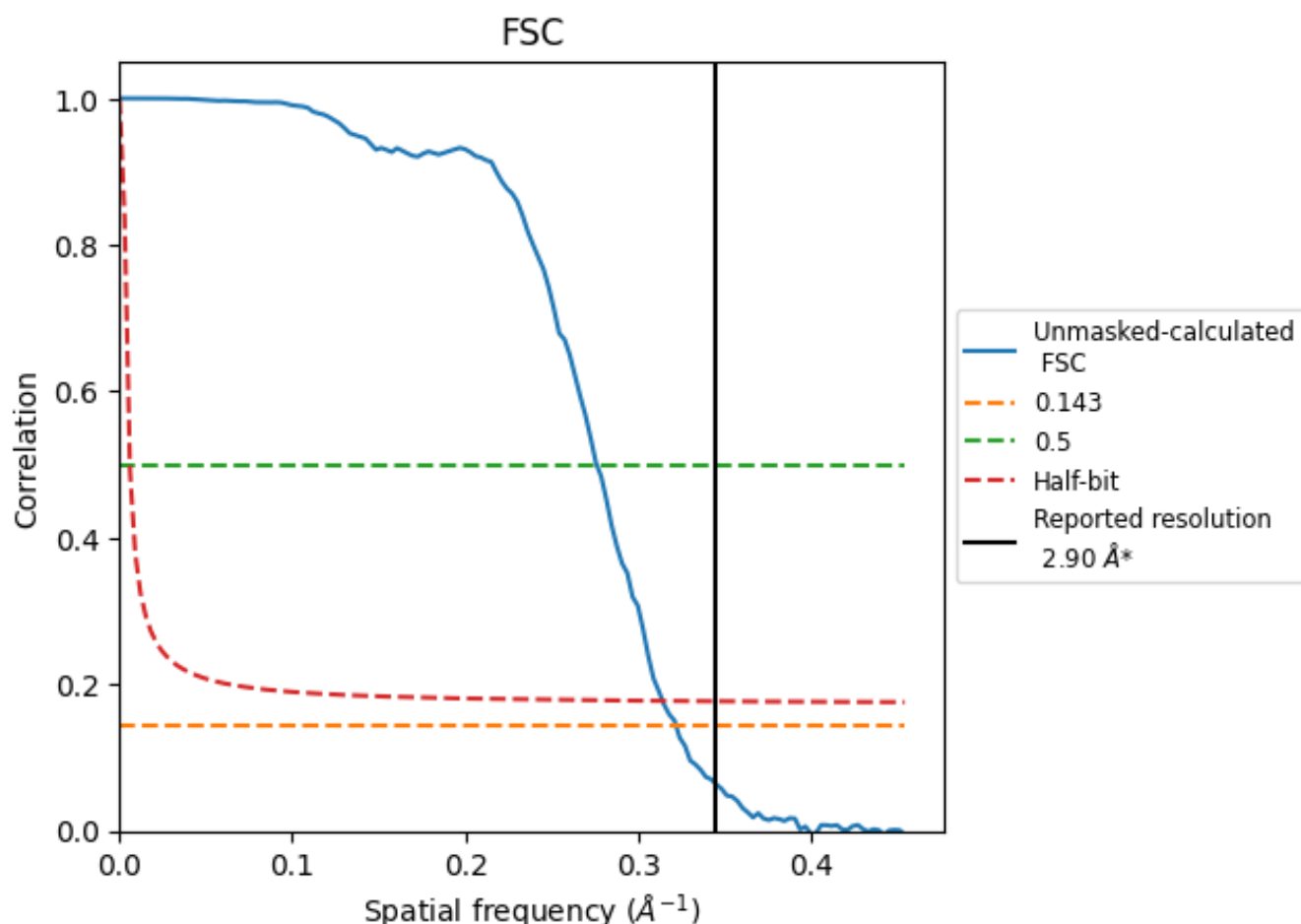


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

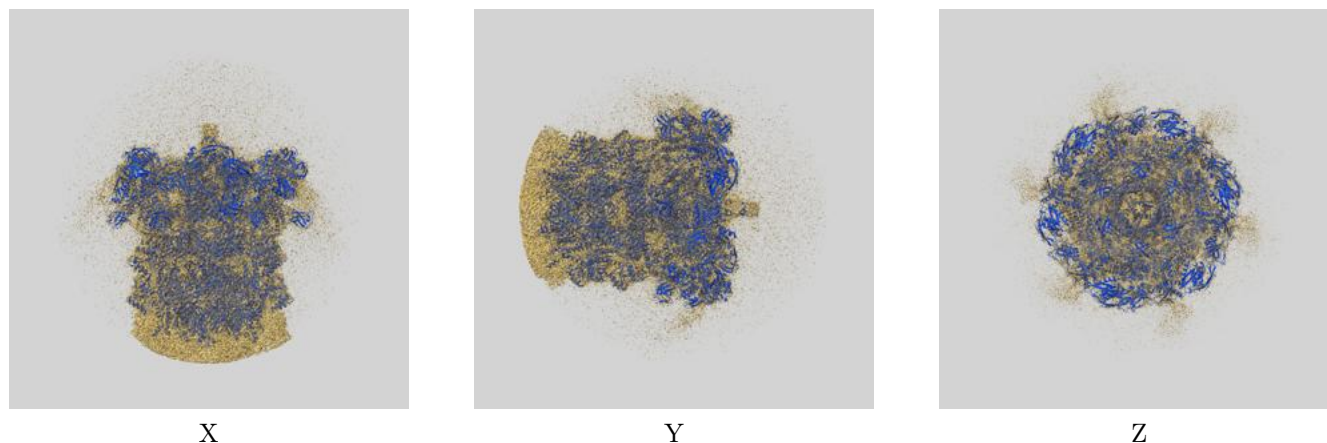
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.10	3.62	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

