



# wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

May 25, 2019 – 12:03 PM EDT

PDB ID : 6O2S  
EMDB ID: : EMD-0614  
Title : Deacetylated Microtubules  
Authors : Eshun-Wilson, L.; Zhang, R.; Portran, D.; Nachury, M.V.; Toso, D.; Lohr, T.;  
Vendruscolo, M.; Bonomi, M.; Fraser, J.S.; Nogales, E.  
Deposited on : 2019-02-24  
Resolution : 4.00 Å(reported)  
Based on PDB ID : 3JAR

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

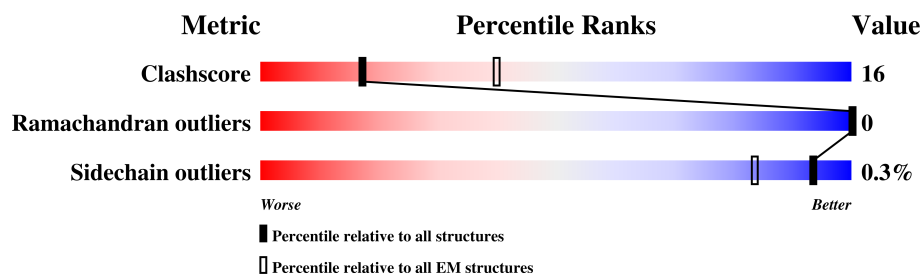
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	1A	451	74%	22% .
1	1B	451	74%	22% .
1	1C	451	73%	23% .
1	1D	451	73%	23% .
1	1E	451	73%	23% .
1	1F	451	73%	23% .
1	1G	451	74%	22% .
1	1I	451	73%	23% .
1	1J	451	73%	23% .














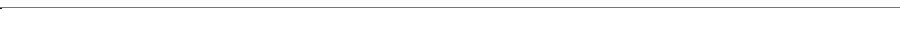


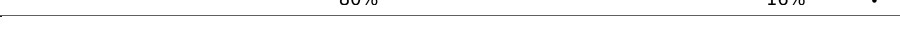
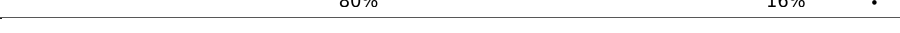







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Mol	Chain	Length	Quality of chain	
1	1K	451		.
1	1L	451		.
1	1M	451		.
1	1N	451		.
1	2A	451		.
1	2B	451		.
1	2C	451		.
1	2D	451		.
1	2E	451		.
1	2F	451		.
1	2G	451		.
1	2I	451		.
1	2J	451		.
1	2K	451		.
1	2L	451		.
1	2M	451		.
1	2N	451		.
1	3A	451		.
1	3B	451		.
1	3C	451		.
1	3D	451		.
1	3E	451		.
1	3F	451		.
1	3G	451		.
1	3I	451		.

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Mol	Chain	Length	Quality of chain	
1	3J	451		•
1	3K	451		•
1	3L	451		•
1	3M	451		•
1	3N	451		•
1	4A	451		•
1	4B	451		•
1	4C	451		•
1	4D	451		•
1	4E	451		•
1	4F	451		•
1	4G	451		•
1	4I	451		•
1	4J	451		•
1	4K	451		•
1	4L	451		•
1	4M	451		•
1	4N	451		•
2	1H	445		•
2	1O	445		•
2	1P	445		•
2	1Q	445		•
2	1R	445		•
2	1S	445		•
2	1T	445		•














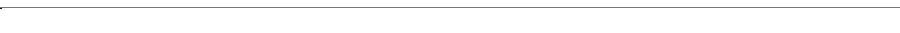


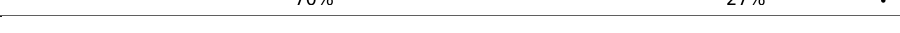



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Mol	Chain	Length	Quality of chain	
2	1U	445	<div><div></div></div>	73% 24% .
2	1V	445	<div><div></div></div>	73% 24% .
2	1W	445	<div><div></div></div>	72% 25% .
2	1X	445	<div><div></div></div>	72% 24% .
2	1Y	445	<div><div></div></div>	73% 23% .
2	1Z	445	<div><div></div></div>	73% 23% .
2	2H	445	<div><div></div></div>	71% 26% .
2	2O	445	<div><div></div></div>	71% 25% .
2	2P	445	<div><div></div></div>	71% 26% .
2	2Q	445	<div><div></div></div>	70% 26% .
2	2R	445	<div><div></div></div>	70% 26% .
2	2S	445	<div><div></div></div>	71% 26% .
2	2T	445	<div><div></div></div>	71% 25% .
2	2U	445	<div><div></div></div>	71% 25% .
2	2V	445	<div><div></div></div>	71% 25% .
2	2W	445	<div><div></div></div>	70% 26% .
2	2X	445	<div><div></div></div>	70% 26% .
2	2Y	445	<div><div></div></div>	72% 25% .
2	2Z	445	<div><div></div></div>	72% 25% .
2	3H	445	<div><div></div></div>	77% 20% .
2	3O	445	<div><div></div></div>	77% 20% .
2	3P	445	<div><div></div></div>	76% 20% .
2	3Q	445	<div><div></div></div>	77% 20% .
2	3R	445	<div><div></div></div>	77% 20% .
2	3S	445	<div><div></div></div>	76% 20% .

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Mol	Chain	Length	Quality of chain
2	3T	445	 77% 20% .
2	3U	445	 76% 20% .
2	3V	445	 76% 20% .
2	3W	445	 76% 21% .
2	3X	445	 76% 20% .
2	3Y	445	 77% 20% .
2	3Z	445	 77% 19% .
2	4H	445	 70% 26% .
2	4O	445	 71% 26% .
2	4P	445	 69% 27% .
2	4Q	445	 69% 27% .
2	4R	445	 69% 27% .
2	4S	445	 69% 27% .
2	4T	445	 69% 27% .
2	4U	445	 69% 27% .
2	4V	445	 70% 27% .
2	4W	445	 70% 27% .
2	4X	445	 69% 27% .
2	4Y	445	 71% 25% .
2	4Z	445	 71% 25% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 354900 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1B	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1C	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1D	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1E	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1F	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1G	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1I	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1J	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1K	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1L	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1M	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	1N	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	2A	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	2B	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	2C	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	2D	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2E	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2F	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2G	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2I	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2J	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2K	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2L	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2M	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	2N	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3A	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3B	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3C	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3D	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3E	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3F	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3G	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3I	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3J	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3K	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3L	434	Total 3396	C 2151	N 577	O 647	S 21	0	0
1	3M	434	Total 3396	C 2151	N 577	O 647	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3N	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4A	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4B	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4C	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4D	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4E	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4F	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4G	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4I	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4J	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4K	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4L	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4M	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		
1	4N	434	Total	C	N	O	S	0	0
			3396	2151	577	647	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1O	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1P	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1Q	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1R	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	1S	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1T	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1U	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1V	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1W	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1X	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1Y	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	1Z	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2O	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2P	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2Q	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2R	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2S	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2T	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2U	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2V	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2W	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2X	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2Y	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	2Z	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

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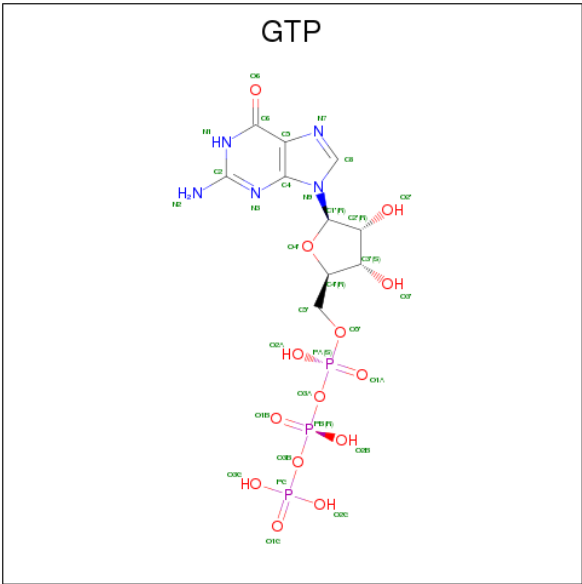
Mol	Chain	Residues	Atoms					AltConf	Trace
2	3H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3O	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3P	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3Q	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3R	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3S	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3T	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3U	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3V	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3W	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3X	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3Y	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	3Z	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4O	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4P	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4Q	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4R	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4S	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4T	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4U	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	4V	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4W	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4X	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4Y	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	4Z	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
3	1A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1F	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
3	1G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	1N	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2F	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	2N	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	3A	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
3	3B	1	Total 32	C 10	N 5	O 14	P 3	0
3	3C	1	Total 32	C 10	N 5	O 14	P 3	0
3	3D	1	Total 32	C 10	N 5	O 14	P 3	0
3	3E	1	Total 32	C 10	N 5	O 14	P 3	0
3	3F	1	Total 32	C 10	N 5	O 14	P 3	0
3	3G	1	Total 32	C 10	N 5	O 14	P 3	0
3	3I	1	Total 32	C 10	N 5	O 14	P 3	0
3	3J	1	Total 32	C 10	N 5	O 14	P 3	0
3	3K	1	Total 32	C 10	N 5	O 14	P 3	0
3	3L	1	Total 32	C 10	N 5	O 14	P 3	0
3	3M	1	Total 32	C 10	N 5	O 14	P 3	0
3	3N	1	Total 32	C 10	N 5	O 14	P 3	0
3	4A	1	Total 32	C 10	N 5	O 14	P 3	0
3	4B	1	Total 32	C 10	N 5	O 14	P 3	0
3	4C	1	Total 32	C 10	N 5	O 14	P 3	0
3	4D	1	Total 32	C 10	N 5	O 14	P 3	0
3	4E	1	Total 32	C 10	N 5	O 14	P 3	0
3	4F	1	Total 32	C 10	N 5	O 14	P 3	0
3	4G	1	Total 32	C 10	N 5	O 14	P 3	0
3	4I	1	Total 32	C 10	N 5	O 14	P 3	0
3	4J	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
3	4K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	4L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	4M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	4N	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	2E	1	Total	Mg	0
			1	1	
4	4F	1	Total	Mg	0
			1	1	
4	1N	1	Total	Mg	0
			1	1	
4	4K	1	Total	Mg	0
			1	1	
4	2I	1	Total	Mg	0
			1	1	
4	2B	1	Total	Mg	0
			1	1	
4	1J	1	Total	Mg	0
			1	1	
4	3L	1	Total	Mg	0
			1	1	
4	1E	1	Total	Mg	0
			1	1	
4	2M	1	Total	Mg	0
			1	1	
4	3I	1	Total	Mg	0
			1	1	
4	3G	1	Total	Mg	0
			1	1	
4	2F	1	Total	Mg	0
			1	1	
4	4I	1	Total	Mg	0
			1	1	
4	4N	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	1A	1	Total 1	Mg 1	0
4	4D	1	Total 1	Mg 1	0
4	3D	1	Total 1	Mg 1	0
4	2J	1	Total 1	Mg 1	0
4	3C	1	Total 1	Mg 1	0
4	2C	1	Total 1	Mg 1	0
4	1M	1	Total 1	Mg 1	0
4	4C	1	Total 1	Mg 1	0
4	1D	1	Total 1	Mg 1	0
4	2N	1	Total 1	Mg 1	0
4	3N	1	Total 1	Mg 1	0
4	2G	1	Total 1	Mg 1	0
4	1I	1	Total 1	Mg 1	0
4	3A	1	Total 1	Mg 1	0
4	3J	1	Total 1	Mg 1	0
4	2K	1	Total 1	Mg 1	0
4	4A	1	Total 1	Mg 1	0
4	3F	1	Total 1	Mg 1	0
4	1L	1	Total 1	Mg 1	0
4	1G	1	Total 1	Mg 1	0
4	4E	1	Total 1	Mg 1	0

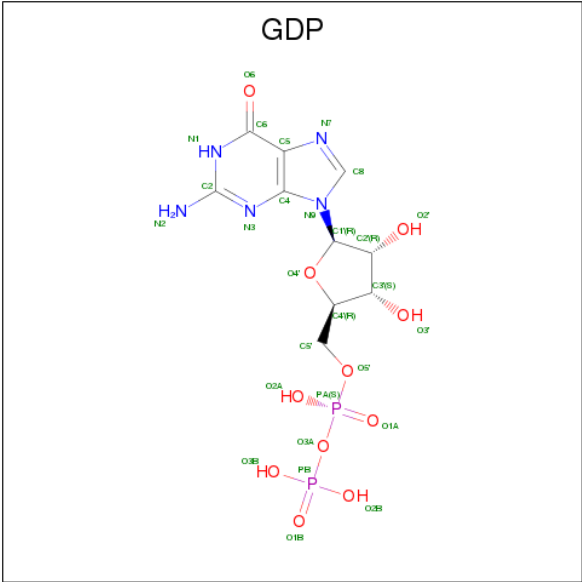
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Mol	Chain	Residues	Atoms		AltConf
4	3K	1	Total 1	Mg 1	0
4	4J	1	Total 1	Mg 1	0
4	3B	1	Total 1	Mg 1	0
4	1C	1	Total 1	Mg 1	0
4	4G	1	Total 1	Mg 1	0
4	2D	1	Total 1	Mg 1	0
4	3M	1	Total 1	Mg 1	0
4	4L	1	Total 1	Mg 1	0
4	3E	1	Total 1	Mg 1	0
4	1F	1	Total 1	Mg 1	0
4	4B	1	Total 1	Mg 1	0
4	4M	1	Total 1	Mg 1	0
4	2A	1	Total 1	Mg 1	0
4	1K	1	Total 1	Mg 1	0
4	1B	1	Total 1	Mg 1	0
4	2L	1	Total 1	Mg 1	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
5	1H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1O	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1V	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1X	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	1Z	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2H	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
5	2O	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2V	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2X	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	2Z	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3O	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3V	1	Total	C	N	O	P	0
			28	10	5	11	2	

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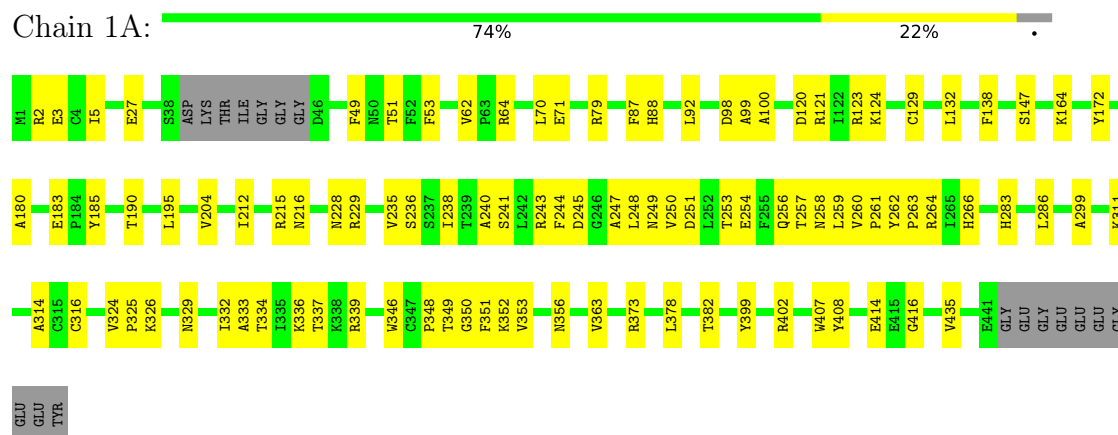
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Mol	Chain	Residues	Atoms					AltConf
5	3W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3X	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	3Z	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4O	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4R	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4S	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4T	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4U	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4V	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4W	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4X	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4Y	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	4Z	1	Total	C	N	O	P	0
			28	10	5	11	2	

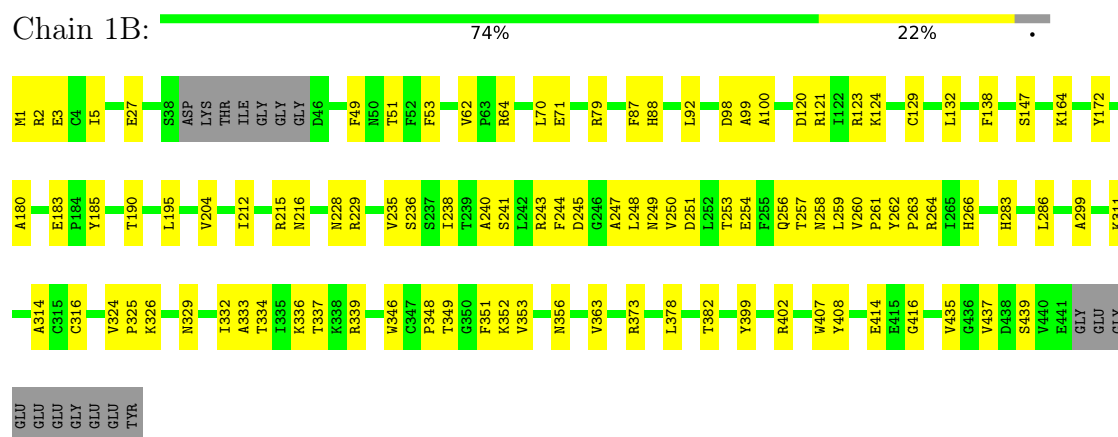
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

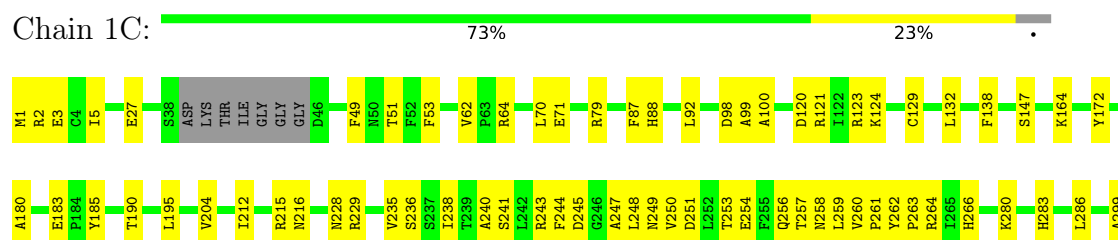
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

