wwPDB EM Validation Summary Report

Dec 8, 2025 – 11:02 PM EST

PDB ID	:	9YA1 / pdb_00009ya1
EMDB ID	:	EMD-72717
Title	:	Cryo-EM structure of intraconoidal microtubule 2 (ICMT2) from Toxoplasma gondii (8-nm repeat)
Authors	:	Zeng, J.; Zhang, R.
Deposited on	:	2025-09-15
Resolution	:	3.52 Å(reported)

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

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

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

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

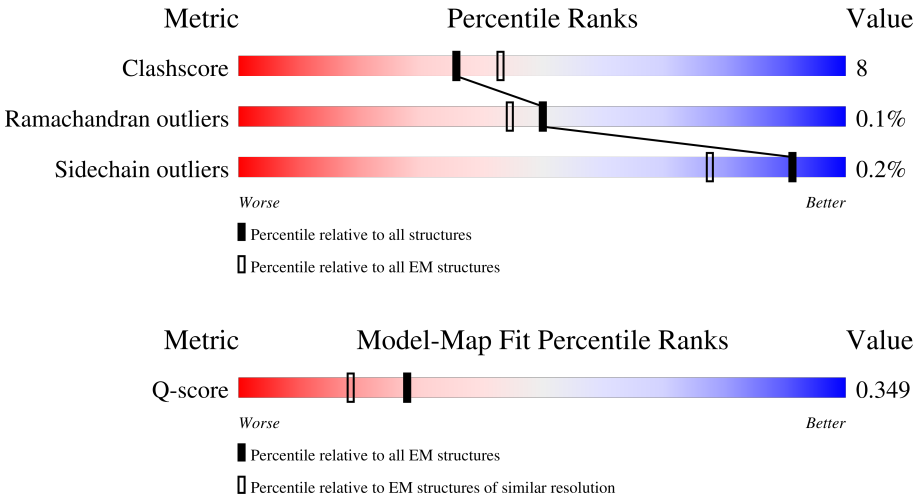
EMDB validation analysis	:	0.0.1.dev129
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.47

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 3.52 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13017 (3.02 - 4.02)

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	1	2041	5% 94%
1	2	2041	5% 94%
2	A	351	15% 83%
2	B	351	15% 83%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	351	15% 83%
2	D	351	14% 83%
2	E	351	14% 83%
2	F	351	13% 84%
2	G	351	5% 16% 83%
2	H	351	13% 84%
2	I	351	14% 83%
2	J	351	15% 83%
2	K	351	13% 83%
3	A0	453	78% 16% 6%
3	A2	453	75% 20% 6%
3	A4	453	77% 17% 6%
3	A6	453	74% 21% 6%
3	A8	453	79% 16% 6%
3	B0	453	78% 17% 6%
3	B2	453	78% 16% 6%
3	B4	453	79% 15% 6%
3	B6	453	79% 15% 6%
3	B8	453	74% 20% 6%
3	C0	453	80% 15% 6%
3	C2	453	77% 17% 6%
3	C4	453	76% 18% 6%
3	C6	453	77% 17% 6%
3	C8	453	81% 13% 6%
3	D0	453	76% 19% 6%

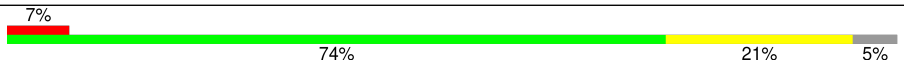
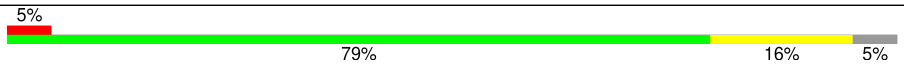
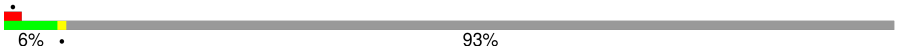
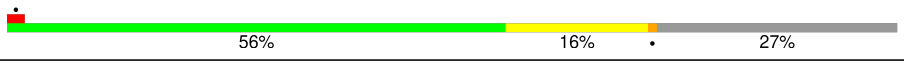
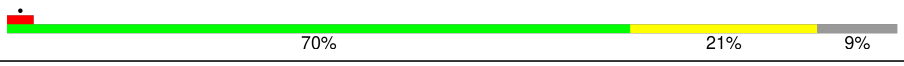
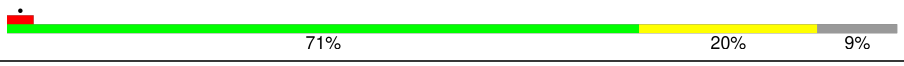
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D2	453	79% 16% 6%
3	D4	453	78% 16% 6%
3	D6	453	75% 19% 6%
3	D8	453	70% 23% 6%
3	E0	453	76% 19% 6%
3	E2	453	78% 16% 6%
3	E4	453	80% 15% 6%
3	E6	453	77% 17% 6%
3	E8	453	10% 78% 17% 6%
3	F0	453	5% 79% 15% 6%
4	A1	449	74% 20% 5%
4	A3	449	5% 71% 23% 5%
4	A5	449	75% 20% 5%
4	A7	449	78% 17% 5%
4	A9	449	74% 20% 5%
4	B1	449	75% 20% 5%
4	B3	449	74% 21% 5%
4	B5	449	79% 16% 5%
4	B7	449	76% 19% 5%
4	B9	449	77% 18% 5%
4	C1	449	73% 21% 5%
4	C3	449	81% 14% 5%
4	C5	449	76% 19% 5%
4	C7	449	80% 15% 5%
4	C9	449	76% 18% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D1	449	
4	D3	449	
4	D5	449	
4	D7	449	
4	D9	449	
4	E1	449	
4	E3	449	
4	E5	449	
4	E7	449	
4	E9	449	
4	F1	449	
5	O	583	
5	P	583	
5	R	583	
6	U	336	
6	V	336	
6	W	336	
6	X	336	
7	a	220	
7	b	220	
7	c	220	
7	d	220	
7	e	220	
7	f	220	
7	g	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	h	220	70% 20% 9%
7	i	220	71% 20% 9%
7	j	220	72% 19% 9%
7	m	220	21% 72% 20% 9%
7	n	220	23% 71% 20% 9%
7	o	220	69% 22% 9%
7	p	220	76% 15% 9%
7	q	220	77% 14% 9%
7	r	220	74% 18% 9%
7	s	220	68% 22% 9%
7	t	220	72% 16% 9%
7	u	220	72% 19% 9%
7	v	220	72% 19% 9%
7	w	220	5% 74% 18% 9%
7	x	220	70% 21% 9%
8	k	189	59% 16% 25%
8	l	189	53% 22% 25%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 226608 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 ICMAP4, TGME49_225340.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	130	Total	C	N	O	S	0	0
			1054	670	185	197	2		
1	2	130	Total	C	N	O	S	0	0
			1054	670	185	197	2		

- Molecule 2 is a protein called Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	B	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	C	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	D	59	Total	C	N	O	S	0	0
			464	306	74	83	1		
2	E	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	F	56	Total	C	N	O	S	0	0
			441	292	70	78	1		
2	G	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	H	56	Total	C	N	O	S	0	0
			441	292	70	78	1		
2	I	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	J	60	Total	C	N	O	S	0	0
			471	311	75	84	1		
2	K	60	Total	C	N	O	S	0	0
			471	311	75	84	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ARG	PRO	conflict	UNP A0A7J6K285
B	93	ARG	PRO	conflict	UNP A0A7J6K285
C	93	ARG	PRO	conflict	UNP A0A7J6K285
D	93	ARG	PRO	conflict	UNP A0A7J6K285
E	93	ARG	PRO	conflict	UNP A0A7J6K285
F	93	ARG	PRO	conflict	UNP A0A7J6K285
G	93	ARG	PRO	conflict	UNP A0A7J6K285
H	93	ARG	PRO	conflict	UNP A0A7J6K285
I	93	ARG	PRO	conflict	UNP A0A7J6K285
J	93	ARG	PRO	conflict	UNP A0A7J6K285
K	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	F0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

- Molecule 4 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	F1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 5 is a protein called TLAP3 (apical cap protein AC5), TGME49_235380.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	171	Total	C	N	O	S	0	0
			1360	844	255	259	2		
5	P	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		
5	R	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		

- Molecule 6 is a protein called TLAP4 (thioredoxin-like associated protein), TGME49_201760.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	22	Total	C	N	O	S	0	0
			182	112	38	31	1		
6	V	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	W	113	Total	C	N	O	S	0	0
			954	592	182	179	1		
6	X	91	Total	C	N	O		0	0
			772	480	144	148			

- Molecule 7 is a protein called TRXL1, TGME49_232410.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	b	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	w	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	x	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

- Molecule 8 is a protein called TRXL2, TGME49_225790.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	141	Total	C	N	O	S	0	0
			1155	747	205	199	4		
8	l	141	Total	C	N	O	S	0	0
			1155	747	205	199	4		

There are 46 discrepancies between the modelled and reference sequences:

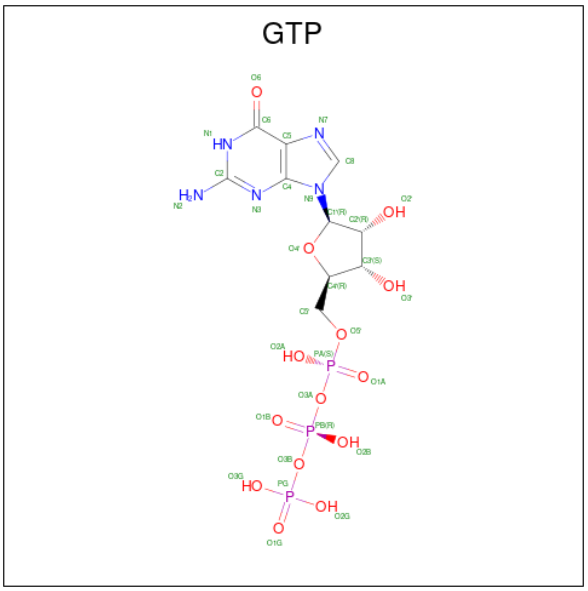
Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	expression tag	UNP A0A7J6K232
k	168	ALA	-	expression tag	UNP A0A7J6K232
k	169	GLN	-	expression tag	UNP A0A7J6K232
k	170	ARG	-	expression tag	UNP A0A7J6K232
k	171	LEU	-	expression tag	UNP A0A7J6K232
k	172	ARG	-	expression tag	UNP A0A7J6K232
k	173	THR	-	expression tag	UNP A0A7J6K232
k	174	LEU	-	expression tag	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
k	175	ASN	-	expression tag	UNP A0A7J6K232
k	176	ASP	-	expression tag	UNP A0A7J6K232
k	177	ALA	-	expression tag	UNP A0A7J6K232
k	178	THR	-	expression tag	UNP A0A7J6K232
k	179	ASP	-	expression tag	UNP A0A7J6K232
k	180	PRO	-	expression tag	UNP A0A7J6K232
k	181	TRP	-	expression tag	UNP A0A7J6K232
k	182	LYS	-	expression tag	UNP A0A7J6K232
k	183	LYS	-	expression tag	UNP A0A7J6K232
k	184	ARG	-	expression tag	UNP A0A7J6K232
k	185	LEU	-	expression tag	UNP A0A7J6K232
k	186	PRO	-	expression tag	UNP A0A7J6K232
k	187	GLN	-	expression tag	UNP A0A7J6K232
k	188	ASN	-	expression tag	UNP A0A7J6K232
k	189	VAL	-	expression tag	UNP A0A7J6K232
l	167	SER	-	expression tag	UNP A0A7J6K232
l	168	ALA	-	expression tag	UNP A0A7J6K232
l	169	GLN	-	expression tag	UNP A0A7J6K232
l	170	ARG	-	expression tag	UNP A0A7J6K232
l	171	LEU	-	expression tag	UNP A0A7J6K232
l	172	ARG	-	expression tag	UNP A0A7J6K232
l	173	THR	-	expression tag	UNP A0A7J6K232
l	174	LEU	-	expression tag	UNP A0A7J6K232
l	175	ASN	-	expression tag	UNP A0A7J6K232
l	176	ASP	-	expression tag	UNP A0A7J6K232
l	177	ALA	-	expression tag	UNP A0A7J6K232
l	178	THR	-	expression tag	UNP A0A7J6K232
l	179	ASP	-	expression tag	UNP A0A7J6K232
l	180	PRO	-	expression tag	UNP A0A7J6K232
l	181	TRP	-	expression tag	UNP A0A7J6K232
l	182	LYS	-	expression tag	UNP A0A7J6K232
l	183	LYS	-	expression tag	UNP A0A7J6K232
l	184	ARG	-	expression tag	UNP A0A7J6K232
l	185	LEU	-	expression tag	UNP A0A7J6K232
l	186	PRO	-	expression tag	UNP A0A7J6K232
l	187	GLN	-	expression tag	UNP A0A7J6K232
l	188	ASN	-	expression tag	UNP A0A7J6K232
l	189	VAL	-	expression tag	UNP A0A7J6K232

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	A8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E7	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
9	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

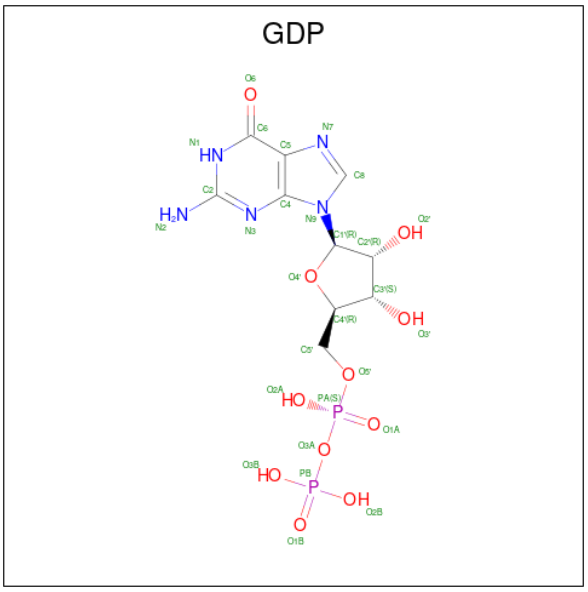
Mol	Chain	Residues	Atoms		AltConf
10	A0	1	Total	Mg	0
			1	1	
10	A2	1	Total	Mg	0
			1	1	
10	A4	1	Total	Mg	0
			1	1	
10	A6	1	Total	Mg	0
			1	1	
10	A8	1	Total	Mg	0
			1	1	
10	B0	1	Total	Mg	0
			1	1	
10	B2	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
10	B4	1	Total Mg 1 1	0
10	B6	1	Total Mg 1 1	0
10	B8	1	Total Mg 1 1	0
10	C0	1	Total Mg 1 1	0
10	C2	1	Total Mg 1 1	0
10	C4	1	Total Mg 1 1	0
10	C6	1	Total Mg 1 1	0
10	C9	1	Total Mg 1 1	0
10	D1	1	Total Mg 1 1	0
10	D3	1	Total Mg 1 1	0
10	D4	1	Total Mg 1 1	0
10	D6	1	Total Mg 1 1	0
10	D8	1	Total Mg 1 1	0
10	E0	1	Total Mg 1 1	0
10	E2	1	Total Mg 1 1	0
10	E4	1	Total Mg 1 1	0
10	E6	1	Total Mg 1 1	0
10	E8	1	Total Mg 1 1	0
10	F0	1	Total Mg 1 1	0

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

Continued from previous page...

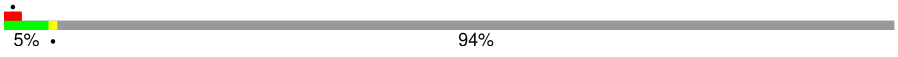
Mol	Chain	Residues	Atoms					AltConf
11	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	O	1	Total	C	N	O	P	0
			28	10	5	11	2	
11	P	1	Total	C	N	O	P	0
			28	10	5	11	2	

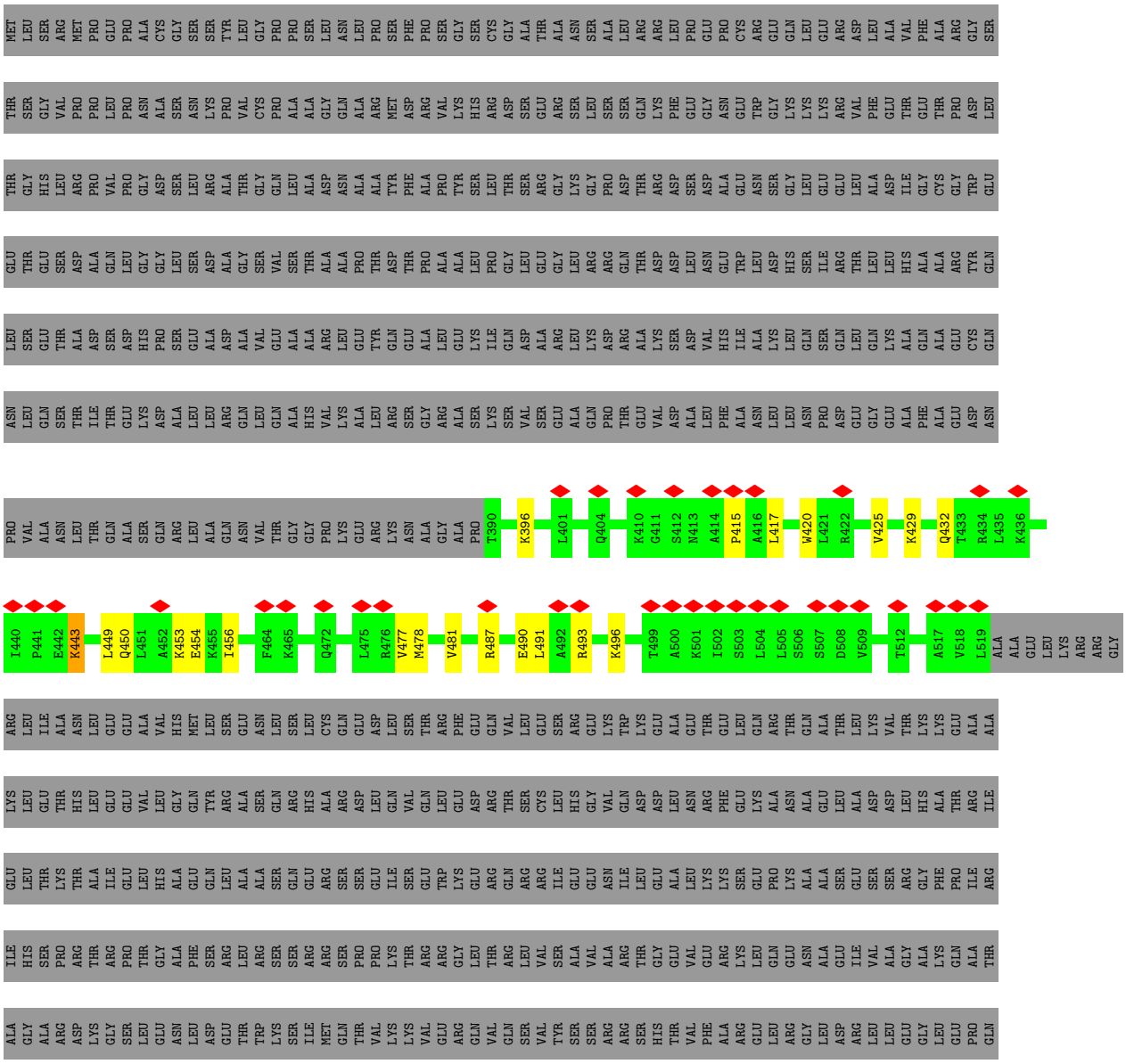
3 Residue-property plots (i)

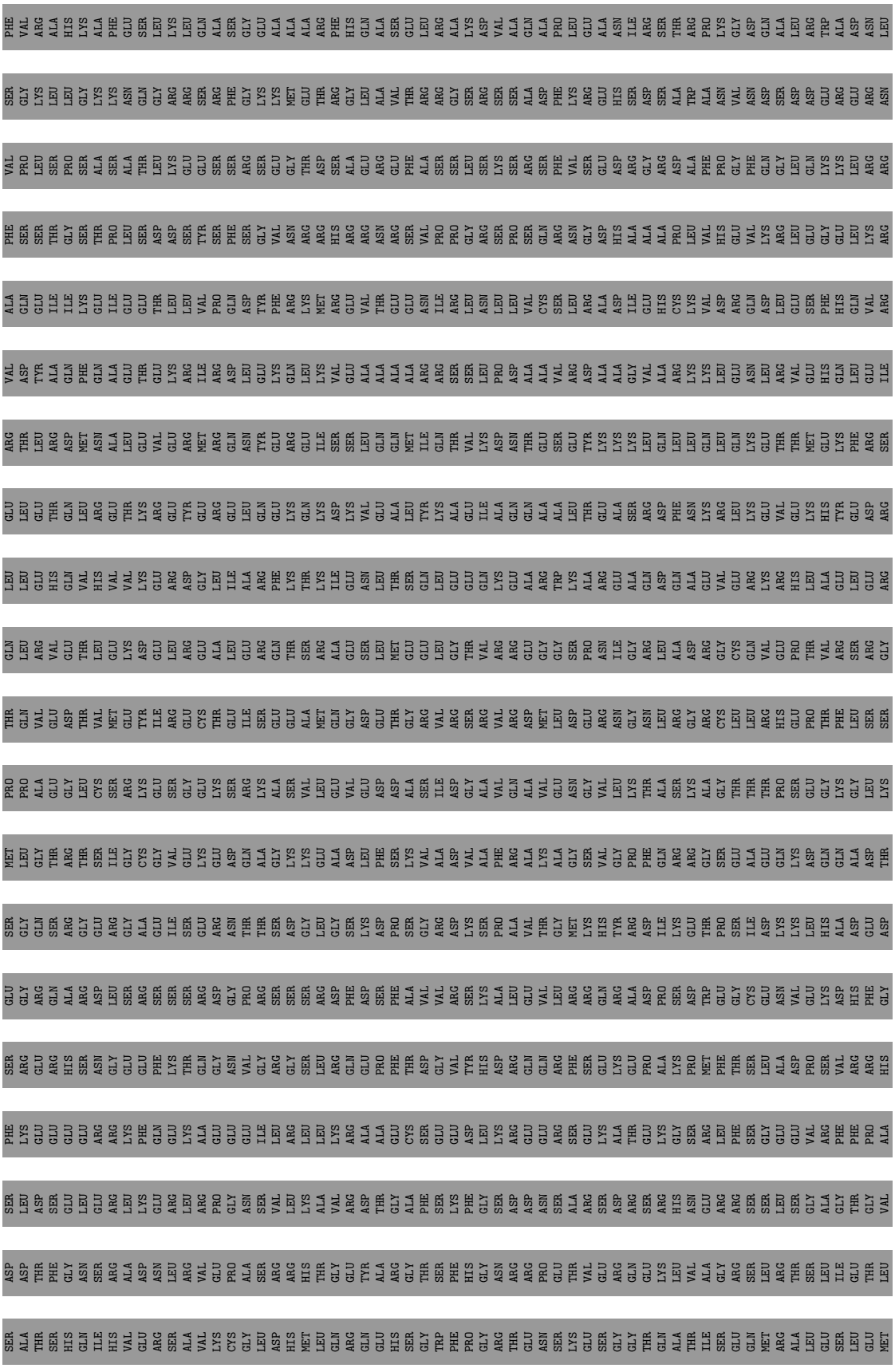
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ICMAP4, TGME49_225340

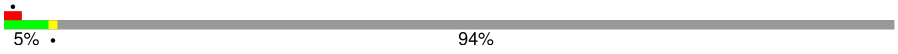
Chain 1:

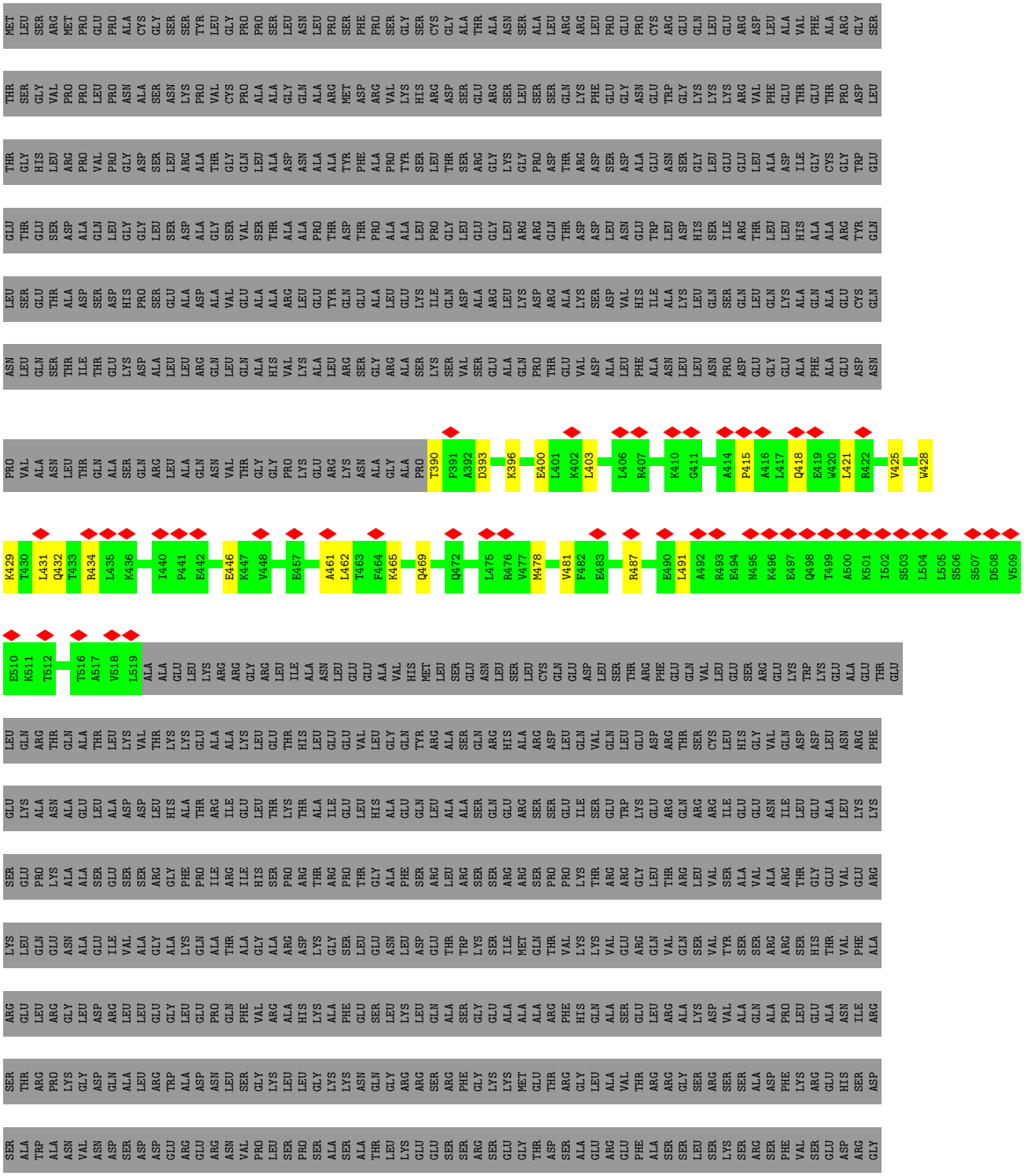


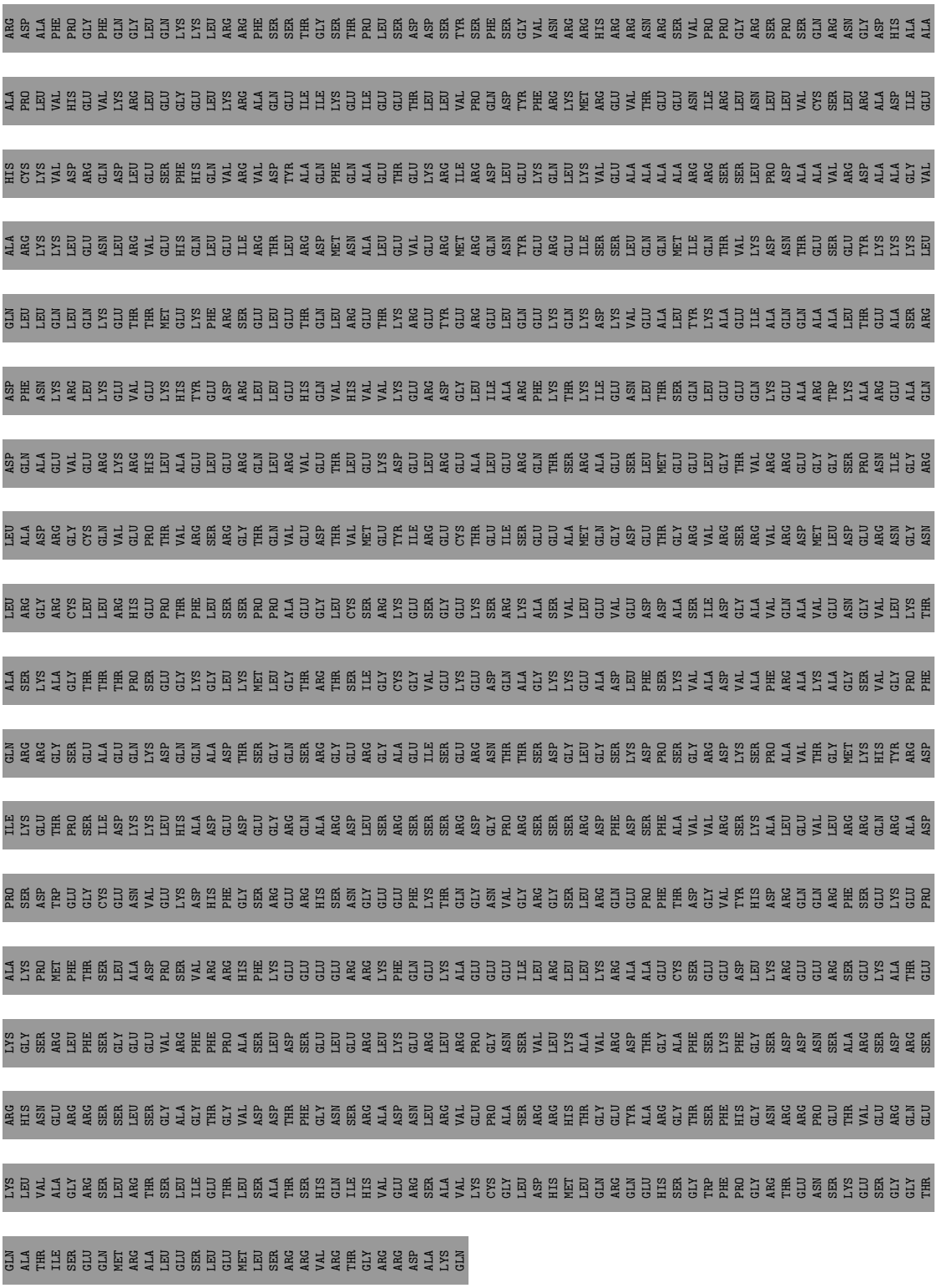



PHE VAL ARG ALA HIS LYS ALA PHE GLU SER LEU LYS LEU GLN ALA SER GLY GLU ALA ALA ARG PHE HIS GLN ALA ASN ILE ARG SER THR ARG PRO LYS GLY ASP GLN ALA LEU ARG TRP ALA ASP ASN LEU
SER GLY LYS LEU LEU PRO GLY LYS LYS ASN GLN GLY ARG ARG SER ARG PHE GLY LYS LYS MET GLU THR ARG GLY LEU ALA ARG GLY ARG ARG ASN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

• Molecule 1: ICMAP4, TGME49_225340

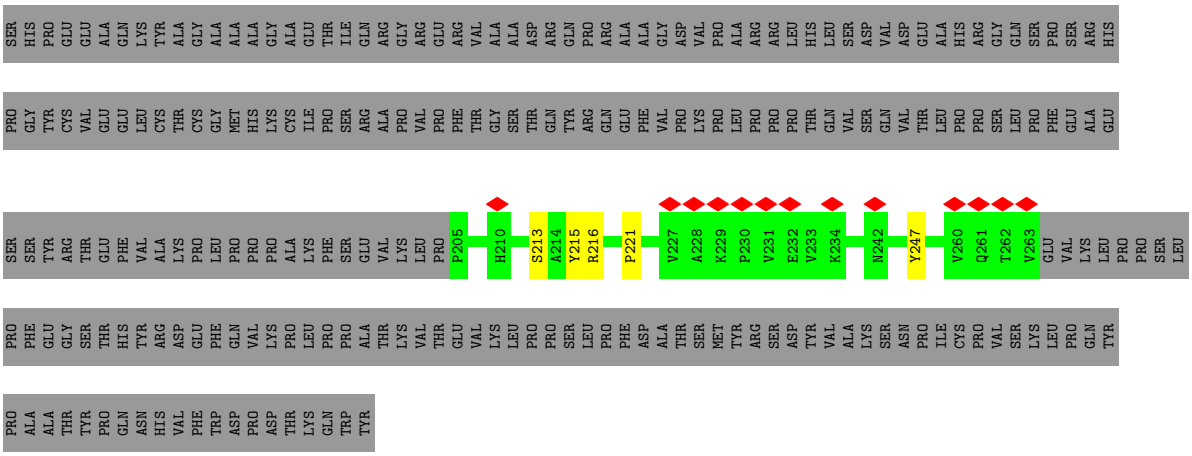
Chain 2: 





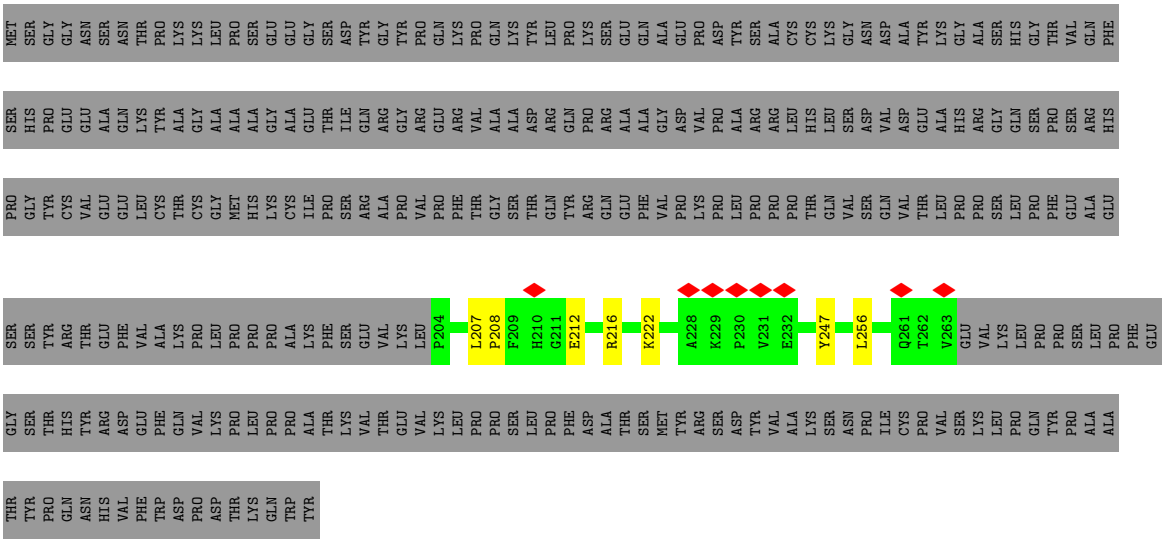
• Molecule 2: Microtubule associated protein SPM1

Chain A:



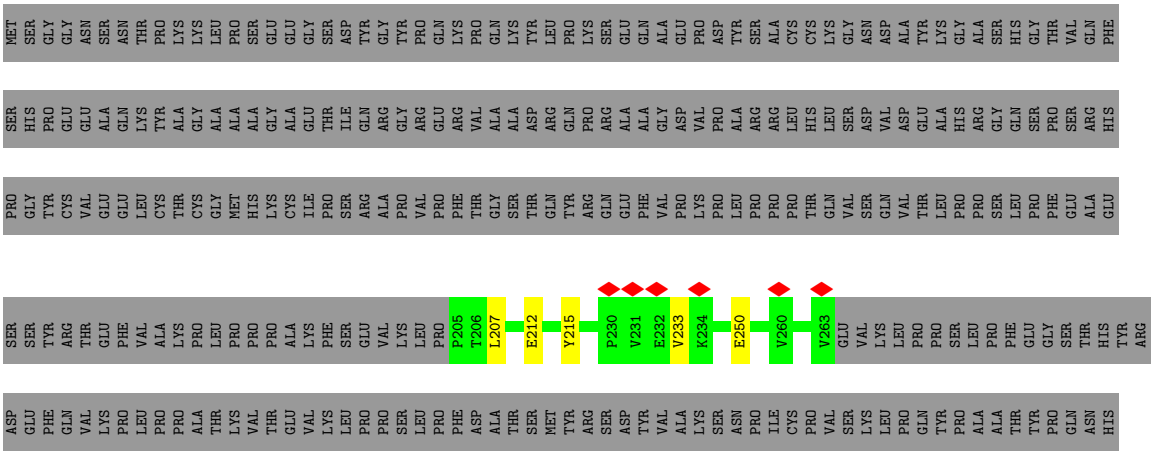
• Molecule 2: Microtubule associated protein SPM1

Chain B:



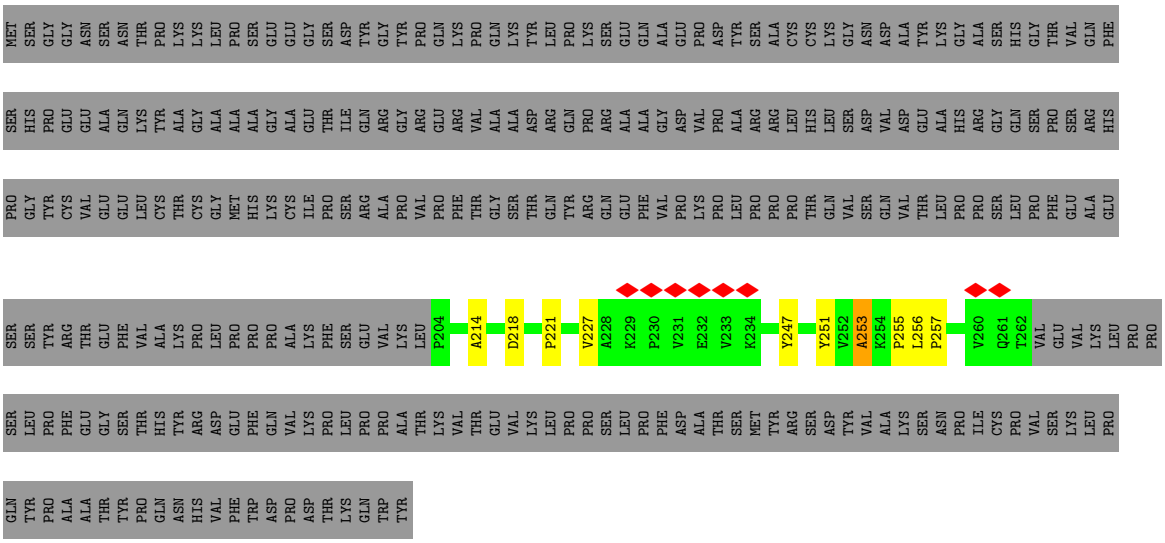
• Molecule 2: Microtubule associated protein SPM1

Chain C:



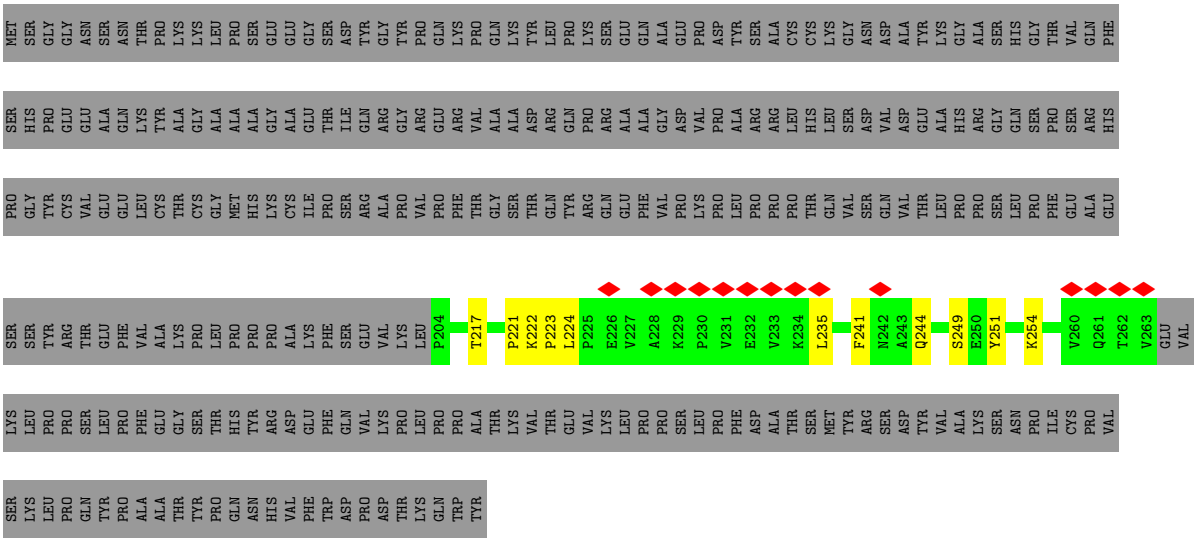
• Molecule 2: Microtubule associated protein SPM1

Chain D:



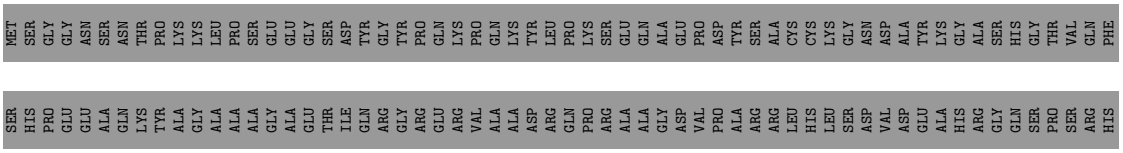
• Molecule 2: Microtubule associated protein SPM1

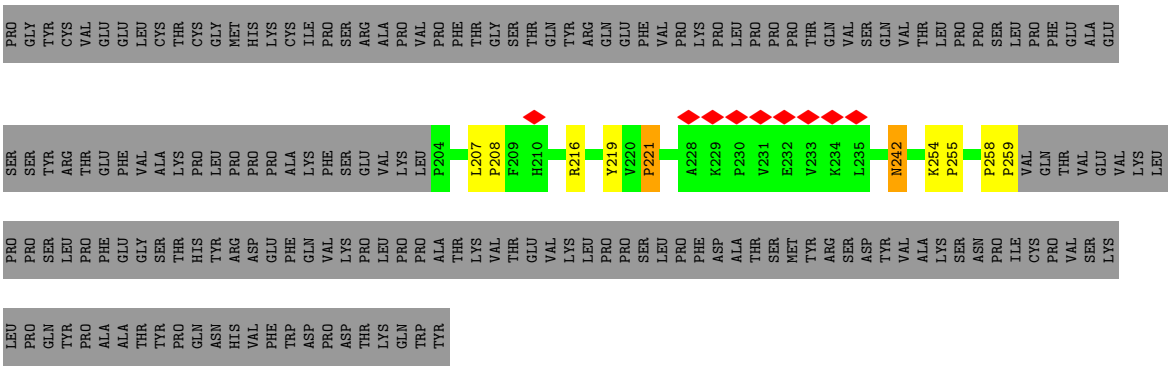
Chain E:



• Molecule 2: Microtubule associated protein SPM1

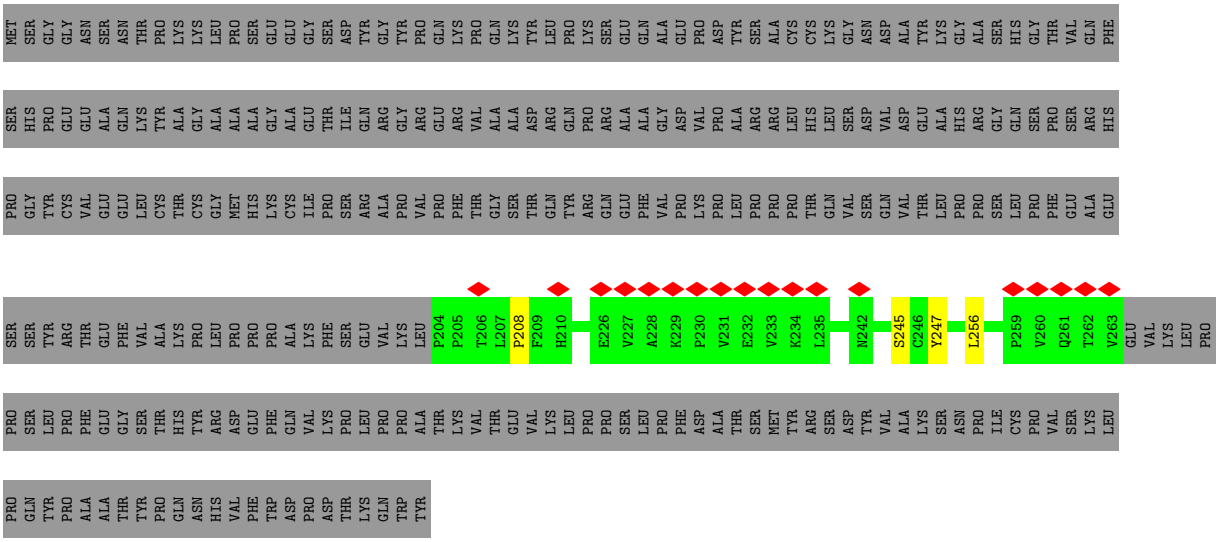
Chain F:





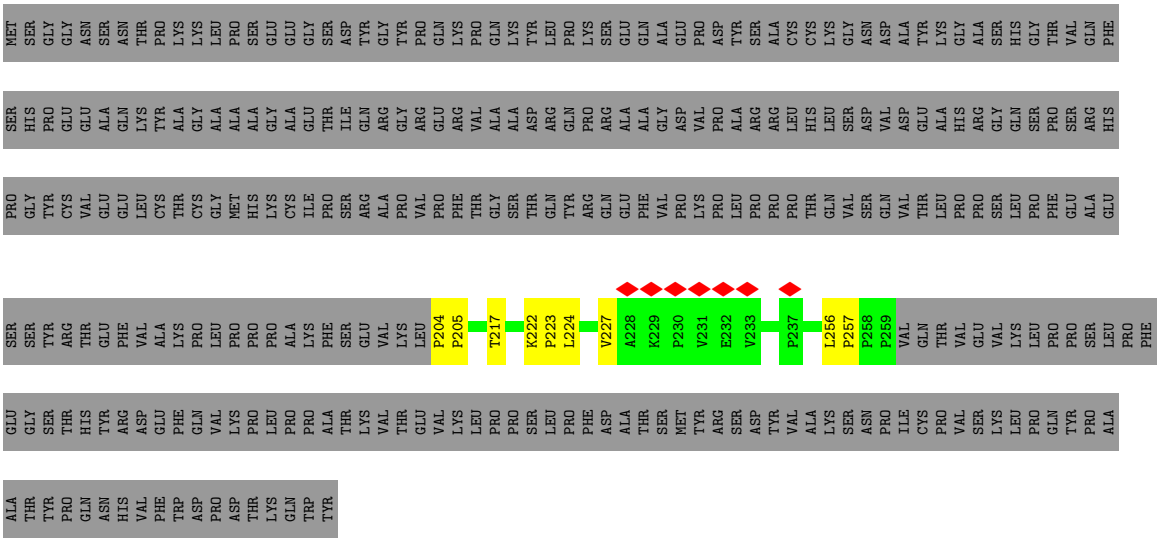
• Molecule 2: Microtubule associated protein SPM1

