Full wwPDB EM Validation Report ⓘ

Jul 20, 2024 – 10:20 am BST

PDB ID	:	8QV2
EMDB ID	:	EMD-18665
Title	:	Structure of the native y-Tubulin Ring Complex (yTuRC) capping microtubule minus ends at the spindle pole body
Authors	:	Dendooven, T.; Yatskevich, S.; Burt, A.; Bellini, D.; Kilmartin, J.; Barford, D.
Deposited on	:	2023-10-17
Resolution	:	9.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

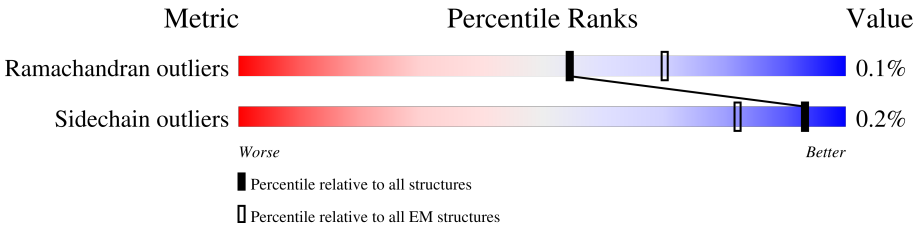
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	473	15% 93% 7%
1	b	473	96%
1	c	473	93% 7%
1	d	473	96%
1	e	473	93% 7%
1	f	473	96%
1	g	473	93% 7%
1	h	473	96%
1	i	473	93% 7%

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Mol	Chain	Length	Quality of chain
1	j	473	96%
1	k	473	93% 7%
1	l	473	96%
1	m	473	93% 7%
1	n	473	96%
2	C	823	5% 84% 16%
2	E	823	85% 15%
2	G	823	85% 15%
2	I	823	85% 15%
2	K	823	85% 15%
2	M	823	85% 15%
2	O	823	85% 15%
3	D	846	76% 23%
3	F	846	79% 21%
3	H	846	79% 21%
3	J	846	79% 21%
3	L	846	79% 21%
3	N	846	79% 21%
3	P	846	6% 79% 21%
4	Ab	447	94% 5%
4	Ac	447	97%
4	Ad	447	97%
4	Ae	447	97%
4	Af	447	97%
4	Ag	447	98%

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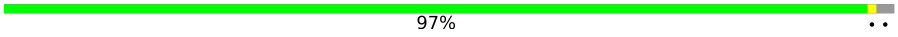
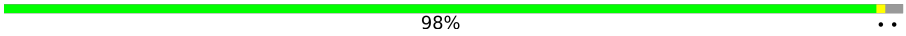
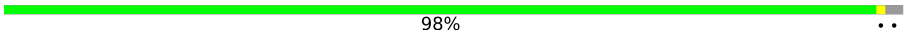
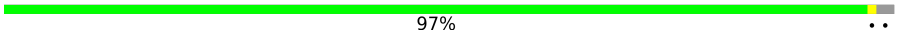
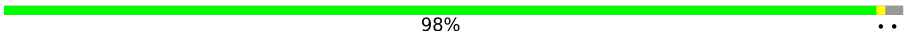
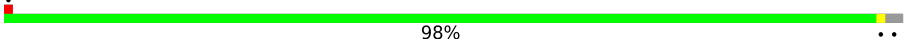
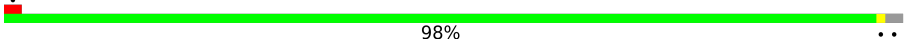
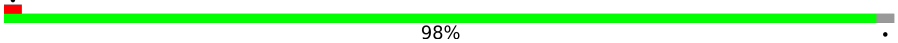
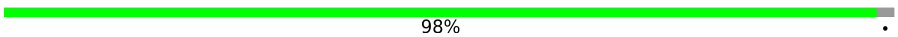
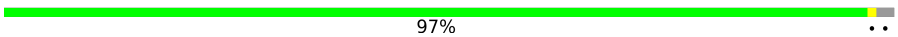
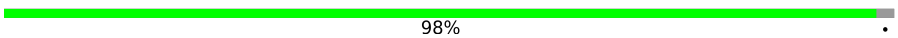
Mol	Chain	Length	Quality of chain
4	Ah	447	
4	Ai	447	
4	Aj	447	
4	Ak	447	
4	Al	447	
4	Am	447	
4	An	447	
4	Ao	447	
4	Ap	447	
4	Aq	447	
4	Ar	447	
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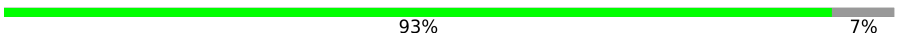
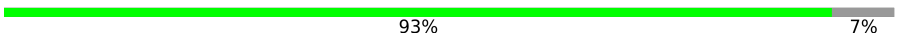
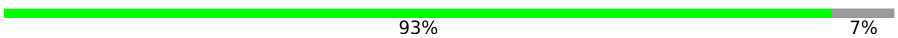
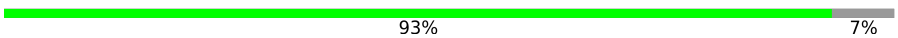
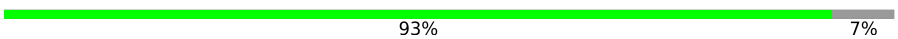
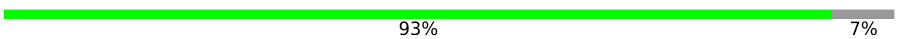
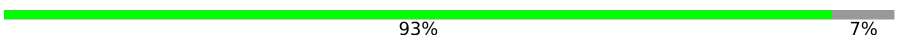
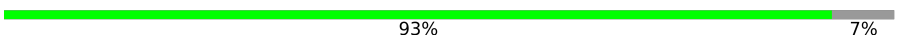
5	Bc	457	
5	Bd	457	
5	Be	457	
5	Bf	457	
5	Bg	457	
5	Bh	457	
5	Bi	457	
5	Bj	457	
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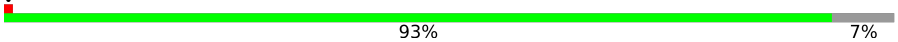
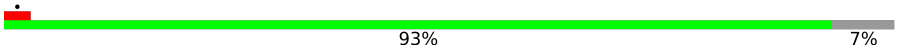
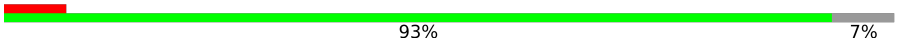
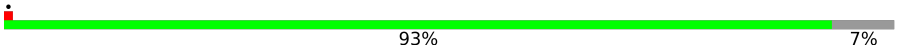
5	Bl	457	
5	Bm	457	
5	Bn	457	
5	Bo	457	

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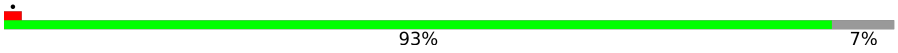
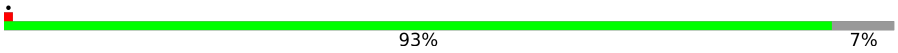
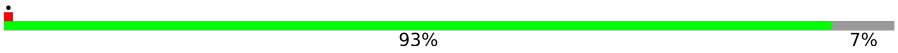
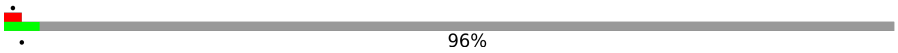
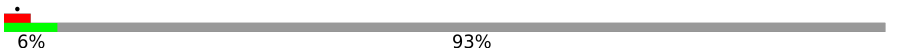
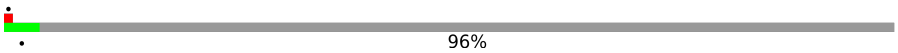
Mol	Chain	Length	Quality of chain
5	Bp	457	
5	Bq	457	
5	Br	457	
6	Sa	944	
6	Sb	944	
6	Sc	944	
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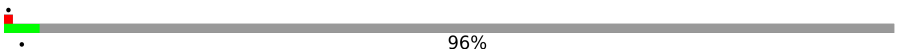
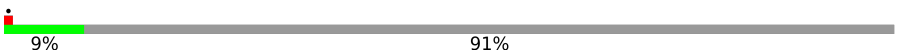
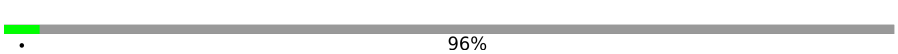
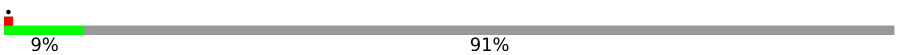
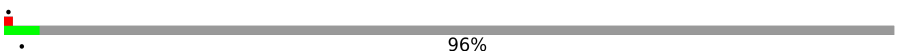
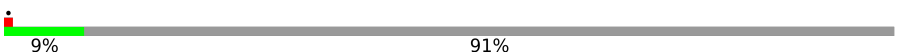
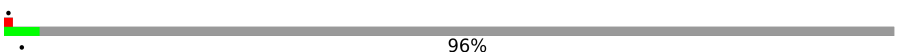
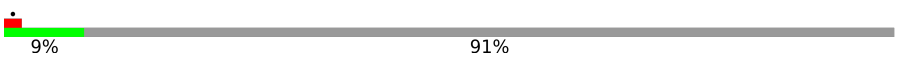
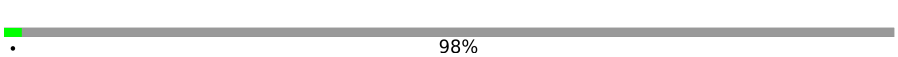
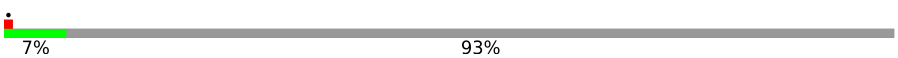
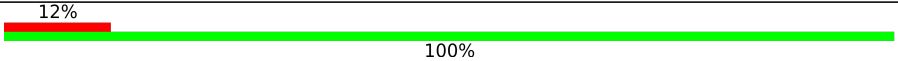
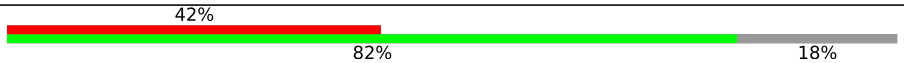
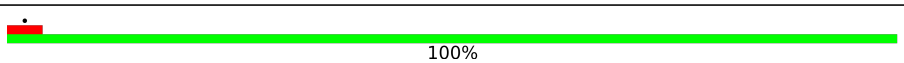
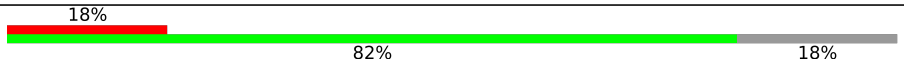
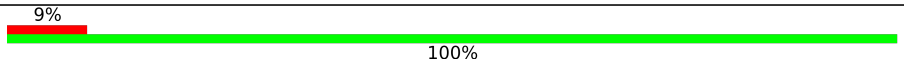
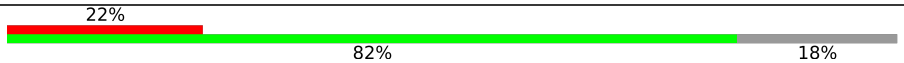
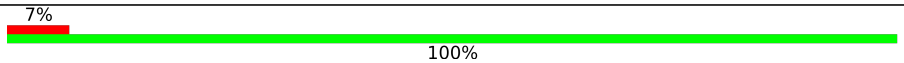
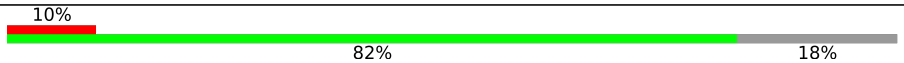
6	Se	944	
6	Sf	944	
6	Sg	944	
6	Sh	944	
6	Si	944	
6	Sj	944	
6	Sk	944	
6	Sl	944	
6	Sm	944	
6	Sn	944	
7	Ua	67	
7	Ub	67	
7	Uc	67	
7	Ud	67	
7	Ue	67	
7	Uf	67	
7	Ug	67	
7	Uh	67	

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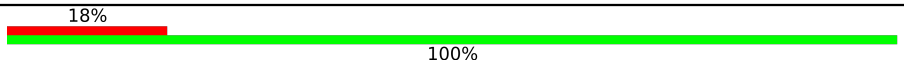
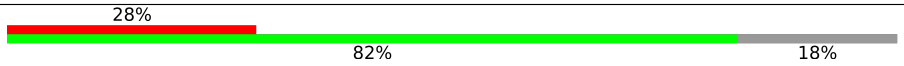
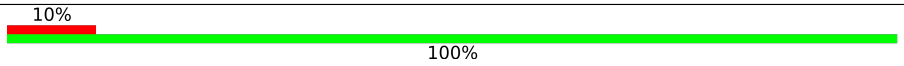
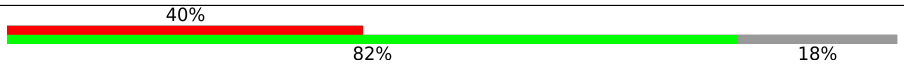
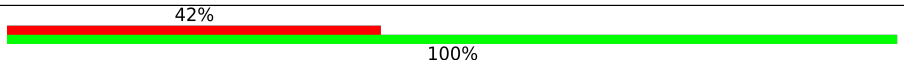
Mol	Chain	Length	Quality of chain
7	Ui	67	
7	Uj	67	
7	Uk	67	
7	Ul	67	
7	Um	67	
7	Un	67	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 255200 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 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	c	441	Total 3448	C 2158	N 585	O 689	S 16	0	0
1	d	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	e	439	Total 3433	C 2149	N 581	O 687	S 16	0	0
1	f	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	g	441	Total 3448	C 2158	N 585	O 689	S 16	0	0
1	h	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	i	439	Total 3433	C 2149	N 581	O 687	S 16	0	0
1	j	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	k	441	Total 3448	C 2158	N 585	O 689	S 16	0	0
1	l	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	m	439	Total 3433	C 2149	N 581	O 687	S 16	0	0
1	n	453	Total 3545	C 2217	N 599	O 712	S 17	0	0
1	a	440	Total 3441	C 2153	N 584	O 688	S 16	0	0

- Molecule 2 is a protein called Spindle pole body component.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	693	Total 5778	C 3716	N 974	O 1059	S 29	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		
2	G	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		
2	I	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		
2	K	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		
2	M	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		
2	O	701	Total	C	N	O	S	0	0
			5847	3760	985	1073	29		

- Molecule 3 is a protein called Spindle pole body component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	651	Total	C	N	O	S	0	0
			5390	3494	886	994	16		
3	F	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		
3	H	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		
3	J	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		
3	L	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		
3	N	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		
3	P	672	Total	C	N	O	S	0	0
			5557	3595	918	1028	16		

- Molecule 4 is a protein called Tubulin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	440	Total	C	N	O	S	0	0
			3438	2167	585	667	19		
4	Ac	440	Total	C	N	O	S	0	0
			3438	2167	585	667	19		
4	Af	440	Total	C	N	O	S	0	0
			3438	2167	585	667	19		
4	Ae	440	Total	C	N	O	S	0	0
			3438	2167	585	667	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ah	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ag	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Aj	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ai	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Al	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ak	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	An	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Am	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ab	423	Total 3312	C 2089	N 563	O 641	S 19	0	0
4	Ap	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ao	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Ar	440	Total 3438	C 2167	N 585	O 667	S 19	0	0
4	Aq	440	Total 3438	C 2167	N 585	O 667	S 19	0	0

- Molecule 5 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Bd	427	Total 3343	C 2098	N 571	O 653	S 21	0	0
5	Bc	427	Total 3343	C 2098	N 571	O 653	S 21	0	0
5	Bf	427	Total 3343	C 2098	N 571	O 653	S 21	0	0
5	Be	427	Total 3343	C 2098	N 571	O 653	S 21	0	0
5	Bh	427	Total 3343	C 2098	N 571	O 653	S 21	0	0
5	Bg	427	Total 3343	C 2098	N 571	O 653	S 21	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
5	Bj	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bi	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bl	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bk	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bn	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bm	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bb	414	Total C N O S 3247 2038 554 634 21	0	0
5	Bp	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bo	427	Total C N O S 3343 2098 571 653 21	0	0
5	Br	427	Total C N O S 3343 2098 571 653 21	0	0
5	Bq	427	Total C N O S 3343 2098 571 653 21	0	0

- Molecule 6 is a protein called Spindle pole body component 110.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	Sc	42	Total C N O 352 215 61 76	0	0
6	Sd	85	Total C N O S 714 439 130 144 1	0	0
6	Se	42	Total C N O 352 215 61 76	0	0
6	Sf	86	Total C N O S 723 444 131 147 1	0	0
6	Sg	42	Total C N O 352 215 61 76	0	0
6	Sh	85	Total C N O S 714 439 130 144 1	0	0
6	Si	42	Total C N O 352 215 61 76	0	0
6	Sj	86	Total C N O S 723 444 131 147 1	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
6	Sk	42	Total C N O 352 215 61 76	0	0
6	Sl	85	Total C N O S 714 439 130 144 1	0	0
6	Sa	42	Total C N O 352 215 61 76	0	0
6	Sb	62	Total C N O 517 318 91 108	0	0
6	Sm	20	Total C N O 171 107 31 33	0	0
6	Sn	64	Total C N O S 545 337 102 105 1	0	0

- Molecule 7 is a protein called Unkown protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	Ue	67	Total C N O 335 201 67 67	0	0
7	Uf	55	Total C N O 275 165 55 55	0	0
7	Ui	67	Total C N O 335 201 67 67	0	0
7	Uj	55	Total C N O 275 165 55 55	0	0
7	Um	67	Total C N O 335 201 67 67	0	0
7	Un	55	Total C N O 275 165 55 55	0	0
7	Ua	67	Total C N O 335 201 67 67	0	0
7	Ub	55	Total C N O 275 165 55 55	0	0
7	Ug	67	Total C N O 335 201 67 67	0	0
7	Uh	55	Total C N O 275 165 55 55	0	0
7	Uk	67	Total C N O 335 201 67 67	0	0
7	Ul	55	Total C N O 275 165 55 55	0	0
7	Uc	67	Total C N O 335 201 67 67	0	0

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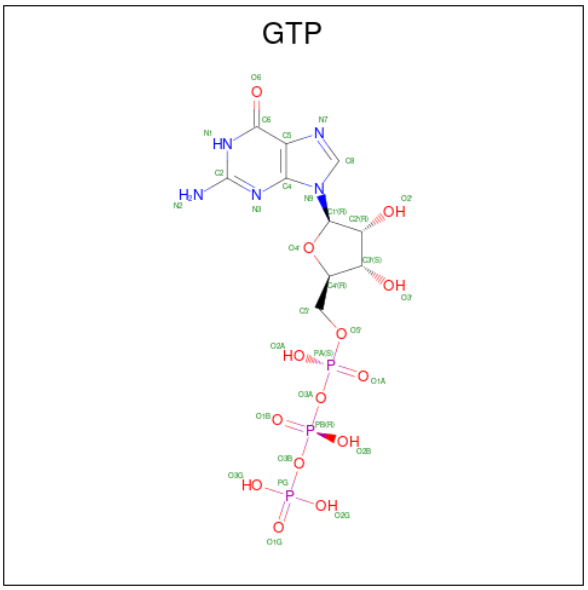
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Ud	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
8	b	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	c	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	d	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	e	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	f	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	g	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	h	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	i	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	j	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	k	1	Total	C	N	O	P	0
			32	10	5	14	3	

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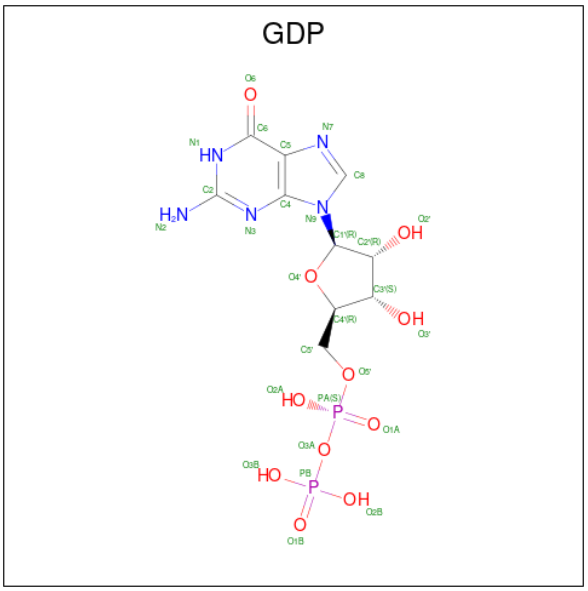
Mol	Chain	Residues	Atoms					AltConf
8	l	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	m	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	n	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	Ue	1	Total	O	0
			1	1	
10	Ui	1	Total	O	0
			1	1	
10	Um	1	Total	O	0
			1	1	
10	Ua	1	Total	O	0
			1	1	
10	Ug	1	Total	O	0
			1	1	

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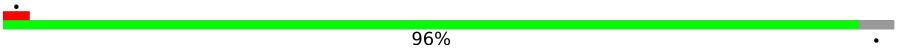
Mol	Chain	Residues	Atoms	AltConf
10	Uk	1	Total O 1 1	0
10	Uc	1	Total O 1 1	0

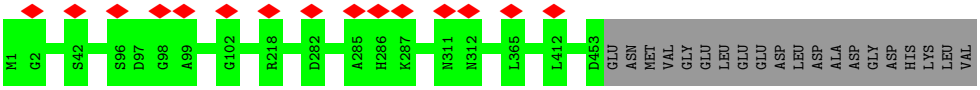
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin gamma chain

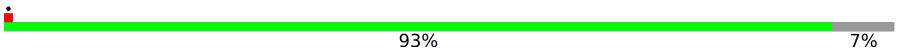
Chain b:

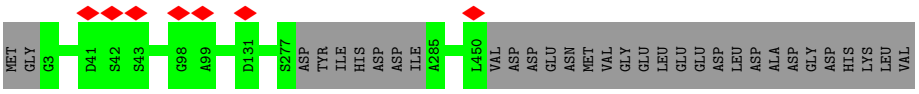




• Molecule 1: Tubulin gamma chain

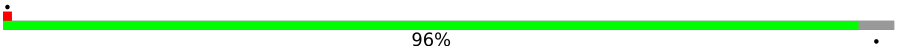
Chain c:

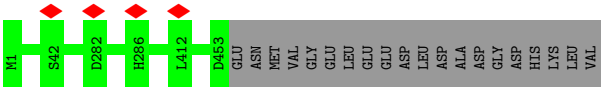




• Molecule 1: Tubulin gamma chain

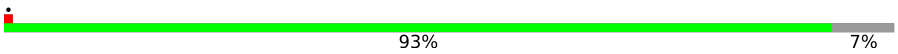
Chain d:

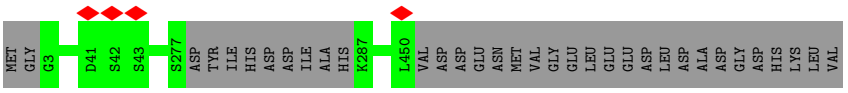




• Molecule 1: Tubulin gamma chain

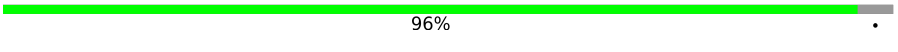
Chain e:

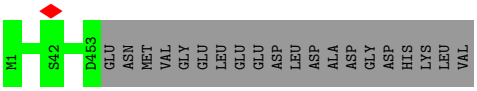




• Molecule 1: Tubulin gamma chain

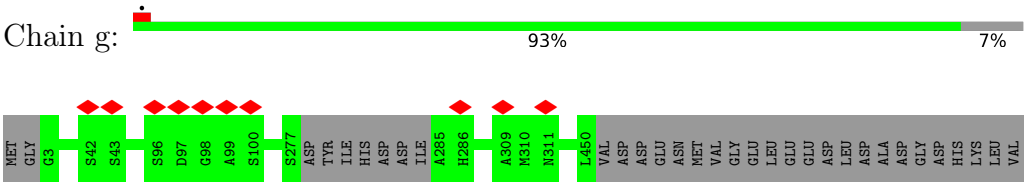
Chain f:





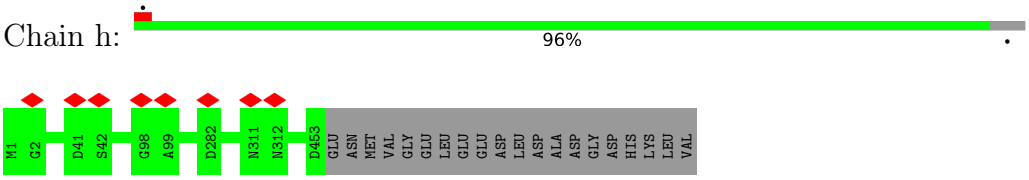
• Molecule 1: Tubulin gamma chain

Chain g:



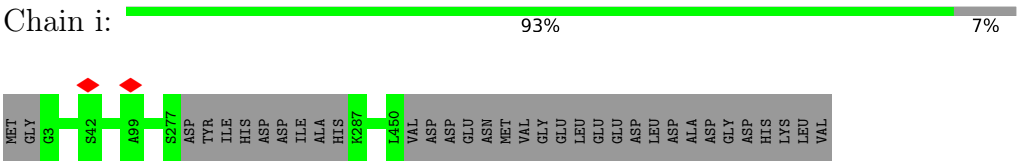
• Molecule 1: Tubulin gamma chain

Chain h:



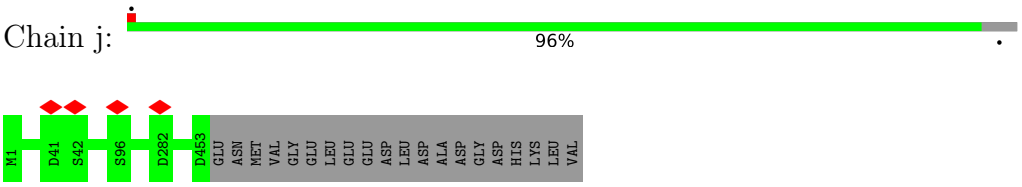
• Molecule 1: Tubulin gamma chain

Chain i:



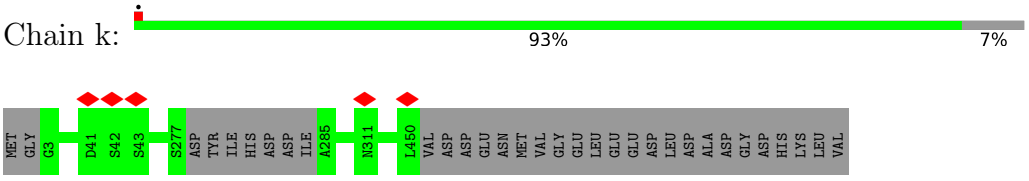
• Molecule 1: Tubulin gamma chain

Chain j:



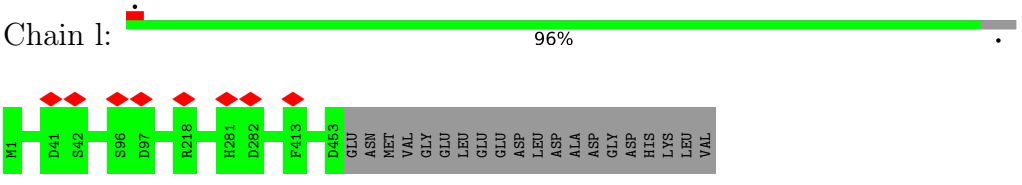
• Molecule 1: Tubulin gamma chain

Chain k:



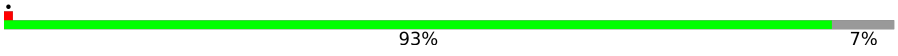
• Molecule 1: Tubulin gamma chain

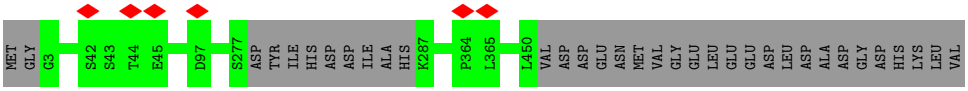
Chain l:



• Molecule 1: Tubulin gamma chain

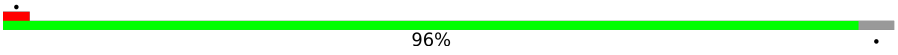
Chain m:

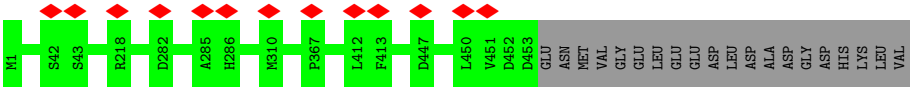




• Molecule 1: Tubulin gamma chain

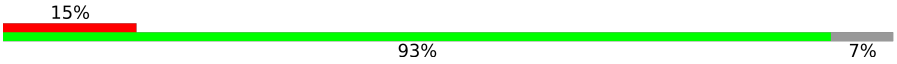
Chain n:

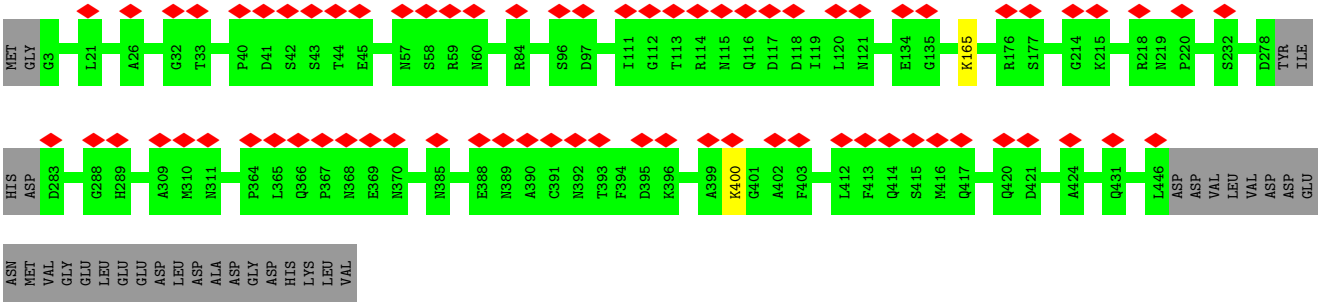




• Molecule 1: Tubulin gamma chain

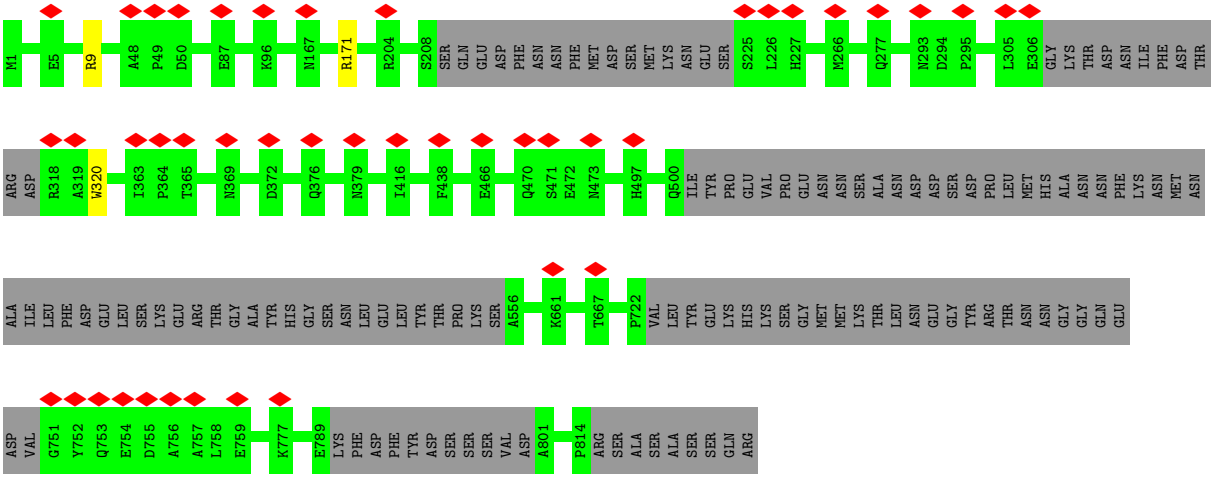
Chain a:





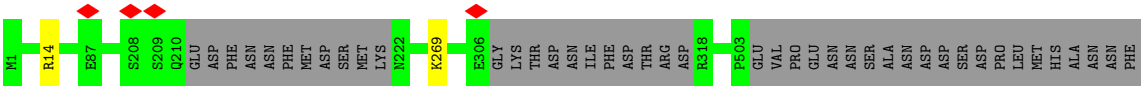
• Molecule 2: Spindle pole body component

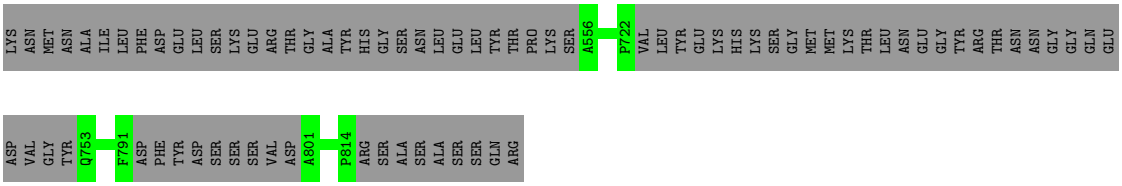
Chain C:



• Molecule 2: Spindle pole body component

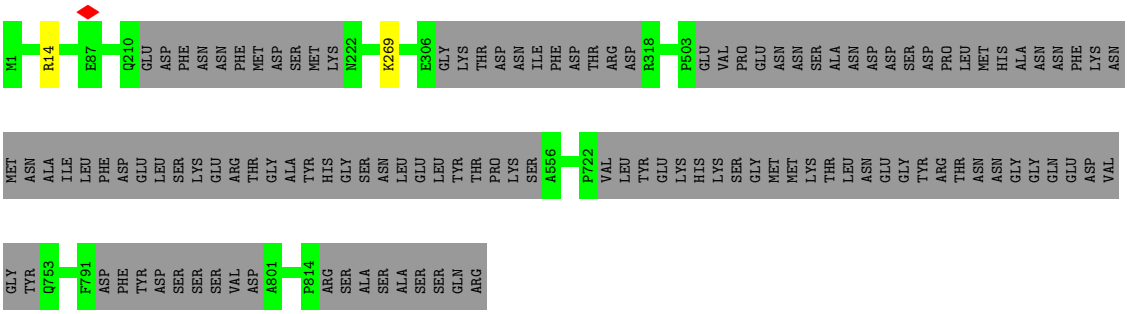
Chain E:





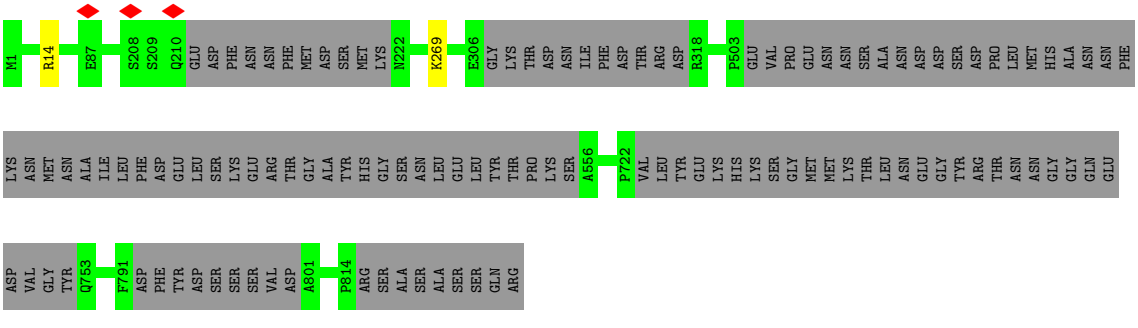
• Molecule 2: Spindle pole body component

Chain G:



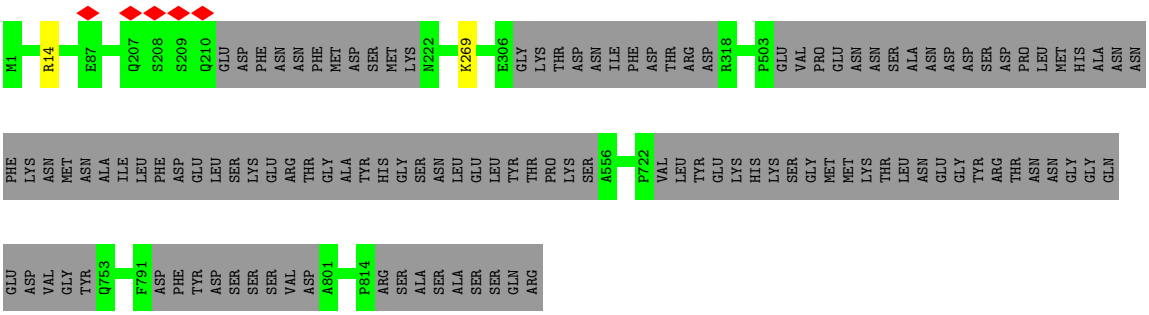
• Molecule 2: Spindle pole body component

Chain I:



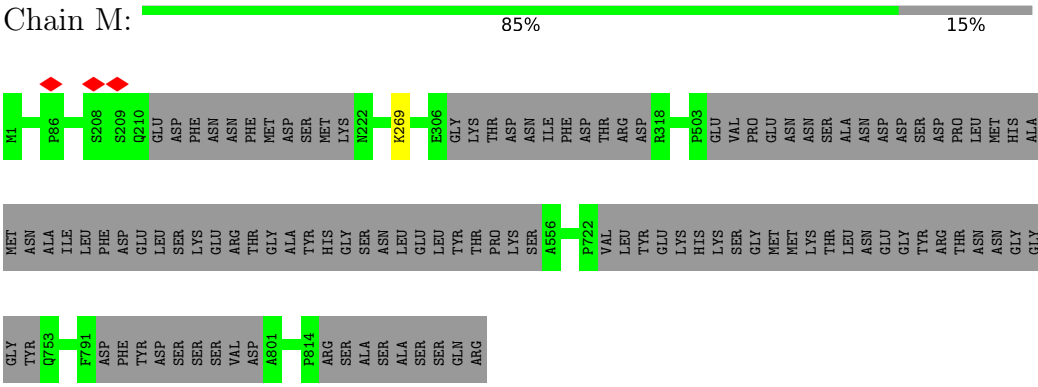
• Molecule 2: Spindle pole body component

Chain K:



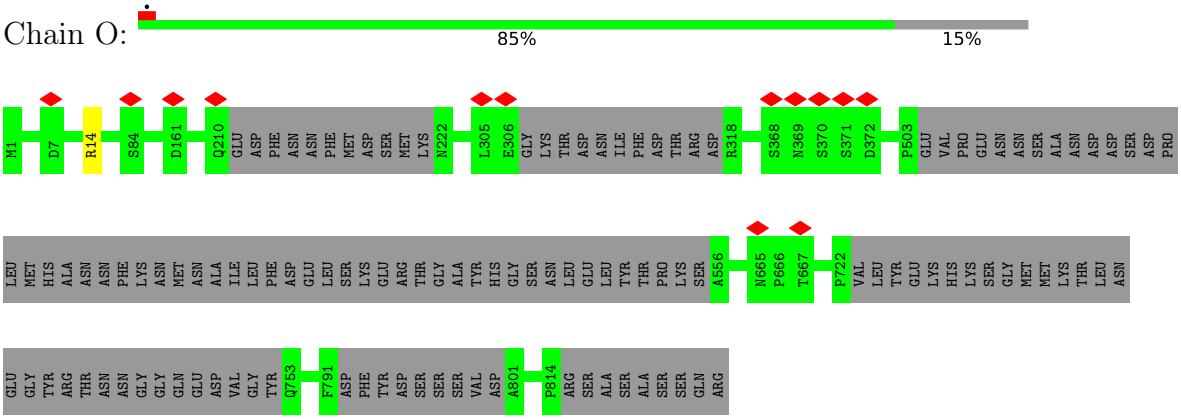
• Molecule 2: Spindle pole body component

Chain M:



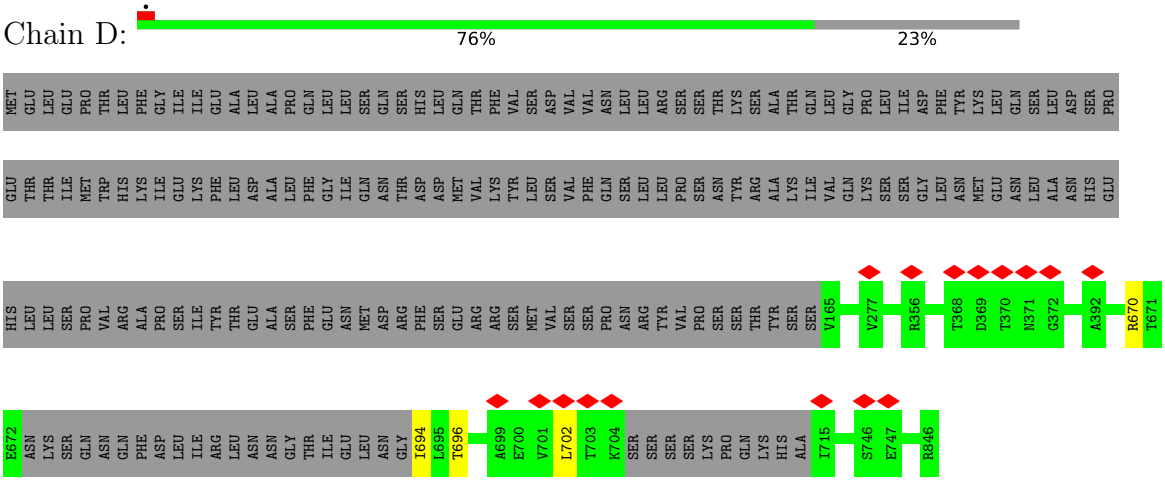
• Molecule 2: Spindle pole body component

Chain O:



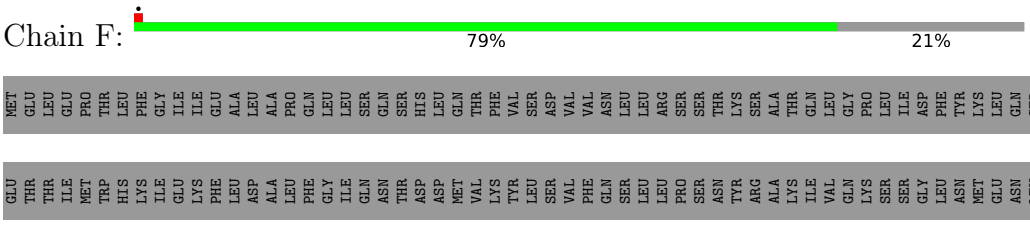
• Molecule 3: Spindle pole body component

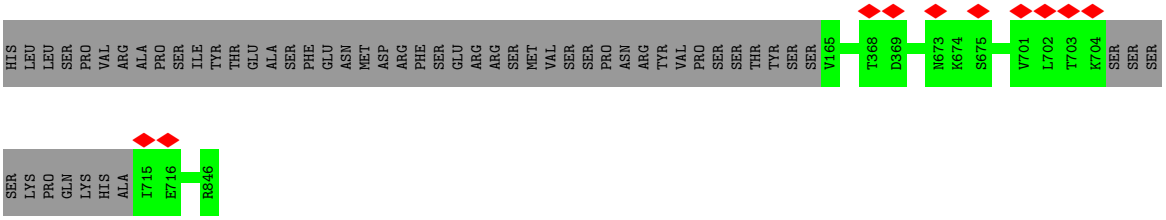
Chain D:



• Molecule 3: Spindle pole body component

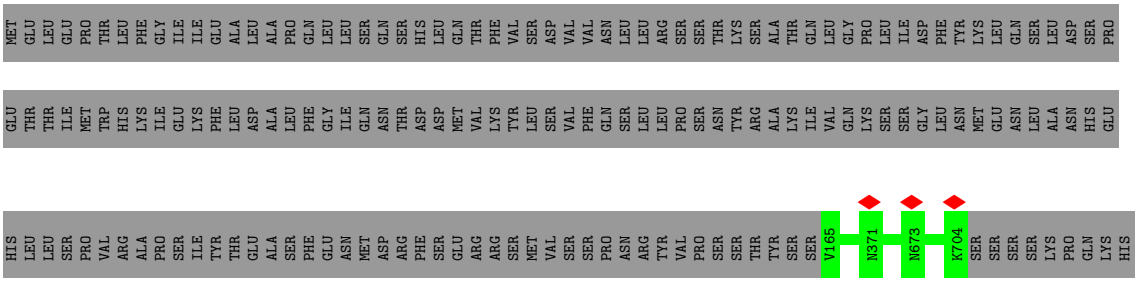
Chain F:





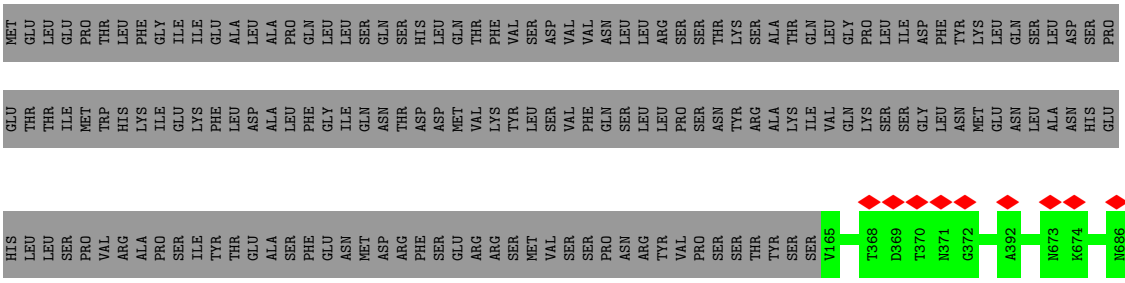
• Molecule 3: Spindle pole body component

Chain H:



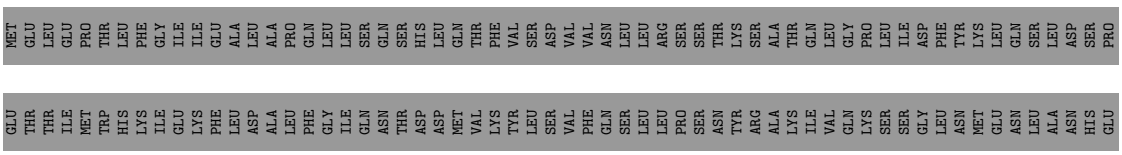
• Molecule 3: Spindle pole body component

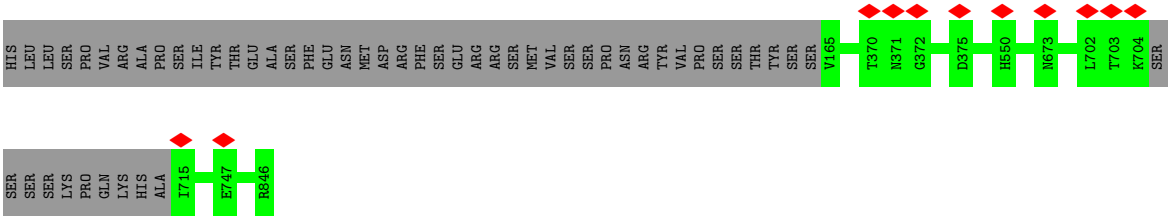
Chain J:



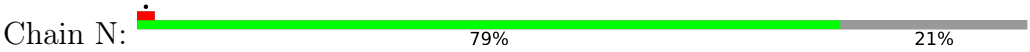
• Molecule 3: Spindle pole body component

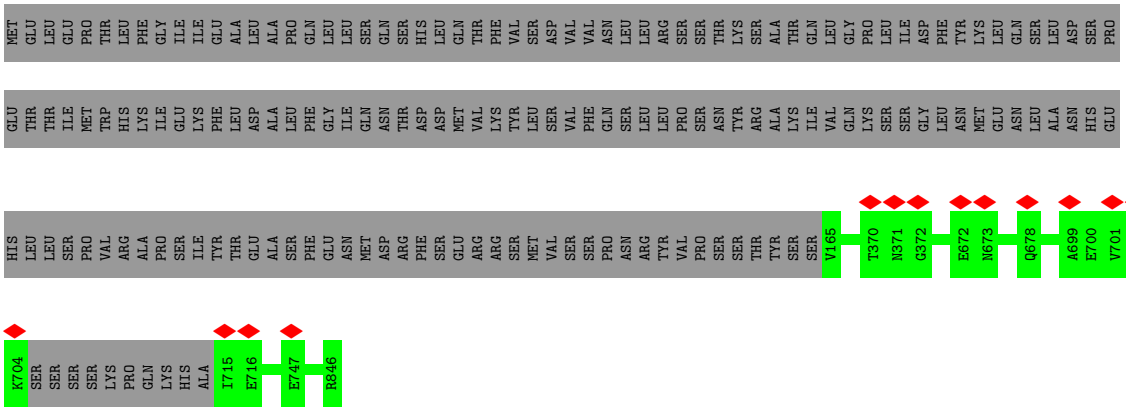
Chain L:



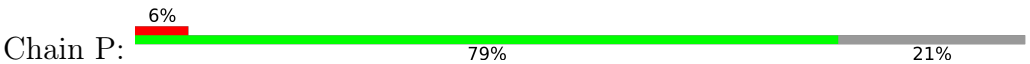


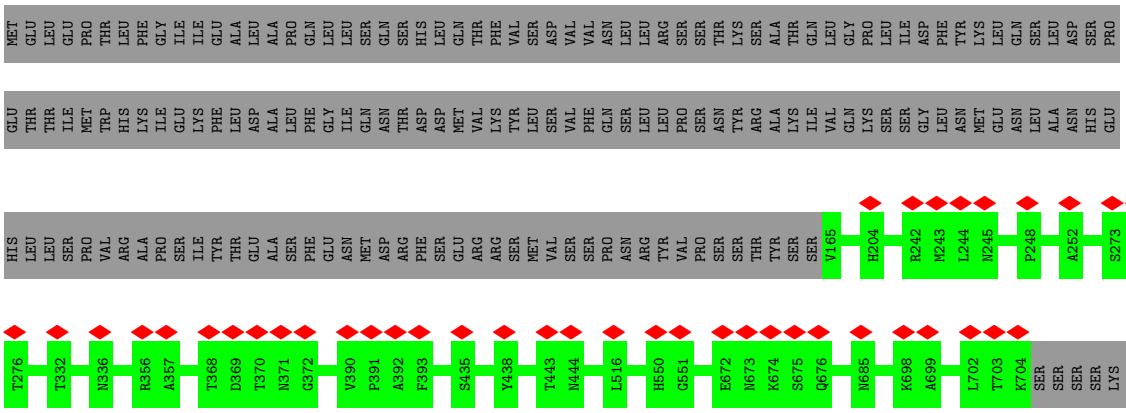
• Molecule 3: Spindle pole body component



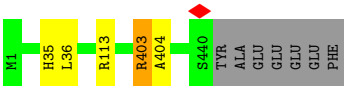


• Molecule 3: Spindle pole body component



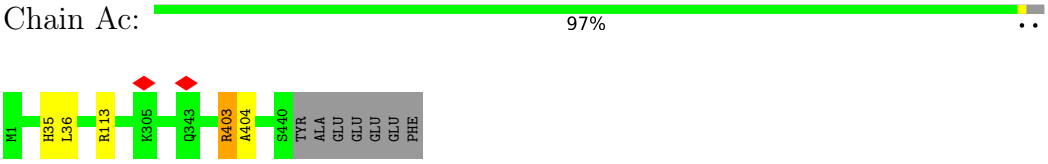


• Molecule 4: Tubulin alpha-1 chain



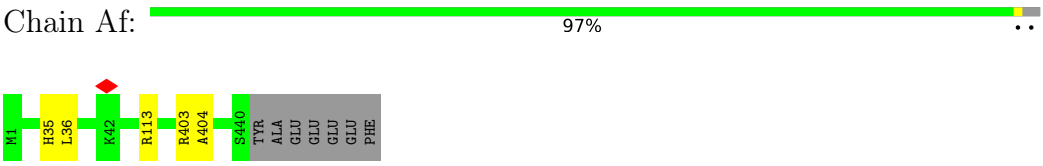
• Molecule 4: Tubulin alpha-1 chain

Chain Ac:



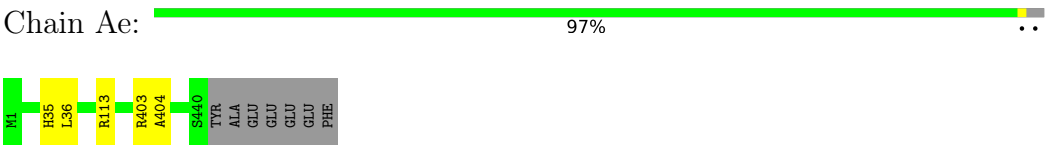
• Molecule 4: Tubulin alpha-1 chain

Chain Af:



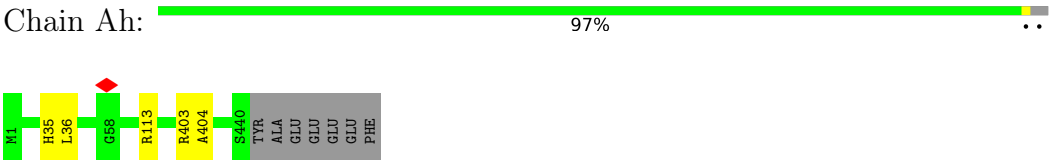
• Molecule 4: Tubulin alpha-1 chain

Chain Ae:



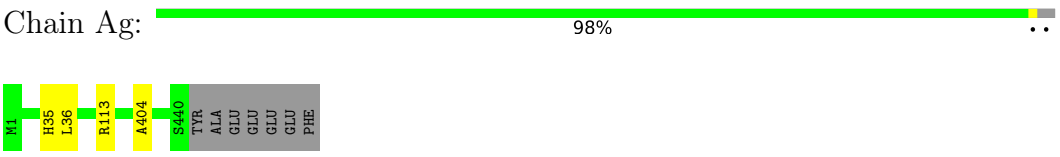
• Molecule 4: Tubulin alpha-1 chain

Chain Ah:



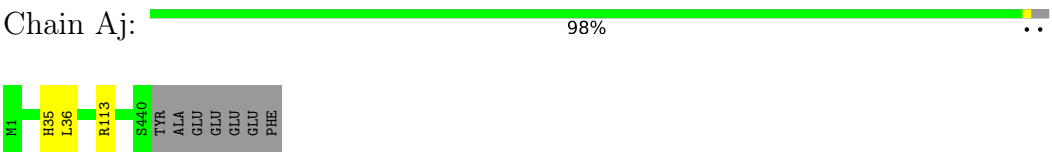
• Molecule 4: Tubulin alpha-1 chain

Chain Ag:



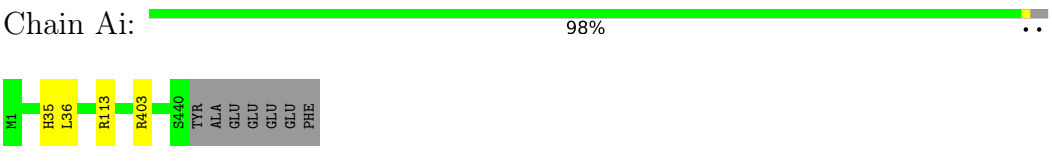
• Molecule 4: Tubulin alpha-1 chain

Chain Aj:



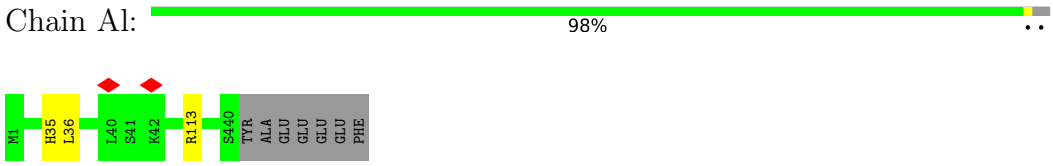
• Molecule 4: Tubulin alpha-1 chain

Chain Ai:



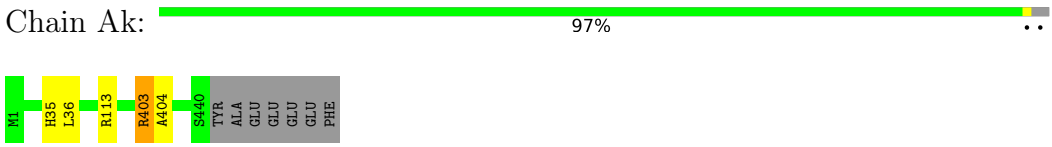
• Molecule 4: Tubulin alpha-1 chain

Chain Al:



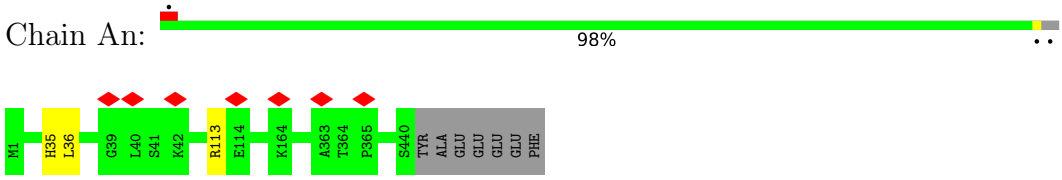
• Molecule 4: Tubulin alpha-1 chain

Chain Ak:



• Molecule 4: Tubulin alpha-1 chain

Chain An:



• Molecule 4: Tubulin alpha-1 chain

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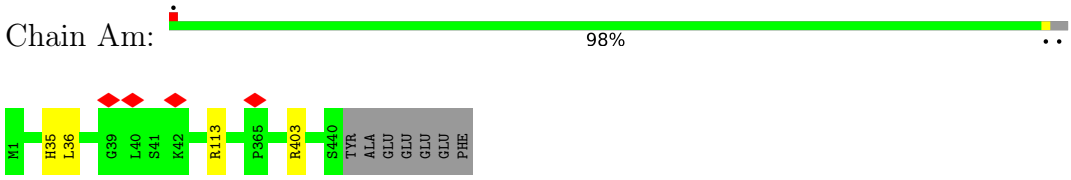

• Molecule 4: Tubulin alpha-1 chain

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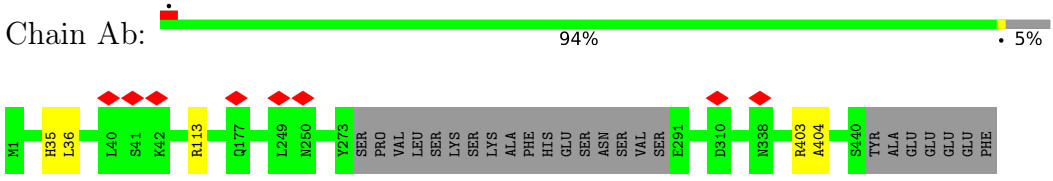
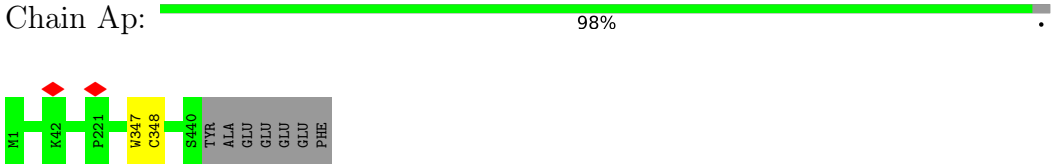


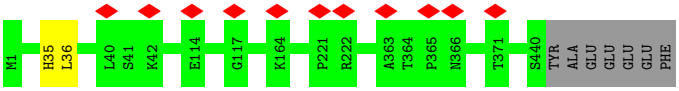
• Molecule 4: Tubulin alpha-1 chain

Chain Ap:



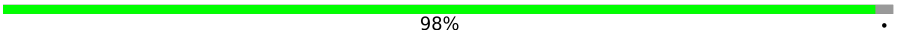
• Molecule 4: Tubulin alpha-1 chain

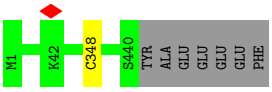
Chain Ao:



• Molecule 4: Tubulin alpha-1 chain

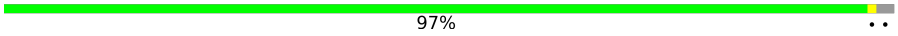
Chain Ar:

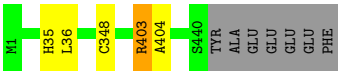




• Molecule 4: Tubulin alpha-1 chain

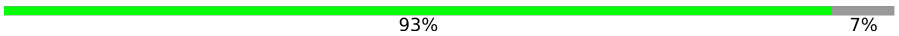
Chain Aq:

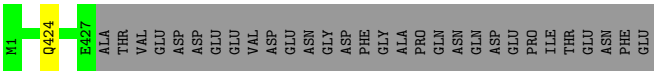




• Molecule 5: Tubulin beta chain

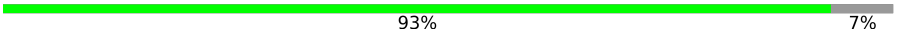
Chain Bd:

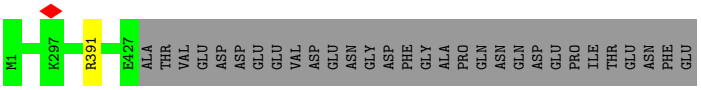




• Molecule 5: Tubulin beta chain

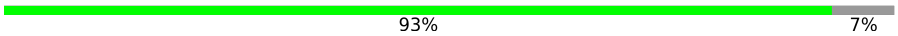
Chain Bc:

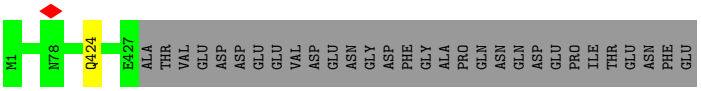




• Molecule 5: Tubulin beta chain

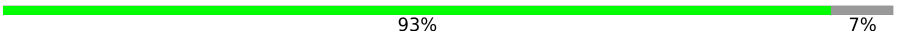
Chain Bf:

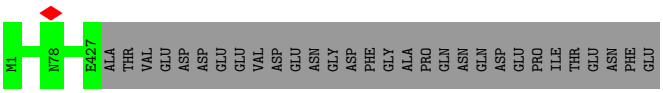




• Molecule 5: Tubulin beta chain

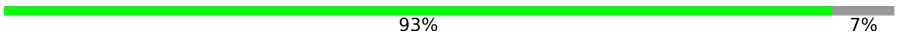
Chain Be:

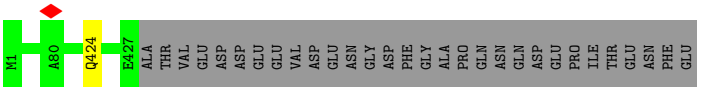




• Molecule 5: Tubulin beta chain

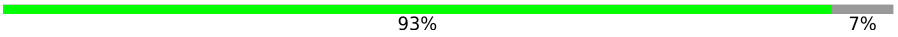
Chain Bh:

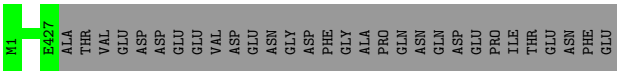




• Molecule 5: Tubulin beta chain

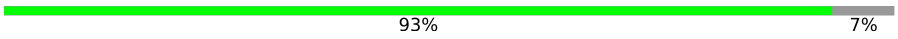
Chain Bg:

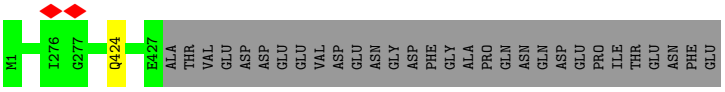




• Molecule 5: Tubulin beta chain

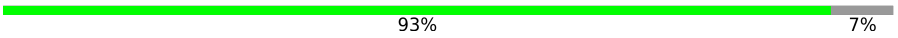
Chain Bj:

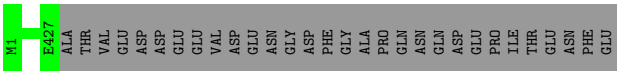




• Molecule 5: Tubulin beta chain

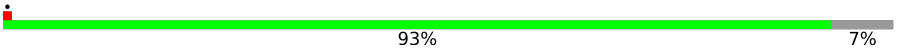
Chain Bi:

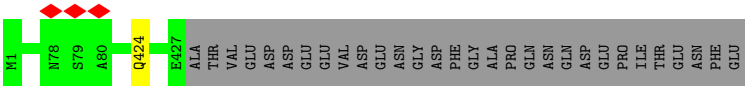




• Molecule 5: Tubulin beta chain

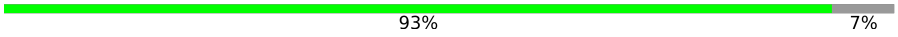
Chain Bl:

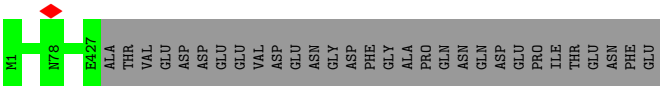




• Molecule 5: Tubulin beta chain

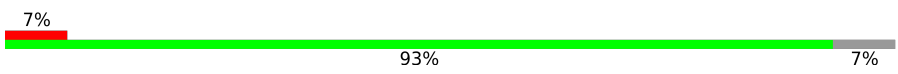
Chain Bk:

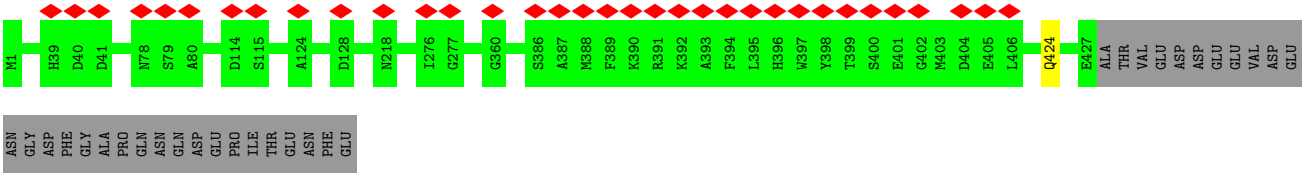




• Molecule 5: Tubulin beta chain

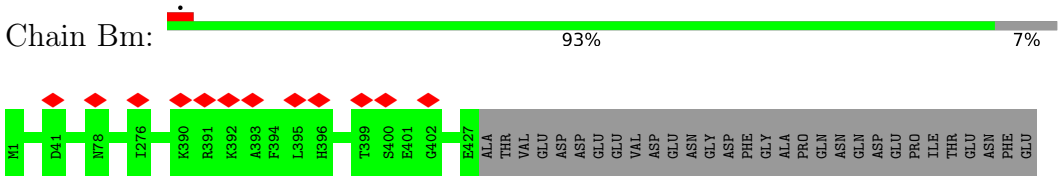
Chain Bn:





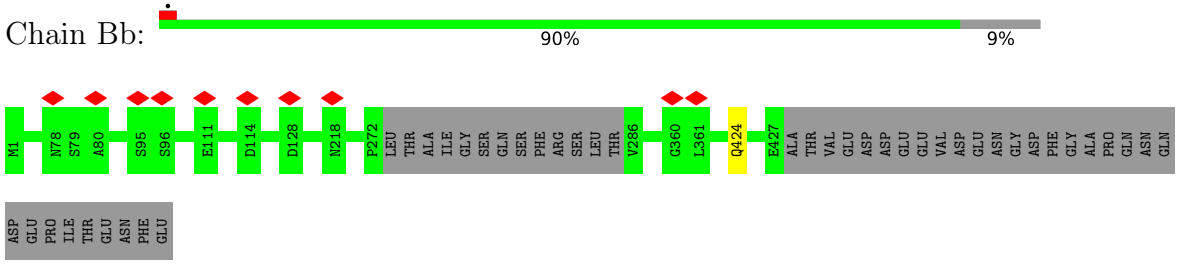
• Molecule 5: Tubulin beta chain

Chain Bm:



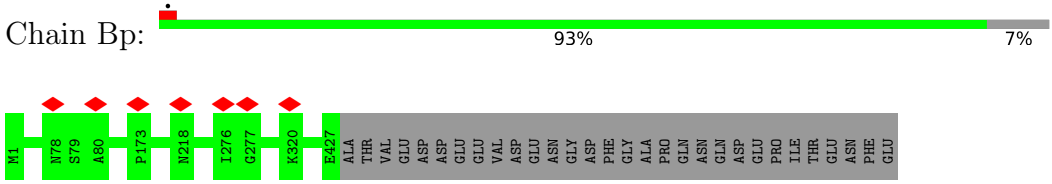
• Molecule 5: Tubulin beta chain

Chain Bb:



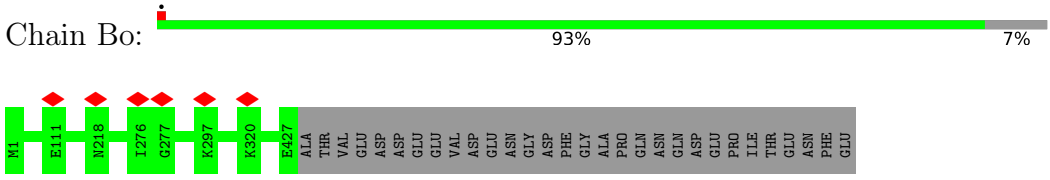
• Molecule 5: Tubulin beta chain

Chain Bp:



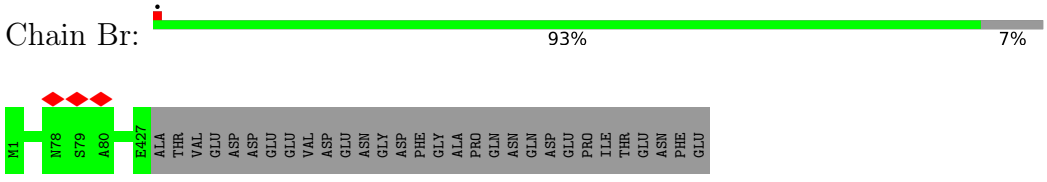
• Molecule 5: Tubulin beta chain

Chain Bo:



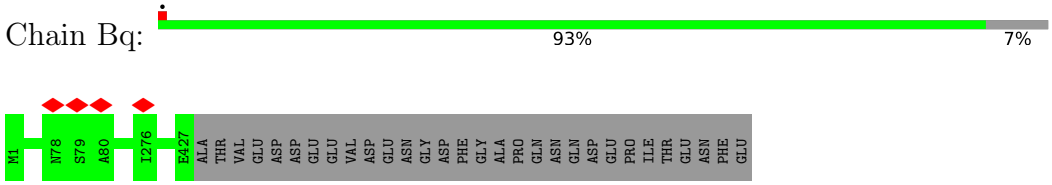
• Molecule 5: Tubulin beta chain

Chain Br:



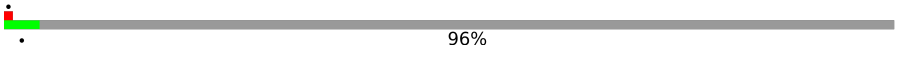
• Molecule 5: Tubulin beta chain

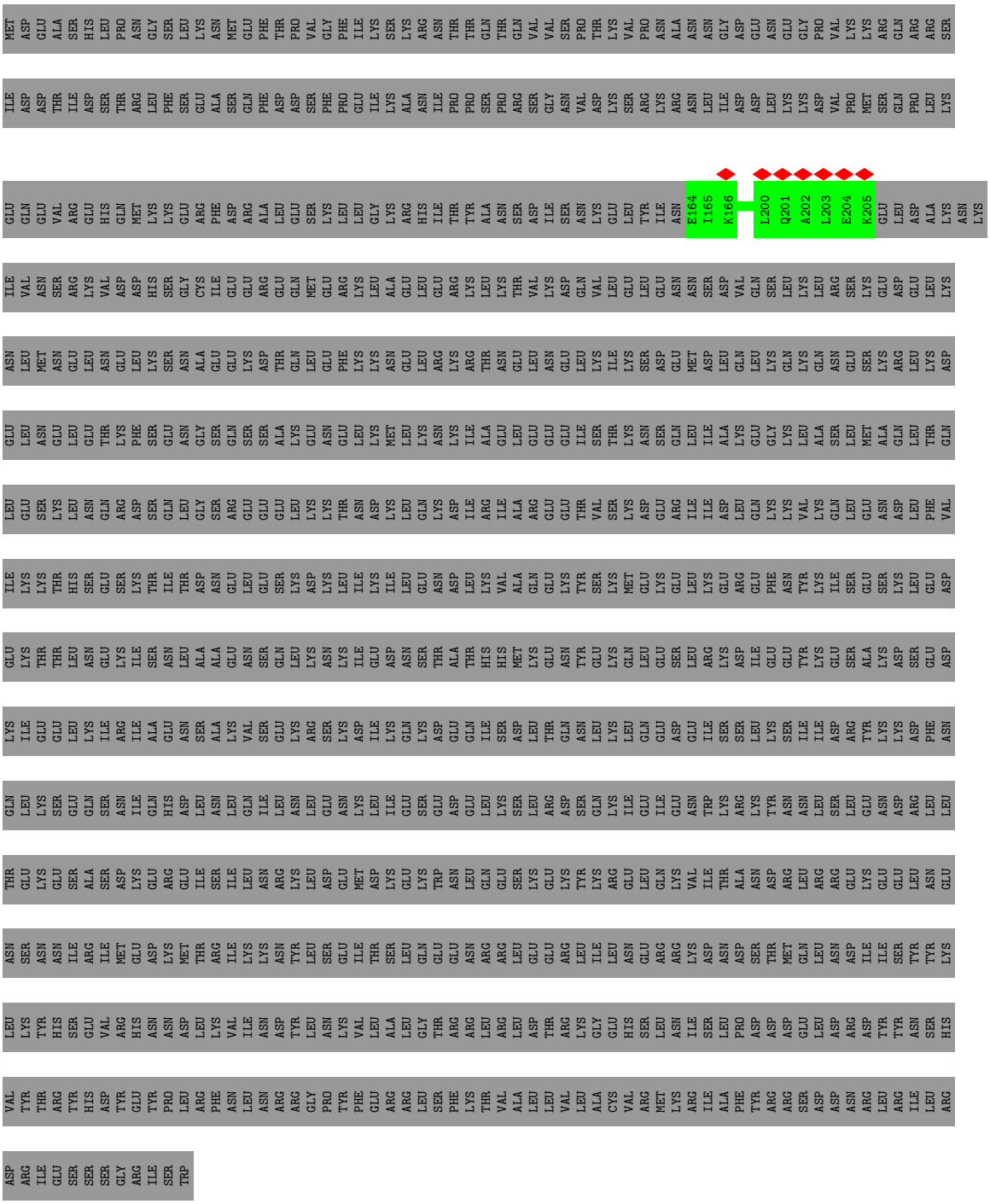
Chain Bq:



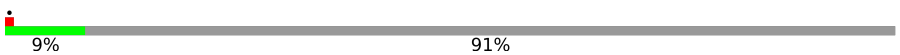
• Molecule 6: Spindle pole body component 110

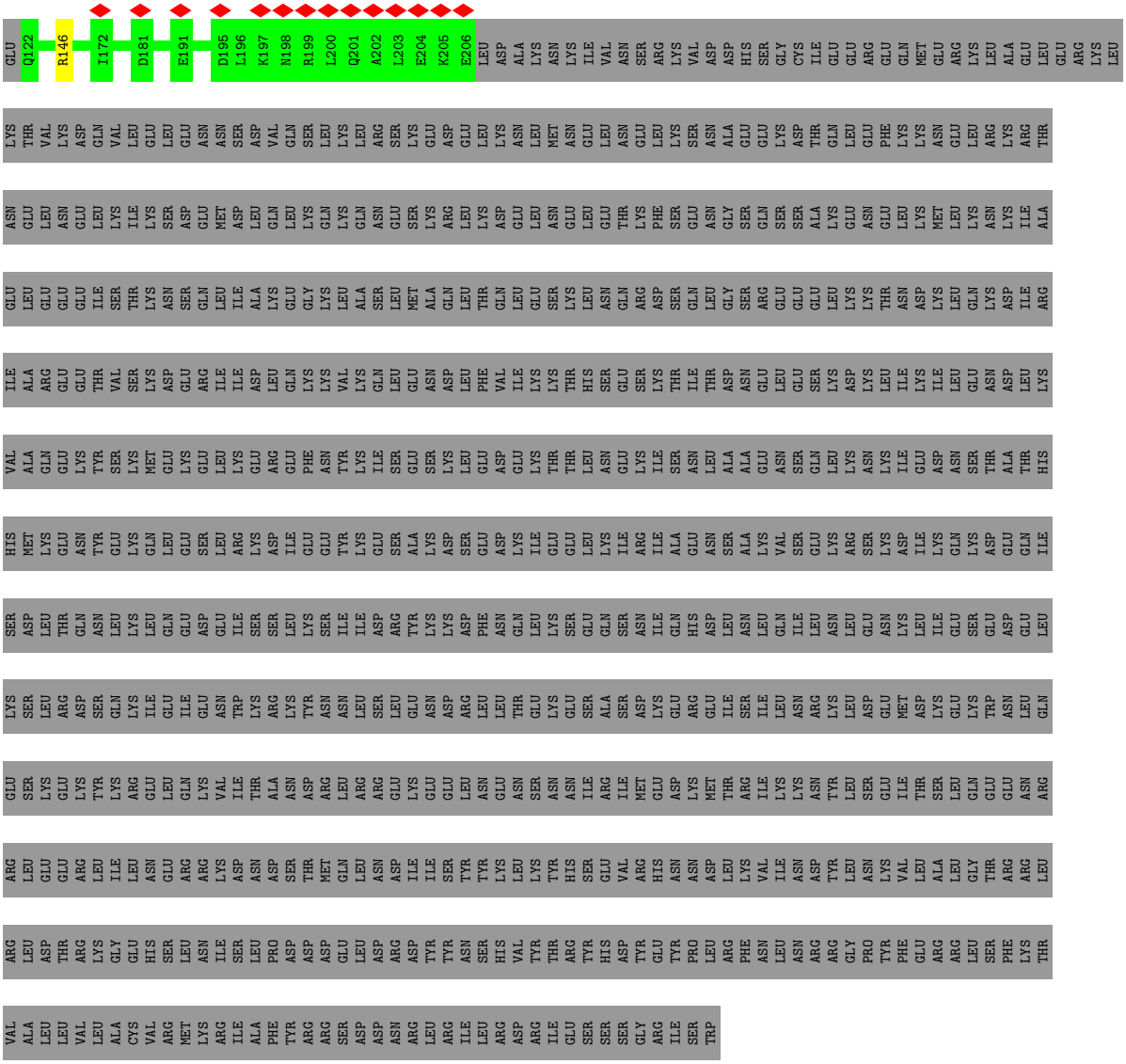
Chain Sc:





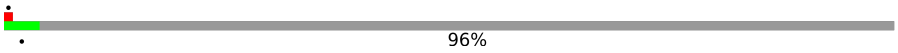
• Molecule 6: Spindle pole body component 110

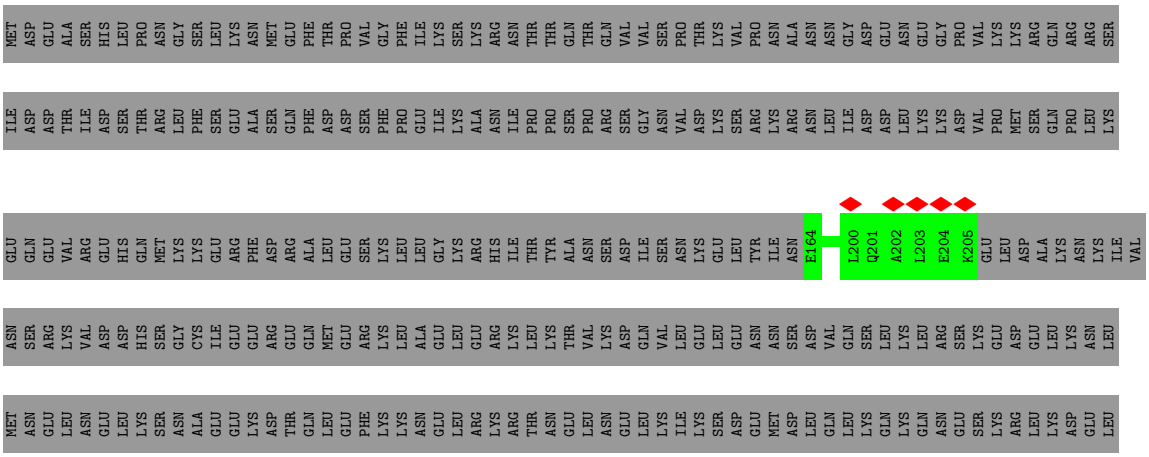


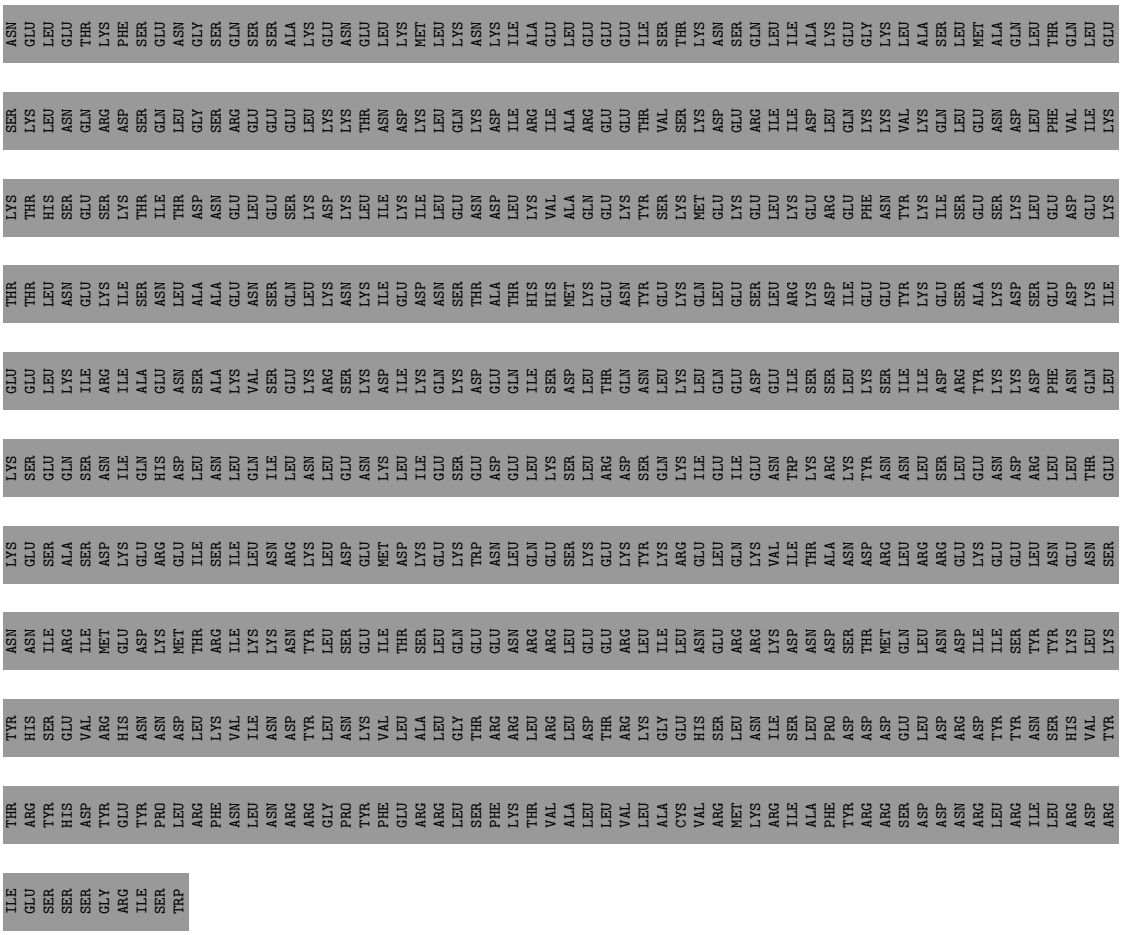


• Molecule 6: Spindle pole body component 110

Chain Se:

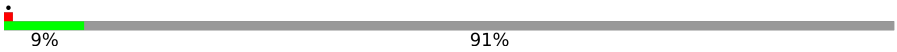


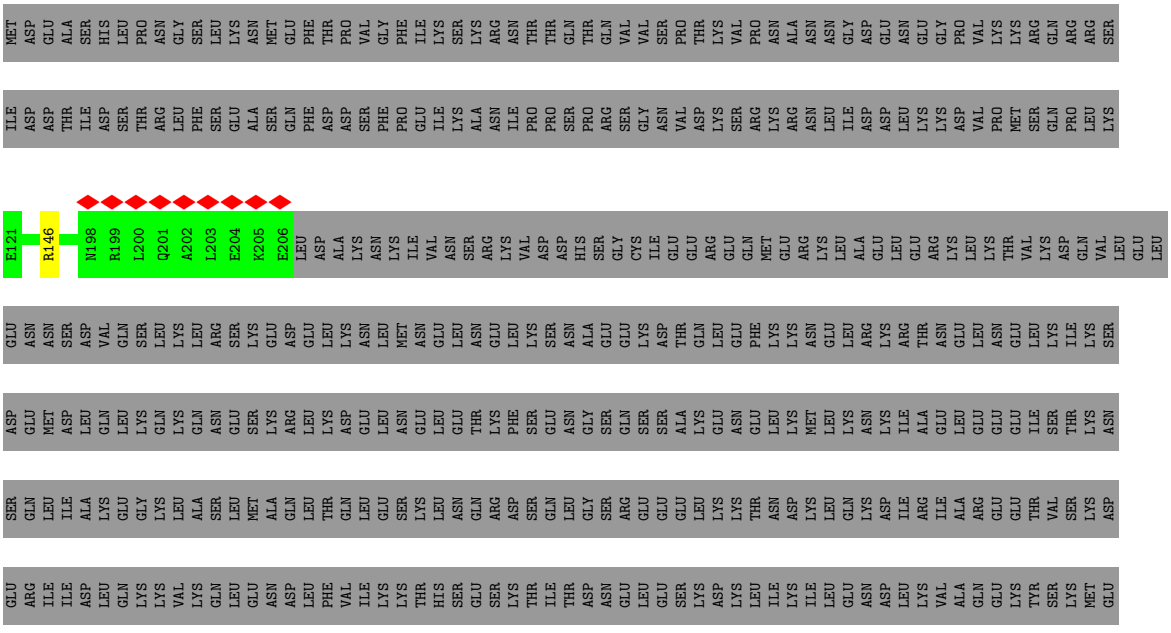




• Molecule 6: Spindle pole body component 110

Chain Sf:





LYS GLU LEU LYS GLU ARG GLU PHE ASN TYR LYS ILE SER GLU SER LYS LEU GLU ASP GLU LYS THR THR LEU ASN GLU LYS ILE SER ASN LEU ALA ALA GLU ASN SER GLN LEU LYS ASN LYS ILE GLU ASP ASN SER THR ALA THR HIS HIS MET LYS GLU ASN TYR GLU LYS GLN LEU

GLU SER LEU ARG LYS ASP ILE GLU GLU TYR LYS GLU SER ALA LYS ASP SER GLU ASP LYS ILE GLU GLU LEU LYS ILE ARG ILE ALA GLU ASN SER ALA LYS VAL SER GLU LYS ARG SER LYS ASP ILE LYS GLN LYS ASP GLU GLN ILE SER ASP LEU THR GLN ASN LEU LYS LEU GLN

GLU ASP GLU ILE SER SER LEU LYS SER ILE ILE ASP ARG TYR LYS LYS ASP PHE ASN GLN LEU LYS SER GLU GLN SER ASN ILE GLN HIS ASP LEU ASN LEU GLN ILE LEU ASN LEU GLU ASN LYS LEU ILE GLU SER GLU ASP GLU LEU LYS SER LEU ARG ASP SER GLN LYS ILE GLU

ILE GLU ASN TRP LYS ARG LYS TYR ASN ASN LEU SER LEU GLU ASN ASP ARG LEU LEU THR GLU LYS GLU SER ALA SER ASP LYS GLU ARG GLU ILE SER ILE LEU ASN ARG LYS LEU ASP GLU MET ASP LYS GLU LYS TRP ASN LEU GLN GLU SER LYS GLU LYS TYR LYS ARG GLU LEU

GLN LYS VAL ILE THR ALA ASN ASP ARG LEU ARG ARG GLU LYS GLU GLU LEU ASN GLU ASN SER ASN ASN ILE ARG ILE MET GLU ASP LYS MET THR ARG ILE LYS LYS ASN TYR LEU SER GLU ILE THR SER LEU GLN GLU GLU ASN ARG ARG LEU GLU GLU ARG LEU ILE LEU ASN GLU

ARG ARG LYS ASP ASN ASP SER THR MET GLN LEU ASN ASP ILE ILE SER TYR TYR LYS LEU LYS TYR HIS SER GLU VAL ARG HIS ASN ASN ASP LEU LYS VAL ILE ASN ASP TYR LEU ASN LYS VAL LEU ALA LEU GLY THR ARG ARG LEU ARG LEU ASP THR ARG LYS GLY GLU HIS SER

LEU ASN ILE SER LEU PRO ASP ASP ASP GLU LEU ASP ARG ASP TYR TYR ASN SER HIS VAL TYR THR ARG TYR HIS ASP TYR GLU TYR PRO LEU ARG PHE ASN LEU ASN ARG ARG GLY PRO TYR PHE GLU ARG ARG LEU SER PHE LYS THR VAL ALA LEU LEU VAL LEU ALA CYS VAL ARG

MET LYS ARG ILE ALA PHE TYR ARG ARG SER ASP ASP ASN ARG LEU ARG ILE LEU ARG ASP ARG ILE GLU SER SER SER GLY ARG ILE SER TRP

- Molecule 6: Spindle pole body component 110

Chain Sg: 96%

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

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

GLU GLN GLU VAL ARG GLU HIS GLN MET LYS LYS GLU ARG PHE ASP ARG ALA LEU GLU SER LYS LEU LEU GLY LYS ARG HIS ILE THR TYR ALA ASN SER ASP ILE SER ASN LYS GLU LEU TYR ILE ASN E164 L200 E204 K205 GLU LEU ASP ALA LYS ASN LYS ILE VAL ASN SER

ARG LYS VAL ASP ASP HIS SER GLY CYS ILE GLU GLU ARG GLU GLN MET GLU ARG LYS LEU ALA GLU LEU GLU ARG LYS LEU LYS THR VAL LYS ASP GLN VAL LEU GLU LEU GLU ASN ASN SER ASP VAL GLN SER LEU LYS LEU ARG SER LYS GLU ASP GLU LEU LYS ASN LEU MET ASN

GLU LEU ASN GLU LEU LYS SER ASN ALA GLU GLU LYS ASP THR GLN LEU GLU PHE LYS LYS ASN GLU LEU ARG LYS ARG THR ASN GLU LEU ASN GLU LEU LYS ILE LYS SER ASP GLU MET ASP LEU GLN LEU LYS GLN LYS GLN ASN GLU SER LYS ARG LEU LYS ASP GLU LEU ASN GLU

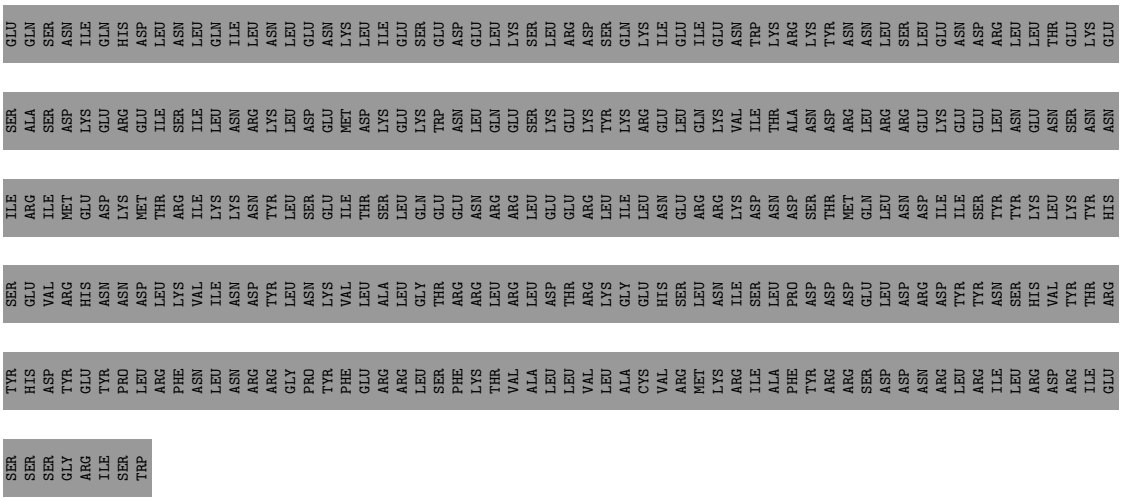
LEU GLU THR LYS PHE SER GLU ASN GLY SER GLN SER SER ALA LYS GLU ASN GLU LEU LYS MET LEU LYS ASN LYS ILE ALA GLU LEU GLU GLU GLU ILE SER THR LYS ASN SER GLN LEU ILE ALA LYS GLU GLY LYS LEU ALA SER LEU MET ALA GLN LEU THR GLN LEU GLU SER LYS

LEU ASN GLN ARG ASP SER GLN LEU GLY SER ARG GLU GLU GLU LEU LYS LYS THR ASN ASP LYS LEU GLN LYS ASP ILE ARG ILE ALA ARG GLU GLU THR VAL SER LYS ASP GLU ARG ILE ILE ASP LEU GLN LYS LYS VAL LYS GLN LEU GLU ASN ASP LEU PHE VAL ILE LYS LYS THR

HIS SER GLU SER LYS THR ILE THR ASP ASN GLU LEU GLU SER LYS ASP LYS LEU ILE LYS ILE LEU GLU ASN ASP LEU LYS VAL ALA GLN GLU LYS TYR SER LYS MET GLU LYS GLU LEU LYS GLU ARG GLU PHE ASN TYR LYS ILE SER GLU SER LYS LEU GLU ASP GLU LYS THR THR

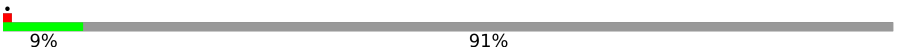
LEU ASN GLU LYS ILE SER ASN LEU ALA ALA GLU ASN SER GLN LEU LYS ASN LYS ILE GLU ASP ASN SER THR ALA THR HIS HIS MET LYS GLU ASN TYR GLU LYS GLN LEU GLU SER LEU ARG LYS ASP ILE GLU GLU TYR LYS GLU SER ALA LYS ASP SER GLU ASP LYS ILE GLU GLU

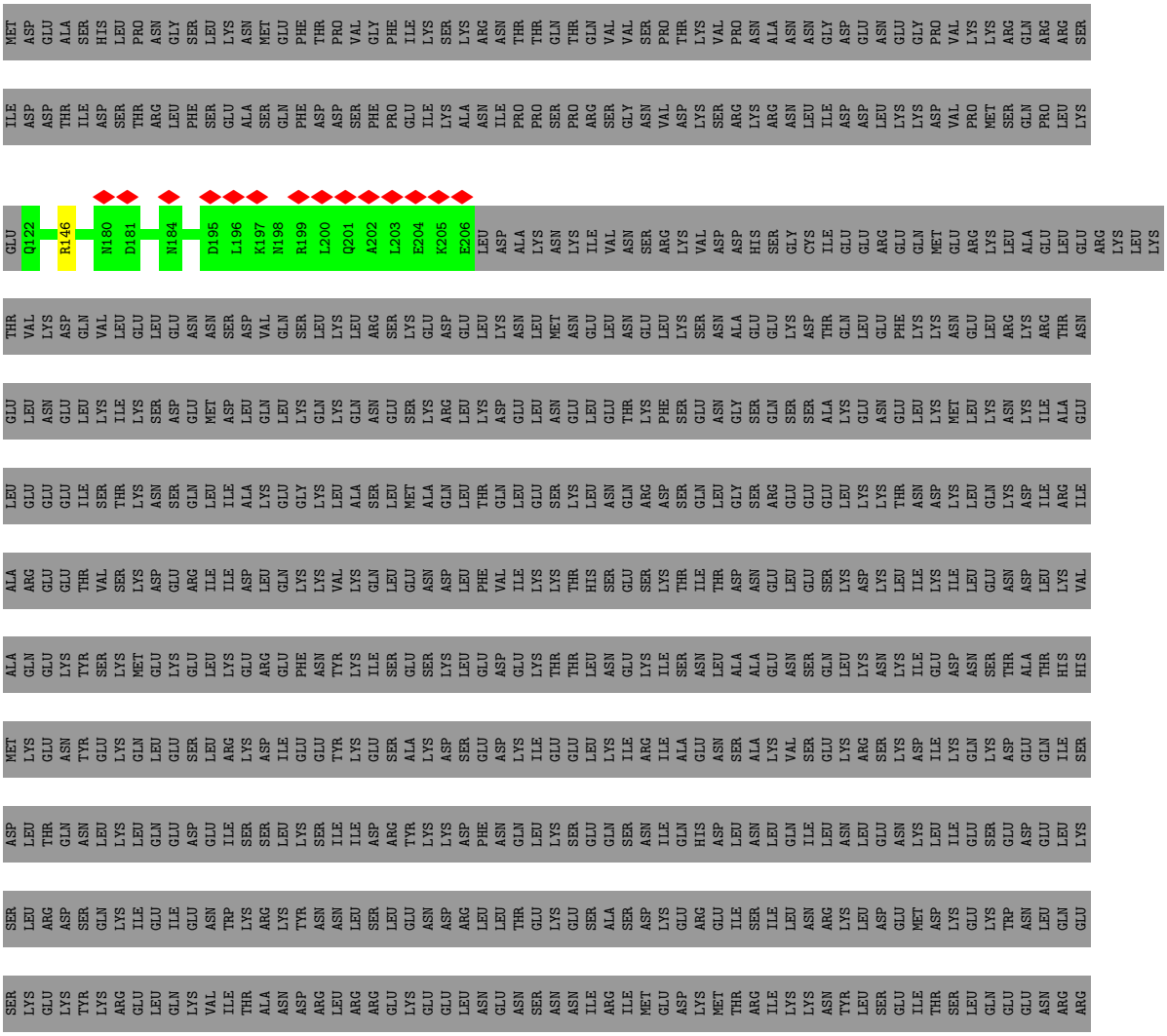
LEU LYS ILE ARG ILE ALA GLU ASN SER ALA LYS VAL SER GLU LYS ARG SER LYS ASP ILE LYS GLN LYS ASP GLU GLN ILE SER ASP LEU THR GLN ASN LEU LYS LEU GLN GLU ASP GLU ILE SER SER LEU LYS SER ILE ILE ASP ARG TYR LYS LYS ASP PHE ASN GLN LEU LYS SER

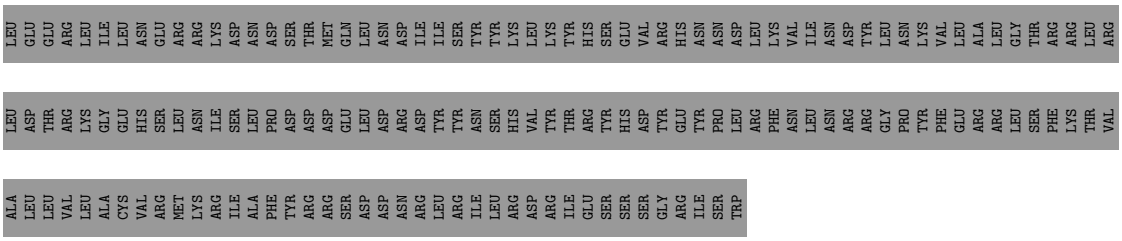


• Molecule 6: Spindle pole body component 110

Chain Sh:

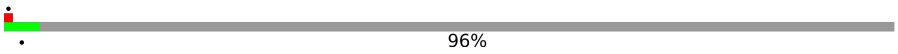


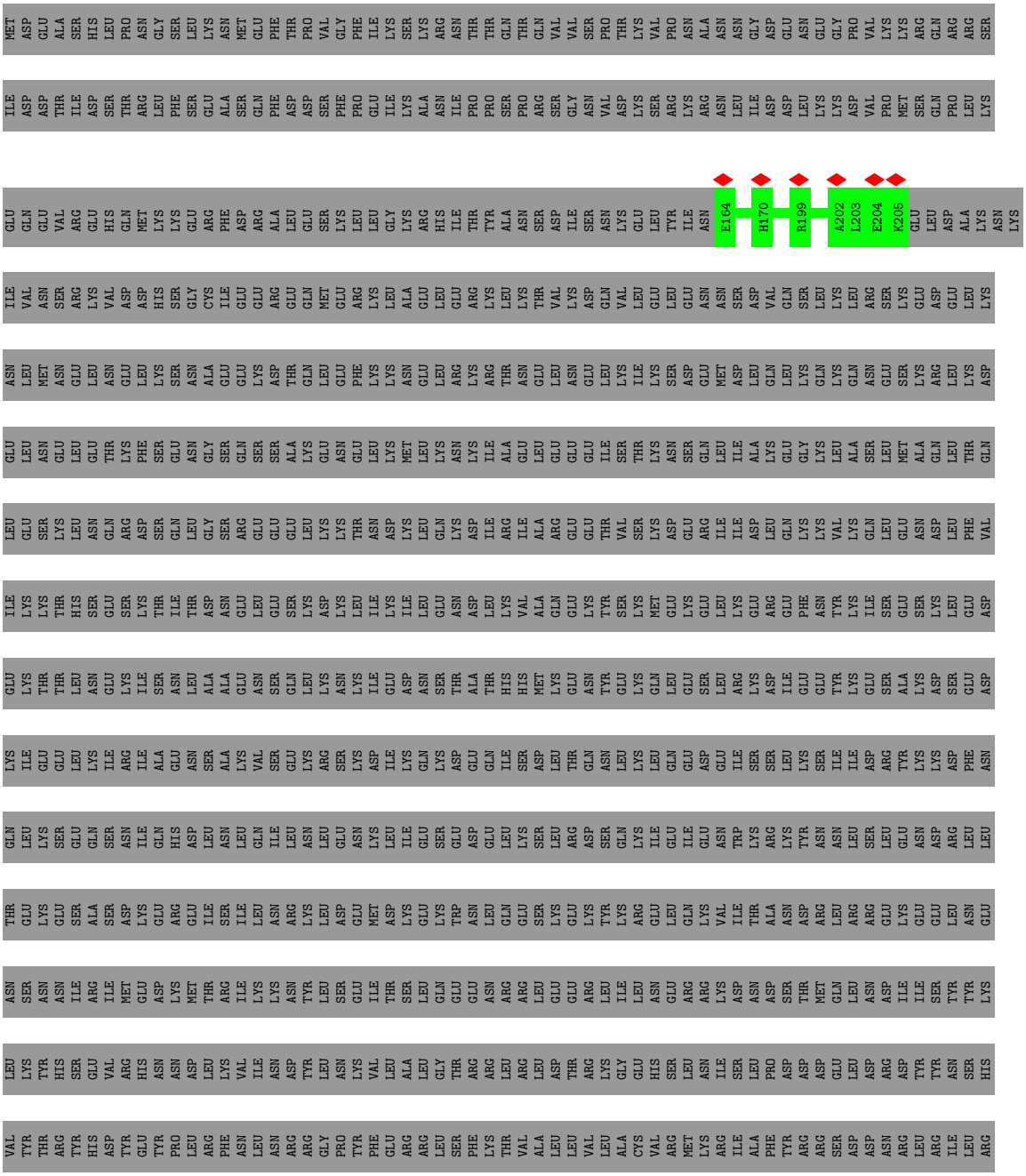




• Molecule 6: Spindle pole body component 110

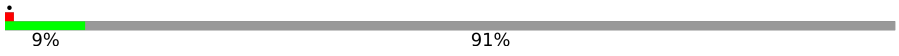
Chain Si:

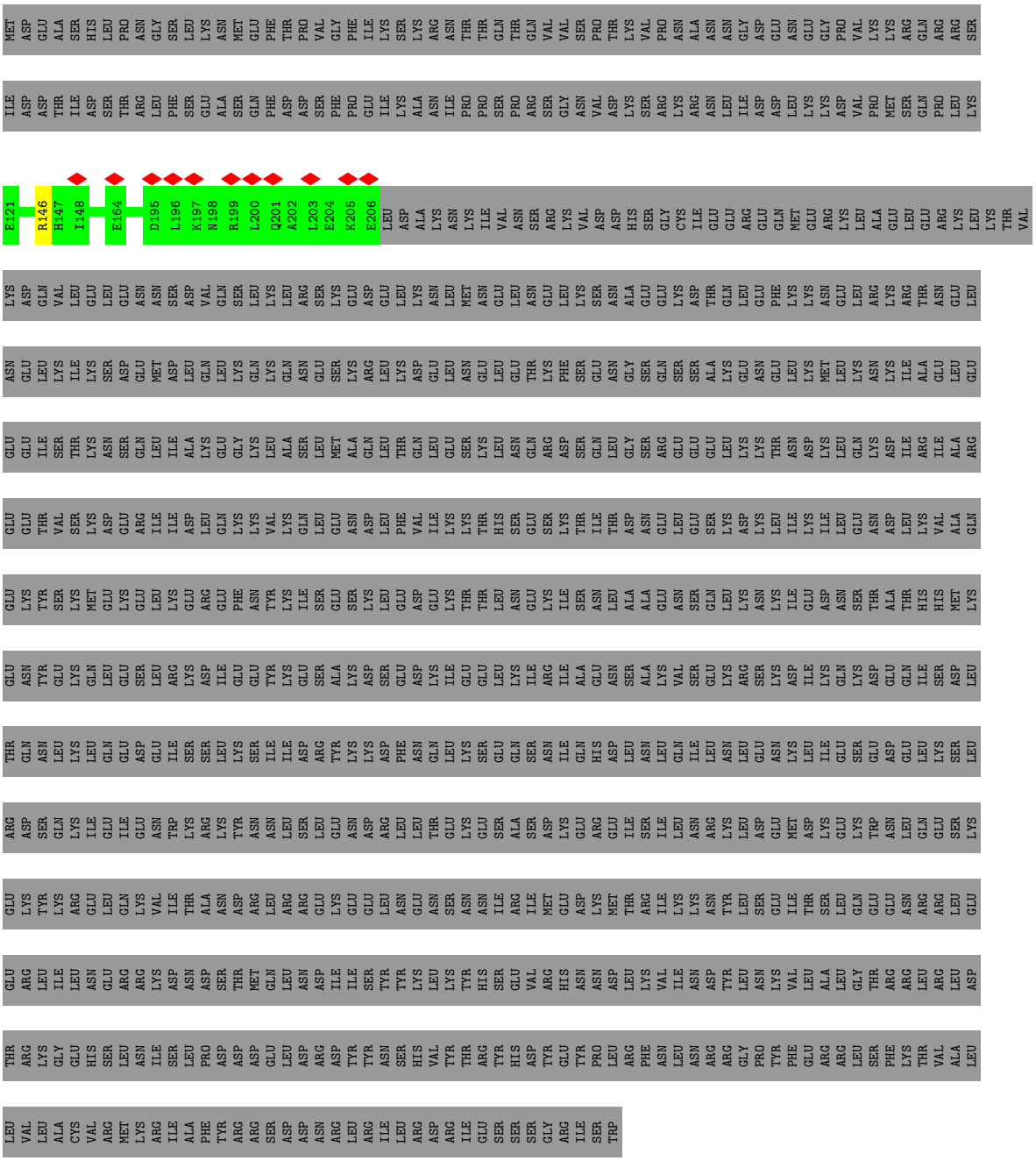




• Molecule 6: Spindle pole body component 110

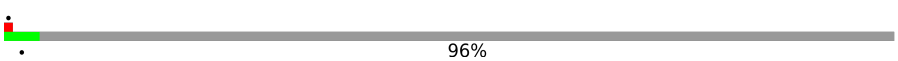
Chain Sj:

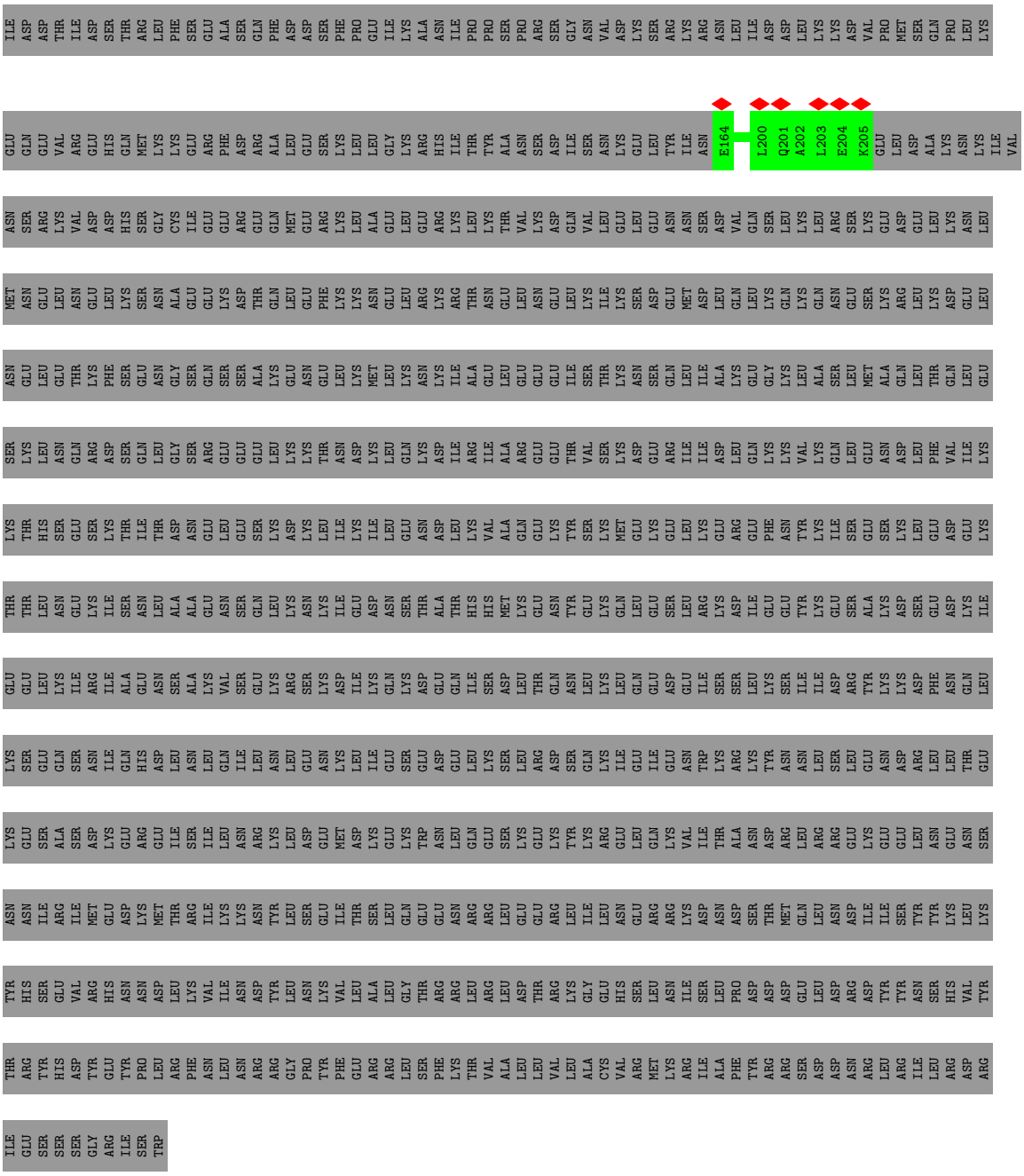




• Molecule 6: Spindle pole body component 110

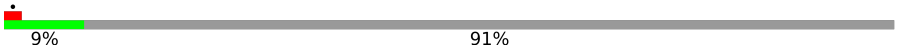
Chain Sk:

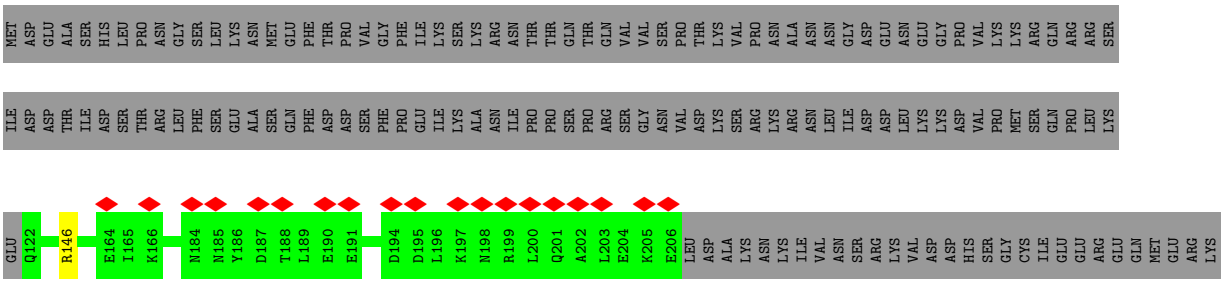


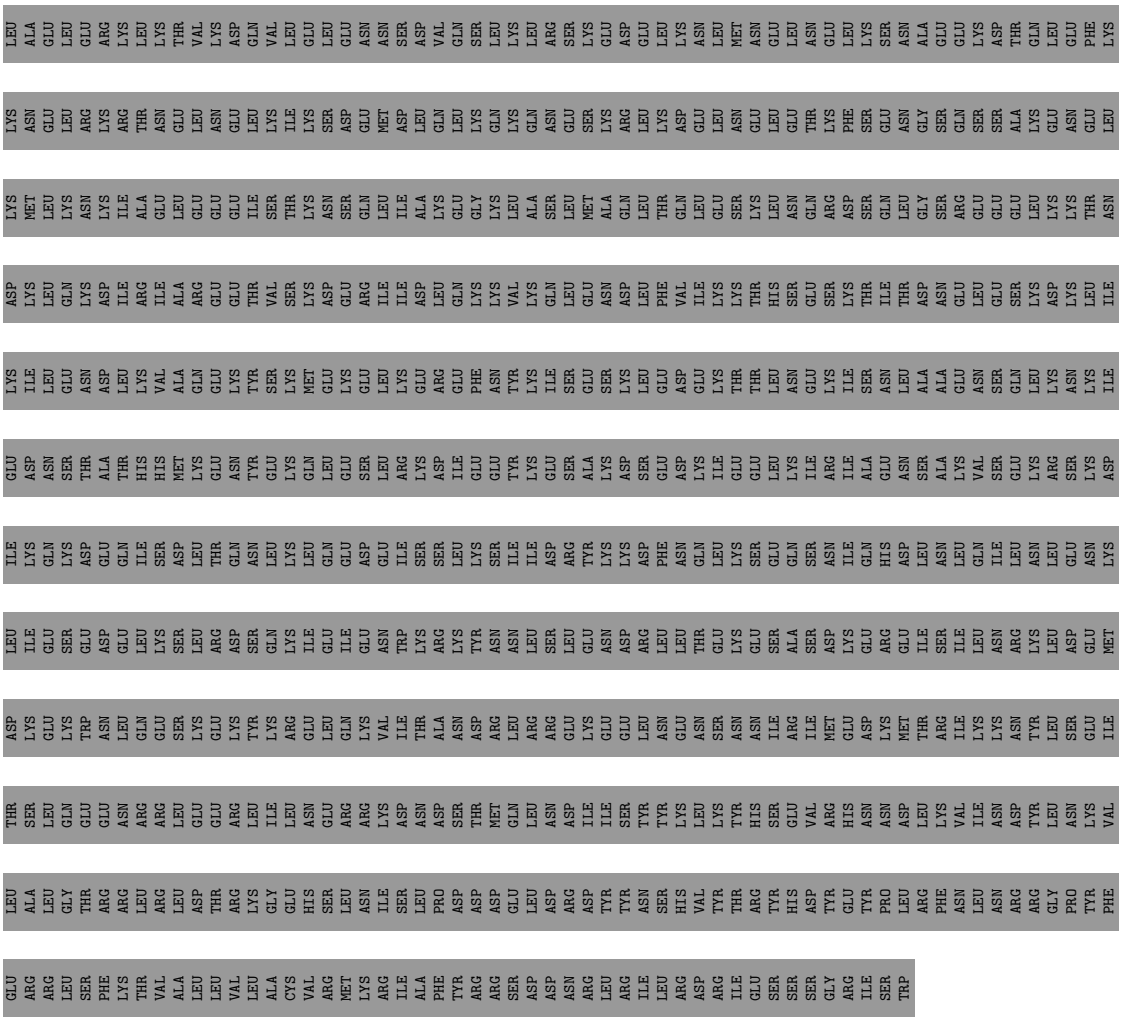


• Molecule 6: Spindle pole body component 110

Chain Sl:

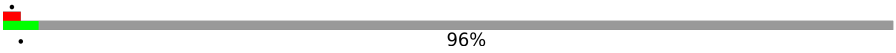


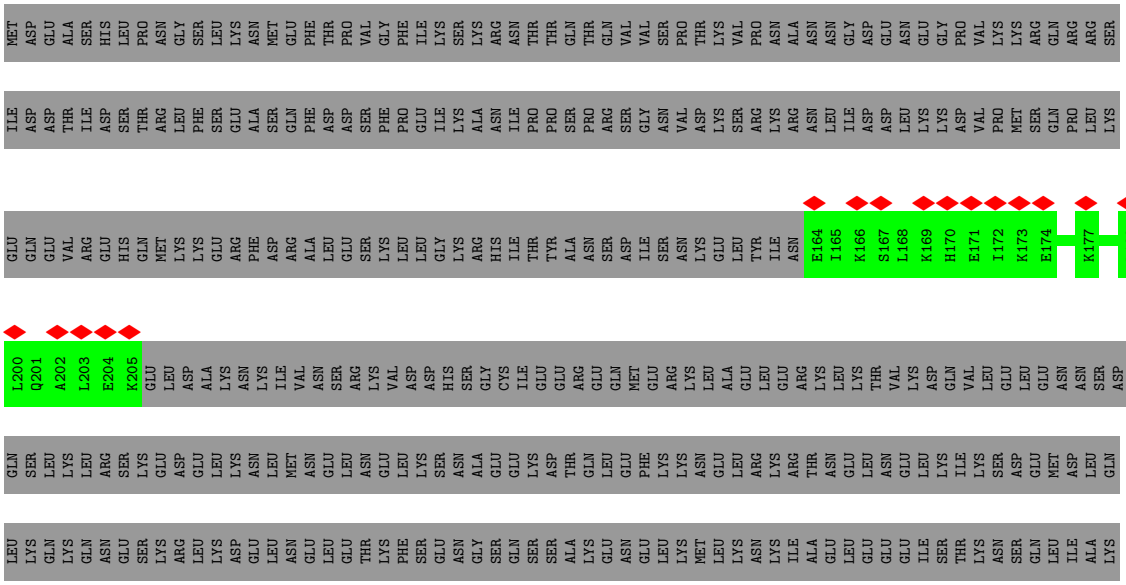




• Molecule 6: Spindle pole body component 110

Chain Sa:





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GLN LYS LYS VAL LYS GLN LEU GLU ASN ASP LEU PHE VAL ILE LYS LYS THR HIS SER GLU SER LYS THR ILE THR ASP ASN GLU LEU GLU SER LYS ASP LYS LEU ILE LYS ILE LEU GLU ASN ASP LEU LYS VAL ALA GLN GLU LYS TYR SER LYS MET GLU LYS GLU LEU LYS GLU ARG

GLU PHE ASN TYR LYS ILE SER GLU SER LYS LEU GLU ASP GLU LYS THR THR LEU ASN GLU LYS ILE SER ASN LEU ALA ALA GLU ASN SER GLN LEU LYS ASN LYS ILE GLU ASP ASN SER THR ALA THR HIS HIS MET LYS GLU ASN TYR GLU LYS GLN LEU GLU SER LEU ARG LYS ASP

ILE GLU GLU TYR LYS GLU SER ALA LYS ASP SER GLU ASP LYS ILE GLU GLU LEU LYS ILE ARG ILE ALA GLU ASN SER ALA LYS VAL SER GLU LYS ARG SER LYS ASP ILE LYS GLN LYS ASP GLU GLN ILE SER ASP LEU THR GLN ASN LEU LYS LEU GLN GLU ASP GLU ILE SER SER

LEU LYS SER ILE ILE ASP ARG TYR LYS LYS ASP PHE ASN GLN LEU LYS SER GLU GLN SER ASN ILE GLN HIS ASP LEU ASN LEU GLN ILE LEU ASN LEU GLU ASN LYS LEU ILE GLU SER GLU ASP GLU LEU LYS SER LEU ARG ASP SER GLN LYS ILE GLU ILE GLU ASN TRP LYS ARG

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

ASN ASP ARG LEU ARG ARG GLU LYS GLU GLU LEU ASN GLU ASN SER ASN ASN ILE ARG ILE MET GLU ASP LYS MET THR ARG ILE LYS LYS ASN TYR LEU SER GLU ILE THR SER LEU GLN GLU GLU ASN ARG ARG LEU GLU GLU ARG LEU ILE LEU ASN GLU ARG ARG LYS ASP ASN ASP

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

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

TYR ARG ARG SER ASP ASP ASN ARG LEU ARG ILE LEU ARG ASP ARG ILE GLU SER SER SER GLY ARG ILE SER TRP

- Molecule 6: Spindle pole body component 110

Chain Sb: 6% 93%

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

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

GLU GLN GLU VAL ARG GLU HIS GLN MET LYS LYS GLU ARG PHE ASP ARG ALA LEU GLU SER LYS LEU LEU GLY K145 R146 D154 I155 S156 L168 E171 I172 K173 R176 K177 D181 T188 E191 E192 T193 D194 D195 L196 K197 N198 R199 L200 Q201 A202 L203 E204 K205 E206

LEU ASP ALA LYS ASN LYS ILE VAL ASN SER ARG LYS VAL ASP ASP HIS SER GLY CYS ILE GLU GLU ARG GLU GLN MET GLU ARG LYS LEU ALA GLU LEU GLU ARG LYS LEU LYS THR VAL LYS ASP GLN VAL LEU GLU LEU GLU ASN ASN SER ASP VAL GLN SER LEU LYS LEU ARG SER

LYS GLU ASP GLU LEU LYS ASN LEU MET ASN GLU LEU ASN GLU LEU LYS SER ASN ALA GLU GLU LYS ASP THR GLN LEU GLU PHE LYS LYS ASN GLU LEU ARG LYS ARG THR ASN GLU LEU ASN GLU LEU LYS ILE LYS SER ASP GLU MET ASP LEU GLN LEU LYS GLN LYS GLN ASN GLU

SER LYS ARG LEU LYS ASP GLU LEU ASN GLU LEU GLU THR LYS PHE SER GLU ASN GLY SER GLN SER SER ALA LYS GLU ASN GLU LEU LYS MET LEU LYS ASN LYS ILE ALA GLU LEU GLU GLU GLU ILE SER THR LYS ASN SER GLN LEU ILE ALA LYS GLU GLY LYS LEU ALA SER LEU

MET ALA GLN LEU THR GLN LEU GLU SER LYS LEU ASN GLN ARG ASP SER GLN LEU GLY SER ARG GLU GLU GLU LEU LYS LYS THR ASN ASP LYS LEU GLN LYS ASP ILE ARG ILE ALA ARG GLU GLU THR VAL SER LYS ASP GLU ARG ILE ILE ASP LEU GLN LYS LYS VAL LYS GLN LEU

GLU ASN ASP LEU PHE VAL ILE LYS LYS THR HIS SER GLU SER LYS THR ILE THR ASP ASN GLU LEU GLU SER LYS ASP LYS LEU ILE LYS ILE LEU GLU ASN ASP LEU LYS VAL ALA GLN GLU LYS TYR SER LYS MET GLU LYS GLU LEU LYS GLU ARG GLU PHE ASN TYR LYS ILE SER

GLU SER LYS LEU GLU ASP GLU LYS THR THR LEU ASN GLU LYS ILE SER ASN LEU ALA ALA GLU ASN SER GLN LEU LYS ASN LYS ILE GLU ASP ASN SER THR ALA THR HIS HIS MET LYS GLU ASN TYR GLU LYS GLN LEU GLU SER LEU ARG LYS ASP ILE GLU GLU TYR LYS GLU SER

ALA LYS ASP SER GLU ASP LYS ILE GLU GLU LEU LYS ILE ARG ILE ALA GLU ASN SER ALA LYS VAL SER GLU LYS ARG SER LYS ASP ILE LYS GLN LYS ASP GLU GLN ILE SER ASP LEU THR GLN ASN LEU LYS LEU GLN GLU ASP GLU ILE SER SER LEU LYS SER ILE ILE ASP ARG

TYR LYS LYS ASP PHE ASN GLN LEU LYS SER GLU GLN SER ASN ILE GLN HIS ASP LEU ASN LEU GLN ILE LEU ASN LEU GLU ASN LYS LEU ILE GLU SER GLU ASP GLU LEU LYS SER LEU ARG ASP SER GLN LYS ILE GLU ILE GLU ASN TRP LYS ARG LYS TYR ASN ASN LEU SER LEU

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

LYS GLU GLU LEU ASN GLU ASN SER ASN ASN ILE ARG ILE MET GLU ASP LYS MET THR ARG ILE LYS LYS ASN TYR LEU SER GLU ILE THR SER LEU GLN GLU GLU ASN ARG ARG LEU GLU GLU ARG LEU ILE LEU ASN GLU ARG ARG LYS ASP ASN ASP SER THR MET GLN LEU ASN ASP

ILE ILE SER TYR TYR LYS LEU LYS TYR HIS SER GLU VAL ARG HIS ASN ASN ASP LEU LYS VAL ILE ASN ASP TYR LEU ASN LYS VAL LEU ALA LEU GLY THR ARG ARG LEU ARG LEU ASP THR ARG LYS GLY GLU HIS SER LEU ASN ILE SER LEU PRO ASP ASP ASP GLU LEU ASP ARG

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

ARG LEU ARG ILE LEU ARG ASP ARG ILE GLU SER SER SER GLY ARG ILE SER TRP

- Molecule 6: Spindle pole body component 110

Chain Sm: 98%

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

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

GLU GLN GLU VAL ARG GLU HIS GLN MET LYS LYS GLU ARG PHE ASP ARG ALA LEU GLU SER LYS LEU LEU GLY LYS ARG HIS ILE THR TYR ALA ASN SER ASP ILE SER ASN LYS GLU LEU TYR ILE ASN E164 I165 K166 K169 D181 T182 L183 ASN ASN TYR ASP THR LEU GLU GLU

GLU THR ASP ASP LEU LYS ASN ARG LEU GLN ALA LEU GLU LYS GLU LEU ASP ALA LYS ASN LYS ILE VAL ASN SER ARG LYS VAL ASP ASP HIS SER GLY CYS ILE GLU GLU ARG GLU GLN MET GLU ARG LYS LEU ALA GLU LEU GLU ARG LYS LEU LYS THR VAL LYS ASP GLN VAL LEU

GLU LEU GLU ASN ASN SER ASP VAL GLN SER LEU LYS LEU ARG SER LYS GLU ASP GLU LEU LYS ASN LEU MET ASN GLU LEU ASN GLU LEU LYS SER ASN ALA GLU GLU LYS ASP THR GLN LEU GLU PHE LYS LYS ASN GLU LEU ARG LYS ARG THR ASN GLU LEU ASN GLU LEU LYS ILE

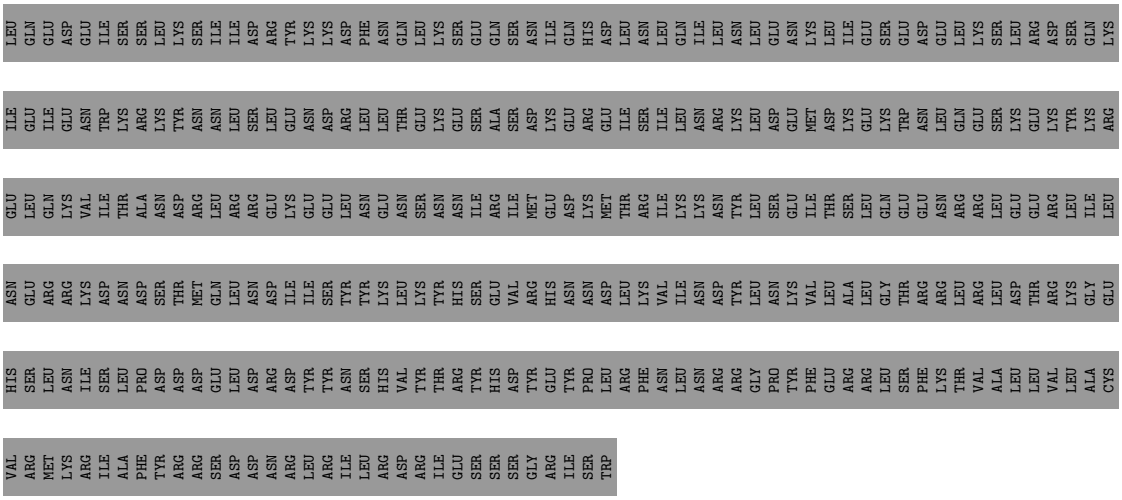
LYS SER ASP GLU MET ASP LEU GLN LEU LYS GLN LYS GLN ASN GLU SER LYS ARG LEU LYS ASP GLU LEU ASN GLU LEU GLU THR LYS PHE SER GLU ASN GLY SER GLN SER SER ALA LYS GLU ASN GLU LEU LYS MET LEU LYS ASN LYS ILE ALA GLU LEU GLU GLU GLU ILE SER THR

LYS ASN SER GLN LEU ILE ALA LYS GLU GLY LYS LEU ALA SER LEU MET ALA GLN LEU THR GLN LEU GLU SER LYS LEU ASN GLN ARG ASP SER GLN LEU GLY SER ARG GLU GLU GLU LEU LYS LYS THR ASN ASP LYS LEU GLN LYS ASP ILE ARG ILE ALA ARG GLU GLU THR VAL SER

LYS ASP GLU ARG ILE ILE ASP LEU GLN LYS LYS VAL LYS GLN LEU GLU ASN ASP LEU PHE VAL ILE LYS LYS THR HIS SER GLU SER LYS THR ILE THR ASP ASN GLU LEU GLU SER LYS ASP LYS LEU ILE LYS ILE LEU GLU ASN ASP LEU LYS VAL ALA GLN GLU LYS TYR SER LYS

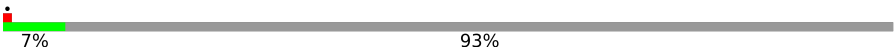
MET GLU LYS GLU LEU LYS GLU ARG GLU PHE ASN TYR LYS ILE SER GLU SER LYS LEU GLU ASP GLU LYS THR THR LEU ASN GLU LYS ILE SER ASN LEU ALA ALA GLU ASN SER GLN LEU LYS ASN LYS ILE GLU ASP ASN SER THR ALA THR HIS HIS MET LYS GLU ASN TYR GLU LYS

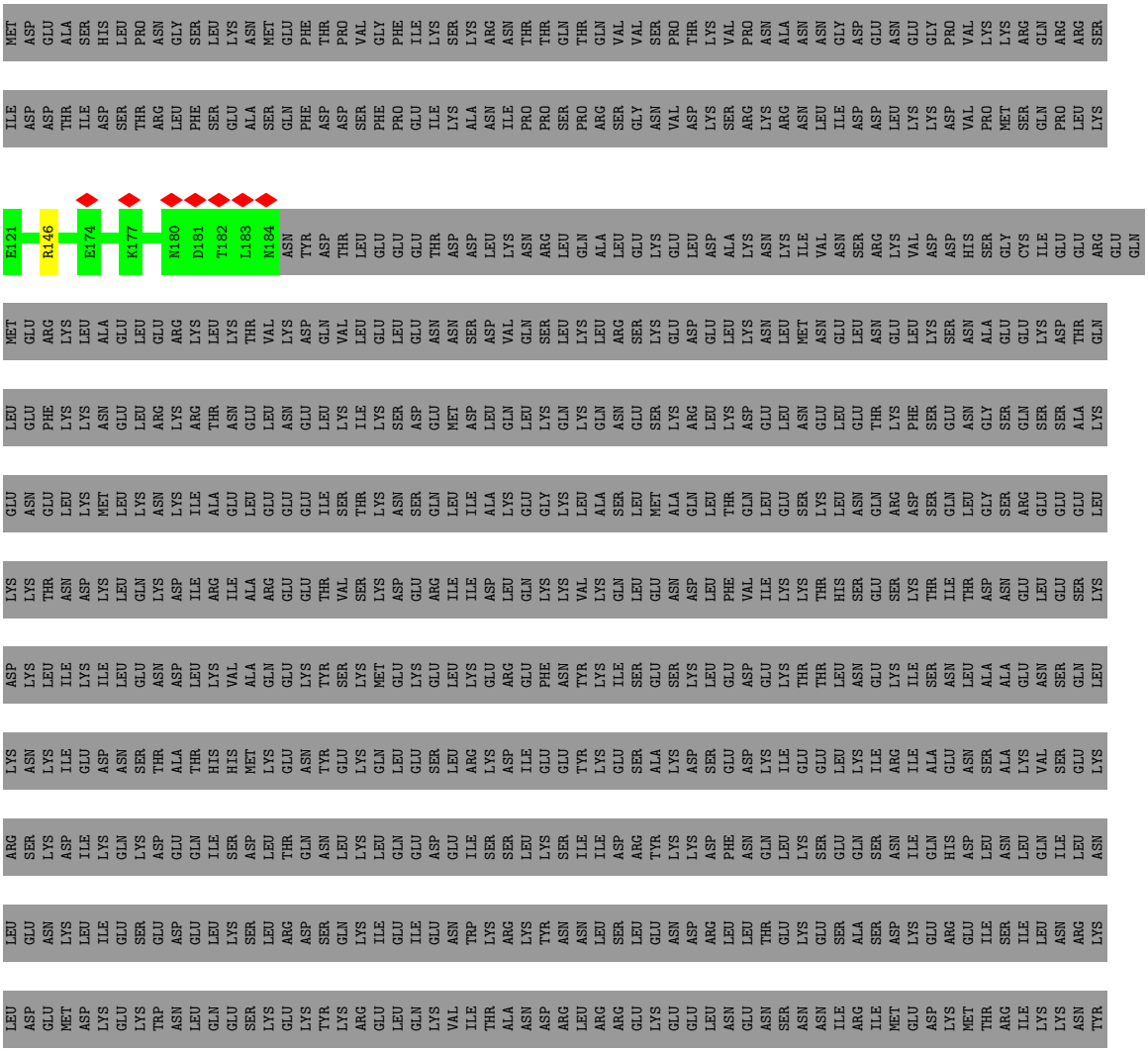
GLN LEU GLU SER LEU ARG LYS ASP ILE GLU GLU TYR LYS GLU SER ALA LYS ASP SER GLU ASP LYS ILE GLU GLU LEU LYS ILE ARG ILE ALA GLU ASN SER ALA LYS VAL SER GLU LYS ARG SER LYS ASP ILE LYS GLN LYS ASP GLU GLN ILE SER ASP LEU THR GLN ASN LEU LYS

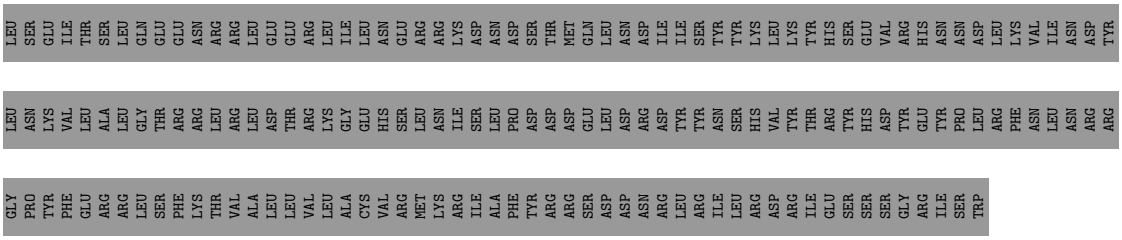


• Molecule 6: Spindle pole body component 110

Chain Sn:

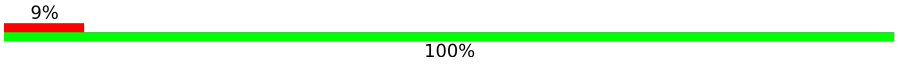


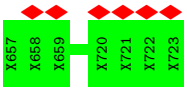




- Molecule 7: Unkown protein

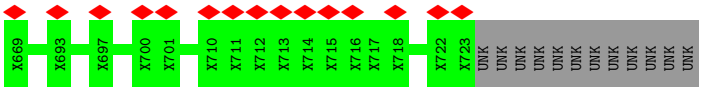
Chain Ue:





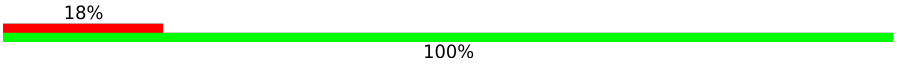
- Molecule 7: Unkown protein

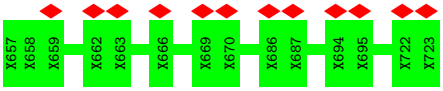
Chain Uf:



- Molecule 7: Unkown protein

Chain Ui:





- Molecule 7: Unkown protein

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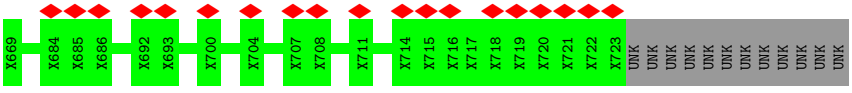