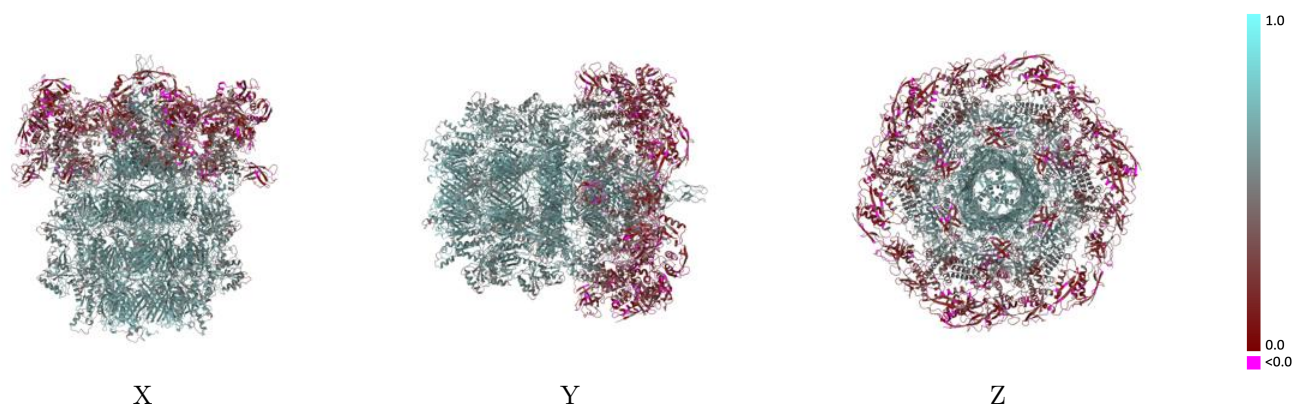
This section contains information regarding the fit between EMDB map EMD-42956 and PDB model 8V3W. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



