



## wwPDB EM Map/Model Validation Report ⓘ

May 5, 2016 – 10:19 PM EDT

PDB ID : 5FM1  
EMDB ID: : EMD-1731  
Title : Structure of gamma-tubulin small complex based on a cryo-EM map, chemical cross-links, and a remotely related structure  
Authors : Greenberg, C.H.; Kollman, J.; Zelter, A.; Johnson, R.; MacCoss, M.J.; Davis, T.N.; Agard, D.A.; Sali, A.  
Deposited on : 2015-10-30  
Resolution : 8.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

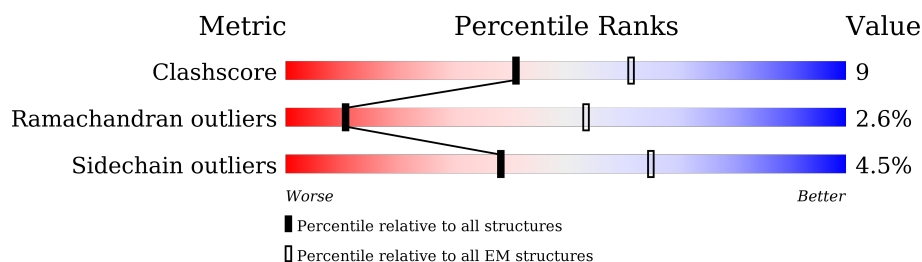
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




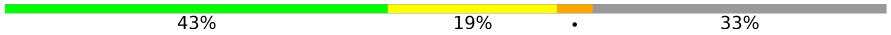
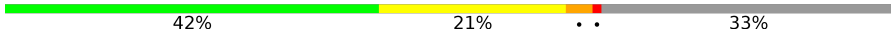
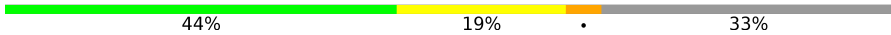
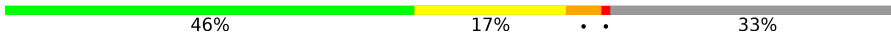
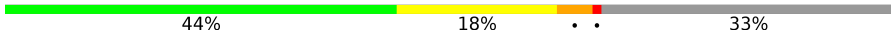
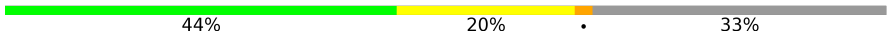
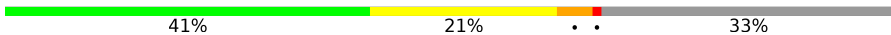
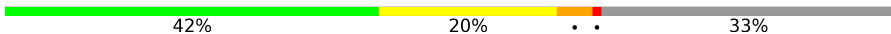
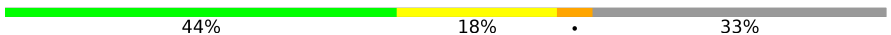
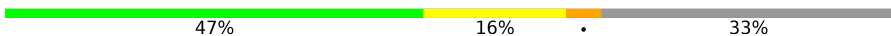














Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1-A	823	
1	10-A	823	
1	2-A	823	
1	3-A	823	
1	4-A	823	
1	5-A	823	
1	6-A	823	
1	7-A	823	
1	8-A	823	
















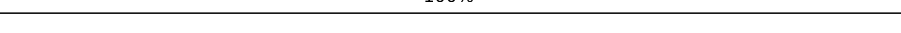
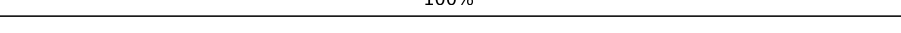
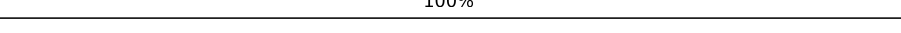
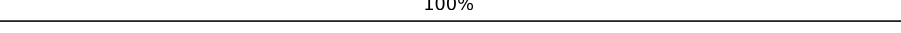
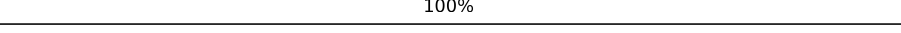
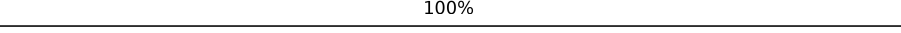
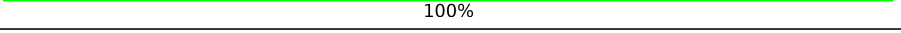
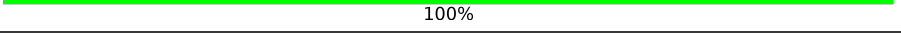
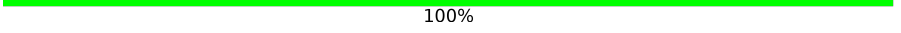
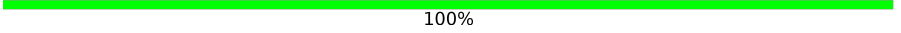
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Mol	Chain	Length	Quality of chain
1	9-A	823	
2	1-B	846	
2	10-B	846	
2	2-B	846	
2	3-B	846	
2	4-B	846	
2	5-B	846	
2	6-B	846	
2	7-B	846	
2	8-B	846	
2	9-B	846	
3	1-C	473	
3	1-D	473	
3	10-C	473	
3	10-D	473	
3	2-C	473	
3	2-D	473	
3	3-C	473	
3	3-D	473	
3	4-C	473	
3	4-D	473	
3	5-C	473	
3	5-D	473	
3	6-C	473	
3	6-D	473	


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Mol	Chain	Length	Quality of chain
3	7-C	473	 66%23%5%6%
3	7-D	473	 65%25%5%6%
3	8-C	473	 64%26%5%6%
3	8-D	473	 67%22%5%6%
3	9-C	473	 65%24%5%6%
3	9-D	473	 65%24%5%6%
4	1-E	44	 100%
4	1-F	44	 98%
4	10-E	44	 95%5%
4	10-F	44	 100%
4	2-E	44	 100%
4	2-F	44	 100%
4	3-E	44	 100%
4	3-F	44	 98%
4	4-E	44	 100%
4	4-F	44	 100%
4	5-E	44	 100%
4	5-F	44	 100%
4	6-E	44	 100%
4	6-F	44	 100%
4	7-E	44	 100%
4	7-F	44	 100%
4	8-E	44	 100%
4	8-F	44	 100%
4	9-E	44	 100%

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Mol	Chain	Length	Quality of chain
4	9-F	44	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 169380 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 SPINDLE POLE BODY COMPONENT SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	2-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	3-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	4-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	5-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	6-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	7-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	8-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	9-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	10-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		

- Molecule 2 is a protein called SPINDLE POLE BODY COMPONENT SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	2-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	3-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	4-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	5-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	7-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	8-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	9-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	10-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

- Molecule 3 is a protein called TUBULIN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	2-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	3-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	4-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	5-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	6-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	7-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	8-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	9-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	10-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	1-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	2-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	3-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	4-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	6-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	7-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	8-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	9-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	10-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		

- Molecule 4 is a protein called SPINDLE POLE BODY COMPONENT 110.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	2-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	3-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	4-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	5-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	6-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	7-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	8-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	9-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	10-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	1-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	2-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	3-F	44	Total	C	N	O	0	0
			220	132	44	44		

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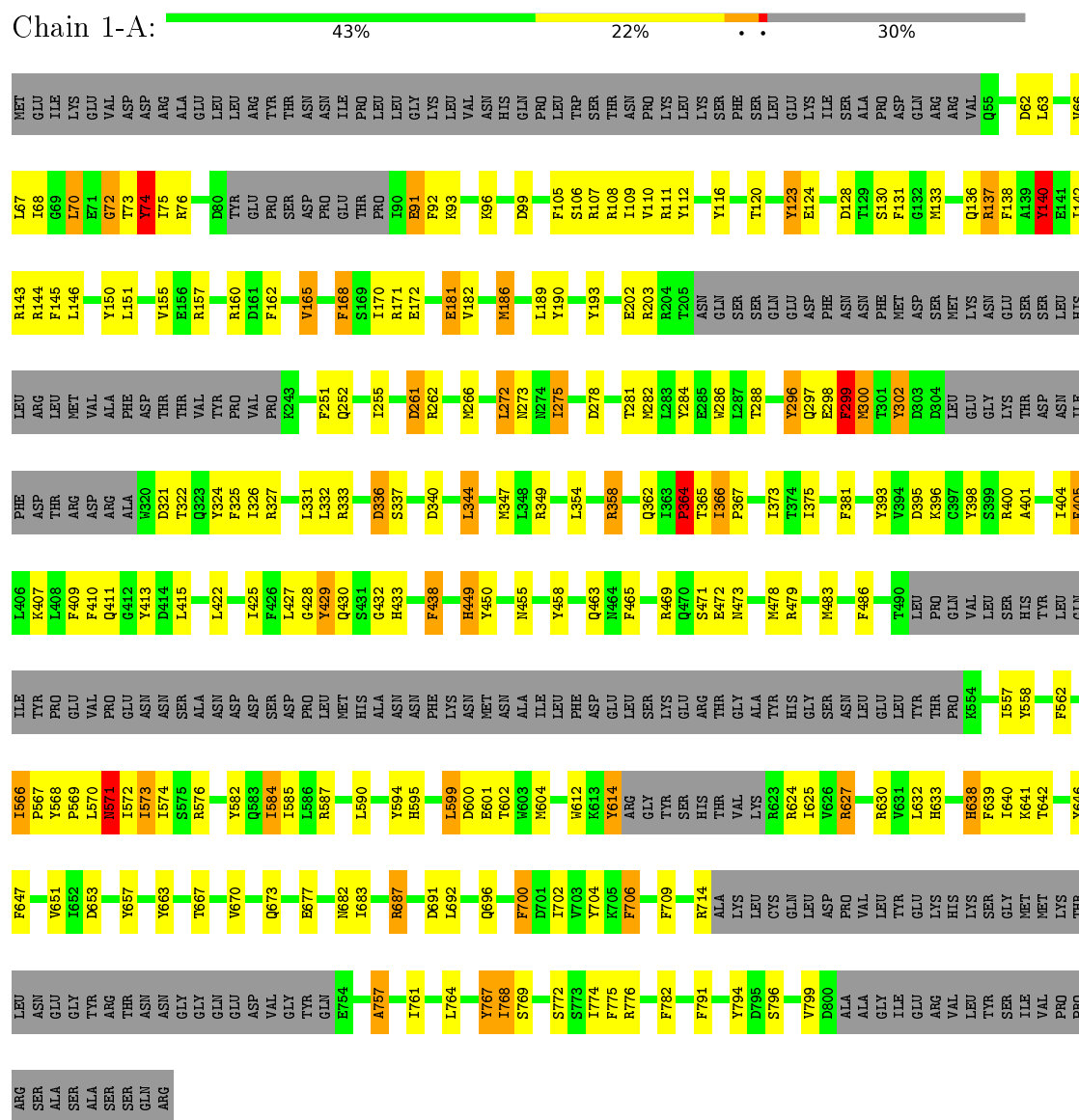
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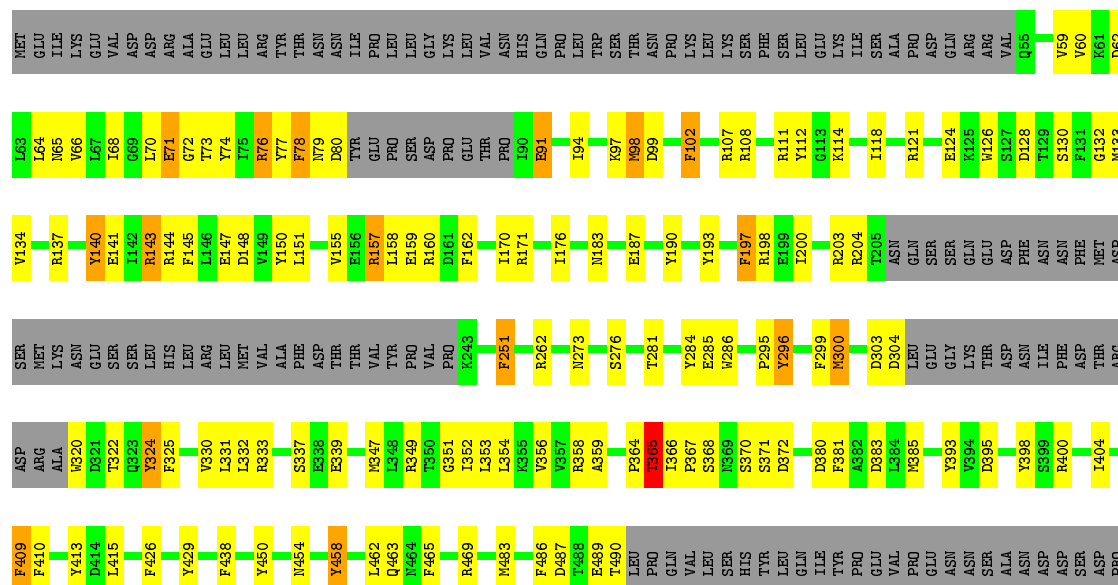
Mol	Chain	Residues	Atoms				AltConf	Trace
4	4-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	5-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	6-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	7-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	8-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	9-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	10-F	44	Total	C	N	O	0	0
			220	132	44	44		