- Molecule 7: Unkown protein

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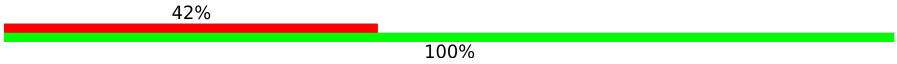
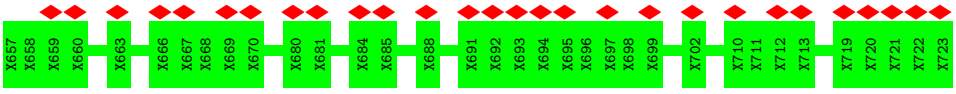
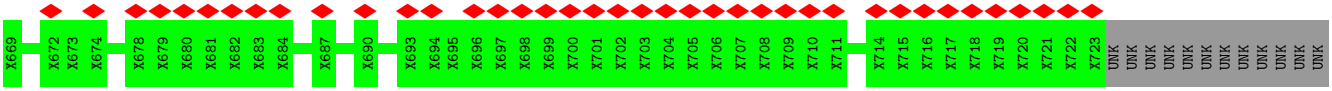




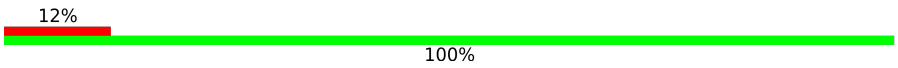
- Molecule 7: Unkown protein

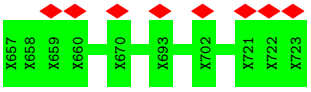
Chain Un:



• Molecule 7: Unkown protein

Chain Ua:





• Molecule 7: Unkown protein

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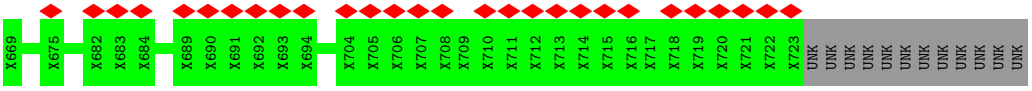
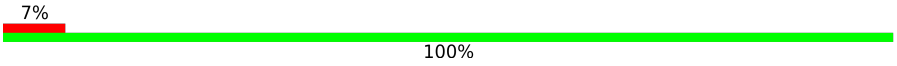
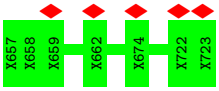


• Molecule 7: Unkown protein

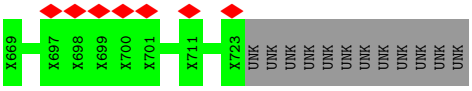
Chain Ug:





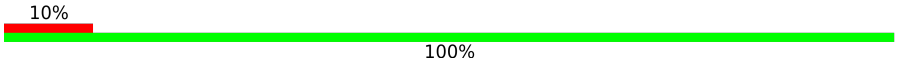
• Molecule 7: Unkown protein

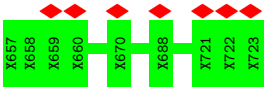
Chain Uh:



• Molecule 7: Unkown protein

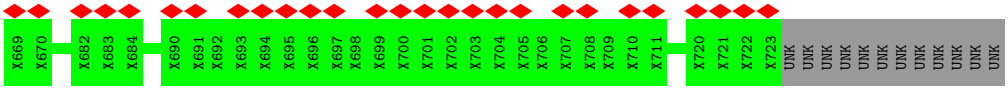
Chain Uk:





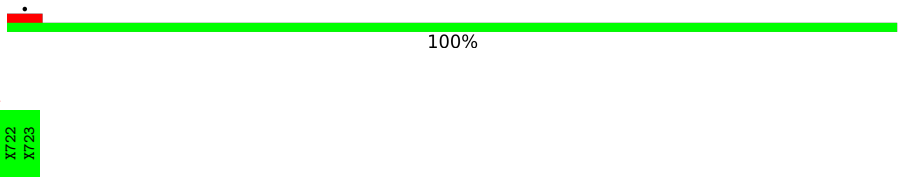
• Molecule 7: Unkown protein

Chain Ul:



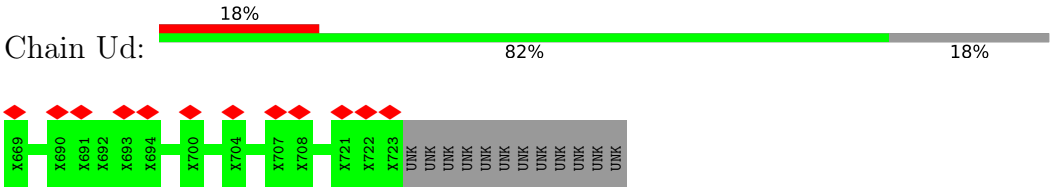
• Molecule 7: Unkown protein

Chain Uc:



• Molecule 7: Unkown protein

Chain Ud:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	7910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	123	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.814	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.243	Depositor
Map size (Å)	554.39996, 554.39996, 554.39996	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.2999997, 3.2999997, 3.2999997	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.24	0/3513	0.41	0/4769
1	b	0.24	0/3620	0.40	0/4917
1	c	0.24	0/3520	0.40	0/4779
1	d	0.24	0/3620	0.40	0/4917
1	e	0.24	0/3504	0.40	0/4757
1	f	0.24	0/3620	0.40	0/4917
1	g	0.24	0/3520	0.40	0/4779
1	h	0.24	0/3620	0.40	0/4917
1	i	0.24	0/3504	0.40	0/4757
1	j	0.24	0/3620	0.39	0/4917
1	k	0.24	0/3520	0.40	0/4779
1	l	0.24	0/3620	0.39	0/4917
1	m	0.24	0/3504	0.40	0/4757
1	n	0.24	0/3620	0.40	0/4917
2	C	0.95	6/5890 (0.1%)	0.42	1/7949 (0.0%)
2	E	0.24	0/5961	0.38	0/8045
2	G	0.23	0/5961	0.38	0/8045
2	I	0.23	0/5961	0.38	0/8045
2	K	0.23	0/5961	0.38	0/8045
2	M	0.23	0/5961	0.38	0/8045
2	O	0.23	0/5961	0.38	0/8045
3	D	0.25	0/5507	0.36	0/7443
3	F	0.24	0/5676	0.37	0/7672
3	H	0.24	0/5676	0.36	0/7672
3	J	0.24	0/5676	0.36	0/7672
3	L	0.24	0/5676	0.36	0/7672
3	N	0.24	0/5676	0.36	0/7672
3	P	0.24	0/5676	0.37	0/7672
4	Ab	0.24	0/3384	0.40	0/4589
4	Ac	0.25	0/3514	0.41	0/4766
4	Ad	0.25	0/3514	0.41	0/4766
4	Ae	0.25	0/3514	0.41	0/4766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	Af	0.24	0/3514	0.41	0/4766
4	Ag	0.25	0/3514	0.41	0/4766
4	Ah	0.24	0/3514	0.41	0/4766
4	Ai	0.24	0/3514	0.39	0/4766
4	Aj	0.24	0/3514	0.39	0/4766
4	Ak	0.24	0/3514	0.40	0/4766
4	Al	0.24	0/3514	0.40	0/4766
4	Am	0.24	0/3514	0.40	0/4766
4	An	0.24	0/3514	0.40	0/4766
4	Ao	0.24	0/3514	0.41	0/4766
4	Ap	0.87	6/3514 (0.2%)	0.41	0/4766
4	Aq	0.24	0/3514	0.41	0/4766
4	Ar	0.24	0/3514	0.39	0/4766
5	Bb	0.25	0/3318	0.42	0/4493
5	Bc	1.23	1/3416 (0.0%)	0.45	2/4627 (0.0%)
5	Bd	0.25	0/3416	0.42	0/4627
5	Be	0.24	0/3416	0.41	0/4627
5	Bf	0.24	0/3416	0.41	0/4627
5	Bg	0.24	0/3416	0.41	0/4627
5	Bh	0.24	0/3416	0.41	0/4627
5	Bi	0.24	0/3416	0.40	0/4627
5	Bj	0.24	0/3416	0.41	0/4627
5	Bk	0.24	0/3416	0.40	0/4627
5	Bl	0.24	0/3416	0.41	0/4627
5	Bm	0.24	0/3416	0.40	0/4627
5	Bn	0.24	0/3416	0.42	0/4627
5	Bo	0.24	0/3416	0.40	0/4627
5	Bp	0.24	0/3416	0.41	0/4627
5	Bq	0.24	0/3416	0.40	0/4627
5	Br	0.24	0/3416	0.41	0/4627
6	Sa	0.23	0/353	0.39	0/471
6	Sb	0.22	0/521	0.39	0/698
6	Sc	0.22	0/353	0.35	0/471
6	Sd	0.22	0/720	0.36	0/960
6	Se	0.22	0/353	0.36	0/471
6	Sf	0.22	0/729	0.35	0/972
6	Sg	0.22	0/353	0.36	0/471
6	Sh	0.22	0/720	0.35	0/960
6	Si	0.21	0/353	0.34	0/471
6	Sj	0.22	0/729	0.36	0/972
6	Sk	0.22	0/353	0.38	0/471
6	Sl	0.22	0/720	0.36	0/960
6	Sm	0.23	0/171	0.35	0/224

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	Sn	0.22	0/550	0.39	0/729
All	All	0.33	13/255704 (0.0%)	0.39	3/346161 (0.0%)

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
4	Ab	0	2
4	Ac	0	2
4	Ad	0	2
4	Ae	0	2
4	Af	0	2
4	Ag	0	2
4	Ah	0	2
4	Ai	0	2
4	Aj	0	2
4	Ak	0	2
4	Al	0	2
4	Am	0	2
4	An	0	2
4	Ao	0	2
4	Ap	0	1
4	Aq	0	3
4	Ar	0	1
5	Bb	0	1
5	Bd	0	1
5	Bf	0	1
5	Bh	0	1
5	Bj	0	1
5	Bl	0	1
5	Bn	0	1
All	All	0	40

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Bc	391	ARG	CB-CG	70.11	3.41	1.52
2	C	320	TRP	CE3-CZ3	51.60	2.26	1.38
4	Ap	347	TRP	CE3-CZ3	33.02	1.94	1.38
2	C	320	TRP	CZ3-CH2	28.17	1.85	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	320	TRP	CE2-CZ2	26.02	1.83	1.39
2	C	320	TRP	CD2-CE2	21.08	1.66	1.41
4	Ap	347	TRP	CZ3-CH2	21.06	1.73	1.40
4	Ap	347	TRP	CE2-CZ2	19.22	1.72	1.39
4	Ap	347	TRP	CD2-CE2	16.31	1.60	1.41
2	C	320	TRP	CZ2-CH2	14.93	1.65	1.37
2	C	320	TRP	CD2-CE3	14.19	1.61	1.40
4	Ap	347	TRP	CD2-CE3	11.46	1.57	1.40
4	Ap	347	TRP	CZ2-CH2	11.16	1.58	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Bc	391	ARG	CA-CB-CG	8.95	133.09	113.40
2	C	320	TRP	CE3-CZ3-CH2	-7.12	113.37	121.20
5	Bc	391	ARG	CB-CG-CD	7.04	129.91	111.60

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Ab	35	HIS	Peptide
4	Ab	36	LEU	Peptide
4	Ac	35	HIS	Peptide
4	Ac	36	LEU	Peptide
4	Ad	35	HIS	Peptide
4	Ad	36	LEU	Peptide
4	Ae	35	HIS	Peptide
4	Ae	36	LEU	Peptide
4	Af	35	HIS	Peptide
4	Af	36	LEU	Peptide
4	Ag	35	HIS	Peptide
4	Ag	36	LEU	Peptide
4	Ah	35	HIS	Peptide
4	Ah	36	LEU	Peptide
4	Ai	35	HIS	Peptide
4	Ai	36	LEU	Peptide
4	Aj	35	HIS	Peptide
4	Aj	36	LEU	Peptide
4	Ak	35	HIS	Peptide
4	Ak	36	LEU	Peptide
4	Al	35	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	Al	36	LEU	Peptide
4	Am	35	HIS	Peptide
4	Am	36	LEU	Peptide
4	An	35	HIS	Peptide
4	An	36	LEU	Peptide
4	Ao	35	HIS	Peptide
4	Ao	36	LEU	Peptide
4	Ap	348	CYS	Peptide
4	Aq	348	CYS	Peptide
4	Aq	35	HIS	Peptide
4	Aq	36	LEU	Peptide
4	Ar	348	CYS	Peptide
5	Bb	424	GLN	Peptide
5	Bd	424	GLN	Peptide
5	Bf	424	GLN	Peptide
5	Bh	424	GLN	Peptide
5	Bj	424	GLN	Peptide
5	Bl	424	GLN	Peptide
5	Bn	424	GLN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	436/473 (92%)	419 (96%)	17 (4%)	0	100	100
1	b	451/473 (95%)	444 (98%)	7 (2%)	0	100	100
1	c	437/473 (92%)	431 (99%)	6 (1%)	0	100	100
1	d	451/473 (95%)	444 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	435/473 (92%)	428 (98%)	7 (2%)	0	100	100
1	f	451/473 (95%)	441 (98%)	10 (2%)	0	100	100
1	g	437/473 (92%)	428 (98%)	9 (2%)	0	100	100
1	h	451/473 (95%)	443 (98%)	8 (2%)	0	100	100
1	i	435/473 (92%)	428 (98%)	7 (2%)	0	100	100
1	j	451/473 (95%)	443 (98%)	8 (2%)	0	100	100
1	k	437/473 (92%)	428 (98%)	9 (2%)	0	100	100
1	l	451/473 (95%)	444 (98%)	7 (2%)	0	100	100
1	m	435/473 (92%)	428 (98%)	7 (2%)	0	100	100
1	n	451/473 (95%)	445 (99%)	6 (1%)	0	100	100
2	C	681/823 (83%)	648 (95%)	33 (5%)	0	100	100
2	E	689/823 (84%)	675 (98%)	14 (2%)	0	100	100
2	G	689/823 (84%)	674 (98%)	15 (2%)	0	100	100
2	I	689/823 (84%)	674 (98%)	15 (2%)	0	100	100
2	K	689/823 (84%)	676 (98%)	13 (2%)	0	100	100
2	M	689/823 (84%)	672 (98%)	17 (2%)	0	100	100
2	O	689/823 (84%)	678 (98%)	11 (2%)	0	100	100
3	D	645/846 (76%)	623 (97%)	22 (3%)	0	100	100
3	F	668/846 (79%)	651 (98%)	17 (2%)	0	100	100
3	H	668/846 (79%)	646 (97%)	22 (3%)	0	100	100
3	J	668/846 (79%)	649 (97%)	19 (3%)	0	100	100
3	L	668/846 (79%)	646 (97%)	22 (3%)	0	100	100
3	N	668/846 (79%)	646 (97%)	22 (3%)	0	100	100
3	P	668/846 (79%)	650 (97%)	18 (3%)	0	100	100
4	Ab	419/447 (94%)	396 (94%)	22 (5%)	1 (0%)	47	81
4	Ac	438/447 (98%)	408 (93%)	28 (6%)	2 (0%)	29	69
4	Ad	438/447 (98%)	408 (93%)	28 (6%)	2 (0%)	29	69
4	Ae	438/447 (98%)	410 (94%)	26 (6%)	2 (0%)	29	69
4	Af	438/447 (98%)	410 (94%)	26 (6%)	2 (0%)	29	69
4	Ag	438/447 (98%)	410 (94%)	27 (6%)	1 (0%)	47	81
4	Ah	438/447 (98%)	412 (94%)	24 (6%)	2 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ai	438/447 (98%)	410 (94%)	28 (6%)	0	100	100
4	Aj	438/447 (98%)	413 (94%)	25 (6%)	0	100	100
4	Ak	438/447 (98%)	411 (94%)	25 (6%)	2 (0%)	29	69
4	Al	438/447 (98%)	414 (94%)	24 (6%)	0	100	100
4	Am	438/447 (98%)	412 (94%)	26 (6%)	0	100	100
4	An	438/447 (98%)	415 (95%)	23 (5%)	0	100	100
4	Ao	438/447 (98%)	413 (94%)	25 (6%)	0	100	100
4	Ap	438/447 (98%)	421 (96%)	17 (4%)	0	100	100
4	Aq	438/447 (98%)	414 (94%)	22 (5%)	2 (0%)	29	69
4	Ar	438/447 (98%)	423 (97%)	15 (3%)	0	100	100
5	Bb	410/457 (90%)	398 (97%)	12 (3%)	0	100	100
5	Bc	425/457 (93%)	415 (98%)	10 (2%)	0	100	100
5	Bd	425/457 (93%)	410 (96%)	15 (4%)	0	100	100
5	Be	425/457 (93%)	411 (97%)	14 (3%)	0	100	100
5	Bf	425/457 (93%)	414 (97%)	11 (3%)	0	100	100
5	Bg	425/457 (93%)	416 (98%)	9 (2%)	0	100	100
5	Bh	425/457 (93%)	413 (97%)	12 (3%)	0	100	100
5	Bi	425/457 (93%)	416 (98%)	9 (2%)	0	100	100
5	Bj	425/457 (93%)	411 (97%)	14 (3%)	0	100	100
5	Bk	425/457 (93%)	417 (98%)	8 (2%)	0	100	100
5	Bl	425/457 (93%)	412 (97%)	13 (3%)	0	100	100
5	Bm	425/457 (93%)	416 (98%)	9 (2%)	0	100	100
5	Bn	425/457 (93%)	412 (97%)	13 (3%)	0	100	100
5	Bo	425/457 (93%)	419 (99%)	6 (1%)	0	100	100
5	Bp	425/457 (93%)	418 (98%)	7 (2%)	0	100	100
5	Bq	425/457 (93%)	420 (99%)	5 (1%)	0	100	100
5	Br	425/457 (93%)	418 (98%)	7 (2%)	0	100	100
6	Sa	40/944 (4%)	40 (100%)	0	0	100	100
6	Sb	60/944 (6%)	60 (100%)	0	0	100	100
6	Sc	40/944 (4%)	40 (100%)	0	0	100	100
6	Sd	83/944 (9%)	81 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Se	40/944 (4%)	40 (100%)	0	0	100	100
6	Sf	84/944 (9%)	82 (98%)	2 (2%)	0	100	100
6	Sg	40/944 (4%)	40 (100%)	0	0	100	100
6	Sh	83/944 (9%)	81 (98%)	2 (2%)	0	100	100
6	Si	40/944 (4%)	40 (100%)	0	0	100	100
6	Sj	84/944 (9%)	82 (98%)	2 (2%)	0	100	100
6	Sk	40/944 (4%)	40 (100%)	0	0	100	100
6	Sl	83/944 (9%)	81 (98%)	2 (2%)	0	100	100
6	Sm	18/944 (2%)	18 (100%)	0	0	100	100
6	Sn	62/944 (7%)	60 (97%)	2 (3%)	0	100	100
All	All	31111/46889 (66%)	30123 (97%)	972 (3%)	16 (0%)	54	86

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Af	404	ALA
4	Ae	404	ALA
4	Ad	404	ALA
4	Ac	404	ALA
4	Ah	404	ALA
4	Ag	404	ALA
4	Aq	404	ALA
4	Ad	403	ARG
4	Ac	403	ARG
4	Af	403	ARG
4	Ah	403	ARG
4	Aq	403	ARG
4	Ae	403	ARG
4	Ak	403	ARG
4	Ak	404	ALA
4	Ab	404	ALA

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	391/420 (93%)	389 (100%)	2 (0%)	88 93
1	b	403/420 (96%)	403 (100%)	0	100 100
1	c	392/420 (93%)	392 (100%)	0	100 100
1	d	403/420 (96%)	403 (100%)	0	100 100
1	e	391/420 (93%)	391 (100%)	0	100 100
1	f	403/420 (96%)	403 (100%)	0	100 100
1	g	392/420 (93%)	392 (100%)	0	100 100
1	h	403/420 (96%)	403 (100%)	0	100 100
1	i	391/420 (93%)	391 (100%)	0	100 100
1	j	403/420 (96%)	403 (100%)	0	100 100
1	k	392/420 (93%)	392 (100%)	0	100 100
1	l	403/420 (96%)	403 (100%)	0	100 100
1	m	391/420 (93%)	391 (100%)	0	100 100
1	n	403/420 (96%)	403 (100%)	0	100 100
2	C	649/766 (85%)	647 (100%)	2 (0%)	92 95
2	E	658/766 (86%)	656 (100%)	2 (0%)	92 95
2	G	658/766 (86%)	656 (100%)	2 (0%)	92 95
2	I	658/766 (86%)	656 (100%)	2 (0%)	92 95
2	K	658/766 (86%)	656 (100%)	2 (0%)	92 95
2	M	658/766 (86%)	657 (100%)	1 (0%)	93 96
2	O	658/766 (86%)	657 (100%)	1 (0%)	93 96
3	D	607/787 (77%)	603 (99%)	4 (1%)	84 90
3	F	626/787 (80%)	626 (100%)	0	100 100
3	H	626/787 (80%)	626 (100%)	0	100 100
3	J	626/787 (80%)	626 (100%)	0	100 100
3	L	626/787 (80%)	626 (100%)	0	100 100
3	N	626/787 (80%)	626 (100%)	0	100 100
3	P	626/787 (80%)	626 (100%)	0	100 100
4	Ab	359/381 (94%)	357 (99%)	2 (1%)	86 92
4	Ac	375/381 (98%)	373 (100%)	2 (0%)	88 93
4	Ad	375/381 (98%)	373 (100%)	2 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Ae	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Af	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ag	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ah	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ai	375/381 (98%)	373 (100%)	2 (0%)	88	93
4	Aj	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ak	375/381 (98%)	373 (100%)	2 (0%)	88	93
4	Al	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Am	375/381 (98%)	373 (100%)	2 (0%)	88	93
4	An	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ao	375/381 (98%)	375 (100%)	0	100	100
4	Ap	375/381 (98%)	375 (100%)	0	100	100
4	Aq	375/381 (98%)	374 (100%)	1 (0%)	92	95
4	Ar	375/381 (98%)	375 (100%)	0	100	100
5	Bb	355/392 (91%)	355 (100%)	0	100	100
5	Bc	366/392 (93%)	366 (100%)	0	100	100
5	Bd	366/392 (93%)	366 (100%)	0	100	100
5	Be	366/392 (93%)	366 (100%)	0	100	100
5	Bf	366/392 (93%)	366 (100%)	0	100	100
5	Bg	366/392 (93%)	366 (100%)	0	100	100
5	Bh	366/392 (93%)	366 (100%)	0	100	100
5	Bi	366/392 (93%)	366 (100%)	0	100	100
5	Bj	366/392 (93%)	366 (100%)	0	100	100
5	Bk	366/392 (93%)	366 (100%)	0	100	100
5	Bl	366/392 (93%)	366 (100%)	0	100	100
5	Bm	366/392 (93%)	366 (100%)	0	100	100
5	Bn	366/392 (93%)	366 (100%)	0	100	100
5	Bo	366/392 (93%)	366 (100%)	0	100	100
5	Bp	366/392 (93%)	366 (100%)	0	100	100
5	Bq	366/392 (93%)	366 (100%)	0	100	100
5	Br	366/392 (93%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	Sa	40/901 (4%)	40 (100%)	0	100 100
6	Sb	58/901 (6%)	57 (98%)	1 (2%)	60 78
6	Sc	40/901 (4%)	40 (100%)	0	100 100
6	Sd	79/901 (9%)	78 (99%)	1 (1%)	69 81
6	Se	40/901 (4%)	40 (100%)	0	100 100
6	Sf	80/901 (9%)	79 (99%)	1 (1%)	69 81
6	Sg	40/901 (4%)	40 (100%)	0	100 100
6	Sh	79/901 (9%)	78 (99%)	1 (1%)	69 81
6	Si	40/901 (4%)	40 (100%)	0	100 100
6	Sj	80/901 (9%)	79 (99%)	1 (1%)	69 81
6	Sk	40/901 (4%)	40 (100%)	0	100 100
6	Sl	79/901 (9%)	78 (99%)	1 (1%)	69 81
6	Sm	20/901 (2%)	20 (100%)	0	100 100
6	Sn	61/901 (7%)	60 (98%)	1 (2%)	62 79
All	All	27867/42506 (66%)	27822 (100%)	45 (0%)	93 96

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	9	ARG
2	C	171	ARG
3	D	670	ARG
3	D	694	ILE
3	D	696	THR
3	D	702	LEU
2	E	14	ARG
2	E	269	LYS
2	G	14	ARG
2	G	269	LYS
2	I	14	ARG
2	I	269	LYS
2	K	14	ARG
2	K	269	LYS
2	M	269	LYS
2	O	14	ARG
1	a	165	LYS
1	a	400	LYS

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Mol	Chain	Res	Type
4	Ad	113	ARG
4	Ad	403	ARG
4	Ac	113	ARG
4	Ac	403	ARG
4	Af	113	ARG
4	Ae	113	ARG
4	Ah	113	ARG
4	Ag	113	ARG
4	Aj	113	ARG
4	Ai	113	ARG
4	Ai	403	ARG
4	Al	113	ARG
4	Ak	113	ARG
4	Ak	403	ARG
4	An	113	ARG
4	Am	113	ARG
4	Am	403	ARG
4	Ab	113	ARG
4	Ab	403	ARG
6	Sd	146	ARG
6	Sf	146	ARG
6	Sh	146	ARG
6	Sj	146	ARG
6	Sl	146	ARG
6	Sb	146	ARG
6	Sn	146	ARG
4	Aq	403	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (426) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	9	GLN
1	b	38	GLN
1	b	81	ASN
1	b	137	GLN
1	b	228	ASN
1	b	303	ASN
1	b	320	ASN
1	b	330	GLN
1	b	339	GLN
1	c	9	GLN
1	c	15	ASN

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Mol	Chain	Res	Type
1	c	229	GLN
1	c	320	ASN
1	c	339	GLN
1	d	9	GLN
1	d	81	ASN
1	d	137	GLN
1	d	140	HIS
1	d	303	ASN
1	d	320	ASN
1	d	330	GLN
1	d	417	GLN
1	e	9	GLN
1	e	15	ASN
1	e	107	ASN
1	e	229	GLN
1	e	320	ASN
1	e	385	ASN
1	f	9	GLN
1	f	137	GLN
1	f	303	ASN
1	f	320	ASN
1	f	330	GLN
1	g	9	GLN
1	g	15	ASN
1	g	107	ASN
1	g	229	GLN
1	g	320	ASN
1	h	9	GLN
1	h	81	ASN
1	h	107	ASN
1	h	137	GLN
1	h	153	ASN
1	h	303	ASN
1	h	312	ASN
1	h	320	ASN
1	h	330	GLN
1	i	9	GLN
1	i	15	ASN
1	i	107	ASN
1	i	229	GLN
1	i	385	ASN
1	j	9	GLN

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Mol	Chain	Res	Type
1	j	137	GLN
1	j	303	ASN
1	j	320	ASN
1	j	330	GLN
1	k	9	GLN
1	k	15	ASN
1	k	107	ASN
1	k	229	GLN
1	k	320	ASN
1	l	9	GLN
1	l	81	ASN
1	l	137	GLN
1	l	140	HIS
1	l	153	ASN
1	l	303	ASN
1	l	320	ASN
1	l	330	GLN
1	m	9	GLN
1	m	15	ASN
1	m	107	ASN
1	m	229	GLN
1	m	320	ASN
1	m	385	ASN
1	n	9	GLN
1	n	81	ASN
1	n	107	ASN
1	n	137	GLN
1	n	303	ASN
1	n	320	ASN
1	n	330	GLN
1	n	392	ASN
2	C	35	ASN
2	C	559	HIS
2	C	648	ASN
3	D	169	GLN
3	D	380	HIS
3	D	534	ASN
3	D	642	GLN
3	D	729	ASN
3	D	808	ASN
2	E	55	GLN
2	E	485	GLN

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Mol	Chain	Res	Type
2	E	665	ASN
2	E	673	GLN
3	F	169	GLN
3	F	206	GLN
3	F	371	ASN
3	F	423	ASN
3	F	534	ASN
3	F	642	GLN
3	F	673	ASN
2	G	55	GLN
2	G	65	ASN
2	G	362	GLN
2	G	411	GLN
2	G	583	GLN
2	G	673	GLN
3	H	169	GLN
3	H	206	GLN
3	H	380	HIS
3	H	642	GLN
3	H	660	ASN
3	H	808	ASN
2	I	65	ASN
2	I	258	ASN
2	I	323	GLN
2	I	411	GLN
2	I	673	GLN
3	J	169	GLN
3	J	206	GLN
3	J	380	HIS
3	J	534	ASN
3	J	642	GLN
3	J	808	ASN
2	K	55	GLN
2	K	362	GLN
2	K	411	GLN
2	K	417	ASN
2	K	485	GLN
2	K	673	GLN
3	L	169	GLN
3	L	206	GLN
3	L	380	HIS
3	L	534	ASN

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Mol	Chain	Res	Type
3	L	642	GLN
3	L	685	ASN
3	L	808	ASN
2	M	55	GLN
2	M	222	ASN
2	M	258	ASN
2	M	485	GLN
2	M	673	GLN
3	N	169	GLN
3	N	206	GLN
3	N	380	HIS
3	N	534	ASN
3	N	642	GLN
3	N	808	ASN
2	O	55	GLN
2	O	379	ASN
2	O	485	GLN
2	O	583	GLN
2	O	665	ASN
3	P	169	GLN
3	P	206	GLN
3	P	269	ASN
3	P	270	ASN
3	P	380	HIS
3	P	423	ASN
3	P	642	GLN
3	P	808	ASN
1	a	9	GLN
1	a	29	HIS
1	a	60	ASN
1	a	103	ASN
1	a	153	ASN
1	a	228	ASN
1	a	355	ASN
1	a	370	ASN
4	Ad	92	GLN
4	Ad	207	ASN
4	Ad	230	ASN
4	Ad	259	ASN
4	Ad	330	GLN
4	Ad	335	GLN
4	Ad	366	ASN

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Mol	Chain	Res	Type
4	Ac	92	GLN
4	Ac	230	ASN
4	Ac	330	GLN
4	Ac	335	GLN
4	Ac	366	ASN
5	Bd	11	GLN
5	Bd	134	GLN
5	Bd	191	GLN
5	Bd	195	HIS
5	Bd	219	GLN
5	Bd	227	ASN
5	Bd	256	ASN
5	Bd	291	GLN
5	Bd	298	ASN
5	Bc	191	GLN
5	Bc	227	ASN
5	Bc	256	ASN
5	Bc	291	GLN
5	Bc	298	ASN
5	Bc	396	HIS
4	Af	92	GLN
4	Af	102	ASN
4	Af	207	ASN
4	Af	227	ASN
4	Af	259	ASN
4	Af	330	GLN
4	Af	335	GLN
4	Af	366	ASN
4	Ae	92	GLN
4	Ae	102	ASN
4	Ae	207	ASN
4	Ae	230	ASN
4	Ae	330	GLN
4	Ae	335	GLN
4	Ae	366	ASN
5	Bf	11	GLN
5	Bf	78	ASN
5	Bf	134	GLN
5	Bf	191	GLN
5	Bf	195	HIS
5	Bf	219	GLN
5	Bf	291	GLN

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Mol	Chain	Res	Type
5	Bf	298	ASN
5	Be	11	GLN
5	Be	191	GLN
5	Be	195	HIS
5	Be	227	ASN
5	Be	291	GLN
5	Be	298	ASN
5	Be	396	HIS
4	Ah	92	GLN
4	Ah	102	ASN
4	Ah	230	ASN
4	Ah	259	ASN
4	Ah	330	GLN
4	Ah	335	GLN
4	Ah	366	ASN
4	Ag	92	GLN
4	Ag	102	ASN
4	Ag	207	ASN
4	Ag	230	ASN
4	Ag	257	GLN
4	Ag	259	ASN
4	Ag	330	GLN
4	Ag	335	GLN
4	Ag	338	ASN
4	Ag	366	ASN
5	Bh	11	GLN
5	Bh	134	GLN
5	Bh	191	GLN
5	Bh	195	HIS
5	Bh	219	GLN
5	Bh	291	GLN
5	Bh	298	ASN
5	Bg	11	GLN
5	Bg	191	GLN
5	Bg	219	GLN
5	Bg	291	GLN
5	Bg	298	ASN
4	Aj	18	ASN
4	Aj	92	GLN
4	Aj	102	ASN
4	Aj	207	ASN
4	Aj	330	GLN

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Mol	Chain	Res	Type
4	Aj	335	GLN
4	Aj	366	ASN
4	Ai	18	ASN
4	Ai	55	HIS
4	Ai	92	GLN
4	Ai	129	GLN
4	Ai	207	ASN
4	Ai	230	ASN
4	Ai	330	GLN
4	Ai	335	GLN
4	Ai	366	ASN
5	Bj	11	GLN
5	Bj	134	GLN
5	Bj	191	GLN
5	Bj	195	HIS
5	Bj	219	GLN
5	Bj	291	GLN
5	Bj	298	ASN
5	Bi	191	GLN
5	Bi	219	GLN
5	Bi	256	ASN
5	Bi	291	GLN
5	Bi	298	ASN
4	Al	18	ASN
4	Al	92	GLN
4	Al	102	ASN
4	Al	207	ASN
4	Al	230	ASN
4	Al	259	ASN
4	Al	330	GLN
4	Al	335	GLN
4	Al	366	ASN
4	Ak	18	ASN
4	Ak	55	HIS
4	Ak	92	GLN
4	Ak	102	ASN
4	Ak	129	GLN
4	Ak	207	ASN
4	Ak	230	ASN
4	Ak	330	GLN
4	Ak	335	GLN
4	Ak	366	ASN

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Mol	Chain	Res	Type
5	Bl	11	GLN
5	Bl	78	ASN
5	Bl	134	GLN
5	Bl	191	GLN
5	Bl	195	HIS
5	Bl	219	GLN
5	Bl	245	GLN
5	Bl	291	GLN
5	Bl	298	ASN
5	Bk	131	GLN
5	Bk	191	GLN
5	Bk	219	GLN
5	Bk	291	GLN
5	Bk	298	ASN
4	An	55	HIS
4	An	102	ASN
4	An	129	GLN
4	An	207	ASN
4	An	259	ASN
4	An	330	GLN
4	An	335	GLN
4	An	366	ASN
4	Am	18	ASN
4	Am	92	GLN
4	Am	102	ASN
4	Am	129	GLN
4	Am	207	ASN
4	Am	230	ASN
4	Am	330	GLN
4	Am	335	GLN
4	Am	366	ASN
5	Bn	48	ASN
5	Bn	78	ASN
5	Bn	134	GLN
5	Bn	191	GLN
5	Bn	219	GLN
5	Bn	245	GLN
5	Bn	291	GLN
5	Bn	298	ASN
5	Bm	11	GLN
5	Bm	78	ASN
5	Bm	190	HIS