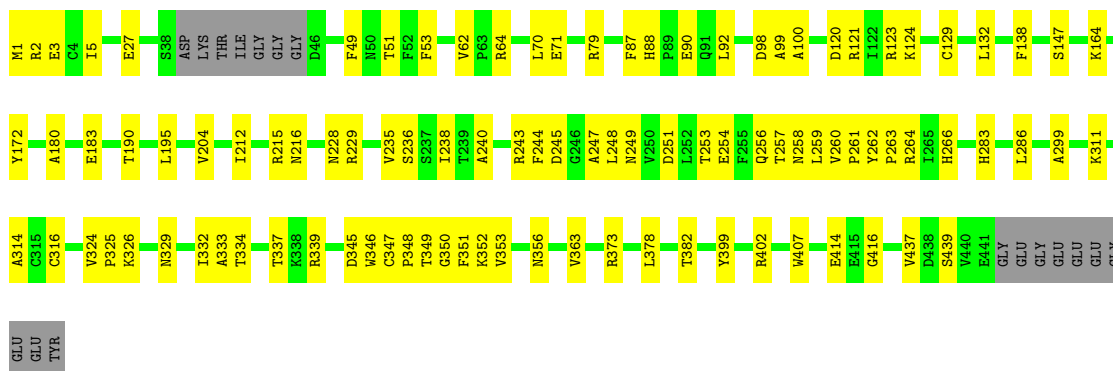




GLU  
GLY  
GLU  
GLU  
GLY  
GLY  
GLU  
TYR

- Molecule 1: Tubulin alpha-1B chain

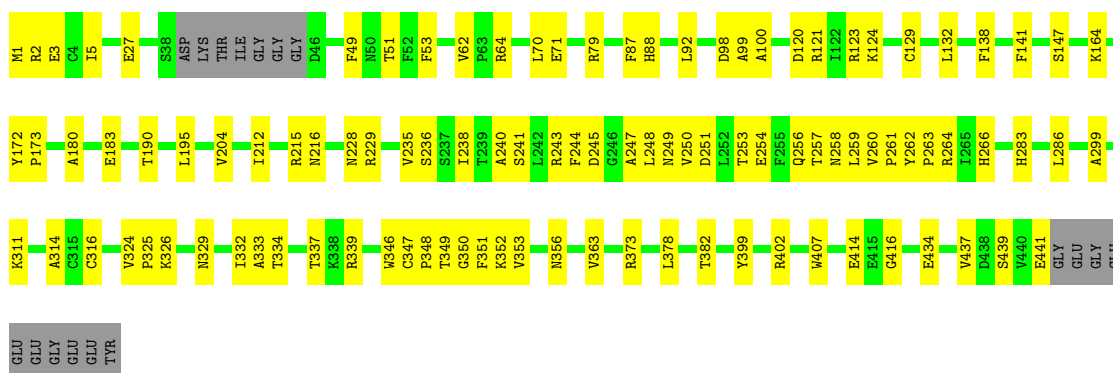
Chain 1G:  74% 22%



GLU  
GLU  
TYR

- Molecule 1: Tubulin alpha-1B chain

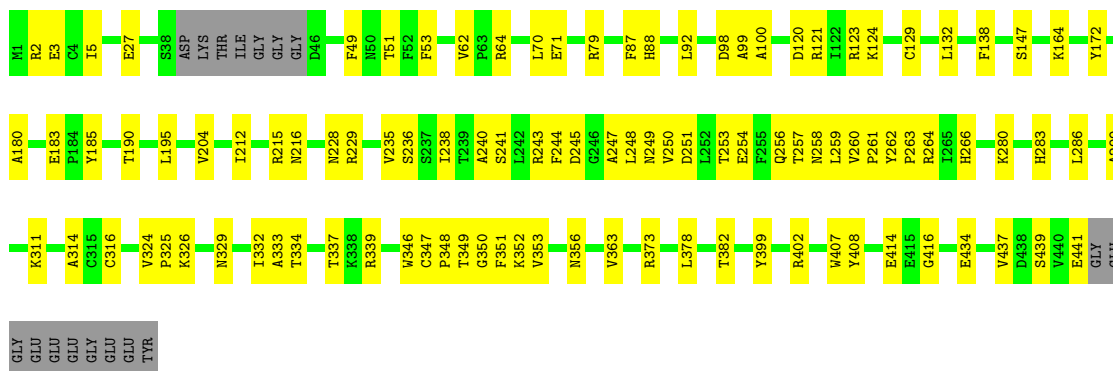
Chain 1I:  73% 23%



GLU  
GLU  
GLY  
GLY  
GLY  
TYR

- Molecule 1: Tubulin alpha-1B chain

Chain 1J:  73% 23%

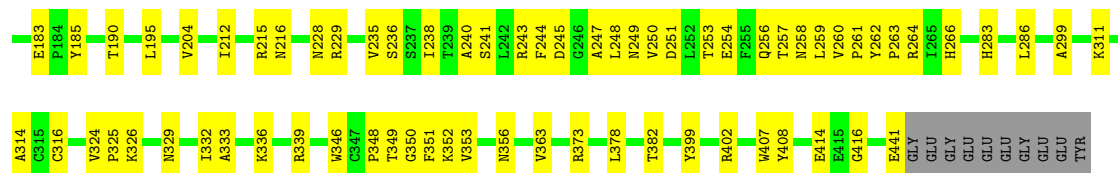


GLY  
GLU  
GLU  
GLY  
GLY  
GLY  
GLY  
TYR

- Molecule 1: Tubulin alpha-1B chain

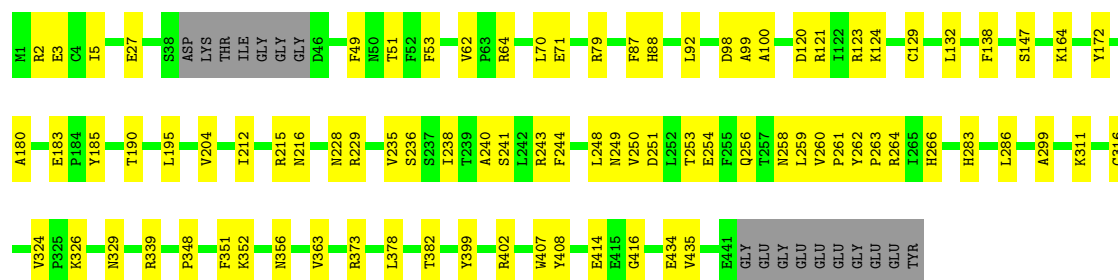






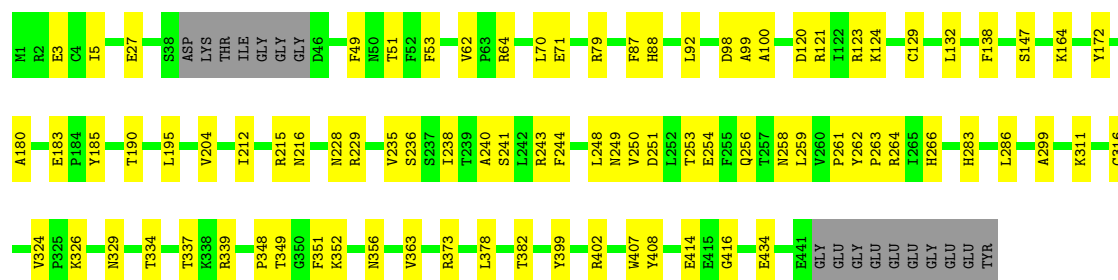
• Molecule 1: Tubulin alpha-1B chain

Chain 2A: 77% 19%



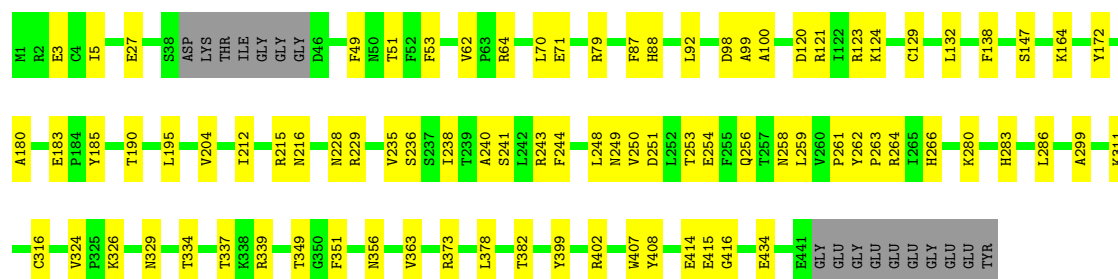
• Molecule 1: Tubulin alpha-1B chain

Chain 2B: 77% 19%



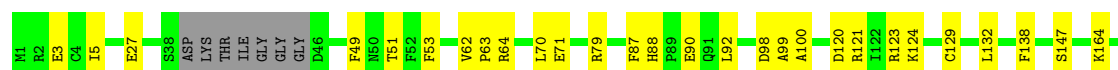
• Molecule 1: Tubulin alpha-1B chain

Chain 2C: 77% 19%



• Molecule 1: Tubulin alpha-1B chain

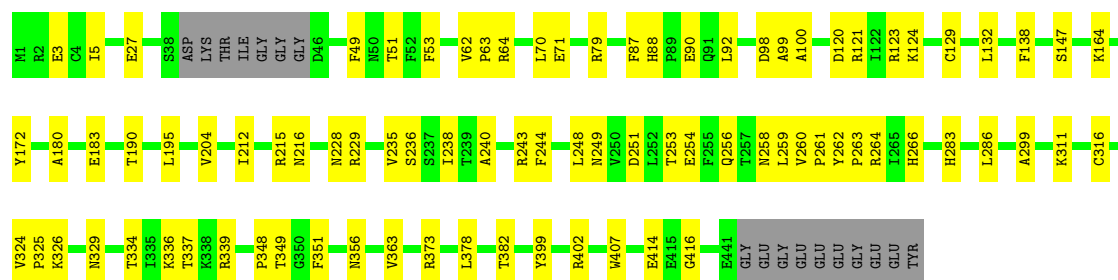
Chain 2D: 77% 19%





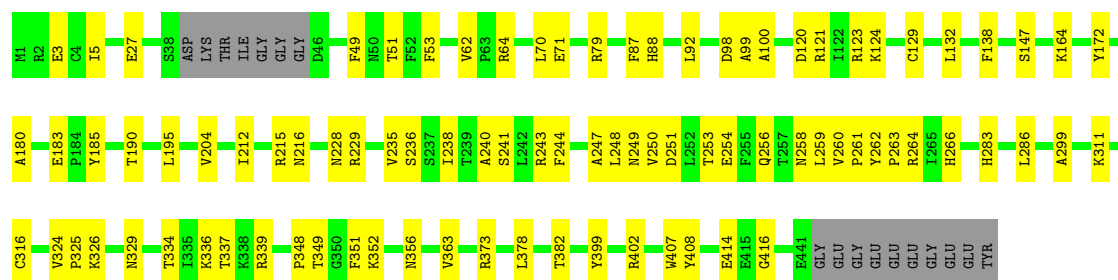
- Molecule 1: Tubulin alpha-1B chain

Chain 2E: 77% 19%



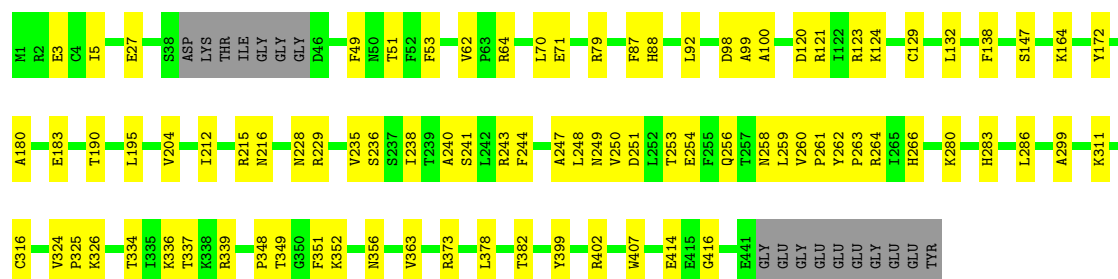
- Molecule 1: Tubulin alpha-1B chain

Chain 2F: 76% 20%



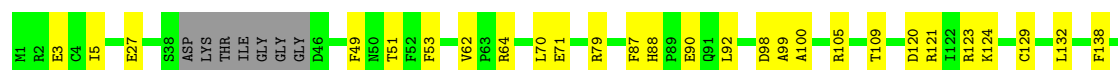
- Molecule 1: Tubulin alpha-1B chain

Chain 2G: 77% 19%



- Molecule 1: Tubulin alpha-1B chain

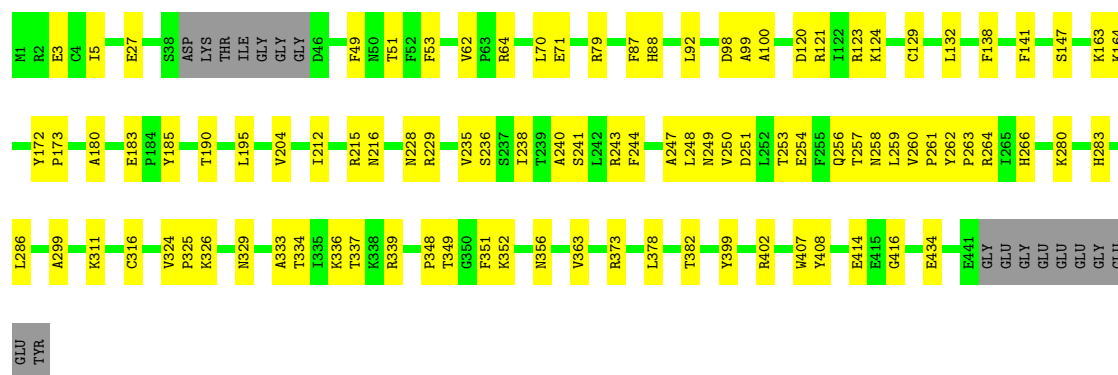
Chain 2I: 75% 21%





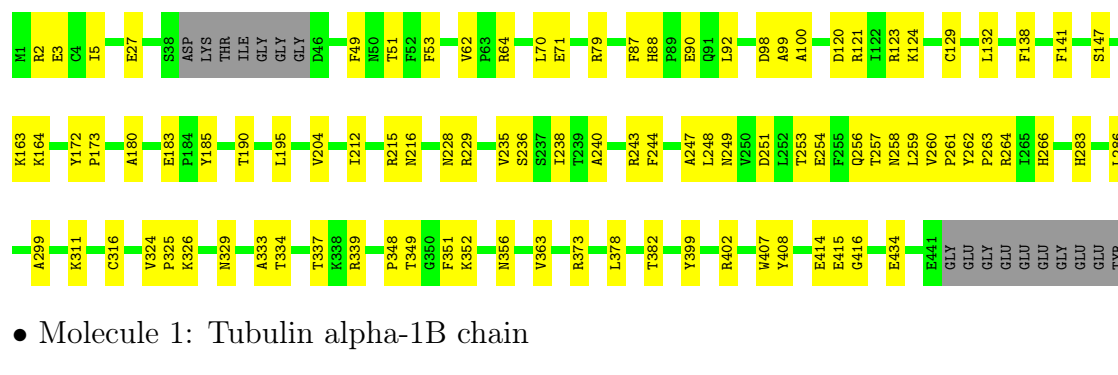
- Molecule 1: Tubulin alpha-1B chain

Chain 2J: 75% 21%



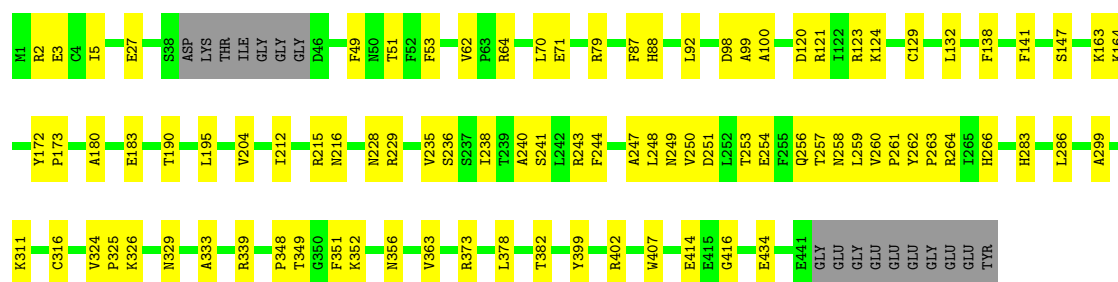
- Molecule 1: Tubulin alpha-1B chain

Chain 2K: 75% 21%




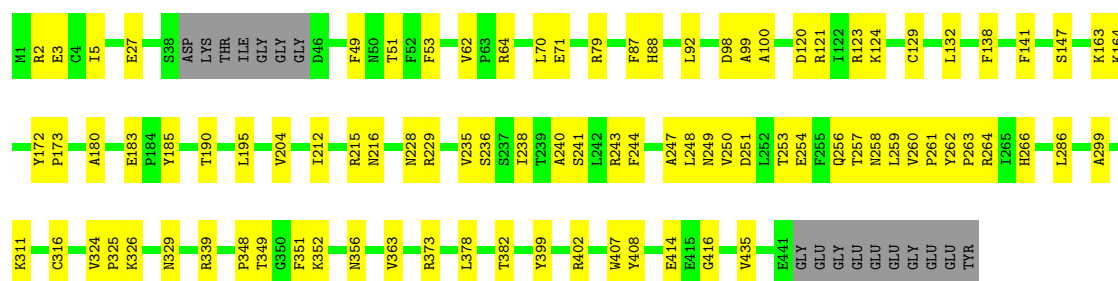
- Molecule 1: Tubulin alpha-1B chain

Chain 2L: 76% 20%




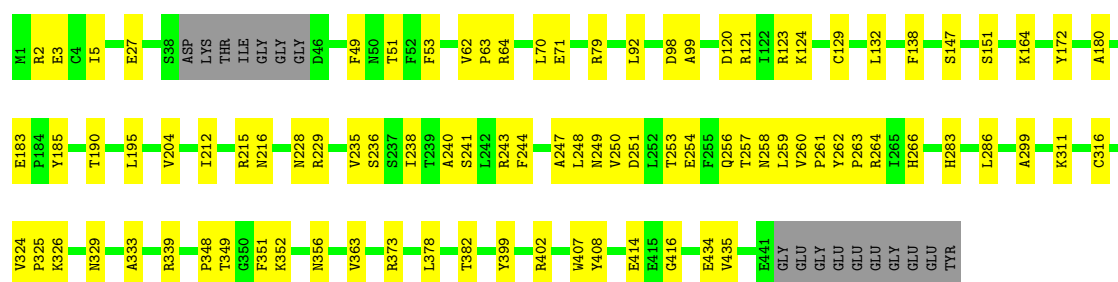
- Molecule 1: Tubulin alpha-1B chain

Chain 2M:  76% 20% .




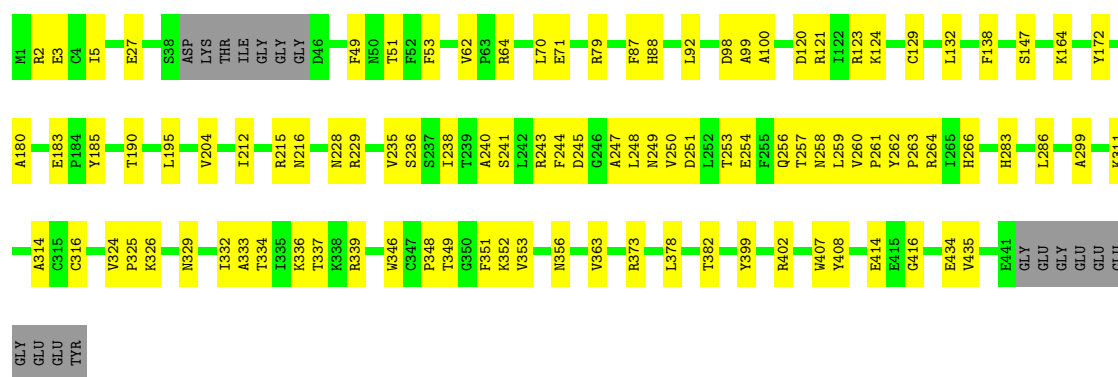
• Molecule 1: Tubulin alpha-1B chain

Chain 2N:  76% 20% .