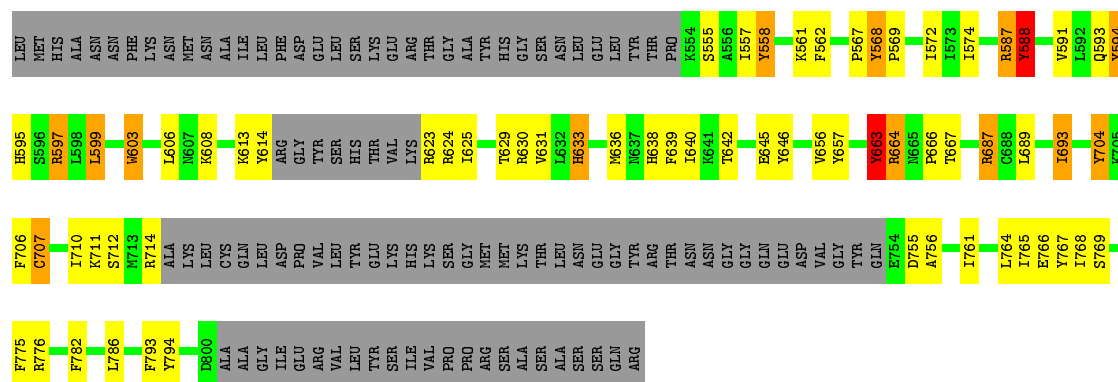
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: SPINDLE POLE BODY COMPONENT SPC97

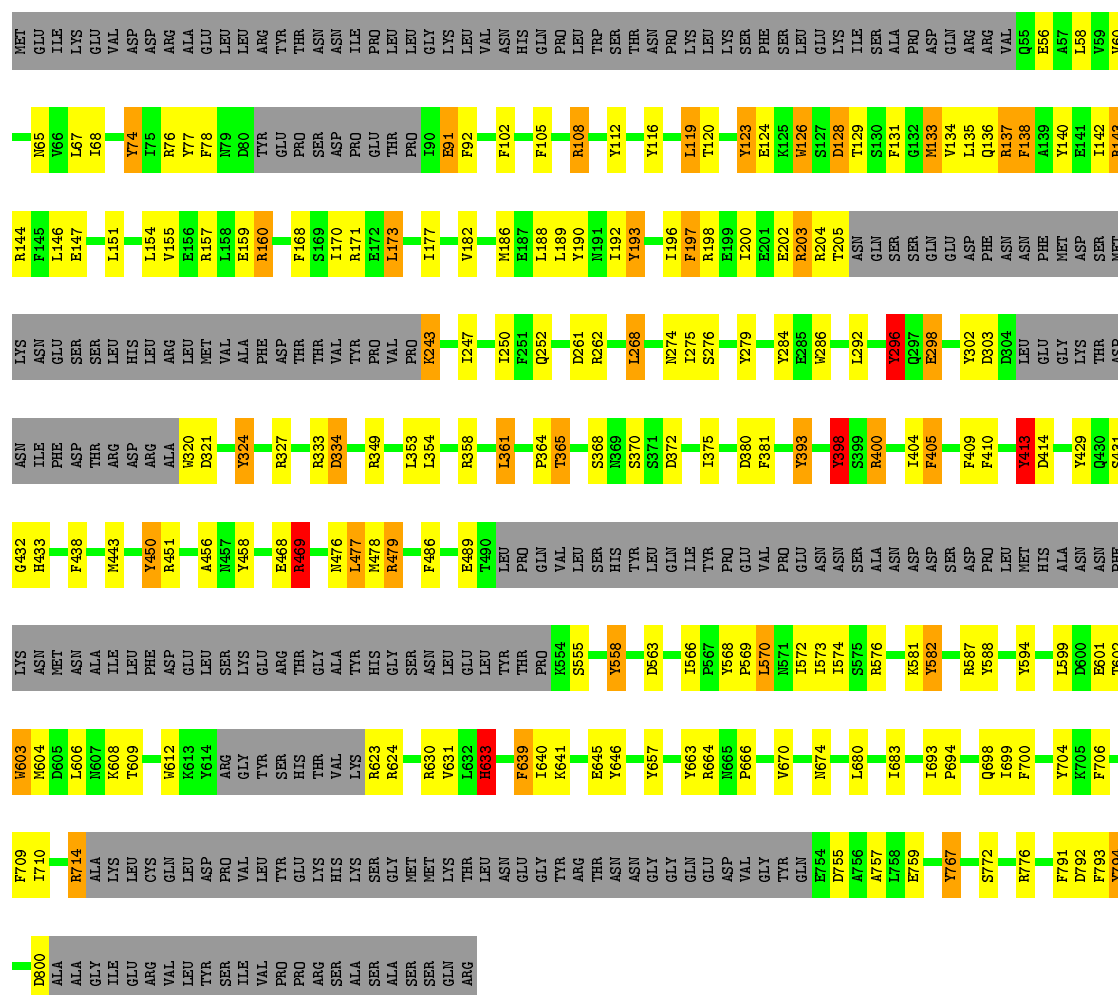






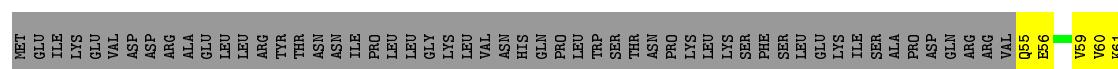
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