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Mol	Chain	Res	Type
5	Bm	191	GLN
5	Bm	219	GLN
5	Bm	256	ASN
5	Bm	291	GLN
5	Bm	298	ASN
4	Ab	18	ASN
4	Ab	74	ASN
4	Ab	92	GLN
4	Ab	207	ASN
4	Ab	259	ASN
4	Ab	330	GLN
4	Ab	335	GLN
4	Ab	338	ASN
4	Ab	366	ASN
5	Bb	134	GLN
5	Bb	191	GLN
5	Bb	195	HIS
5	Bb	212	GLN
5	Bb	256	ASN
5	Bb	291	GLN
5	Bb	396	HIS
6	Sd	152	ASN
6	Sd	170	HIS
6	Sf	152	ASN
6	Sh	152	ASN
6	Sh	180	ASN
6	Sj	152	ASN
6	Sl	152	ASN
6	Sb	185	ASN
6	Sb	201	GLN
6	Sm	180	ASN
6	Sn	152	ASN
4	Ap	18	ASN
4	Ap	129	GLN
4	Ap	234	GLN
4	Ap	330	GLN
4	Ap	381	ASN
4	Ao	74	ASN
4	Ao	92	GLN
4	Ao	102	ASN
4	Ao	129	GLN
4	Ao	177	GLN

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Mol	Chain	Res	Type
4	Ao	259	ASN
4	Ao	294	ASN
4	Ao	366	ASN
5	Bp	11	GLN
5	Bp	37	HIS
5	Bp	191	GLN
5	Bp	219	GLN
5	Bp	227	ASN
5	Bo	134	GLN
5	Bo	191	GLN
5	Bo	291	GLN
5	Bo	334	GLN
5	Bo	350	GLN
4	Ar	18	ASN
4	Ar	234	GLN
4	Ar	343	GLN
4	Ar	381	ASN
4	Aq	74	ASN
4	Aq	92	GLN
4	Aq	102	ASN
4	Aq	129	GLN
4	Aq	259	ASN
4	Aq	335	GLN
4	Aq	366	ASN
5	Br	48	ASN
5	Br	191	GLN
5	Br	219	GLN
5	Br	227	ASN
5	Br	291	GLN
5	Br	298	ASN
5	Bq	78	ASN
5	Bq	134	GLN
5	Bq	191	GLN
5	Bq	279	GLN
5	Bq	291	GLN
5	Bq	334	GLN
5	Bq	350	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
8	GTP	h	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.67	7 (21%)
8	GTP	f	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.65	7 (21%)
8	GTP	d	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.66	7 (21%)
8	GTP	j	501	-	26,34,34	1.11	2 (7%)	32,54,54	1.66	7 (21%)
8	GTP	e	501	-	26,34,34	1.10	2 (7%)	32,54,54	1.61	7 (21%)
8	GTP	b	501	-	26,34,34	1.11	2 (7%)	32,54,54	1.66	7 (21%)
8	GTP	g	501	-	26,34,34	1.11	2 (7%)	32,54,54	1.61	7 (21%)
8	GTP	l	501	-	26,34,34	1.11	2 (7%)	32,54,54	1.62	7 (21%)
8	GTP	k	501	-	26,34,34	1.10	2 (7%)	32,54,54	1.62	7 (21%)
8	GTP	c	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.61	7 (21%)
8	GTP	m	501	-	26,34,34	1.10	2 (7%)	32,54,54	1.63	7 (21%)
8	GTP	i	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.62	7 (21%)
8	GTP	n	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.66	7 (21%)
9	GDP	a	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)

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
8	GTP	h	501	-	-	5/18/38/38	0/3/3/3
8	GTP	f	501	-	-	4/18/38/38	0/3/3/3
8	GTP	d	501	-	-	4/18/38/38	0/3/3/3
8	GTP	j	501	-	-	4/18/38/38	0/3/3/3
8	GTP	e	501	-	-	5/18/38/38	0/3/3/3
8	GTP	b	501	-	-	4/18/38/38	0/3/3/3
8	GTP	g	501	-	-	5/18/38/38	0/3/3/3
8	GTP	l	501	-	-	4/18/38/38	0/3/3/3
8	GTP	k	501	-	-	5/18/38/38	0/3/3/3
8	GTP	c	501	-	-	4/18/38/38	0/3/3/3
8	GTP	m	501	-	-	4/18/38/38	0/3/3/3
8	GTP	i	501	-	-	4/18/38/38	0/3/3/3
8	GTP	n	501	-	-	5/18/38/38	0/3/3/3
9	GDP	a	501	-	-	3/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	d	501	GTP	C5-C6	-4.06	1.39	1.47
8	j	501	GTP	C5-C6	-4.02	1.39	1.47
8	f	501	GTP	C5-C6	-4.01	1.39	1.47
8	n	501	GTP	C5-C6	-4.00	1.39	1.47
8	b	501	GTP	C5-C6	-4.00	1.39	1.47
8	h	501	GTP	C5-C6	-3.99	1.39	1.47
8	c	501	GTP	C5-C6	-3.99	1.39	1.47
8	i	501	GTP	C5-C6	-3.98	1.39	1.47
8	g	501	GTP	C5-C6	-3.94	1.39	1.47
8	e	501	GTP	C5-C6	-3.94	1.39	1.47
8	k	501	GTP	C5-C6	-3.94	1.39	1.47
8	l	501	GTP	C5-C6	-3.93	1.39	1.47
8	m	501	GTP	C5-C6	-3.93	1.39	1.47
9	a	501	GDP	C6-N1	-2.57	1.34	1.37
8	f	501	GTP	C2-N3	2.28	1.38	1.33
8	c	501	GTP	C2-N3	2.27	1.38	1.33
8	h	501	GTP	C2-N3	2.25	1.38	1.33
8	i	501	GTP	C2-N3	2.24	1.38	1.33
8	m	501	GTP	C2-N3	2.24	1.38	1.33
8	n	501	GTP	C2-N3	2.23	1.38	1.33
8	k	501	GTP	C2-N3	2.23	1.38	1.33
8	b	501	GTP	C2-N3	2.22	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	g	501	GTP	C2-N3	2.22	1.38	1.33
8	d	501	GTP	C2-N3	2.20	1.38	1.33
8	l	501	GTP	C2-N3	2.19	1.38	1.33
8	j	501	GTP	C2-N3	2.18	1.38	1.33
8	e	501	GTP	C2-N3	2.13	1.38	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	n	501	GTP	PA-O3A-PB	-3.91	119.40	132.83
8	b	501	GTP	PA-O3A-PB	-3.91	119.42	132.83
8	d	501	GTP	PA-O3A-PB	-3.90	119.44	132.83
8	h	501	GTP	PA-O3A-PB	-3.90	119.45	132.83
8	j	501	GTP	PA-O3A-PB	-3.89	119.47	132.83
8	f	501	GTP	PA-O3A-PB	-3.80	119.77	132.83
8	l	501	GTP	PA-O3A-PB	-3.78	119.84	132.83
8	k	501	GTP	PA-O3A-PB	-3.76	119.92	132.83
8	i	501	GTP	PA-O3A-PB	-3.73	120.02	132.83
9	a	501	GDP	PA-O3A-PB	-3.73	120.03	132.83
8	m	501	GTP	PA-O3A-PB	-3.72	120.08	132.83
8	e	501	GTP	PA-O3A-PB	-3.71	120.10	132.83
8	c	501	GTP	PA-O3A-PB	-3.70	120.12	132.83
8	g	501	GTP	PA-O3A-PB	-3.70	120.13	132.83
8	l	501	GTP	PB-O3B-PG	-3.68	120.20	132.83
8	h	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
8	j	501	GTP	PB-O3B-PG	-3.63	120.37	132.83
8	n	501	GTP	PB-O3B-PG	-3.60	120.47	132.83
8	b	501	GTP	PB-O3B-PG	-3.57	120.59	132.83
8	k	501	GTP	PB-O3B-PG	-3.56	120.59	132.83
8	m	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
8	c	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
8	f	501	GTP	PB-O3B-PG	-3.55	120.66	132.83
8	i	501	GTP	PB-O3B-PG	-3.54	120.66	132.83
8	g	501	GTP	PB-O3B-PG	-3.53	120.70	132.83
8	d	501	GTP	PB-O3B-PG	-3.53	120.72	132.83
8	e	501	GTP	PB-O3B-PG	-3.53	120.73	132.83
9	a	501	GDP	C3'-C2'-C1'	3.50	106.25	100.98
8	f	501	GTP	C3'-C2'-C1'	3.46	106.18	100.98
8	h	501	GTP	C3'-C2'-C1'	3.39	106.08	100.98
8	j	501	GTP	C3'-C2'-C1'	3.37	106.05	100.98
8	b	501	GTP	C3'-C2'-C1'	3.35	106.02	100.98
8	h	501	GTP	C5-C6-N1	3.33	119.84	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	d	501	GTP	C5-C6-N1	3.32	119.82	113.95
8	n	501	GTP	C5-C6-N1	3.32	119.82	113.95
8	d	501	GTP	C3'-C2'-C1'	3.31	105.97	100.98
8	n	501	GTP	C3'-C2'-C1'	3.31	105.97	100.98
8	b	501	GTP	C5-C6-N1	3.31	119.80	113.95
8	j	501	GTP	C5-C6-N1	3.31	119.79	113.95
8	g	501	GTP	C5-C6-N1	3.30	119.79	113.95
8	i	501	GTP	C5-C6-N1	3.30	119.78	113.95
8	m	501	GTP	C5-C6-N1	3.29	119.77	113.95
8	f	501	GTP	C5-C6-N1	3.29	119.76	113.95
8	c	501	GTP	C5-C6-N1	3.28	119.75	113.95
8	l	501	GTP	C5-C6-N1	3.26	119.71	113.95
8	k	501	GTP	C5-C6-N1	3.24	119.67	113.95
8	e	501	GTP	C5-C6-N1	3.24	119.67	113.95
8	m	501	GTP	C3'-C2'-C1'	3.21	105.81	100.98
8	e	501	GTP	C3'-C2'-C1'	3.19	105.79	100.98
8	l	501	GTP	C3'-C2'-C1'	3.19	105.78	100.98
8	i	501	GTP	C3'-C2'-C1'	3.18	105.77	100.98
8	k	501	GTP	C3'-C2'-C1'	3.16	105.74	100.98
8	g	501	GTP	C3'-C2'-C1'	3.16	105.74	100.98
8	c	501	GTP	C3'-C2'-C1'	3.14	105.71	100.98
8	d	501	GTP	C8-N7-C5	3.03	108.76	102.99
8	h	501	GTP	C8-N7-C5	3.02	108.75	102.99
8	k	501	GTP	C8-N7-C5	3.02	108.74	102.99
8	m	501	GTP	C8-N7-C5	3.01	108.72	102.99
8	c	501	GTP	C8-N7-C5	2.99	108.69	102.99
8	g	501	GTP	C2-N1-C6	-2.99	119.60	125.10
8	g	501	GTP	C8-N7-C5	2.98	108.67	102.99
8	f	501	GTP	C8-N7-C5	2.98	108.67	102.99
8	d	501	GTP	C2-N1-C6	-2.98	119.61	125.10
8	i	501	GTP	C2-N1-C6	-2.98	119.61	125.10
8	b	501	GTP	C8-N7-C5	2.98	108.66	102.99
8	i	501	GTP	C8-N7-C5	2.96	108.62	102.99
8	n	501	GTP	C8-N7-C5	2.96	108.62	102.99
8	e	501	GTP	C2-N1-C6	-2.95	119.66	125.10
8	j	501	GTP	C2-N1-C6	-2.95	119.66	125.10
8	m	501	GTP	C2-N1-C6	-2.95	119.66	125.10
8	j	501	GTP	C8-N7-C5	2.95	108.61	102.99
8	n	501	GTP	C2-N1-C6	-2.94	119.69	125.10
8	c	501	GTP	C2-N1-C6	-2.93	119.70	125.10
8	e	501	GTP	C8-N7-C5	2.93	108.57	102.99
8	h	501	GTP	C2-N1-C6	-2.92	119.72	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	l	501	GTP	C8-N7-C5	2.92	108.55	102.99
8	l	501	GTP	C2-N1-C6	-2.91	119.73	125.10
8	k	501	GTP	C2-N1-C6	-2.90	119.76	125.10
8	b	501	GTP	C2-N1-C6	-2.90	119.77	125.10
8	f	501	GTP	C2-N1-C6	-2.89	119.78	125.10
9	a	501	GDP	C5-C6-N1	2.32	118.05	113.95
9	a	501	GDP	C8-N7-C5	2.32	107.41	102.99
8	d	501	GTP	O6-C6-C5	-2.25	119.97	124.37
8	h	501	GTP	O6-C6-C5	-2.23	120.02	124.37
8	k	501	GTP	O6-C6-C5	-2.21	120.05	124.37
8	m	501	GTP	O6-C6-C5	-2.21	120.05	124.37
8	j	501	GTP	O6-C6-C5	-2.21	120.06	124.37
8	b	501	GTP	O6-C6-C5	-2.20	120.08	124.37
8	n	501	GTP	O6-C6-C5	-2.19	120.09	124.37
8	g	501	GTP	O6-C6-C5	-2.18	120.11	124.37
8	l	501	GTP	O6-C6-C5	-2.18	120.12	124.37
8	f	501	GTP	O6-C6-C5	-2.18	120.12	124.37
8	e	501	GTP	O6-C6-C5	-2.17	120.13	124.37
8	i	501	GTP	O6-C6-C5	-2.14	120.19	124.37
8	c	501	GTP	O6-C6-C5	-2.14	120.19	124.37

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	b	501	GTP	C5'-O5'-PA-O3A
8	b	501	GTP	C5'-O5'-PA-O2A
8	c	501	GTP	C5'-O5'-PA-O1A
8	c	501	GTP	C5'-O5'-PA-O2A
8	d	501	GTP	C5'-O5'-PA-O3A
8	d	501	GTP	C5'-O5'-PA-O2A
8	e	501	GTP	C5'-O5'-PA-O1A
8	e	501	GTP	C5'-O5'-PA-O2A
8	f	501	GTP	C5'-O5'-PA-O1A
8	f	501	GTP	C5'-O5'-PA-O2A
8	g	501	GTP	C5'-O5'-PA-O1A
8	g	501	GTP	C5'-O5'-PA-O2A
8	h	501	GTP	C5'-O5'-PA-O1A
8	h	501	GTP	C5'-O5'-PA-O2A
8	i	501	GTP	C5'-O5'-PA-O1A
8	i	501	GTP	C5'-O5'-PA-O2A
8	j	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
8	j	501	GTP	C5'-O5'-PA-O2A
8	k	501	GTP	C5'-O5'-PA-O1A
8	k	501	GTP	C5'-O5'-PA-O2A
8	l	501	GTP	C5'-O5'-PA-O1A
8	l	501	GTP	C5'-O5'-PA-O2A
8	m	501	GTP	C5'-O5'-PA-O1A
8	n	501	GTP	C5'-O5'-PA-O1A
8	n	501	GTP	C5'-O5'-PA-O2A
9	a	501	GDP	C5'-O5'-PA-O1A
8	f	501	GTP	C4'-C5'-O5'-PA
8	j	501	GTP	C4'-C5'-O5'-PA
8	m	501	GTP	C4'-C5'-O5'-PA
8	e	501	GTP	C5'-O5'-PA-O3A
8	g	501	GTP	C5'-O5'-PA-O3A
8	b	501	GTP	PB-O3A-PA-O1A
8	b	501	GTP	C4'-C5'-O5'-PA
8	d	501	GTP	C4'-C5'-O5'-PA
8	g	501	GTP	C4'-C5'-O5'-PA
8	k	501	GTP	C4'-C5'-O5'-PA
8	l	501	GTP	C4'-C5'-O5'-PA
8	n	501	GTP	C4'-C5'-O5'-PA
8	m	501	GTP	C5'-O5'-PA-O2A
8	c	501	GTP	C4'-C5'-O5'-PA
8	e	501	GTP	C4'-C5'-O5'-PA
8	h	501	GTP	C4'-C5'-O5'-PA
8	i	501	GTP	C4'-C5'-O5'-PA
8	g	501	GTP	PB-O3A-PA-O1A
8	d	501	GTP	PB-O3A-PA-O1A
8	e	501	GTP	PB-O3A-PA-O1A
8	h	501	GTP	PB-O3A-PA-O1A
8	k	501	GTP	PB-O3A-PA-O1A
8	n	501	GTP	PB-O3A-PA-O1A
8	c	501	GTP	C5'-O5'-PA-O3A
8	f	501	GTP	C5'-O5'-PA-O3A
8	h	501	GTP	C5'-O5'-PA-O3A
8	i	501	GTP	C5'-O5'-PA-O3A
8	j	501	GTP	C5'-O5'-PA-O3A
8	k	501	GTP	C5'-O5'-PA-O3A
8	l	501	GTP	C5'-O5'-PA-O3A
8	m	501	GTP	C5'-O5'-PA-O3A
8	n	501	GTP	C5'-O5'-PA-O3A
9	a	501	GDP	C5'-O5'-PA-O3A

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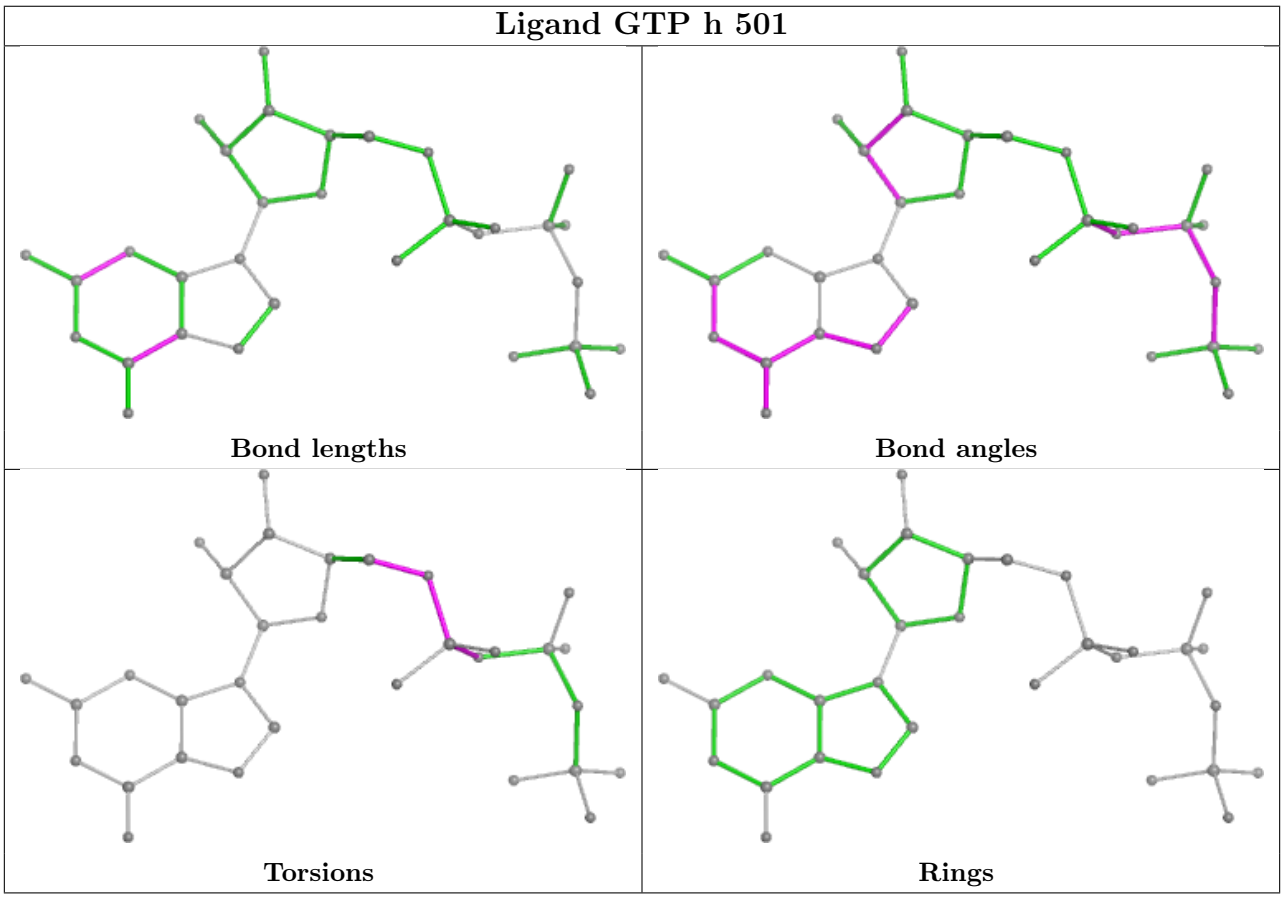
Mol	Chain	Res	Type	Atoms
9	a	501	GDP	O4'-C4'-C5'-O5'

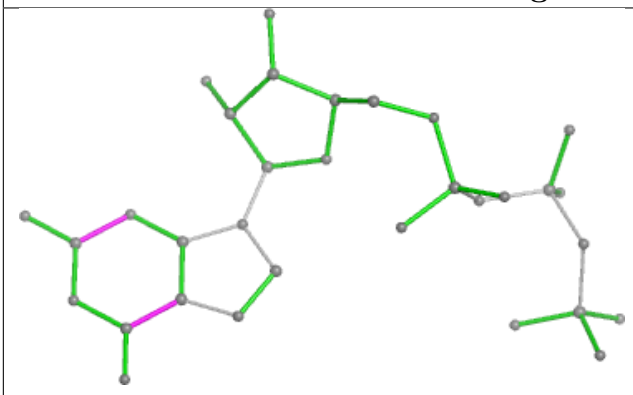
There are no ring outliers.

No monomer is involved in short contacts.

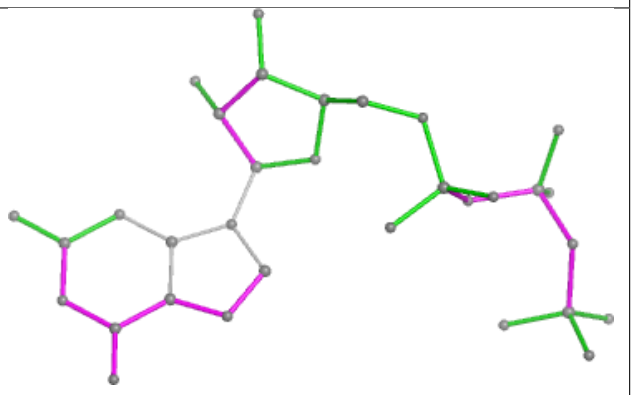
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



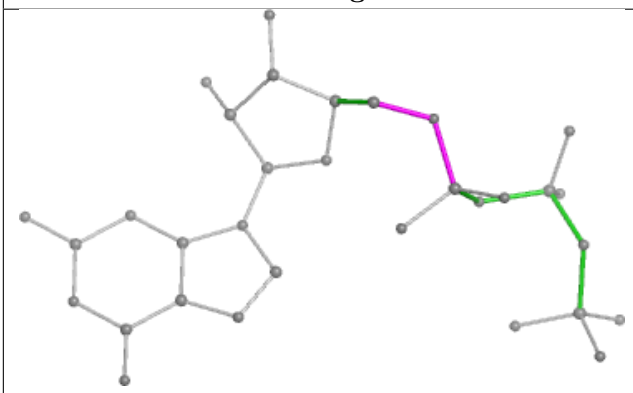
Ligand GTP f 501



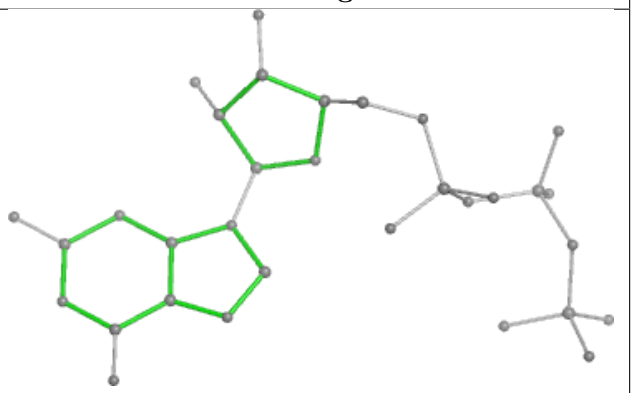
Bond lengths



Bond angles

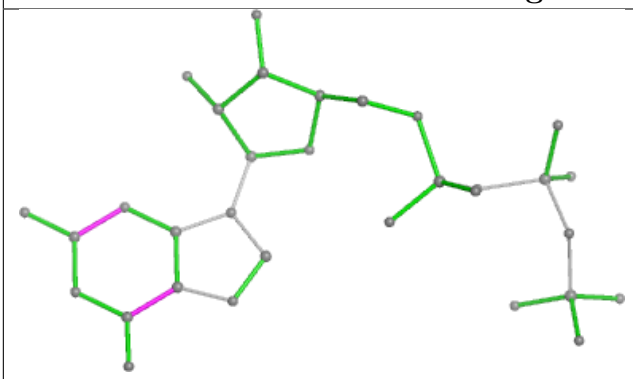


Torsions

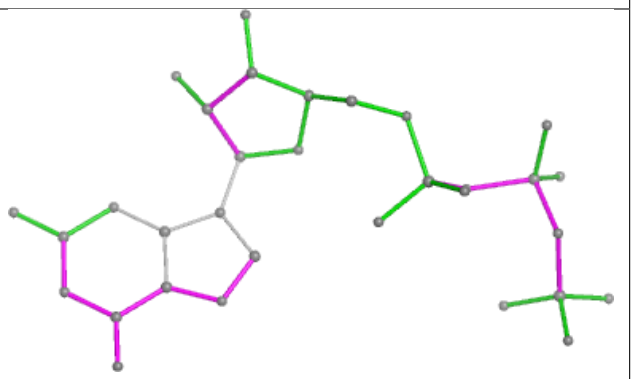


Rings

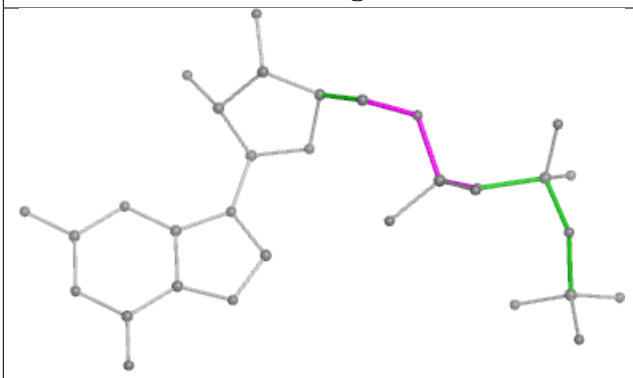
Ligand GTP d 501



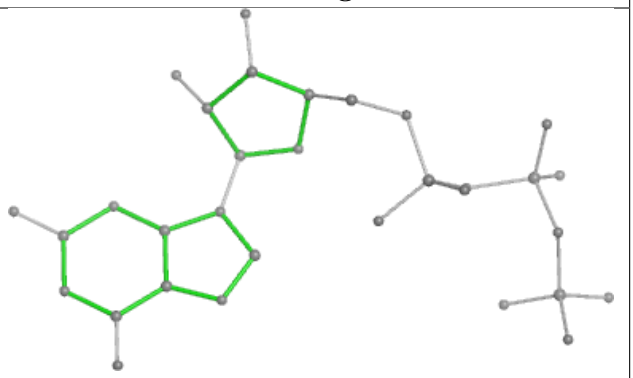
Bond lengths



Bond angles

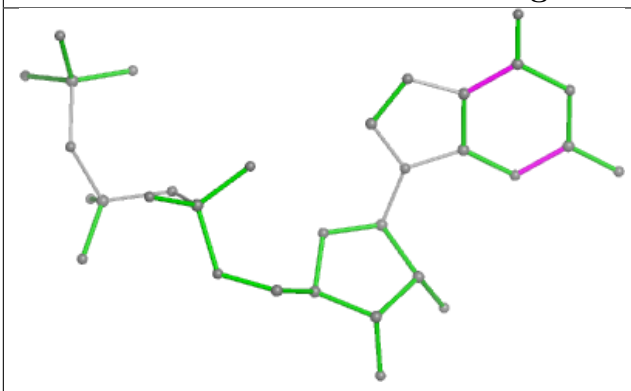


Torsions

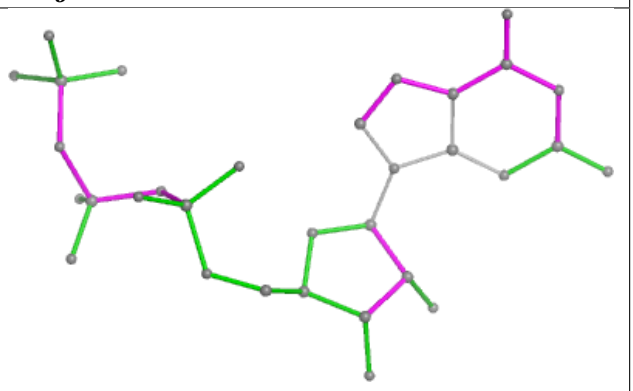


Rings

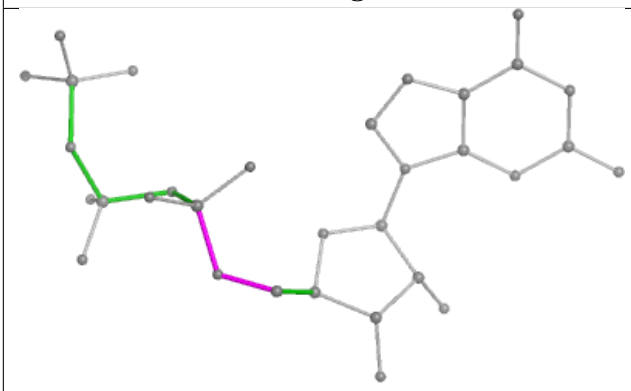
Ligand GTP j 501



Bond lengths



Bond angles



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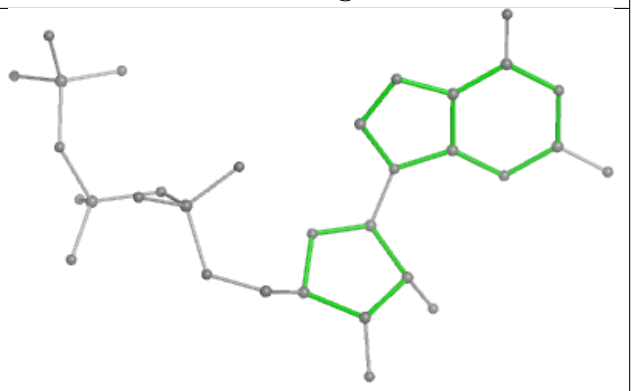
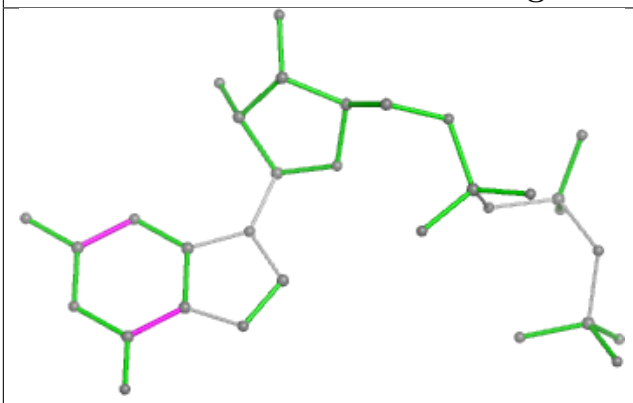


Rings

Ligand GTP e 501



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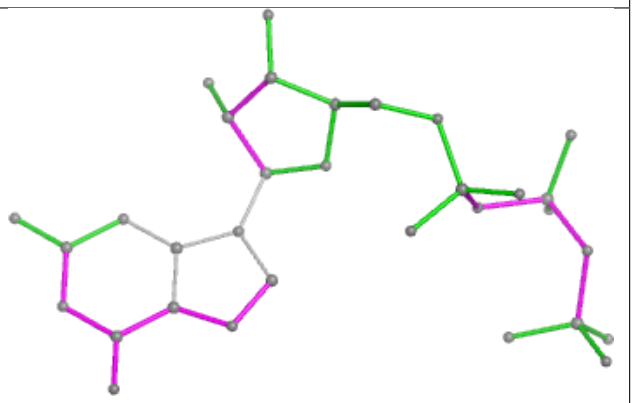
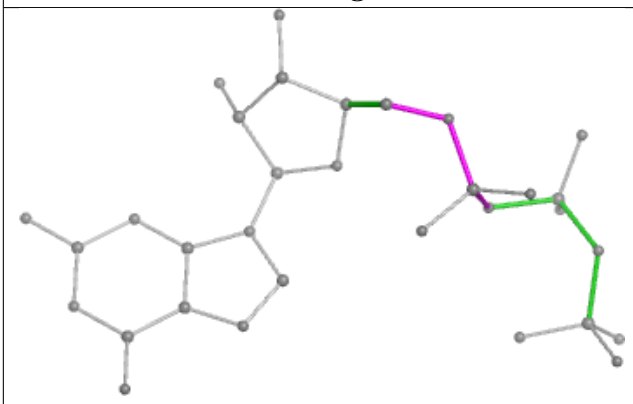
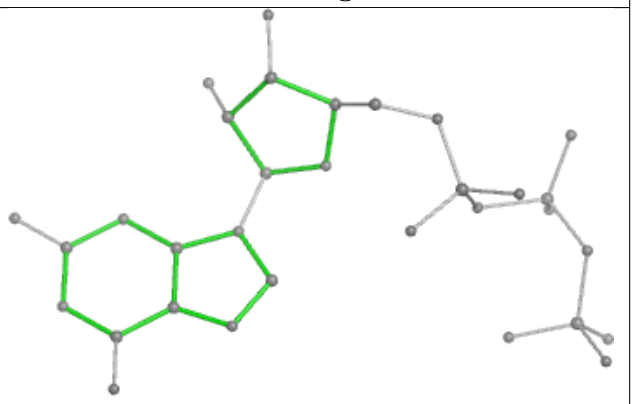