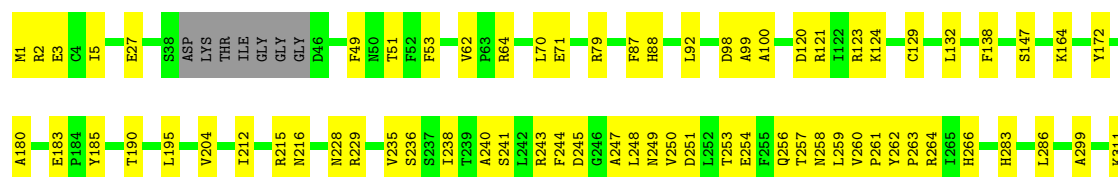
• Molecule 1: Tubulin alpha-1B chain

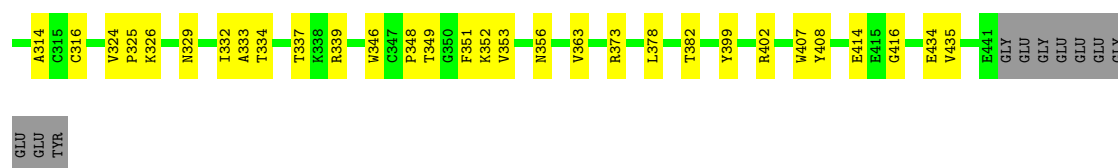
Chain 3A:  74% 22% .



• Molecule 1: Tubulin alpha-1B chain

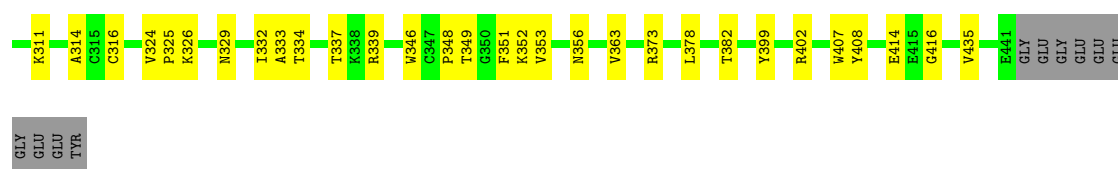
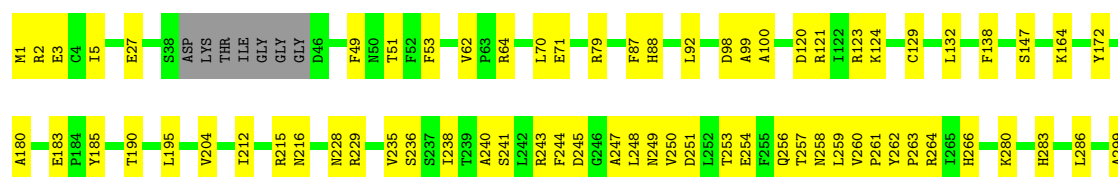
Chain 3B:  74% 22% .





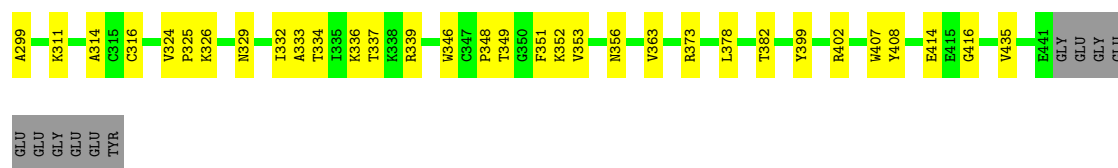
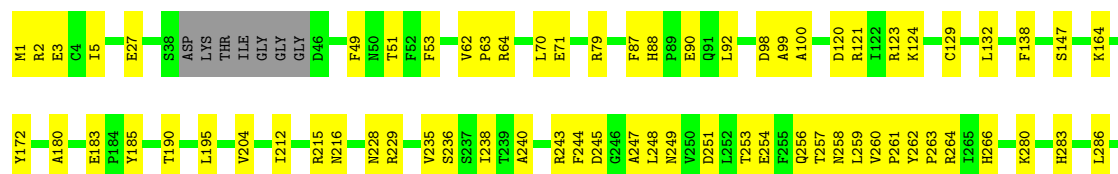
- Molecule 1: Tubulin alpha-1B chain

Chain 3C: 74% 22%



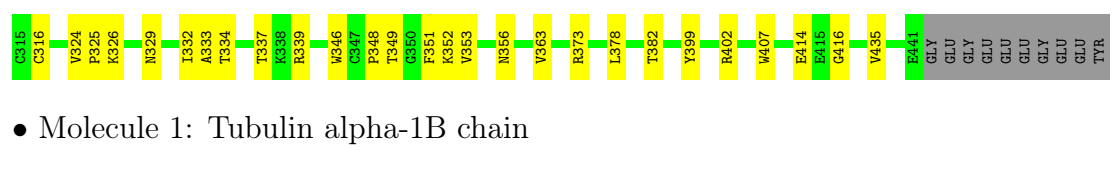
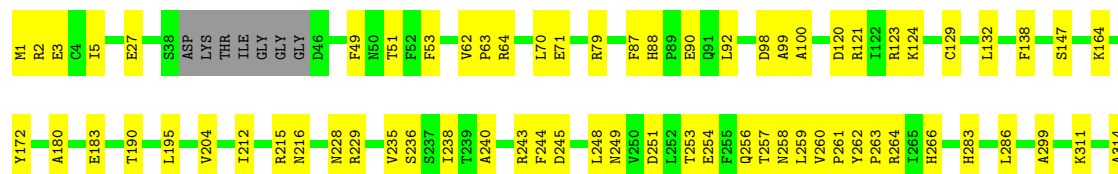
- Molecule 1: Tubulin alpha-1B chain

Chain 3D: 74% 22%

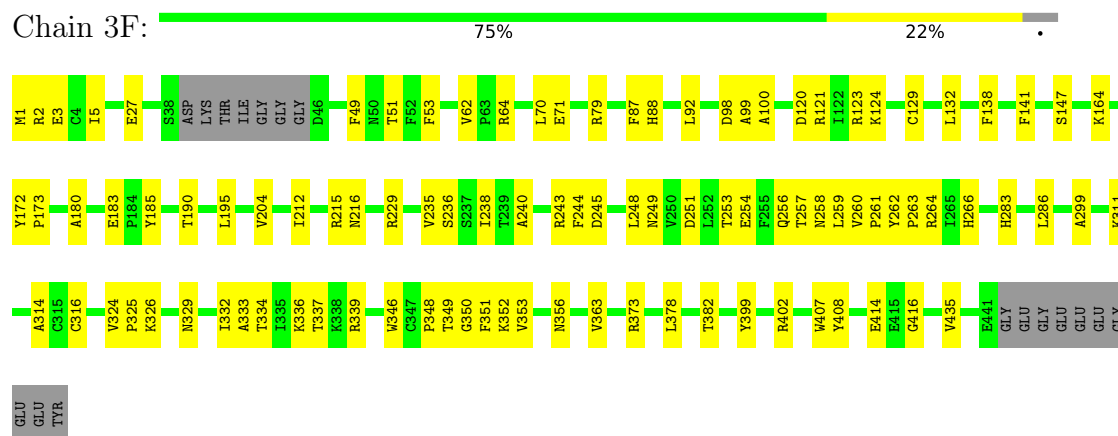


- Molecule 1: Tubulin alpha-1B chain

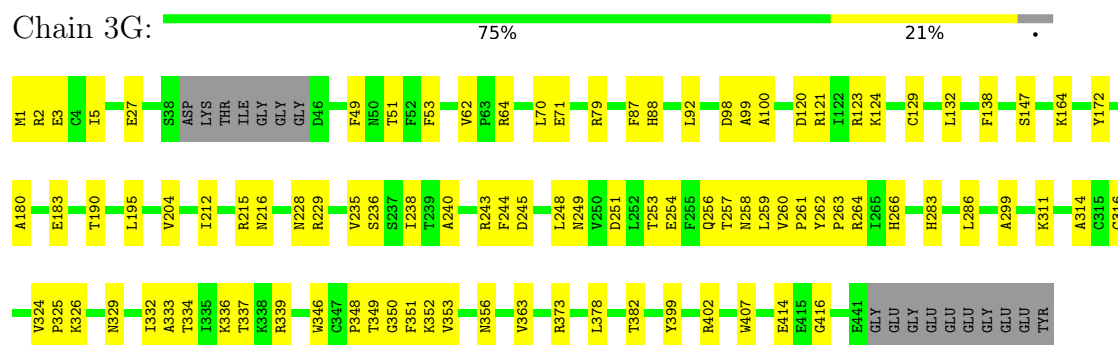
Chain 3E: 75% 21%



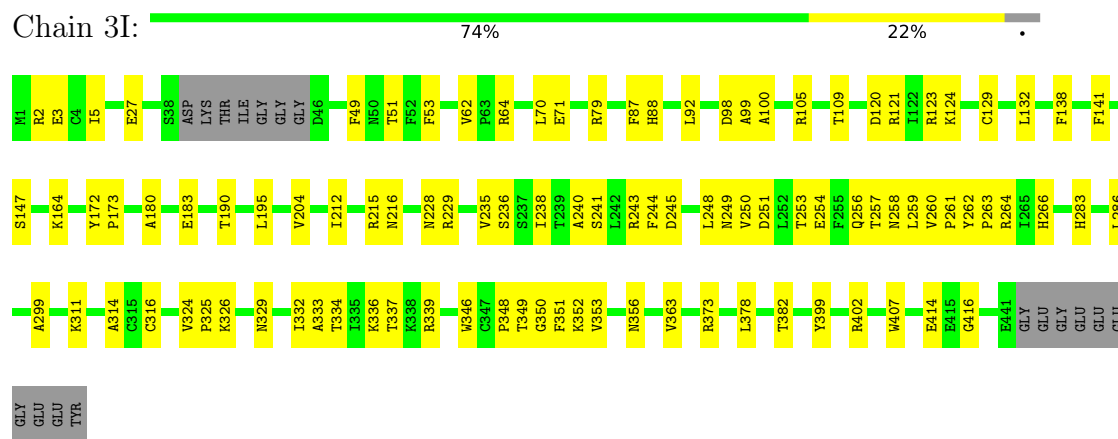
- Molecule 1: Tubulin alpha-1B chain



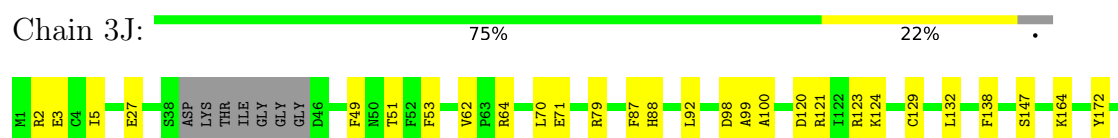
• Molecule 1: Tubulin alpha-1B chain

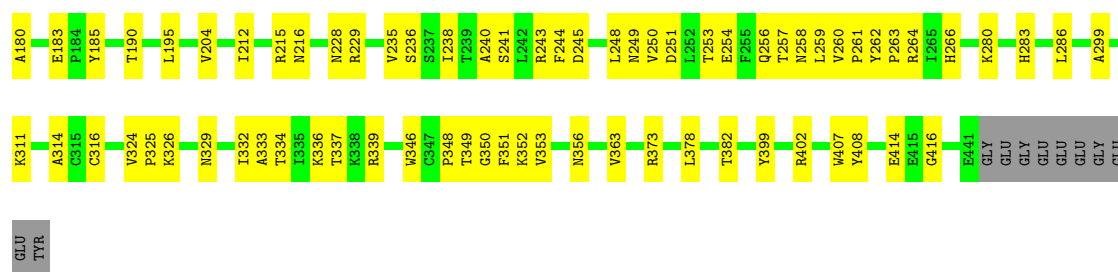


• Molecule 1: Tubulin alpha-1B chain



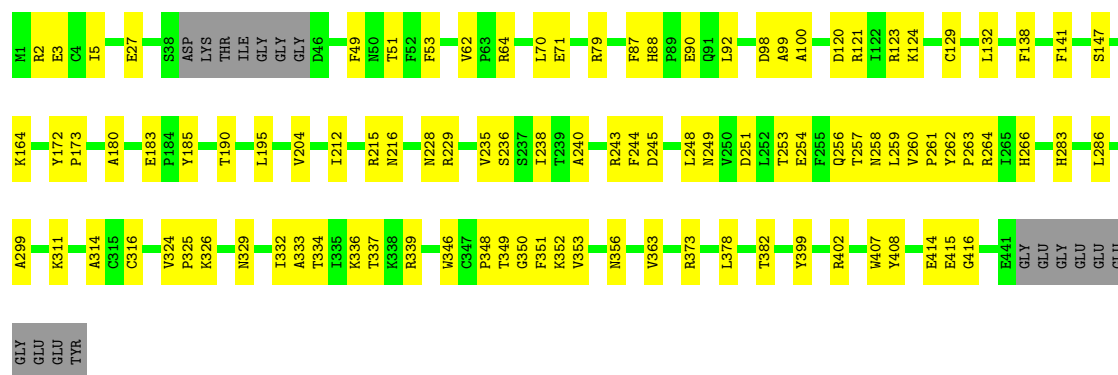
• Molecule 1: Tubulin alpha-1B chain





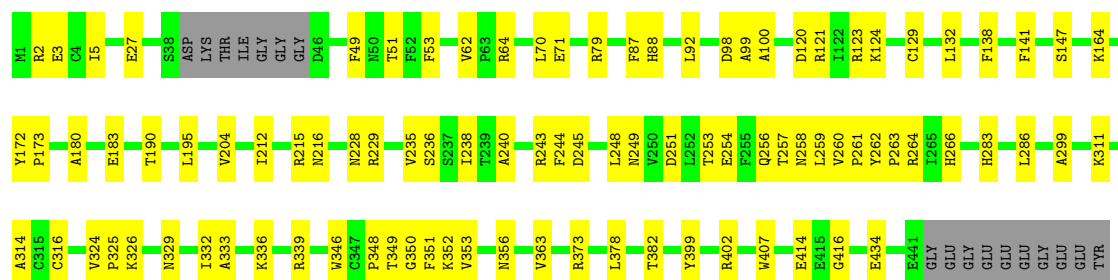
• Molecule 1: Tubulin alpha-1B chain

Chain 3K: 74% 22%



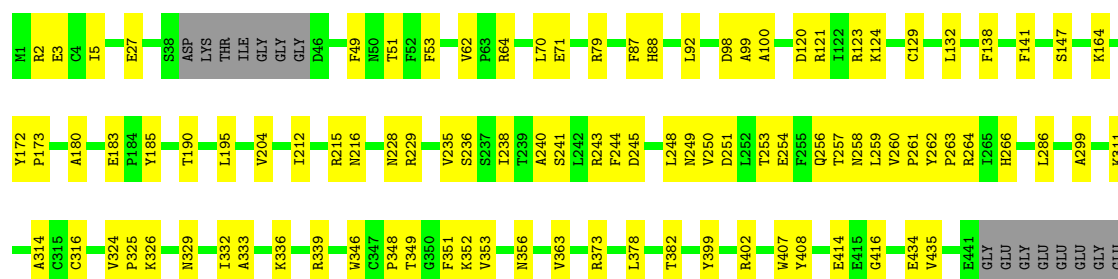
• Molecule 1: Tubulin alpha-1B chain

Chain 3L: 75% 21%




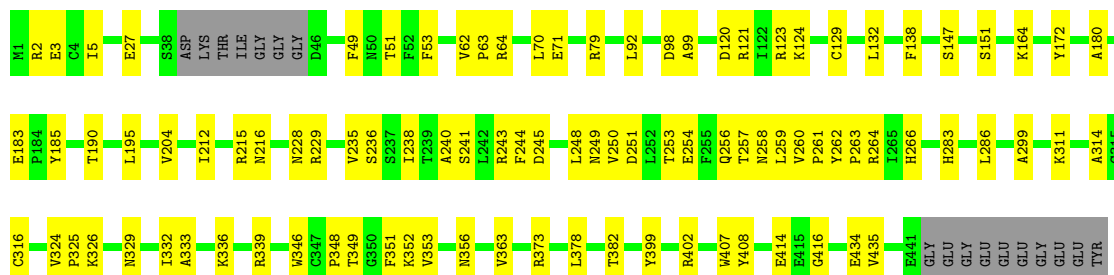
• Molecule 1: Tubulin alpha-1B chain

Chain 3M: 75% 22%


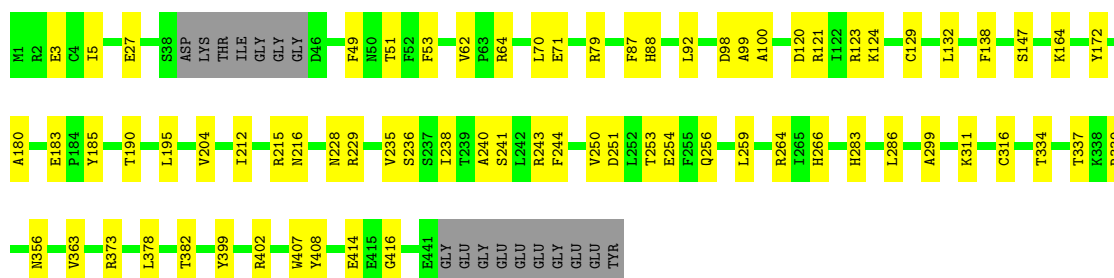


GLU  
TYR


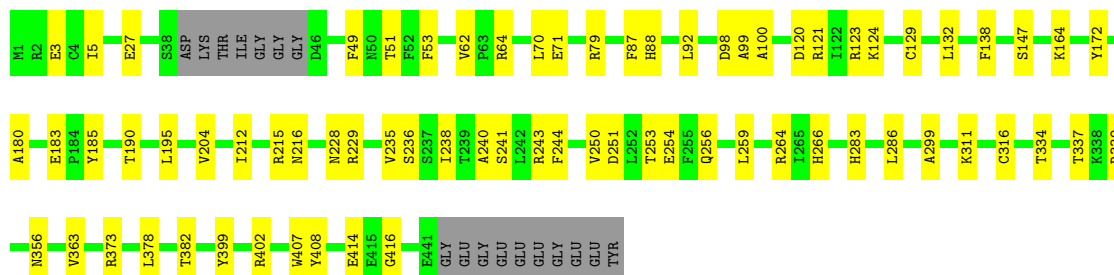
- Molecule 1: Tubulin alpha-1B chain

Chain 3N:  75% 21% .


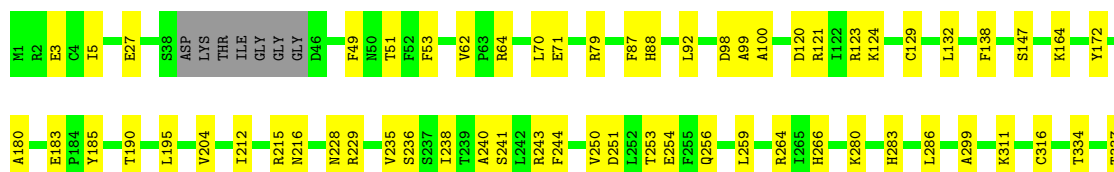
- Molecule 1: Tubulin alpha-1B chain

Chain 4A:  80% 16% .

- Molecule 1: Tubulin alpha-1B chain

Chain 4B:  80% 16% .