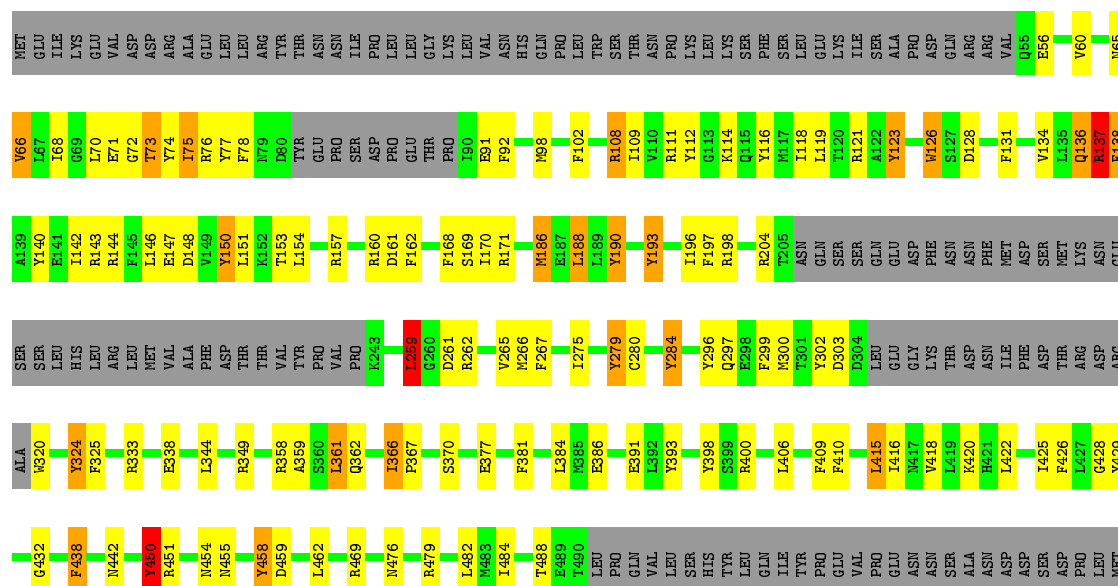
Chain 4-A: 47% 18% 30%



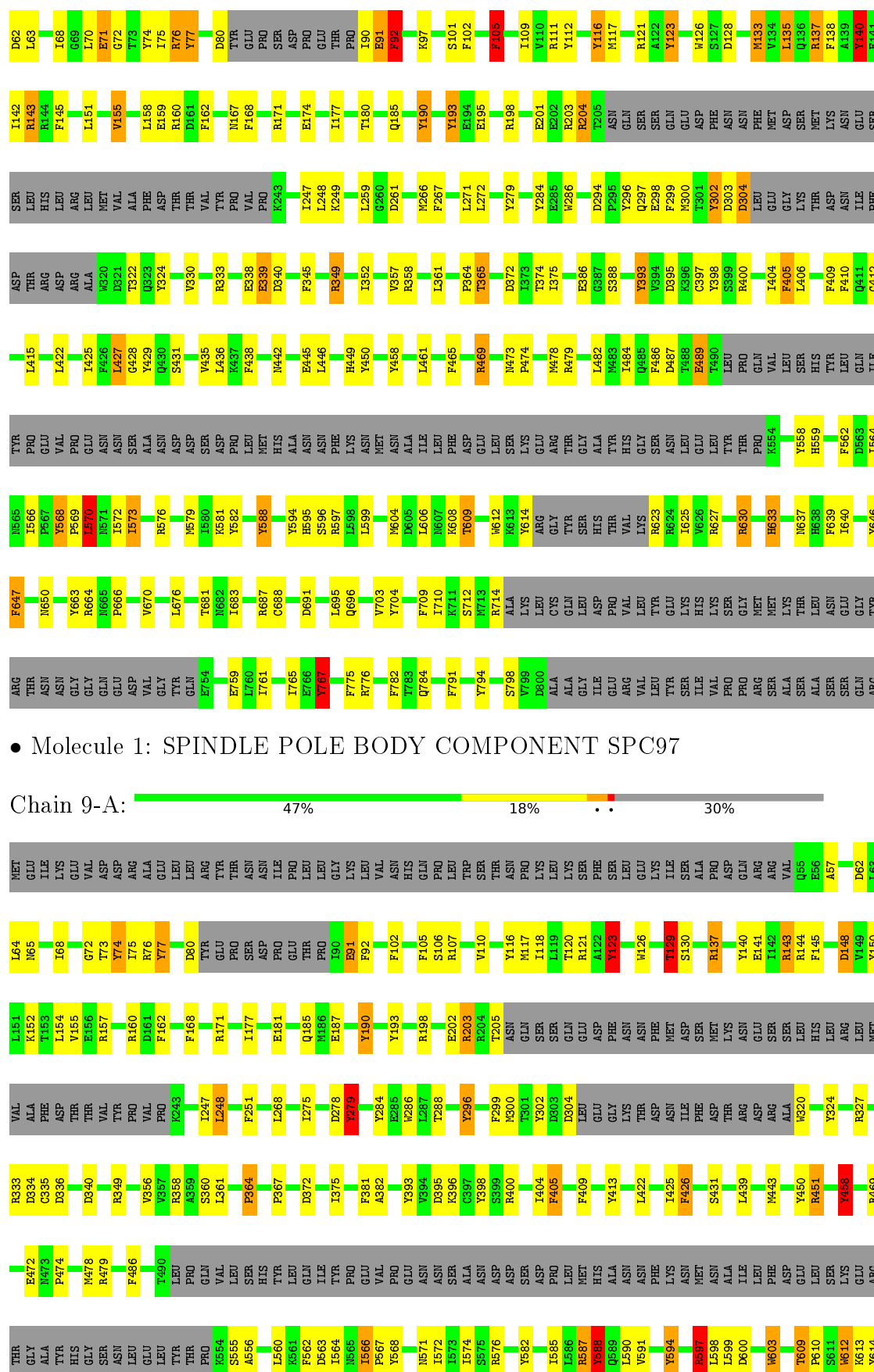
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 5-A: 44% 20% 5% 30%







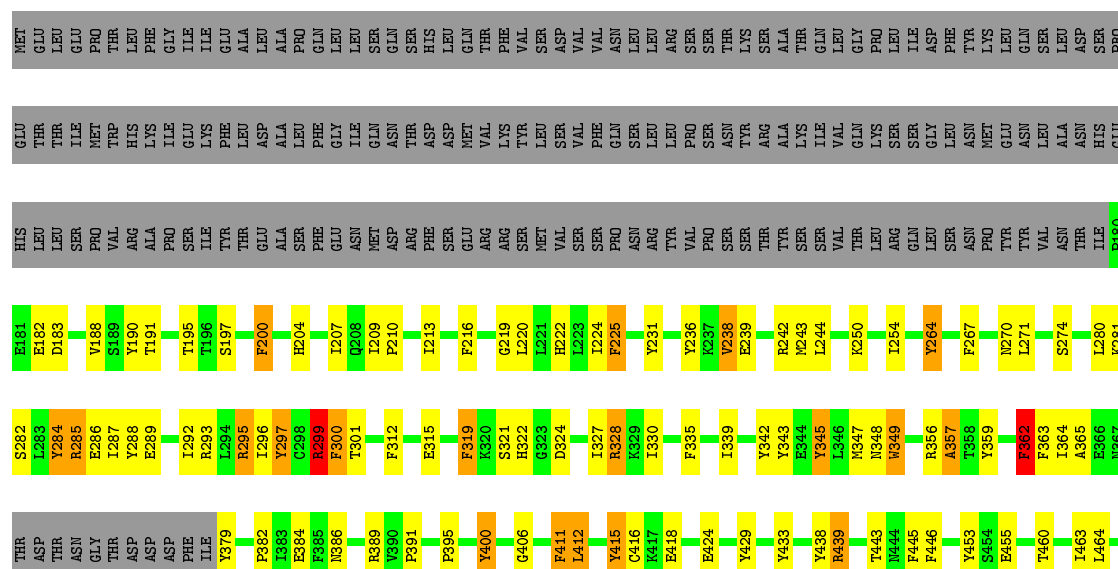


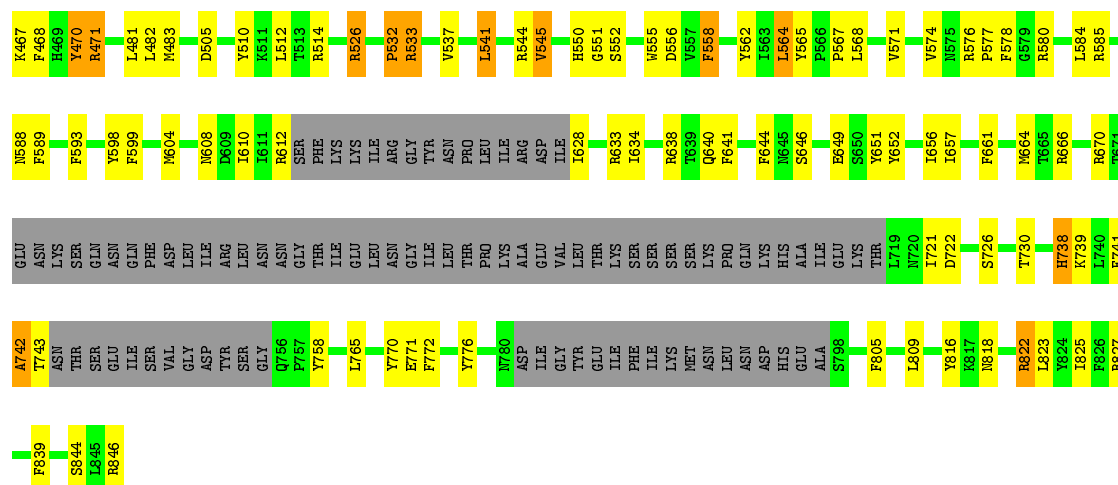






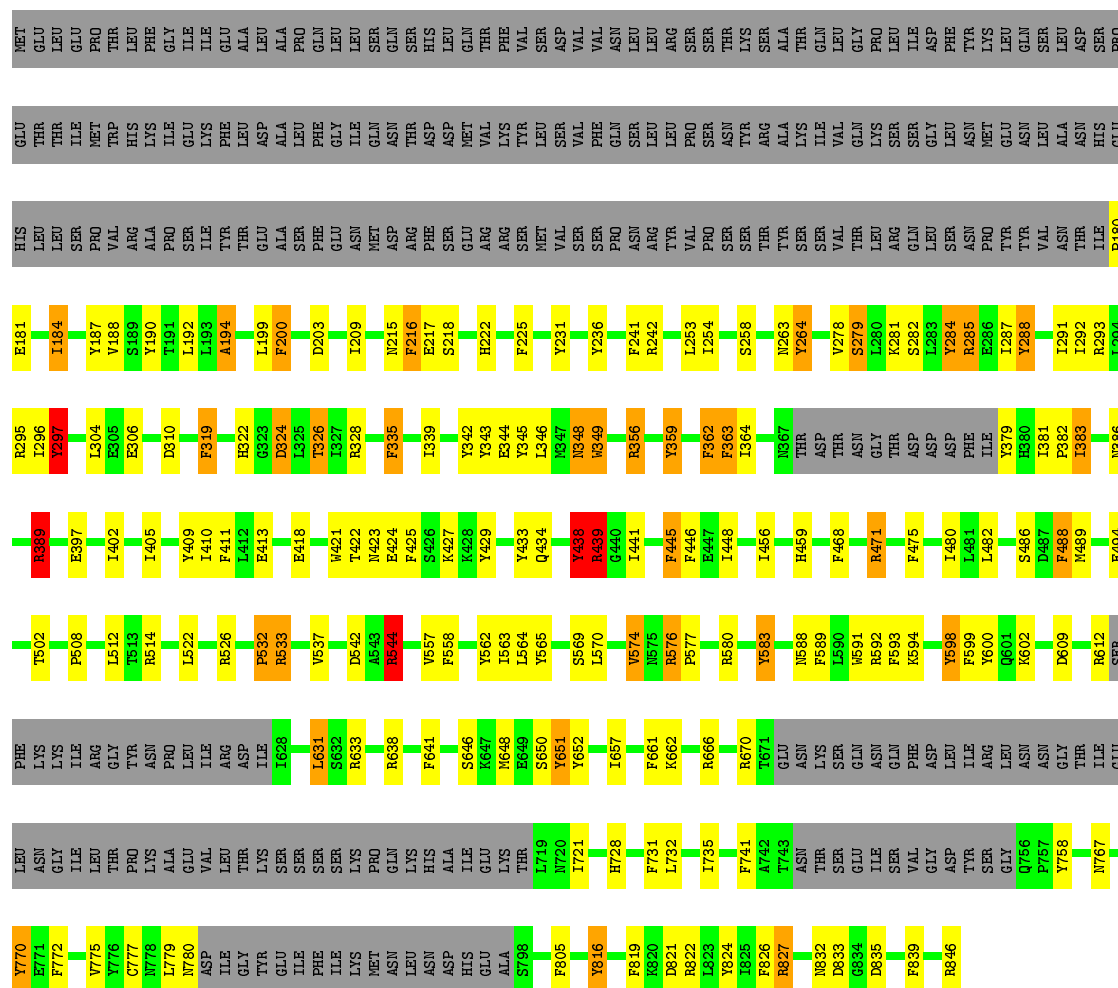
Chain 2-B: 





• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

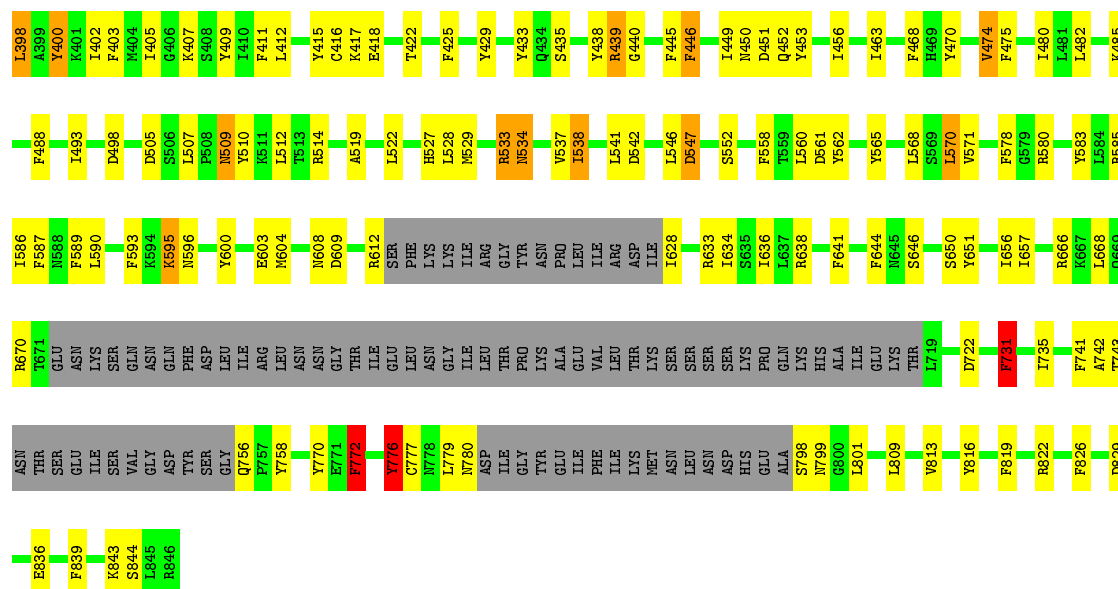
Chain 3-B: 46% 17% 33%



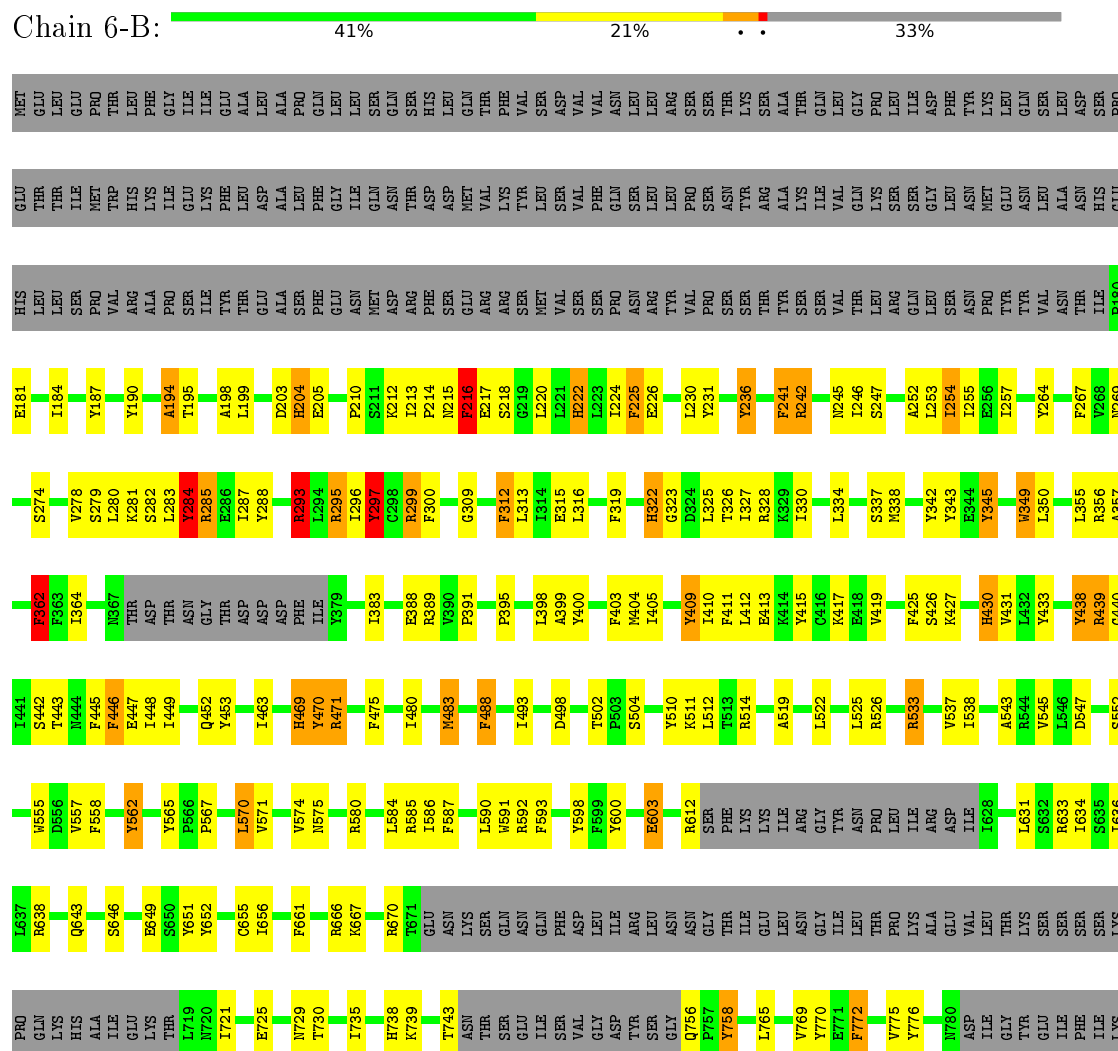
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 4-B: 44% 18% 33%

[illegible]



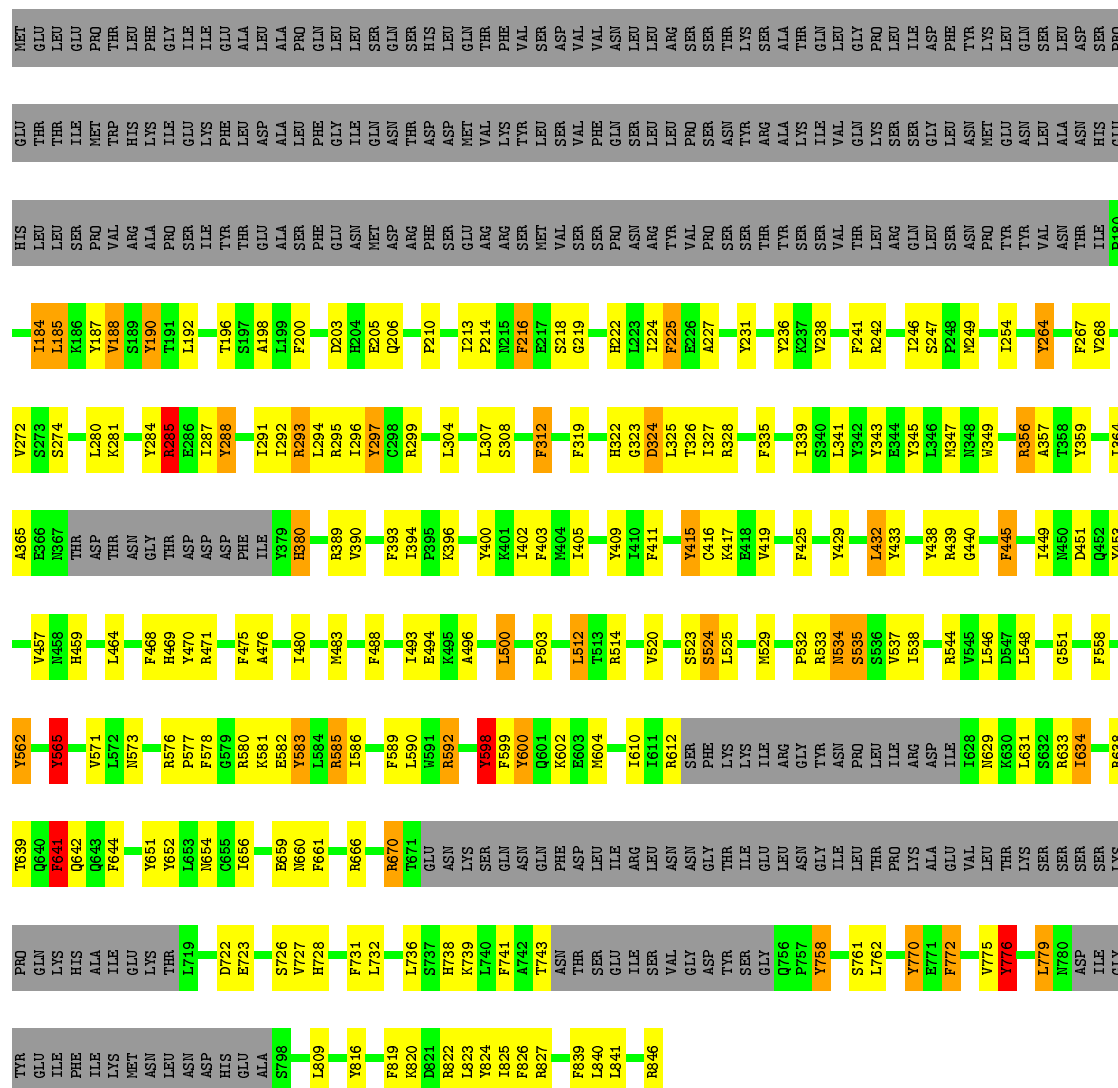
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98