Chain G:



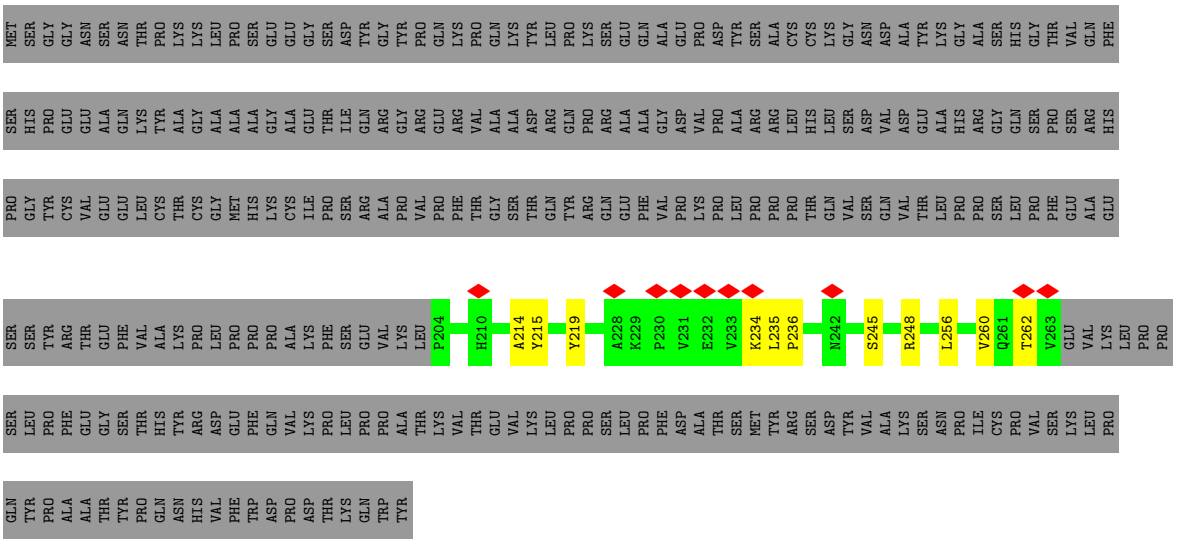
• Molecule 2: Microtubule associated protein SPM1

Chain H:



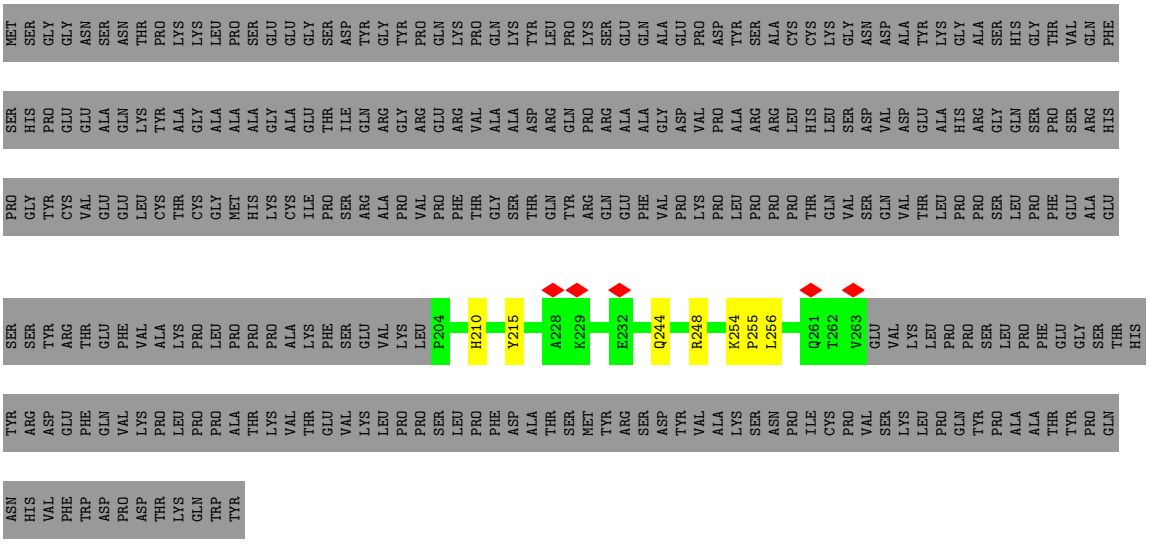
• Molecule 2: Microtubule associated protein SPM1

Chain I:



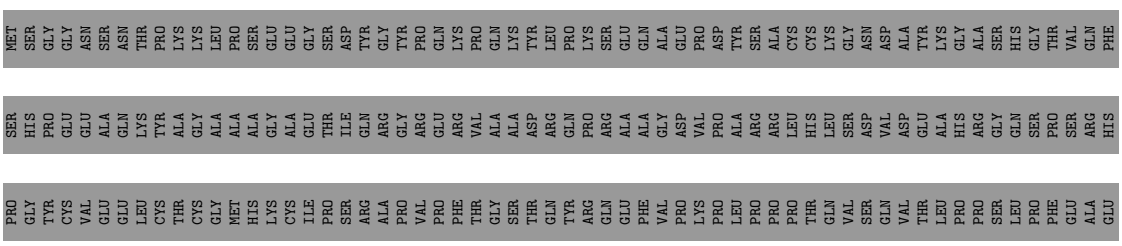
• Molecule 2: Microtubule associated protein SPM1

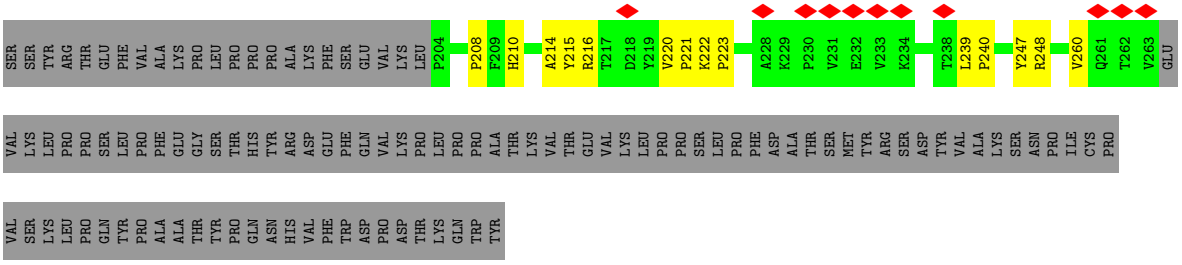
Chain J:



• Molecule 2: Microtubule associated protein SPM1

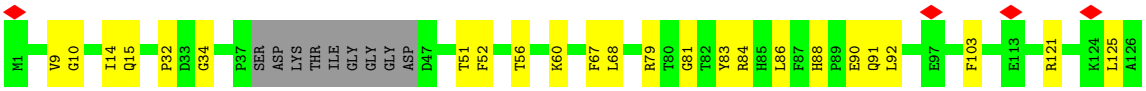
Chain K:

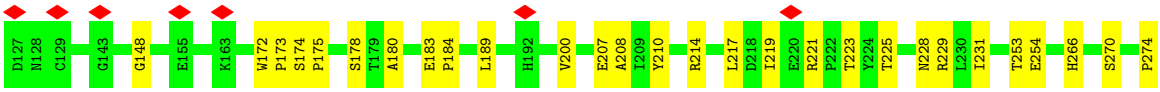


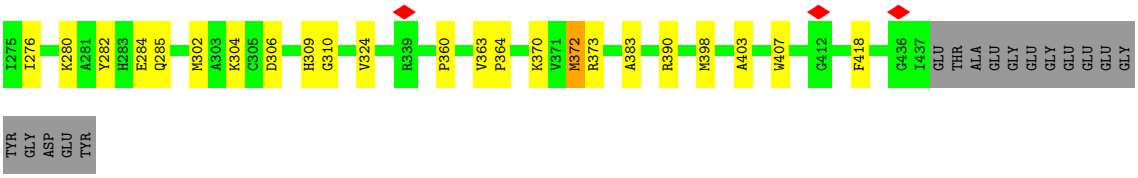


• Molecule 3: Tubulin alpha chain

Chain A0:

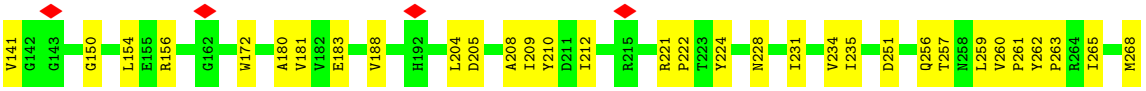


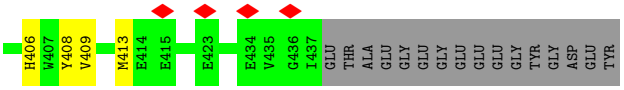




• Molecule 3: Tubulin alpha chain

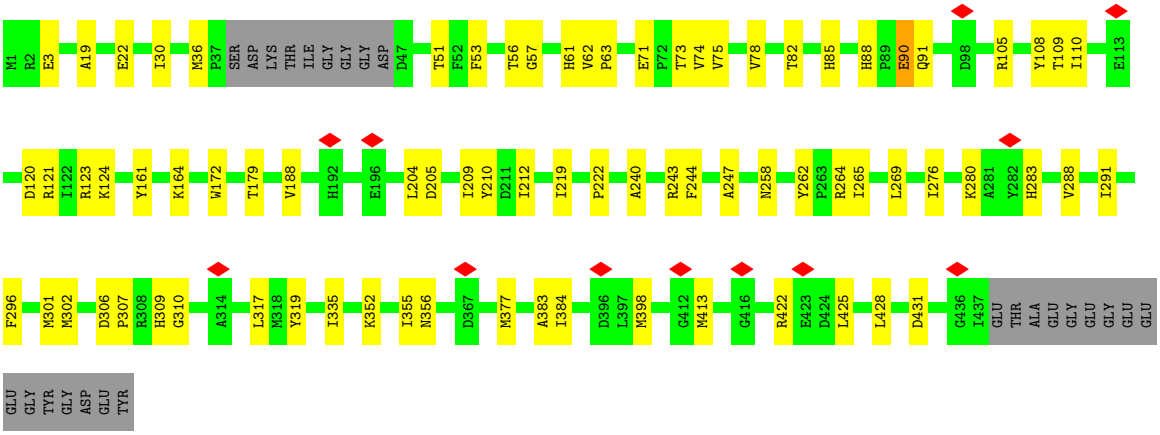
Chain A2:





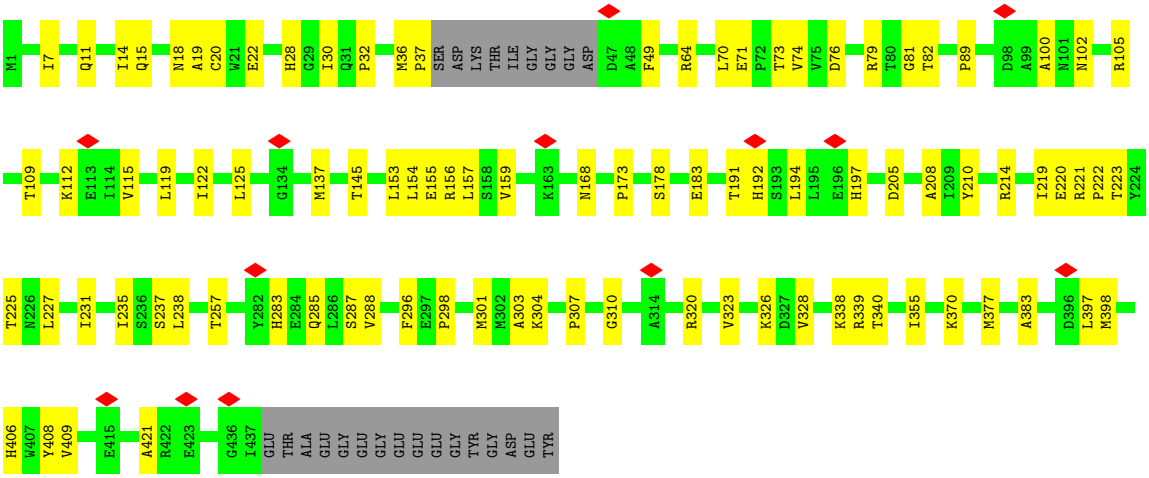
• Molecule 3: Tubulin alpha chain

Chain A4:



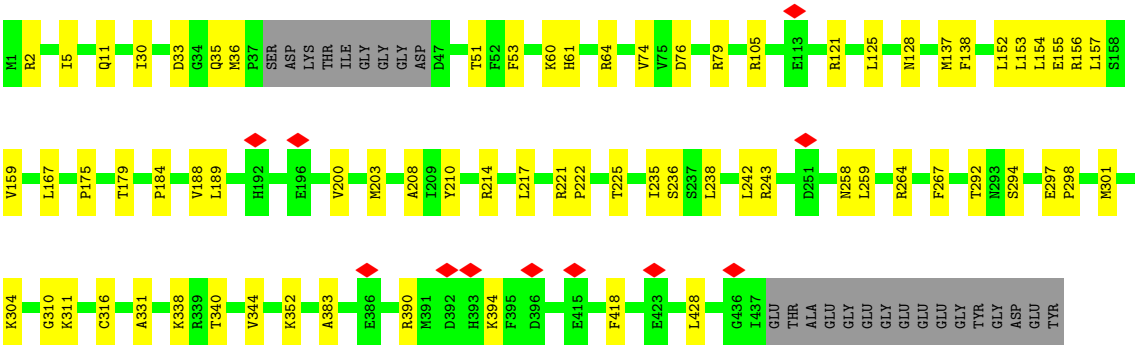
• Molecule 3: Tubulin alpha chain

Chain A6:



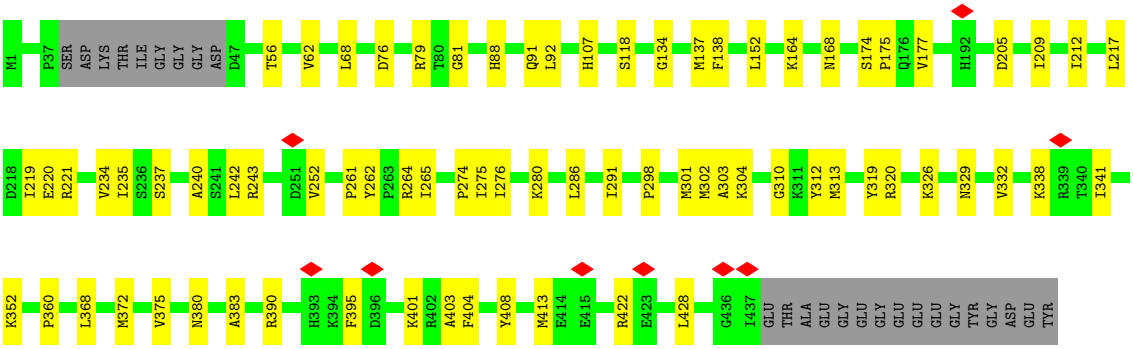
• Molecule 3: Tubulin alpha chain

Chain A8:



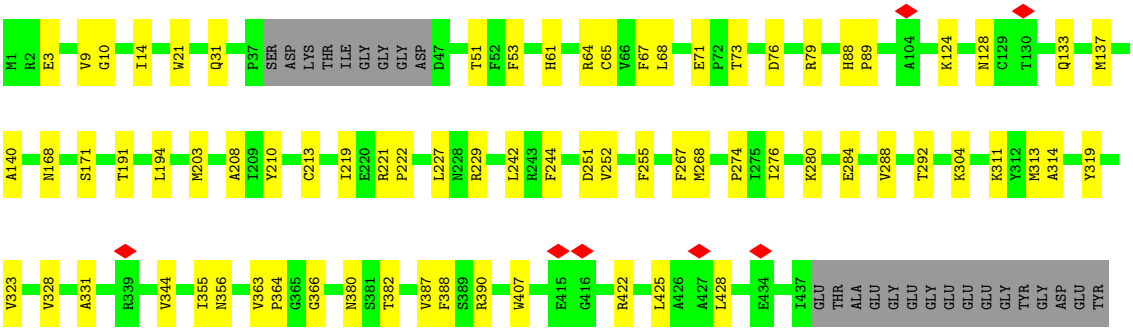
• Molecule 3: Tubulin alpha chain

Chain B0:



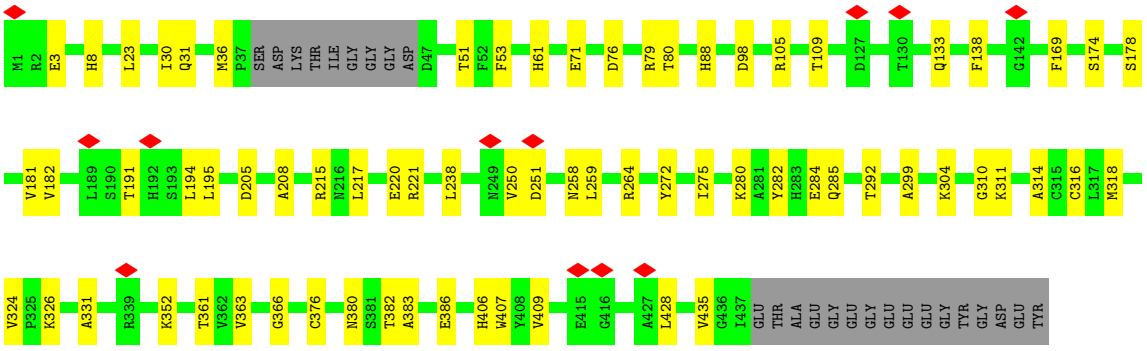
• Molecule 3: Tubulin alpha chain

Chain B2:



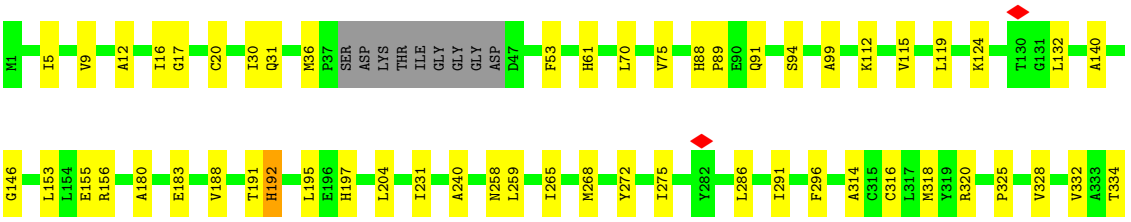
• Molecule 3: Tubulin alpha chain

Chain B4:



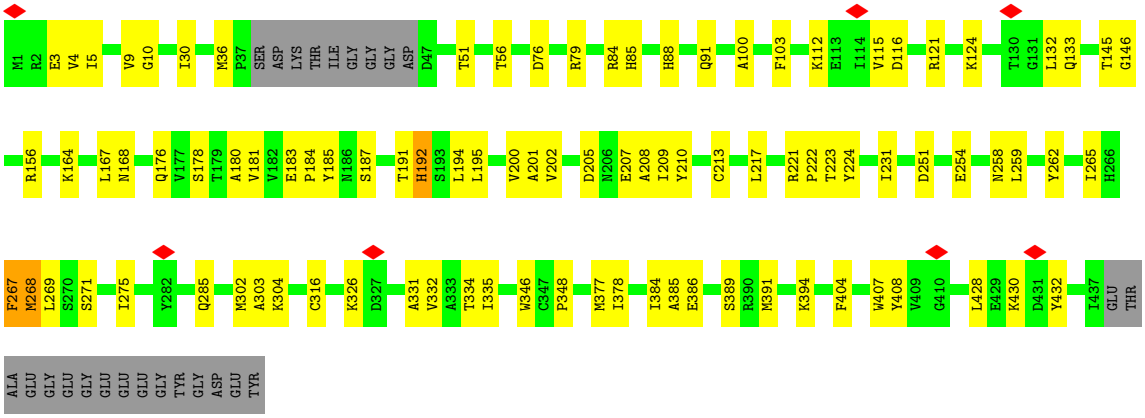
• Molecule 3: Tubulin alpha chain

Chain B6:



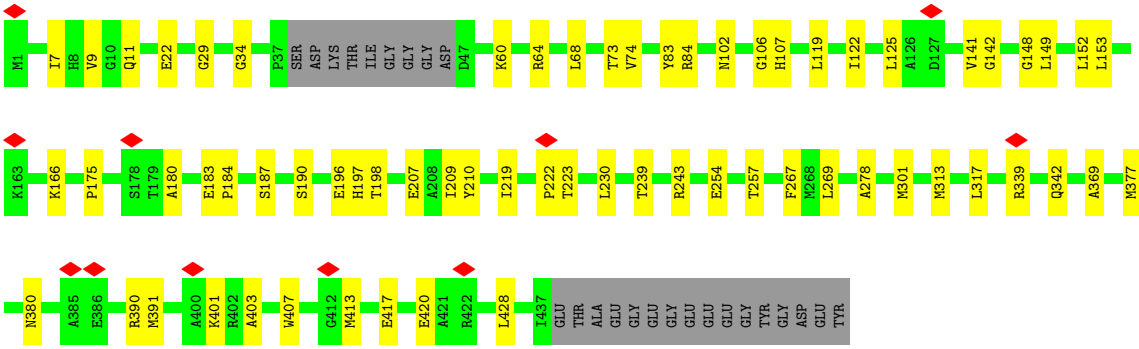
• Molecule 3: Tubulin alpha chain

Chain B8:



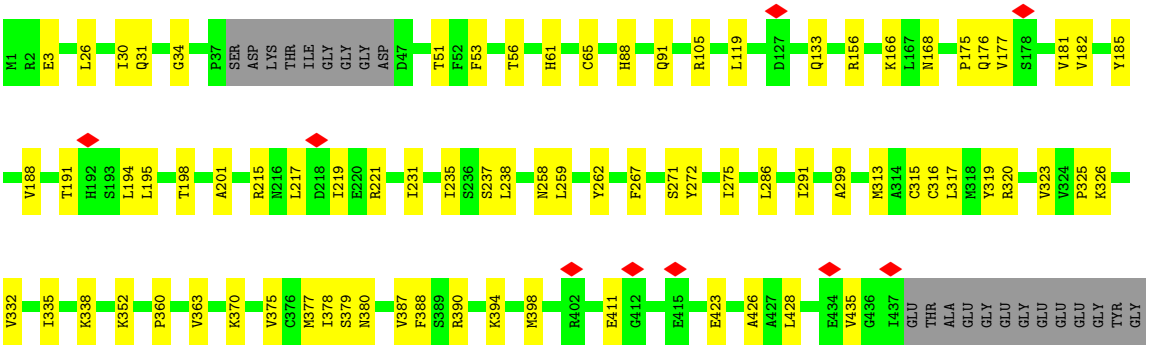
• Molecule 3: Tubulin alpha chain

Chain C0:



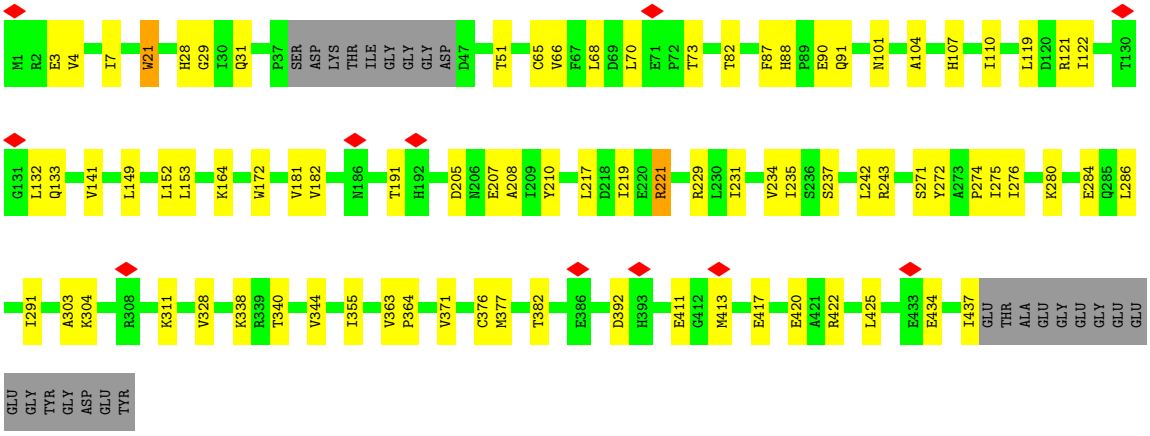
• Molecule 3: Tubulin alpha chain

Chain C2:



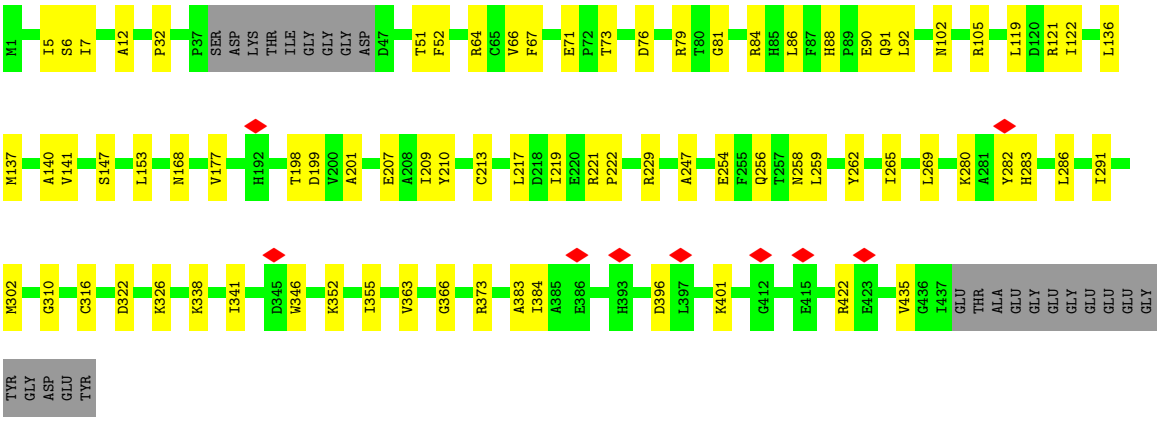
• Molecule 3: Tubulin alpha chain

Chain C4:



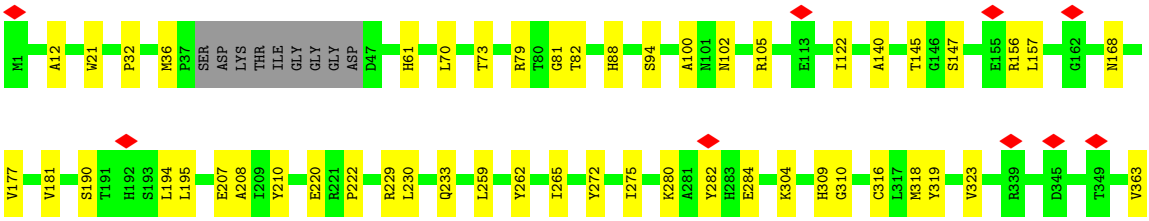
• Molecule 3: Tubulin alpha chain

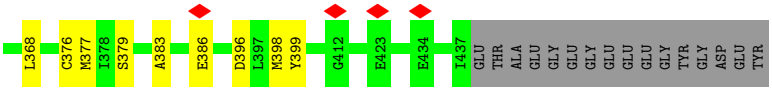
Chain C6:



• Molecule 3: Tubulin alpha chain

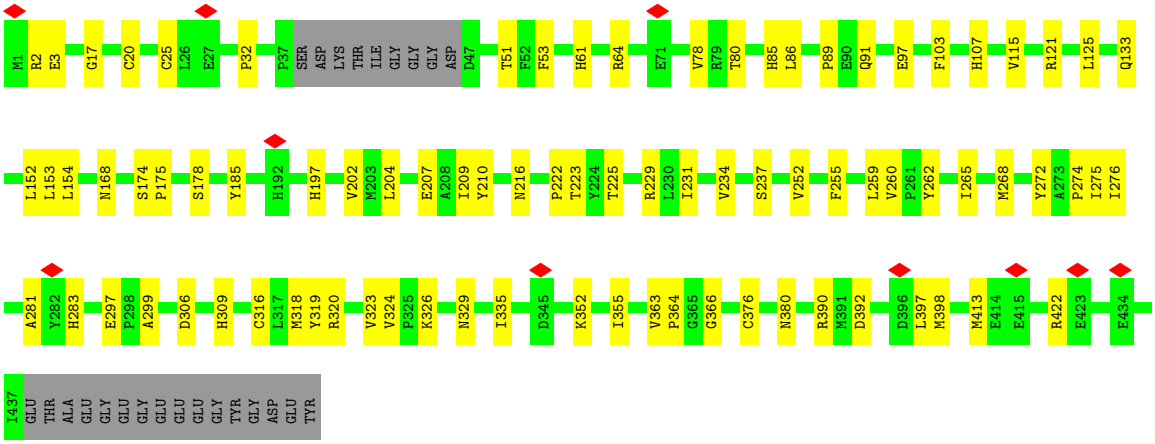
Chain C8:





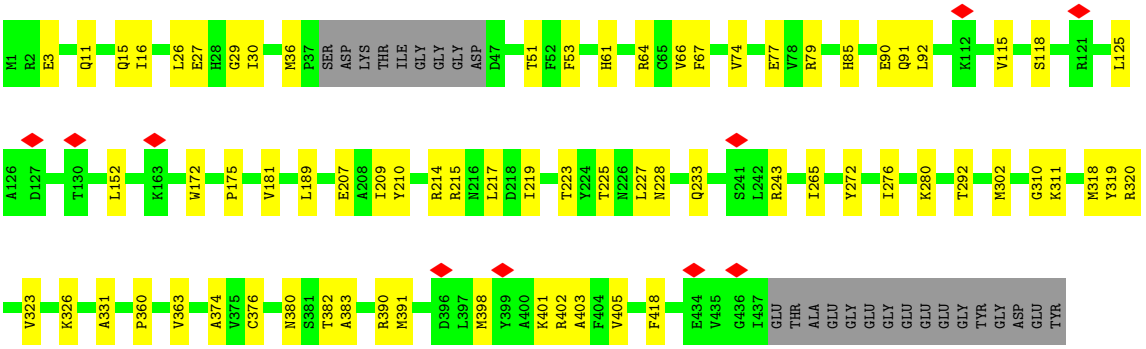
• Molecule 3: Tubulin alpha chain

Chain D0:



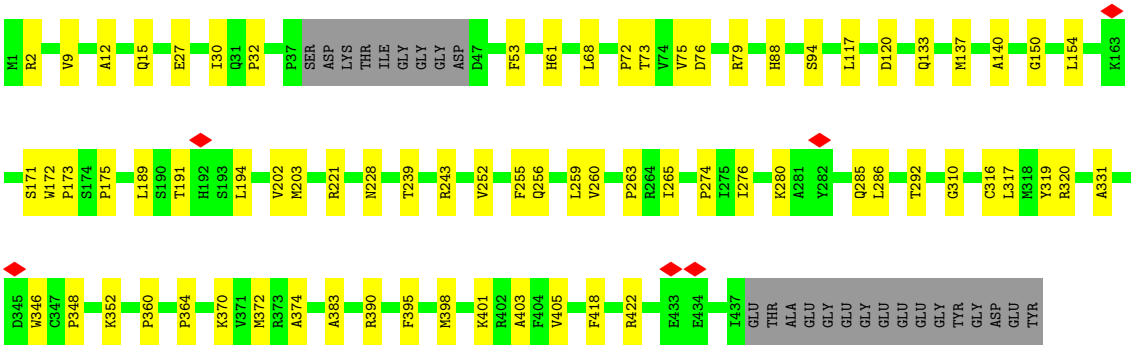
• Molecule 3: Tubulin alpha chain

Chain D2:



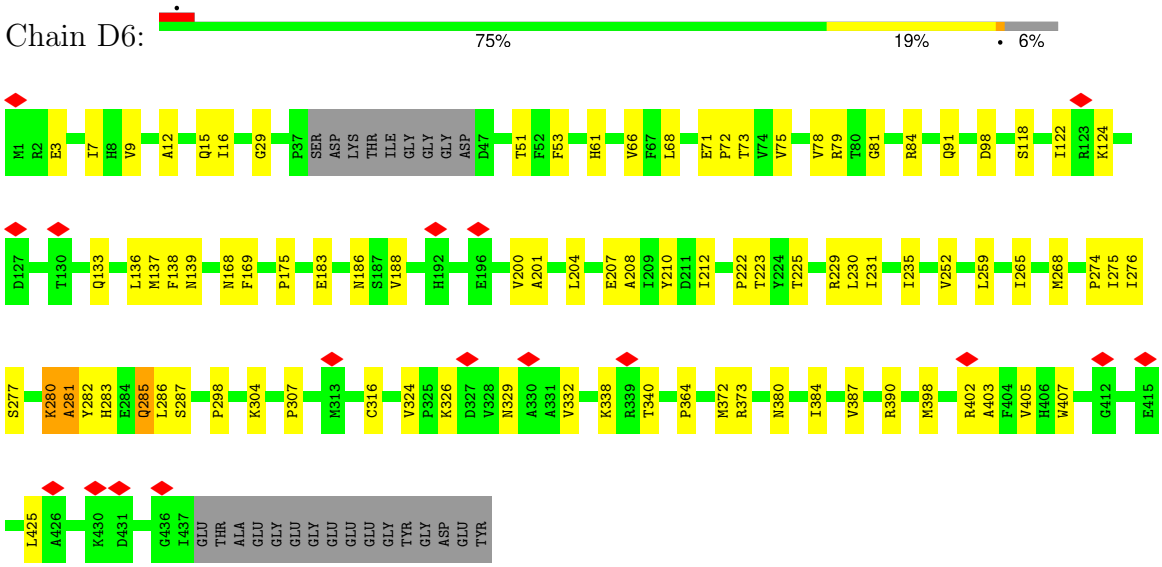
• Molecule 3: Tubulin alpha chain

Chain D4:



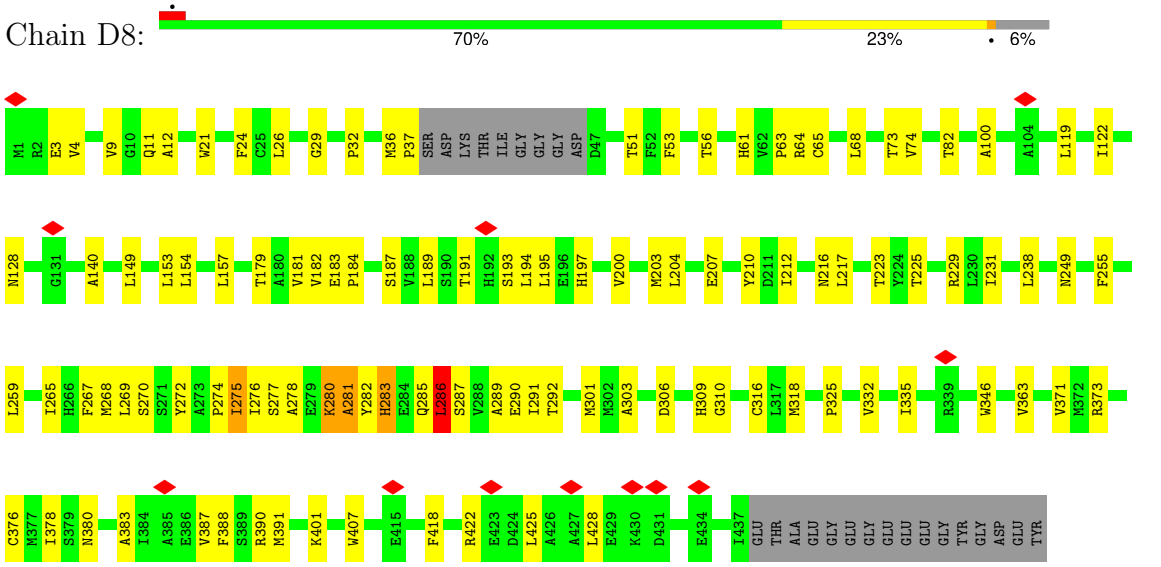
• Molecule 3: Tubulin alpha chain

Chain D6:



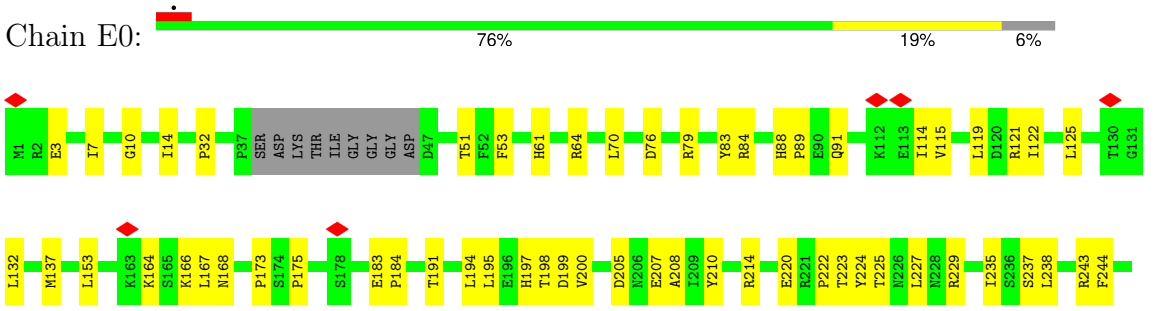
• Molecule 3: Tubulin alpha chain

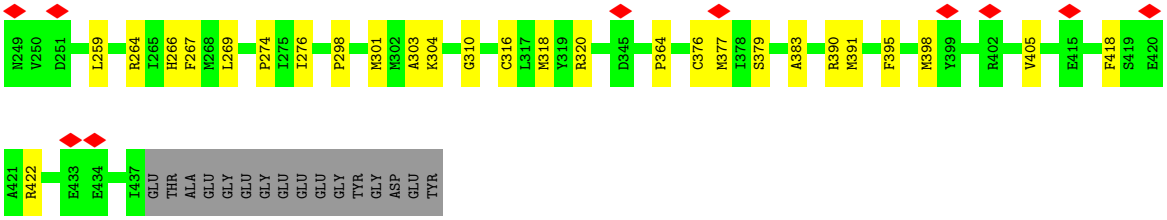
Chain D8:



• Molecule 3: Tubulin alpha chain

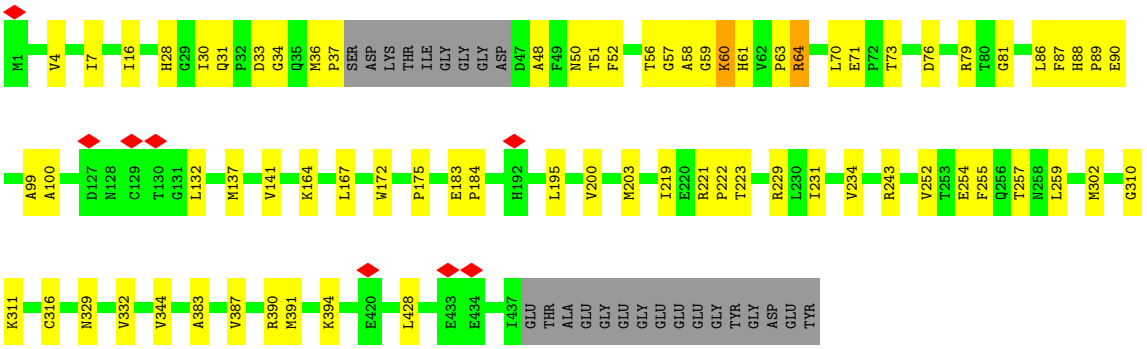
Chain E0:





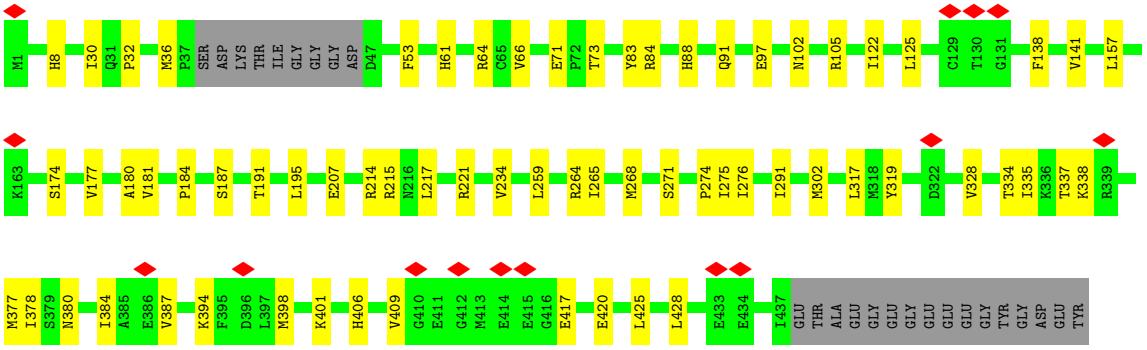
• Molecule 3: Tubulin alpha chain

Chain E2:



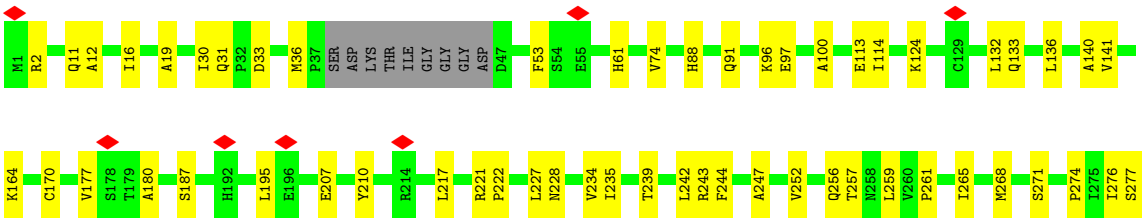
• Molecule 3: Tubulin alpha chain

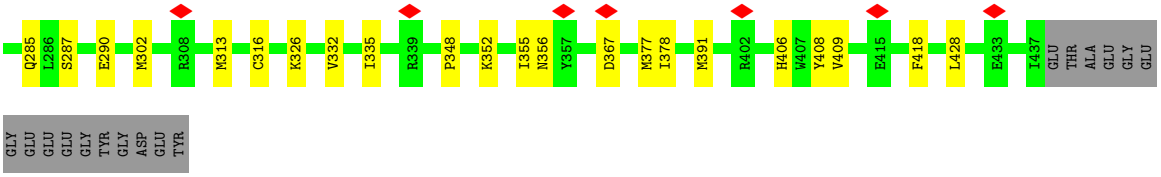
Chain E4:



• Molecule 3: Tubulin alpha chain

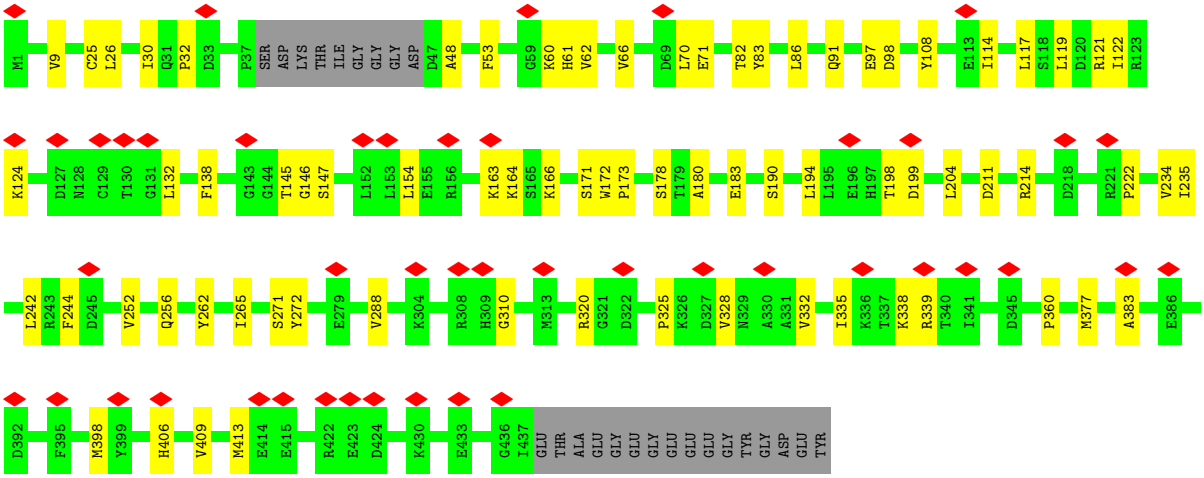
Chain E6:





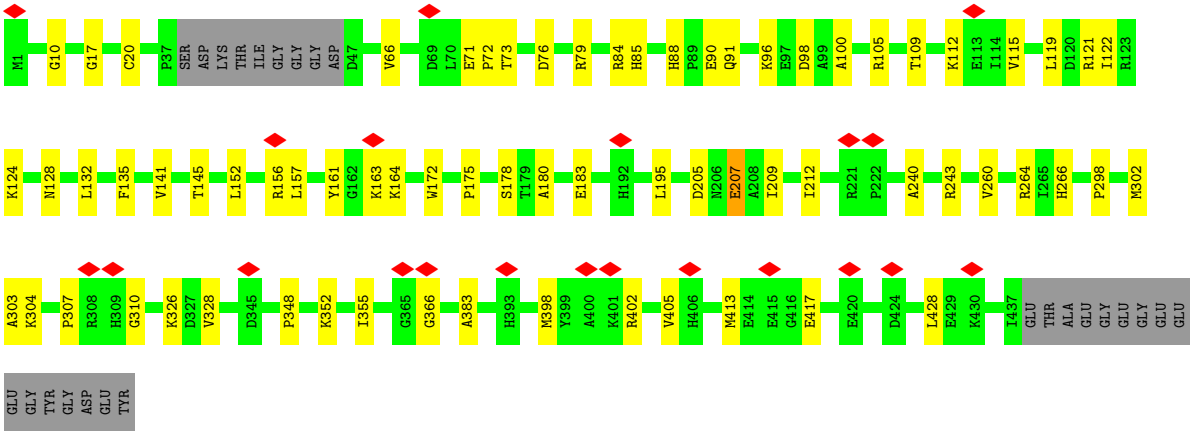
• Molecule 3: Tubulin alpha chain

Chain E8:



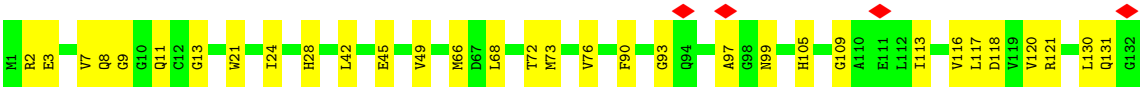
• Molecule 3: Tubulin alpha chain

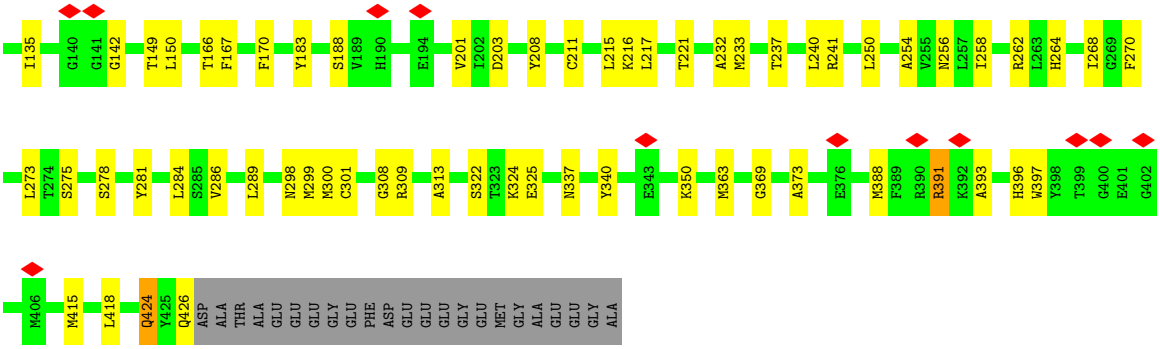
Chain F0:



• Molecule 4: Tubulin beta chain

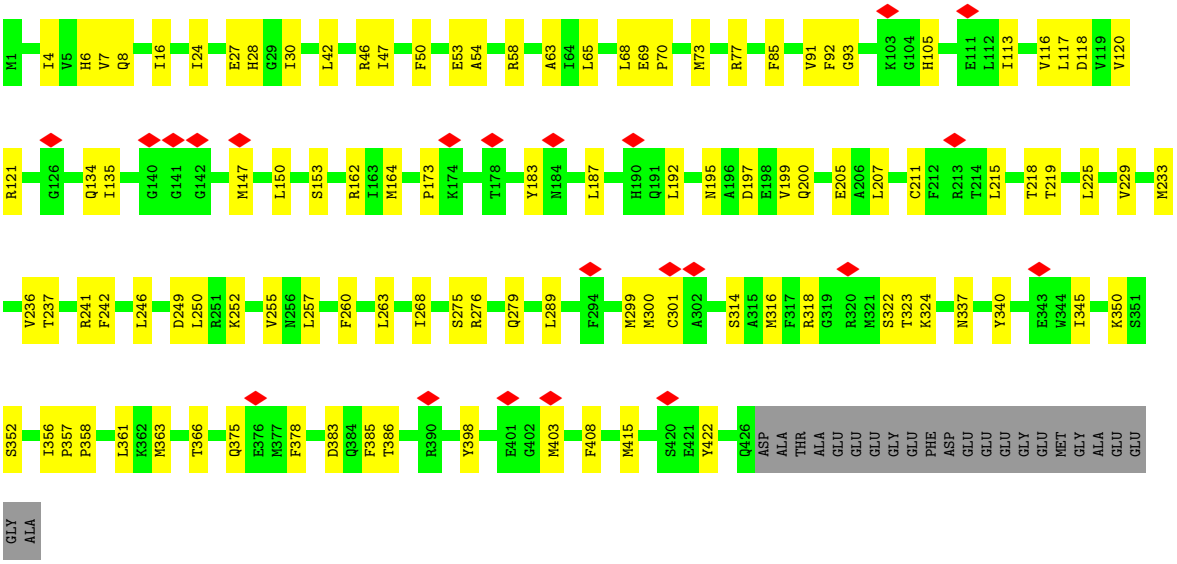
Chain A1:





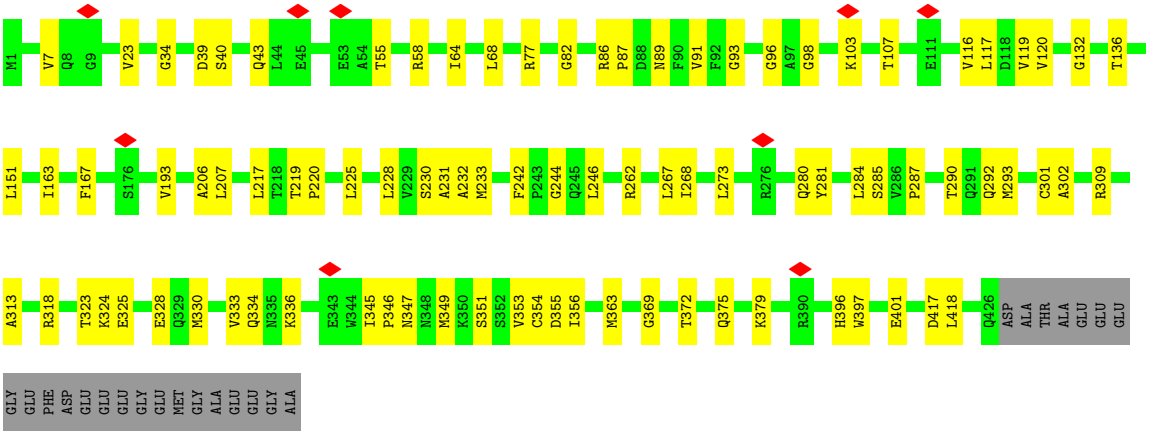
• Molecule 4: Tubulin beta chain

Chain A3:



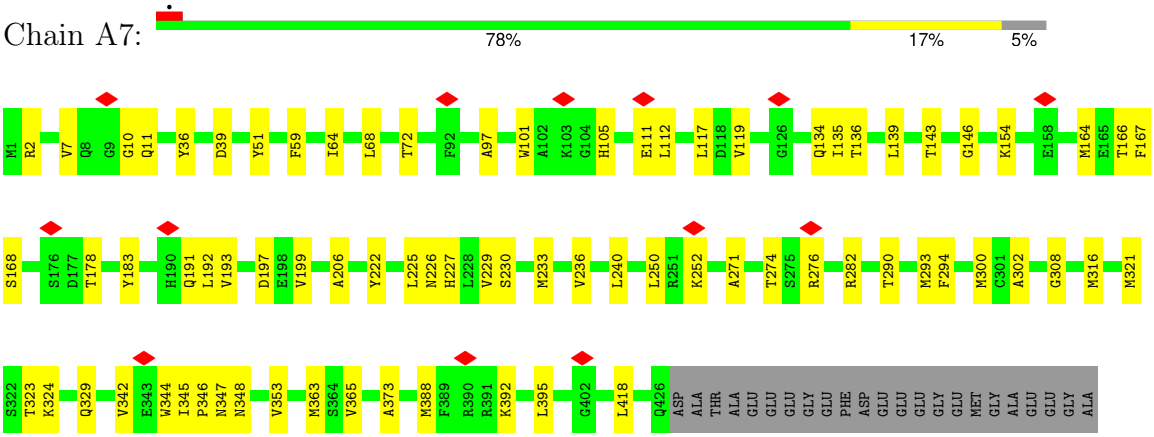
• Molecule 4: Tubulin beta chain

Chain A5:



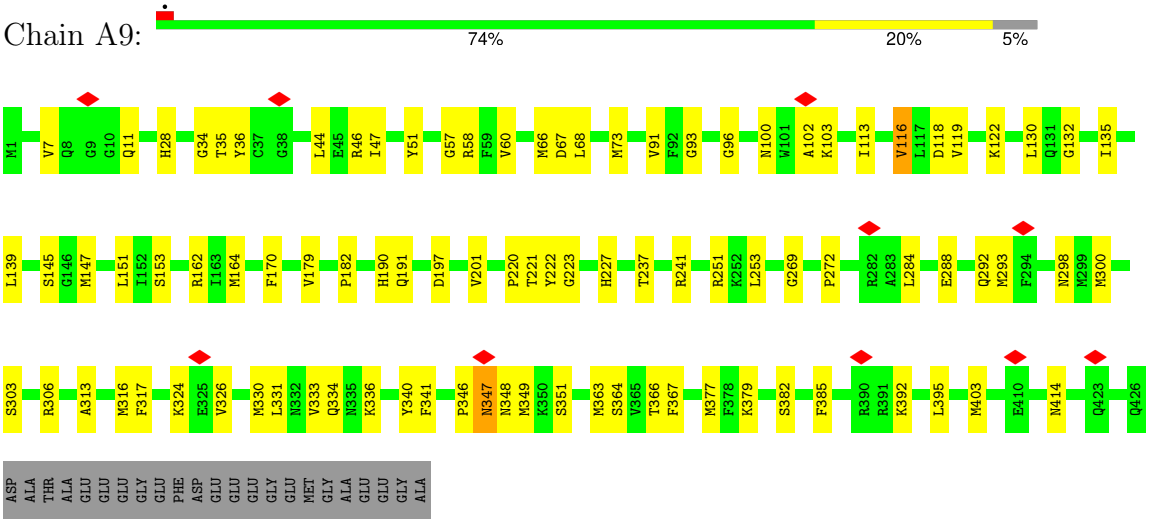
• Molecule 4: Tubulin beta chain

Chain A7:



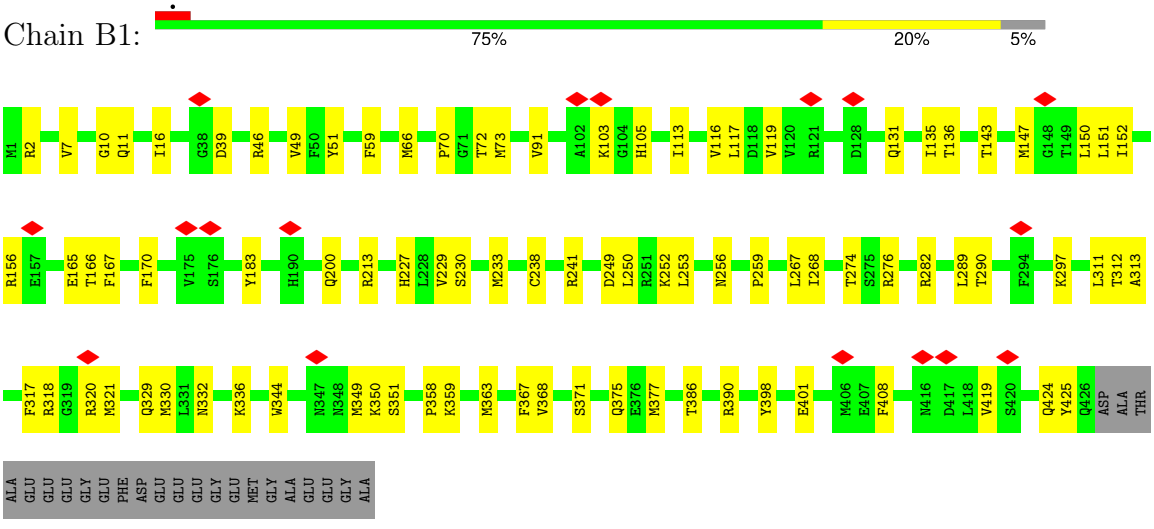
• Molecule 4: Tubulin beta chain

Chain A9:



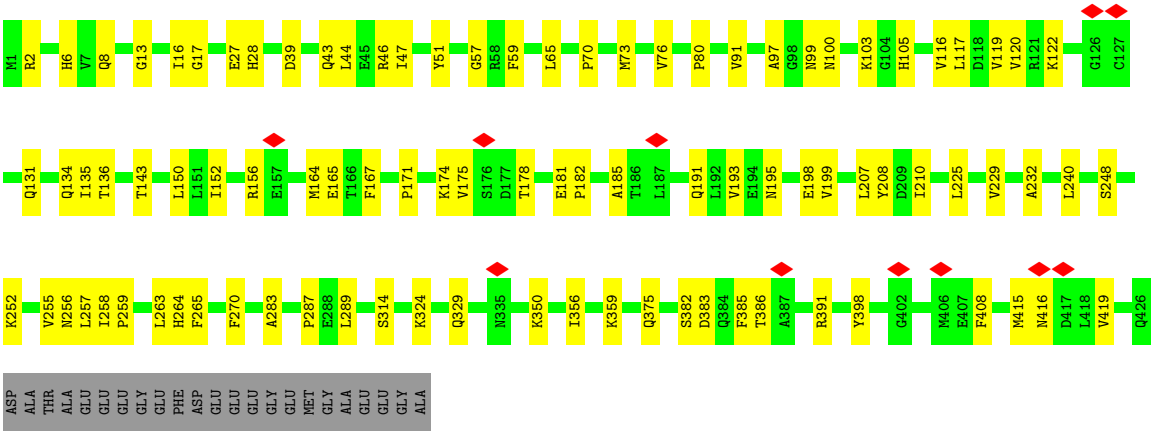
• Molecule 4: Tubulin beta chain

Chain B1:



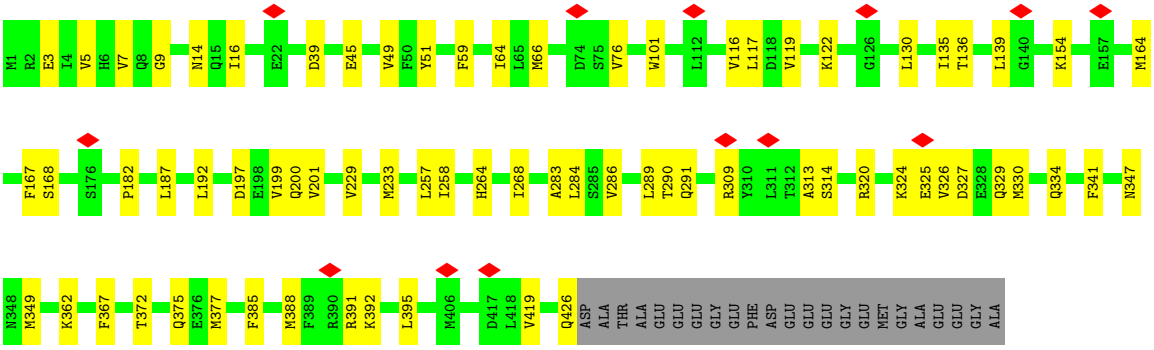
• Molecule 4: Tubulin beta chain

Chain B3:



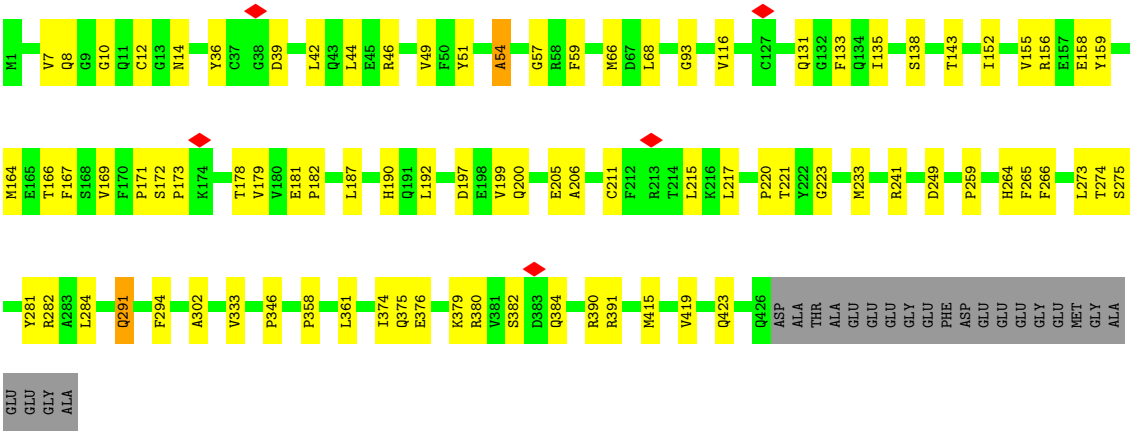
• Molecule 4: Tubulin beta chain

Chain B5:



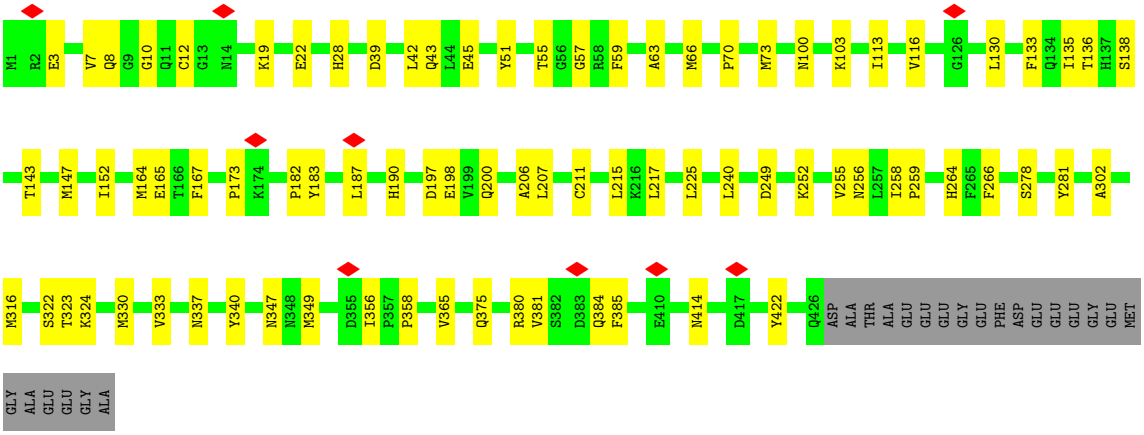
• Molecule 4: Tubulin beta chain

Chain B7:



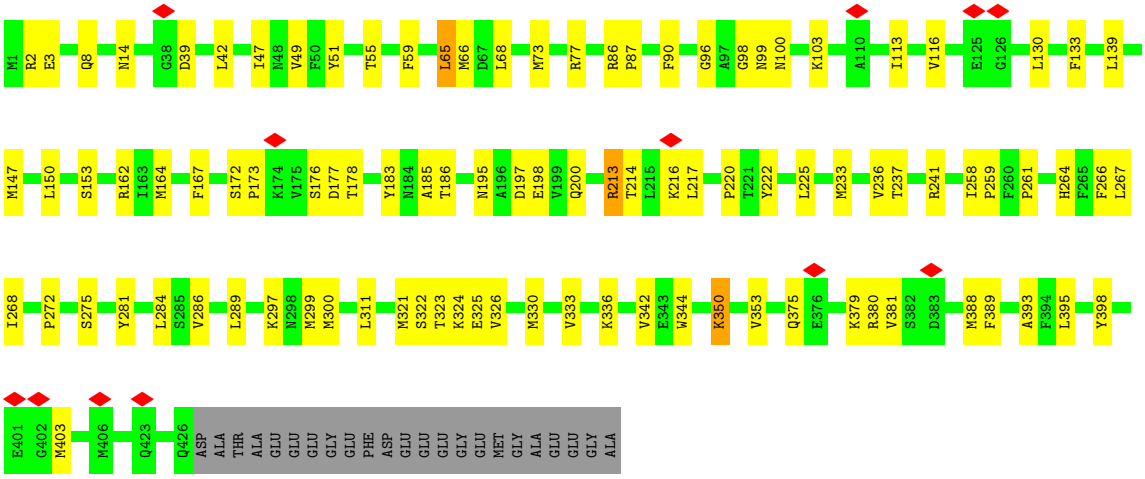
• Molecule 4: Tubulin beta chain

Chain B9:



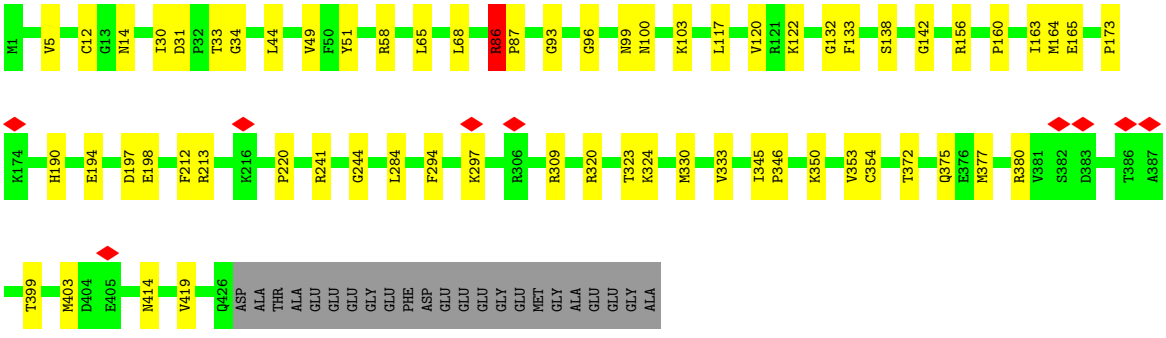
• Molecule 4: Tubulin beta chain

Chain C1:



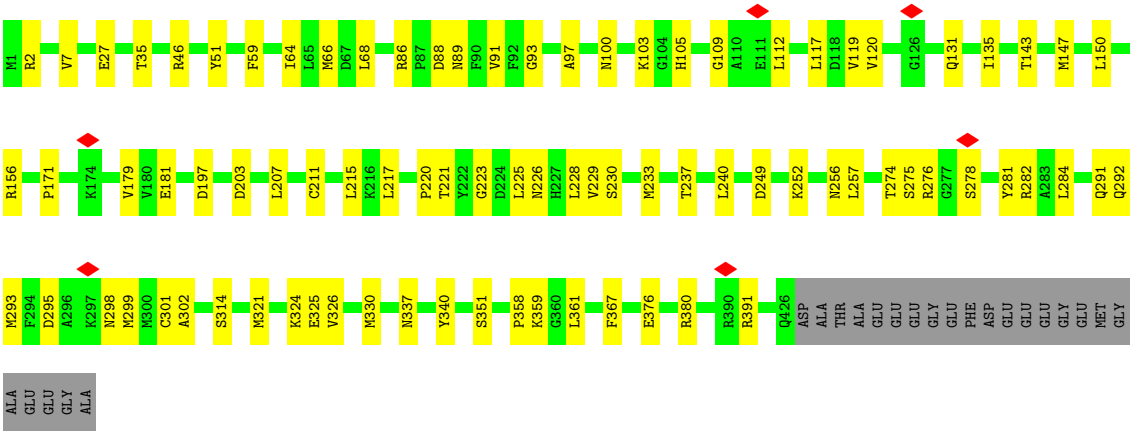
• Molecule 4: Tubulin beta chain

Chain C3:



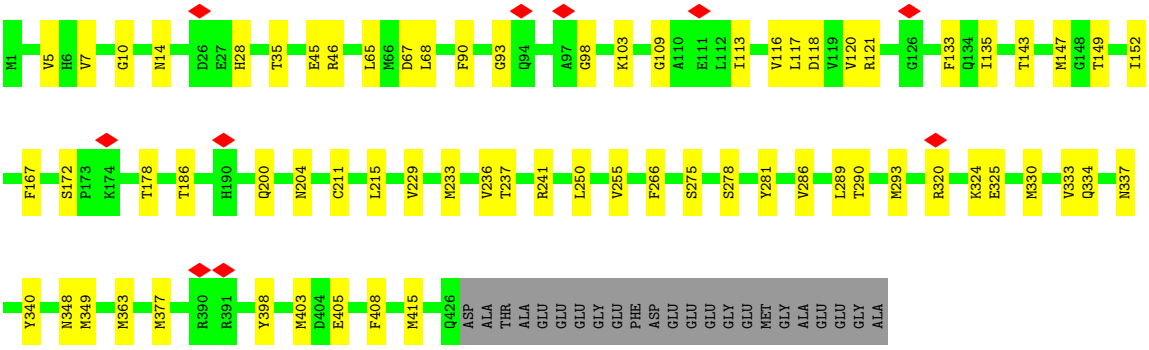
• Molecule 4: Tubulin beta chain

Chain C5:



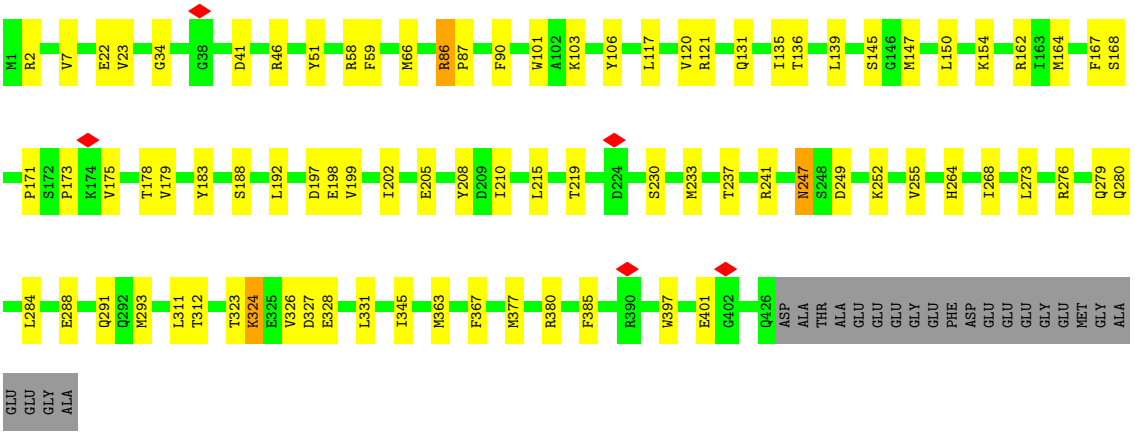
• Molecule 4: Tubulin beta chain

Chain C7:



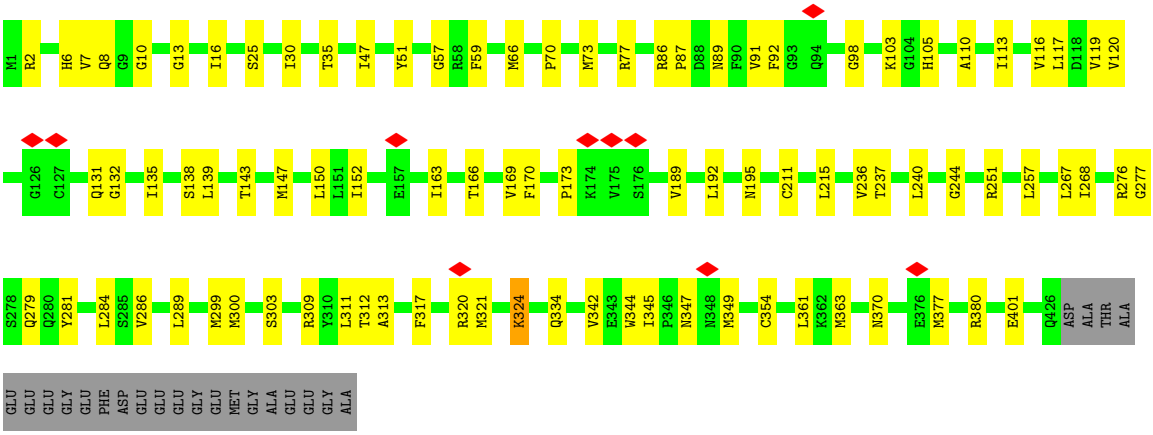
• Molecule 4: Tubulin beta chain

Chain C9:



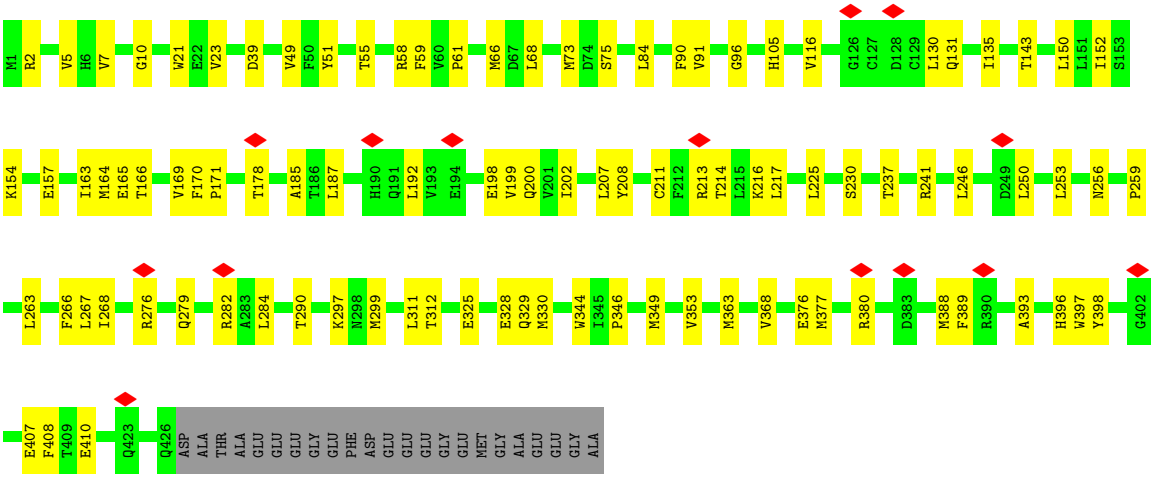
• Molecule 4: Tubulin beta chain

Chain D1:



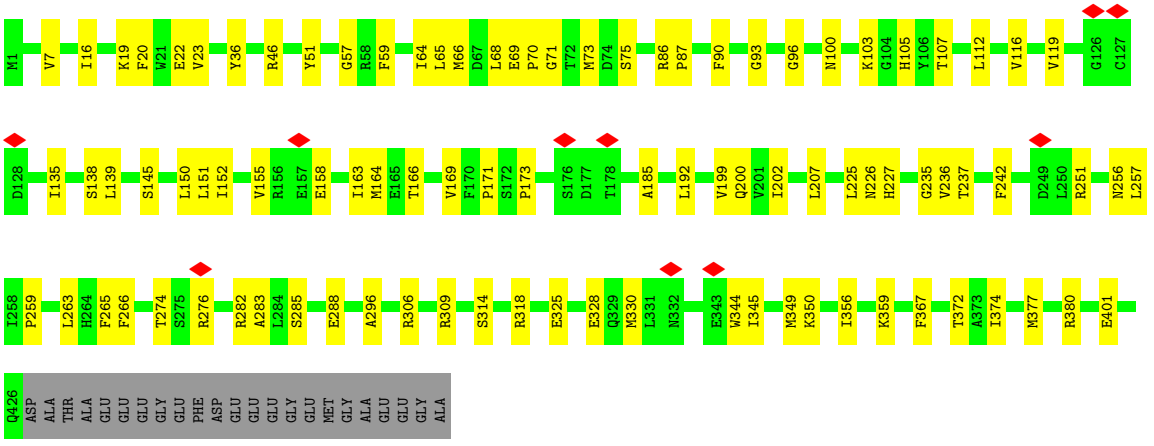
• Molecule 4: Tubulin beta chain

Chain D3:



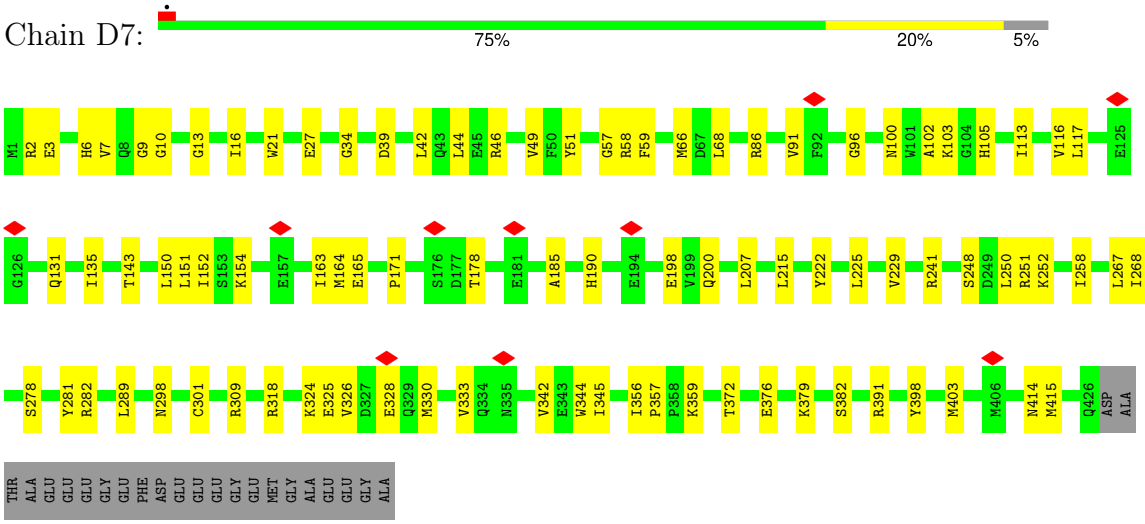
• Molecule 4: Tubulin beta chain

Chain D5:



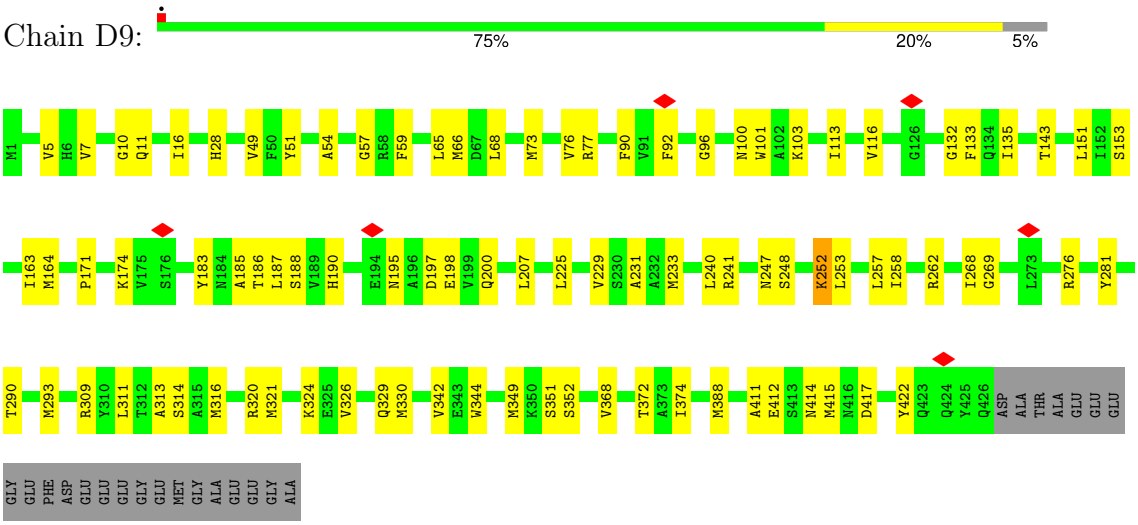
• Molecule 4: Tubulin beta chain

Chain D7:



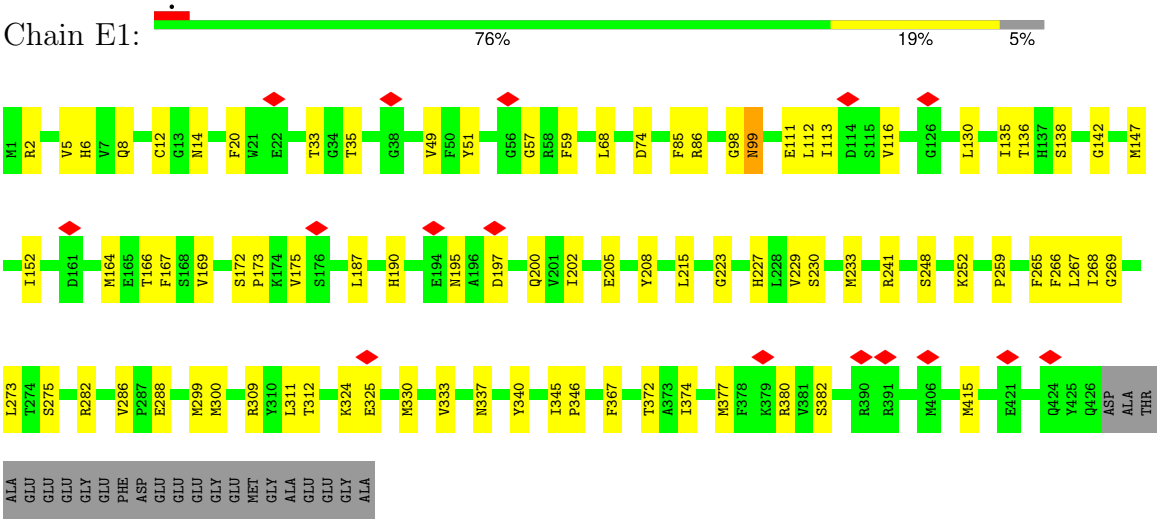
• Molecule 4: Tubulin beta chain

Chain D9:



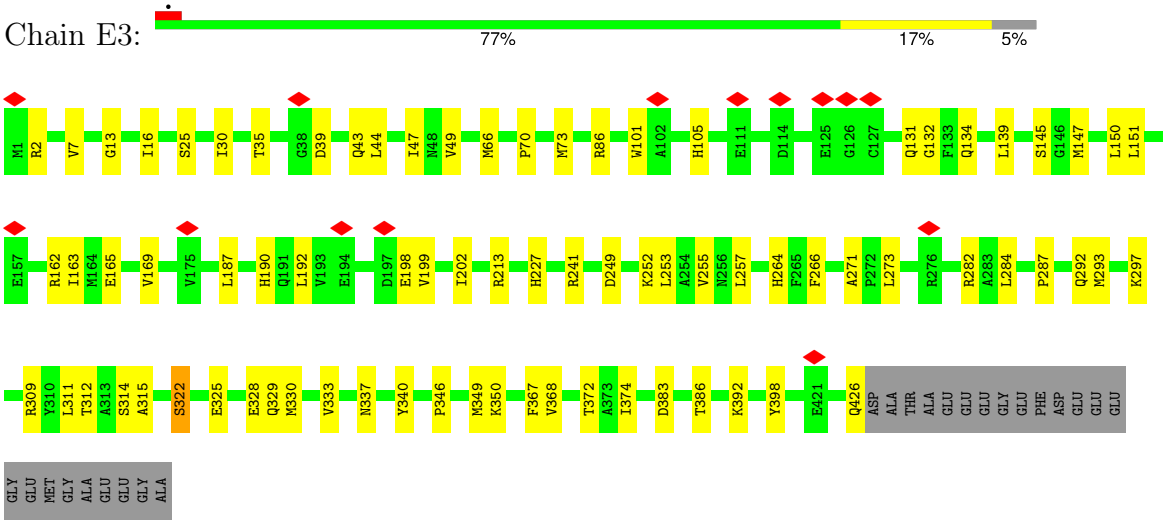
• Molecule 4: Tubulin beta chain

Chain E1:



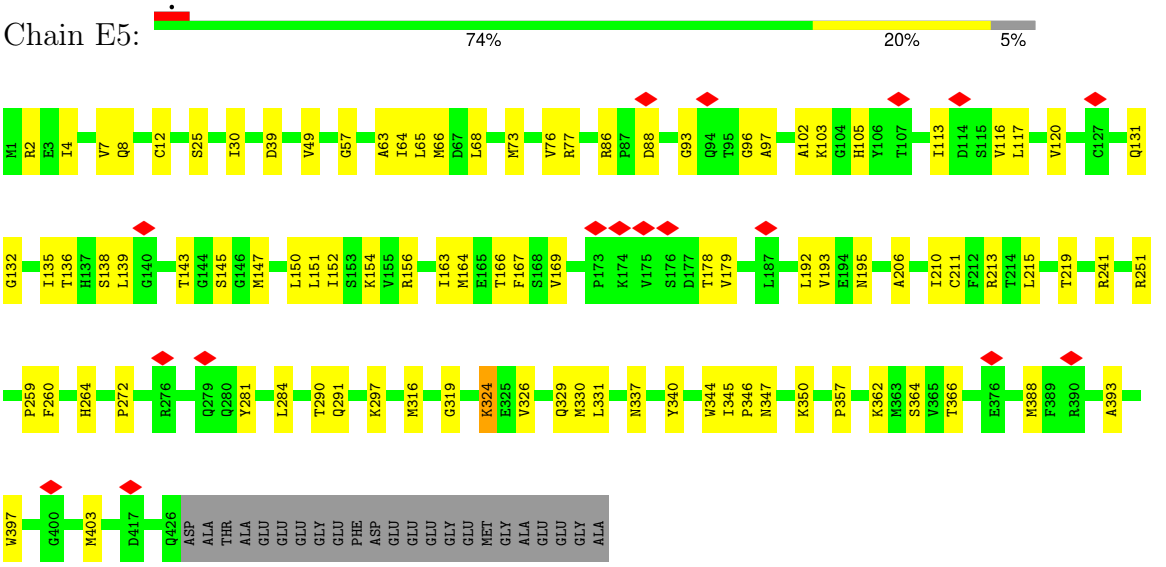
• Molecule 4: Tubulin beta chain

Chain E3:



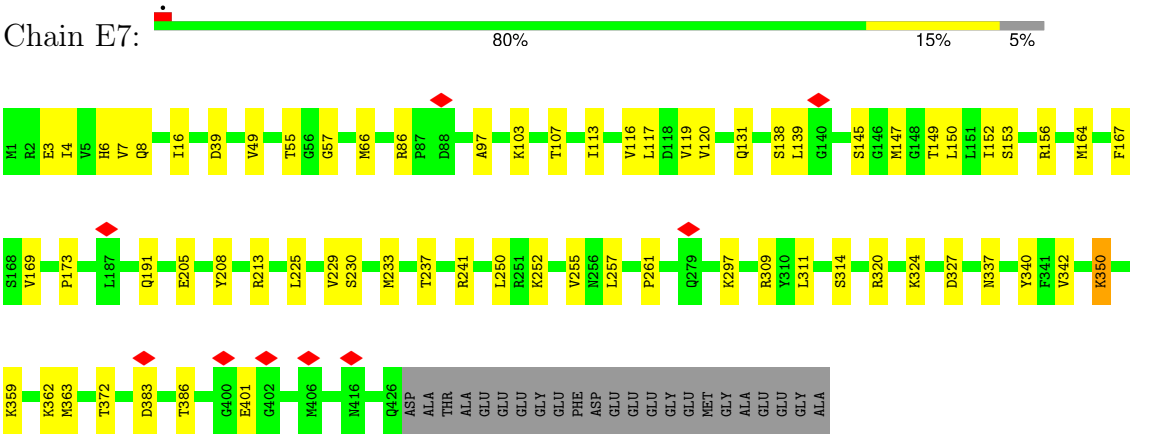
• Molecule 4: Tubulin beta chain

Chain E5:



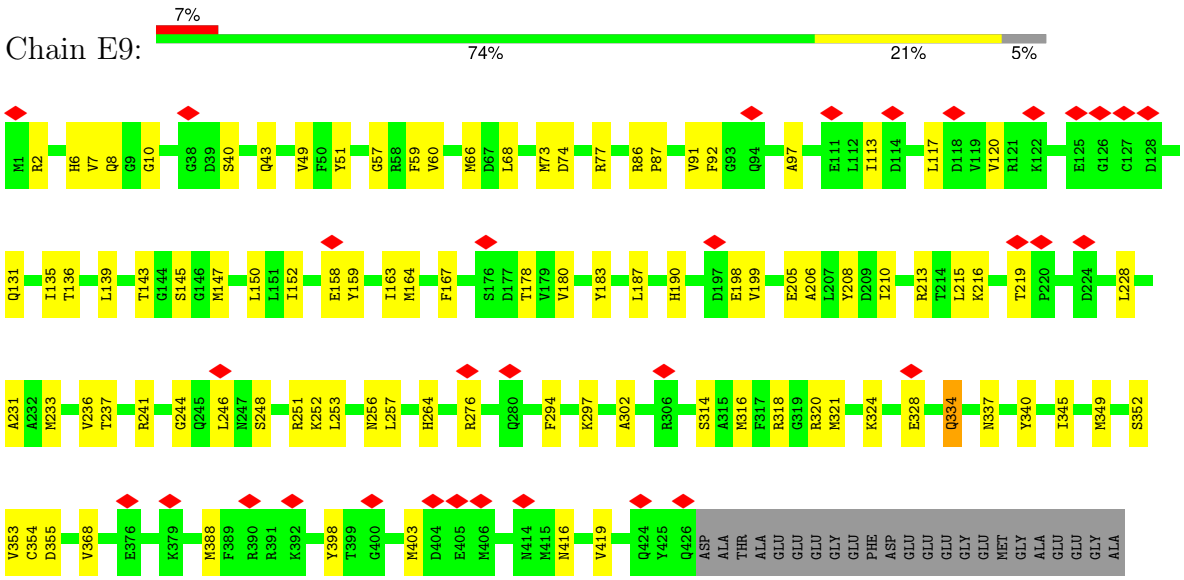
• Molecule 4: Tubulin beta chain

Chain E7:



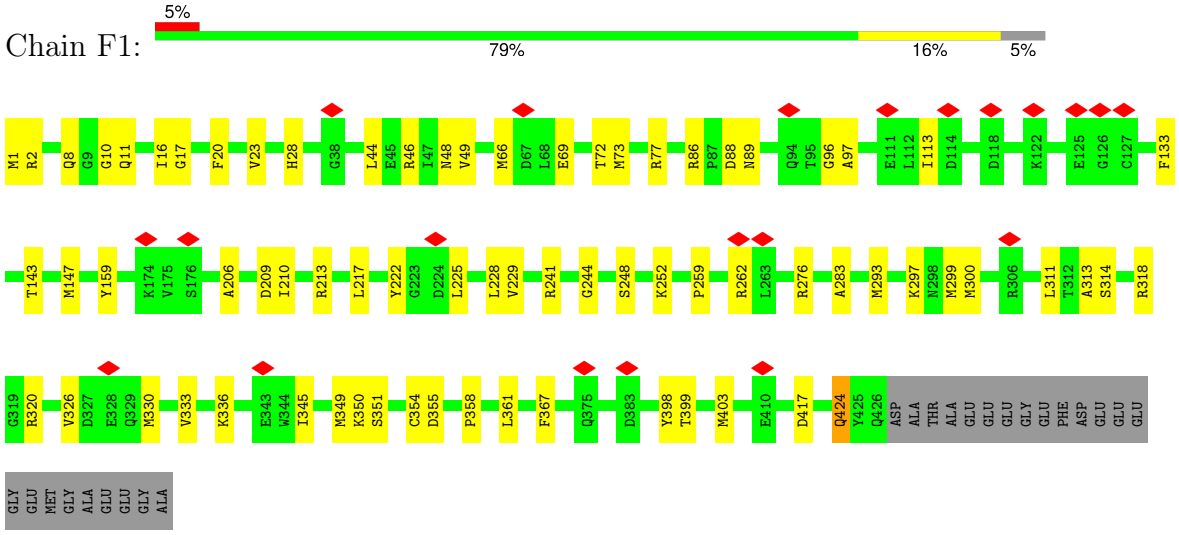
• Molecule 4: Tubulin beta chain

Chain E9:



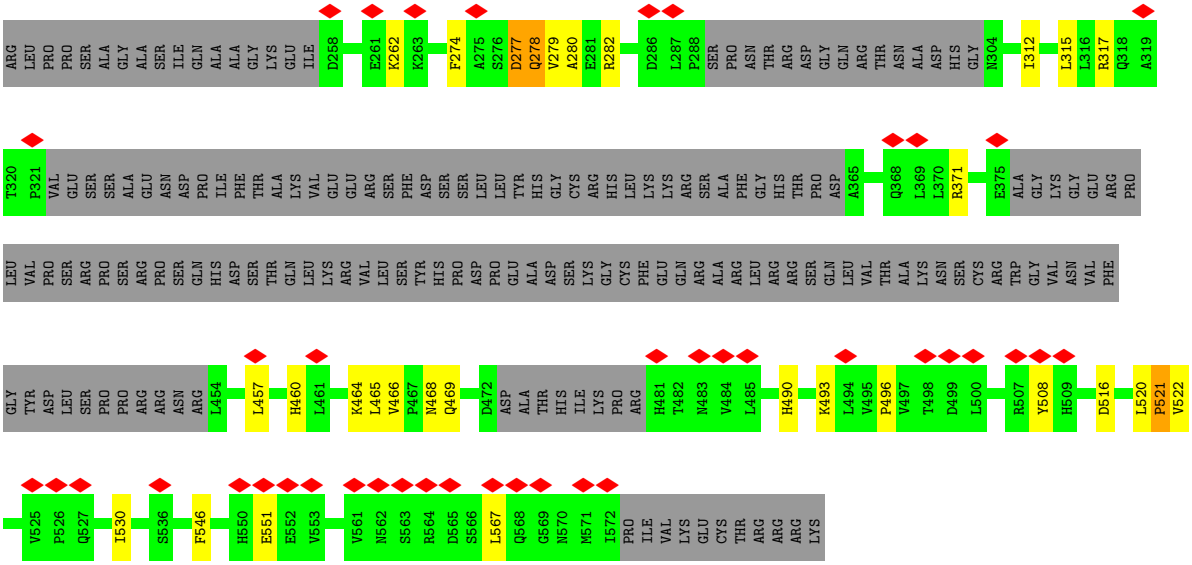
• Molecule 4: Tubulin beta chain

Chain F1:



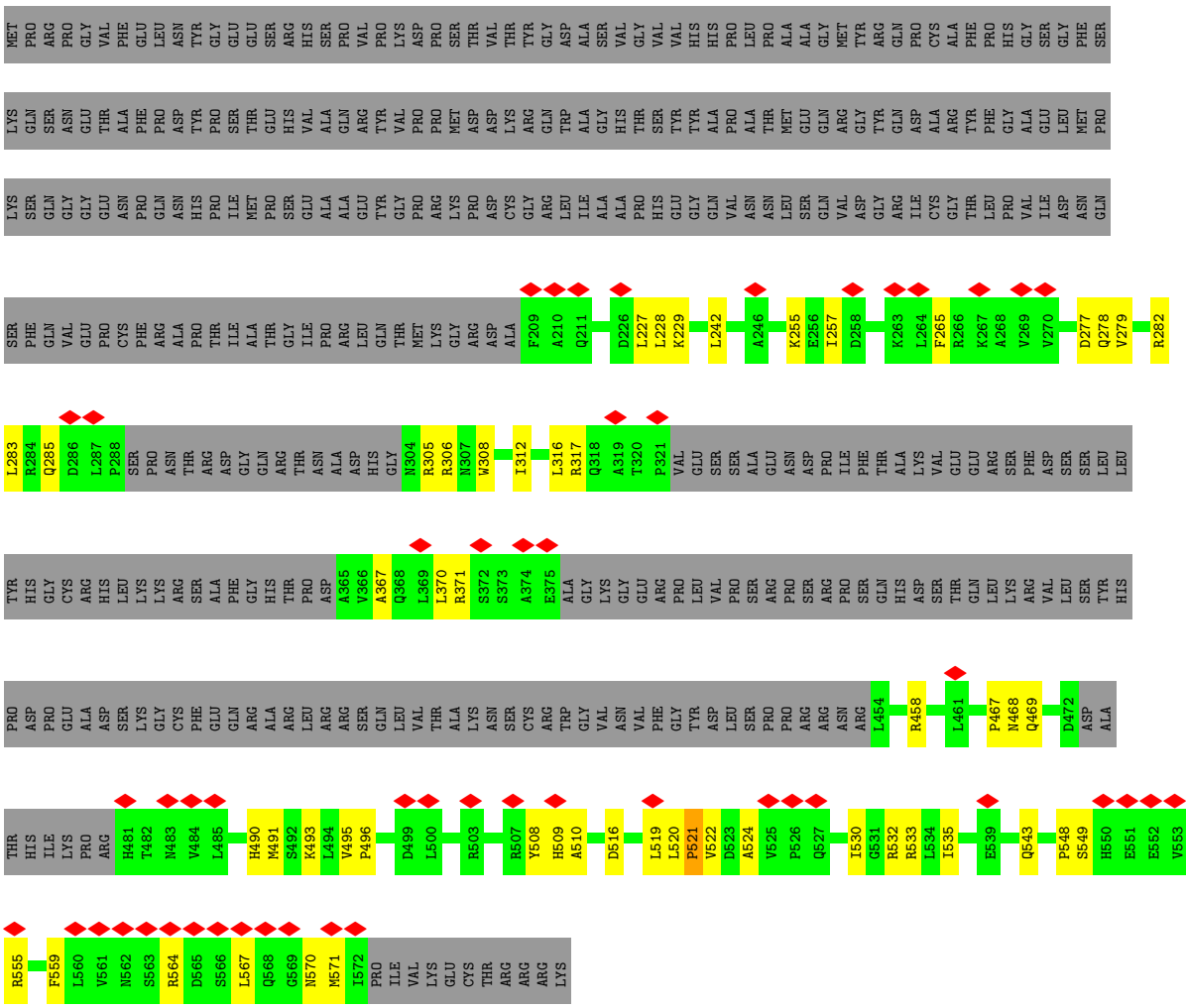
• Molecule 5: TLAP3 (apical cap protein AC5), TGME49_235380

Chain O:



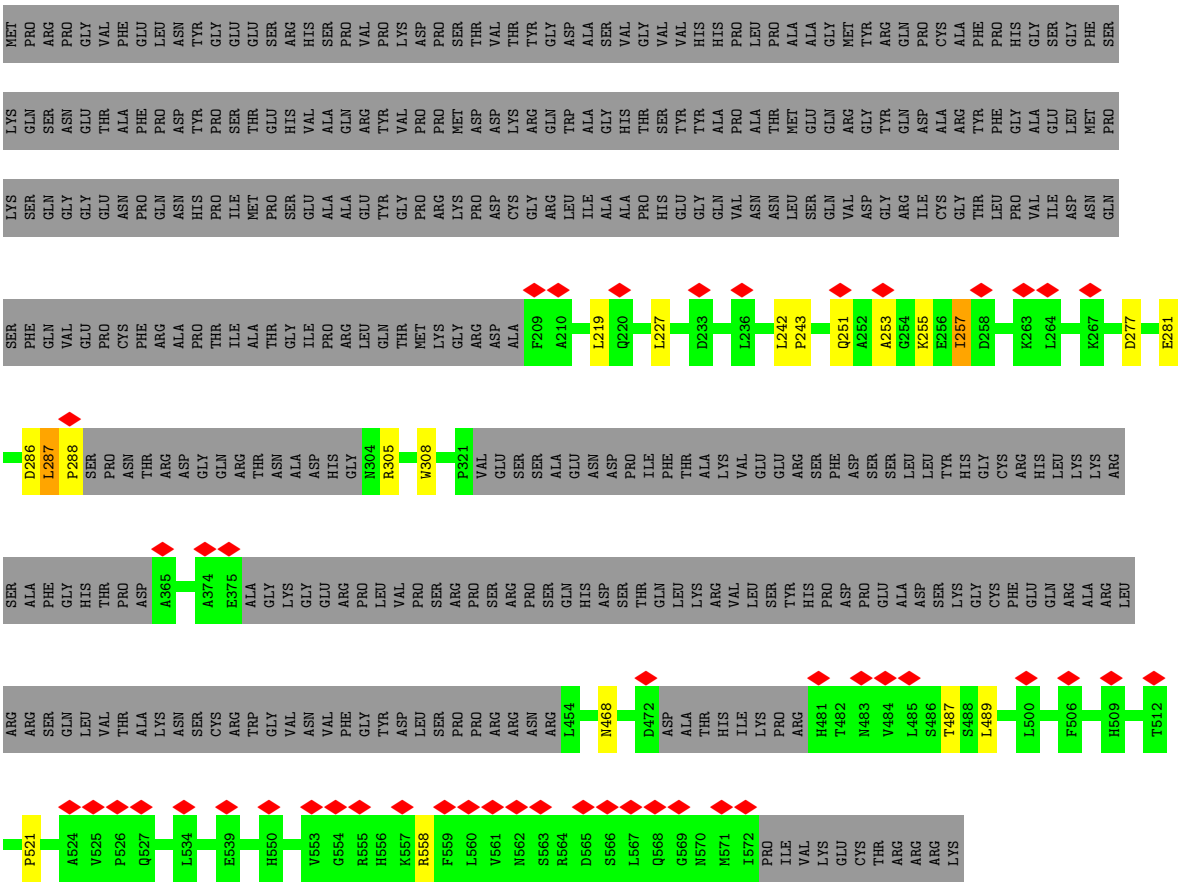
• Molecule 5: TLAP3 (apical cap protein AC5), TGME49_235380

Chain P:



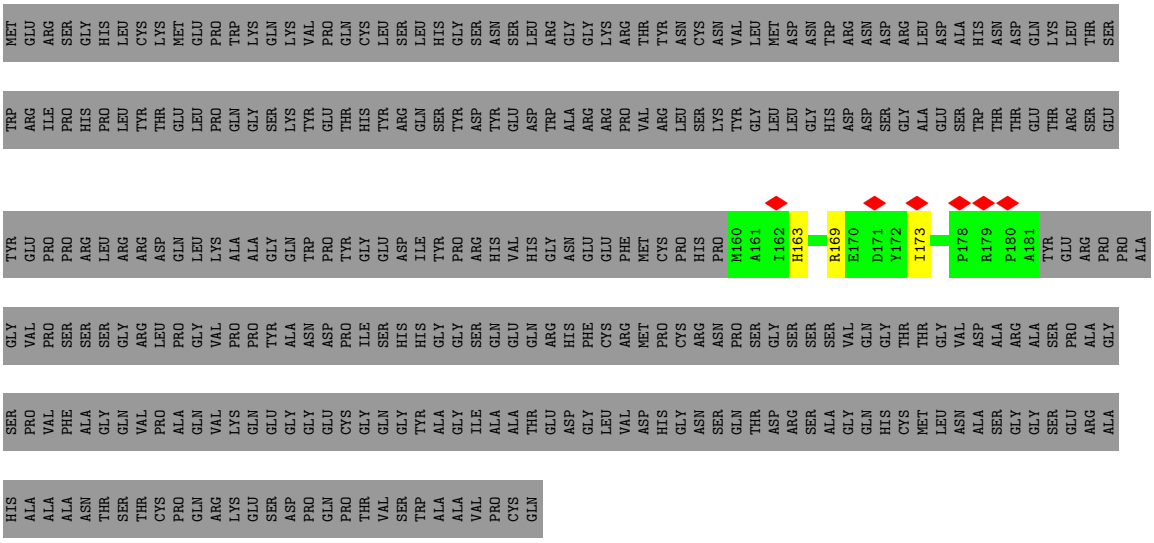
• Molecule 5: TLAP3 (apical cap protein AC5), TGME49_235380

Chain R:



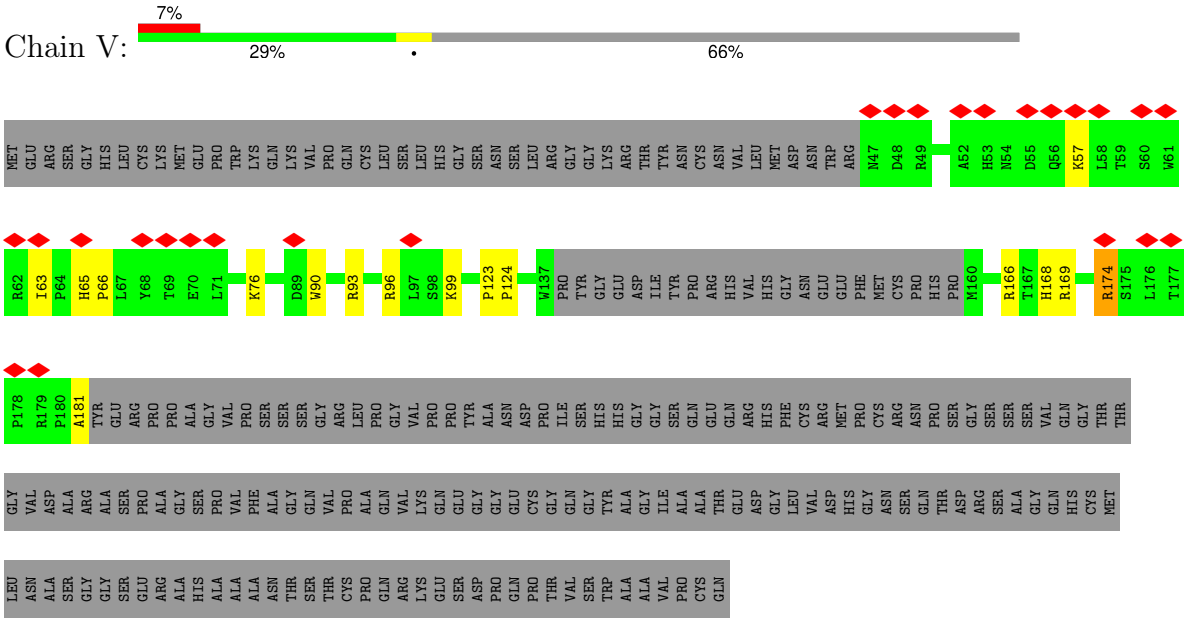
• Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760

Chain U:



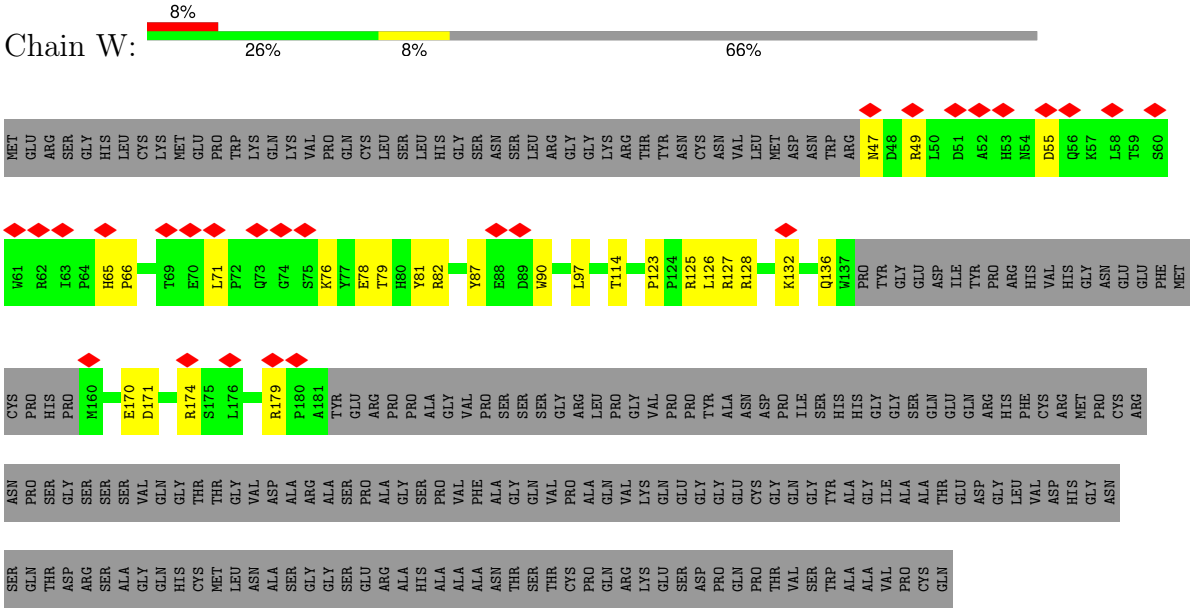
• Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760

Chain V:



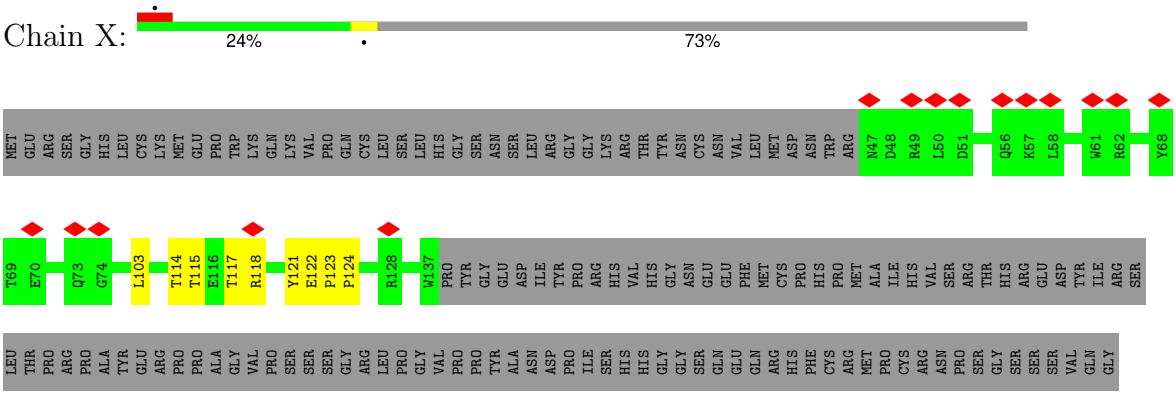
• Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760

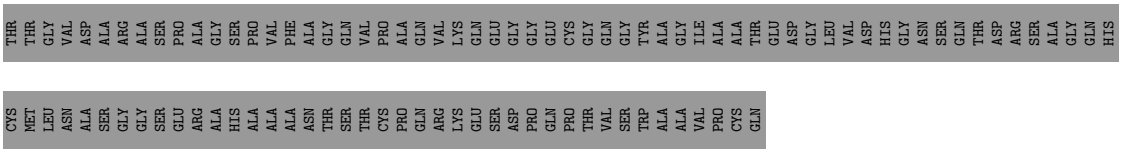
Chain W:



• Molecule 6: TLAP4 (thioredoxin-like associated protein), TGME49_201760

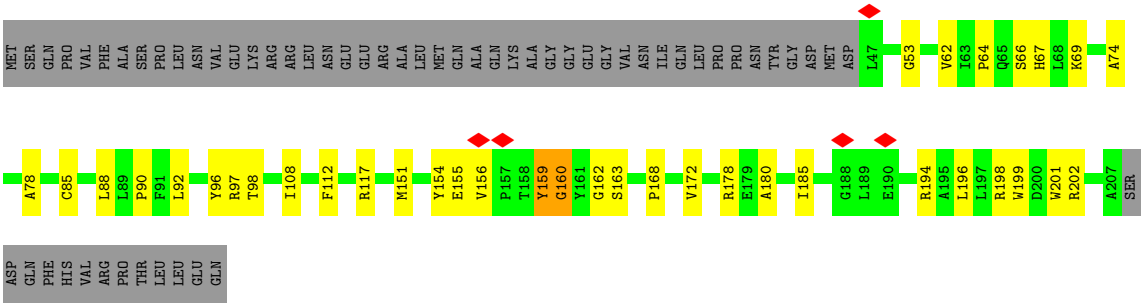
Chain X:





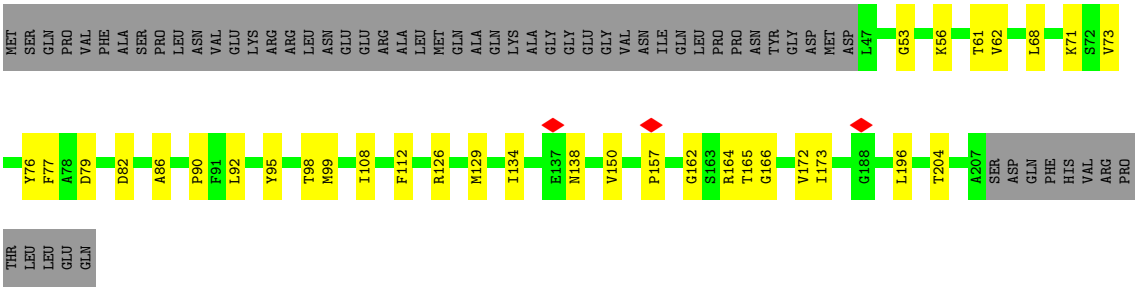
• Molecule 7: TRXL1, TGME49_232410

Chain a:



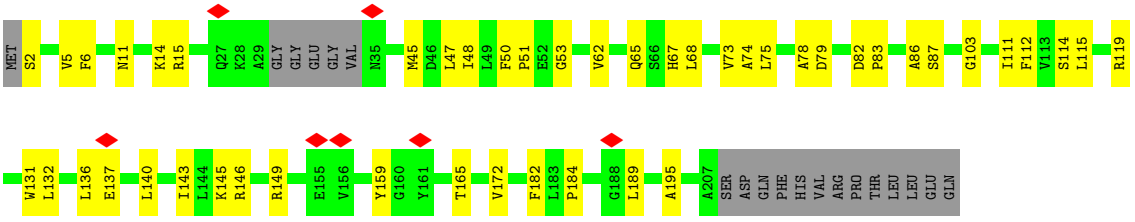
• Molecule 7: TRXL1, TGME49_232410

Chain b:



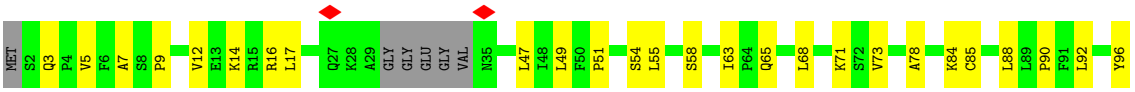
• Molecule 7: TRXL1, TGME49_232410

Chain c:

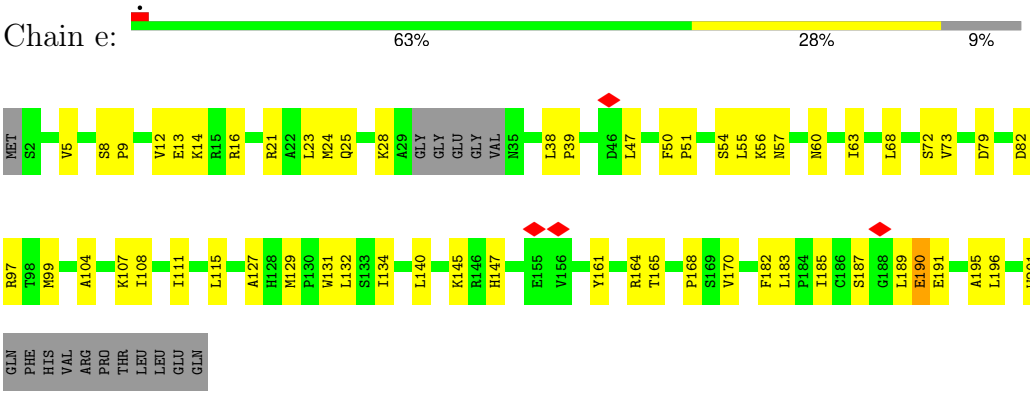


• Molecule 7: TRXL1, TGME49_232410

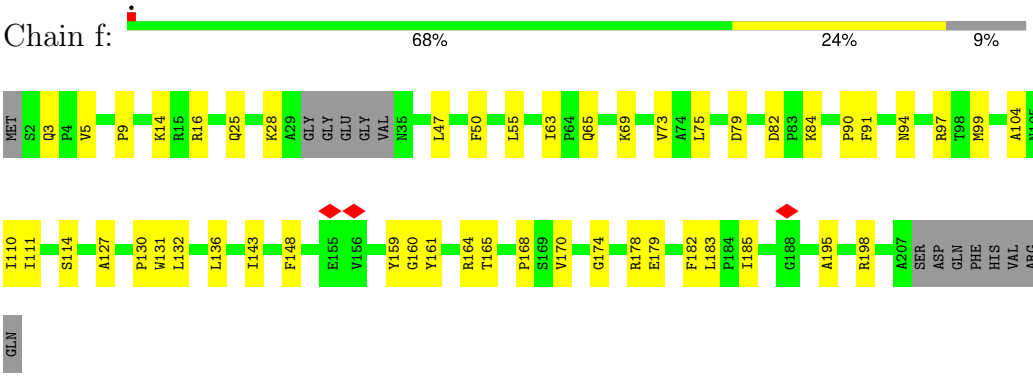
Chain d:



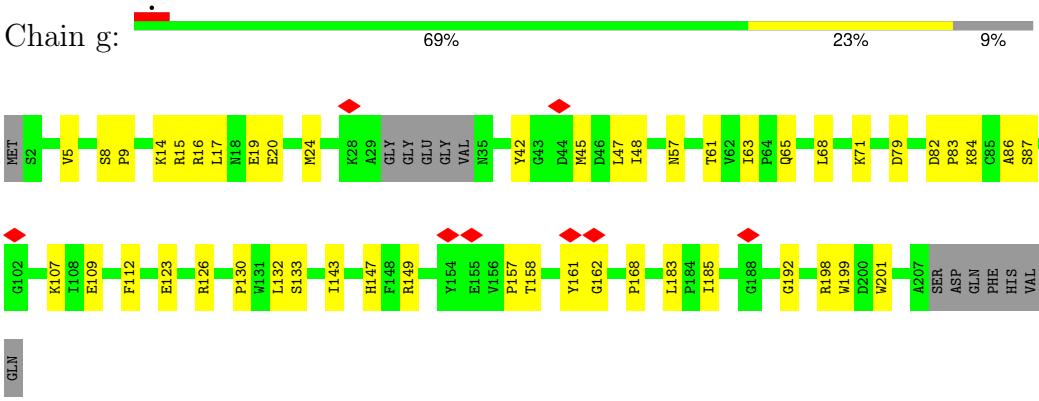
• Molecule 7: TRXL1, TGME49_232410



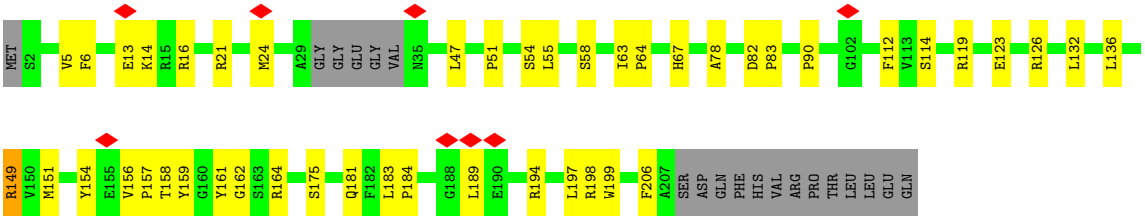
• Molecule 7: TRXL1, TGME49_232410



• Molecule 7: TRXL1, TGME49_232410

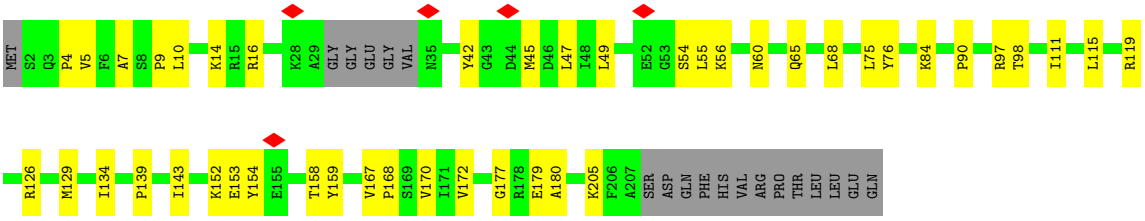


• Molecule 7: TRXL1, TGME49_232410



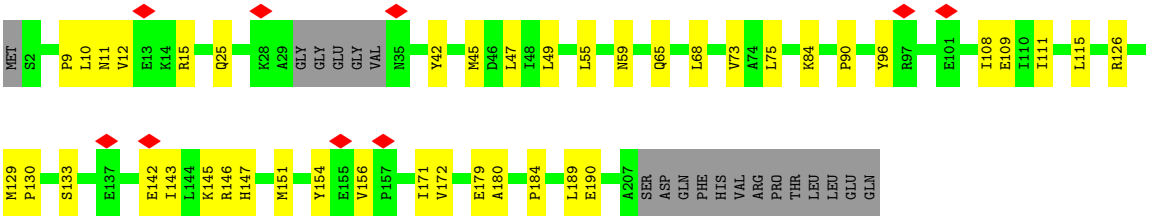
• Molecule 7: TRXL1, TGME49_232410

Chain i:



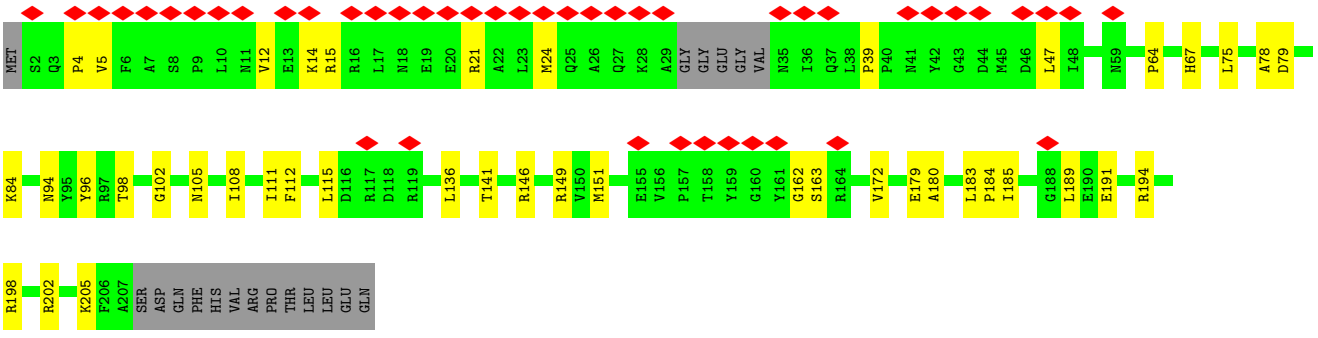
• Molecule 7: TRXL1, TGME49_232410

Chain j:



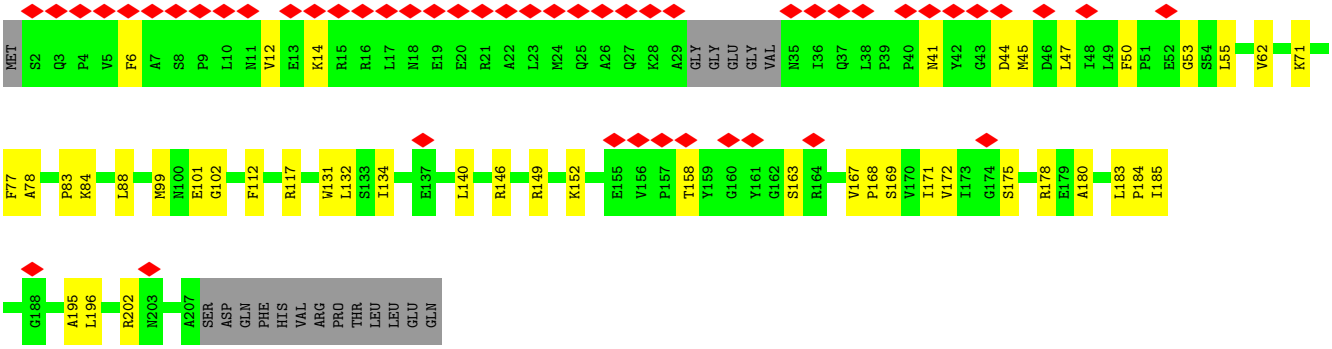
• Molecule 7: TRXL1, TGME49_232410

Chain m:



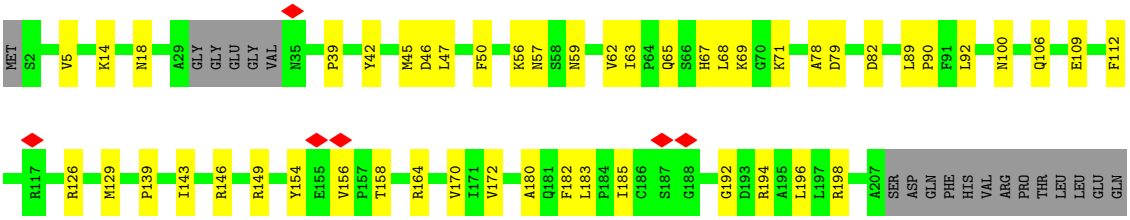
• Molecule 7: TRXL1, TGME49_232410

Chain n:



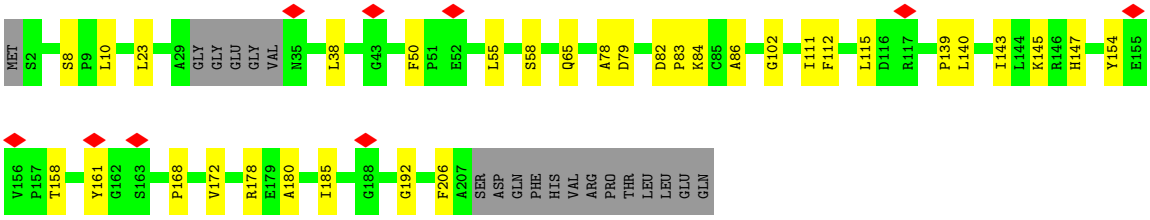
• Molecule 7: TRXL1, TGME49_232410

Chain o:



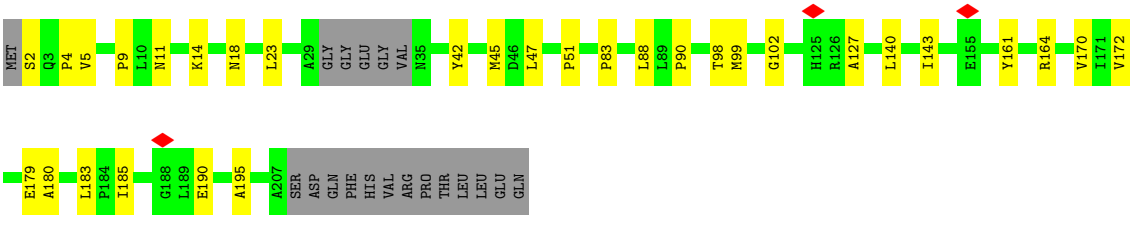
• Molecule 7: TRXL1, TGME49_232410

Chain p:



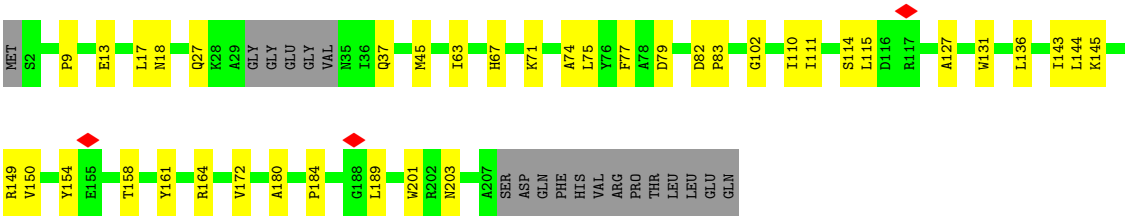
• Molecule 7: TRXL1, TGME49_232410

Chain q:



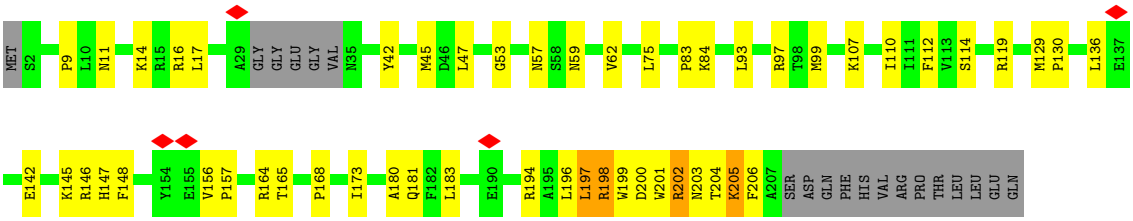
• Molecule 7: TRXL1, TGME49_232410

Chain r:



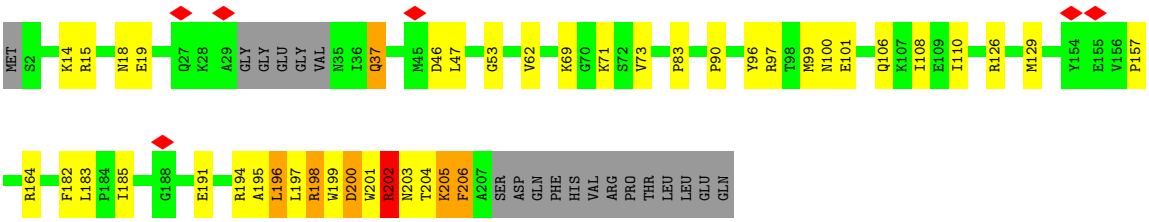
• Molecule 7: TRXL1, TGME49_232410

Chain s:



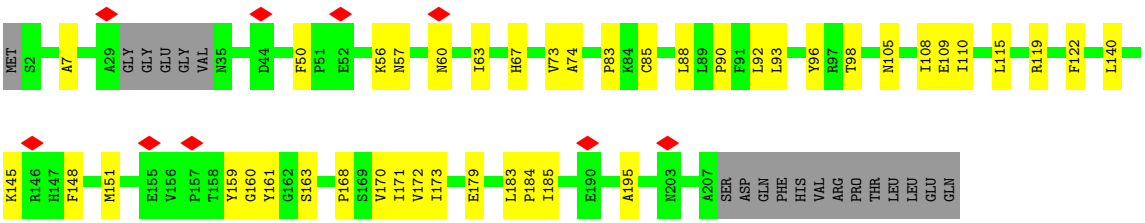
• Molecule 7: TRXL1, TGME49_232410

Chain t:



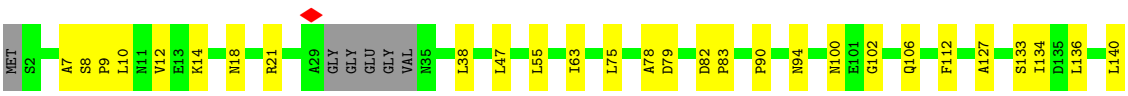
• Molecule 7: TRXL1, TGME49_232410

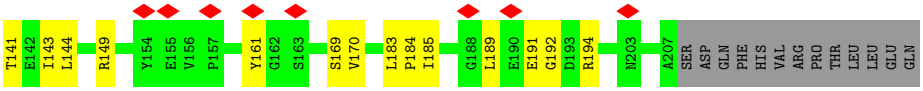
Chain u:



• Molecule 7: TRXL1, TGME49_232410

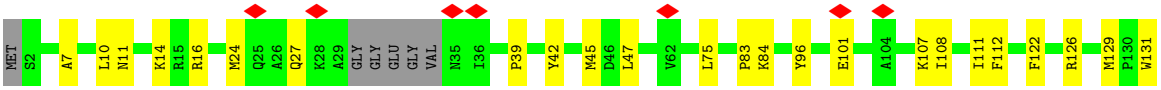
Chain v:

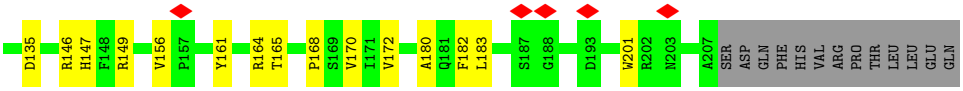




• Molecule 7: TRXL1, TGME49_232410

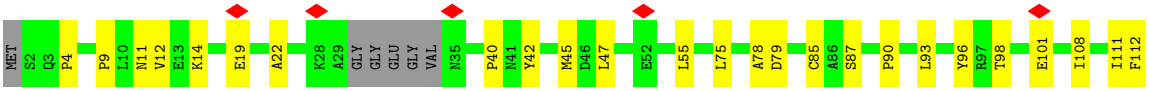
Chain w:

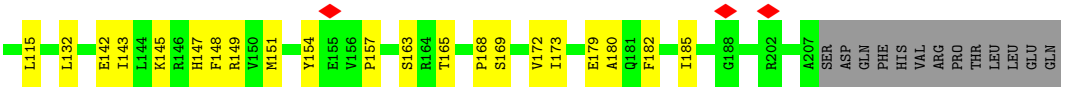




• Molecule 7: TRXL1, TGME49_232410

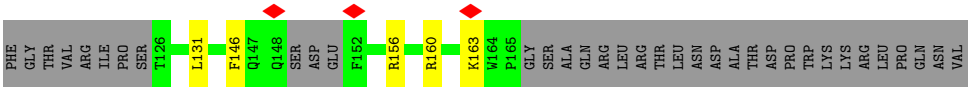
Chain x:





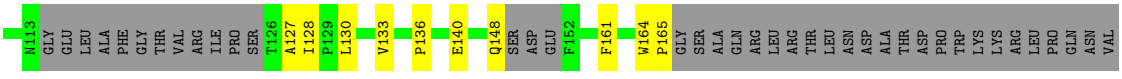
• Molecule 8: TRXL2, TGME49_225790

Chain k:



• Molecule 8: TRXL2, TGME49_225790

Chain l:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.133	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 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	1	0.28	0/1069	0.78	1/1440 (0.1%)
1	2	0.22	0/1069	0.65	0/1440
2	A	0.20	0/483	0.51	0/667
2	B	0.20	0/491	0.51	0/679
2	C	0.21	0/483	0.53	0/667
2	D	0.37	1/484 (0.2%)	0.64	0/669
2	E	0.19	0/491	0.70	2/679 (0.3%)
2	F	0.26	0/461	0.61	0/637
2	G	0.22	0/491	0.62	2/679 (0.3%)
2	H	0.26	0/461	0.57	0/637
2	I	0.29	0/491	0.58	0/679
2	J	0.25	0/491	0.52	0/679
2	K	0.21	0/491	0.60	0/679
3	A0	0.21	0/3398	0.57	2/4606 (0.0%)
3	A2	0.23	0/3398	0.62	0/4606
3	A4	0.21	0/3398	0.53	0/4606
3	A6	0.23	0/3398	0.60	0/4606
3	A8	0.22	0/3398	0.58	2/4606 (0.0%)
3	B0	0.21	0/3398	0.57	0/4606
3	B2	0.21	0/3398	0.56	0/4606
3	B4	0.22	0/3398	0.57	0/4606
3	B6	0.20	0/3398	0.54	0/4606
3	B8	0.24	0/3398	0.58	1/4606 (0.0%)
3	C0	0.24	0/3398	0.59	0/4606
3	C2	0.24	0/3398	0.60	0/4606
3	C4	0.25	0/3398	0.62	0/4606
3	C6	0.23	0/3398	0.58	1/4606 (0.0%)
3	C8	0.22	0/3398	0.56	1/4606 (0.0%)
3	D0	0.24	0/3398	0.58	0/4606
3	D2	0.21	0/3398	0.54	0/4606
3	D4	0.23	0/3398	0.56	0/4606
3	D6	0.23	0/3398	0.55	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	D8	0.29	0/3398	0.60	0/4606
3	E0	0.22	0/3398	0.56	0/4606
3	E2	0.32	0/3398	0.63	0/4606
3	E4	0.21	0/3398	0.54	0/4606
3	E6	0.22	0/3398	0.53	0/4606
3	E8	0.20	0/3398	0.55	0/4606
3	F0	0.22	0/3398	0.61	0/4606
4	A1	0.23	0/3404	0.61	1/4606 (0.0%)
4	A3	0.22	0/3404	0.60	1/4606 (0.0%)
4	A5	0.23	0/3404	0.59	2/4606 (0.0%)
4	A7	0.22	0/3404	0.56	0/4606
4	A9	0.23	0/3404	0.61	1/4606 (0.0%)
4	B1	0.23	0/3404	0.61	0/4606
4	B3	0.24	0/3404	0.61	0/4606
4	B5	0.23	0/3404	0.58	0/4606
4	B7	0.22	0/3404	0.58	2/4606 (0.0%)
4	B9	0.23	0/3404	0.60	0/4606
4	C1	0.27	0/3404	0.68	2/4606 (0.0%)
4	C3	0.23	0/3404	0.59	1/4606 (0.0%)
4	C5	0.26	0/3404	0.64	0/4606
4	C7	0.22	0/3404	0.56	0/4606
4	C9	0.25	0/3404	0.66	3/4606 (0.1%)
4	D1	0.22	0/3404	0.57	1/4606 (0.0%)
4	D3	0.24	0/3404	0.59	0/4606
4	D5	0.23	0/3404	0.55	0/4606
4	D7	0.22	0/3404	0.60	1/4606 (0.0%)
4	D9	0.21	0/3404	0.55	1/4606 (0.0%)
4	E1	0.22	0/3404	0.58	2/4606 (0.0%)
4	E3	0.24	0/3404	0.56	0/4606
4	E5	0.23	0/3404	0.59	1/4606 (0.0%)
4	E7	0.21	0/3404	0.56	1/4606 (0.0%)
4	E9	0.22	0/3404	0.58	0/4606
4	F1	0.24	0/3404	0.63	1/4606 (0.0%)
5	O	0.26	0/1383	0.73	0/1871
5	P	0.24	0/1776	0.73	1/2403 (0.0%)
5	R	0.22	0/1776	0.67	0/2403
6	U	0.23	0/186	0.69	0/251
6	V	0.25	0/982	0.58	0/1332
6	W	0.30	0/982	0.76	0/1332
6	X	0.22	0/796	0.61	0/1081
7	a	0.28	0/1321	0.65	0/1788
7	b	0.30	0/1321	0.66	0/1788
7	c	0.26	0/1645	0.63	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	d	0.25	0/1645	0.64	2/2225 (0.1%)
7	e	0.25	0/1645	0.66	1/2225 (0.0%)
7	f	0.25	0/1645	0.63	0/2225
7	g	0.25	0/1645	0.63	0/2225
7	h	0.23	0/1645	0.64	1/2225 (0.0%)
7	i	0.22	0/1645	0.60	0/2225
7	j	0.23	0/1645	0.58	1/2225 (0.0%)
7	m	0.24	0/1645	0.62	0/2225
7	n	0.23	0/1645	0.59	0/2225
7	o	0.24	0/1645	0.61	0/2225
7	p	0.24	0/1645	0.60	2/2225 (0.1%)
7	q	0.25	0/1645	0.58	1/2225 (0.0%)
7	r	0.23	0/1645	0.56	0/2225
7	s	0.32	0/1645	0.66	1/2225 (0.0%)
7	t	0.32	0/1645	0.66	0/2225
7	u	0.22	0/1645	0.54	0/2225
7	v	0.24	0/1645	0.65	3/2225 (0.1%)
7	w	0.23	0/1645	0.62	0/2225
7	x	0.22	0/1645	0.59	0/2225
8	k	0.22	0/1184	0.57	1/1600 (0.1%)
8	l	0.26	0/1184	0.69	0/1600
All	All	0.24	1/230099 (0.0%)	0.60	47/311692 (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
1	1	0	1
2	F	0	1
3	A0	0	2
3	A4	0	1
3	B2	0	1
3	B8	0	1
3	C4	0	3
3	C8	0	2
3	E2	0	1
3	F0	0	1
4	A1	0	1
4	A7	0	1
4	A9	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	C1	0	3
4	C3	0	2
4	C5	0	1
4	C9	0	2
4	E3	0	1
5	O	0	1
6	V	0	2
6	W	0	1
7	a	0	1
7	d	0	1
7	e	0	1
7	g	0	1
7	p	0	1
7	s	0	2
7	t	0	3
8	l	0	2
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	253	ALA	C-N	-5.42	1.25	1.33