- Molecule 1: Tubulin alpha-1B chain

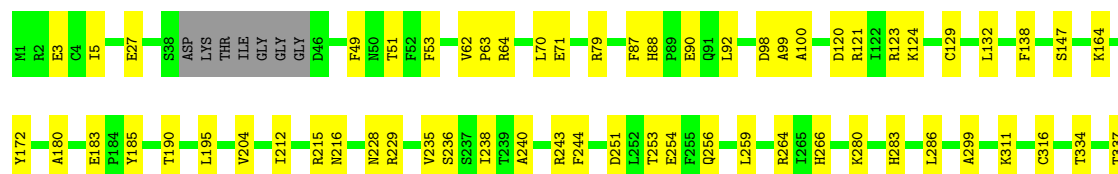
Chain 4C:  80% 16% .





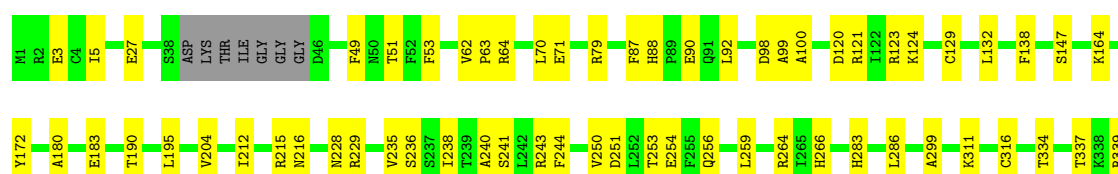
• Molecule 1: Tubulin alpha-1B chain

Chain 4D: 80% 16% •



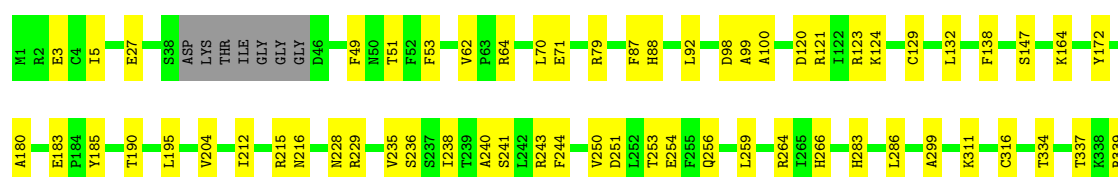
• Molecule 1: Tubulin alpha-1B chain

Chain 4E: 80% 16% •



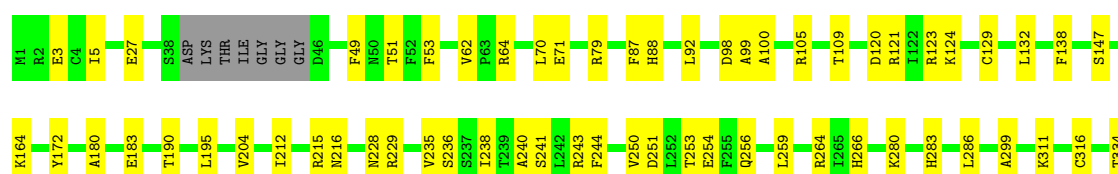
• Molecule 1: Tubulin alpha-1B chain

Chain 4F: 80% 16% •



• Molecule 1: Tubulin alpha-1B chain

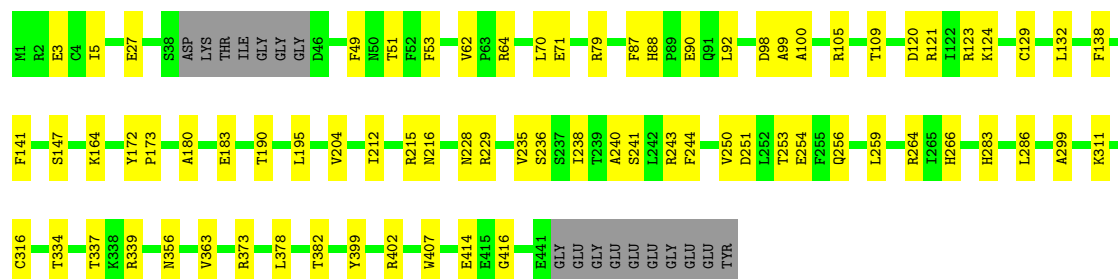
Chain 4G: 80% 16% •





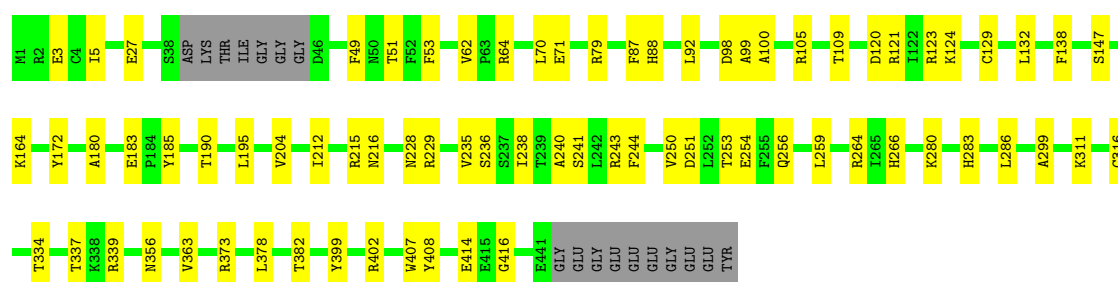
• Molecule 1: Tubulin alpha-1B chain

Chain 4I: 80% 17%



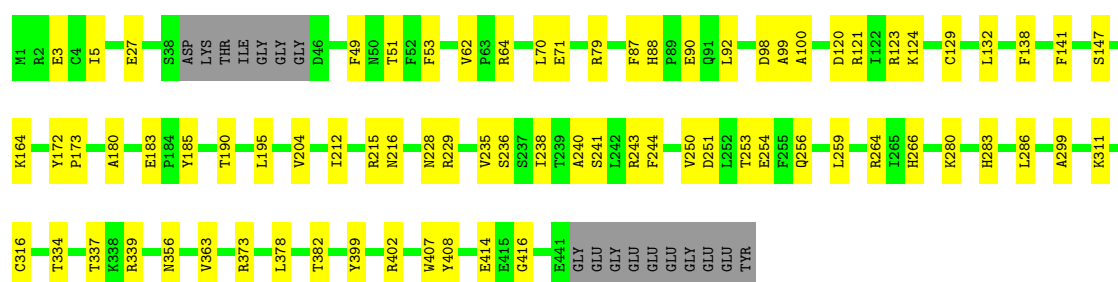
• Molecule 1: Tubulin alpha-1B chain

Chain 4J: 80% 17%



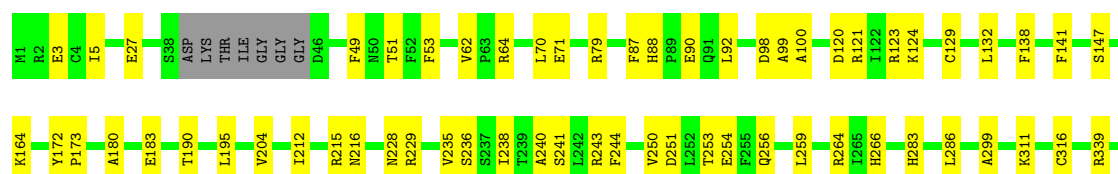
• Molecule 1: Tubulin alpha-1B chain

Chain 4K: 79% 17%



• Molecule 1: Tubulin alpha-1B chain

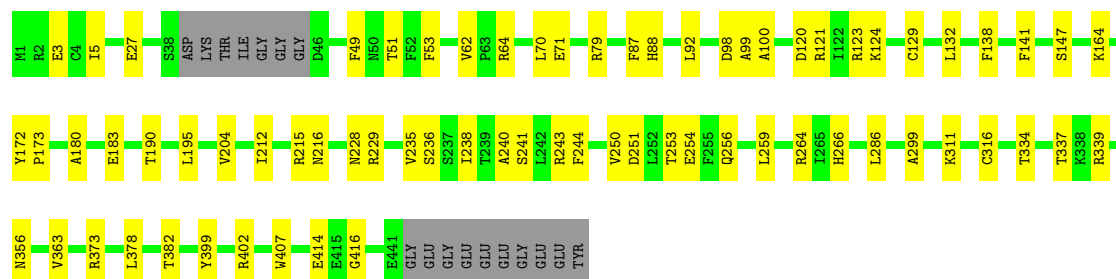
Chain 4L: 80% 16%





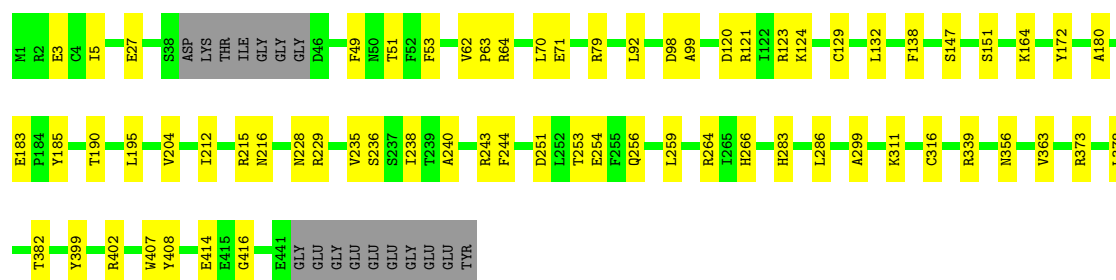
• Molecule 1: Tubulin alpha-1B chain

Chain 4M: 80% 16% .



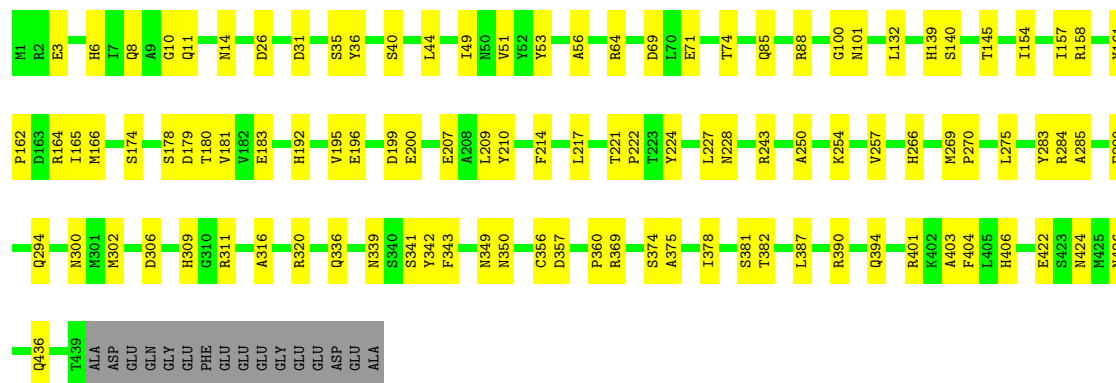
• Molecule 1: Tubulin alpha-1B chain

Chain 4N: 81% 15% .



• Molecule 2: Tubulin beta chain

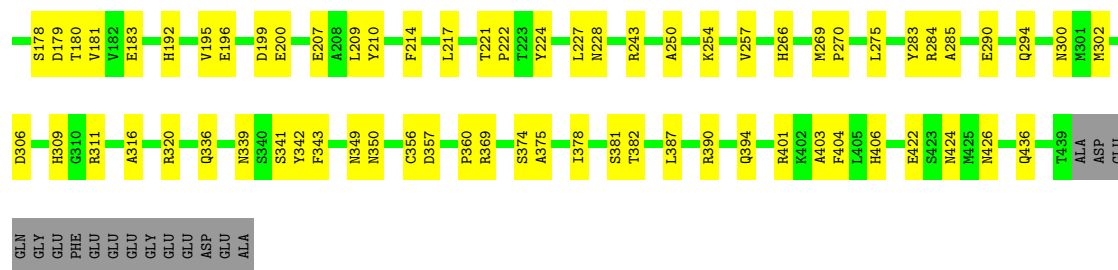
Chain 1H: 73% 23% .



• Molecule 2: Tubulin beta chain

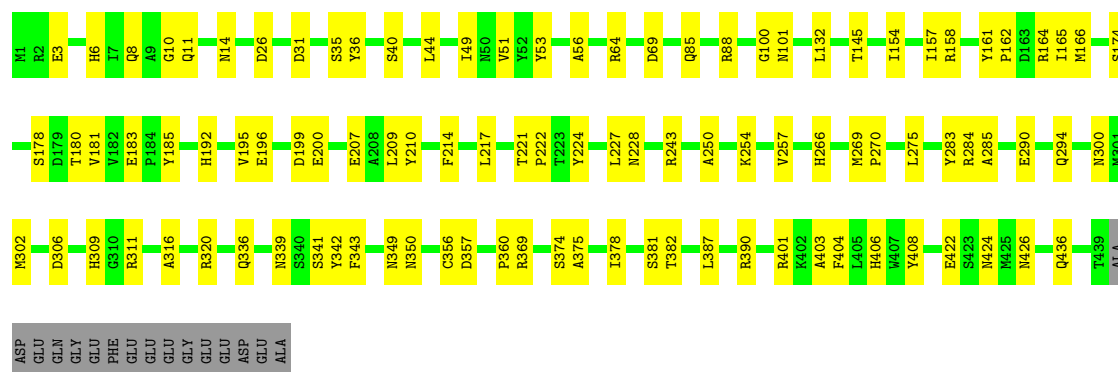
Chain 1O: 74% 22% .





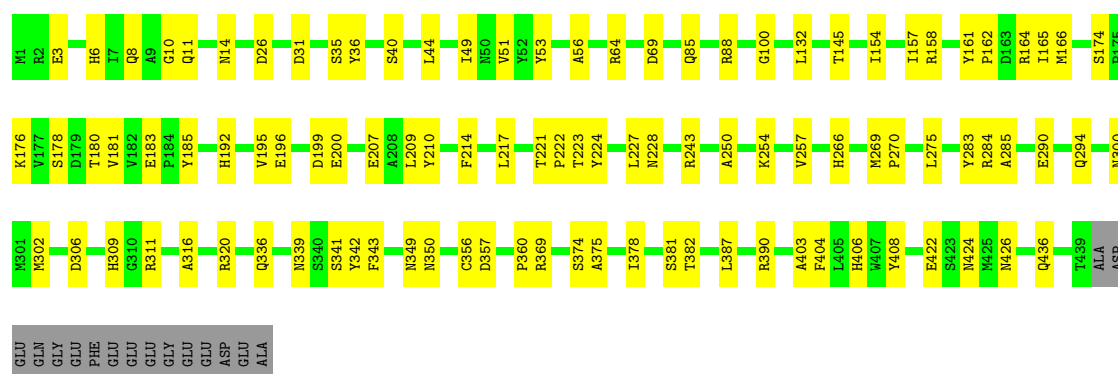
• Molecule 2: Tubulin beta chain

Chain 1P: 74% 22% .



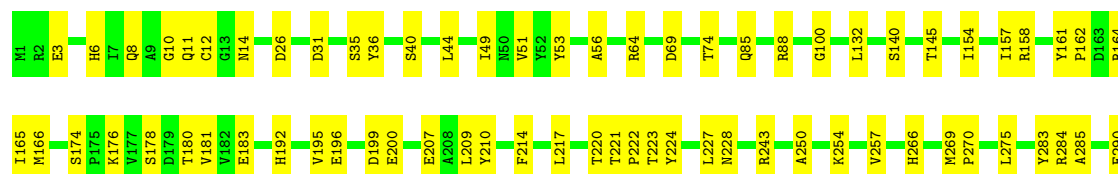
• Molecule 2: Tubulin beta chain

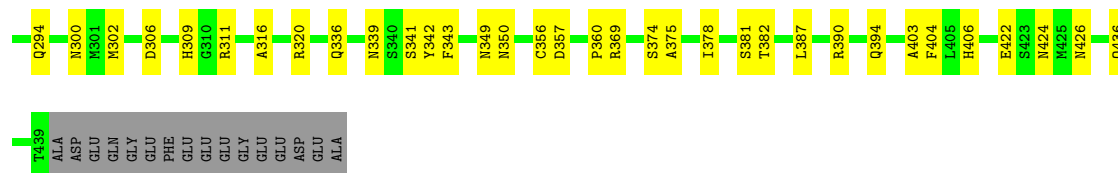
Chain 1Q: 74% 22% .



• Molecule 2: Tubulin beta chain

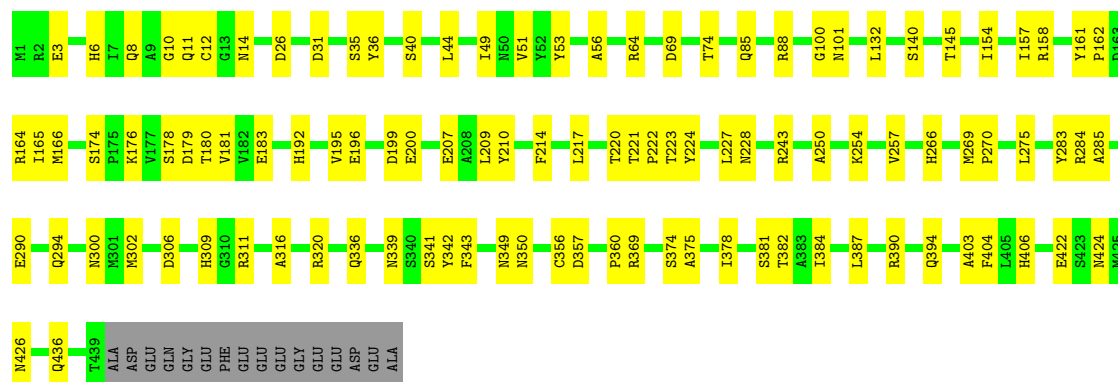
Chain 1R: 73% 23% .