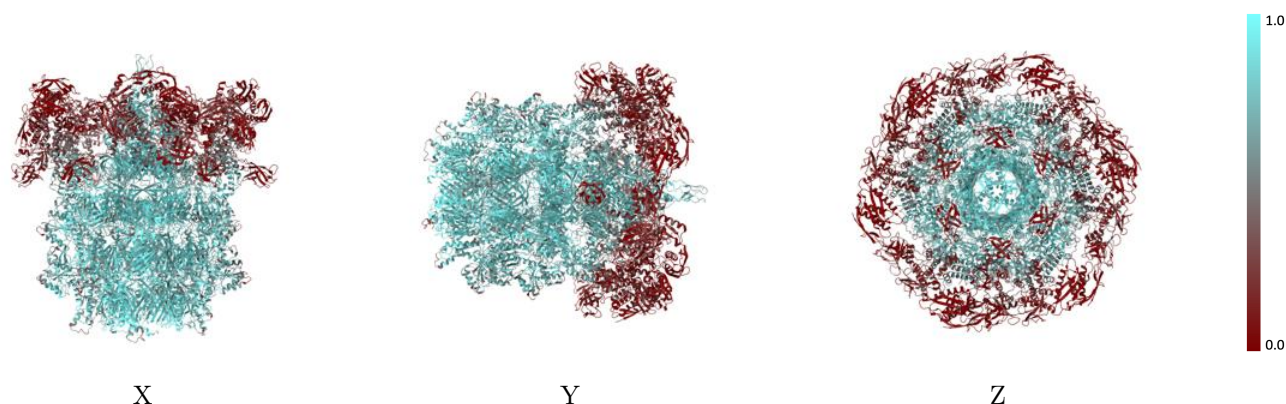
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



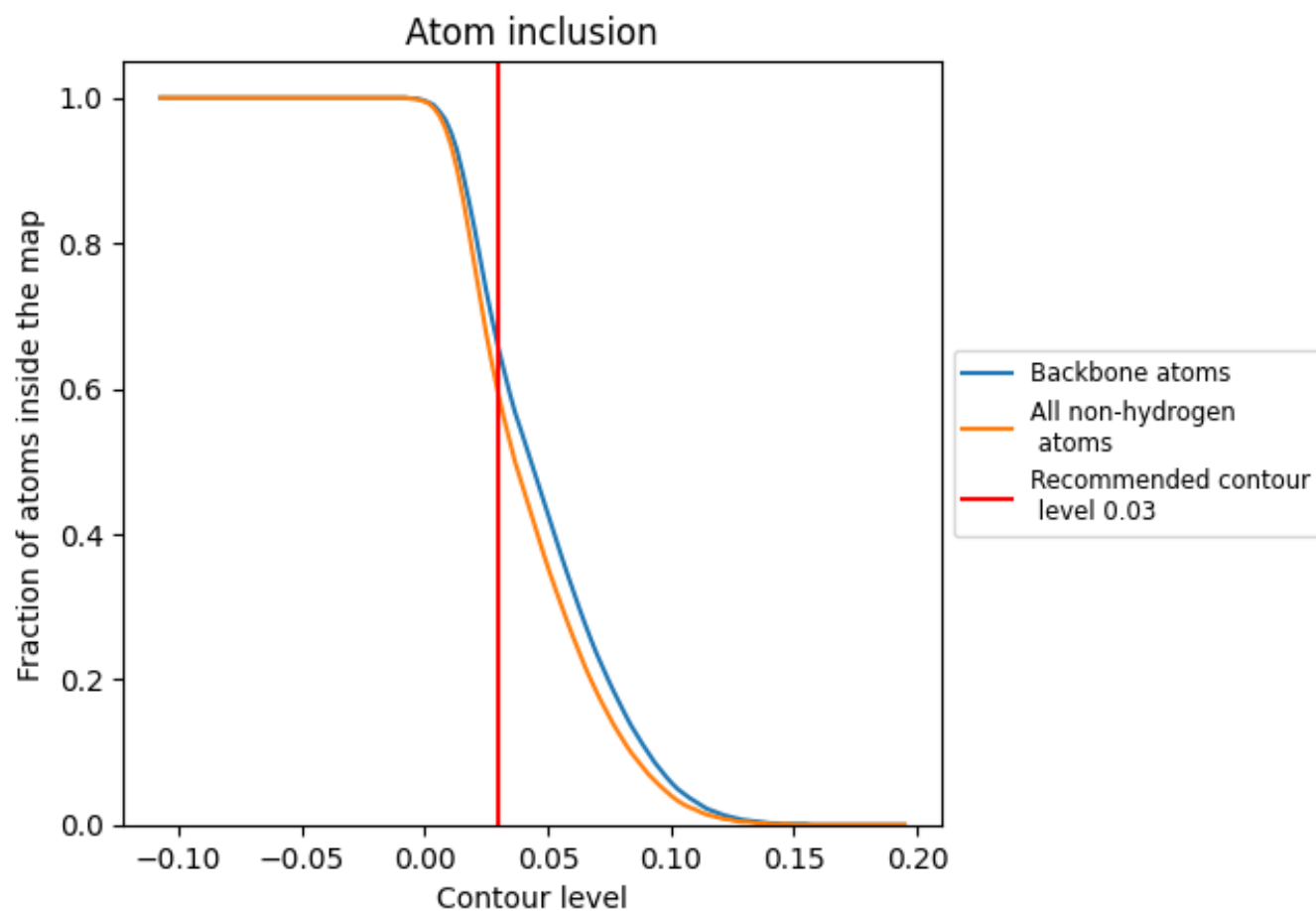
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



























