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	221	PRO	CA-C-N	8.74	133.75	121.61
2	E	221	PRO	C-N-CA	8.74	133.75	121.61
4	A5	396	HIS	CA-C-N	8.30	136.63	122.26
4	A5	396	HIS	C-N-CA	8.30	136.63	122.26
4	A1	391	ARG	CA-CB-CG	6.83	127.77	114.10

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	443	LYS	Peptide
3	A0	372	MET	Peptide
3	A0	90	GLU	Peptide
4	A1	391	ARG	Sidechain
3	A4	90	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1054	0	1111	15	0
1	2	1054	0	1111	15	0
2	A	464	0	469	5	0
2	B	471	0	476	6	0
2	C	464	0	469	5	0
2	D	464	0	467	11	0
2	E	471	0	476	9	0
2	F	441	0	443	9	0
2	G	471	0	476	3	0
2	H	441	0	443	5	0
2	I	471	0	476	8	0
2	J	471	0	476	6	0
2	K	471	0	476	12	0
3	A0	3325	0	3252	52	0
3	A2	3325	0	3252	66	0
3	A4	3325	0	3252	56	0
3	A6	3325	0	3252	63	0
3	A8	3325	0	3251	48	0
3	B0	3325	0	3252	53	0
3	B2	3325	0	3251	50	0
3	B4	3325	0	3252	48	0
3	B6	3325	0	3252	43	0
3	B8	3325	0	3252	72	0
3	C0	3325	0	3252	41	0
3	C2	3325	0	3252	53	0
3	C4	3325	0	3252	58	0
3	C6	3325	0	3252	56	0
3	C8	3325	0	3252	39	0
3	D0	3325	0	3252	63	0
3	D2	3325	0	3252	45	0
3	D4	3325	0	3252	50	0
3	D6	3325	0	3251	59	0
3	D8	3325	0	3251	81	0
3	E0	3325	0	3251	54	0
3	E2	3325	0	3252	51	0
3	E4	3325	0	3252	45	0
3	E6	3325	0	3252	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E8	3325	0	3252	46	0
3	F0	3325	0	3252	50	0
4	A1	3331	0	3207	67	0
4	A3	3331	0	3209	71	0
4	A5	3331	0	3207	65	0
4	A7	3331	0	3207	47	0
4	A9	3331	0	3207	71	0
4	B1	3331	0	3209	58	0
4	B3	3331	0	3207	60	0
4	B5	3331	0	3207	47	0
4	B7	3331	0	3209	63	0
4	B9	3331	0	3209	55	0
4	C1	3331	0	3209	73	0
4	C3	3331	0	3209	43	0
4	C5	3331	0	3209	59	0
4	C7	3331	0	3209	44	0
4	C9	3331	0	3209	66	0
4	D1	3331	0	3209	65	0
4	D3	3331	0	3207	77	0
4	D5	3331	0	3207	60	0
4	D7	3331	0	3207	63	0
4	D9	3331	0	3207	58	0
4	E1	3331	0	3207	57	0
4	E3	3331	0	3209	53	0
4	E5	3331	0	3207	75	0
4	E7	3331	0	3205	46	0
4	E9	3331	0	3207	70	0
4	F1	3331	0	3207	50	0
5	O	1360	0	1354	25	0
5	P	1744	0	1734	48	0
5	R	1744	0	1736	15	0
6	U	182	0	183	3	0
6	V	954	0	899	13	0
6	W	954	0	899	23	0
6	X	772	0	716	7	0
7	a	1289	0	1274	28	0
7	b	1289	0	1274	23	0
7	c	1608	0	1590	33	0
7	d	1608	0	1590	26	0
7	e	1608	0	1590	44	0
7	f	1608	0	1590	37	0
7	g	1608	0	1590	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	1608	0	1590	33	0
7	i	1608	0	1590	28	0
7	j	1608	0	1590	29	0
7	m	1608	0	1590	31	0
7	n	1608	0	1590	34	0
7	o	1608	0	1590	30	0
7	p	1608	0	1590	22	0
7	q	1608	0	1590	23	0
7	r	1608	0	1590	28	0
7	s	1608	0	1590	36	0
7	t	1608	0	1590	29	0
7	u	1608	0	1590	25	0
7	v	1608	0	1590	25	0
7	w	1608	0	1590	23	0
7	x	1608	0	1590	29	0
8	k	1155	0	1155	19	0
8	l	1155	0	1155	29	0
9	A0	32	0	12	0	0
9	A2	32	0	12	0	0
9	A4	32	0	12	0	0
9	A6	32	0	12	0	0
9	A8	32	0	12	0	0
9	B0	32	0	12	0	0
9	B2	32	0	12	0	0
9	B4	32	0	12	0	0
9	B6	32	0	12	0	0
9	B8	32	0	12	0	0
9	C0	32	0	12	0	0
9	C2	32	0	12	0	0
9	C4	32	0	12	0	0
9	C6	32	0	12	0	0
9	C8	32	0	12	0	0
9	D0	32	0	12	0	0
9	D2	32	0	12	0	0
9	D4	32	0	12	0	0
9	D6	32	0	12	0	0
9	D8	32	0	12	0	0
9	E0	32	0	12	0	0
9	E2	32	0	12	0	0
9	E4	32	0	12	0	0
9	E7	32	0	12	1	0
9	E8	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F0	32	0	12	0	0
10	A0	1	0	0	0	0
10	A2	1	0	0	0	0
10	A4	1	0	0	0	0
10	A6	1	0	0	0	0
10	A8	1	0	0	0	0
10	B0	1	0	0	0	0
10	B2	1	0	0	0	0
10	B4	1	0	0	0	0
10	B6	1	0	0	0	0
10	B8	1	0	0	0	0
10	C0	1	0	0	0	0
10	C2	1	0	0	0	0
10	C4	1	0	0	0	0
10	C6	1	0	0	0	0
10	C9	1	0	0	0	0
10	D1	1	0	0	0	0
10	D3	1	0	0	0	0
10	D4	1	0	0	0	0
10	D6	1	0	0	0	0
10	D8	1	0	0	0	0
10	E0	1	0	0	0	0
10	E2	1	0	0	0	0
10	E4	1	0	0	0	0
10	E6	1	0	0	0	0
10	E8	1	0	0	0	0
10	F0	1	0	0	0	0
11	A1	28	0	12	0	0
11	A3	28	0	12	0	0
11	A5	28	0	12	0	0
11	A7	28	0	12	0	0
11	B3	28	0	12	0	0
11	B5	28	0	12	0	0
11	B7	28	0	12	0	0
11	B9	28	0	12	0	0
11	C1	28	0	12	0	0
11	C3	28	0	12	0	0
11	C5	28	0	12	0	0
11	C7	28	0	12	1	0
11	C9	28	0	12	1	0
11	D1	28	0	12	0	0
11	D3	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D5	28	0	12	0	0
11	D7	28	0	12	1	0
11	D9	28	0	12	0	0
11	E1	28	0	12	0	0
11	E3	28	0	12	0	0
11	E5	28	0	12	0	0
11	E7	28	0	12	0	0
11	E9	28	0	12	0	0
11	F1	28	0	12	0	0
11	O	28	0	12	0	0
11	P	28	0	12	0	0
All	All	226608	0	220121	3381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3381 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:v:100:ASN:HD21	7:v:106:GLN:HG2	1.43	0.84
4:C1:8:GLN:HE21	4:C1:14:ASN:HA	1.42	0.81
4:C5:179:VAL:H	3:C6:352:LYS:HZ1	1.29	0.81
4:A5:68:LEU:HB3	4:A5:96:GLY:HA2	1.63	0.80
4:B1:213:ARG:HH22	4:B1:297:LYS:HB3	1.47	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	128/2041 (6%)	120 (94%)	8 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	128/2041 (6%)	122 (95%)	6 (5%)	0	100	100
2	A	57/351 (16%)	46 (81%)	11 (19%)	0	100	100
2	B	58/351 (16%)	54 (93%)	4 (7%)	0	100	100
2	C	57/351 (16%)	48 (84%)	9 (16%)	0	100	100
2	D	57/351 (16%)	49 (86%)	7 (12%)	1 (2%)	7	34
2	E	58/351 (16%)	51 (88%)	7 (12%)	0	100	100
2	F	54/351 (15%)	48 (89%)	6 (11%)	0	100	100
2	G	58/351 (16%)	55 (95%)	3 (5%)	0	100	100
2	H	54/351 (15%)	48 (89%)	5 (9%)	1 (2%)	6	33
2	I	58/351 (16%)	54 (93%)	4 (7%)	0	100	100
2	J	58/351 (16%)	48 (83%)	10 (17%)	0	100	100
2	K	58/351 (16%)	52 (90%)	5 (9%)	1 (2%)	7	35
3	A0	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	A2	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	A4	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
3	A6	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
3	A8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	B0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	B2	424/453 (94%)	413 (97%)	11 (3%)	0	100	100
3	B4	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	B6	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
3	B8	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	C0	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
3	C2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
3	C4	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	C6	424/453 (94%)	394 (93%)	30 (7%)	0	100	100
3	C8	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
3	D0	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
3	D2	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	D4	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
3	D6	424/453 (94%)	408 (96%)	14 (3%)	2 (0%)	25	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D8	424/453 (94%)	401 (95%)	20 (5%)	3 (1%)	19 53
3	E0	424/453 (94%)	409 (96%)	15 (4%)	0	100 100
3	E2	424/453 (94%)	400 (94%)	21 (5%)	3 (1%)	19 53
3	E4	424/453 (94%)	404 (95%)	20 (5%)	0	100 100
3	E6	424/453 (94%)	408 (96%)	16 (4%)	0	100 100
3	E8	424/453 (94%)	404 (95%)	20 (5%)	0	100 100
3	F0	424/453 (94%)	395 (93%)	29 (7%)	0	100 100
4	A1	424/449 (94%)	394 (93%)	30 (7%)	0	100 100
4	A3	424/449 (94%)	399 (94%)	25 (6%)	0	100 100
4	A5	424/449 (94%)	398 (94%)	26 (6%)	0	100 100
4	A7	424/449 (94%)	403 (95%)	21 (5%)	0	100 100
4	A9	424/449 (94%)	401 (95%)	23 (5%)	0	100 100
4	B1	424/449 (94%)	403 (95%)	21 (5%)	0	100 100
4	B3	424/449 (94%)	403 (95%)	21 (5%)	0	100 100
4	B5	424/449 (94%)	402 (95%)	22 (5%)	0	100 100
4	B7	424/449 (94%)	403 (95%)	21 (5%)	0	100 100
4	B9	424/449 (94%)	398 (94%)	26 (6%)	0	100 100
4	C1	424/449 (94%)	391 (92%)	33 (8%)	0	100 100
4	C3	424/449 (94%)	401 (95%)	23 (5%)	0	100 100
4	C5	424/449 (94%)	404 (95%)	20 (5%)	0	100 100
4	C7	424/449 (94%)	394 (93%)	30 (7%)	0	100 100
4	C9	424/449 (94%)	398 (94%)	26 (6%)	0	100 100
4	D1	424/449 (94%)	403 (95%)	21 (5%)	0	100 100
4	D3	424/449 (94%)	404 (95%)	20 (5%)	0	100 100
4	D5	424/449 (94%)	401 (95%)	23 (5%)	0	100 100
4	D7	424/449 (94%)	405 (96%)	19 (4%)	0	100 100
4	D9	424/449 (94%)	407 (96%)	17 (4%)	0	100 100
4	E1	424/449 (94%)	402 (95%)	22 (5%)	0	100 100
4	E3	424/449 (94%)	406 (96%)	18 (4%)	0	100 100
4	E5	424/449 (94%)	402 (95%)	22 (5%)	0	100 100
4	E7	424/449 (94%)	401 (95%)	23 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	E9	424/449 (94%)	394 (93%)	30 (7%)	0	100 100
4	F1	424/449 (94%)	395 (93%)	29 (7%)	0	100 100
5	O	161/583 (28%)	125 (78%)	31 (19%)	5 (3%)	3 25
5	P	210/583 (36%)	169 (80%)	34 (16%)	7 (3%)	3 23
5	R	210/583 (36%)	172 (82%)	33 (16%)	5 (2%)	5 29
6	U	20/336 (6%)	16 (80%)	4 (20%)	0	100 100
6	V	109/336 (32%)	91 (84%)	18 (16%)	0	100 100
6	W	109/336 (32%)	81 (74%)	28 (26%)	0	100 100
6	X	89/336 (26%)	75 (84%)	14 (16%)	0	100 100
7	a	159/220 (72%)	139 (87%)	19 (12%)	1 (1%)	22 55
7	b	159/220 (72%)	140 (88%)	19 (12%)	0	100 100
7	c	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
7	d	197/220 (90%)	183 (93%)	14 (7%)	0	100 100
7	e	197/220 (90%)	184 (93%)	13 (7%)	0	100 100
7	f	197/220 (90%)	183 (93%)	14 (7%)	0	100 100
7	g	197/220 (90%)	184 (93%)	13 (7%)	0	100 100
7	h	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
7	i	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
7	j	197/220 (90%)	187 (95%)	10 (5%)	0	100 100
7	m	197/220 (90%)	182 (92%)	15 (8%)	0	100 100
7	n	197/220 (90%)	177 (90%)	20 (10%)	0	100 100
7	o	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
7	p	197/220 (90%)	182 (92%)	15 (8%)	0	100 100
7	q	197/220 (90%)	185 (94%)	12 (6%)	0	100 100
7	r	197/220 (90%)	190 (96%)	7 (4%)	0	100 100
7	s	197/220 (90%)	181 (92%)	14 (7%)	2 (1%)	13 45
7	t	197/220 (90%)	181 (92%)	12 (6%)	4 (2%)	6 32
7	u	197/220 (90%)	186 (94%)	11 (6%)	0	100 100
7	v	197/220 (90%)	179 (91%)	18 (9%)	0	100 100
7	w	197/220 (90%)	188 (95%)	9 (5%)	0	100 100
7	x	197/220 (90%)	182 (92%)	15 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	k	135/189 (71%)	129 (96%)	6 (4%)	0	100 100
8	l	135/189 (71%)	113 (84%)	21 (16%)	1 (1%)	19 53
All	All	28367/39706 (71%)	26656 (94%)	1675 (6%)	36 (0%)	50 79

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D6	281	ALA
3	D8	286	LEU
5	O	277	ASP
5	O	468	ASN
5	P	277	ASP

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	1	119/1735 (7%)	119 (100%)	0	100 100
1	2	119/1735 (7%)	118 (99%)	1 (1%)	79 87
2	A	54/305 (18%)	54 (100%)	0	100 100
2	B	55/305 (18%)	55 (100%)	0	100 100
2	C	54/305 (18%)	54 (100%)	0	100 100
2	D	54/305 (18%)	54 (100%)	0	100 100
2	E	55/305 (18%)	55 (100%)	0	100 100
2	F	51/305 (17%)	50 (98%)	1 (2%)	50 71
2	G	55/305 (18%)	55 (100%)	0	100 100
2	H	51/305 (17%)	51 (100%)	0	100 100
2	I	55/305 (18%)	55 (100%)	0	100 100
2	J	55/305 (18%)	55 (100%)	0	100 100
2	K	55/305 (18%)	55 (100%)	0	100 100
3	A0	359/379 (95%)	358 (100%)	1 (0%)	91 96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A2	359/379 (95%)	359 (100%)	0	100	100
3	A4	359/379 (95%)	359 (100%)	0	100	100
3	A6	359/379 (95%)	359 (100%)	0	100	100
3	A8	359/379 (95%)	359 (100%)	0	100	100
3	B0	359/379 (95%)	359 (100%)	0	100	100
3	B2	359/379 (95%)	359 (100%)	0	100	100
3	B4	359/379 (95%)	359 (100%)	0	100	100
3	B6	359/379 (95%)	358 (100%)	1 (0%)	91	96
3	B8	359/379 (95%)	358 (100%)	1 (0%)	91	96
3	C0	359/379 (95%)	359 (100%)	0	100	100
3	C2	359/379 (95%)	358 (100%)	1 (0%)	91	96
3	C4	359/379 (95%)	359 (100%)	0	100	100
3	C6	359/379 (95%)	359 (100%)	0	100	100
3	C8	359/379 (95%)	359 (100%)	0	100	100
3	D0	359/379 (95%)	359 (100%)	0	100	100
3	D2	359/379 (95%)	359 (100%)	0	100	100
3	D4	359/379 (95%)	359 (100%)	0	100	100
3	D6	359/379 (95%)	357 (99%)	2 (1%)	84	91
3	D8	359/379 (95%)	354 (99%)	5 (1%)	62	79
3	E0	359/379 (95%)	358 (100%)	1 (0%)	91	96
3	E2	359/379 (95%)	358 (100%)	1 (0%)	91	96
3	E4	359/379 (95%)	359 (100%)	0	100	100
3	E6	359/379 (95%)	359 (100%)	0	100	100
3	E8	359/379 (95%)	359 (100%)	0	100	100
3	F0	359/379 (95%)	359 (100%)	0	100	100
4	A1	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	A3	364/381 (96%)	364 (100%)	0	100	100
4	A5	364/381 (96%)	364 (100%)	0	100	100
4	A7	364/381 (96%)	364 (100%)	0	100	100
4	A9	364/381 (96%)	364 (100%)	0	100	100
4	B1	364/381 (96%)	364 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B3	364/381 (96%)	364 (100%)	0	100	100
4	B5	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	B7	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	B9	364/381 (96%)	364 (100%)	0	100	100
4	C1	364/381 (96%)	364 (100%)	0	100	100
4	C3	364/381 (96%)	364 (100%)	0	100	100
4	C5	364/381 (96%)	364 (100%)	0	100	100
4	C7	364/381 (96%)	364 (100%)	0	100	100
4	C9	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	D1	364/381 (96%)	364 (100%)	0	100	100
4	D3	364/381 (96%)	364 (100%)	0	100	100
4	D5	364/381 (96%)	364 (100%)	0	100	100
4	D7	364/381 (96%)	364 (100%)	0	100	100
4	D9	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	E1	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	E3	364/381 (96%)	364 (100%)	0	100	100
4	E5	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	E7	364/381 (96%)	364 (100%)	0	100	100
4	E9	364/381 (96%)	363 (100%)	1 (0%)	91	96
4	F1	364/381 (96%)	362 (100%)	2 (0%)	86	92
5	O	156/502 (31%)	156 (100%)	0	100	100
5	P	194/502 (39%)	194 (100%)	0	100	100
5	R	194/502 (39%)	194 (100%)	0	100	100
6	U	20/280 (7%)	20 (100%)	0	100	100
6	V	101/280 (36%)	101 (100%)	0	100	100
6	W	101/280 (36%)	101 (100%)	0	100	100
6	X	81/280 (29%)	81 (100%)	0	100	100
7	a	139/190 (73%)	139 (100%)	0	100	100
7	b	139/190 (73%)	139 (100%)	0	100	100
7	c	174/190 (92%)	174 (100%)	0	100	100
7	d	174/190 (92%)	174 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	e	174/190 (92%)	174 (100%)	0	100 100
7	f	174/190 (92%)	174 (100%)	0	100 100
7	g	174/190 (92%)	174 (100%)	0	100 100
7	h	174/190 (92%)	174 (100%)	0	100 100
7	i	174/190 (92%)	174 (100%)	0	100 100
7	j	174/190 (92%)	173 (99%)	1 (1%)	84 91
7	m	174/190 (92%)	174 (100%)	0	100 100
7	n	174/190 (92%)	174 (100%)	0	100 100
7	o	174/190 (92%)	174 (100%)	0	100 100
7	p	174/190 (92%)	174 (100%)	0	100 100
7	q	174/190 (92%)	174 (100%)	0	100 100
7	r	174/190 (92%)	172 (99%)	2 (1%)	70 83
7	s	174/190 (92%)	169 (97%)	5 (3%)	37 63
7	t	174/190 (92%)	169 (97%)	5 (3%)	37 63
7	u	174/190 (92%)	174 (100%)	0	100 100
7	v	174/190 (92%)	173 (99%)	1 (1%)	84 91
7	w	174/190 (92%)	174 (100%)	0	100 100
7	x	174/190 (92%)	174 (100%)	0	100 100
8	k	124/164 (76%)	123 (99%)	1 (1%)	79 87
8	l	124/164 (76%)	124 (100%)	0	100 100
All	All	24483/33719 (73%)	24443 (100%)	40 (0%)	91 97

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	r	37	GLN
7	t	196	LEU
7	s	11	ASN
7	s	202	ARG
7	t	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 289 such sidechains are listed below:

Mol	Chain	Res	Type
4	F1	337	ASN
7	v	100	ASN
5	O	469	GLN
7	f	37	GLN
4	B9	332	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 26 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	GTP	A4	501	10	29,34,34	1.19	2 (6%)	35,54,54	1.25	4 (11%)
11	GDP	B3	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.05	1 (3%)
11	GDP	E1	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.19	4 (13%)
9	GTP	D2	501	10	29,34,34	1.24	2 (6%)	35,54,54	1.46	5 (14%)
9	GTP	D4	501	10	29,34,34	1.25	2 (6%)	35,54,54	1.48	6 (17%)
9	GTP	D8	501	10	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
9	GTP	A2	502	-	29,34,34	1.16	2 (6%)	35,54,54	1.35	3 (8%)
11	GDP	D1	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GTP	D6	501	10	29,34,34	1.18	2 (6%)	35,54,54	1.33	4 (11%)
11	GDP	C5	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
11	GDP	C9	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	3 (10%)
9	GTP	E8	501	10	29,34,34	1.19	2 (6%)	35,54,54	1.35	4 (11%)
9	GTP	C2	501	10	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
9	GTP	A0	501	10	29,34,34	1.20	2 (6%)	35,54,54	1.34	4 (11%)
11	GDP	C1	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.18	2 (6%)
11	GDP	D5	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
9	GTP	B2	501	10	29,34,34	1.18	2 (6%)	35,54,54	1.29	4 (11%)
11	GDP	E9	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	2 (6%)
9	GTP	B8	502	10	29,34,34	1.19	2 (6%)	35,54,54	1.31	4 (11%)
11	GDP	B9	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	2 (6%)
11	GDP	F1	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
11	GDP	P	601	-	25,30,30	0.99	1 (4%)	30,47,47	1.18	2 (6%)
9	GTP	B4	501	10	29,34,34	1.19	2 (6%)	35,54,54	1.32	4 (11%)
9	GTP	C6	501	10	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
9	GTP	E2	501	10	29,34,34	1.20	2 (6%)	35,54,54	1.31	4 (11%)
9	GTP	F0	501	10	29,34,34	1.26	2 (6%)	35,54,54	1.32	4 (11%)
9	GTP	B6	501	10	29,34,34	1.22	2 (6%)	35,54,54	1.39	5 (14%)
11	GDP	C3	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	1 (3%)
11	GDP	O	601	-	25,30,30	1.03	1 (4%)	30,47,47	1.19	3 (10%)
11	GDP	E5	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	3 (10%)
11	GDP	B7	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
9	GTP	A8	501	10	29,34,34	1.20	2 (6%)	35,54,54	1.34	5 (14%)
9	GTP	E0	501	10	29,34,34	1.21	2 (6%)	35,54,54	1.32	3 (8%)
9	GTP	D0	501	10	29,34,34	1.16	1 (3%)	35,54,54	1.38	4 (11%)
9	GTP	C4	501	10	29,34,34	1.28	2 (6%)	35,54,54	1.28	4 (11%)
9	GTP	B0	501	10	29,34,34	1.20	2 (6%)	35,54,54	1.31	3 (8%)
9	GTP	C8	501	10	29,34,34	1.19	2 (6%)	35,54,54	1.37	4 (11%)
9	GTP	E4	501	10	29,34,34	1.23	2 (6%)	35,54,54	1.38	7 (20%)
9	GTP	E7	501	-	29,34,34	1.19	2 (6%)	35,54,54	1.43	7 (20%)
11	GDP	D3	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.15	4 (13%)
11	GDP	D9	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	3 (10%)
9	GTP	A6	501	10	29,34,34	1.15	2 (6%)	35,54,54	1.31	3 (8%)
11	GDP	E7	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	GDP	D7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
11	GDP	A5	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
11	GDP	E3	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
11	GDP	A1	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.25	3 (10%)
11	GDP	A7	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.11	3 (10%)
11	GDP	B5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
9	GTP	C0	501	10	29,34,34	1.27	4 (13%)	35,54,54	1.37	6 (17%)
11	GDP	A3	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.19	3 (10%)
11	GDP	C7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.21	2 (6%)

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
9	GTP	A4	501	10	-	8/18/38/38	0/3/3/3
11	GDP	B3	501	-	-	3/12/32/32	0/3/3/3
11	GDP	E1	501	-	-	0/12/32/32	0/3/3/3
9	GTP	D2	501	10	-	8/18/38/38	0/3/3/3
9	GTP	D4	501	10	-	3/18/38/38	0/3/3/3
9	GTP	D8	501	10	-	5/18/38/38	0/3/3/3
9	GTP	A2	502	-	-	9/18/38/38	0/3/3/3
11	GDP	D1	502	-	-	3/12/32/32	0/3/3/3
9	GTP	D6	501	10	-	6/18/38/38	0/3/3/3
11	GDP	C5	501	-	-	1/12/32/32	0/3/3/3
11	GDP	C9	502	-	-	2/12/32/32	0/3/3/3
9	GTP	E8	501	10	-	8/18/38/38	0/3/3/3
9	GTP	C2	501	10	-	4/18/38/38	0/3/3/3
9	GTP	A0	501	10	-	6/18/38/38	0/3/3/3
11	GDP	C1	501	-	-	0/12/32/32	0/3/3/3
11	GDP	D5	501	-	-	3/12/32/32	0/3/3/3
9	GTP	B2	501	10	-	5/18/38/38	0/3/3/3
11	GDP	E9	501	-	-	8/12/32/32	0/3/3/3
9	GTP	B8	502	10	-	6/18/38/38	0/3/3/3
11	GDP	B9	501	-	-	6/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GDP	F1	501	-	-	3/12/32/32	0/3/3/3
11	GDP	P	601	-	-	6/12/32/32	0/3/3/3
9	GTP	B4	501	10	-	6/18/38/38	0/3/3/3
9	GTP	C6	501	10	-	5/18/38/38	0/3/3/3
9	GTP	E2	501	10	-	5/18/38/38	0/3/3/3
9	GTP	F0	501	10	-	7/18/38/38	0/3/3/3
9	GTP	B6	501	10	-	4/18/38/38	0/3/3/3
11	GDP	C3	501	-	-	3/12/32/32	0/3/3/3
11	GDP	O	601	-	-	5/12/32/32	0/3/3/3
11	GDP	E5	501	-	-	0/12/32/32	0/3/3/3
11	GDP	B7	501	-	-	3/12/32/32	0/3/3/3
9	GTP	A8	501	10	-	5/18/38/38	0/3/3/3
9	GTP	E0	501	10	-	3/18/38/38	0/3/3/3
9	GTP	D0	501	10	-	3/18/38/38	0/3/3/3
9	GTP	C4	501	10	-	4/18/38/38	0/3/3/3
9	GTP	B0	501	10	-	7/18/38/38	0/3/3/3
9	GTP	C8	501	10	-	3/18/38/38	0/3/3/3
9	GTP	E4	501	10	-	10/18/38/38	0/3/3/3
9	GTP	E7	501	-	-	9/18/38/38	0/3/3/3
11	GDP	D3	502	-	-	4/12/32/32	0/3/3/3
11	GDP	D9	501	-	-	3/12/32/32	0/3/3/3
9	GTP	A6	501	10	-	6/18/38/38	0/3/3/3
11	GDP	E7	502	-	-	2/12/32/32	0/3/3/3
11	GDP	D7	501	-	-	5/12/32/32	0/3/3/3
11	GDP	A5	501	-	-	2/12/32/32	0/3/3/3
11	GDP	E3	501	-	-	3/12/32/32	0/3/3/3
11	GDP	A1	501	-	-	5/12/32/32	0/3/3/3
11	GDP	A7	501	-	-	7/12/32/32	0/3/3/3
11	GDP	B5	501	-	-	2/12/32/32	0/3/3/3
9	GTP	C0	501	10	-	9/18/38/38	0/3/3/3
11	GDP	A3	501	-	-	6/12/32/32	0/3/3/3
11	GDP	C7	501	-	-	5/12/32/32	0/3/3/3

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D2	501	GTP	C5-C6	-4.64	1.38	1.47
9	C4	501	GTP	C5-C6	-4.46	1.38	1.47
9	E4	501	GTP	C5-C6	-4.41	1.38	1.47
9	C2	501	GTP	C5-C6	-4.38	1.38	1.47
9	B8	502	GTP	C5-C6	-4.35	1.38	1.47

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B0	501	GTP	C8-N7-C5	3.90	109.18	102.55
9	D4	501	GTP	C8-N7-C5	3.89	109.17	102.55
9	D0	501	GTP	C8-N7-C5	3.86	109.12	102.55
9	E7	501	GTP	C8-N7-C5	3.86	109.12	102.55
9	A2	502	GTP	C8-N7-C5	3.84	109.09	102.55

There are no chirality outliers.

5 of 244 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A0	501	GTP	PB-O3A-PA-O5'
9	A2	502	GTP	C5'-O5'-PA-O3A
9	A2	502	GTP	C5'-O5'-PA-O1A
9	A2	502	GTP	C5'-O5'-PA-O2A
9	A4	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

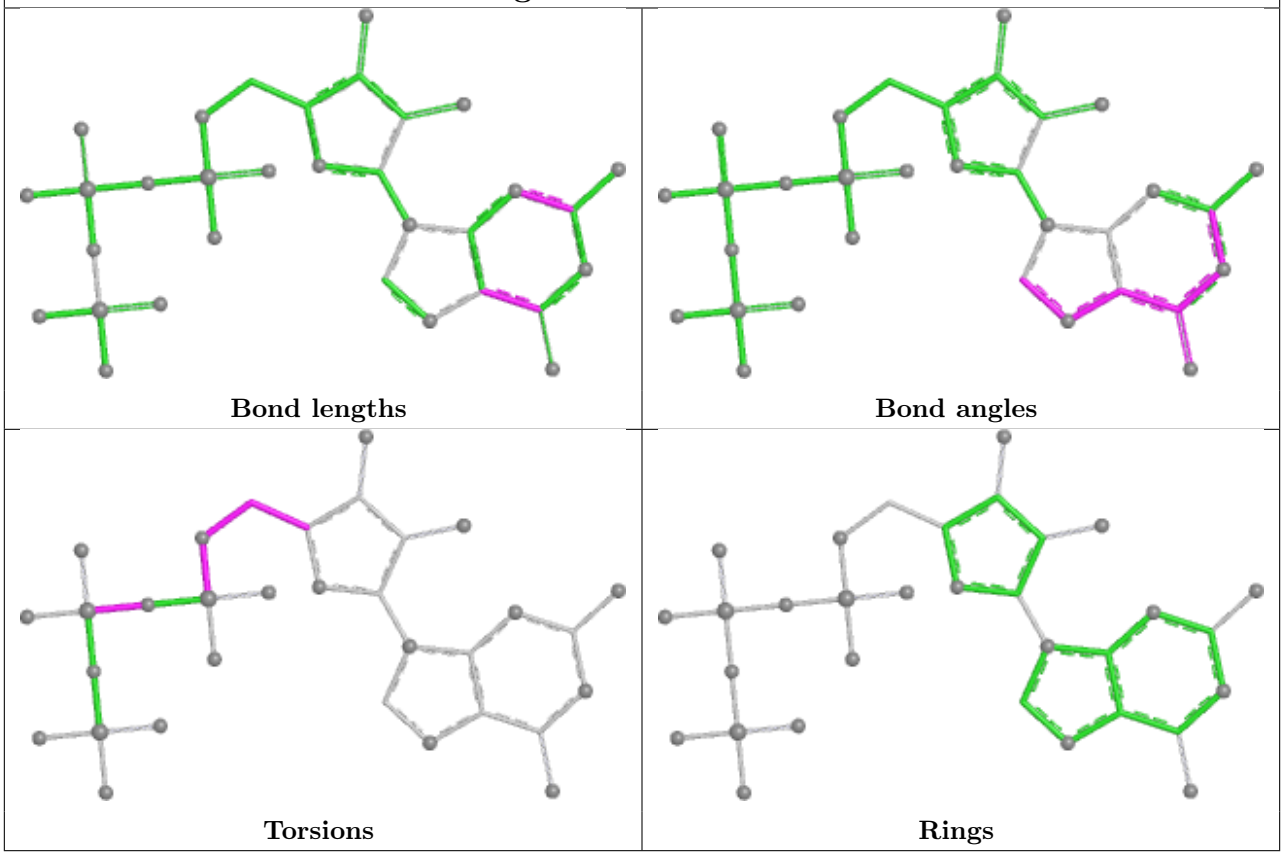
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C9	502	GDP	1	0
9	E7	501	GTP	1	0
11	D7	501	GDP	1	0
11	C7	501	GDP	1	0

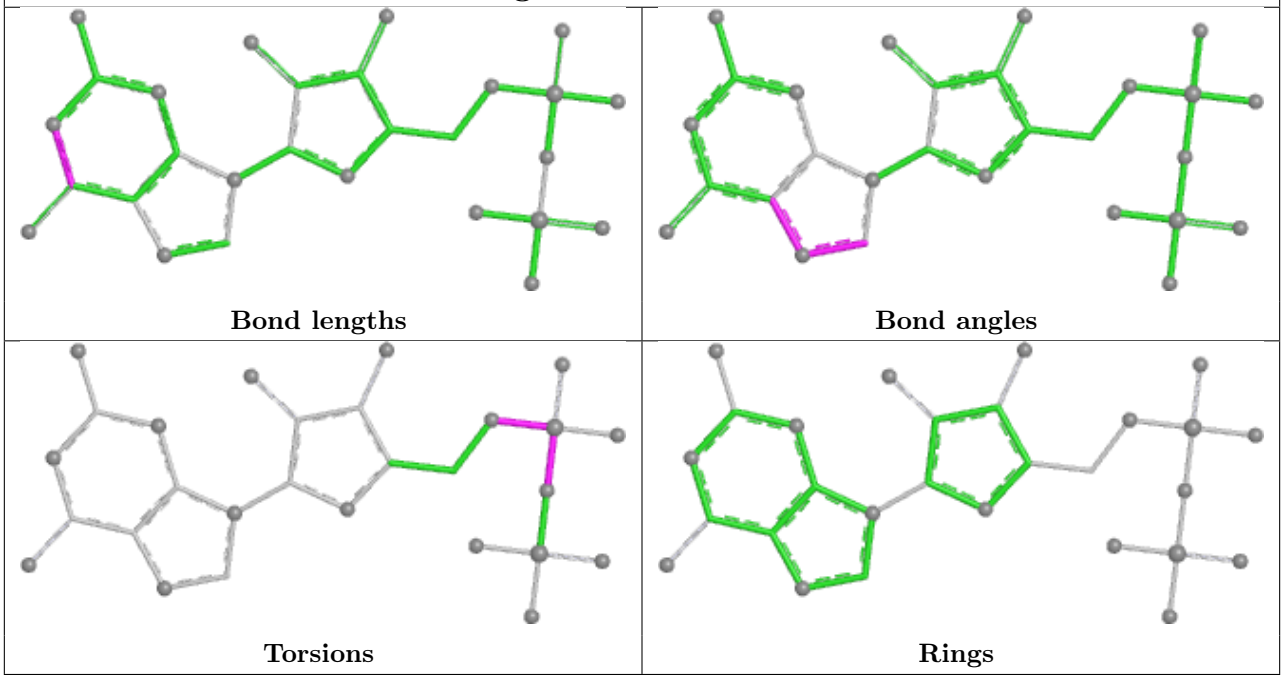
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

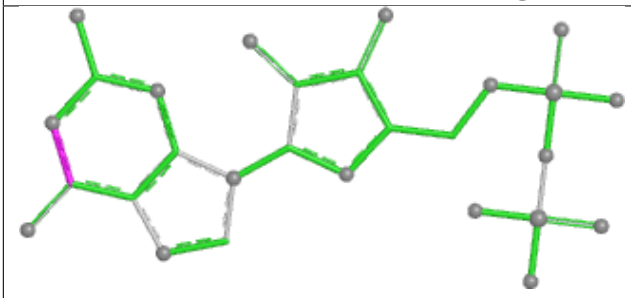
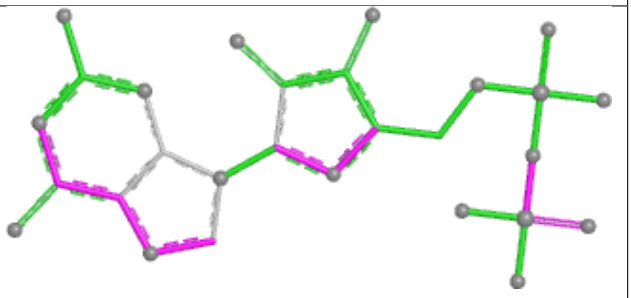
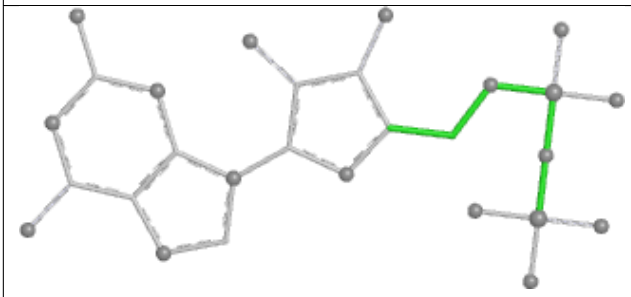
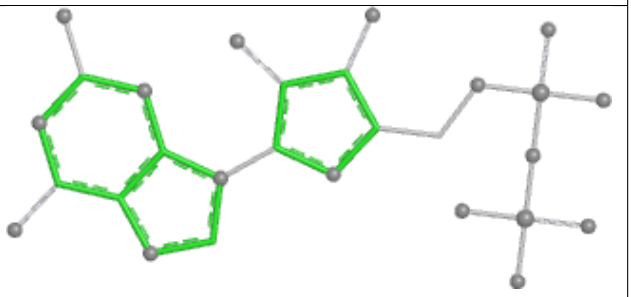
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

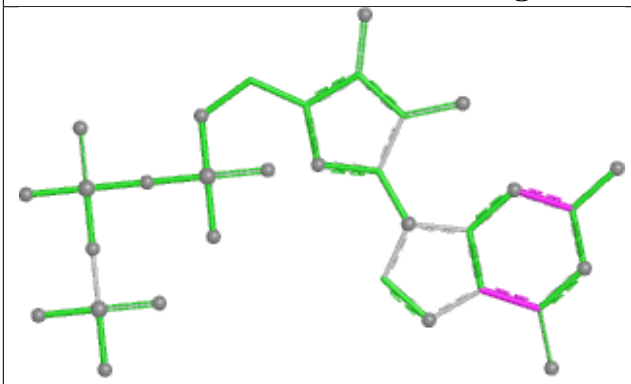
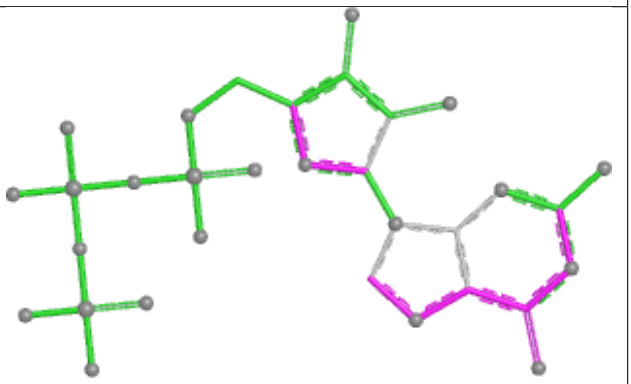
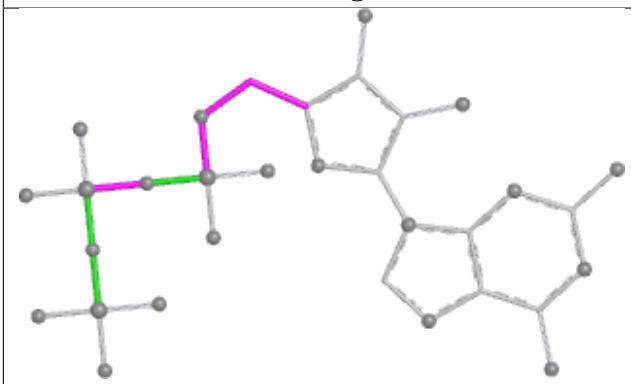
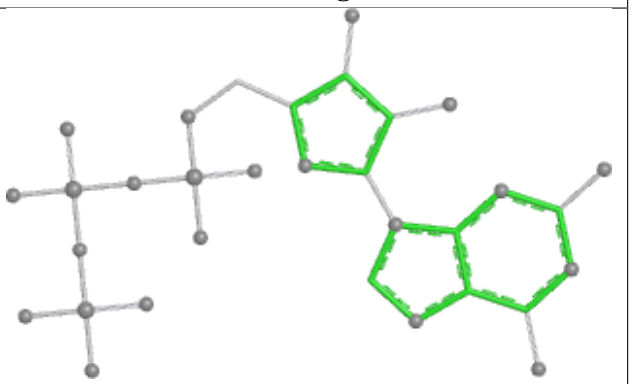
Ligand GTP A4 501



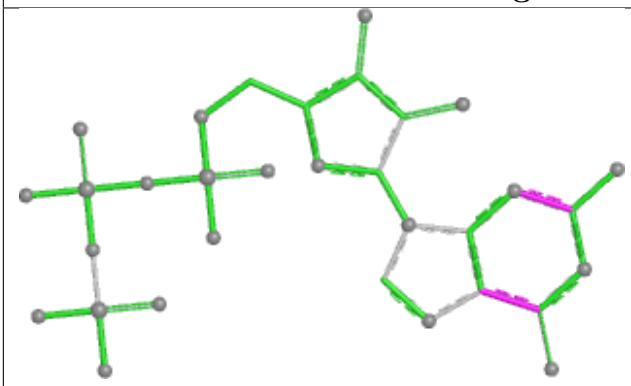
Ligand GDP B3 501



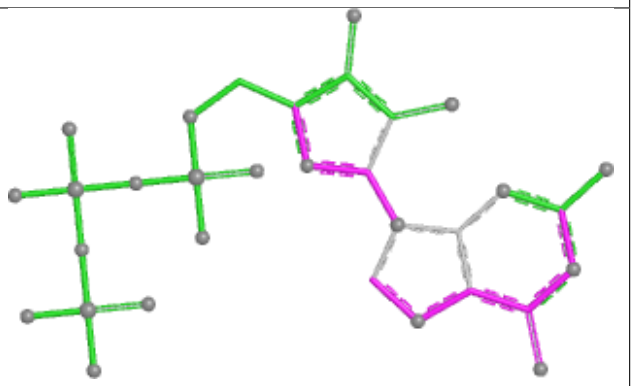
Ligand GDP E1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GTP D2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