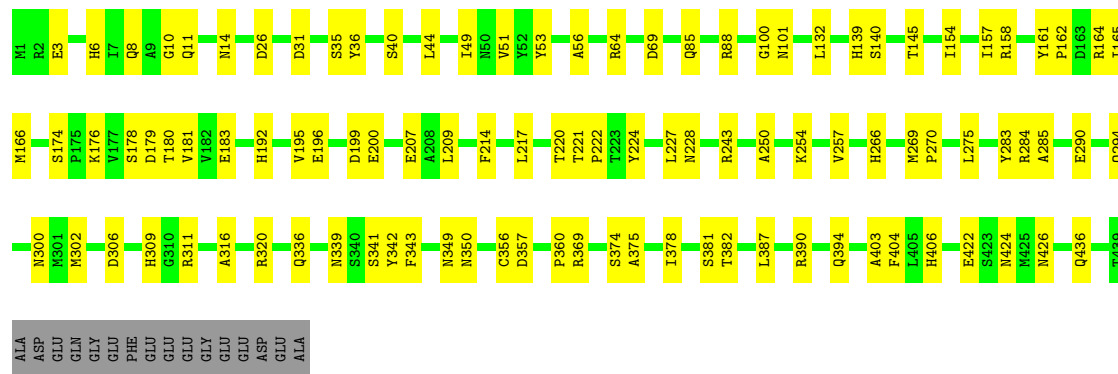
• Molecule 2: Tubulin beta chain

Chain 1S: 73% 24%



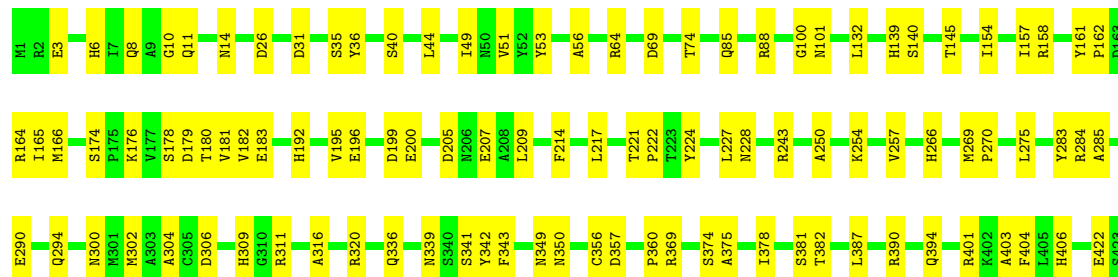
• Molecule 2: Tubulin beta chain

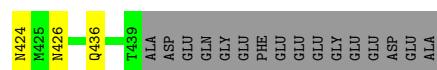
Chain 1T: 73% 23%



• Molecule 2: Tubulin beta chain

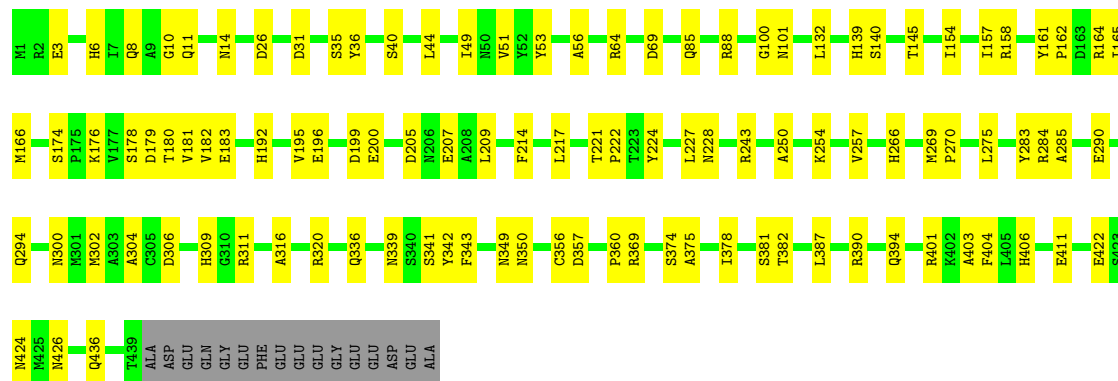
Chain 1U: 73% 24%





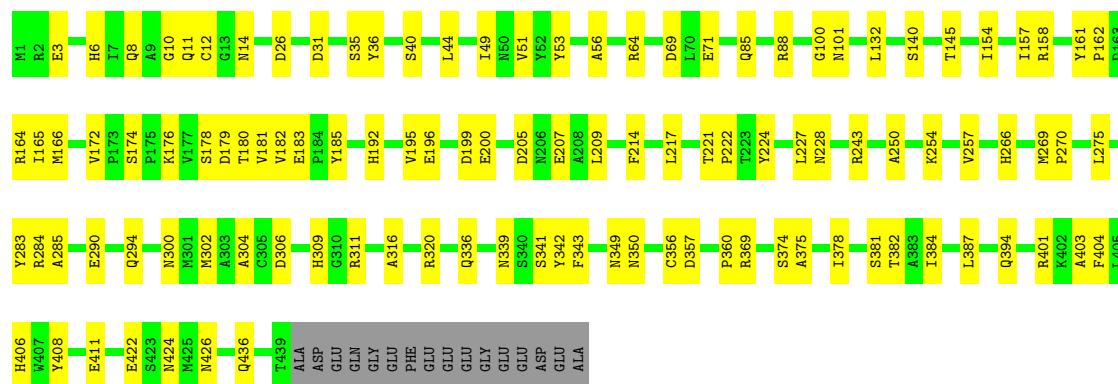
• Molecule 2: Tubulin beta chain

Chain 1V: 73% 24% .



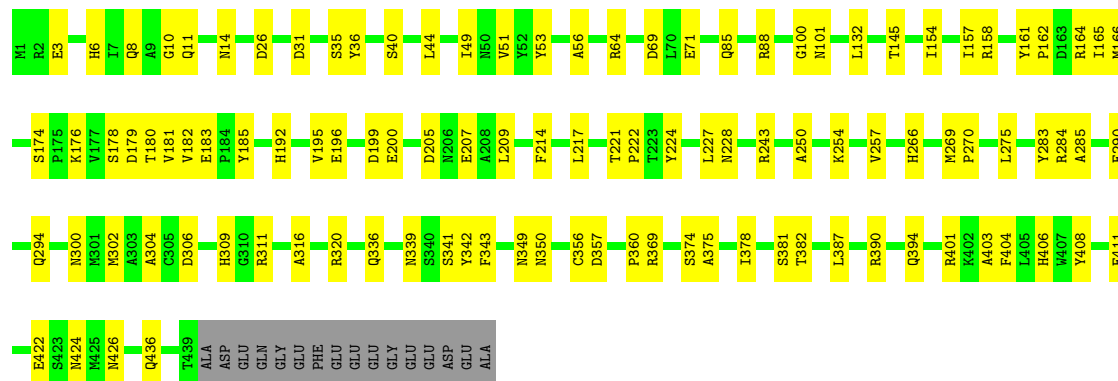
• Molecule 2: Tubulin beta chain

Chain 1W: 72% 25% .

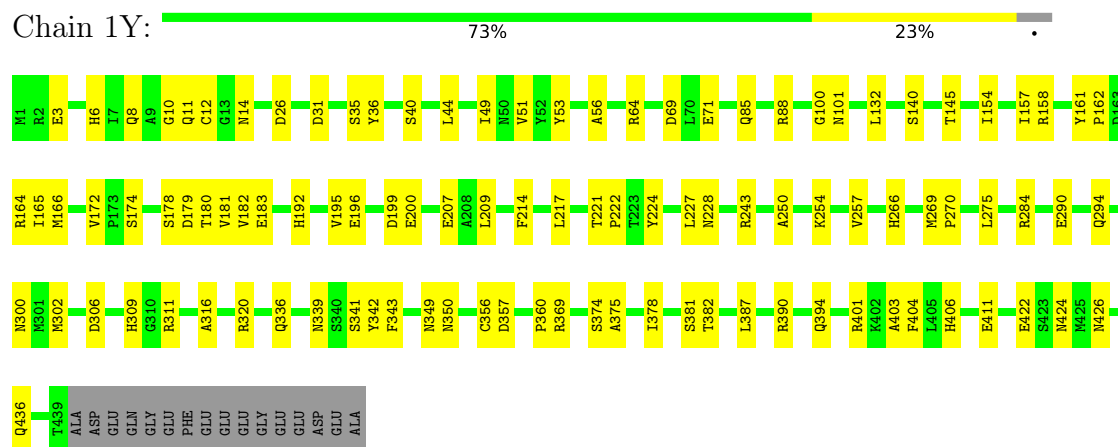


• Molecule 2: Tubulin beta chain

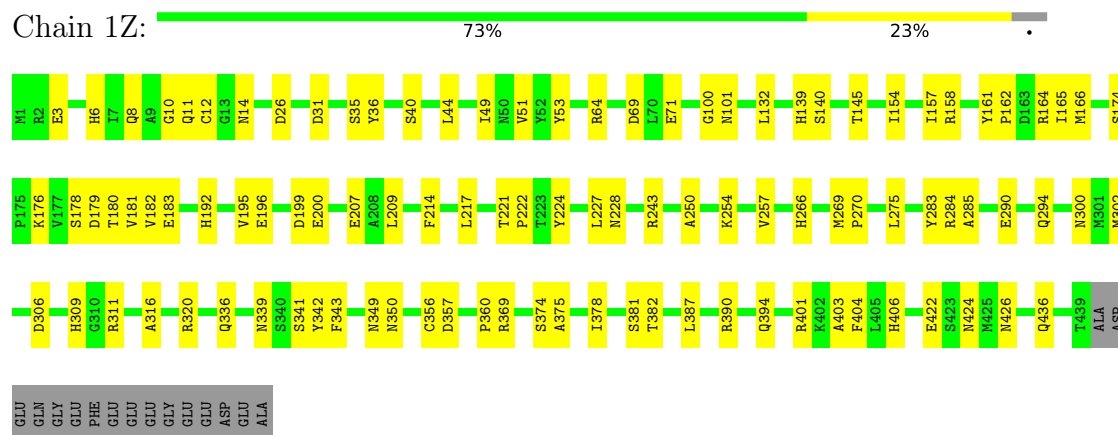
Chain 1X: 72% 24% .



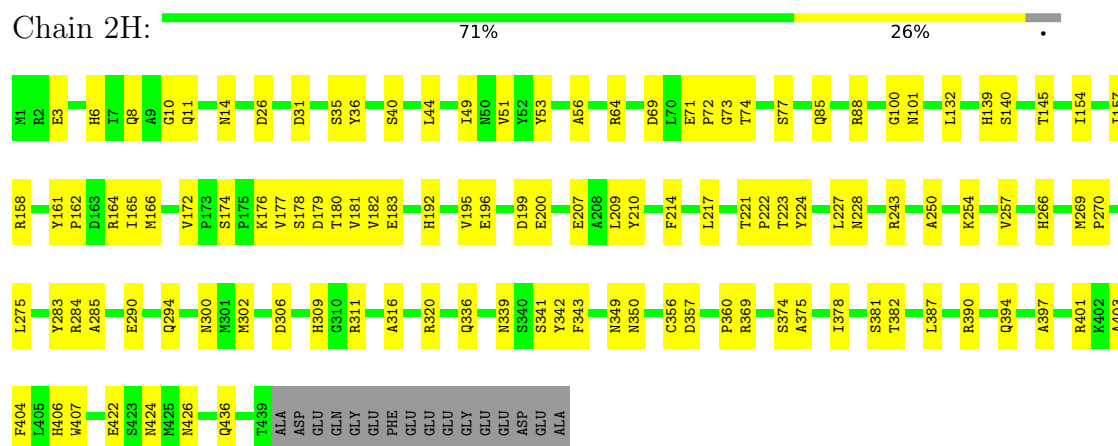
• Molecule 2: Tubulin beta chain



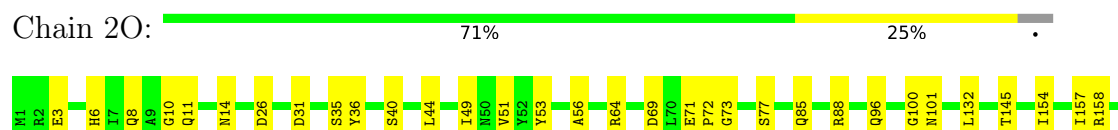
- Molecule 2: Tubulin beta chain

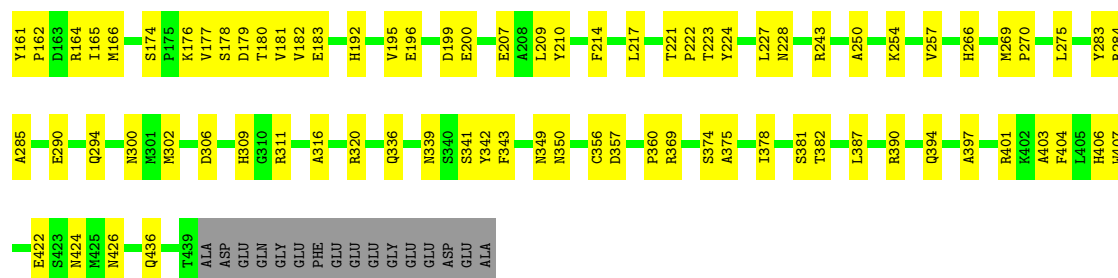


- Molecule 2: Tubulin beta chain



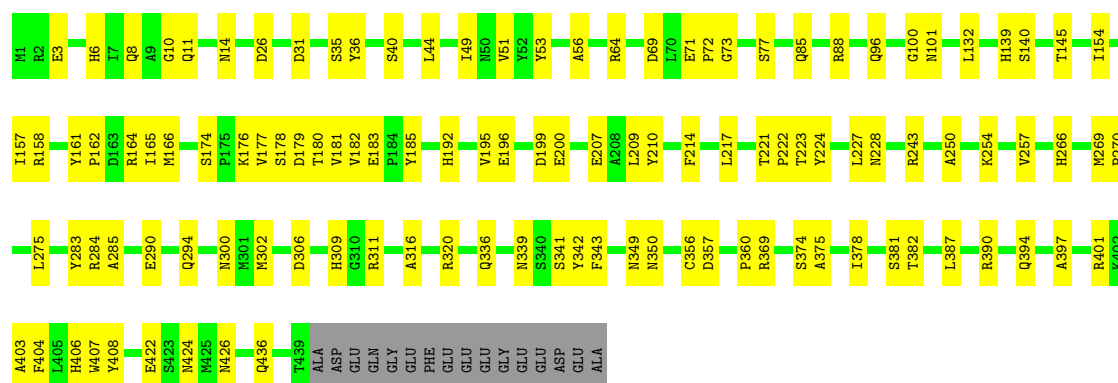
- Molecule 2: Tubulin beta chain





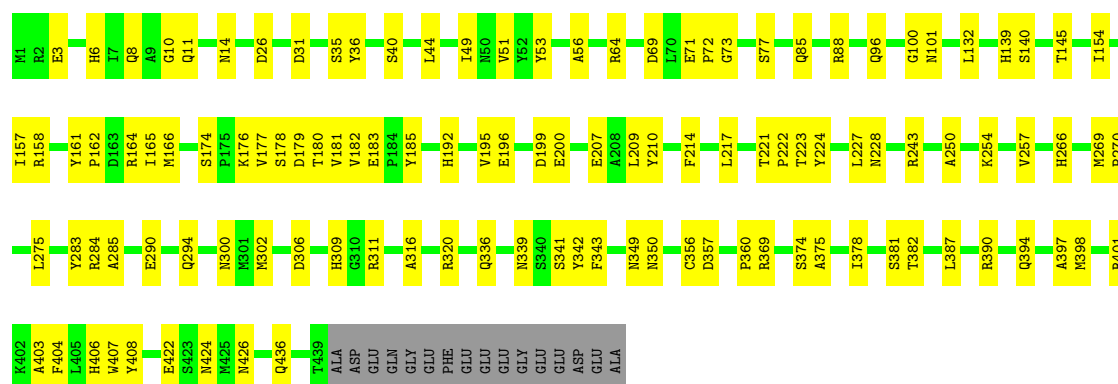
• Molecule 2: Tubulin beta chain

Chain 2P: 71% 26% .



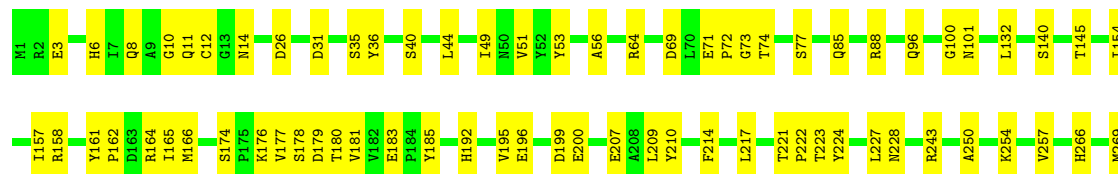
• Molecule 2: Tubulin beta chain

Chain 2Q: 70% 26% .



• Molecule 2: Tubulin beta chain

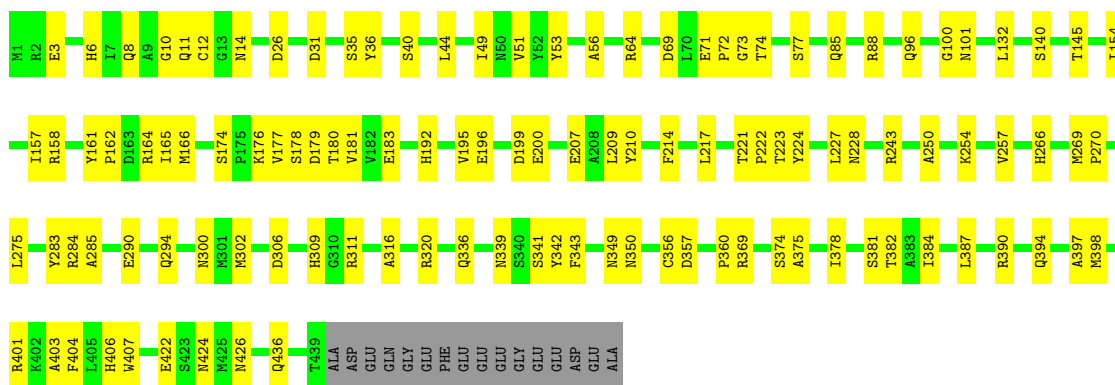
Chain 2R: 70% 26% .





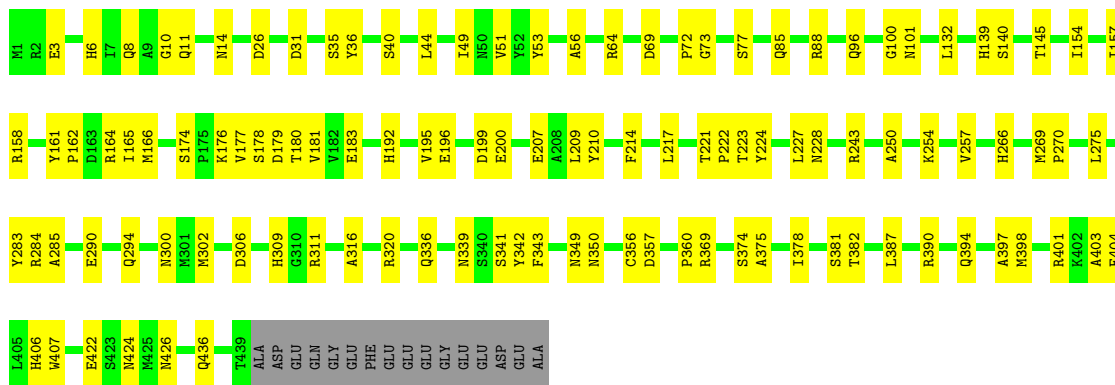
- Molecule 2: Tubulin beta chain

Chain 2S:  71% 26% .



- Molecule 2: Tubulin beta chain

Chain 2T:  71% 25% .



- Molecule 2: Tubulin beta chain

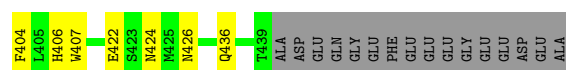
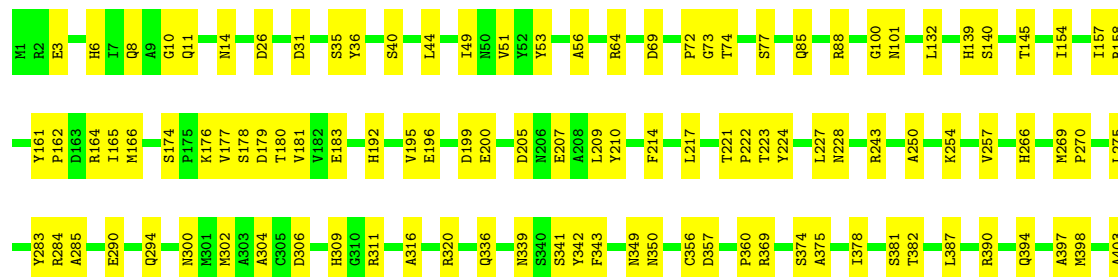
Chain 2U:  71% 25% .