The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5920	 0.4720
0	 0.2120	 0.2450
1	 0.7300	 0.5630
2	 0.8490	 0.6050
3	 0.2390	 0.2770
4	 0.3670	 0.3590
5	 0.9490	 0.6690
6	 0.3260	 0.3250
7	 0.9150	 0.6540
8	 0.7840	 0.5730
9	 0.9160	 0.6570
A	 0.2120	 0.2520
AA	 0.7800	 0.5750
B	 0.8790	 0.6290
C	 0.8280	 0.5910
D	 0.7290	 0.5590
E	 0.2330	 0.2820
F	 0.8660	 0.6160
G	 0.9390	 0.6690
H	 0.5210	 0.4210
I	 0.9470	 0.6740
J	 0.2160	 0.2460
K	 0.7290	 0.5620
L	 0.8410	 0.6050
M	 0.2480	 0.2770
N	 0.3640	 0.3580
O	 0.8580	 0.6160
P	 0.9520	 0.6660
Q	 0.3270	 0.3230
R	 0.9090	 0.6510
S	 0.7860	 0.5720
T	 0.9530	 0.6750
U	 0.2120	 0.2580
V	 0.8850	 0.6250
W	 0.8390	 0.5990



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Chain	Atom inclusion	Q-score
X	 0.7320	 0.5630
Y	 0.2360	 0.2840
Z	 0.9450	 0.6730
a	 0.9170	 0.6580
b	 0.5250	 0.4260
c	 0.7760	 0.5720
d	 0.9460	 0.6740
e	 0.2120	 0.2500
f	 0.7290	 0.5630
g	 0.8460	 0.6100
h	 0.2560	 0.2840
i	 0.3790	 0.3610
j	 0.8650	 0.6190
k	 0.9530	 0.6720
l	 0.3360	 0.3270
m	 0.9120	 0.6570
n	 0.7840	 0.5750
o	 0.9540	 0.6750
p	 0.9170	 0.6600
q	 0.7790	 0.5760
r	 0.2150	 0.2560
s	 0.8850	 0.6240
t	 0.8370	 0.5980
u	 0.7270	 0.5600
v	 0.2360	 0.2860
w	 0.9420	 0.6700
x	 0.5210	 0.4240
y	 0.9600	 0.6760
z	 0.9470	 0.6710