Bond angles

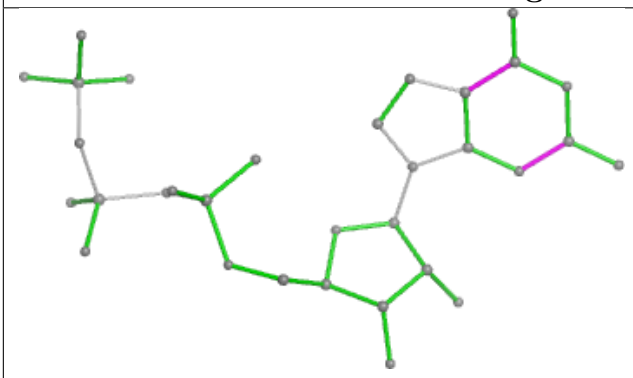


Torsions



Rings

Ligand GTP b 501



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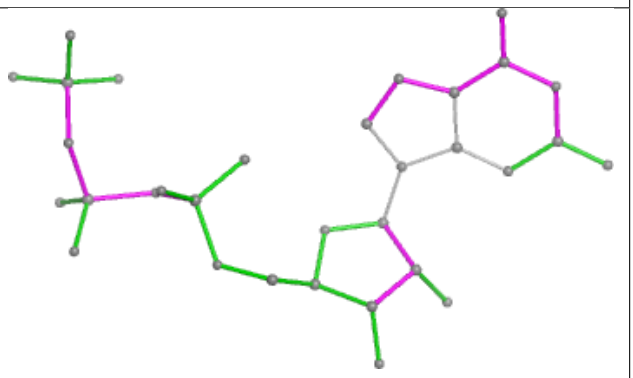

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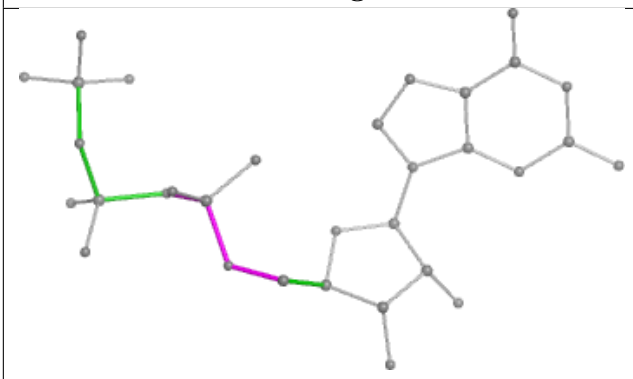

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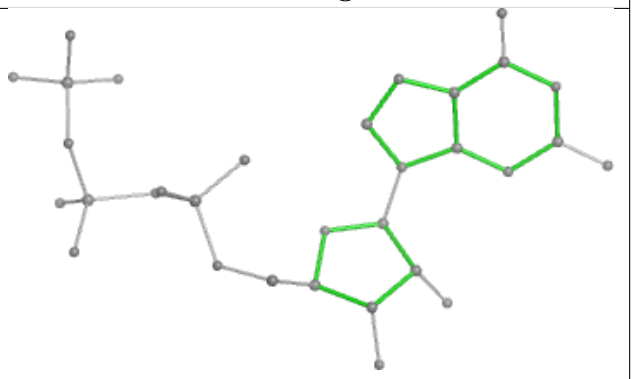
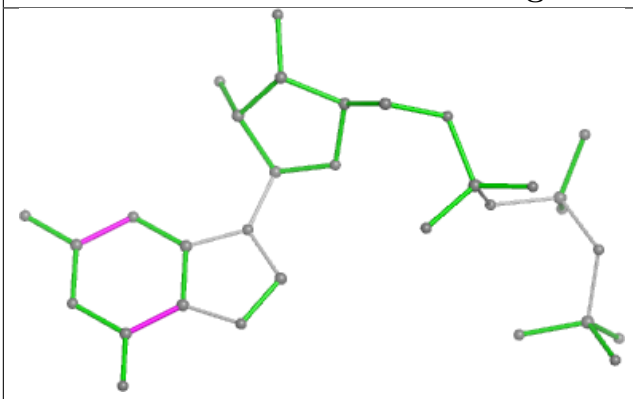


Rings

Ligand GTP g 501



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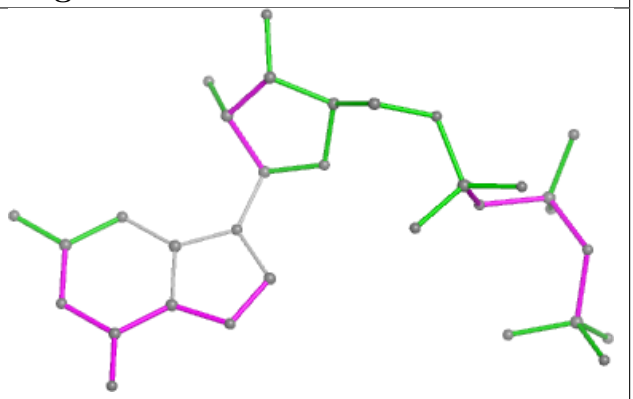

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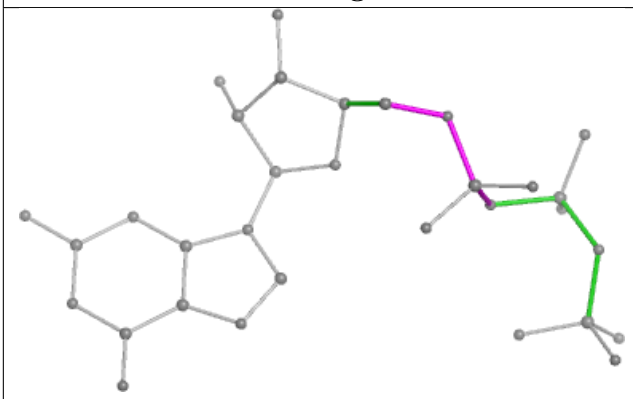

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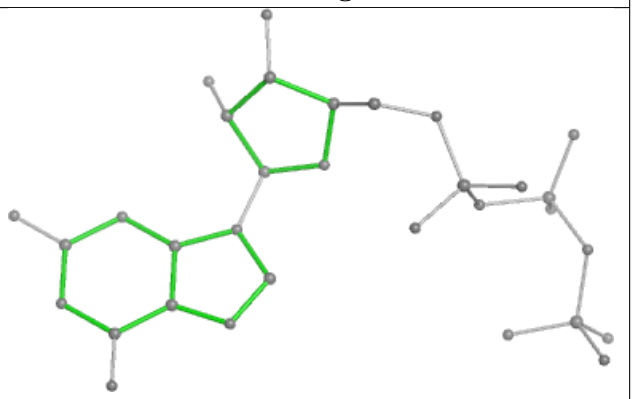
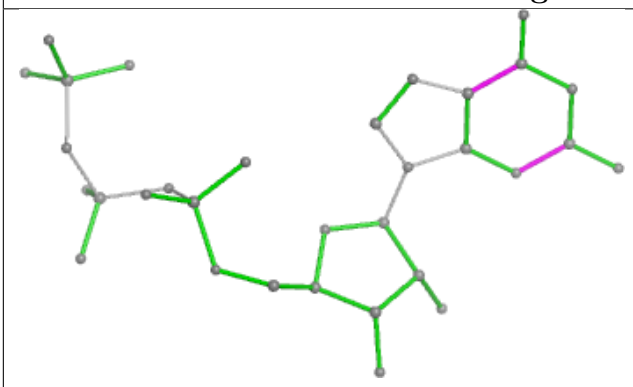


Rings

Ligand GTP l 501



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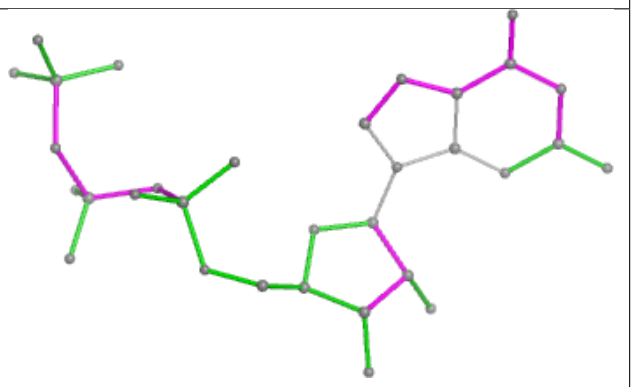

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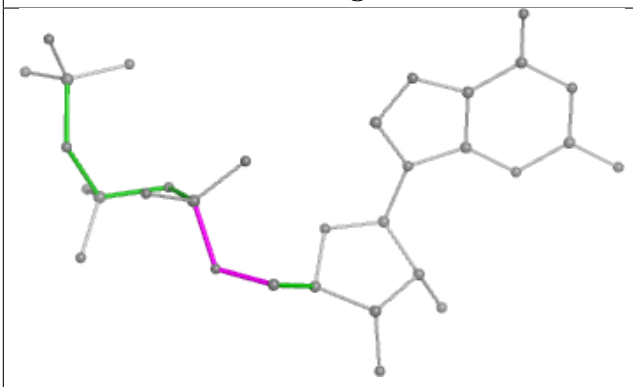

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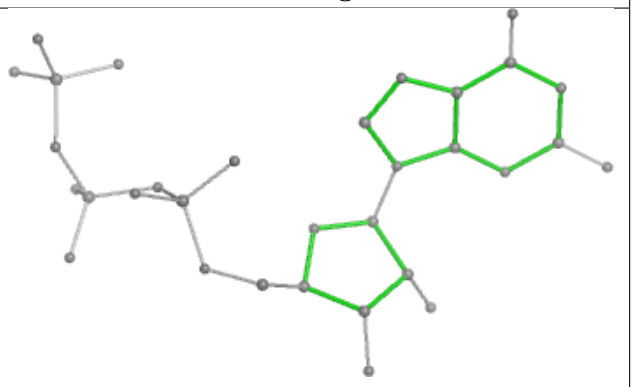
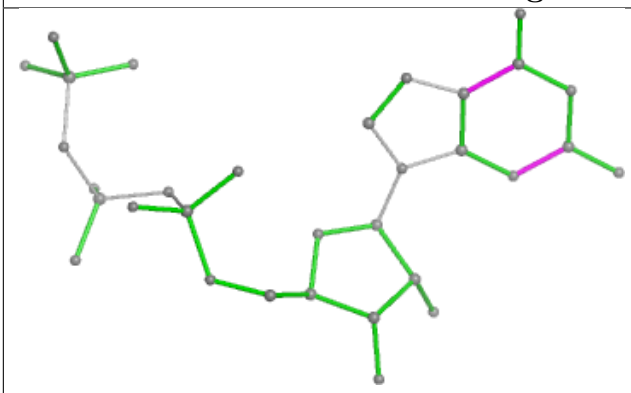


Rings

Ligand GTP k 501



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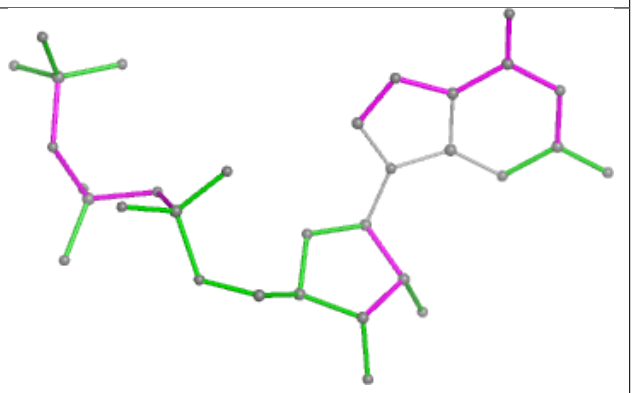
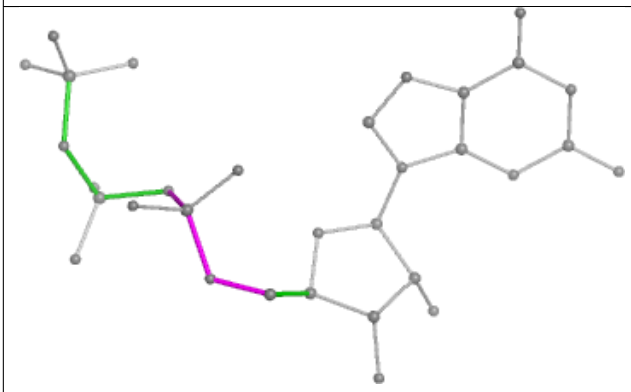


Bond angles



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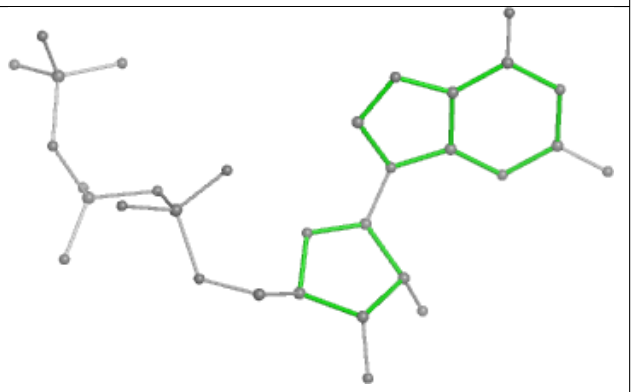
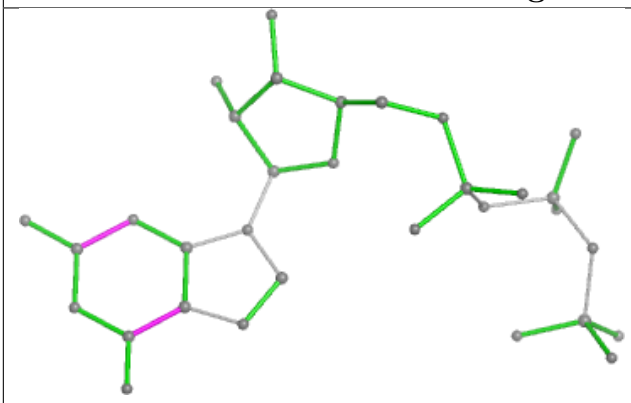
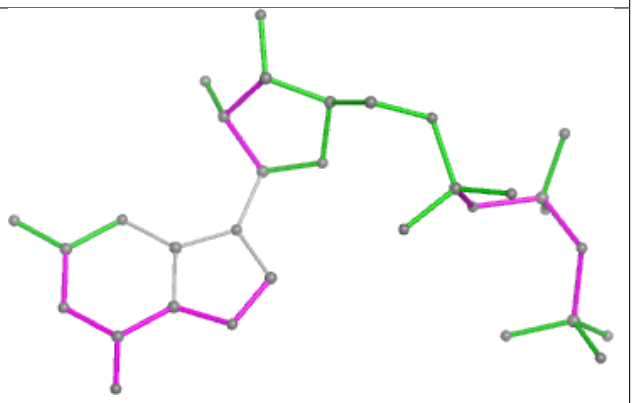


Rings

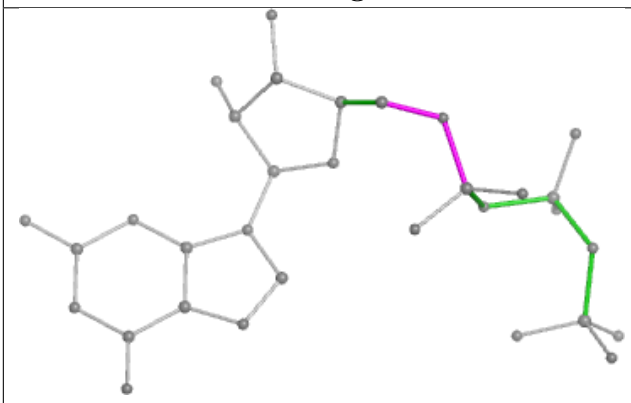
Ligand GTP c 501



Bond lengths



Bond angles



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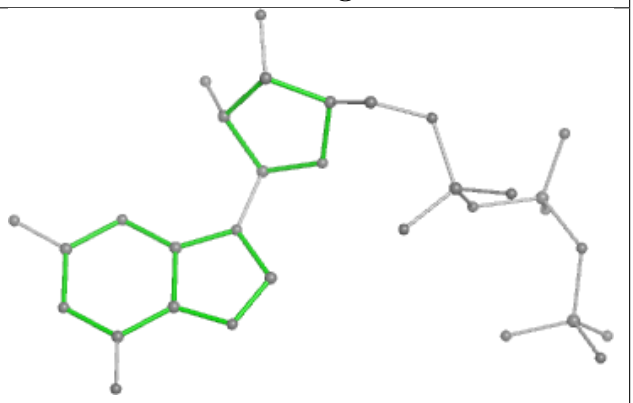
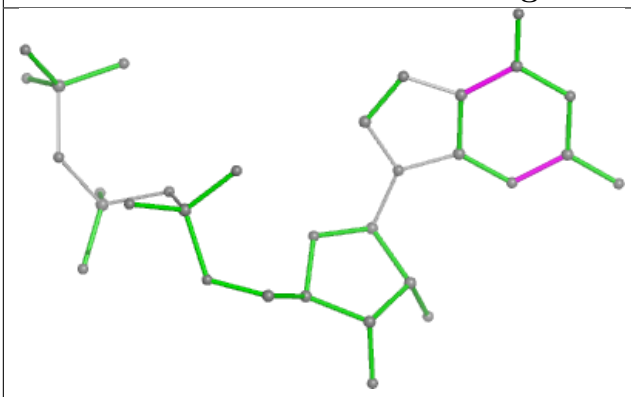
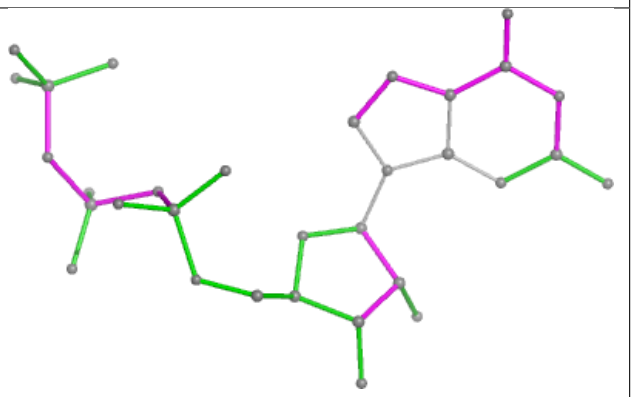


Rings

Ligand GTP m 501



Bond lengths



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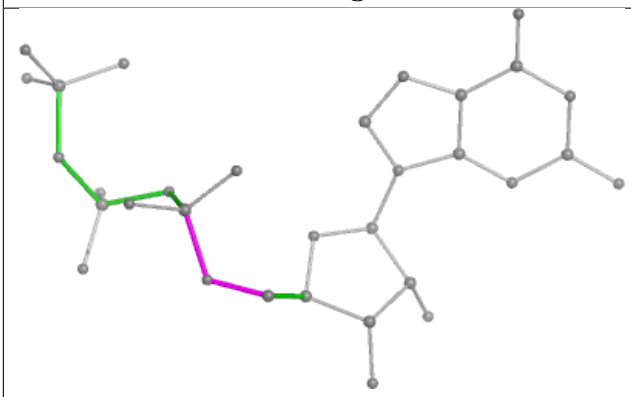

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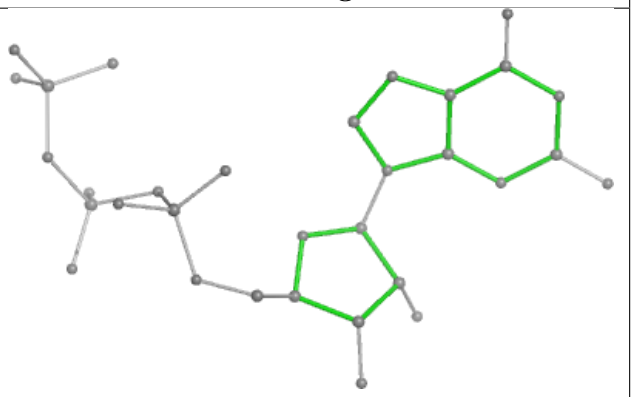
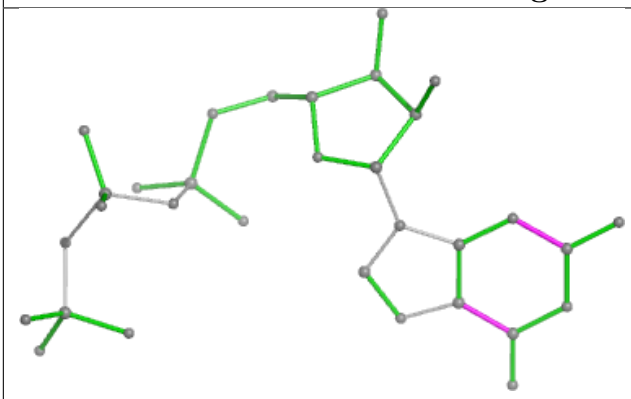
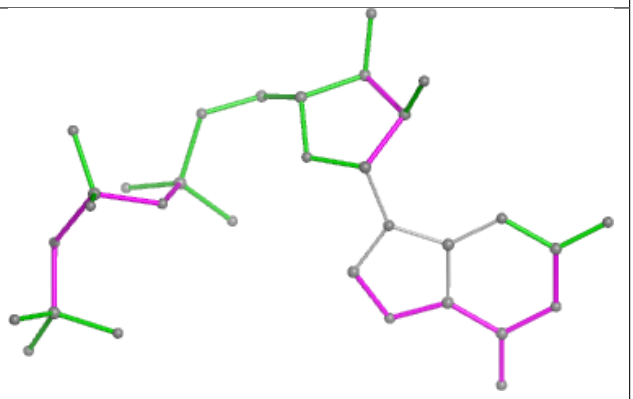


Rings

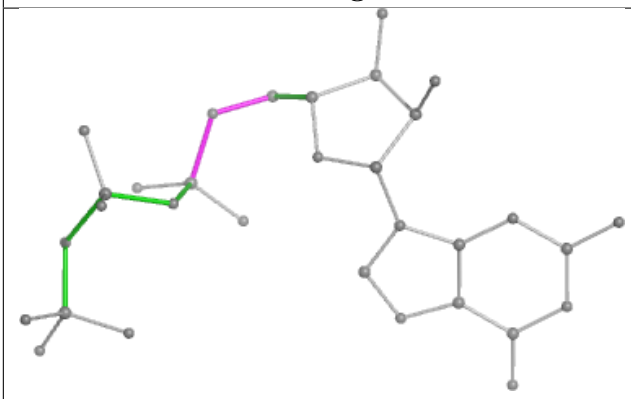
Ligand GTP i 501



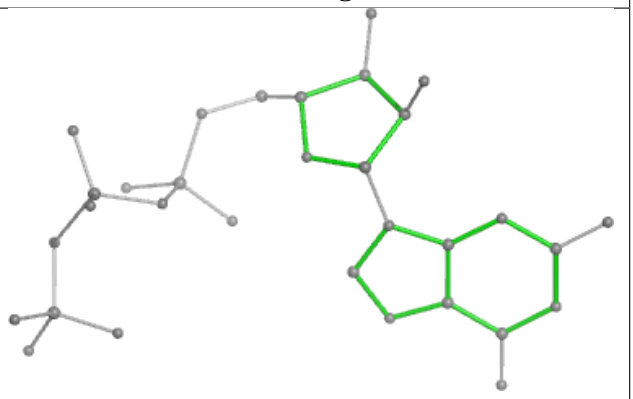
Bond lengths



Bond angles

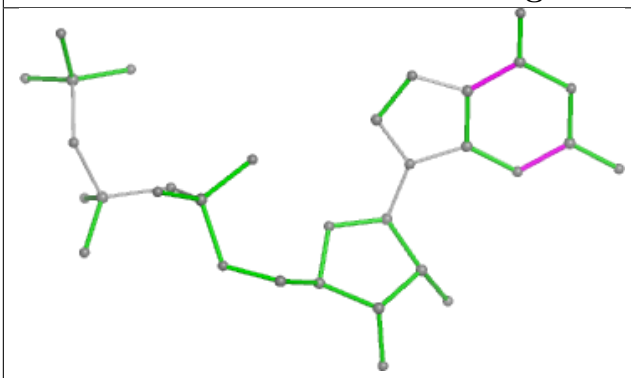


Torsions

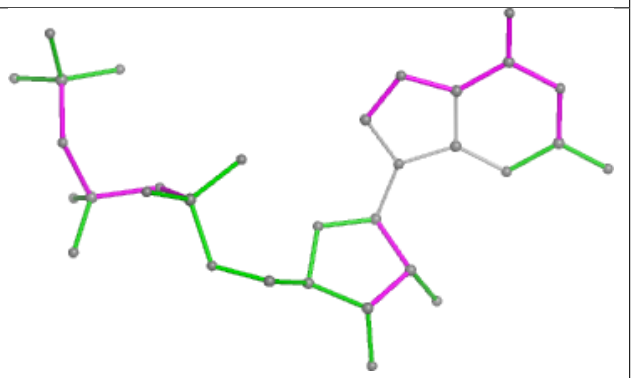


Rings

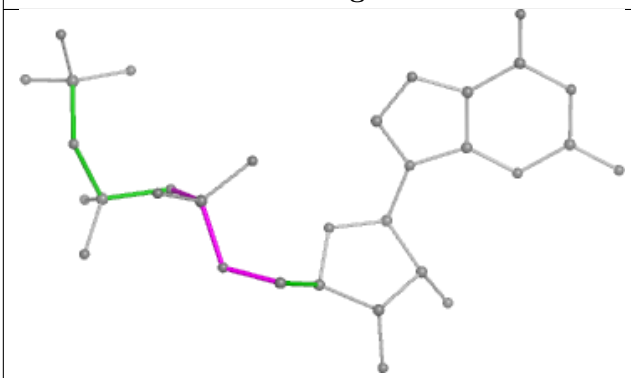
Ligand GTP n 501



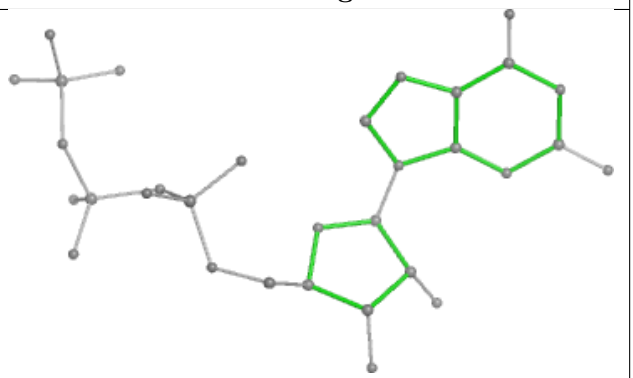
Bond lengths



Bond angles

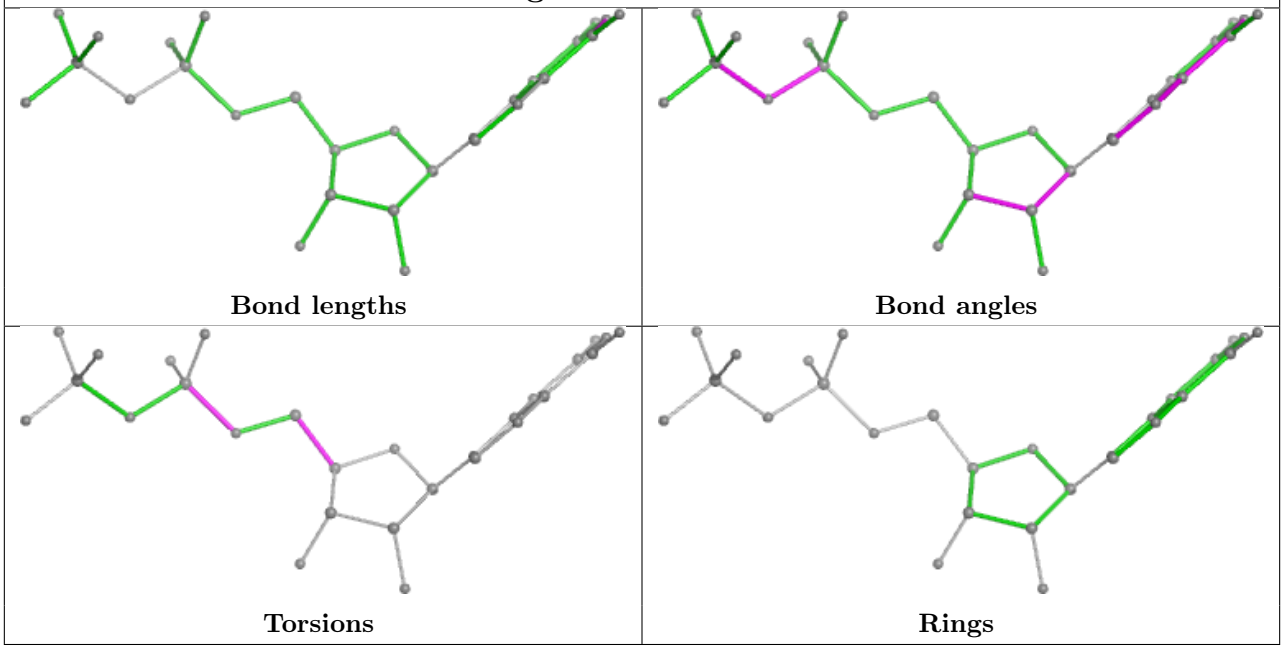


Torsions



Rings

Ligand GDP a 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

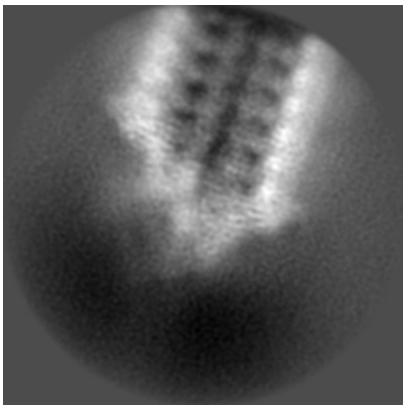
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18665. These allow visual inspection of the internal detail of the map and identification of artifacts.

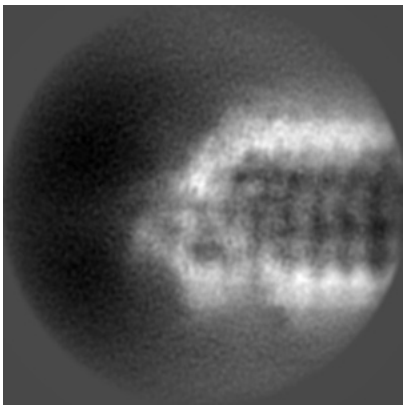
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

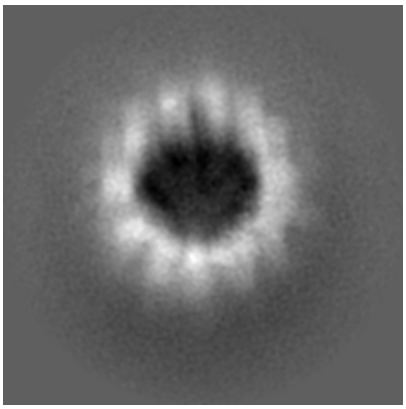
6.1.1 Primary map



X

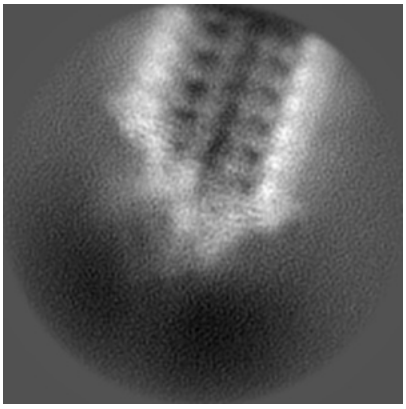


Y

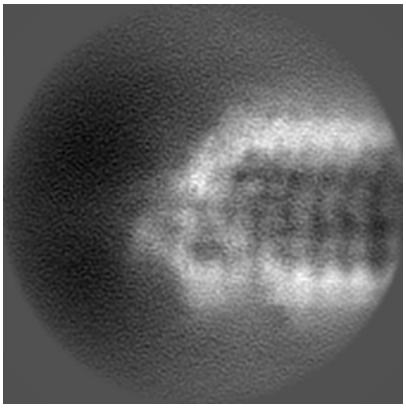


Z

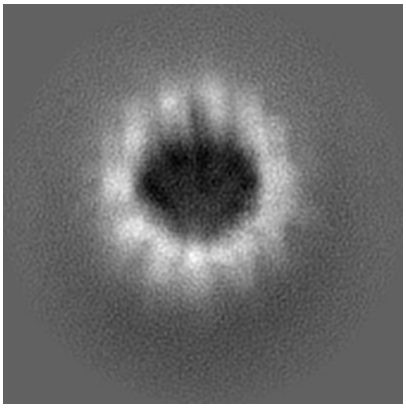
6.1.2 Raw map



X



Y

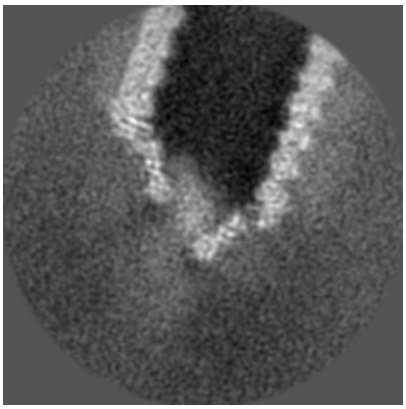


Z

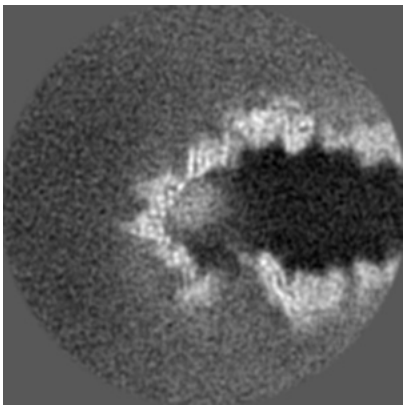
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