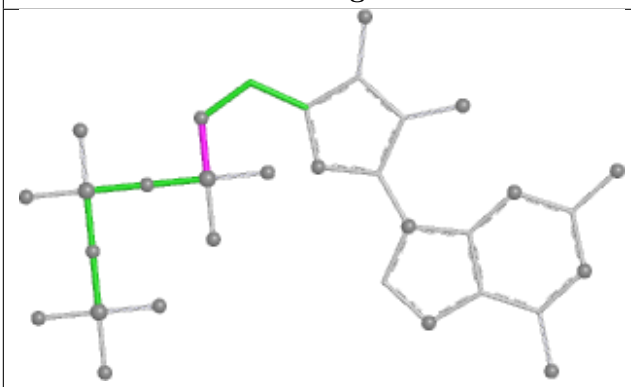
Ligand GTP D4 501



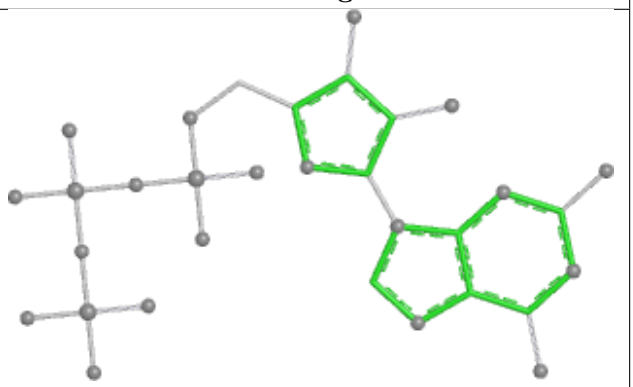
Bond lengths



Bond angles

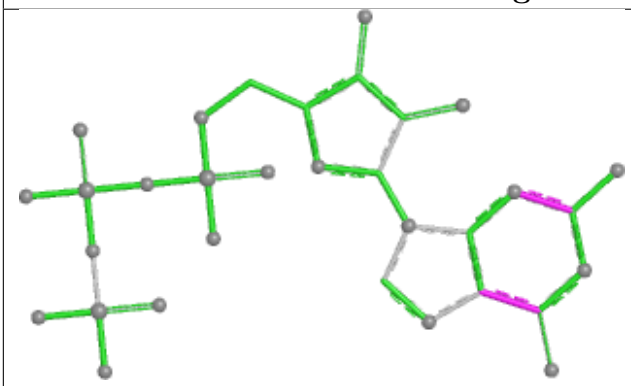


Torsions

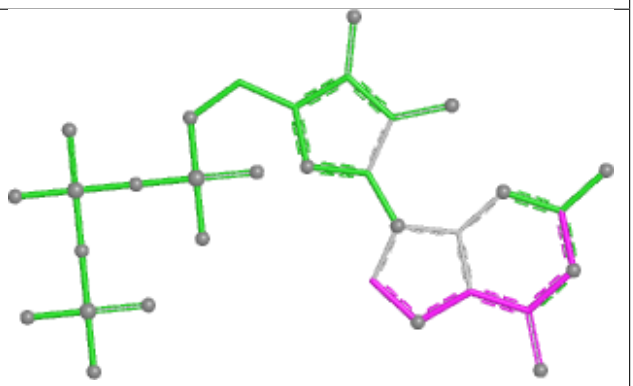


Rings

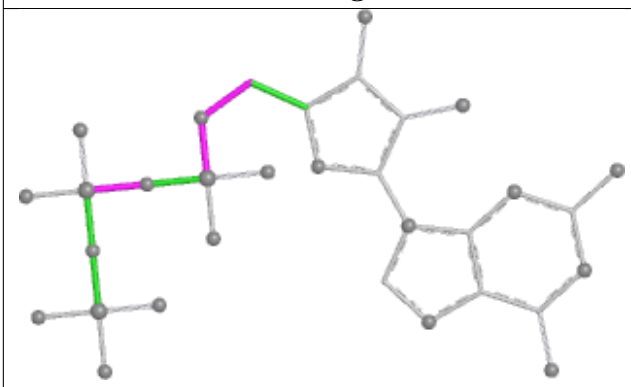
Ligand GTP D8 501



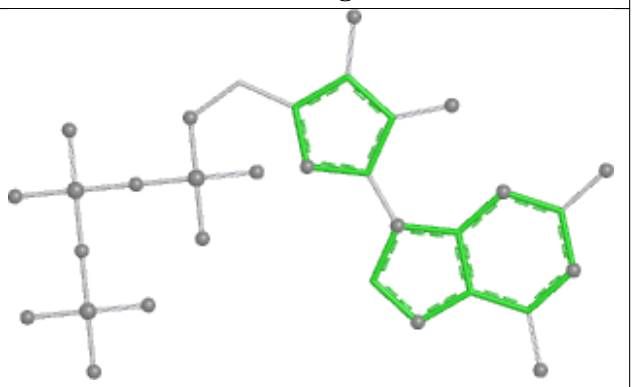
Bond lengths



Bond angles

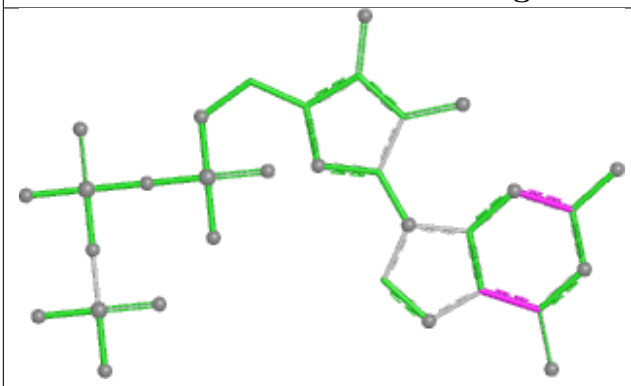


Torsions

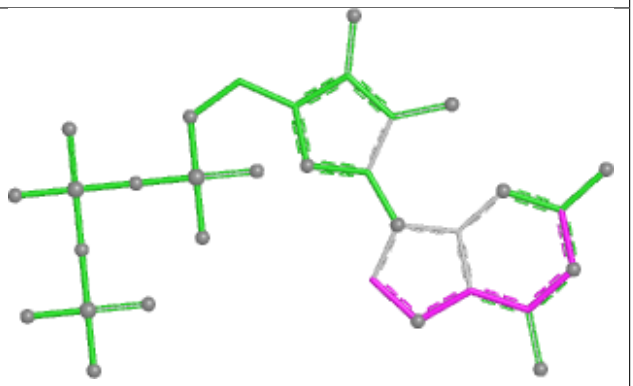


Rings

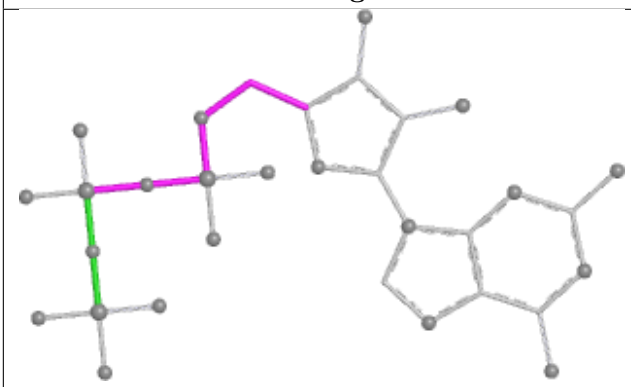
Ligand GTP A2 502



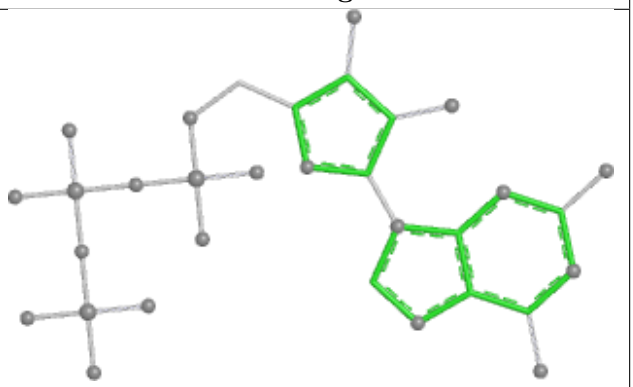
Bond lengths



Bond angles

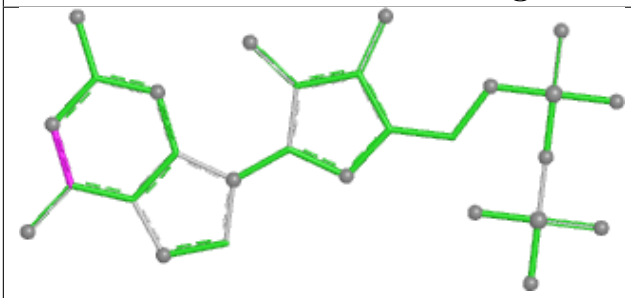


Torsions

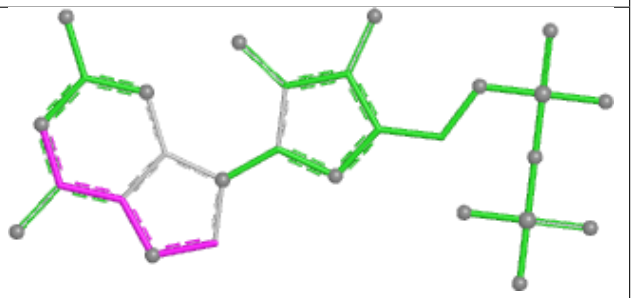


Rings

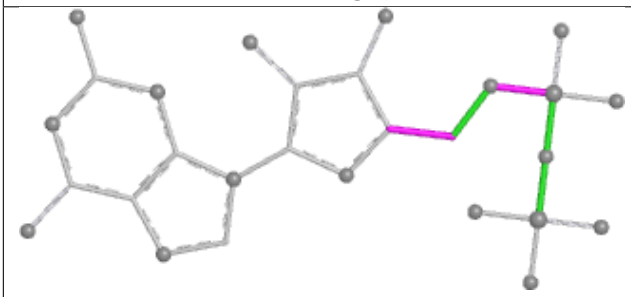
Ligand GDP D1 502



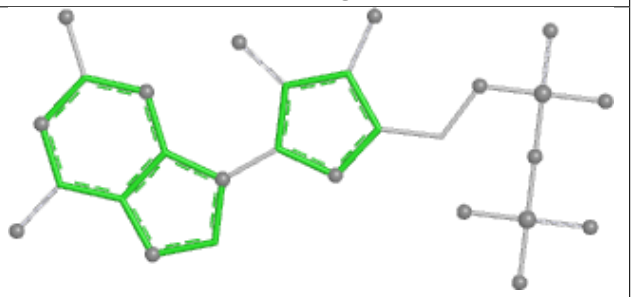
Bond lengths



Bond angles

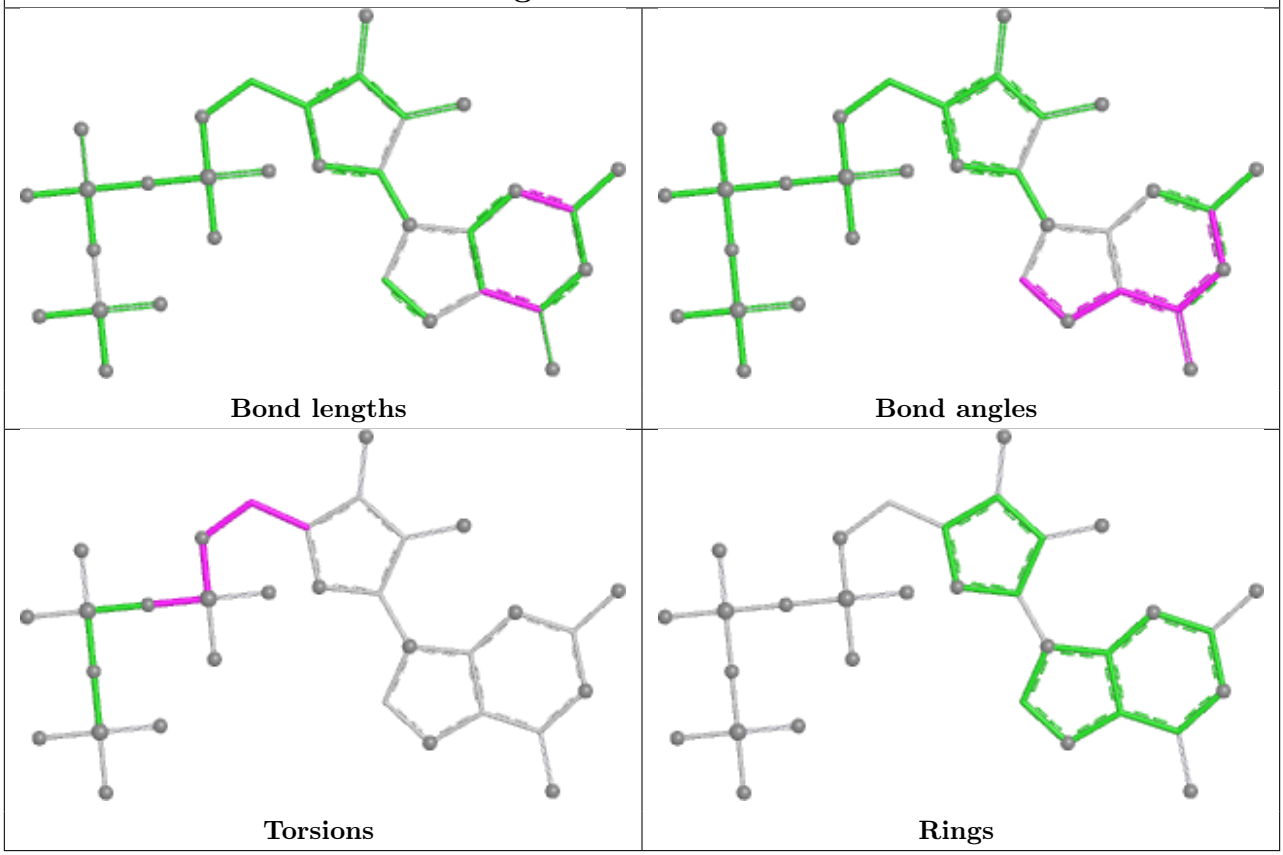


Torsions

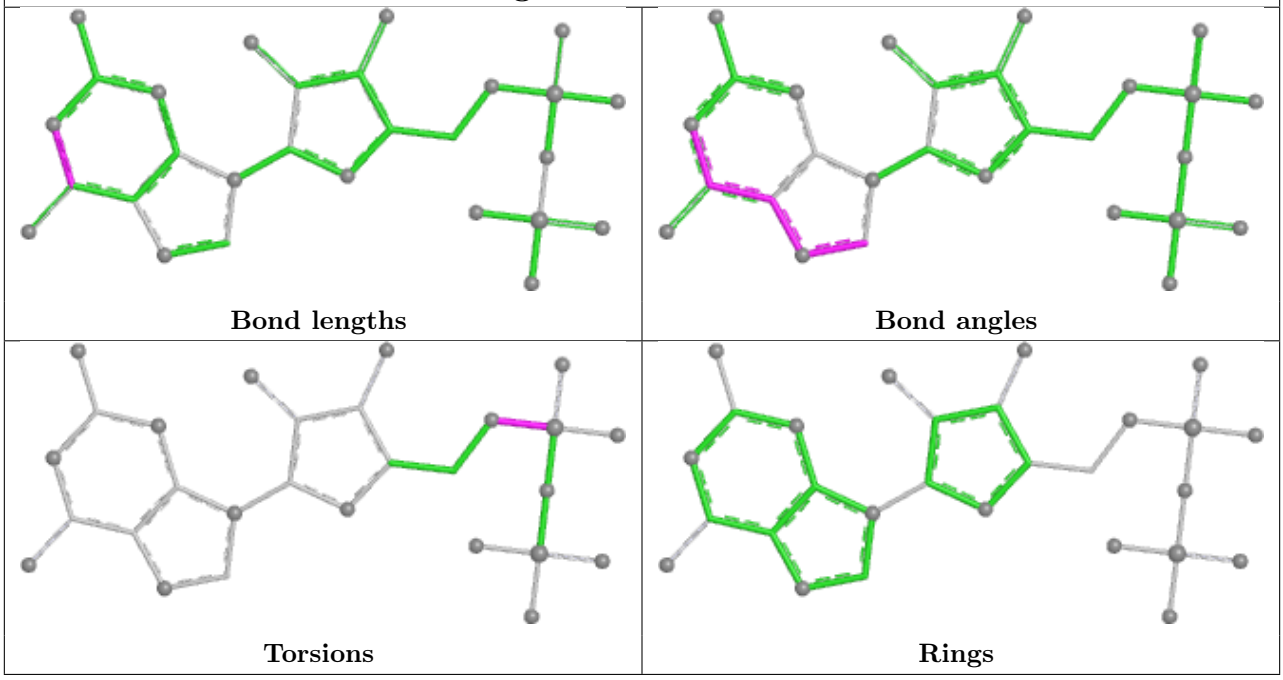


Rings

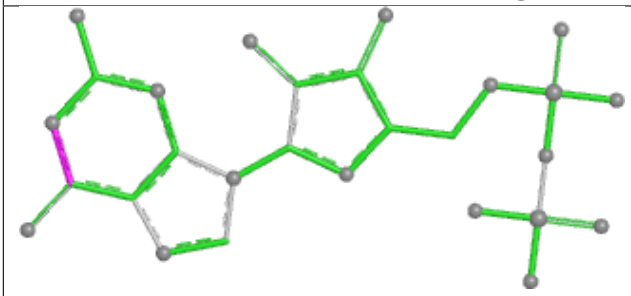
Ligand GTP D6 501



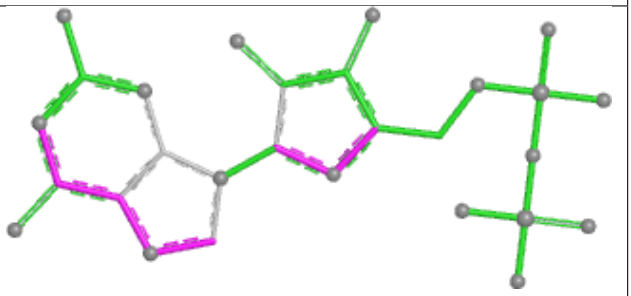
Ligand GDP C5 501



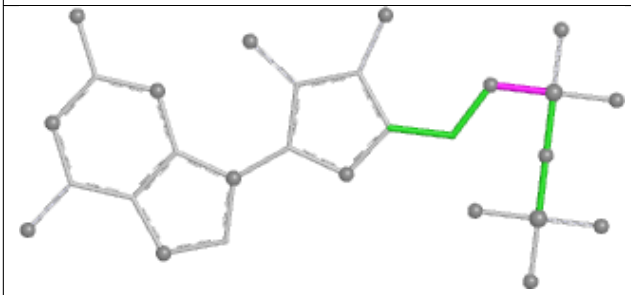
Ligand GDP C9 502



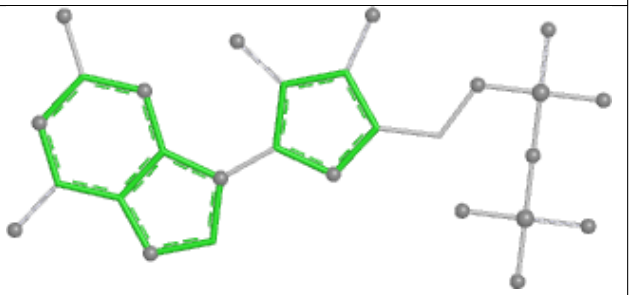
Bond lengths



Bond angles

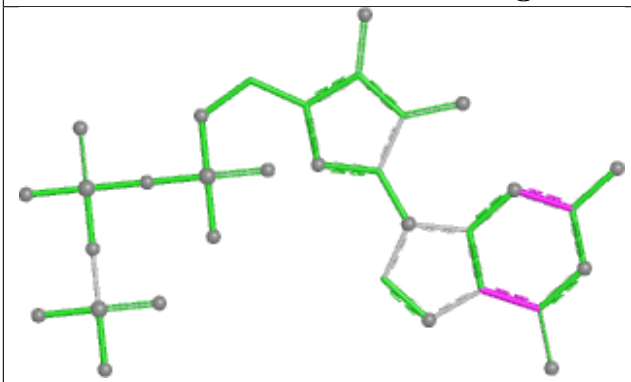


Torsions

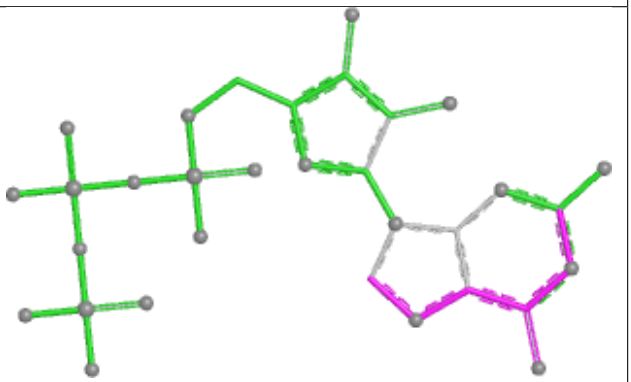


Rings

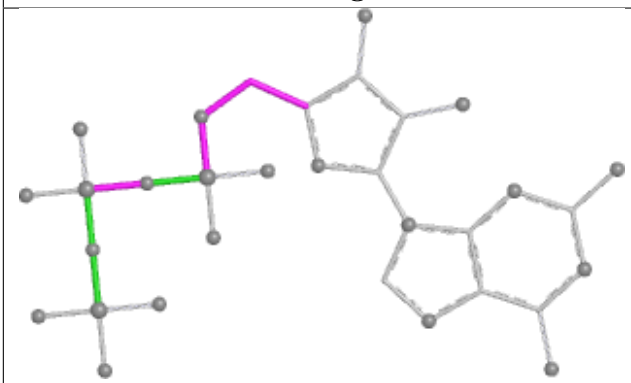
Ligand GTP E8 501



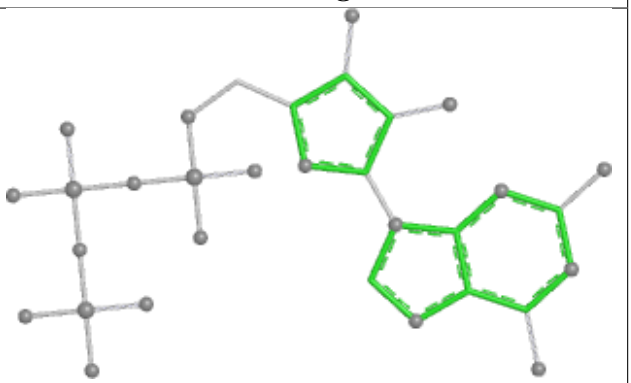
Bond lengths



Bond angles

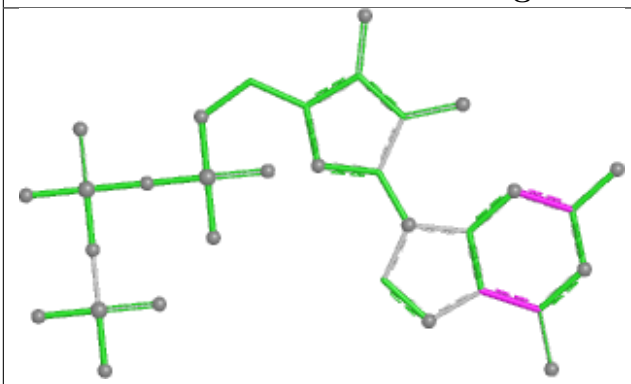


Torsions

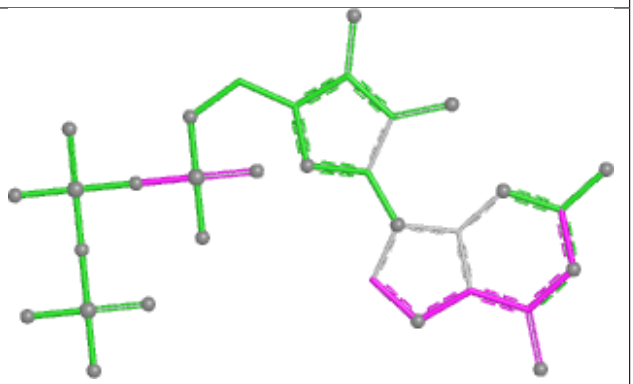


Rings

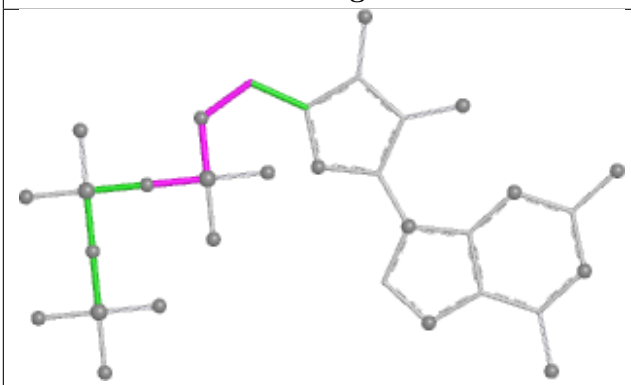
Ligand GTP C2 501



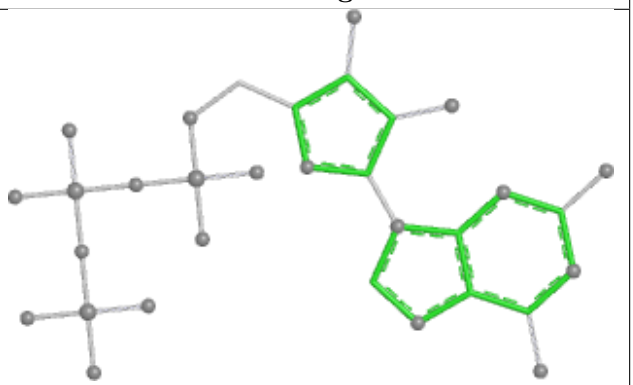
Bond lengths



Bond angles

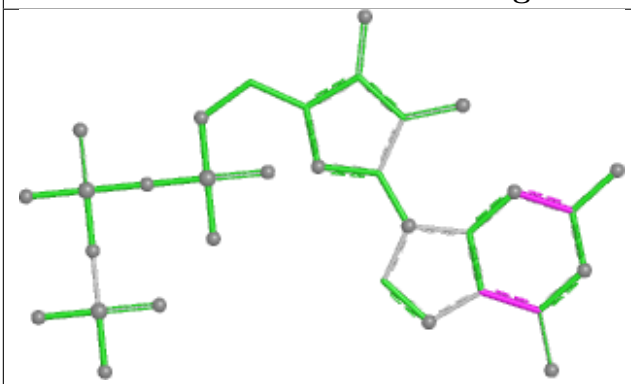


Torsions

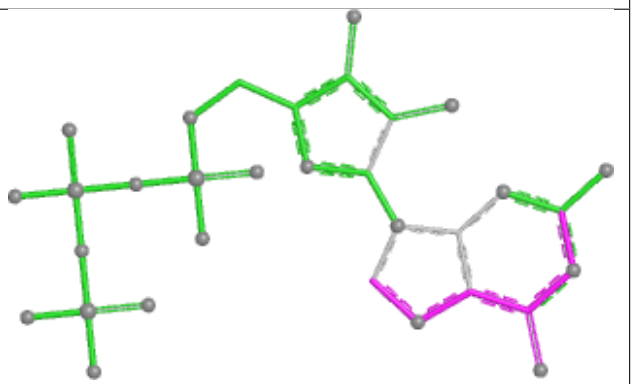


Rings

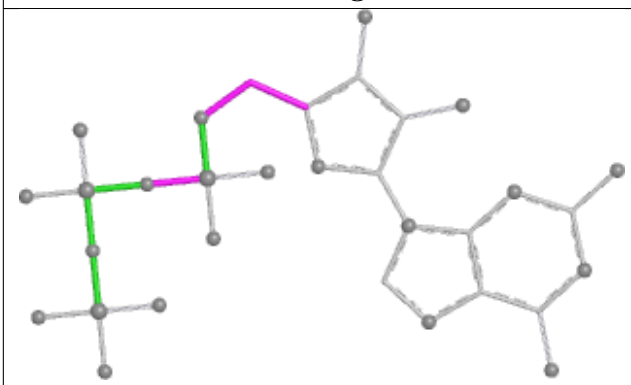
Ligand GTP A0 501



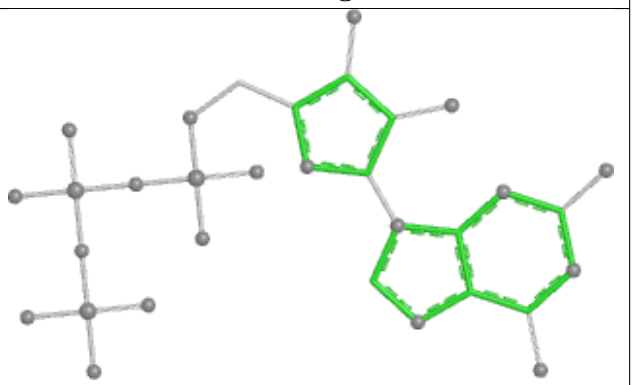
Bond lengths



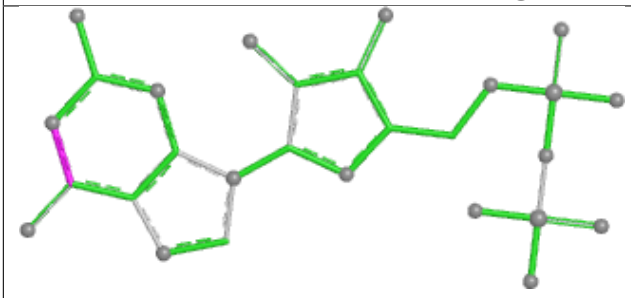
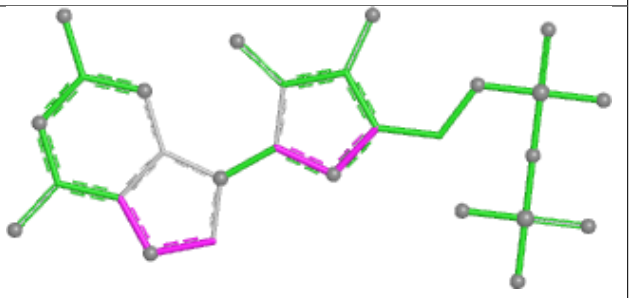
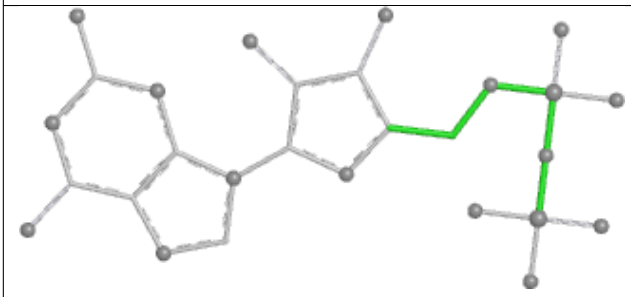
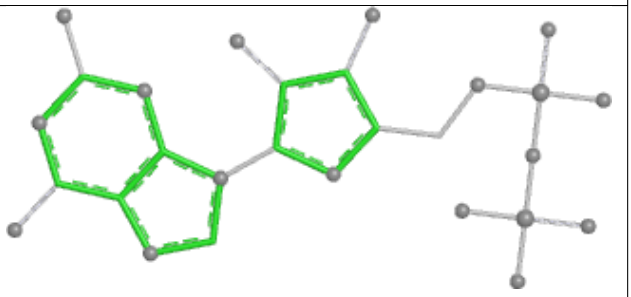
Bond angles

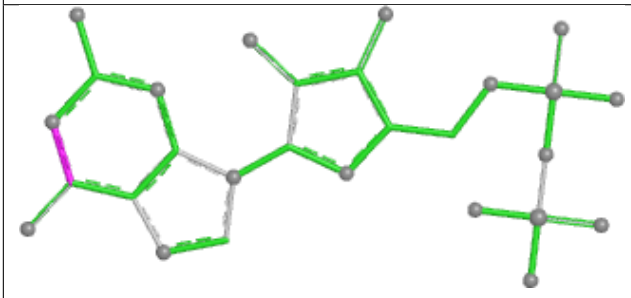
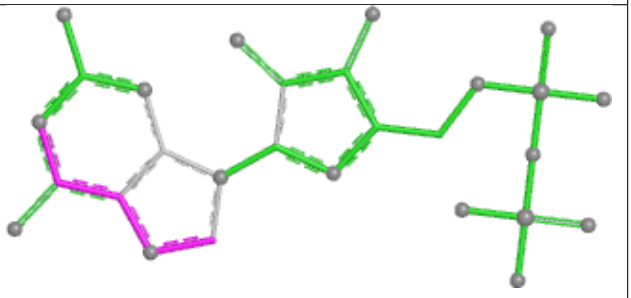
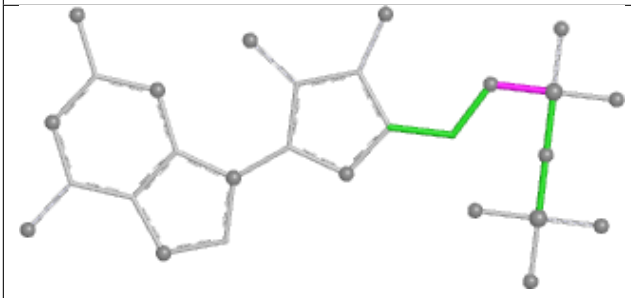
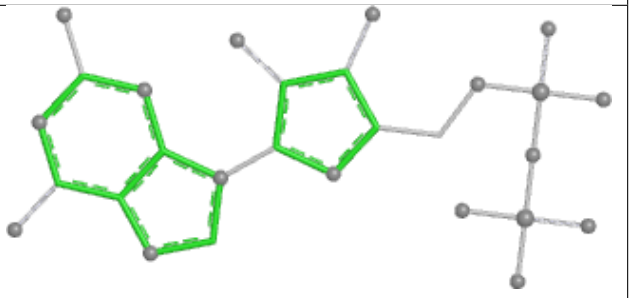


Torsions

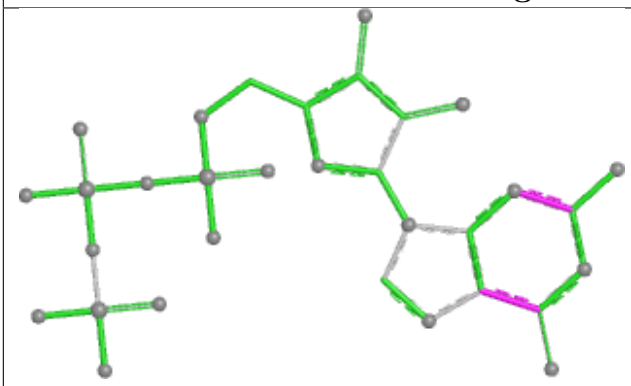


Rings

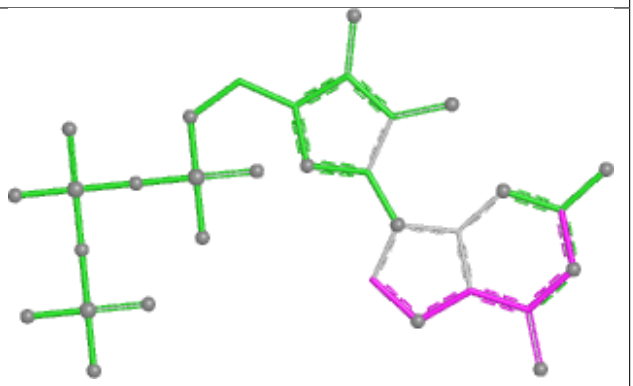
Ligand GDP C1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

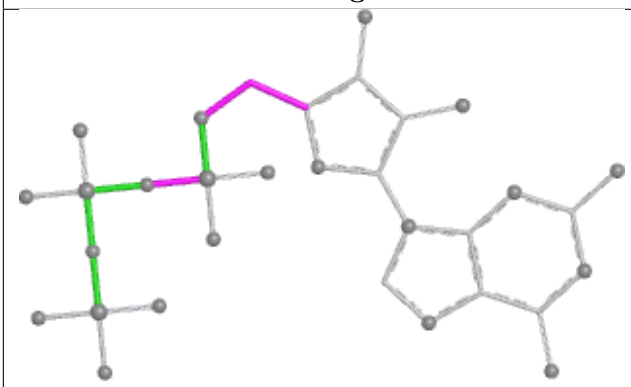
Ligand GTP B2 501



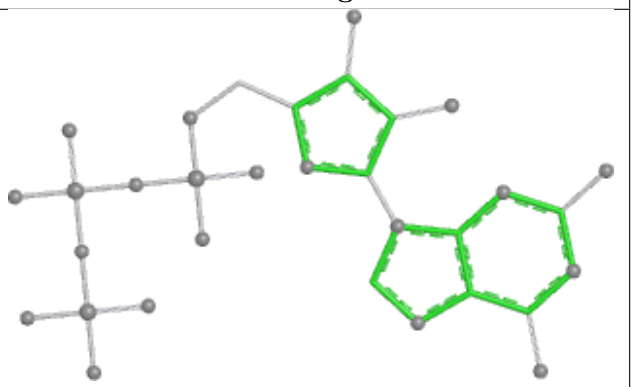
Bond lengths



Bond angles

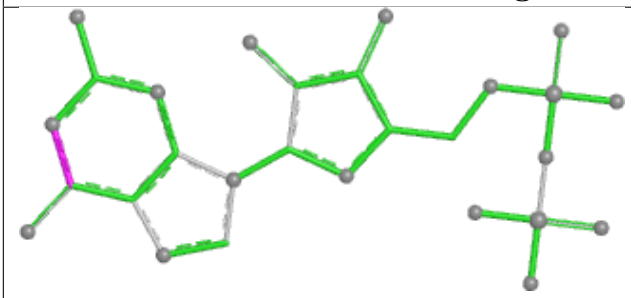


Torsions

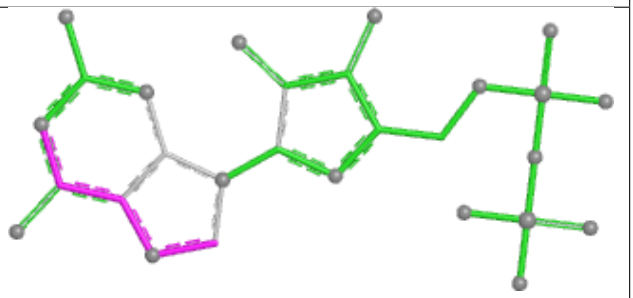


Rings

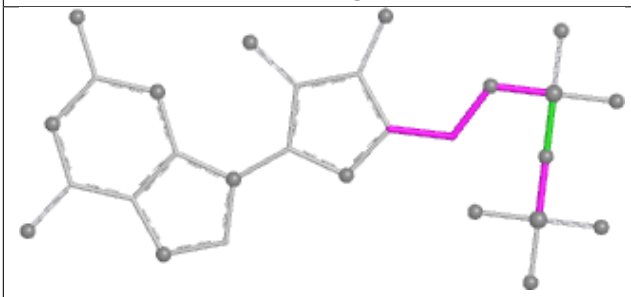
Ligand GDP E9 501



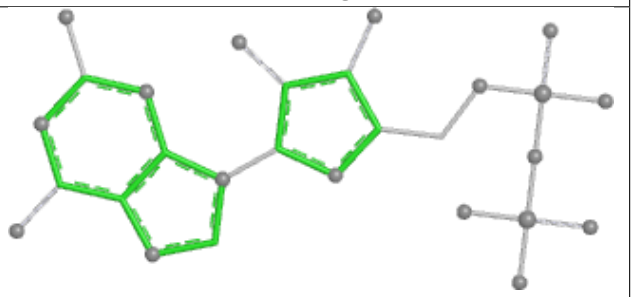
Bond lengths



Bond angles

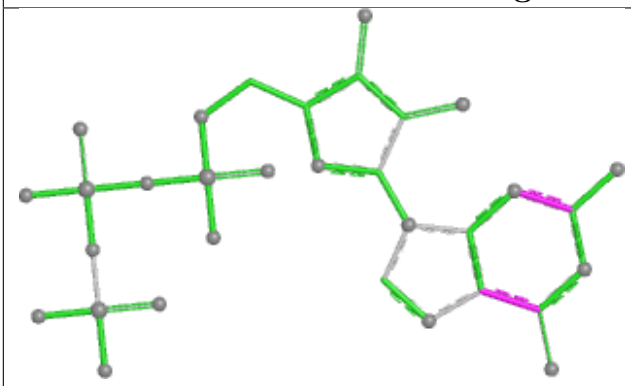


Torsions

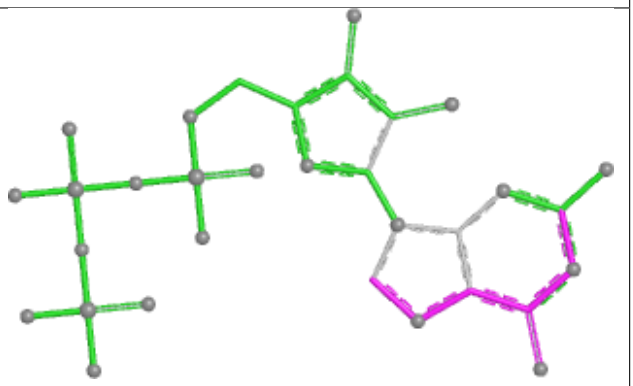


Rings

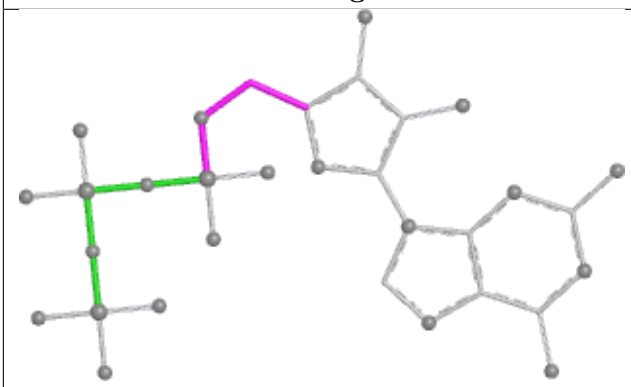
Ligand GTP B8 502



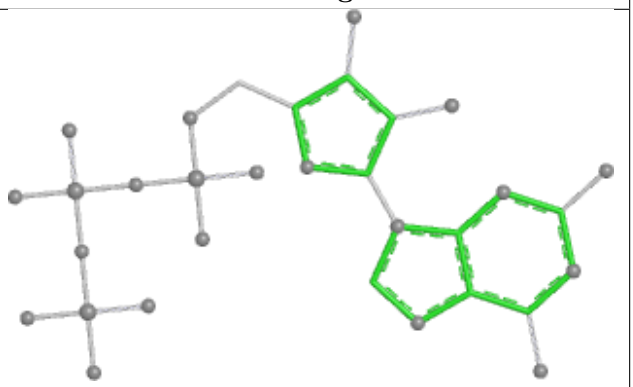
Bond lengths



Bond angles

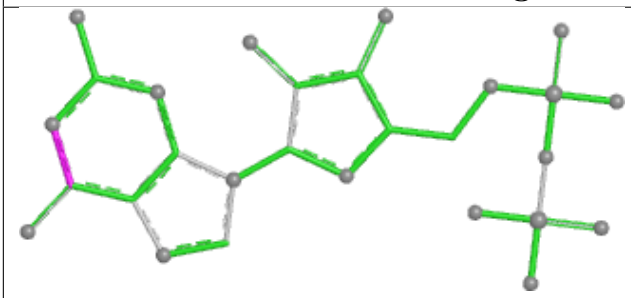


Torsions

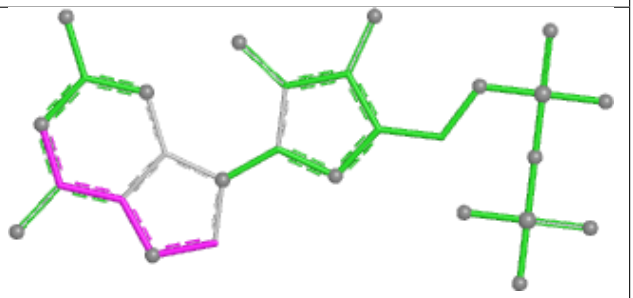


Rings

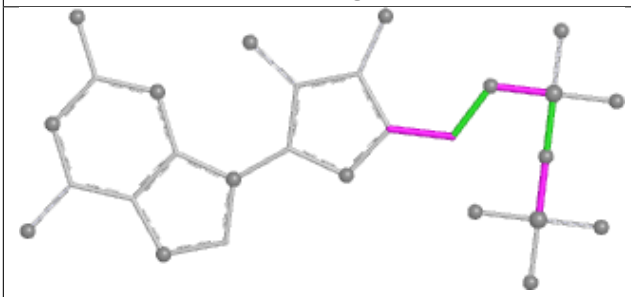
Ligand GDP B9 501



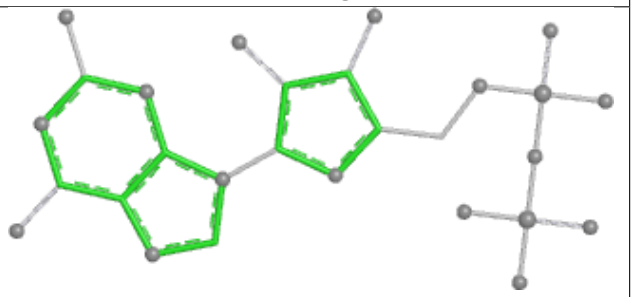
Bond lengths



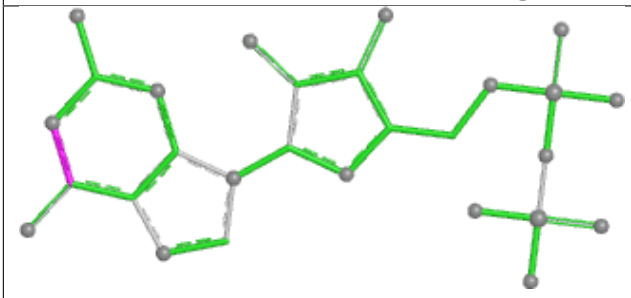
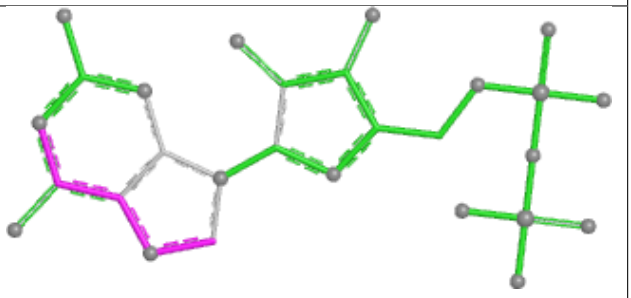
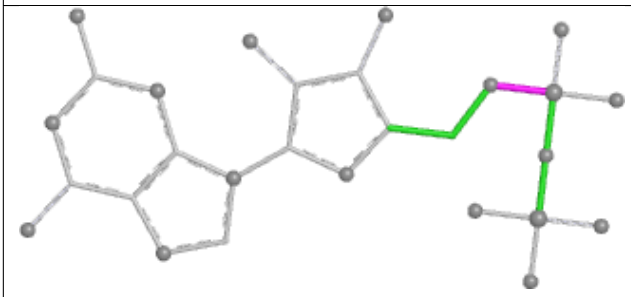
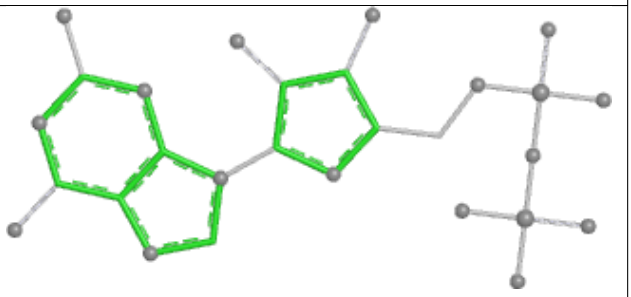
Bond angles

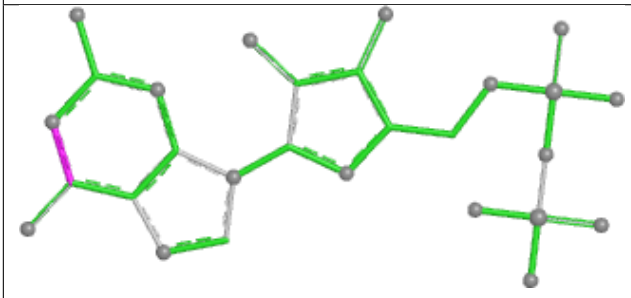
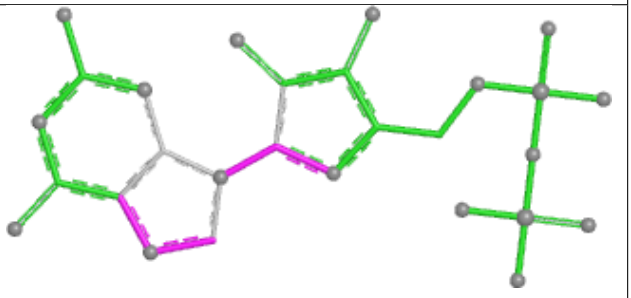
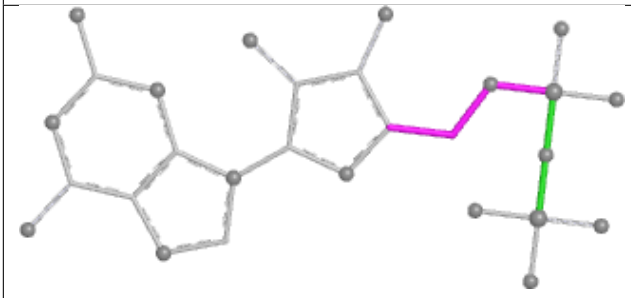
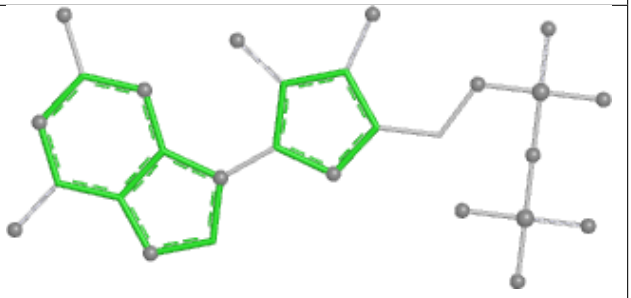