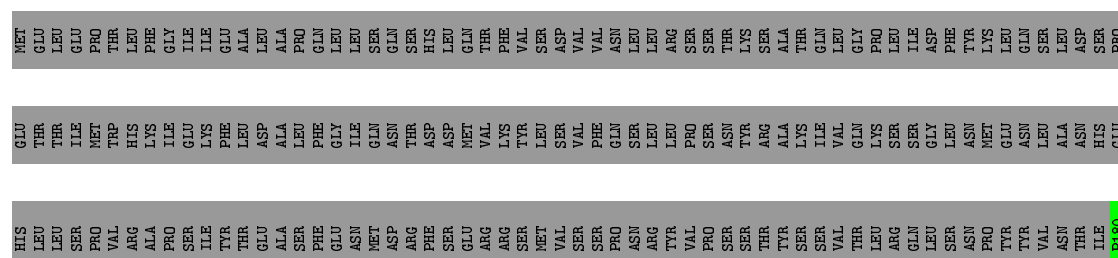
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 7-B: 42% 20% 33%



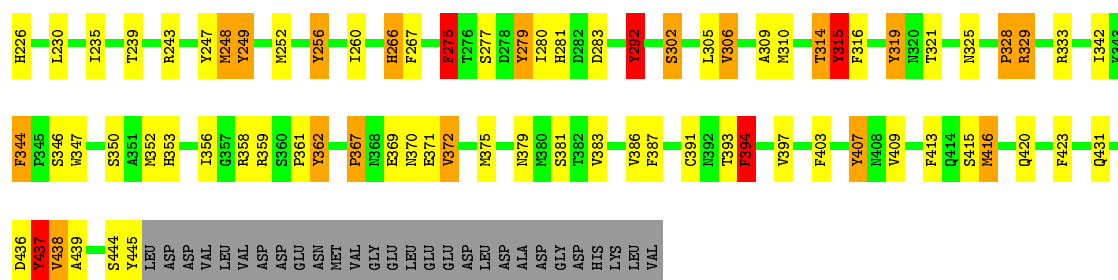
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 8-B: 44% 18% 33%



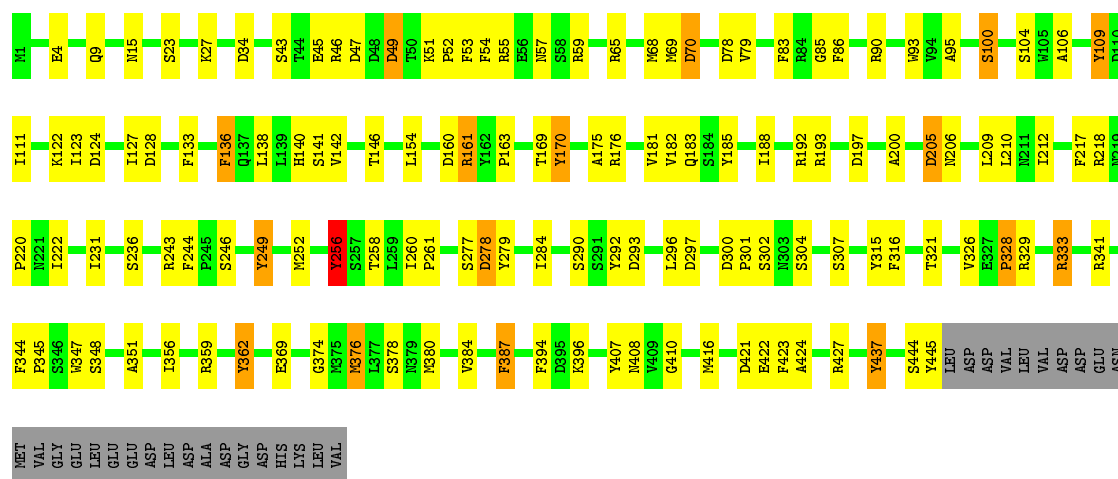






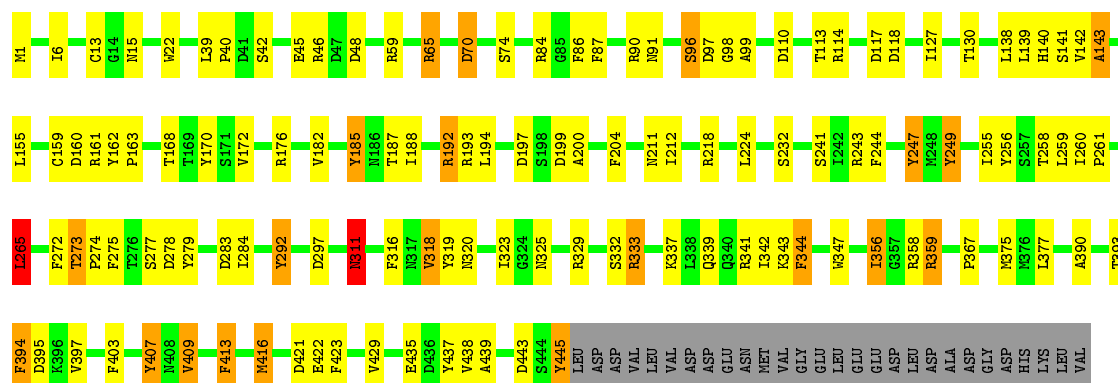
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 1-D: 66% 25% 6%



• Molecule 3: TUBULIN GAMMA CHAIN

Chain 2-C: 67% 22% 6%

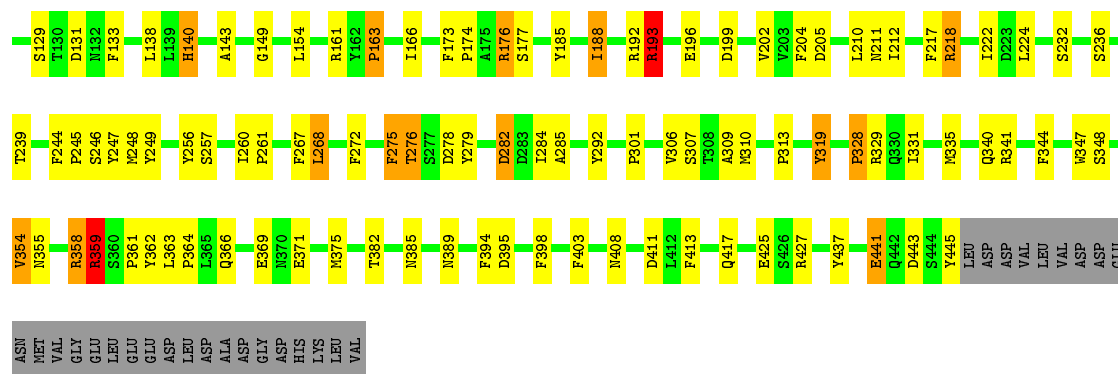


• Molecule 3: TUBULIN GAMMA CHAIN

Chain 2-D: 65% 25% 6%

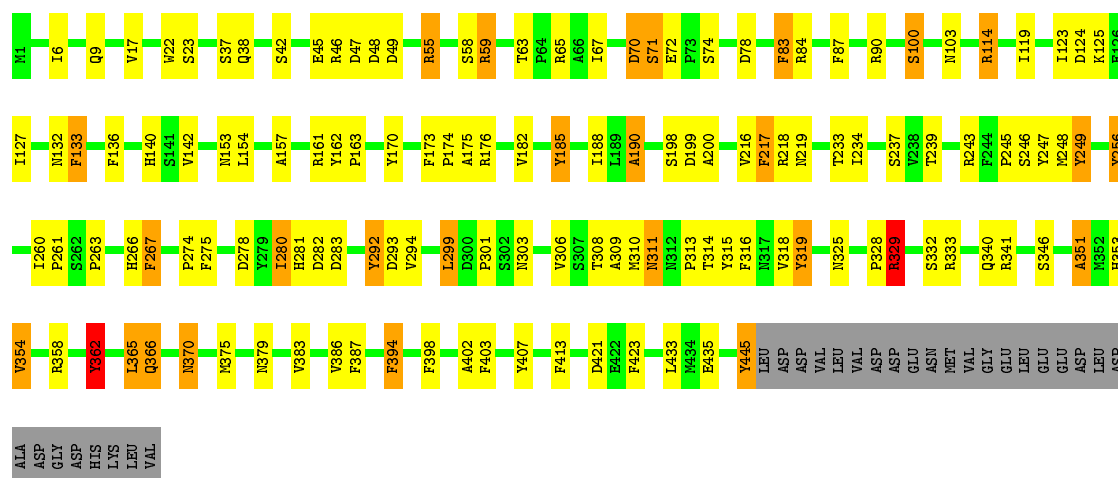






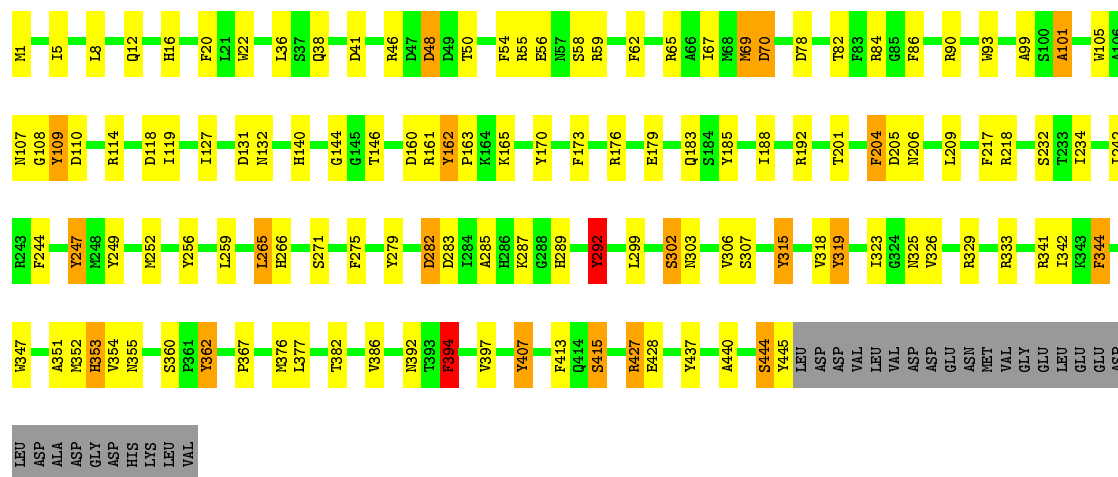
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 3-C: 66% 23% 5% 6%