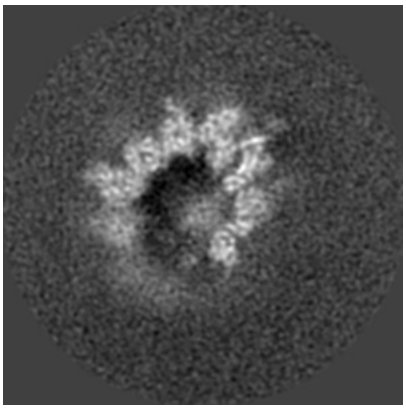
6.2.1 Primary map



X Index: 84

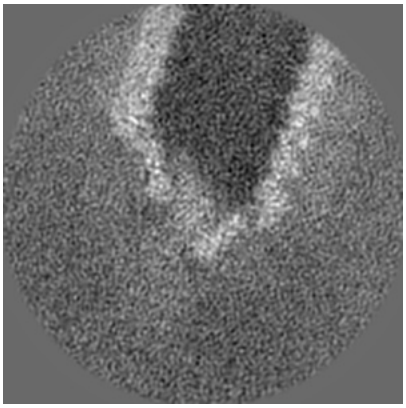


Y Index: 84

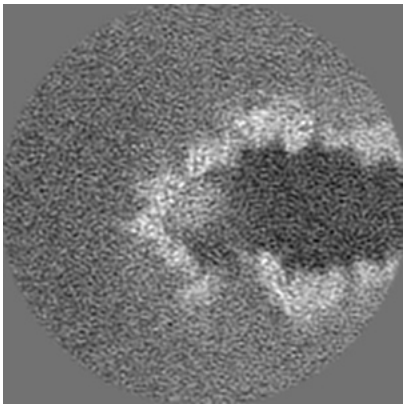


Z Index: 84

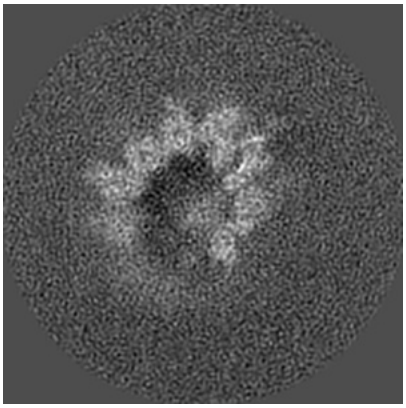
6.2.2 Raw map



X Index: 84



Y Index: 84

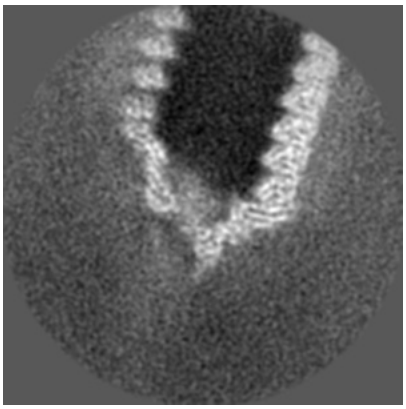


Z Index: 84

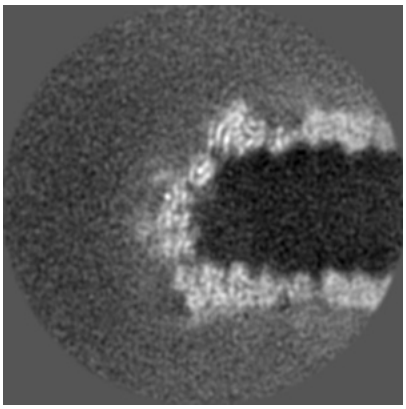
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

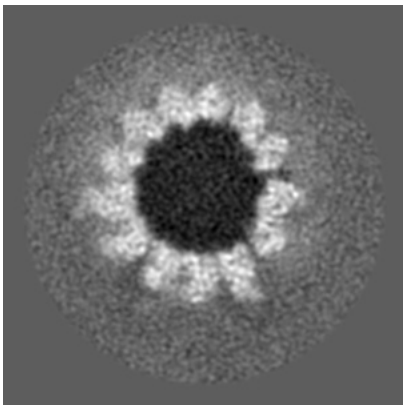
6.3.1 Primary map



X Index: 89

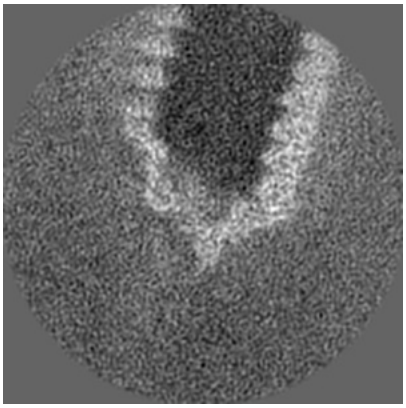


Y Index: 94

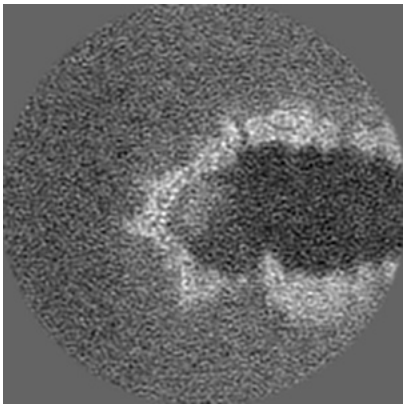


Z Index: 124

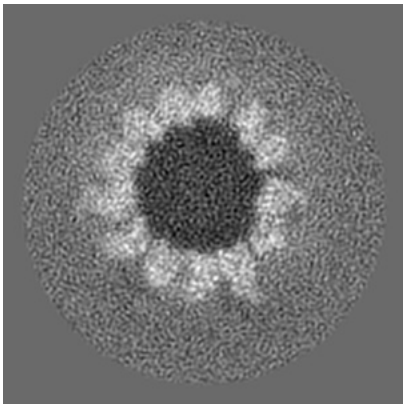
6.3.2 Raw map



X Index: 89



Y Index: 86

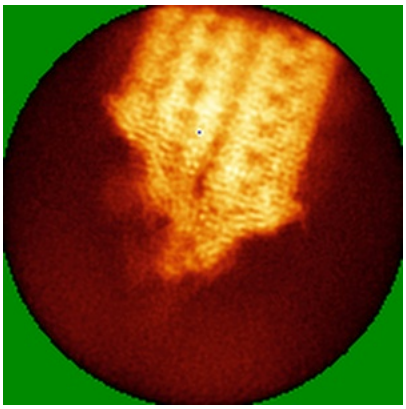


Z Index: 123

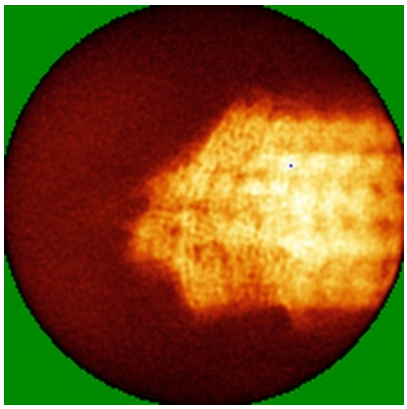
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

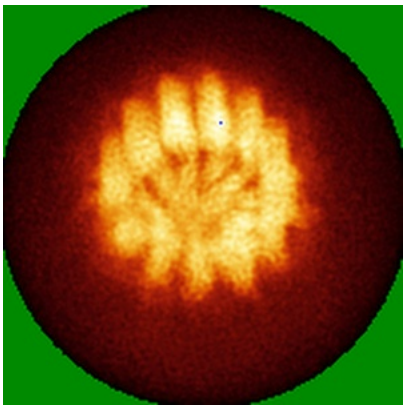
6.4.1 Primary map



X

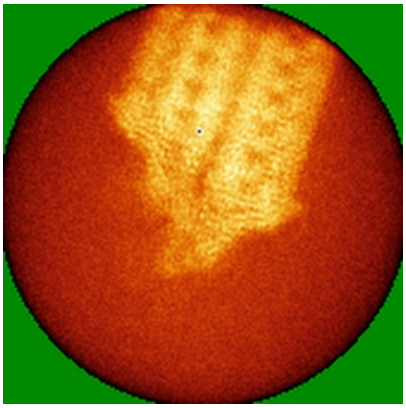


Y

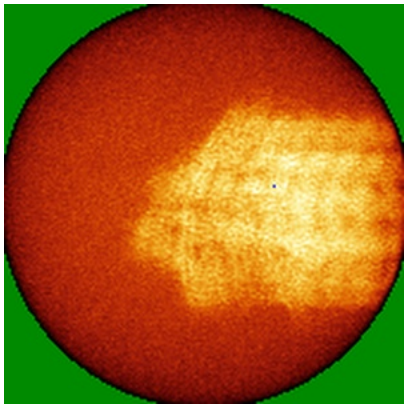


Z

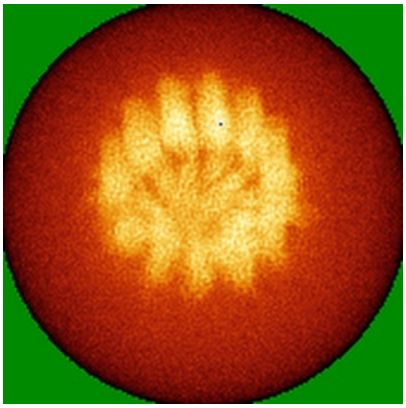
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

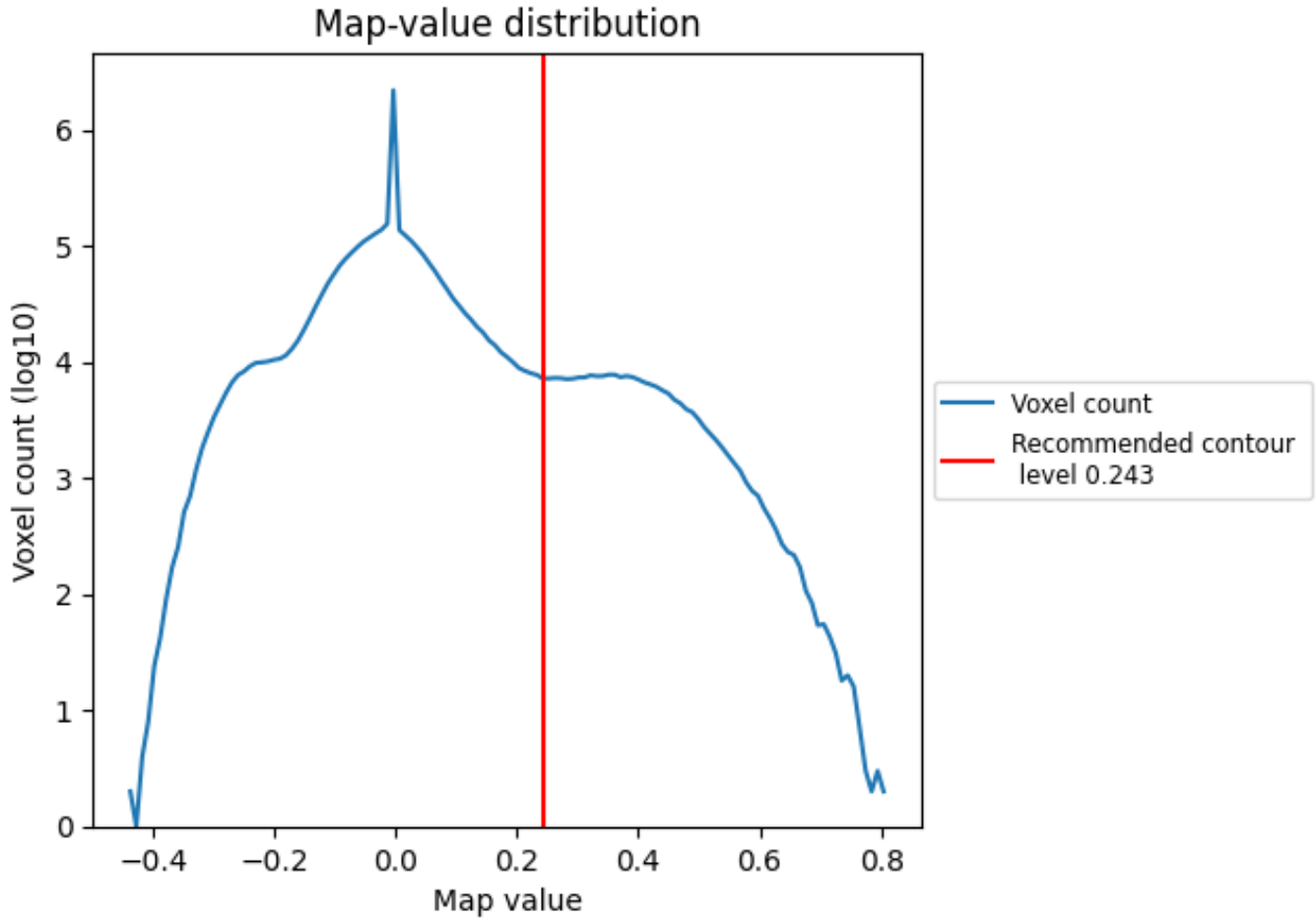
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

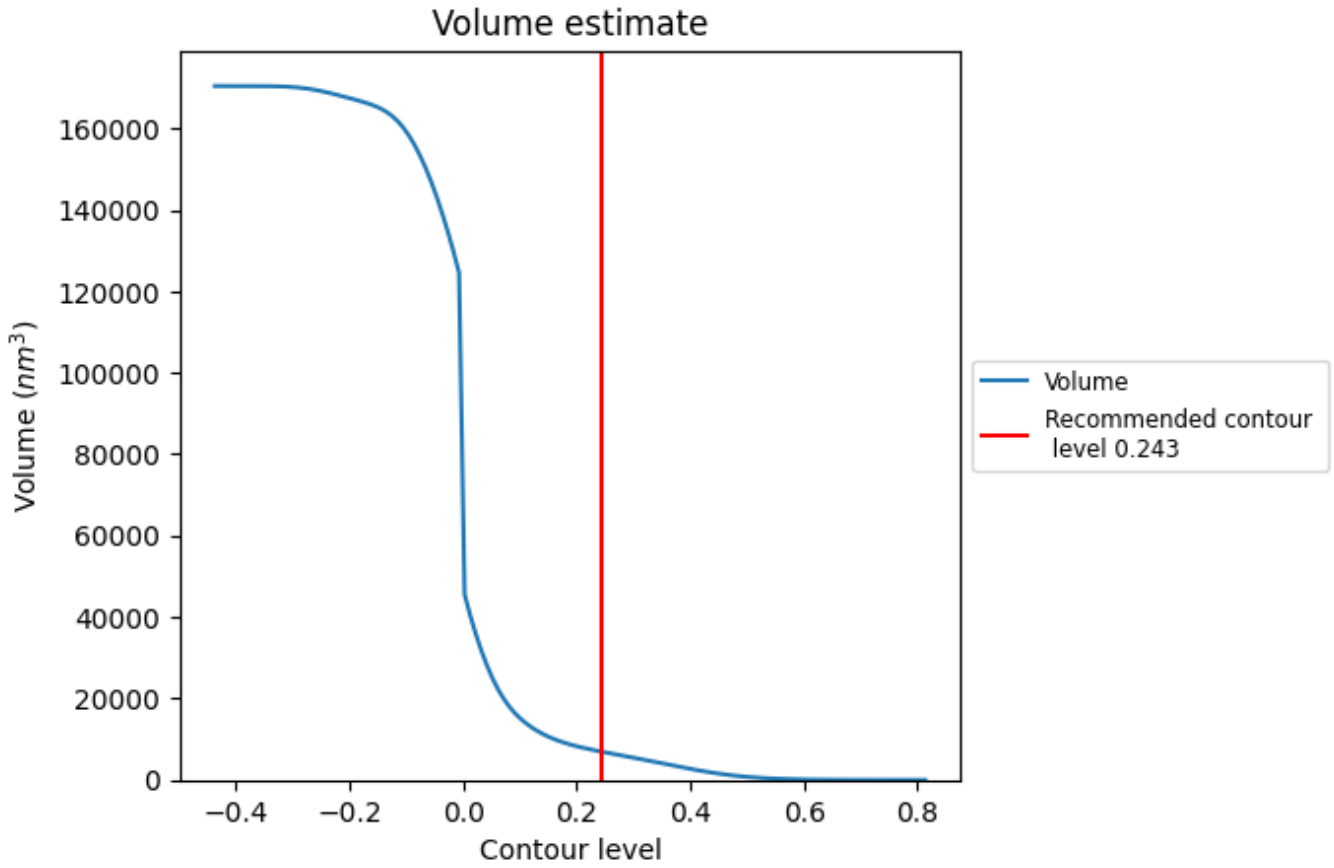
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

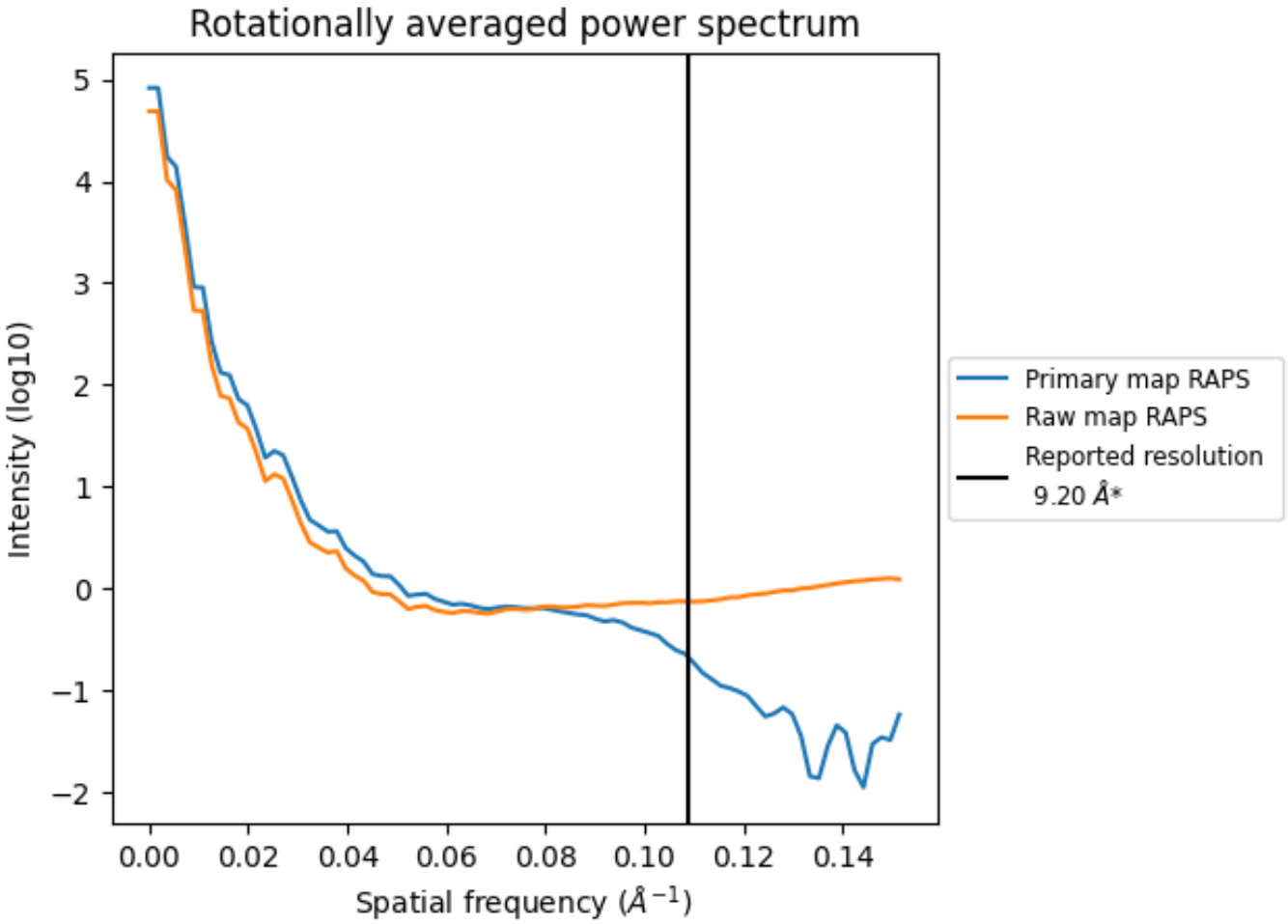
7.2 Volume estimate



The volume at the recommended contour level is 6972 nm^3; this corresponds to an approximate mass of 6298 kDa.

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

7.3 Rotationally averaged power spectrum (i)

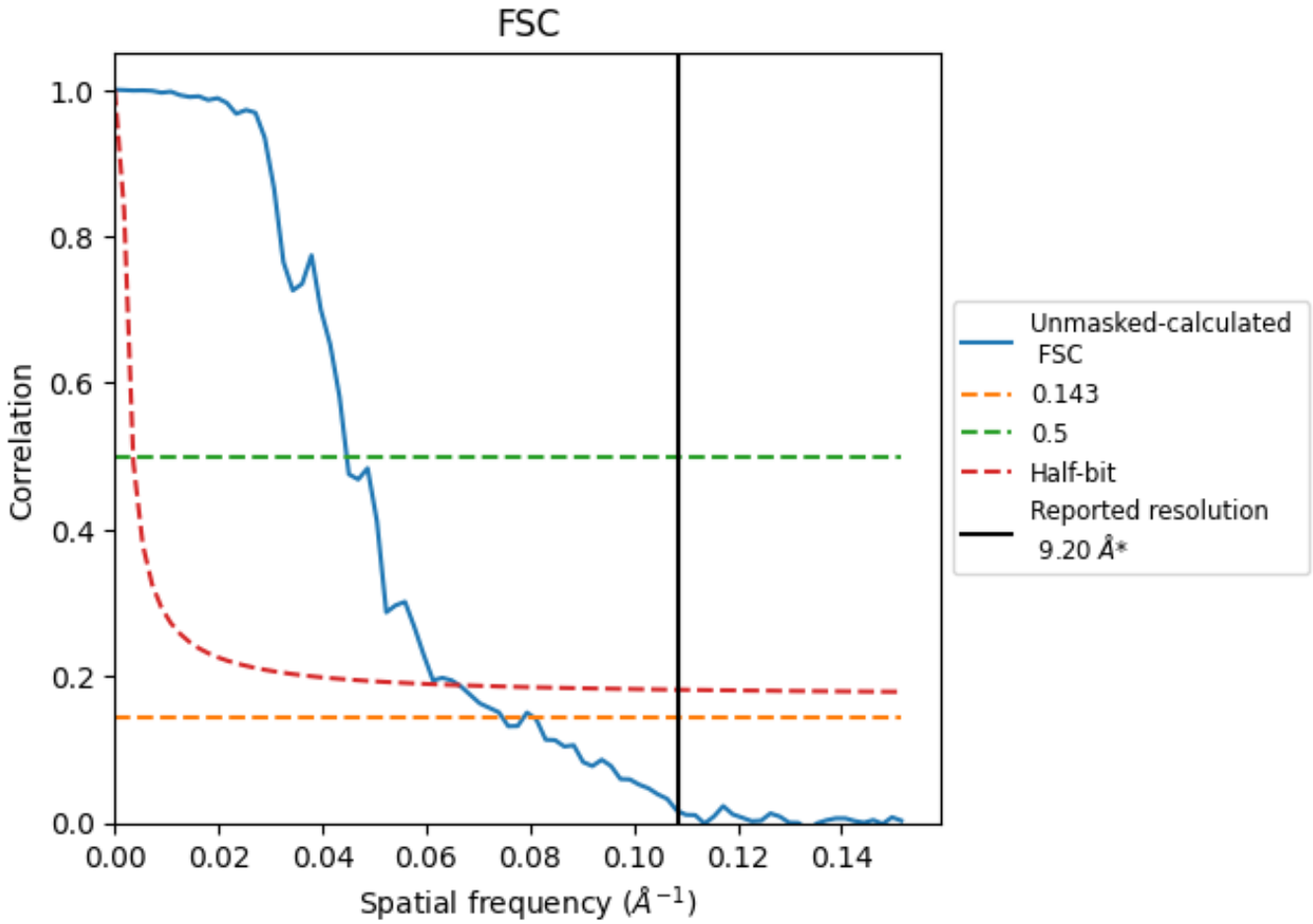


*Reported resolution corresponds to spatial frequency of 0.109 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.109 Å^{-1}

8.2 Resolution estimates (i)

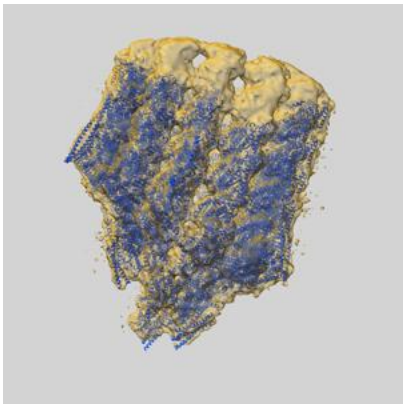
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.39	22.37	15.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.39 differs from the reported value 9.2 by more than 10 %

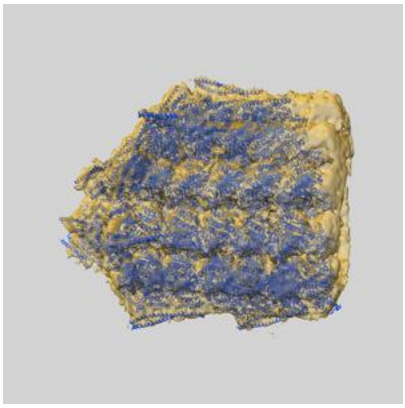
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18665 and PDB model 8QV2. Per-residue inclusion information can be found in section 3 on page 15.

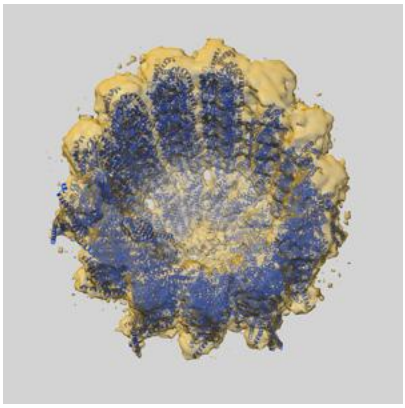
9.1 Map-model overlay



X



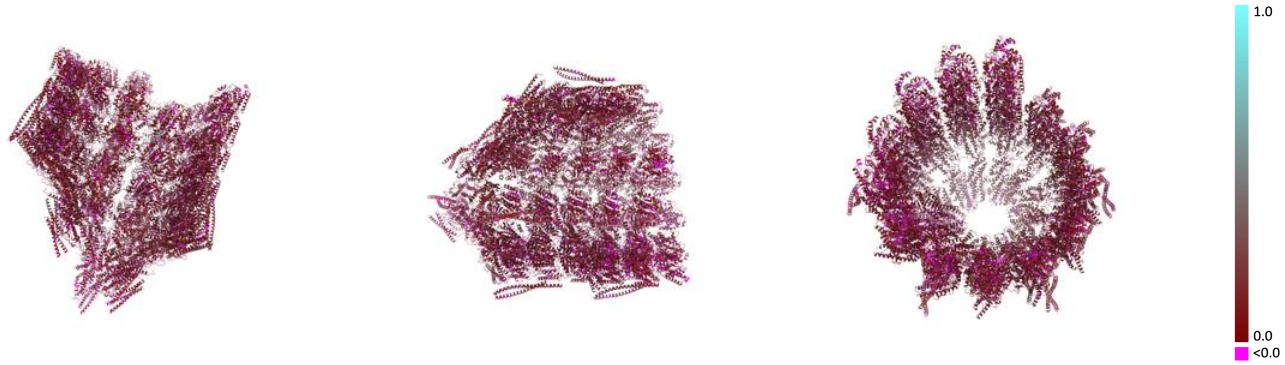
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

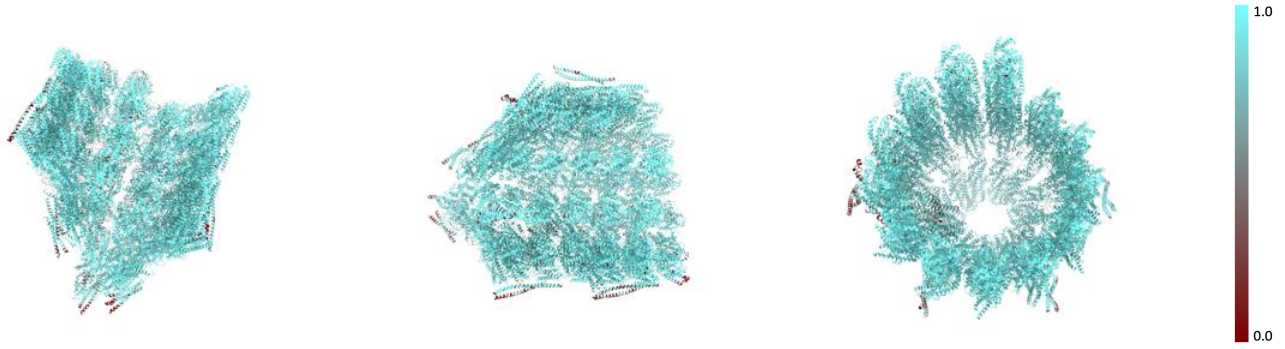
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

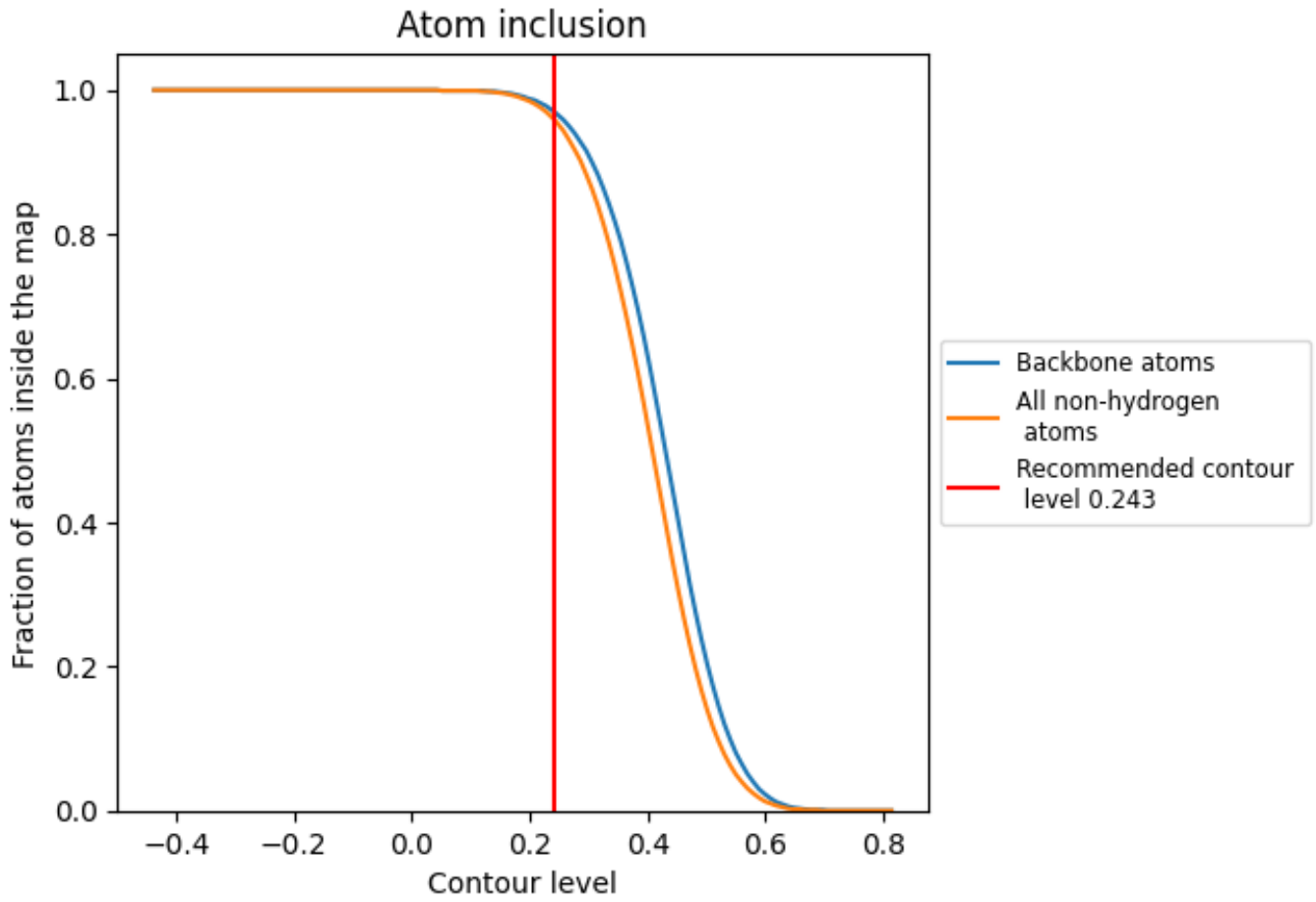
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.243).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.1120
Ab	0.9440	0.1110
Ac	0.9720	0.1250
Ad	0.9880	0.1140
Ae	0.9940	0.1170
Af	0.9880	0.1180
Ag	0.9860	0.1160
Ah	0.9790	0.1150
Ai	0.9870	0.1150
Aj	0.9910	0.1020
Ak	0.9880	0.1080
Al	0.9900	0.0960
Am	0.9730	0.0950
An	0.9640	0.0940
Ao	0.9520	0.0980
Ap	0.9870	0.1090
Aq	0.9920	0.0910
Ar	0.9890	0.1050
Bb	0.9670	0.1060
Bc	0.9830	0.1210
Bd	0.9910	0.1180
Be	0.9910	0.1130
Bf	0.9940	0.1190
Bg	0.9900	0.1190
Bh	0.9800	0.1190
Bi	0.9850	0.1030
Bj	0.9860	0.1090
Bk	0.9840	0.1030
Bl	0.9850	0.0960
Bm	0.9530	0.0870
Bn	0.8850	0.0870
Bo	0.9550	0.0980
Bp	0.9610	0.0930
Bq	0.9810	0.1080
Br	0.9800	0.0970

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Chain	Atom inclusion	Q-score
C	0.8970	0.0510
D	0.9500	0.1130
E	0.9780	0.1230
F	0.9750	0.1350
G	0.9860	0.1310
H	0.9740	0.1320
I	0.9820	0.1320
J	0.9640	0.1390
K	0.9770	0.1360
L	0.9680	0.1340
M	0.9820	0.1290
N	0.9630	0.1240
O	0.9490	0.1110
P	0.8820	0.1170
Sa	0.5480	0.0830
Sb	0.5750	0.0560
Sc	0.7580	0.0840
Sd	0.8080	0.0790
Se	0.8440	0.1210
Sf	0.8570	0.1040
Sg	0.8820	0.1220
Sh	0.8240	0.1100
Si	0.8100	0.0930
Sj	0.8550	0.0980
Sk	0.7870	0.1070
Sl	0.7450	0.0870
Sm	0.7280	0.1040
Sn	0.8090	0.0680
Ua	0.8810	0.1450
Ub	0.4550	0.1070
Uc	0.9370	0.1680
Ud	0.7850	0.1590
Ue	0.8840	0.1860
Uf	0.7420	0.1810
Ug	0.9070	0.1510
Uh	0.8440	0.1800
Ui	0.8240	0.1680
Uj	0.6150	0.1720
Uk	0.8660	0.1610
Ul	0.5340	0.1570
Um	0.5490	0.1280
Un	0.3450	0.0990

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Chain	Atom inclusion	Q-score
a	0.7820	0.0430
b	0.9450	0.1000
c	0.9670	0.1090
d	0.9830	0.1120
e	0.9850	0.1230
f	0.9810	0.1180
g	0.9620	0.1230
h	0.9670	0.1140
i	0.9750	0.1140
j	0.9820	0.1150
k	0.9800	0.1030
l	0.9750	0.1010
m	0.9700	0.1050
n	0.9450	0.0920