Torsions

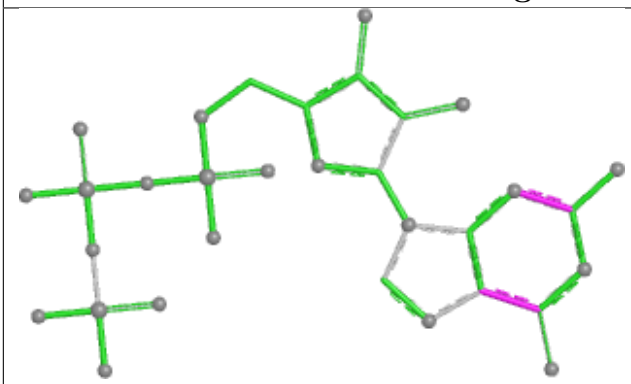


Rings

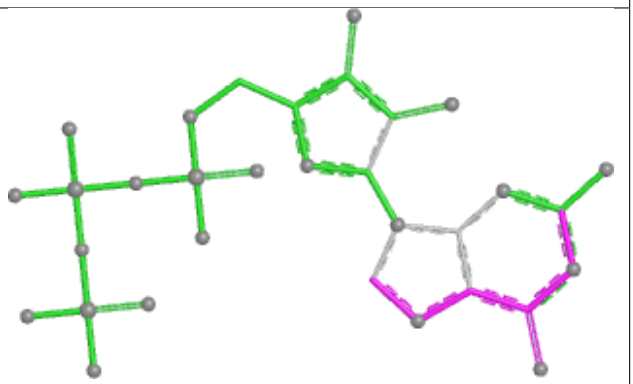
Ligand GDP F1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP P 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

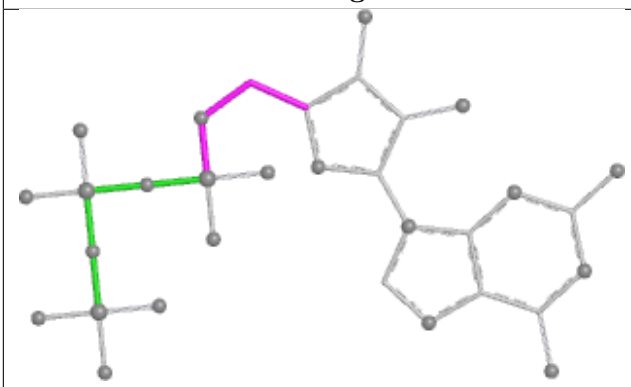
Ligand GTP B4 501



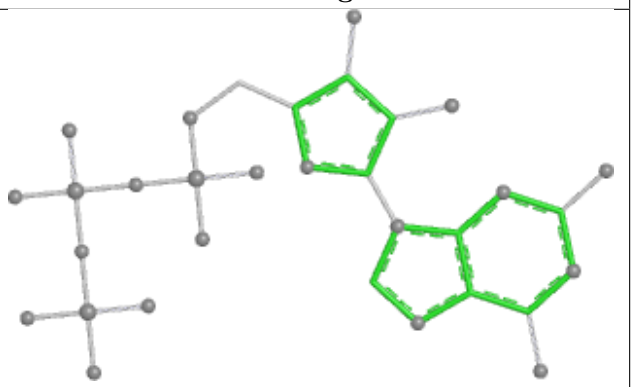
Bond lengths



Bond angles

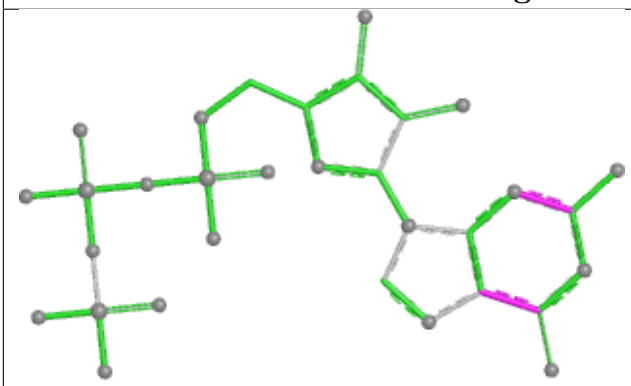


Torsions

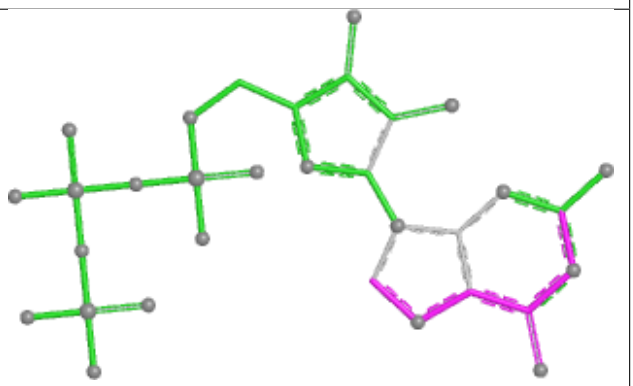


Rings

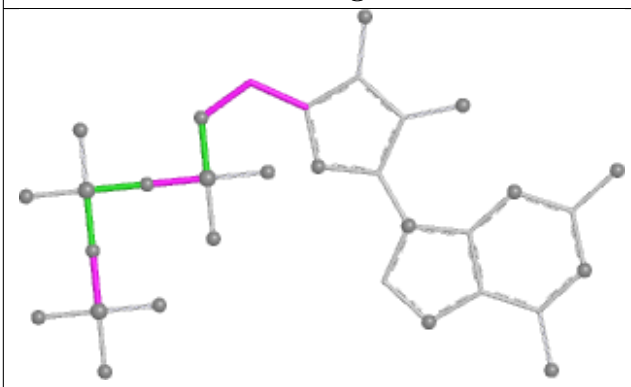
Ligand GTP C6 501



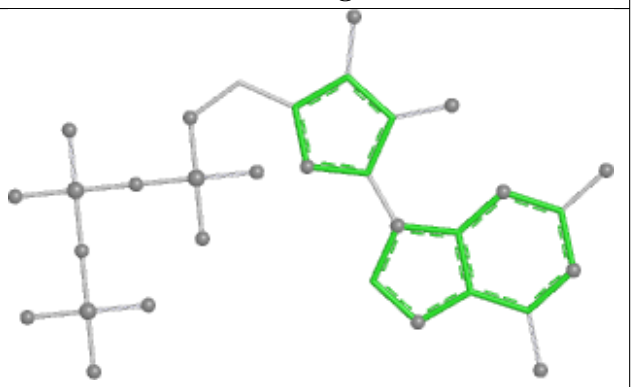
Bond lengths



Bond angles

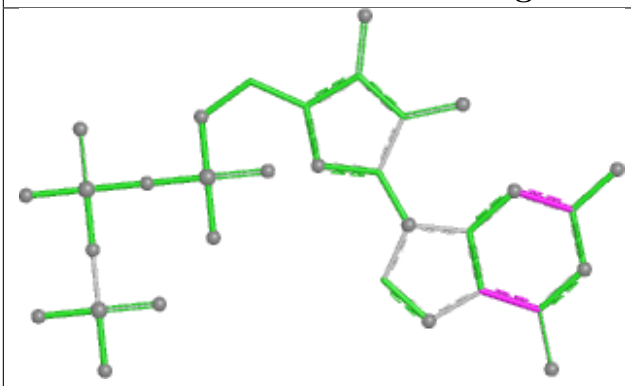


Torsions

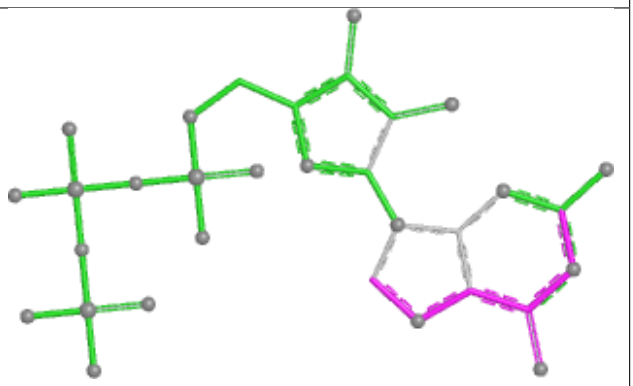


Rings

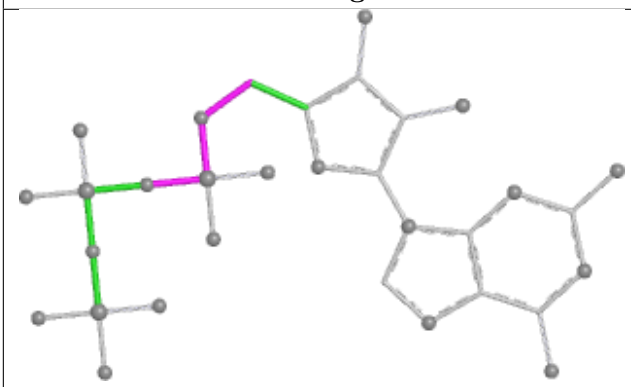
Ligand GTP E2 501



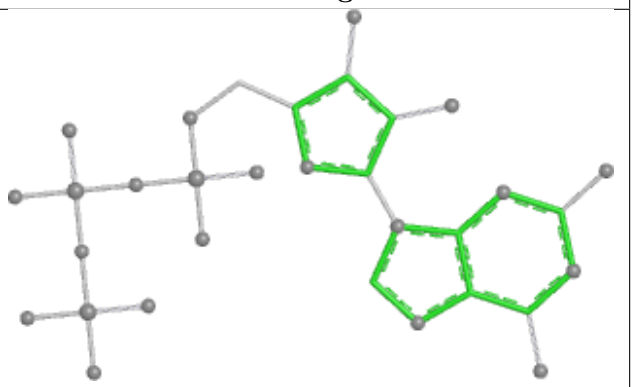
Bond lengths



Bond angles

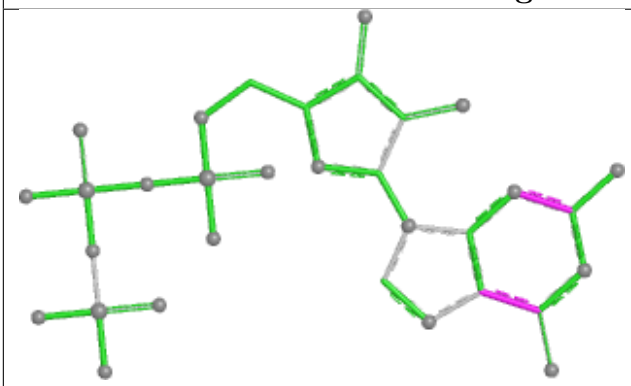


Torsions

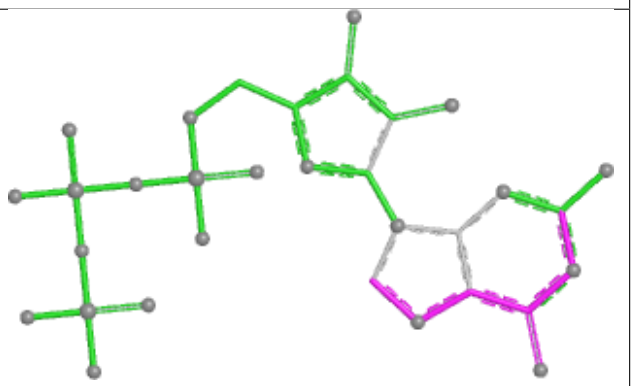


Rings

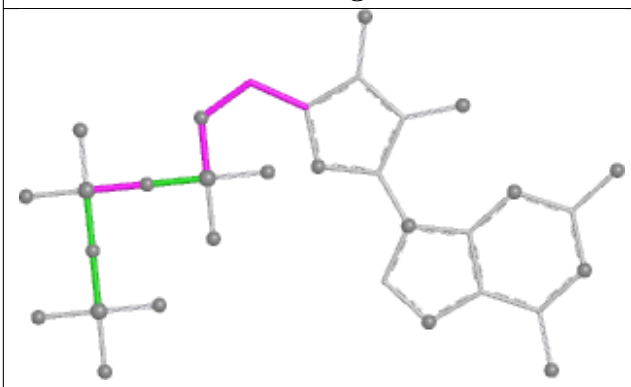
Ligand GTP F0 501



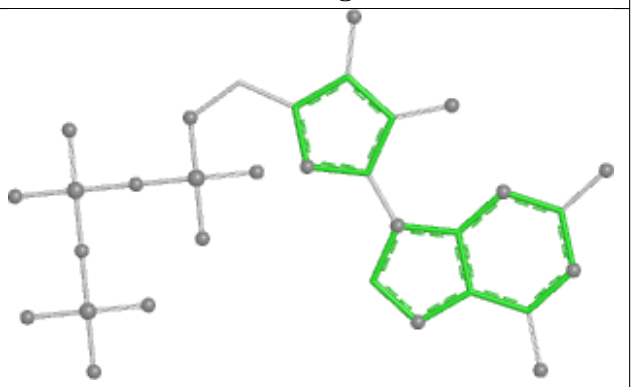
Bond lengths



Bond angles

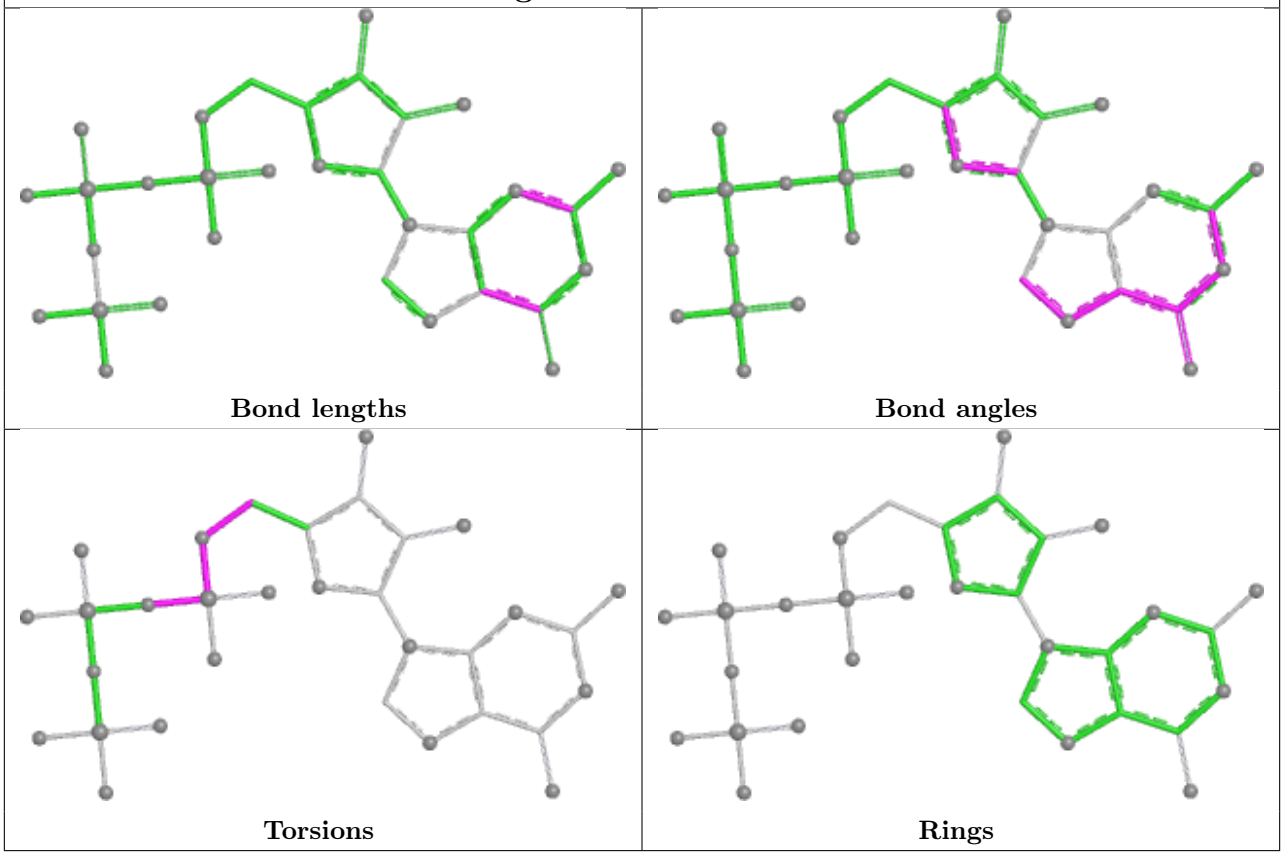


Torsions

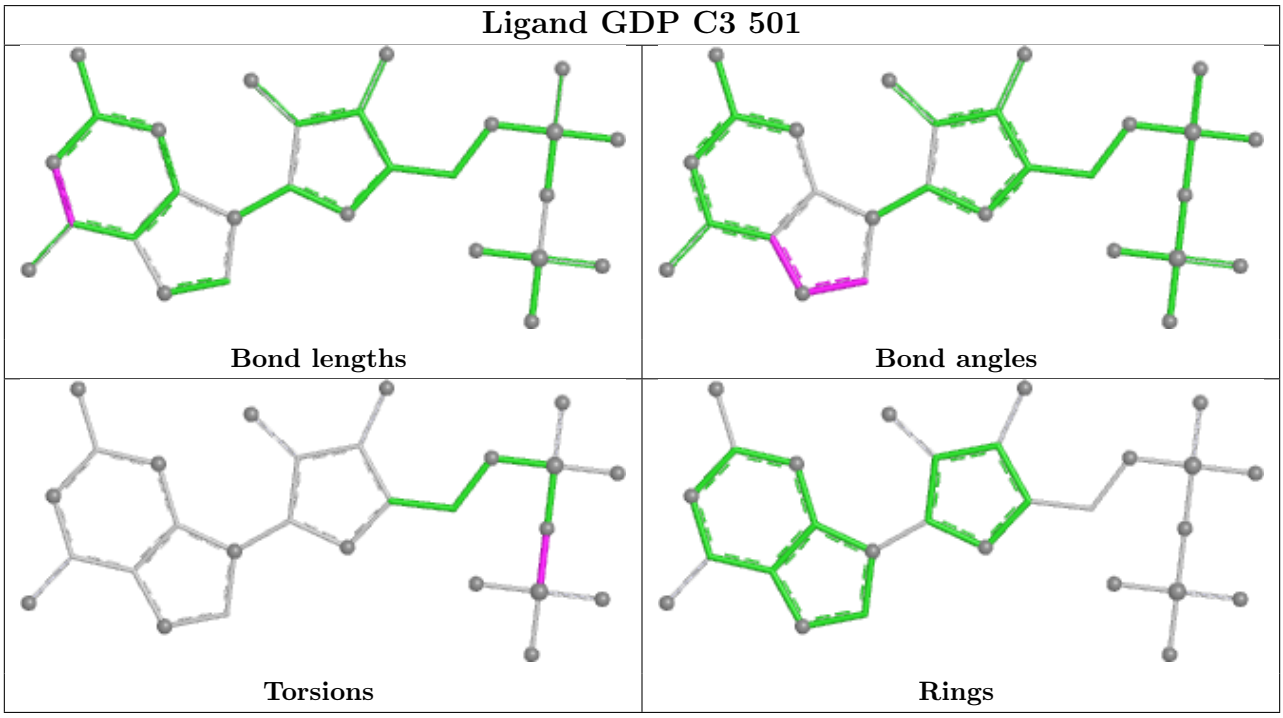


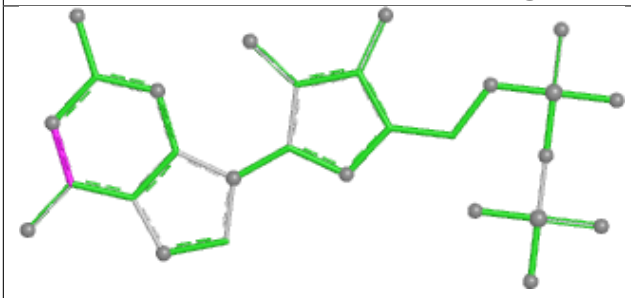
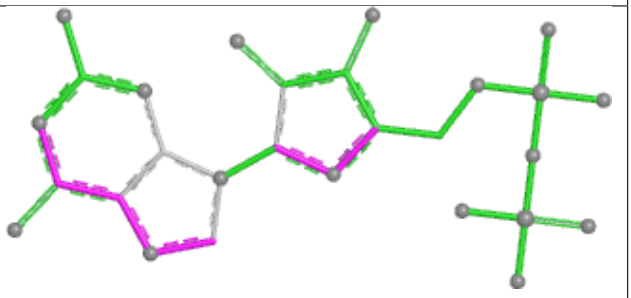
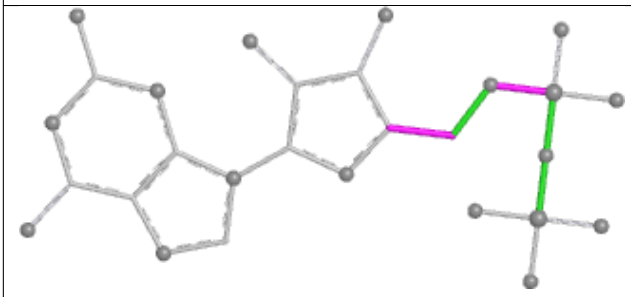
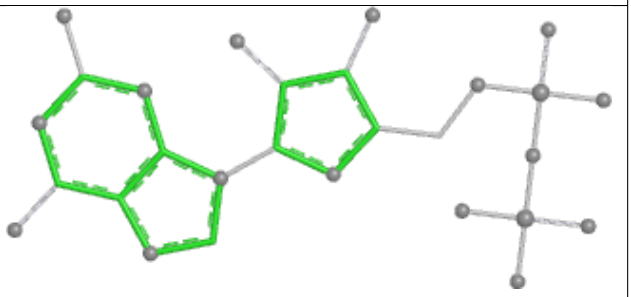
Rings

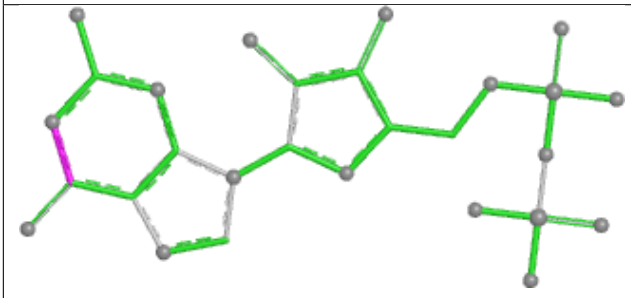
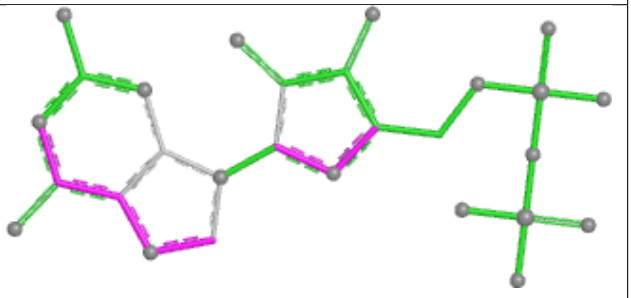
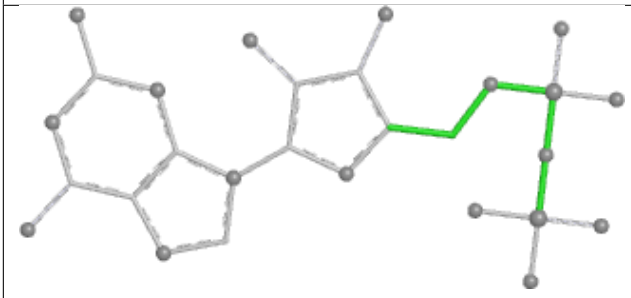
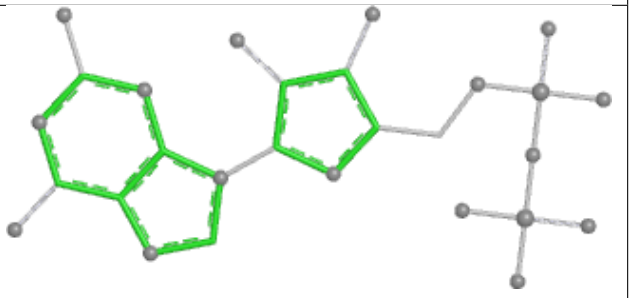
Ligand GTP B6 501

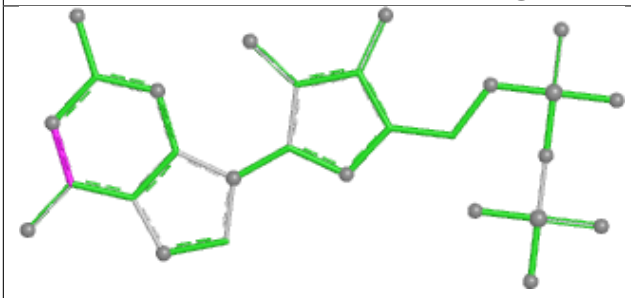
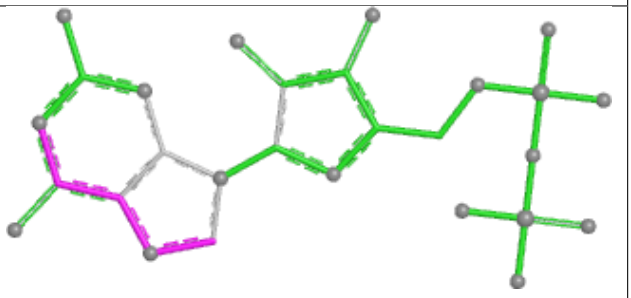
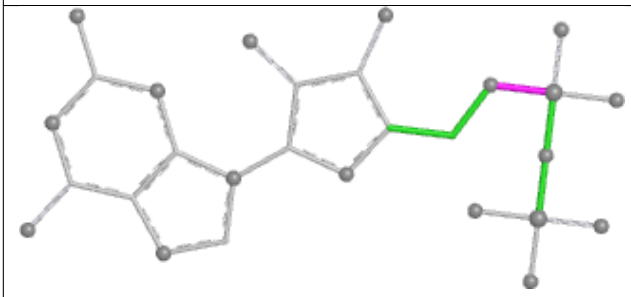
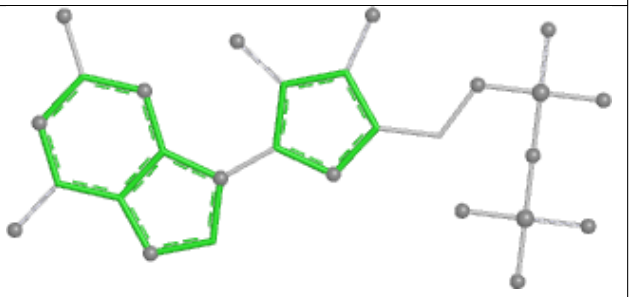


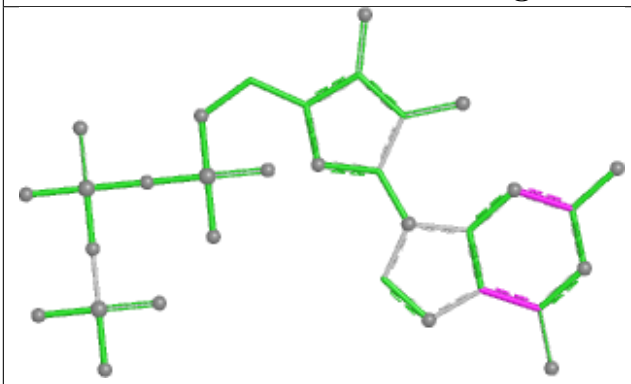
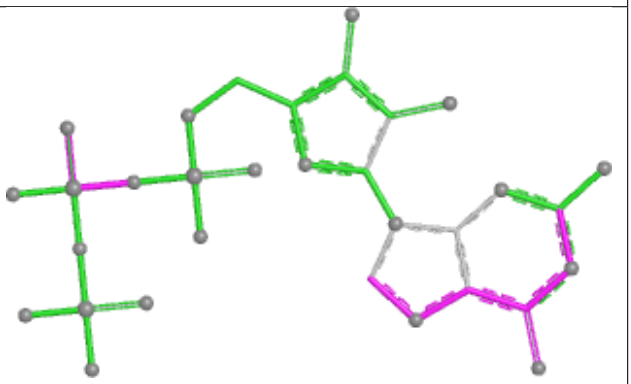
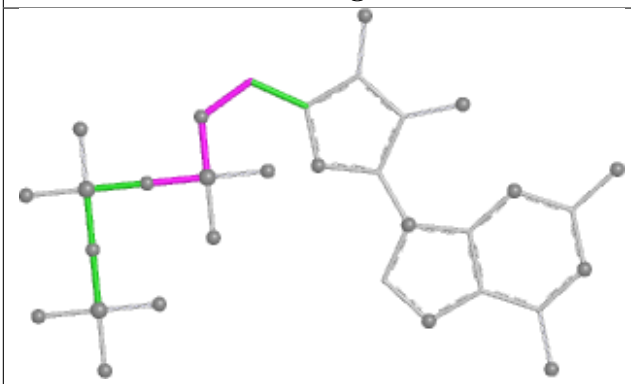
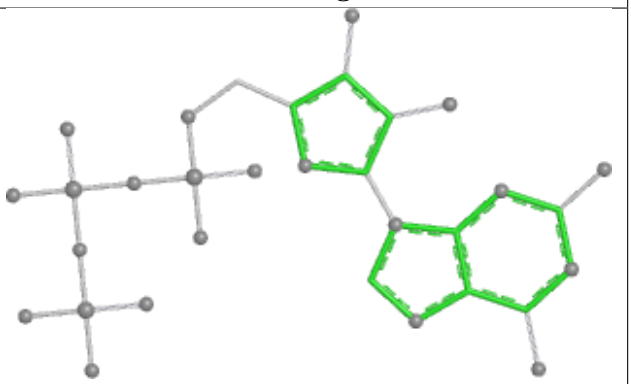
Ligand GDP C3 501



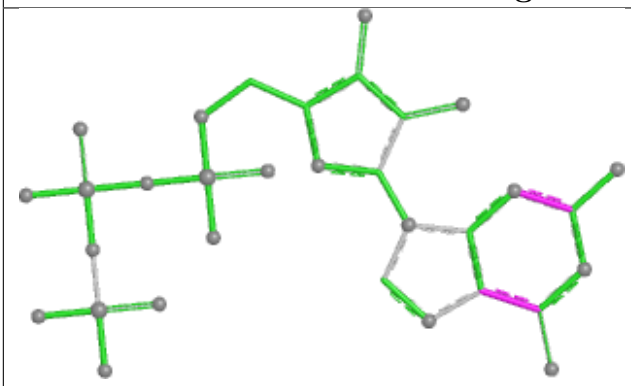
Ligand GDP O 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP E5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

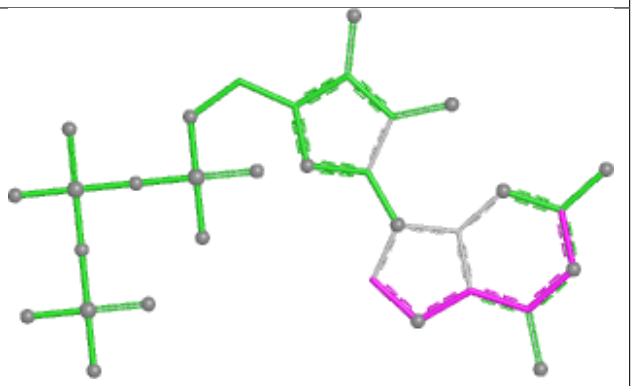
Ligand GDP B7 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GTP A8 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