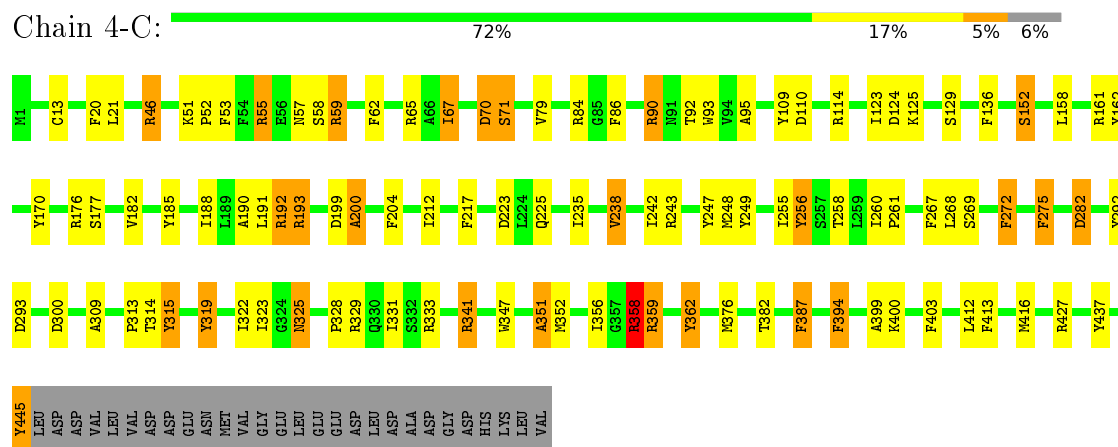


### • Molecule 3: TUBULIN GAMMA CHAIN

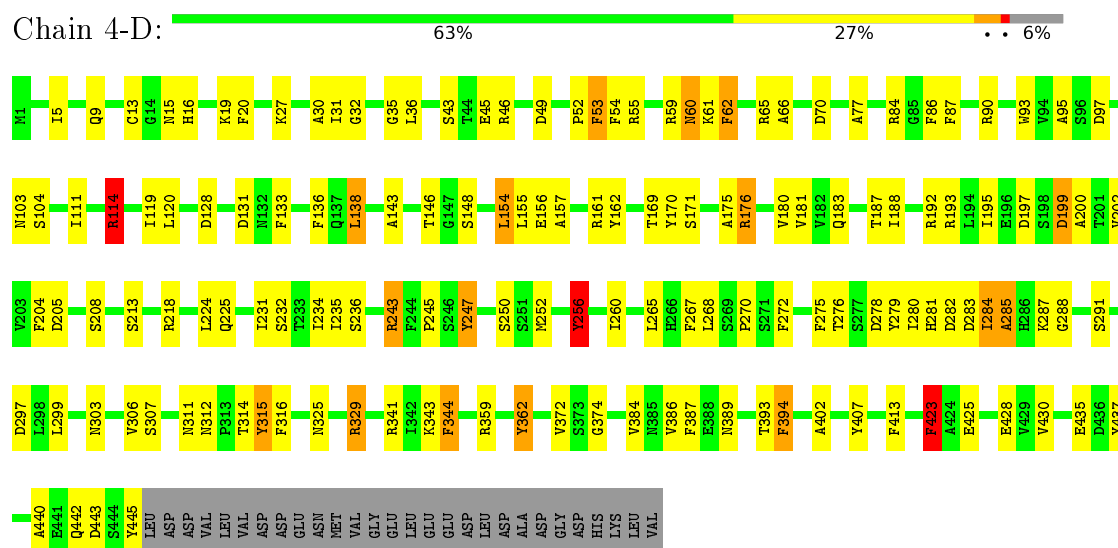
Chain 3-D: 67% 22% 6%



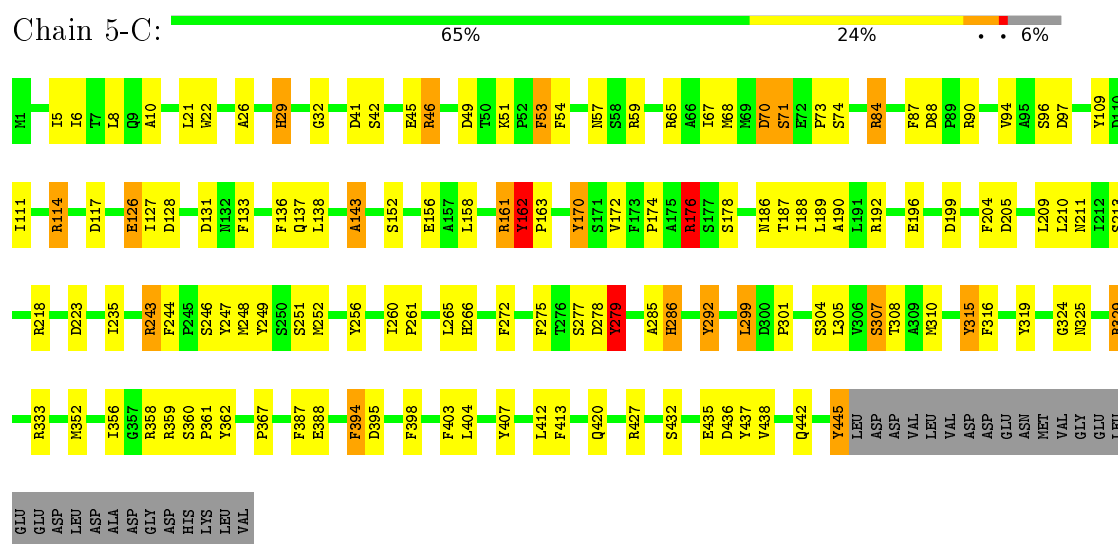
### • Molecule 3: TUBULIN GAMMA CHAIN



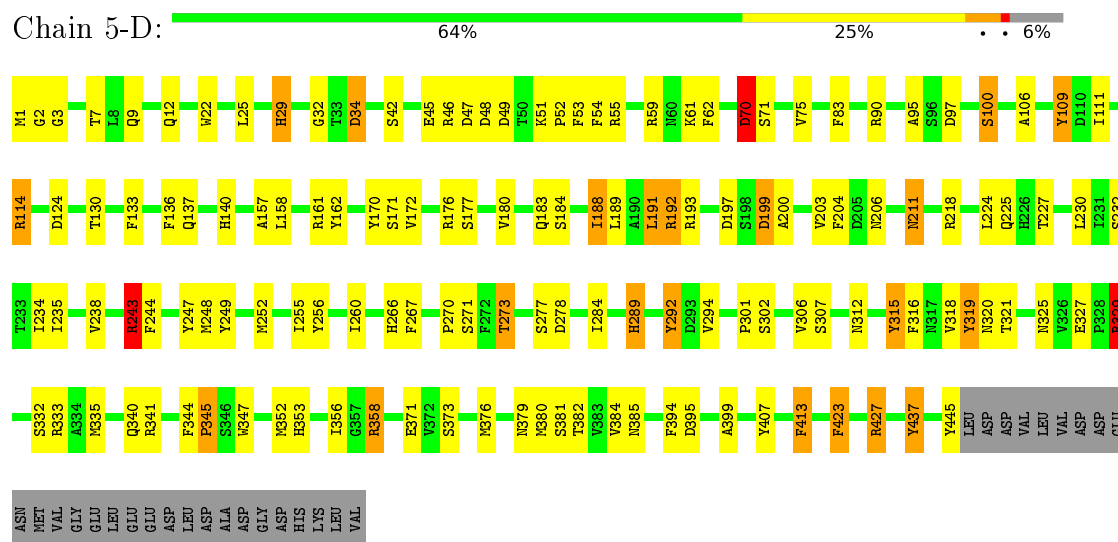
• Molecule 3: TUBULIN GAMMA CHAIN



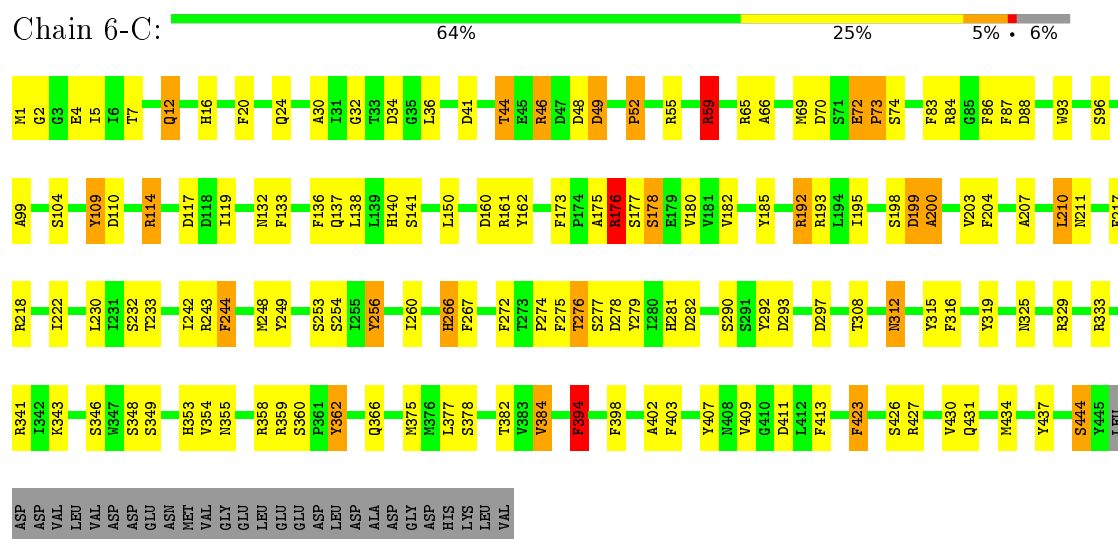
• Molecule 3: TUBULIN GAMMA CHAIN



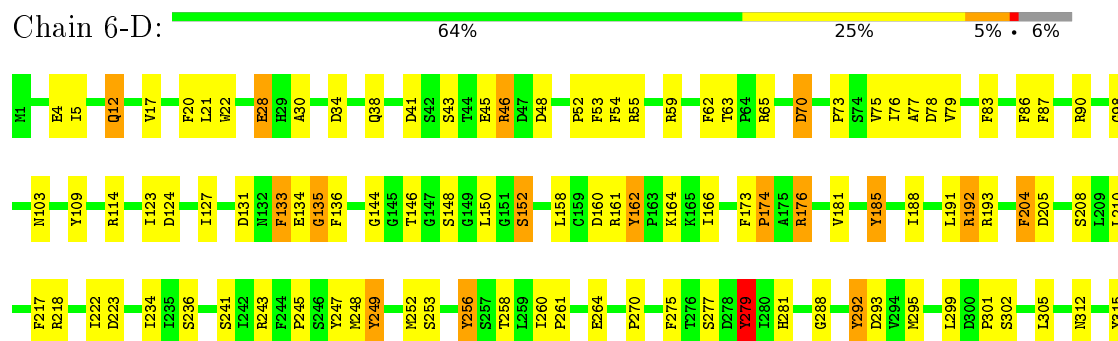
- Molecule 3: TUBULIN GAMMA CHAIN



- Molecule 3: TUBULIN GAMMA CHAIN

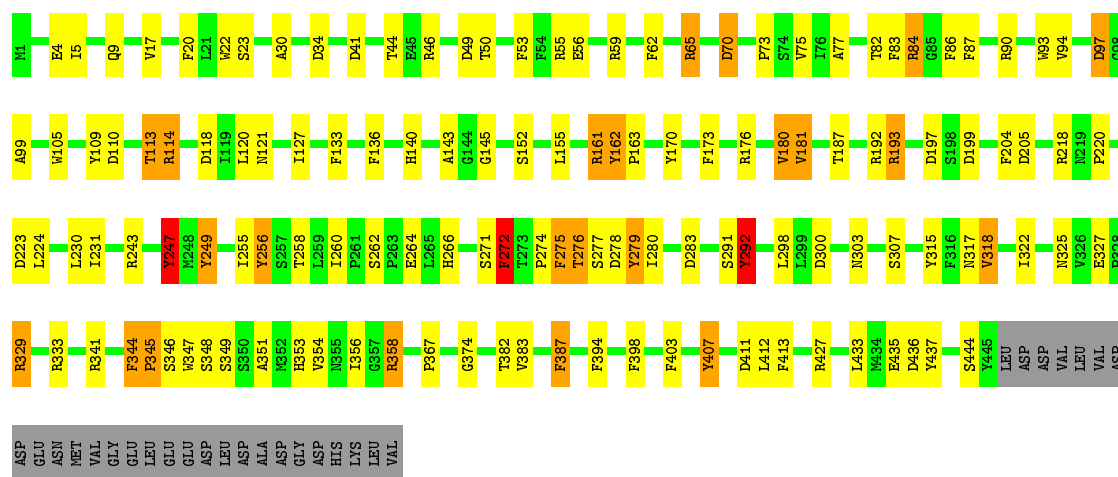


- Molecule 3: TUBULIN GAMMA CHAIN



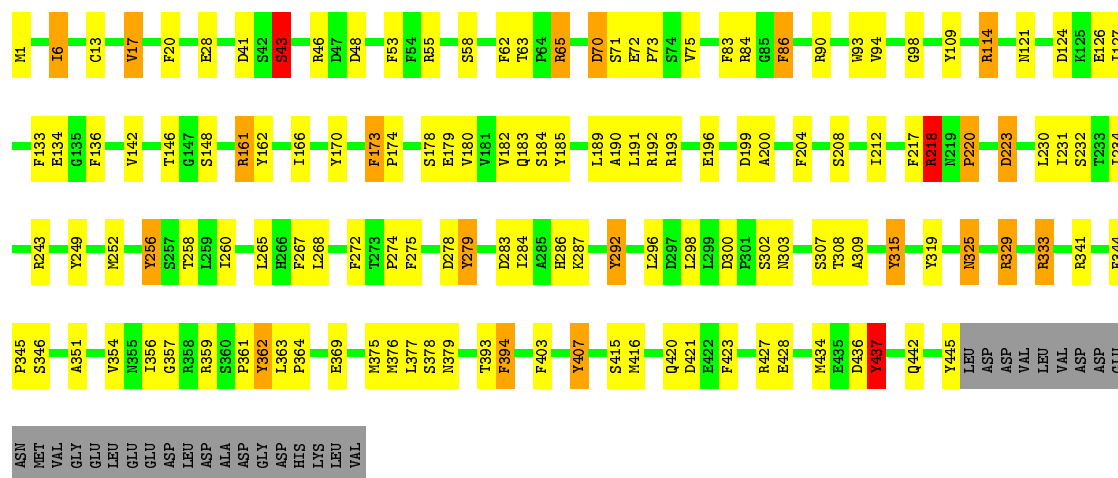
- Molecule 3: TUBULIN GAMMA CHAIN

Chain 7-C:  66% 23% 5% • 6%



- Molecule 3: TUBULIN GAMMA CHAIN

Chain 7-D:  65% 25% . . 6%



- Molecule 3: TUBULIN GAMMA CHAIN

Chain 8-C:  64% 26% 6%







LEU ASP ASP VAL LEU VAL ASP ASP GLU ASN MET VAL GLY LEU LEU GLU ASP LEU ASP ALA ASP GLY ASP HIS LEU VAL


- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 1-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 1-F:  98%

 X1 X28 X44

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-F:  100%

There are no outlier residues recorded for this chain.


- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-F:  98%

 X1 X21 X44

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-E:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-F:  100%



There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-E:  95% 5%



- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-F:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60000	Depositor
Image detector	TVIPS TEMCAM-F816	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	1-A	1.71	38/4917 (0.8%)	2.02	155/6616 (2.3%)
1	10-A	1.75	47/4917 (1.0%)	2.05	150/6616 (2.3%)
1	2-A	1.77	53/4917 (1.1%)	1.95	137/6616 (2.1%)
1	3-A	1.69	39/4917 (0.8%)	1.95	144/6616 (2.2%)
1	4-A	1.75	55/4917 (1.1%)	1.99	142/6616 (2.1%)
1	5-A	1.73	45/4917 (0.9%)	1.96	127/6616 (1.9%)
1	6-A	1.77	59/4917 (1.2%)	1.99	132/6616 (2.0%)
1	7-A	1.74	42/4917 (0.9%)	2.03	143/6616 (2.2%)
1	8-A	1.75	45/4917 (0.9%)	1.99	130/6616 (2.0%)
1	9-A	1.72	47/4917 (1.0%)	1.97	132/6616 (2.0%)
2	1-B	1.74	49/4803 (1.0%)	2.00	139/6481 (2.1%)
2	10-B	1.74	46/4803 (1.0%)	1.93	132/6481 (2.0%)
2	2-B	1.76	53/4803 (1.1%)	1.93	115/6481 (1.8%)
2	3-B	1.74	54/4803 (1.1%)	1.98	129/6481 (2.0%)
2	4-B	1.74	50/4803 (1.0%)	1.93	123/6481 (1.9%)
2	5-B	1.75	44/4803 (0.9%)	2.01	137/6481 (2.1%)
2	6-B	1.75	50/4803 (1.0%)	2.01	138/6481 (2.1%)
2	7-B	1.75	49/4803 (1.0%)	1.94	130/6481 (2.0%)