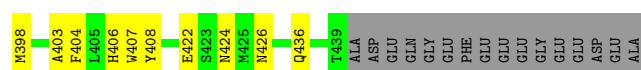
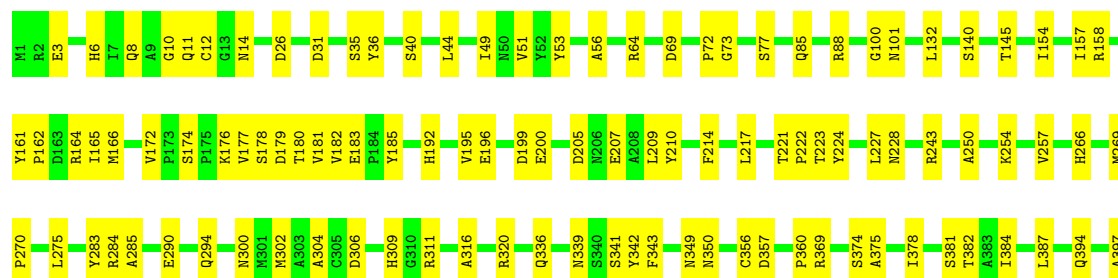
• Molecule 2: Tubulin beta chain

Chain 2V: 71% 25% .



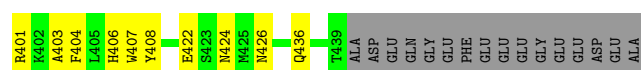
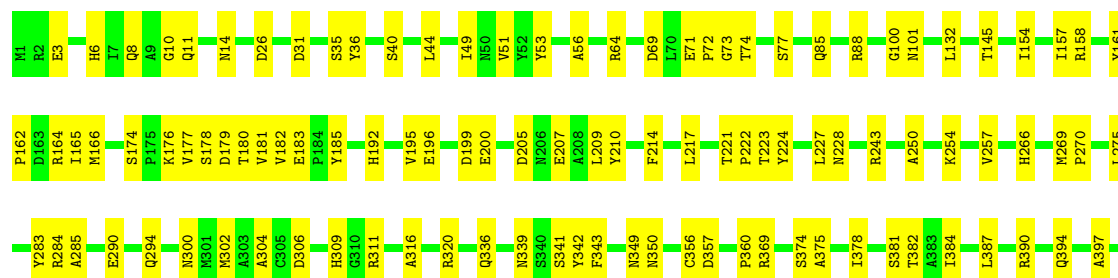
• Molecule 2: Tubulin beta chain

Chain 2W: 70% 26% .



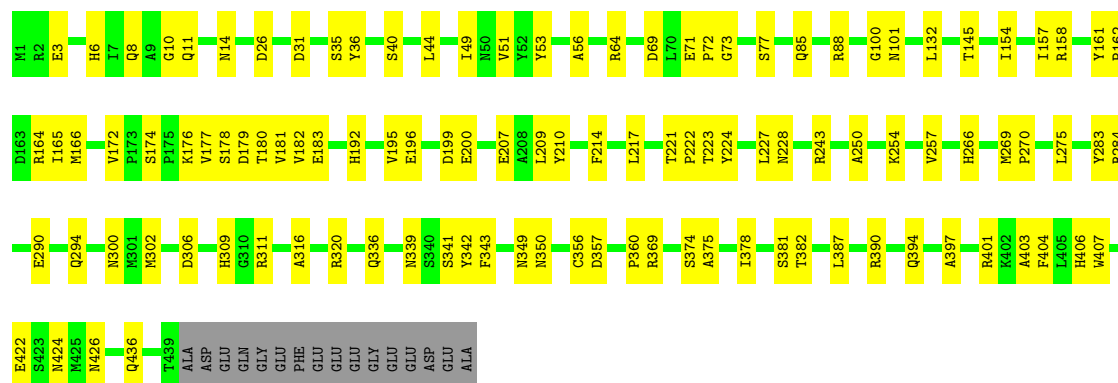
• Molecule 2: Tubulin beta chain

Chain 2X: 70% 26% .



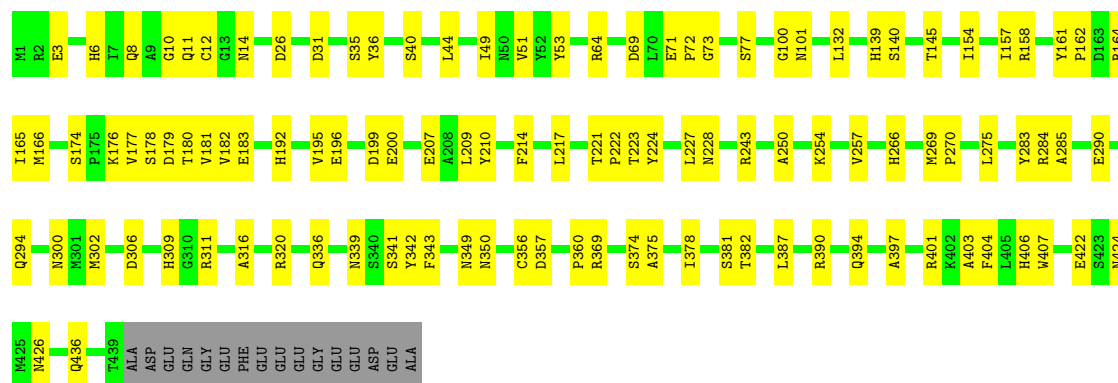
• Molecule 2: Tubulin beta chain

Chain 2Y:  72% 25% .




• Molecule 2: Tubulin beta chain

Chain 2Z:  72% 25% .




• Molecule 2: Tubulin beta chain

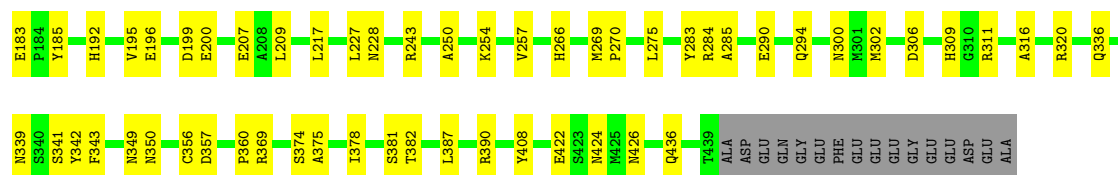
Chain 3H:  77% 20% .



• Molecule 2: Tubulin beta chain

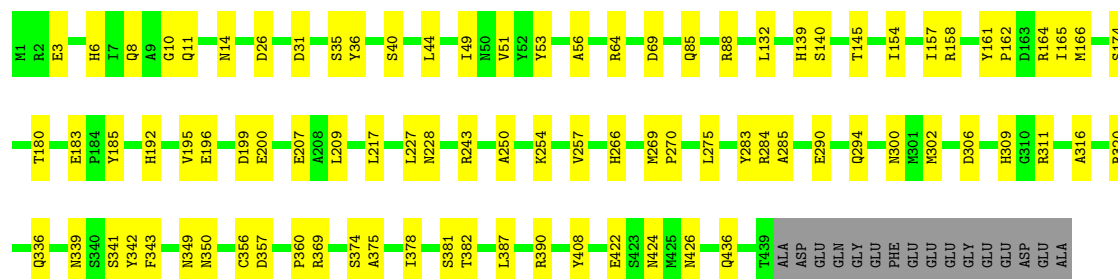
Chain 3O:  77% 20% .





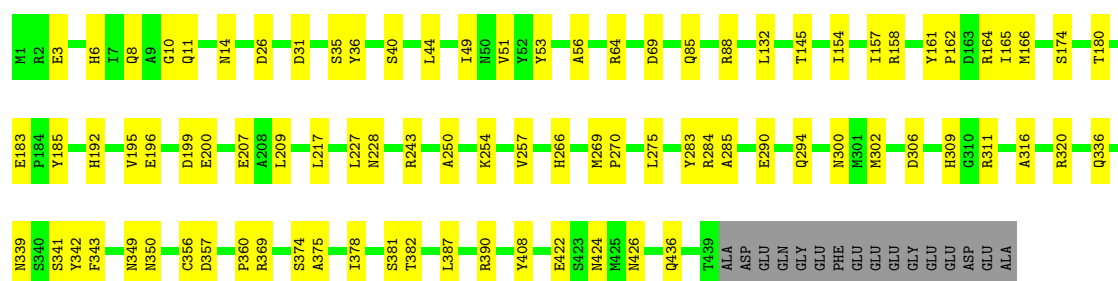
• Molecule 2: Tubulin beta chain

Chain 3P: 76% 20%



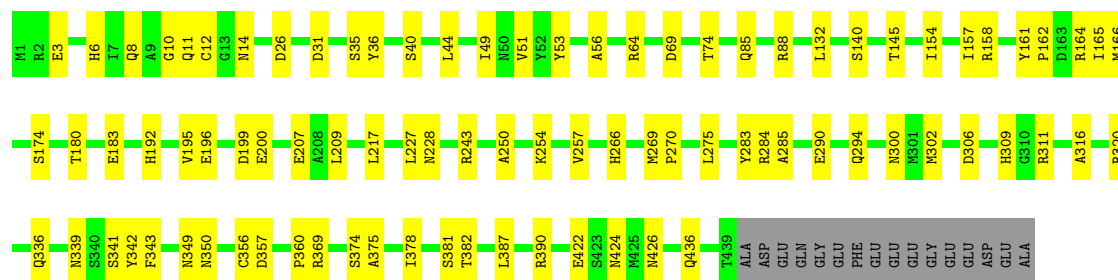
• Molecule 2: Tubulin beta chain

Chain 3Q: 77% 20%



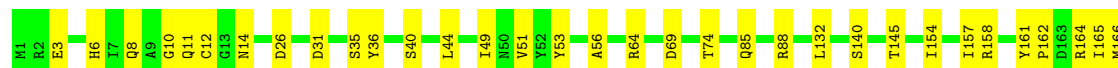
• Molecule 2: Tubulin beta chain

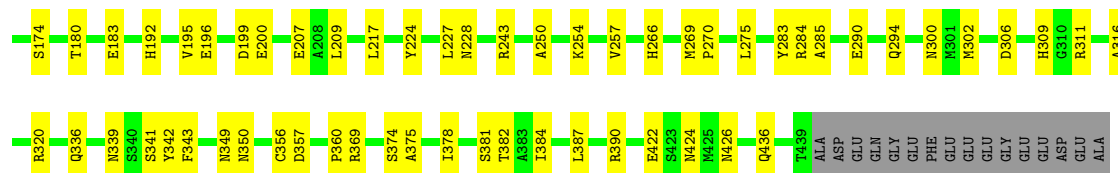
Chain 3R: 77% 20%



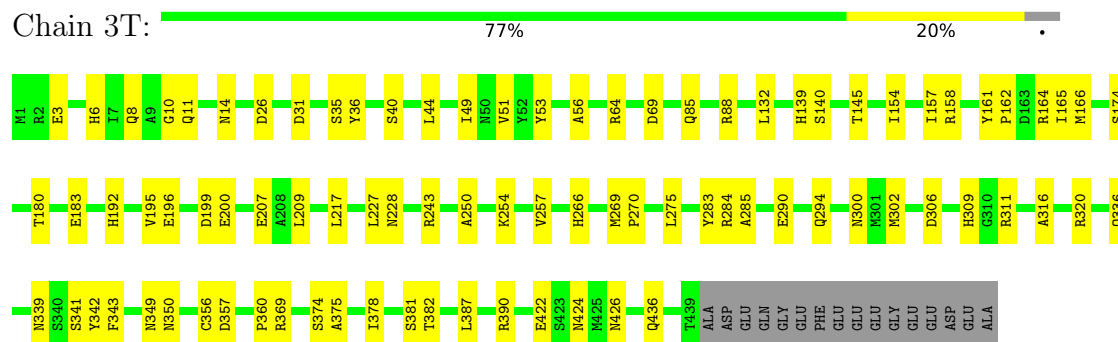
• Molecule 2: Tubulin beta chain

Chain 3S: 76% 20%

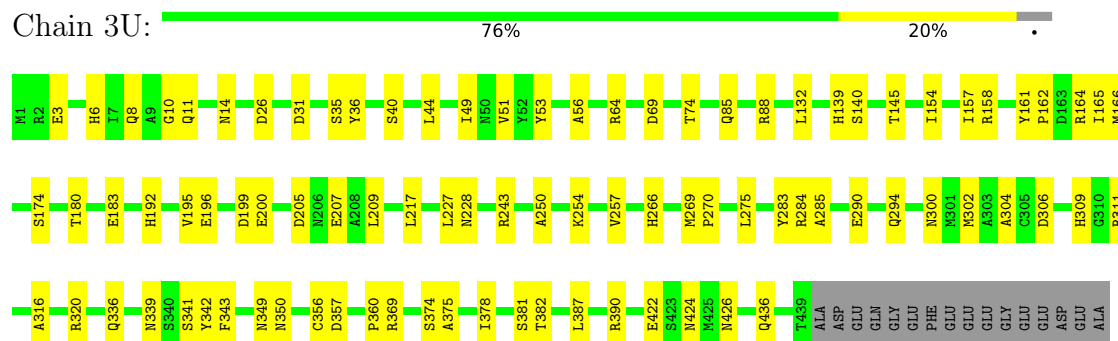




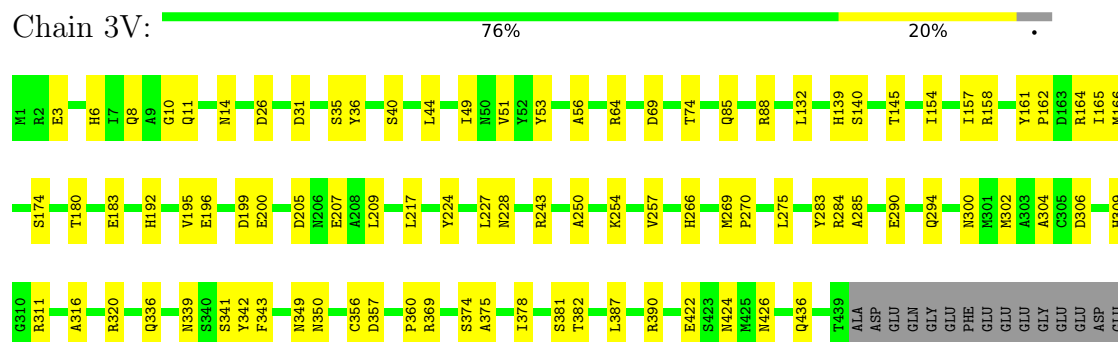
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



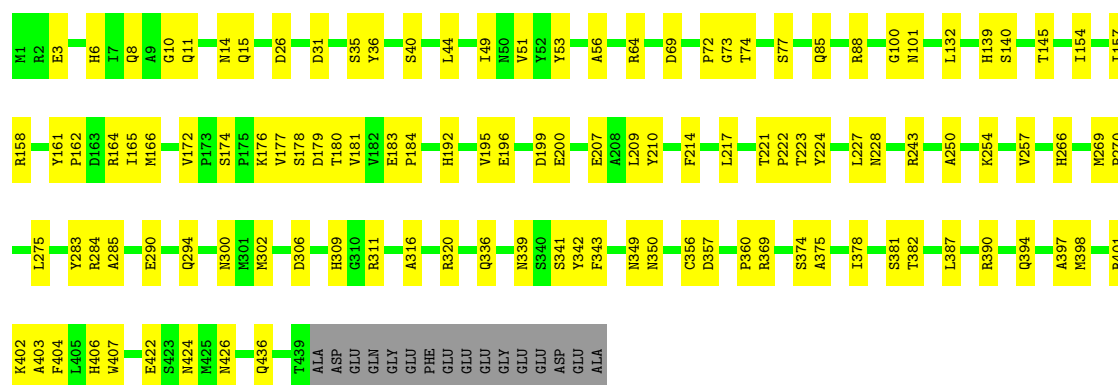
ALA

- Molecule 2: Tubulin beta chain



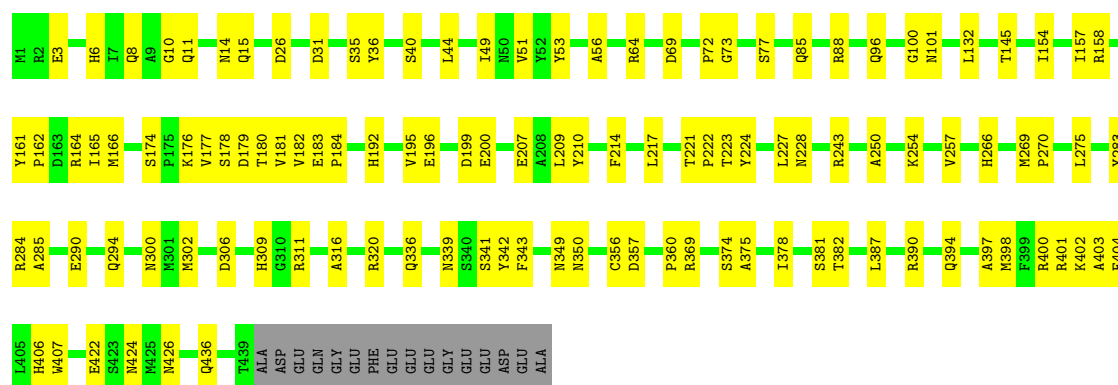


Chain 4H:  70% 26% .



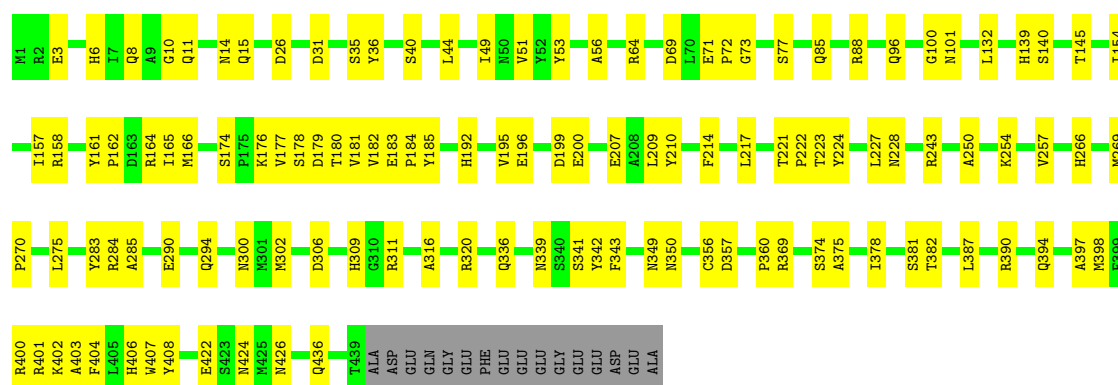
• Molecule 2: Tubulin beta chain

Chain 4O:  71% 26% .



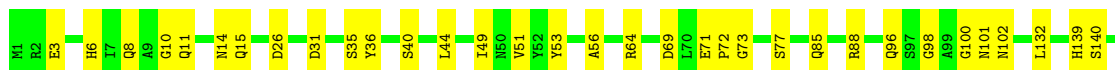
• Molecule 2: Tubulin beta chain

Chain 4P:  69% 27% .