2	8-B	1.73	40/4803 (0.8%)	1.96	118/6481 (1.8%)
2	9-B	1.72	33/4803 (0.7%)	1.98	134/6481 (2.1%)
3	1-C	1.71	22/3558 (0.6%)	1.96	95/4831 (2.0%)
3	1-D	1.72	36/3558 (1.0%)	1.93	99/4831 (2.0%)
3	10-C	1.74	32/3558 (0.9%)	1.98	100/4831 (2.1%)
3	10-D	1.74	35/3558 (1.0%)	1.93	90/4831 (1.9%)
3	2-C	1.72	23/3558 (0.6%)	2.00	104/4831 (2.2%)
3	2-D	1.70	30/3558 (0.8%)	1.96	89/4831 (1.8%)
3	3-C	1.70	30/3558 (0.8%)	1.94	96/4831 (2.0%)
3	3-D	1.73	25/3558 (0.7%)	1.92	81/4831 (1.7%)
3	4-C	1.71	27/3558 (0.8%)	2.00	83/4831 (1.7%)
3	4-D	1.76	35/3558 (1.0%)	2.02	110/4831 (2.3%)
3	5-C	1.74	34/3558 (1.0%)	1.95	92/4831 (1.9%)
3	5-D	1.69	23/3558 (0.6%)	1.89	72/4831 (1.5%)
3	6-C	1.77	42/3558 (1.2%)	1.95	93/4831 (1.9%)
3	6-D	1.72	36/3558 (1.0%)	1.99	98/4831 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
3	7-C	1.75	44/3558 (1.2%)	2.01	96/4831 (2.0%)
3	7-D	1.70	28/3558 (0.8%)	1.94	99/4831 (2.0%)
3	8-C	1.73	28/3558 (0.8%)	1.93	99/4831 (2.0%)
3	8-D	1.72	31/3558 (0.9%)	1.92	83/4831 (1.7%)
3	9-C	1.73	39/3558 (1.1%)	2.02	109/4831 (2.3%)
3	9-D	1.69	32/3558 (0.9%)	1.99	94/4831 (1.9%)
All	All	1.73	1570/168360 (0.9%)	1.97	4569/227590 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	19
1	10-A	0	20
1	2-A	0	16
1	3-A	0	15
1	4-A	0	16
1	5-A	0	18
1	6-A	0	24
1	7-A	0	19
1	8-A	0	21
1	9-A	0	19
2	1-B	0	25
2	10-B	0	25
2	2-B	0	18
2	3-B	0	17
2	4-B	0	21
2	5-B	0	7
2	6-B	0	19
2	7-B	0	23
2	8-B	0	28
2	9-B	0	15
3	1-C	0	15
3	1-D	0	9
3	10-C	0	11
3	10-D	0	17
3	2-C	0	9
3	2-D	0	6
3	3-C	0	16
3	3-D	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4-C	0	13
3	4-D	0	13
3	5-C	0	8
3	5-D	0	10
3	6-C	0	12
3	6-D	1	8
3	7-C	0	9
3	7-D	0	11
3	8-C	0	9
3	8-D	0	14
3	9-C	0	8
3	9-D	0	14
All	All	1	609

The worst 5 of 1570 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-D	279	TYR	CG-CD1	10.47	1.52	1.39
3	4-D	43	SER	CA-CB	9.95	1.67	1.52
3	10-C	148	SER	CA-CB	9.75	1.67	1.52
3	1-D	341	ARG	NE-CZ	9.66	1.45	1.33
1	8-A	333	ARG	CZ-NH1	9.58	1.45	1.33

The worst 5 of 4569 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	714	ARG	NE-CZ-NH1	20.47	130.54	120.30
2	9-B	343	TYR	CB-CG-CD2	-18.96	109.62	121.00
3	9-C	427	ARG	NE-CZ-NH2	-18.13	111.23	120.30
3	5-C	333	ARG	NE-CZ-NH1	18.03	129.32	120.30
3	7-C	84	ARG	NE-CZ-NH1	17.76	129.18	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	6-D	73	PRO	CA

5 of 609 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	112	TYR	Sidechain
1	1-A	123	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	1-A	140	TYR	Sidechain
1	1-A	181	GLU	Peptide
1	1-A	74	TYR	Sidechain