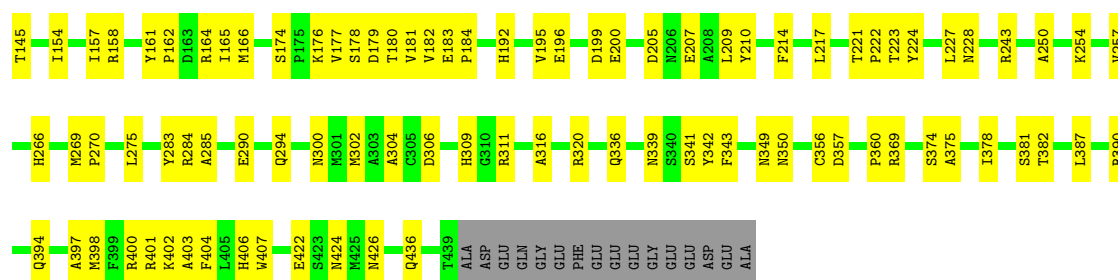


• Molecule 2: Tubulin beta chain

Chain 4Q:  69% 27% .

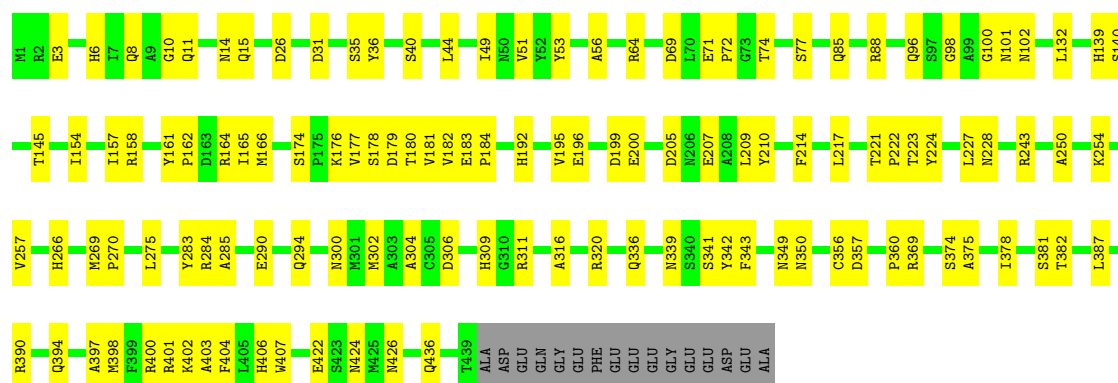






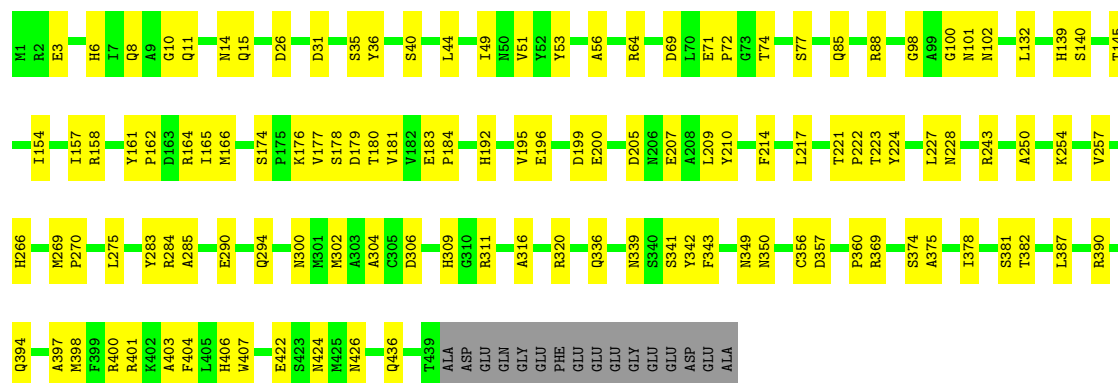
• Molecule 2: Tubulin beta chain

Chain 4U: 69% 27% .



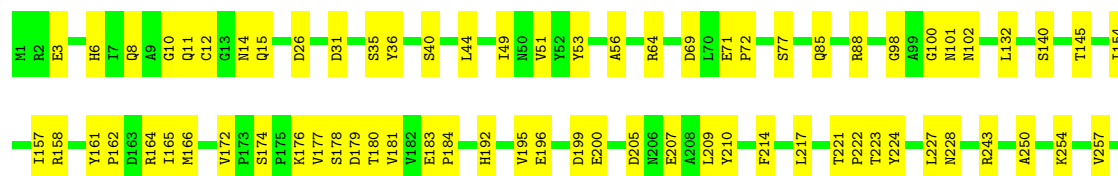
• Molecule 2: Tubulin beta chain

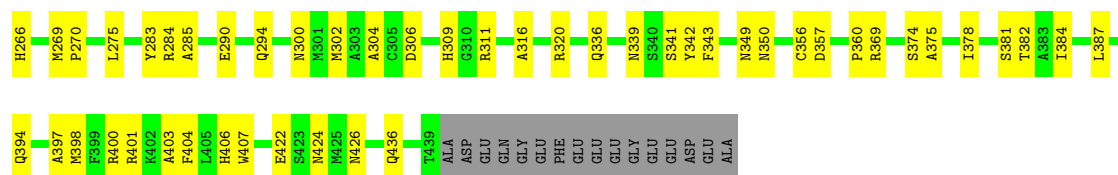
Chain 4V: 70% 27% .



• Molecule 2: Tubulin beta chain

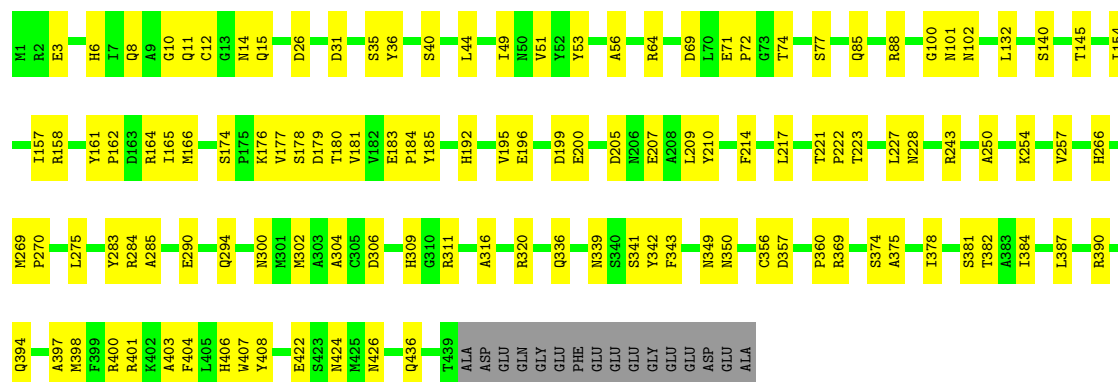
Chain 4W: 70% 27% .





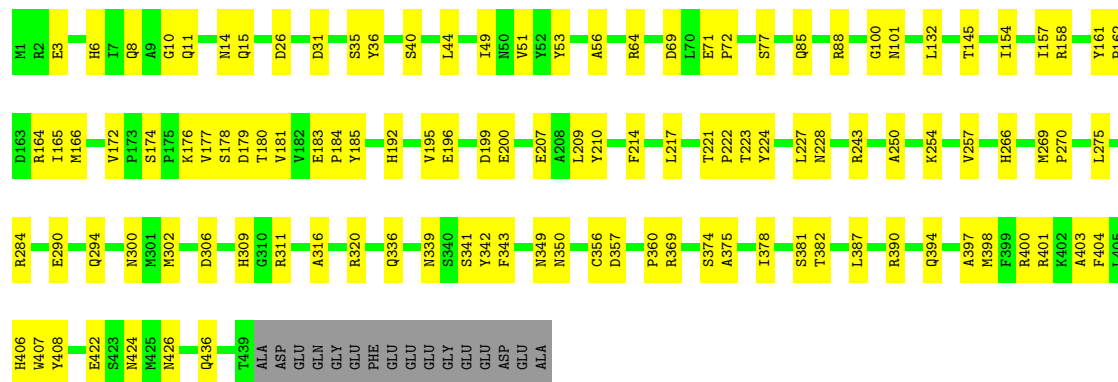
• Molecule 2: Tubulin beta chain

Chain 4X: 69% 27%



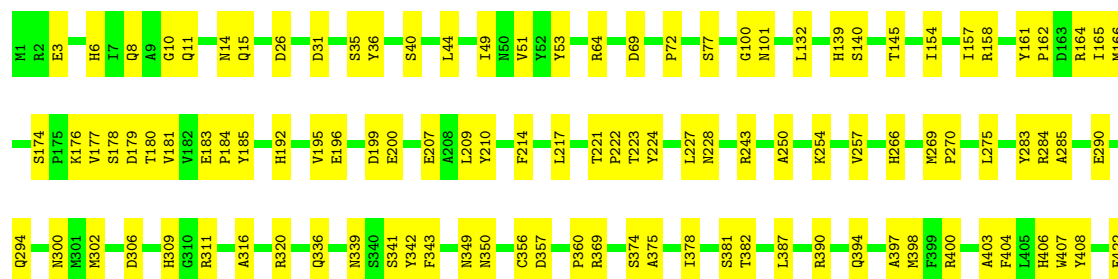
• Molecule 2: Tubulin beta chain

Chain 4Y: 71% 25%



• Molecule 2: Tubulin beta chain

Chain 4Z: 71% 25%



S423	I424	I425	I426	Q436	T439	ALA	ASP	GLU	GLN	GLY	GLU	PHE	GLU	GLU	GLU	GLY	GLU	GLU	ASP	GLU	ALA
------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-27.7°, rise=9.3 Å, axial sym=C1	Depositor
Number of segments used	24692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1422.3	Depositor
Maximum defocus (nm)	2706.1	Depositor
Magnification	23364	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG

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	1A	0.33	0/3473	0.50	0/4716
1	1B	0.33	0/3473	0.50	0/4716
1	1C	0.33	0/3473	0.50	0/4716
1	1D	0.33	0/3473	0.50	0/4716
1	1E	0.33	0/3473	0.50	0/4716
1	1F	0.33	0/3473	0.50	0/4716
1	1G	0.33	0/3473	0.50	0/4716
1	1I	0.33	0/3473	0.50	0/4716
1	1J	0.33	0/3473	0.50	0/4716
1	1K	0.33	0/3473	0.50	0/4716
1	1L	0.33	0/3473	0.50	0/4716
1	1M	0.33	0/3473	0.50	0/4716
1	1N	0.33	0/3473	0.50	0/4716
1	2A	0.33	0/3473	0.50	0/4716
1	2B	0.33	0/3473	0.50	0/4716
1	2C	0.33	0/3473	0.50	0/4716
1	2D	0.33	0/3473	0.50	0/4716
1	2E	0.33	0/3473	0.50	0/4716
1	2F	0.33	0/3473	0.50	0/4716
1	2G	0.33	0/3473	0.50	0/4716
1	2I	0.33	0/3473	0.50	0/4716
1	2J	0.33	0/3473	0.50	0/4716
1	2K	0.33	0/3473	0.50	0/4716
1	2L	0.33	0/3473	0.50	0/4716
1	2M	0.33	0/3473	0.50	0/4716
1	2N	0.33	0/3473	0.50	0/4716
1	3A	0.33	0/3473	0.50	0/4716
1	3B	0.33	0/3473	0.50	0/4716
1	3C	0.33	0/3473	0.50	0/4716
1	3D	0.33	0/3473	0.51	0/4716
1	3E	0.33	0/3473	0.50	0/4716
1	3F	0.33	0/3473	0.50	0/4716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	3G	0.33	0/3473	0.50	0/4716
1	3I	0.33	0/3473	0.50	0/4716
1	3J	0.33	0/3473	0.50	0/4716
1	3K	0.33	0/3473	0.50	0/4716
1	3L	0.33	0/3473	0.50	0/4716
1	3M	0.33	0/3473	0.51	0/4716
1	3N	0.33	0/3473	0.50	0/4716
1	4A	0.33	0/3473	0.50	0/4716
1	4B	0.33	0/3473	0.50	0/4716
1	4C	0.33	0/3473	0.50	0/4716
1	4D	0.33	0/3473	0.50	0/4716
1	4E	0.33	0/3473	0.50	0/4716
1	4F	0.33	0/3473	0.51	0/4716
1	4G	0.33	0/3473	0.50	0/4716
1	4I	0.33	0/3473	0.50	0/4716
1	4J	0.33	0/3473	0.50	0/4716
1	4K	0.33	0/3473	0.50	0/4716
1	4L	0.33	0/3473	0.50	0/4716
1	4M	0.33	0/3473	0.50	0/4716
1	4N	0.33	0/3473	0.50	0/4716
2	1H	0.33	0/3443	0.52	0/4666
2	1O	0.33	0/3443	0.52	0/4666
2	1P	0.33	0/3443	0.52	0/4666
2	1Q	0.34	0/3443	0.52	0/4666
2	1R	0.33	0/3443	0.52	0/4666
2	1S	0.33	0/3443	0.52	0/4666
2	1T	0.33	0/3443	0.52	0/4666
2	1U	0.33	0/3443	0.52	0/4666
2	1V	0.33	0/3443	0.52	0/4666
2	1W	0.33	0/3443	0.52	0/4666
2	1X	0.33	0/3443	0.52	0/4666
2	1Y	0.33	0/3443	0.52	0/4666
2	1Z	0.33	0/3443	0.52	0/4666
2	2H	0.33	0/3443	0.52	0/4666
2	2O	0.33	0/3443	0.52	0/4666
2	2P	0.33	0/3443	0.52	0/4666
2	2Q	0.33	0/3443	0.52	0/4666
2	2R	0.33	0/3443	0.52	0/4666
2	2S	0.33	0/3443	0.52	0/4666
2	2T	0.34	0/3443	0.52	0/4666
2	2U	0.34	0/3443	0.52	0/4666
2	2V	0.34	0/3443	0.52	0/4666
2	2W	0.34	0/3443	0.52	0/4666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	2X	0.33	0/3443	0.52	0/4666
2	2Y	0.34	0/3443	0.52	0/4666
2	2Z	0.33	0/3443	0.52	0/4666
2	3H	0.34	0/3443	0.52	0/4666
2	3O	0.33	0/3443	0.52	0/4666
2	3P	0.33	0/3443	0.52	0/4666
2	3Q	0.33	0/3443	0.52	0/4666
2	3R	0.33	0/3443	0.52	0/4666
2	3S	0.33	0/3443	0.52	0/4666
2	3T	0.33	0/3443	0.52	0/4666
2	3U	0.33	0/3443	0.52	0/4666
2	3V	0.33	0/3443	0.52	0/4666
2	3W	0.33	0/3443	0.52	0/4666
2	3X	0.33	0/3443	0.52	0/4666
2	3Y	0.33	0/3443	0.52	0/4666
2	3Z	0.33	0/3443	0.52	0/4666
2	4H	0.34	0/3443	0.52	0/4666
2	4O	0.34	0/3443	0.52	0/4666
2	4P	0.34	0/3443	0.52	0/4666
2	4Q	0.33	0/3443	0.52	0/4666
2	4R	0.33	0/3443	0.52	0/4666
2	4S	0.33	0/3443	0.52	0/4666
2	4T	0.33	0/3443	0.52	0/4666
2	4U	0.33	0/3443	0.52	0/4666
2	4V	0.33	0/3443	0.52	0/4666
2	4W	0.33	0/3443	0.52	0/4666
2	4X	0.34	0/3443	0.52	0/4666
2	4Y	0.33	0/3443	0.52	0/4666
2	4Z	0.33	0/3443	0.52	0/4666
All	All	0.33	0/359632	0.51	0/487864

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

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	1A	3396	0	3301	252	0
1	1B	3396	0	3301	306	0
1	1C	3396	0	3301	350	0
1	1D	3396	0	3301	372	0
1	1E	3396	0	3301	387	0
1	1F	3396	0	3301	371	0
1	1G	3396	0	3301	341	0
1	1I	3396	0	3301	308	0
1	1J	3396	0	3301	260	0
1	1K	3396	0	3301	230	0
1	1L	3396	0	3301	214	0
1	1M	3396	0	3301	224	0
1	1N	3396	0	3301	223	0
1	2A	3396	0	3301	111	0
1	2B	3396	0	3301	98	0
1	2C	3396	0	3301	97	0
1	2D	3396	0	3301	110	0
1	2E	3396	0	3301	121	0
1	2F	3396	0	3301	145	0
1	2G	3396	0	3301	158	0
1	2I	3396	0	3301	180	0
1	2J	3396	0	3301	197	0
1	2K	3396	0	3300	199	0
1	2L	3396	0	3300	188	0
1	2M	3396	0	3300	179	0
1	2N	3396	0	3301	146	0
1	3A	3396	0	3301	204	0
1	3B	3396	0	3301	206	0
1	3C	3396	0	3301	207	0
1	3D	3396	0	3301	219	0
1	3E	3396	0	3301	224	0
1	3F	3396	0	3301	238	0
1	3G	3396	0	3301	233	0
1	3I	3396	0	3301	232	0
1	3J	3396	0	3301	226	0
1	3K	3396	0	3301	225	0
1	3L	3396	0	3301	212	0
1	3M	3396	0	3301	202	0
1	3N	3396	0	3301	197	0
1	4A	3396	0	3301	51	0
1	4B	3396	0	3301	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4C	3396	0	3301	53	0
1	4D	3396	0	3301	53	0
1	4E	3396	0	3301	52	0
1	4F	3396	0	3301	51	0
1	4G	3396	0	3301	52	0
1	4I	3396	0	3301	53	0
1	4J	3396	0	3301	53	0
1	4K	3396	0	3301	54	0
1	4L	3396	0	3301	52	0
1	4M	3396	0	3301	46	0
1	4N	3396	0	3301	45	0
2	1H	3368	0	3246	112	0
2	1O	3368	0	3246	96	0
2	1P	3368	0	3246	94	0
2	1Q	3368	0	3246	107	0
2	1R	3368	0	3246	122	0
2	1S	3368	0	3246	148	0
2	1T	3368	0	3246	157	0
2	1U	3368	0	3246	179	0
2	1V	3368	0	3246	196	0
2	1W	3368	0	3245	199	0
2	1X	3368	0	3245	189	0
2	1Y	3368	0	3245	181	0
2	1Z	3368	0	3246	148	0
2	2H	3368	0	3246	204	0
2	2O	3368	0	3245	201	0
2	2P	3368	0	3245	203	0
2	2Q	3368	0	3245	214	0
2	2R	3368	0	3245	222	0
2	2S	3368	0	3245	238	0
2	2T	3368	0	3245	231	0
2	2U	3368	0	3245	229	0
2	2V	3368	0	3245	225	0
2	2W	3368	0	3245	223	0
2	2X	3368	0	3245	214	0
2	2Y	3368	0	3246	207	0
2	2Z	3368	0	3246	198	0
2	3H	3368	0	3246	51	0
2	3O	3368	0	3246	50	0
2	3P	3368	0	3246	51	0
2	3Q	3368	0	3246	50	0
2	3R	3368	0	3246	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3S	3368	0	3246	54	0
2	3T	3368	0	3246	50	0
2	3U	3368	0	3246	52	0
2	3V	3368	0	3246	53	0
2	3W	3368	0	3246	53	0
2	3X	3368	0	3246	52	0
2	3Y	3368	0	3246	50	0
2	3Z	3368	0	3246	49	0
2	4H	3368	0	3243	250	0
2	4O	3368	0	3243	299	0
2	4P	3368	0	3243	343	0
2	4Q	3368	0	3243	367	0
2	4R	3368	0	3243	382	0
2	4S	3368	0	3243	370	0
2	4T	3368	0	3245	339	0
2	4U	3368	0	3246	307	0
2	4V	3368	0	3246	259	0
2	4W	3368	0	3246	227	0
2	4X	3368	0	3246	217	0
2	4Y	3368	0	3246	226	0
2	4Z	3368	0	3244	220	0
3	1A	32	0	12	2	0
3	1B	32	0	12	2	0
3	1C	32	0	12	2	0
3	1D	32	0	12	2	0
3	1E	32	0	12	2	0
3	1F	32	0	12	1	0
3	1G	32	0	12	2	0
3	1I	32	0	12	2	0
3	1J	32	0	12	2	0
3	1K	32	0	12	2	0
3	1L	32	0	12	2	0
3	1M	32	0	12	2	0
3	1N	32	0	12	1	0
3	2A	32	0	12	2	0
3	2B	32	0	12	2	0
3	2C	32	0	12	2	0
3	2D	32	0	12	2	0
3	2E	32	0	12	2	0
3	2F	32	0	12	2	0
3	2G	32	0	12	2	0
3	2I	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2J	32	0	12	2	0
3	2K	32	0	12	2	0
3	2L	32	0	12	2	0
3	2M	32	0	12	2	0
3	2N	32	0	12	1	0
3	3A	32	0	12	2	0
3	3B	32	0	12	2	0
3	3C	32	0	12	2	0
3	3D	32	0	12	2	0
3	3E	32	0	12	2	0
3	3F	32	0	12	1	0
3	3G	32	0	12	2	0
3	3I	32	0	12	2	0
3	3J	32	0	12	2	0
3	3K	32	0	12	2	0
3	3L	32	0	12	2	0
3	3M	32	0	12	2	0
3	3N	32	0	12	1	0
3	4A	32	0	12	2	0
3	4B	32	0	12	2	0
3	4C	32	0	12	2	0
3	4D	32	0	12	2	0
3	4E	32	0	12	2	0
3	4F	32	0	12	2	0
3	4G	32	0	12	2	0
3	4I	32	0	12	2	0
3	4J	32	0	12	2	0
3	4K	32	0	12	2	0
3	4L	32	0	12	2	0
3	4M	32	0	12	2	0
3	4N	32	0	12	1	0
4	1A	1	0	0	0	0
4	1B	1	0	0	0	0
4	1C	1	0	0	0	0
4	1D	1	0	0	0	0
4	1E	1	0	0	0	0
4	1F	1	0	0	0	0
4	1G	1	0	0	0	0
4	1I	1	0	0	0	0
4	1J	1	0	0	0	0
4	1K	1	0	0	0	0
4	1L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1M	1	0	0	0	0
4	1N	1	0	0	0	0
4	2A	1	0	0	0	0
4	2B	1	0	0	0	0
4	2C	1	0	0	0	0
4	2D	1	0	0	0	0
4	2E	1	0	0	0	0
4	2F	1	0	0	0	0
4	2G	1	0	0	0	0
4	2I	1	0	0	0	0
4	2J	1	0	0	0	0
4	2K	1	0	0	0	0
4	2L	1	0	0	0	0
4	2M	1	0	0	0	0
4	2N	1	0	0	0	0
4	3A	1	0	0	0	0
4	3B	1	0	0	0	0
4	3C	1	0	0	0	0
4	3D	1	0	0	0	0
4	3E	1	0	0	0	0
4	3F	1	0	0	0	0
4	3G	1	0	0	0	0
4	3I	1	0	0	0	0
4	3J	1	0	0	0	0
4	3K	1	0	0	0	0
4	3L	1	0	0	0	0
4	3M	1	0	0	0	0
4	3N	1	0	0	0	0
4	4A	1	0	0	0	0
4	4B	1	0	0	0	0
4	4C	1	0	0	0	0
4	4D	1	0	0	0	0
4	4E	1	0	0	0	0
4	4F	1	0	0	0	0
4	4G	1	0	0	0	0
4	4I	1	0	0	0	0
4	4J	1	0	0	0	0
4	4K	1	0	0	0	0
4	4L	1	0	0	0	0
4	4M	1	0	0	0	0
4	4N	1	0	0	0	0
5	1H	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1O	28	0	12	2	0
5	1P	28	0	12	2	0
5	1Q	28	0	12	2	0
5	1R	28	0	12	2	0
5	1S	28	0	12	2	0
5	1T	28	0	12	2	0
5	1U	28	0	12	2	0
5	1V	28	0	12	2	0
5	1W	28	0	12	2	0
5	1X	28	0	12	3	0
5	1Y	28	0	12	3	0
5	1Z	28	0	12	2	0
5	2H	28	0	12	3	0
5	2O	28	0	12	4	0
5	2P	28	0	12	5	0
5	2Q	28	0	12	5	0
5	2R	28	0	12	6	0
5	2S	28	0	12	6	0
5	2T	28	0	12	5	0
5	2U	28	0	12	5	0
5	2V	28	0	12	4	0
5	2W	28	0	12	4	0
5	2X	28	0	12	4	0
5	2Y	28	0	12	3	0
5	2Z	28	0	12	3	0
5	3H	28	0	12	2	0
5	3O	28	0	12	2	0
5	3P	28	0	12	2	0
5	3Q	28	0	12	2	0
5	3R	28	0	12	2	0
5	3S	28	0	12	2	0
5	3T	28	0	12	2	0
5	3U	28	0	12	2	0
5	3V	28	0	12	2	0
5	3W	28	0	12	2	0
5	3X	28	0	12	2	0
5	3Y	28	0	12	2	0
5	3Z	28	0	12	2	0
5	4H	28	0	12	5	0
5	4O	28	0	12	6	0
5	4P	28	0	12	7	0
5	4Q	28	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4R	28	0	12	6	0
5	4S	28	0	12	6	0
5	4T	28	0	12	6	0
5	4U	28	0	12	4	0
5	4V	28	0	12	4	0
5	4W	28	0	12	4	0
5	4X	28	0	12	4	0
5	4Y	28	0	12	4	0
5	4Z	28	0	12	4	0
All	All	354900	0	341655	11466	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 16.

The worst 5 of 11466 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)
2:2W:406:HIS:CD2	1:3K:263:PRO:HD3	1.46	1.50
1:1G:262:TYR:HA	2:4T:406:HIS:CD2	1.47	1.49
2:2U:406:HIS:CD2	1:3I:263:PRO:HD3	1.47	1.49
2:2V:406:HIS:CD2	1:3J:263:PRO:HD3	1.45	1.49
1:1I:262:TYR:HA	2:4U:406:HIS:CD2	1.49	1.47

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1B	430/451 (95%)	413 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1C	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1D	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1E	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1F	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1G	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1I	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1J	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1K	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1L	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1M	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	1N	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2A	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2B	430/451 (95%)	414 (96%)	16 (4%)	0	100	100
1	2C	430/451 (95%)	414 (96%)	16 (4%)	0	100	100
1	2D	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2E	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2F	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2G	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2I	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2J	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2K	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2L	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2M	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	2N	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3A	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3B	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3C	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3D	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3E	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3F	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3G	430/451 (95%)	413 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3I	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3J	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3K	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3L	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3M	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	3N	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4A	430/451 (95%)	414 (96%)	16 (4%)	0	100	100
1	4B	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4C	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4D	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4E	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4F	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4G	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4I	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4J	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4K	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4L	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4M	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
1	4N	430/451 (95%)	413 (96%)	17 (4%)	0	100	100
2	1H	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1O	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1P	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1Q	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1R	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1S	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1T	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1U	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1V	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1W	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1X	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	1Y	427/445 (96%)	409 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1Z	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2H	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2O	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2P	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2Q	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2R	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2S	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2T	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2U	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2V	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2W	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2X	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2Y	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	2Z	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3H	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3O	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3P	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3Q	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3R	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3S	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3T	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3U	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3V	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3W	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3X	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3Y	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	3Z	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4H	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4O	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4P	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4Q	427/445 (96%)	409 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4R	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4S	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4T	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4U	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4V	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4W	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4X	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4Y	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
2	4Z	427/445 (96%)	409 (96%)	18 (4%)	0	100	100
All	All	44564/46592 (96%)	42747 (96%)	1817 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1B	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1C	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1D	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1E	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1F	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1G	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1I	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1J	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1K	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1L	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	1M	366/379 (97%)	365 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1N	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2A	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2B	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2C	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2D	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2E	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2F	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2G	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2I	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2J	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2K	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2L	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2M	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	2N	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3A	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3B	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3C	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3D	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3E	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3F	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3G	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3I	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3J	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3K	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3L	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3M	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	3N	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4A	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4B	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4C	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4D	366/379 (97%)	365 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4E	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4F	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4G	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4I	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4J	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4K	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4L	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4M	366/379 (97%)	365 (100%)	1 (0%)	93	96
1	4N	366/379 (97%)	365 (100%)	1 (0%)	93	96
2	1H	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1O	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1P	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1Q	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1R	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1S	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1T	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1U	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1V	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1W	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1X	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1Y	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	1Z	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2H	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2O	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2P	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2Q	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2R	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2S	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2T	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2U	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2V	368/381 (97%)	367 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2W	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2X	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2Y	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	2Z	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3H	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3O	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3P	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3Q	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3R	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3S	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3T	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3U	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3V	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3W	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3X	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3Y	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	3Z	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4H	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4O	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4P	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4Q	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4R	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4S	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4T	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4U	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4V	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4W	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4X	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4Y	368/381 (97%)	367 (100%)	1 (0%)	93	96
2	4Z	368/381 (97%)	367 (100%)	1 (0%)	93	96
All	All	38168/39520 (97%)	38064 (100%)	104 (0%)	93	96

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2V	300	ASN
1	3G	339	ARG
2	4S	300	ASN
2	2W	300	ASN
1	3A	339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 794 such sidechains are listed below:

Mol	Chain	Res	Type
2	2U	101	ASN
1	3F	8	HIS
2	4T	206	ASN
2	2V	101	ASN
2	2Z	8	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 156 ligands modelled in this entry, 52 are monoatomic - leaving 104 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	1A	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	1B	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1C	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1D	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1E	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1F	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1G	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
5	GDP	1H	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
3	GTP	1I	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1J	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1K	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	1L	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1M	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	1N	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
5	GDP	1O	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	1P	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	1Q	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	1R	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	1S	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.11	7 (25%)
5	GDP	1T	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	1U	501	-	24,30,30	1.13	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	1V	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.11	7 (25%)
5	GDP	1W	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	1X	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	1Y	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	1Z	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.09	7 (25%)
3	GTP	2A	501	4	26,34,34	0.93	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2B	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	2C	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2D	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2E	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2F	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2G	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.89	6 (20%)
5	GDP	2H	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
3	GTP	2I	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.89	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	2J	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2K	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2L	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	2M	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	2N	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
5	GDP	2O	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	2P	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	2Q	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2R	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2S	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	2T	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	2U	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2V	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	2W	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2X	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2Y	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	2Z	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
3	GTP	3A	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3B	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3C	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3D	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3E	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3F	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3G	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.89	6 (20%)
5	GDP	3H	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
3	GTP	3I	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3J	501	4	26,34,34	0.93	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3K	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3L	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3M	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	3N	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
5	GDP	3O	501	-	24,30,30	1.13	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3P	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3Q	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3R	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GDP	3S	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3T	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3U	501	-	24,30,30	1.13	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3V	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3W	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3X	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	3Y	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	3Z	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
3	GTP	4A	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	4B	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.89	6 (20%)
3	GTP	4C	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	4D	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.89	6 (20%)
3	GTP	4E	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.89	6 (20%)
3	GTP	4F	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	4G	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
5	GDP	4H	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.11	7 (25%)
3	GTP	4I	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	4J	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	4K	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	4L	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.90	6 (20%)
3	GTP	4M	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	4N	501	4	26,34,34	0.94	1 (3%)	29,54,54	1.89	6 (20%)
5	GDP	4O	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4P	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4Q	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4R	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	4S	501	-	24,30,30	1.11	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4T	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4U	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4V	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4W	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	4X	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)
5	GDP	4Y	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.09	7 (25%)
5	GDP	4Z	501	-	24,30,30	1.12	2 (8%)	27,47,47	2.10	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	1A	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1B	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1C	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1D	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1E	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1F	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	1H	501	-	-	0/12/32/32	0/3/3/3
3	GTP	1I	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1L	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1M	501	4	-	0/18/38/38	0/3/3/3
3	GTP	1N	501	4	-	0/18/38/38	0/3/3/3
5	GDP	1O	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1P	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1Q	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1R	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1S	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1T	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1U	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1V	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1W	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1X	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1Y	501	-	-	0/12/32/32	0/3/3/3
5	GDP	1Z	501	-	-	0/12/32/32	0/3/3/3
3	GTP	2A	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2B	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2C	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2D	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2E	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2F	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	2H	501	-	-	0/12/32/32	0/3/3/3
3	GTP	2I	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2L	501	4	-	0/18/38/38	0/3/3/3
3	GTP	2M	501	4	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	2N	501	4	-	0/18/38/38	0/3/3/3
5	GDP	2O	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2P	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2Q	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2R	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2S	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2T	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2U	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2V	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2W	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2X	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2Y	501	-	-	0/12/32/32	0/3/3/3
5	GDP	2Z	501	-	-	0/12/32/32	0/3/3/3
3	GTP	3A	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3B	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3C	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3D	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3E	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3F	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	3H	501	-	-	0/12/32/32	0/3/3/3
3	GTP	3I	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3L	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3M	501	4	-	0/18/38/38	0/3/3/3
3	GTP	3N	501	4	-	0/18/38/38	0/3/3/3
5	GDP	3O	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3P	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3Q	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3R	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3S	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3T	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3U	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3V	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3W	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3X	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3Y	501	-	-	0/12/32/32	0/3/3/3
5	GDP	3Z	501	-	-	0/12/32/32	0/3/3/3
3	GTP	4A	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4B	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4C	501	4	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	4D	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4E	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4F	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	4H	501	-	-	0/12/32/32	0/3/3/3
3	GTP	4I	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4L	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4M	501	4	-	0/18/38/38	0/3/3/3
3	GTP	4N	501	4	-	0/18/38/38	0/3/3/3
5	GDP	4O	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4P	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4Q	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4R	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4S	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4T	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4U	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4V	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4W	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4X	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4Y	501	-	-	0/12/32/32	0/3/3/3
5	GDP	4Z	501	-	-	0/12/32/32	0/3/3/3

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4C	501	GTP	C6-N1	2.60	1.37	1.33
3	1A	501	GTP	C6-N1	2.61	1.37	1.33
3	2A	501	GTP	C6-N1	2.63	1.37	1.33
3	1C	501	GTP	C6-N1	2.64	1.37	1.33
3	1B	501	GTP	C6-N1	2.64	1.37	1.33

The worst 5 of 676 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4J	501	GTP	N3-C2-N1	-5.11	120.34	127.25
3	1A	501	GTP	N3-C2-N1	-5.10	120.35	127.25
3	2J	501	GTP	N3-C2-N1	-5.10	120.36	127.25
3	2L	501	GTP	N3-C2-N1	-5.10	120.36	127.25
3	4C	501	GTP	N3-C2-N1	-5.09	120.36	127.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

104 monomers are involved in 275 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1A	501	GTP	2	0
3	1B	501	GTP	2	0
3	1C	501	GTP	2	0
3	1D	501	GTP	2	0
3	1E	501	GTP	2	0
3	1F	501	GTP	1	0
3	1G	501	GTP	2	0
5	1H	501	GDP	2	0
3	1I	501	GTP	2	0
3	1J	501	GTP	2	0
3	1K	501	GTP	2	0
3	1L	501	GTP	2	0
3	1M	501	GTP	2	0
3	1N	501	GTP	1	0
5	1O	501	GDP	2	0
5	1P	501	GDP	2	0
5	1Q	501	GDP	2	0
5	1R	501	GDP	2	0
5	1S	501	GDP	2	0
5	1T	501	GDP	2	0
5	1U	501	GDP	2	0
5	1V	501	GDP	2	0
5	1W	501	GDP	2	0
5	1X	501	GDP	3	0
5	1Y	501	GDP	3	0
5	1Z	501	GDP	2	0
3	2A	501	GTP	2	0
3	2B	501	GTP	2	0
3	2C	501	GTP	2	0
3	2D	501	GTP	2	0
3	2E	501	GTP	2	0
3	2F	501	GTP	2	0
3	2G	501	GTP	2	0
5	2H	501	GDP	3	0
3	2I	501	GTP	2	0
3	2J	501	GTP	2	0
3	2K	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2L	501	GTP	2	0
3	2M	501	GTP	2	0
3	2N	501	GTP	1	0
5	2O	501	GDP	4	0
5	2P	501	GDP	5	0
5	2Q	501	GDP	5	0
5	2R	501	GDP	6	0
5	2S	501	GDP	6	0
5	2T	501	GDP	5	0
5	2U	501	GDP	5	0
5	2V	501	GDP	4	0
5	2W	501	GDP	4	0
5	2X	501	GDP	4	0
5	2Y	501	GDP	3	0
5	2Z	501	GDP	3	0
3	3A	501	GTP	2	0
3	3B	501	GTP	2	0
3	3C	501	GTP	2	0
3	3D	501	GTP	2	0
3	3E	501	GTP	2	0
3	3F	501	GTP	1	0
3	3G	501	GTP	2	0
5	3H	501	GDP	2	0
3	3I	501	GTP	2	0
3	3J	501	GTP	2	0
3	3K	501	GTP	2	0
3	3L	501	GTP	2	0
3	3M	501	GTP	2	0
3	3N	501	GTP	1	0
5	3O	501	GDP	2	0
5	3P	501	GDP	2	0
5	3Q	501	GDP	2	0
5	3R	501	GDP	2	0
5	3S	501	GDP	2	0
5	3T	501	GDP	2	0
5	3U	501	GDP	2	0
5	3V	501	GDP	2	0
5	3W	501	GDP	2	0
5	3X	501	GDP	2	0
5	3Y	501	GDP	2	0
5	3Z	501	GDP	2	0
3	4A	501	GTP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4B	501	GTP	2	0
3	4C	501	GTP	2	0
3	4D	501	GTP	2	0
3	4E	501	GTP	2	0
3	4F	501	GTP	2	0
3	4G	501	GTP	2	0
5	4H	501	GDP	5	0
3	4I	501	GTP	2	0
3	4J	501	GTP	2	0
3	4K	501	GTP	2	0
3	4L	501	GTP	2	0
3	4M	501	GTP	2	0
3	4N	501	GTP	1	0
5	4O	501	GDP	6	0
5	4P	501	GDP	7	0
5	4Q	501	GDP	6	0
5	4R	501	GDP	6	0
5	4S	501	GDP	6	0
5	4T	501	GDP	6	0
5	4U	501	GDP	4	0
5	4V	501	GDP	4	0
5	4W	501	GDP	4	0
5	4X	501	GDP	4	0
5	4Y	501	GDP	4	0
5	4Z	501	GDP	4	0

## 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.