## 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	1-A	4831	0	4863	190	0
1	2-A	4831	0	4863	139	0
1	3-A	4831	0	4863	114	0
1	4-A	4831	0	4862	119	0
1	5-A	4831	0	4863	124	0
1	6-A	4831	0	4862	112	0
1	7-A	4831	0	4863	112	0
1	8-A	4831	0	4862	142	0
1	9-A	4831	0	4863	146	0
1	10-A	4831	0	4863	153	0
2	1-B	4701	0	4727	182	0
2	2-B	4701	0	4731	142	0
2	3-B	4701	0	4731	119	0
2	4-B	4701	0	4729	135	0
2	5-B	4701	0	4729	144	0
2	6-B	4701	0	4729	177	0
2	7-B	4701	0	4729	124	0
2	8-B	4701	0	4731	179	0
2	9-B	4701	0	4727	123	0
2	10-B	4701	0	4729	134	0
3	1-C	3483	0	3340	46	0
3	1-D	3483	0	3340	37	0
3	2-C	3483	0	3340	40	0
3	2-D	3483	0	3340	48	0
3	3-C	3483	0	3340	50	0
3	3-D	3483	0	3340	40	0
3	4-C	3483	0	3340	53	0
3	4-D	3483	0	3340	42	0
3	5-C	3483	0	3340	32	0
3	5-D	3483	0	3340	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6-C	3483	0	3340	26	0
3	6-D	3483	0	3340	62	0
3	7-C	3483	0	3340	31	0
3	7-D	3483	0	3340	46	0
3	8-C	3483	0	3340	23	0
3	8-D	3483	0	3340	44	0
3	9-C	3483	0	3340	28	0
3	9-D	3483	0	3340	40	0
3	10-C	3483	0	3340	44	0
3	10-D	3483	0	3340	27	0
4	1-E	220	0	46	0	0
4	1-F	220	0	46	1	0
4	2-E	220	0	46	0	0
4	2-F	220	0	46	0	0
4	3-E	220	0	46	0	0
4	3-F	220	0	46	1	0
4	4-E	220	0	46	0	0
4	4-F	220	0	46	0	0
4	5-E	220	0	46	0	0
4	5-F	220	0	46	0	0
4	6-E	220	0	46	0	0
4	6-F	220	0	46	0	0
4	7-E	220	0	46	0	0
4	7-F	220	0	46	0	0
4	8-E	220	0	46	0	0
4	8-F	220	0	46	0	0
4	9-E	220	0	46	0	0
4	9-F	220	0	46	0	0
4	10-E	220	0	46	2	0
4	10-F	220	0	46	0	0
All	All	169380	0	163639	2991	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 2991 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:A:68:ILE:HD13	2:B:216:PHE:CG	1.27	1.67
2:B:405:ILE:CG2	2:B:456:ILE:HD12	1.28	1.57
1:A:68:ILE:CD1	2:B:216:PHE:HB3	1.21	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE2	2:B:322:HIS:NE2	1.71	1.54
1:A:68:ILE:HD13	2:B:216:PHE:CB	1.30	1.53

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	561/823 (68%)	518 (92%)	20 (4%)	23 (4%)	3	35
1	2-A	561/823 (68%)	534 (95%)	17 (3%)	10 (2%)	11	53
1	3-A	561/823 (68%)	522 (93%)	23 (4%)	16 (3%)	6	43
1	4-A	561/823 (68%)	529 (94%)	20 (4%)	12 (2%)	9	50
1	5-A	561/823 (68%)	525 (94%)	20 (4%)	16 (3%)	6	43
1	6-A	561/823 (68%)	538 (96%)	13 (2%)	10 (2%)	11	53
1	7-A	561/823 (68%)	529 (94%)	23 (4%)	9 (2%)	12	56
1	8-A	561/823 (68%)	523 (93%)	23 (4%)	15 (3%)	6	45
1	9-A	561/823 (68%)	530 (94%)	23 (4%)	8 (1%)	14	58
1	10-A	561/823 (68%)	521 (93%)	29 (5%)	11 (2%)	9	51
2	1-B	553/846 (65%)	519 (94%)	23 (4%)	11 (2%)	9	51
2	2-B	553/846 (65%)	520 (94%)	21 (4%)	12 (2%)	8	49
2	3-B	553/846 (65%)	521 (94%)	20 (4%)	12 (2%)	8	49
2	4-B	553/846 (65%)	515 (93%)	28 (5%)	10 (2%)	11	53
2	5-B	553/846 (65%)	516 (93%)	30 (5%)	7 (1%)	15	60
2	6-B	553/846 (65%)	513 (93%)	27 (5%)	13 (2%)	7	47
2	7-B	553/846 (65%)	514 (93%)	23 (4%)	16 (3%)	6	43
2	8-B	553/846 (65%)	525 (95%)	19 (3%)	9 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9-B	553/846 (65%)	521 (94%)	24 (4%)	8 (1%)	14	58
2	10-B	553/846 (65%)	517 (94%)	22 (4%)	14 (2%)	7	46
3	1-C	443/473 (94%)	392 (88%)	32 (7%)	19 (4%)	3	34
3	1-D	443/473 (94%)	404 (91%)	28 (6%)	11 (2%)	7	46
3	2-C	443/473 (94%)	400 (90%)	30 (7%)	13 (3%)	6	43
3	2-D	443/473 (94%)	411 (93%)	22 (5%)	10 (2%)	8	48
3	3-C	443/473 (94%)	384 (87%)	37 (8%)	22 (5%)	3	31
3	3-D	443/473 (94%)	402 (91%)	27 (6%)	14 (3%)	5	41
3	4-C	443/473 (94%)	399 (90%)	35 (8%)	9 (2%)	9	51
3	4-D	443/473 (94%)	392 (88%)	38 (9%)	13 (3%)	6	43
3	5-C	443/473 (94%)	408 (92%)	19 (4%)	16 (4%)	4	38
3	5-D	443/473 (94%)	399 (90%)	36 (8%)	8 (2%)	11	53
3	6-C	443/473 (94%)	396 (89%)	36 (8%)	11 (2%)	7	46
3	6-D	443/473 (94%)	400 (90%)	29 (6%)	14 (3%)	5	41
3	7-C	443/473 (94%)	406 (92%)	26 (6%)	11 (2%)	7	46
3	7-D	443/473 (94%)	393 (89%)	34 (8%)	16 (4%)	4	38
3	8-C	443/473 (94%)	399 (90%)	27 (6%)	17 (4%)	4	37
3	8-D	443/473 (94%)	395 (89%)	32 (7%)	16 (4%)	4	38
3	9-C	443/473 (94%)	396 (89%)	35 (8%)	12 (3%)	6	45
3	9-D	443/473 (94%)	399 (90%)	32 (7%)	12 (3%)	6	45
3	10-C	443/473 (94%)	404 (91%)	27 (6%)	12 (3%)	6	45
3	10-D	443/473 (94%)	390 (88%)	38 (9%)	15 (3%)	5	40
All	All	20000/26150 (76%)	18419 (92%)	1068 (5%)	513 (3%)	11	45

5 of 513 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	91	GLU
1	1-A	99	ASP
1	1-A	261	ASP
1	1-A	322	THR
1	1-A	364	PRO

### 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	1-A	542/766 (71%)	513 (95%)	29 (5%)	27	64
1	2-A	542/766 (71%)	509 (94%)	33 (6%)	23	60
1	3-A	542/766 (71%)	520 (96%)	22 (4%)	37	71
1	4-A	542/766 (71%)	518 (96%)	24 (4%)	35	69
1	5-A	542/766 (71%)	519 (96%)	23 (4%)	36	70
1	6-A	542/766 (71%)	511 (94%)	31 (6%)	25	62
1	7-A	542/766 (71%)	514 (95%)	28 (5%)	29	65
1	8-A	542/766 (71%)	510 (94%)	32 (6%)	24	61
1	9-A	542/766 (71%)	520 (96%)	22 (4%)	37	71
1	10-A	542/766 (71%)	513 (95%)	29 (5%)	27	64
2	1-B	528/787 (67%)	511 (97%)	17 (3%)	46	76
2	2-B	528/787 (67%)	508 (96%)	20 (4%)	40	73
2	3-B	528/787 (67%)	508 (96%)	20 (4%)	40	73
2	4-B	528/787 (67%)	501 (95%)	27 (5%)	29	66
2	5-B	528/787 (67%)	504 (96%)	24 (4%)	34	69
2	6-B	528/787 (67%)	504 (96%)	24 (4%)	34	69
2	7-B	528/787 (67%)	500 (95%)	28 (5%)	28	64
2	8-B	528/787 (67%)	519 (98%)	9 (2%)	68	87
2	9-B	528/787 (67%)	507 (96%)	21 (4%)	38	71
2	10-B	528/787 (67%)	496 (94%)	32 (6%)	23	60
3	1-C	395/420 (94%)	373 (94%)	22 (6%)	26	62
3	1-D	395/420 (94%)	383 (97%)	12 (3%)	48	77
3	2-C	395/420 (94%)	377 (95%)	18 (5%)	33	68
3	2-D	395/420 (94%)	376 (95%)	19 (5%)	31	67
3	3-C	395/420 (94%)	385 (98%)	10 (2%)	55	81
3	3-D	395/420 (94%)	380 (96%)	15 (4%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4-C	395/420 (94%)	381 (96%)	14 (4%)	43	74
3	4-D	395/420 (94%)	387 (98%)	8 (2%)	63	85
3	5-C	395/420 (94%)	379 (96%)	16 (4%)	37	71
3	5-D	395/420 (94%)	367 (93%)	28 (7%)	18	55
3	6-C	395/420 (94%)	373 (94%)	22 (6%)	26	62
3	6-D	395/420 (94%)	382 (97%)	13 (3%)	45	76
3	7-C	395/420 (94%)	377 (95%)	18 (5%)	33	68
3	7-D	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	8-C	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	8-D	395/420 (94%)	375 (95%)	20 (5%)	29	66
3	9-C	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	9-D	395/420 (94%)	379 (96%)	16 (4%)	37	71
3	10-C	395/420 (94%)	383 (97%)	12 (3%)	48	77
3	10-D	395/420 (94%)	376 (95%)	19 (5%)	31	67
All	All	18600/23930 (78%)	17772 (96%)	828 (4%)	38	69

5 of 828 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5-D	29	HIS
3	6-C	141	SER
2	10-B	180	PRO
3	5-D	211	ASN
1	6-A	603	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 264 such sidechains are listed below:

Mol	Chain	Res	Type
2	5-B	642	GLN
2	6-B	222	HIS
2	10-B	430	HIS
2	5-B	780	ASN
3	5-D	289	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.