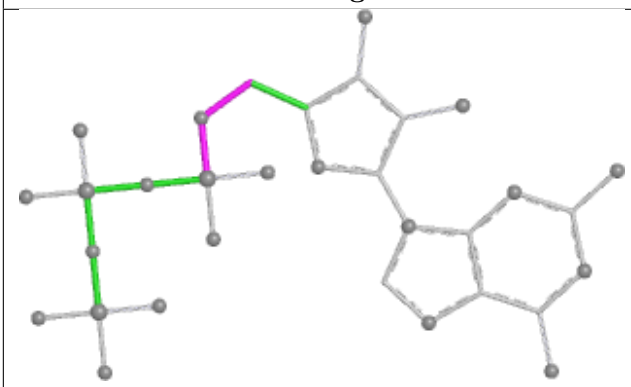
Ligand GTP E0 501



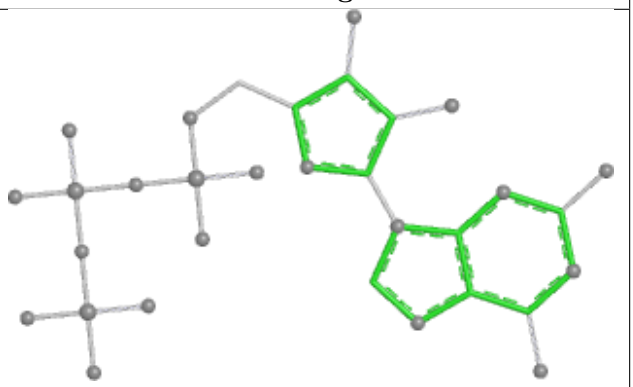
Bond lengths



Bond angles

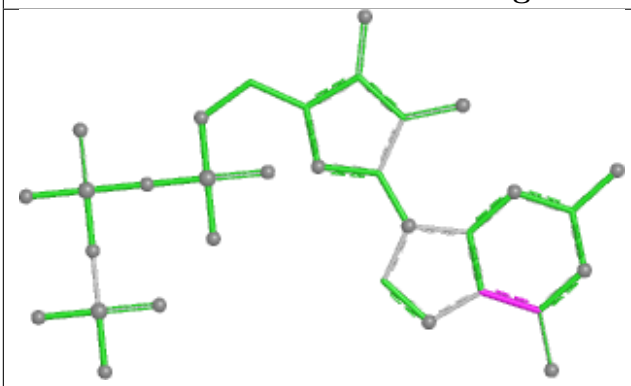


Torsions

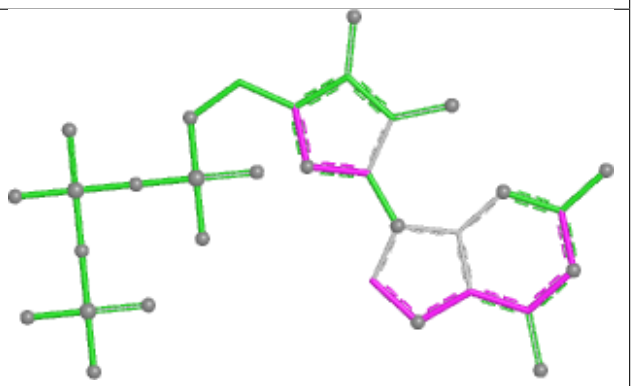


Rings

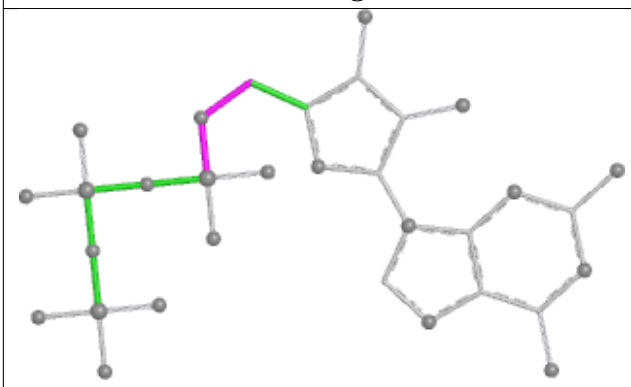
Ligand GTP D0 501



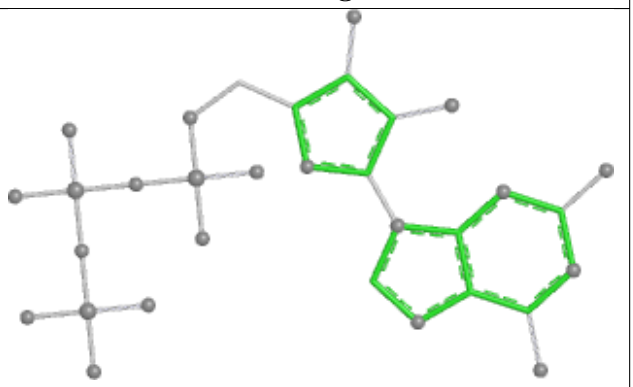
Bond lengths



Bond angles

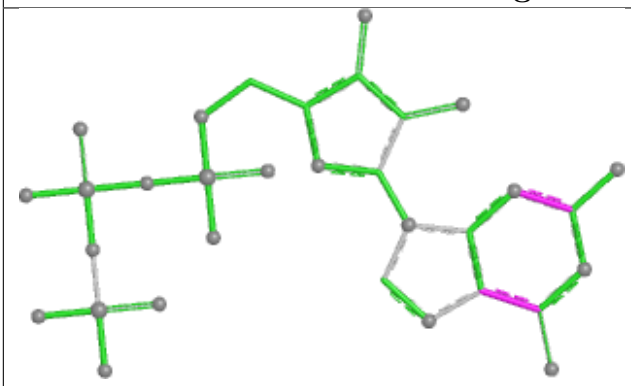


Torsions

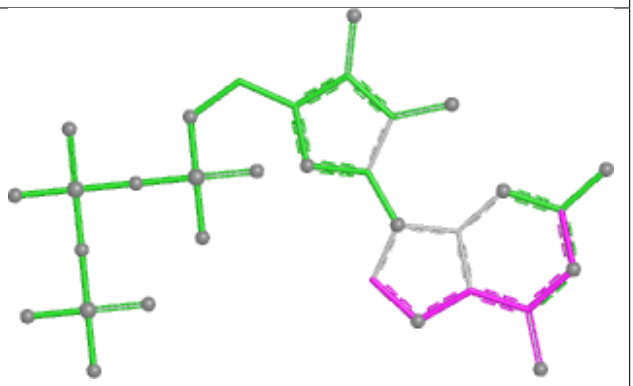


Rings

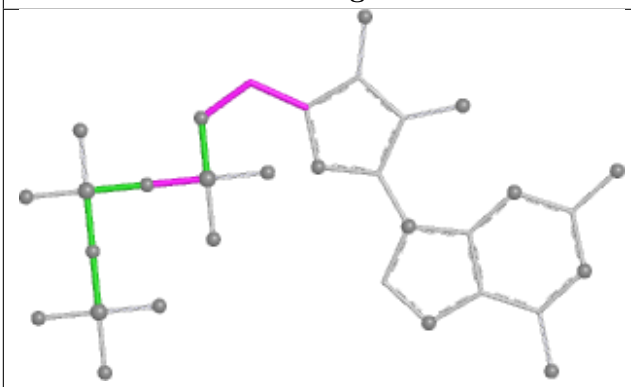
Ligand GTP C4 501



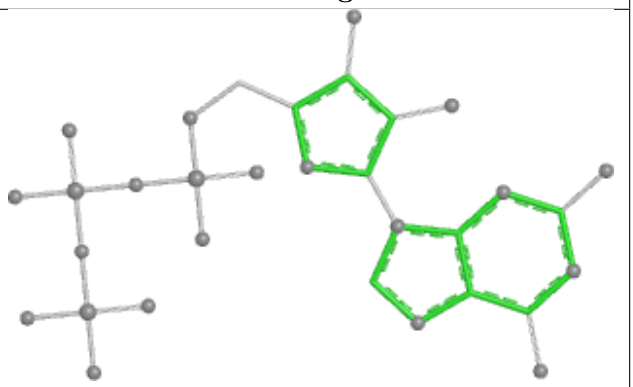
Bond lengths



Bond angles

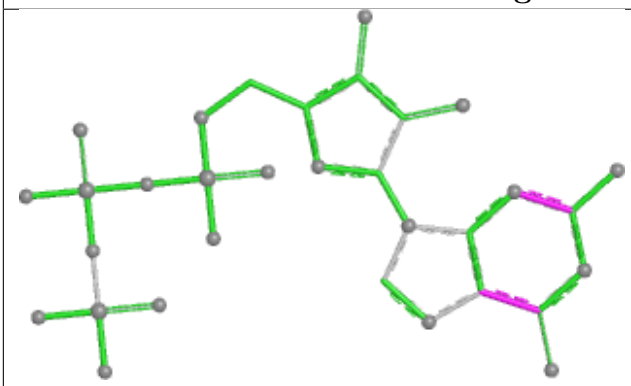


Torsions

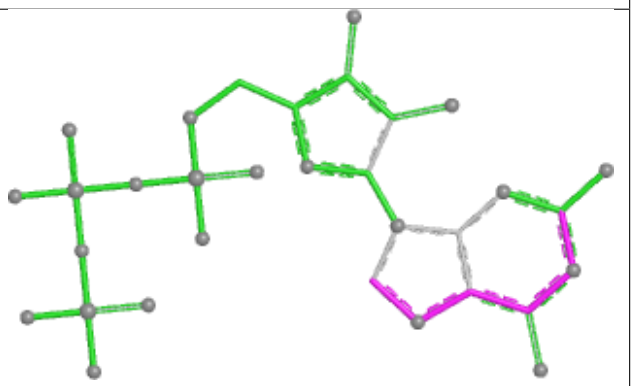


Rings

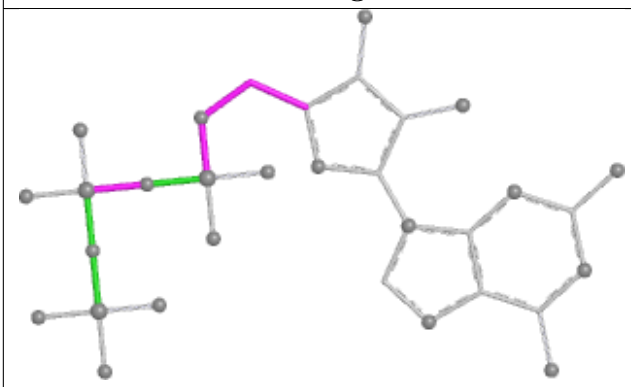
Ligand GTP B0 501



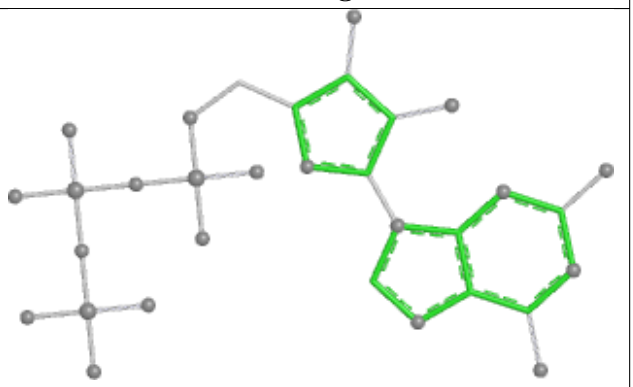
Bond lengths



Bond angles

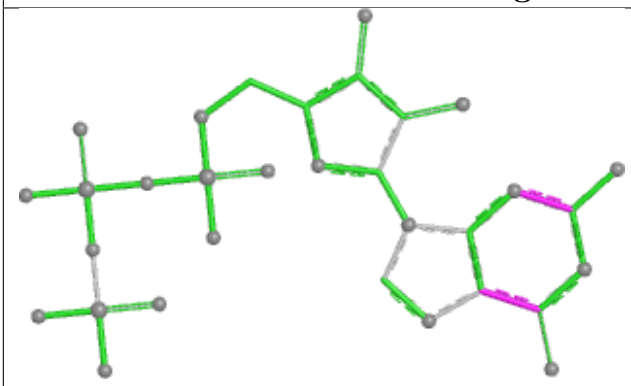


Torsions

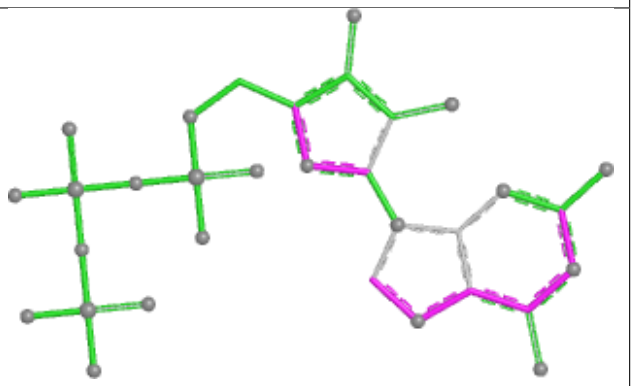


Rings

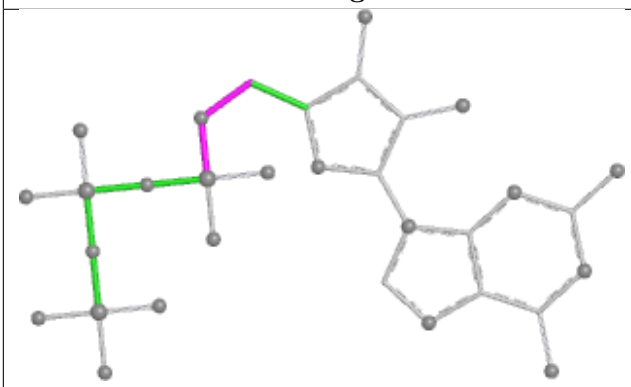
Ligand GTP C8 501



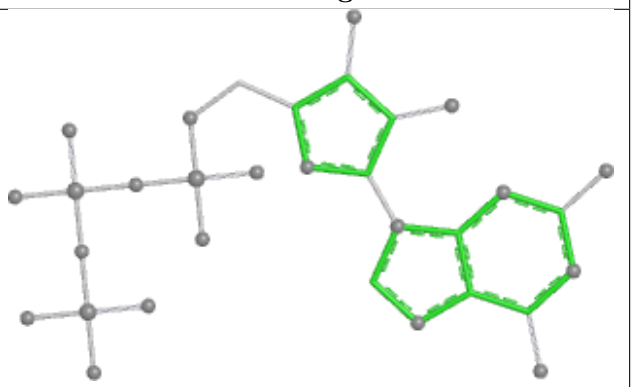
Bond lengths



Bond angles

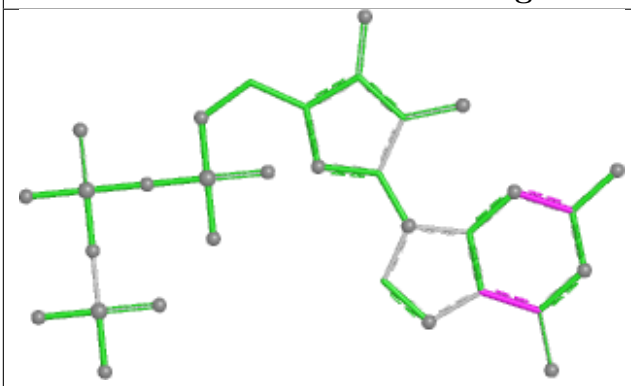


Torsions

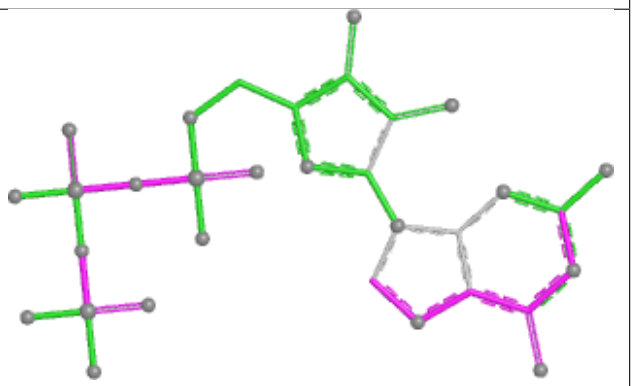


Rings

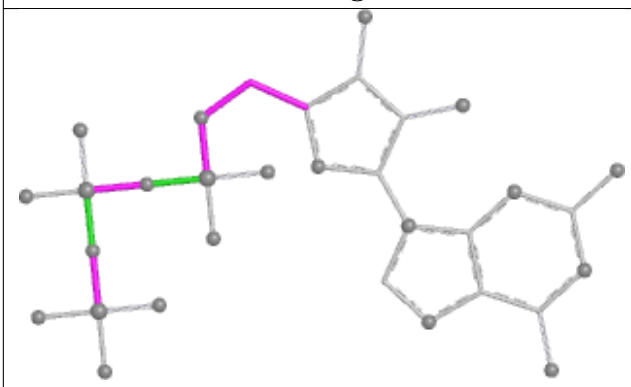
Ligand GTP E4 501



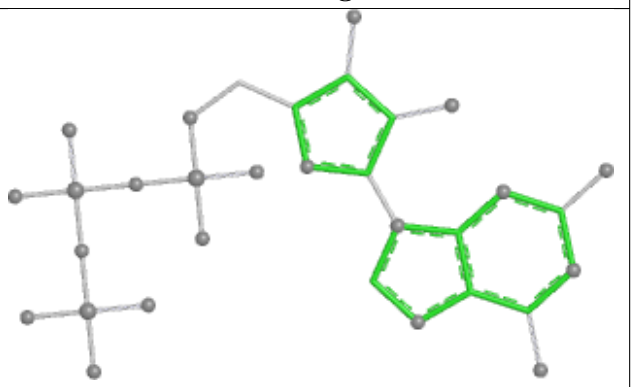
Bond lengths



Bond angles

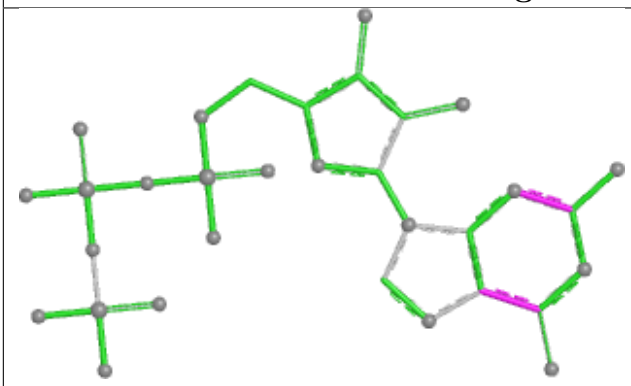


Torsions

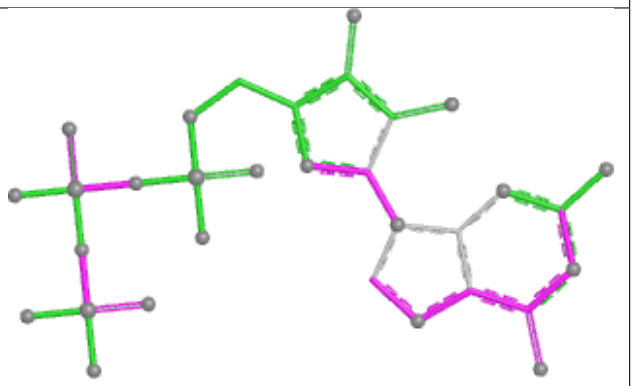


Rings

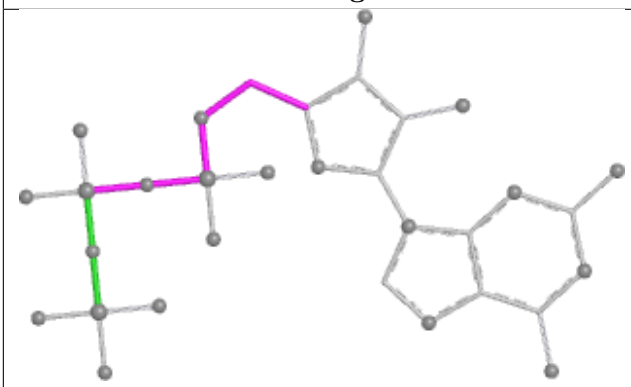
Ligand GTP E7 501



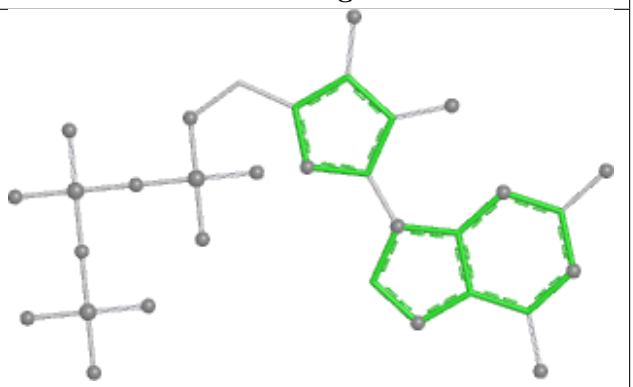
Bond lengths



Bond angles

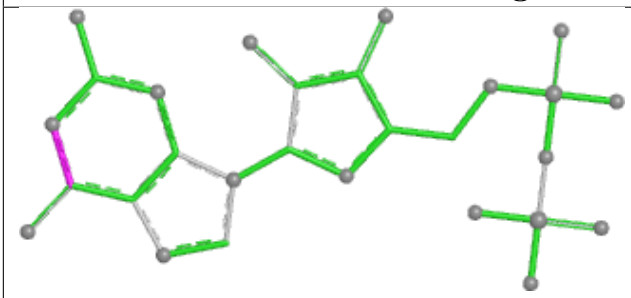


Torsions

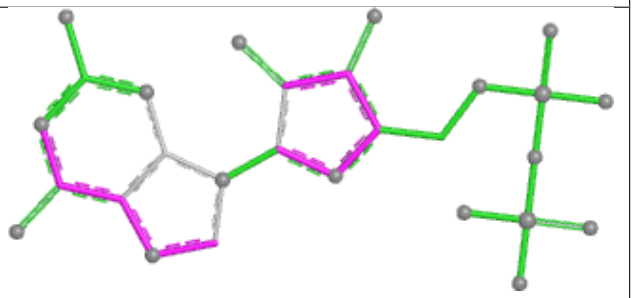


Rings

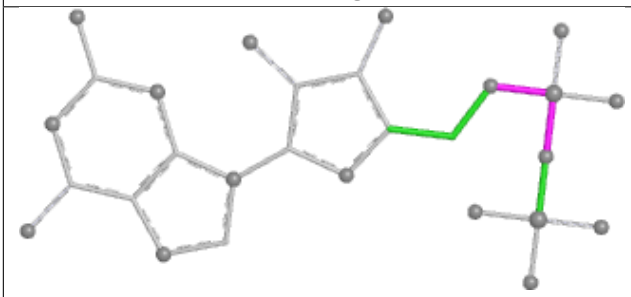
Ligand GDP D3 502



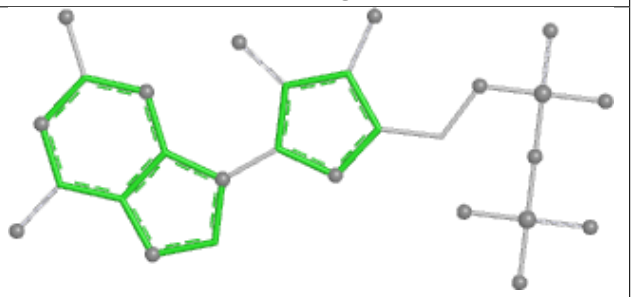
Bond lengths



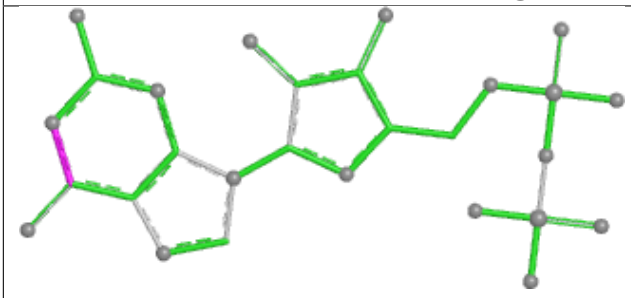
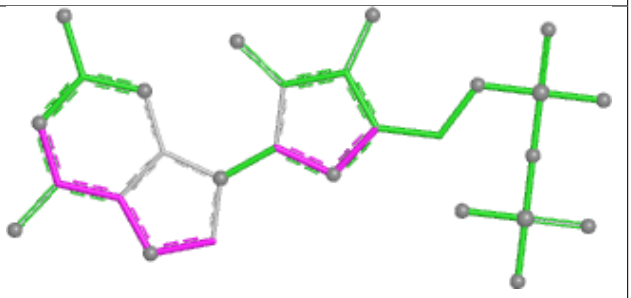
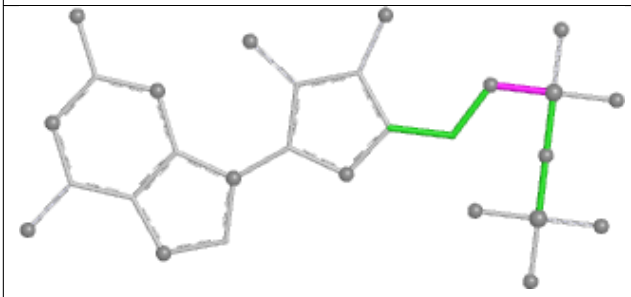
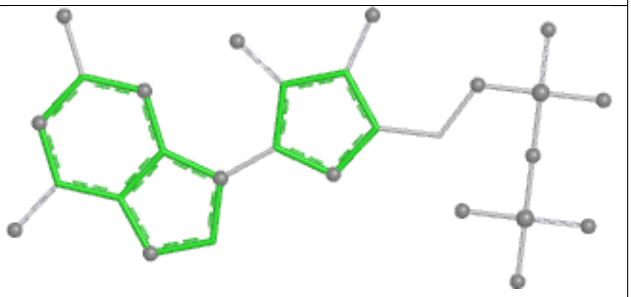
Bond angles

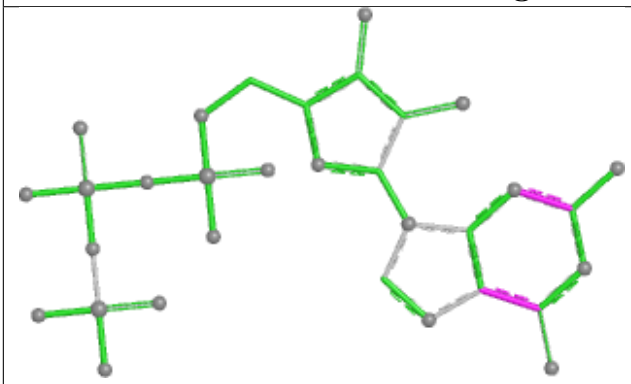
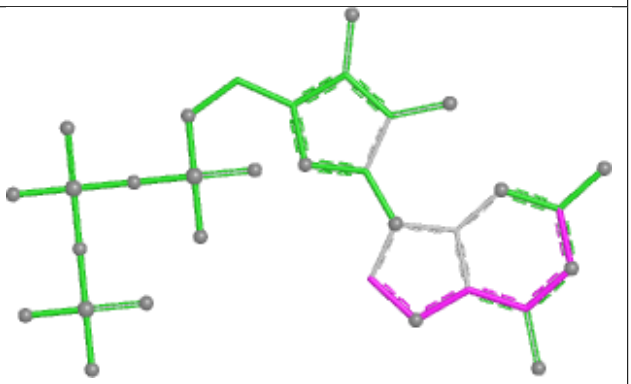
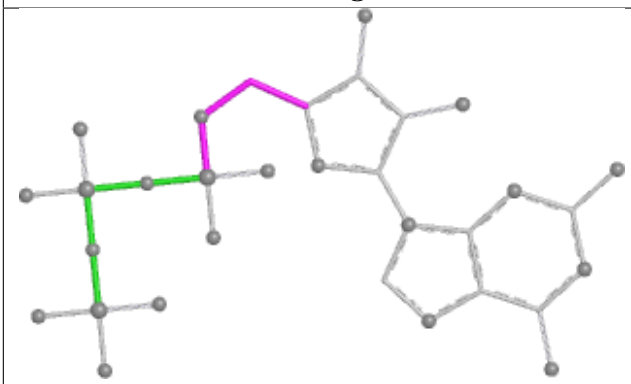
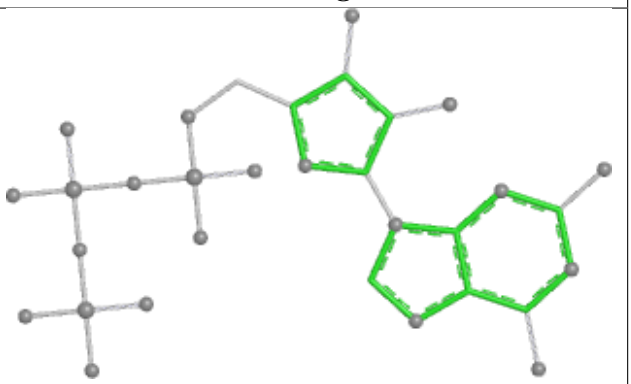


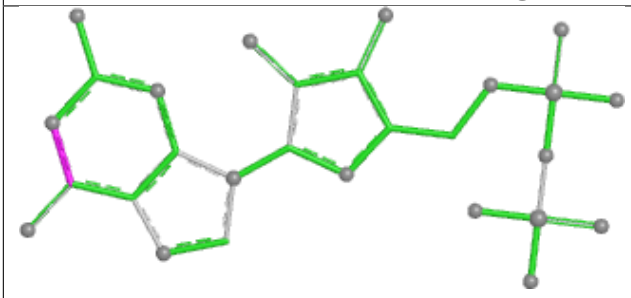
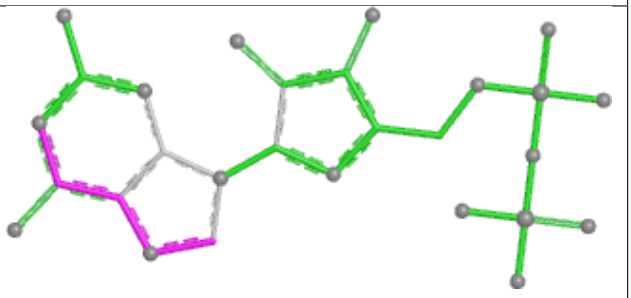
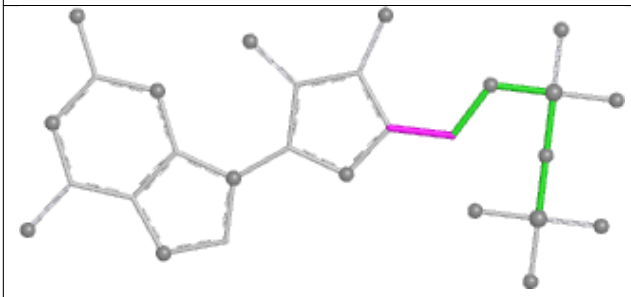
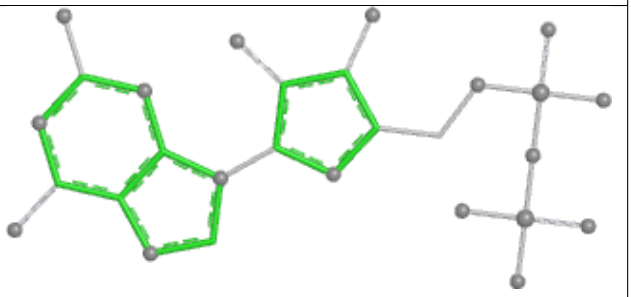
Torsions

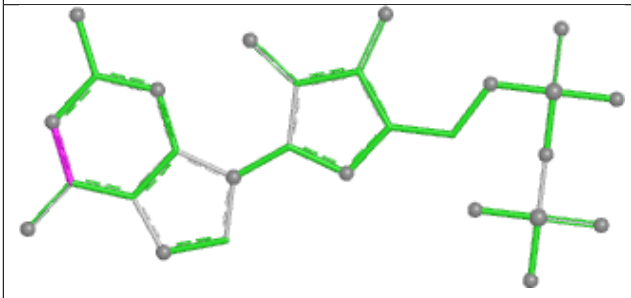
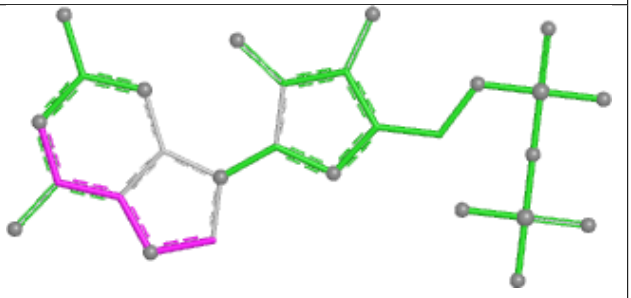
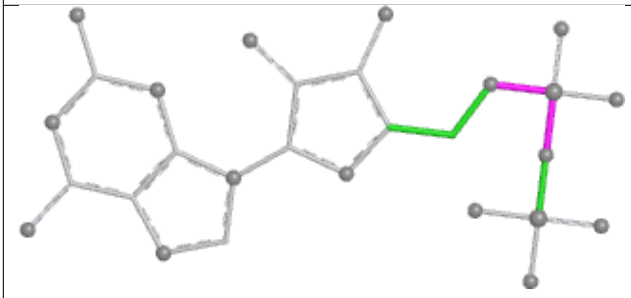
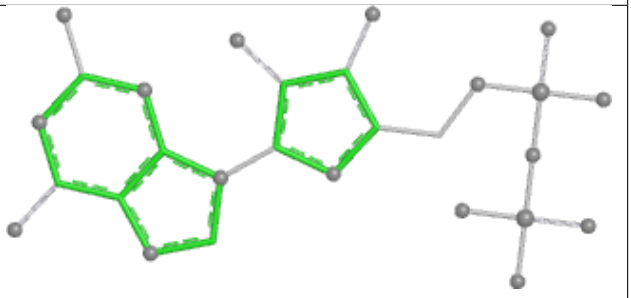


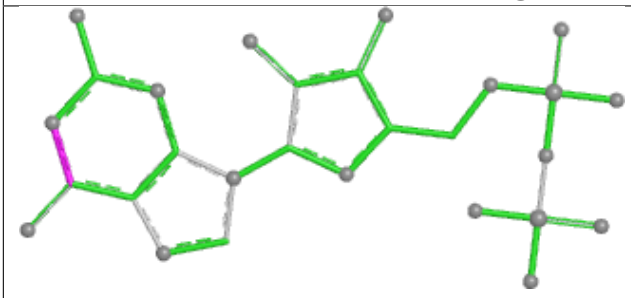
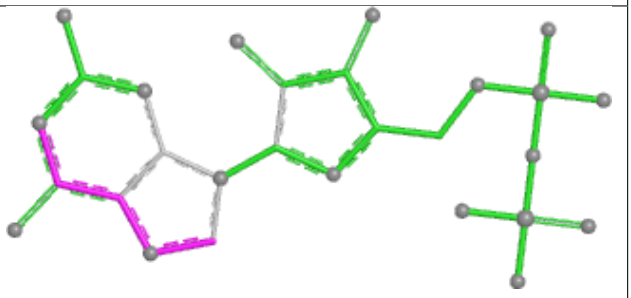
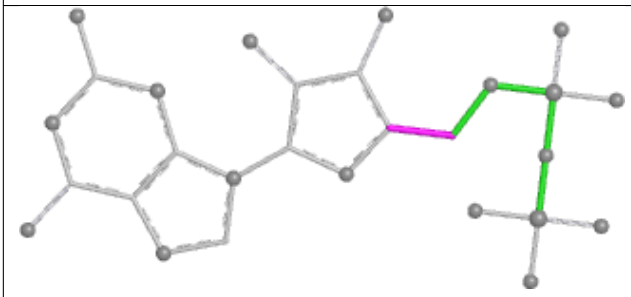
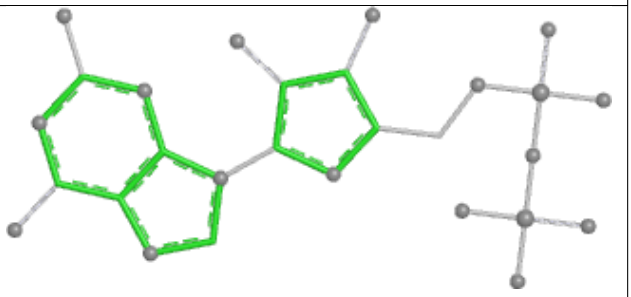
Rings

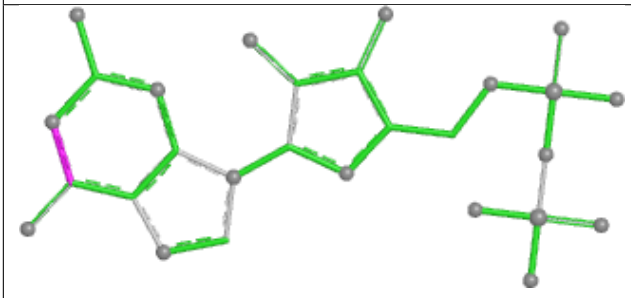
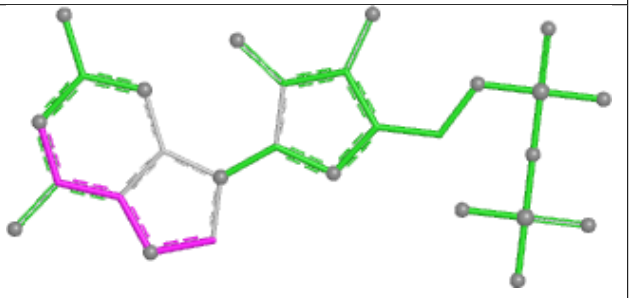
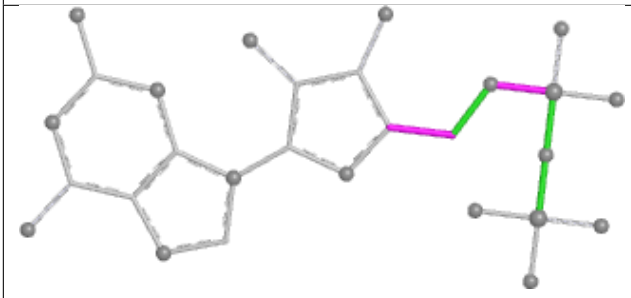
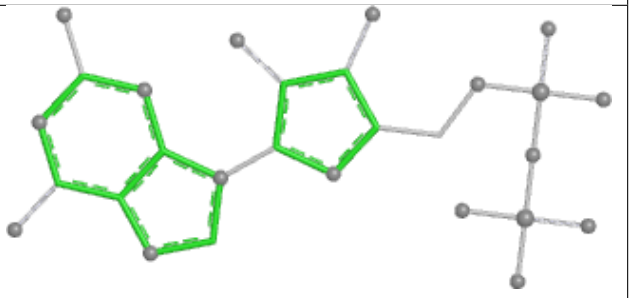
Ligand GDP D9 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

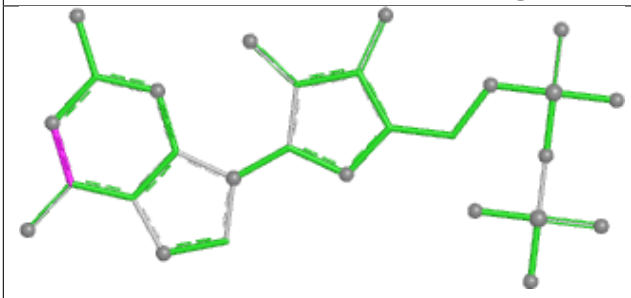
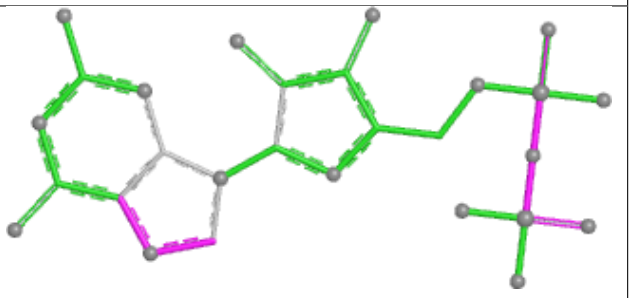
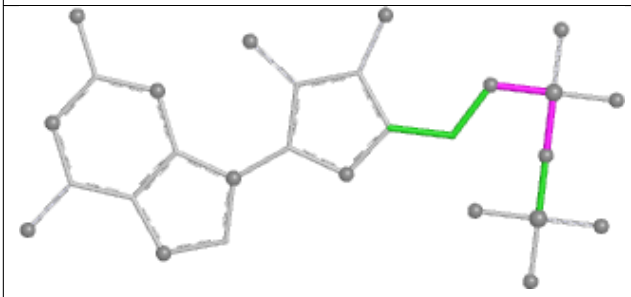
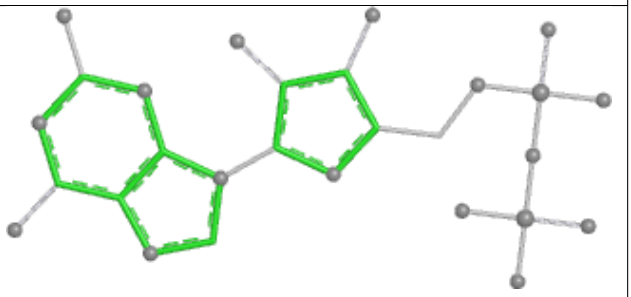
Ligand GTP A6 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

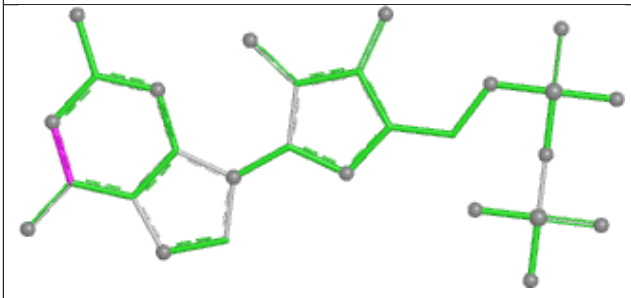
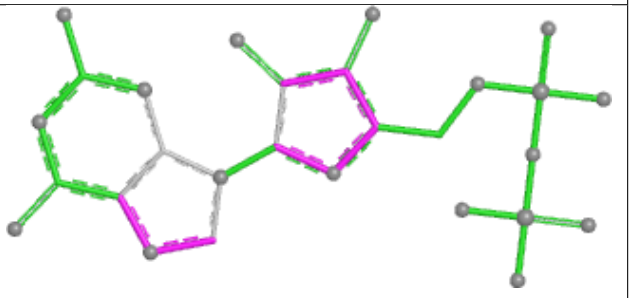
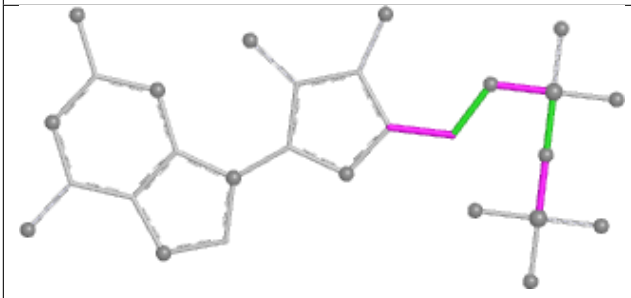
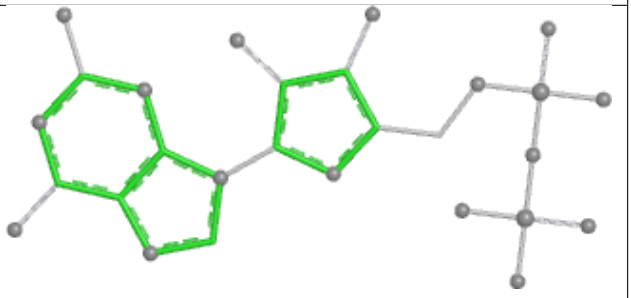
Ligand GDP E7 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

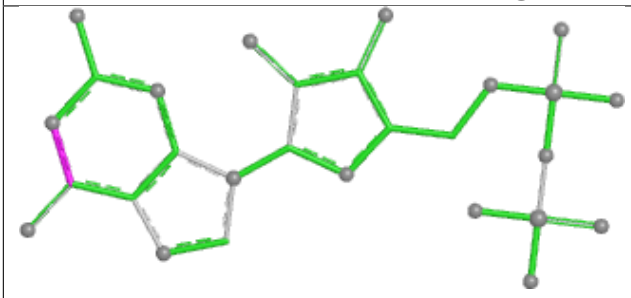
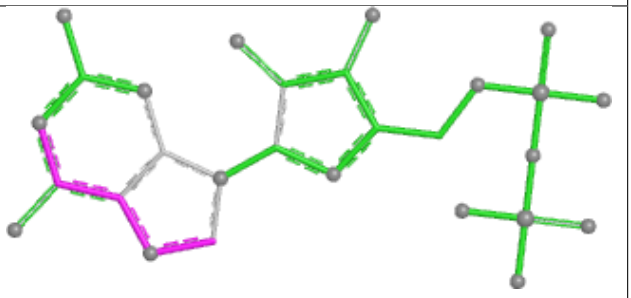
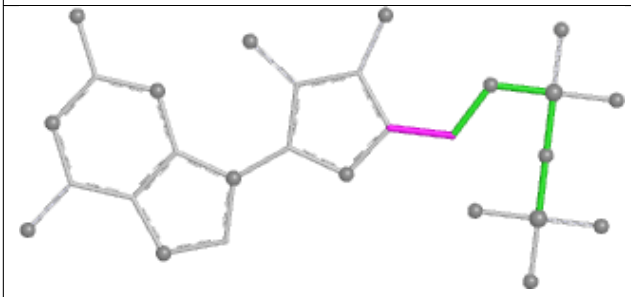
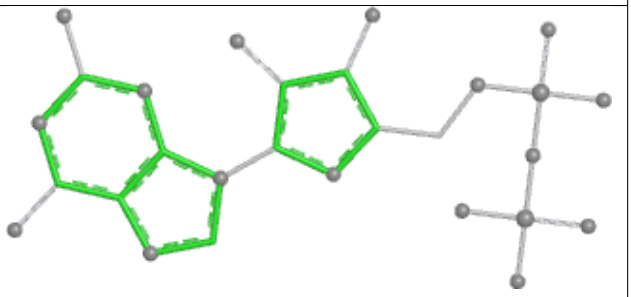
Ligand GDP D7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

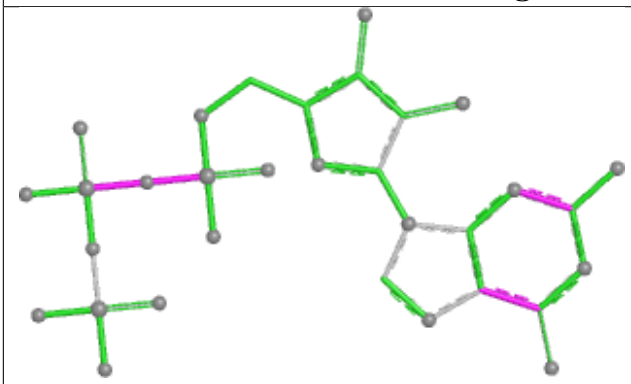
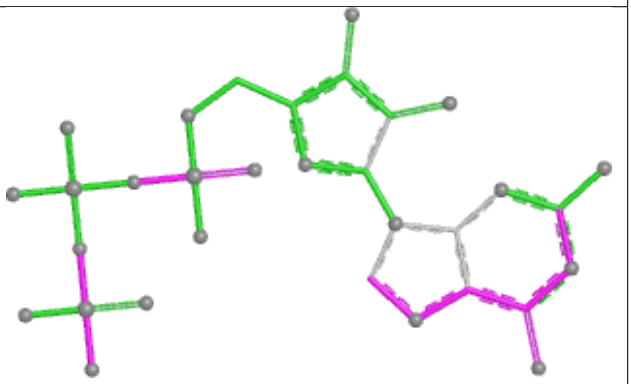
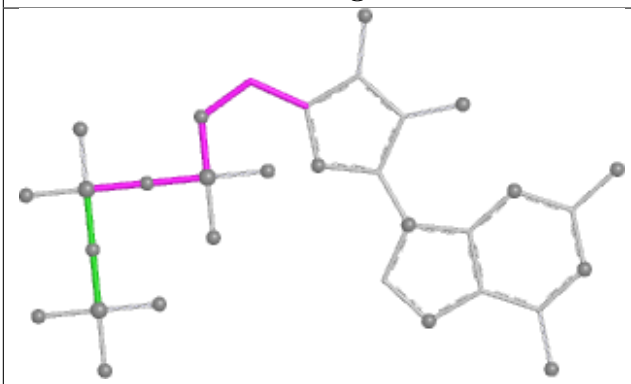
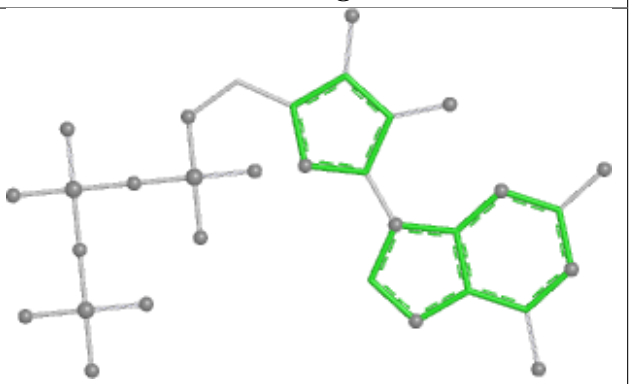
Ligand GDP A5 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP E3 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

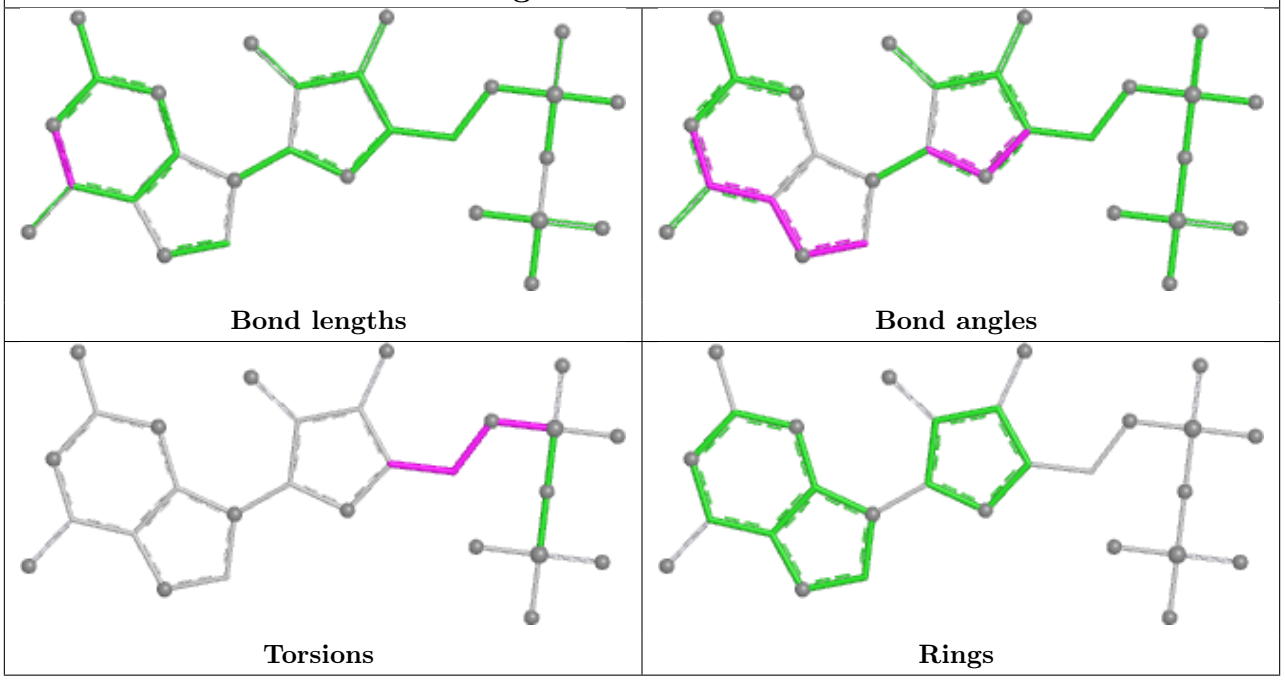
Ligand GDP A1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP A7 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

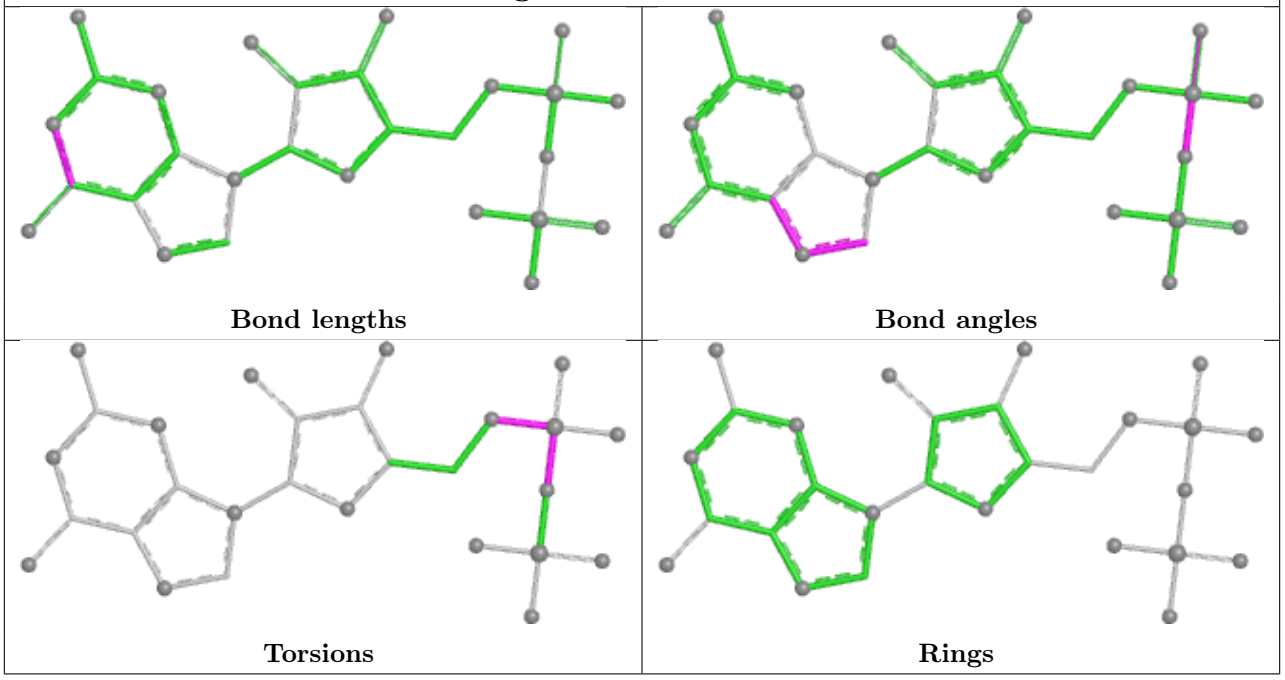
Ligand GDP B5 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GTP C0 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP A3 501



Ligand GDP C7 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.

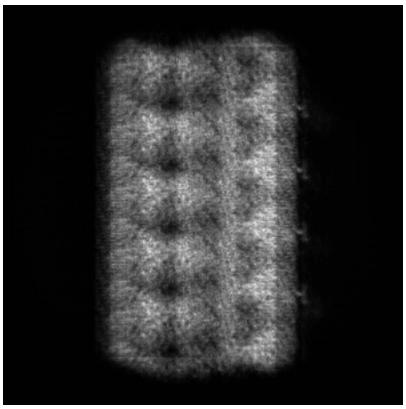
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72717. These allow visual inspection of the internal detail of the map and identification of artifacts.

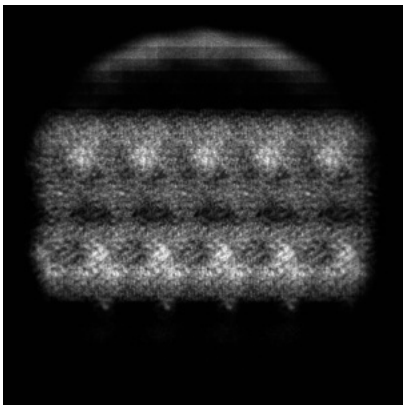
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

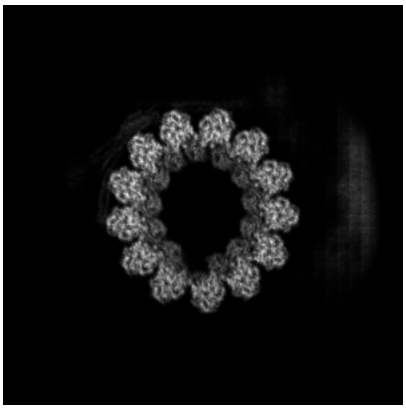
6.1.1 Primary map



X

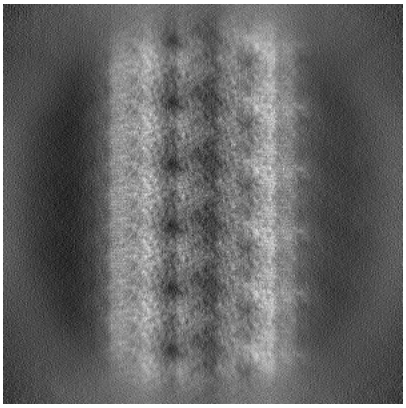


Y

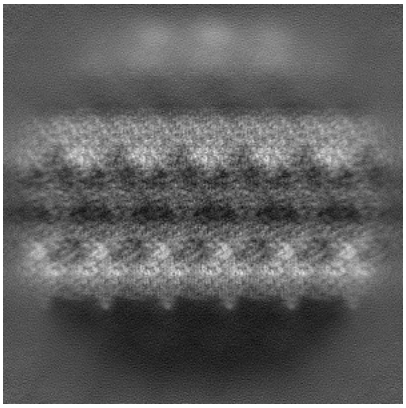


Z

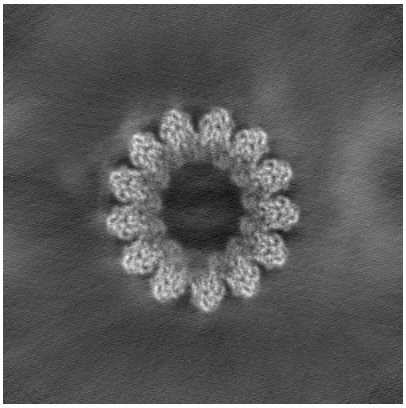
6.1.2 Raw map



X



Y

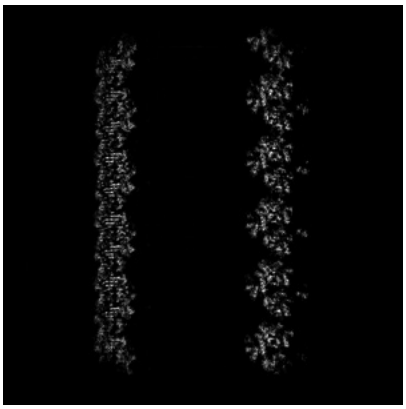


Z

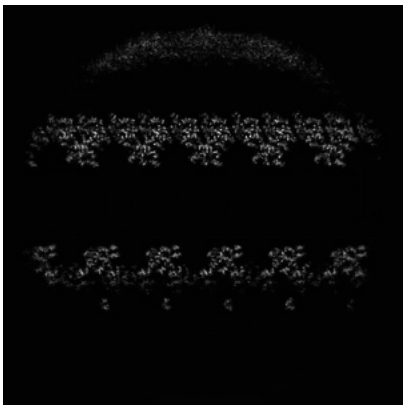
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

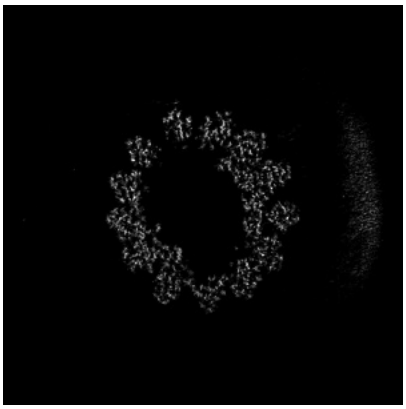
6.2.1 Primary map



X Index: 200

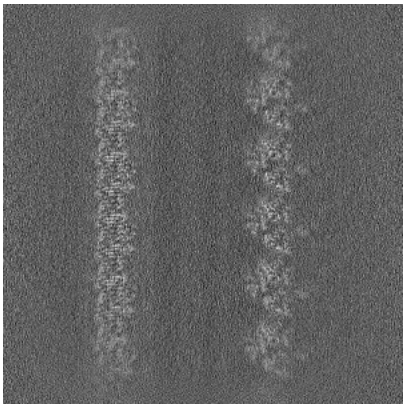


Y Index: 200

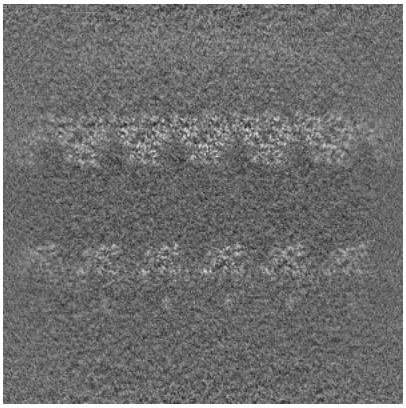


Z Index: 200

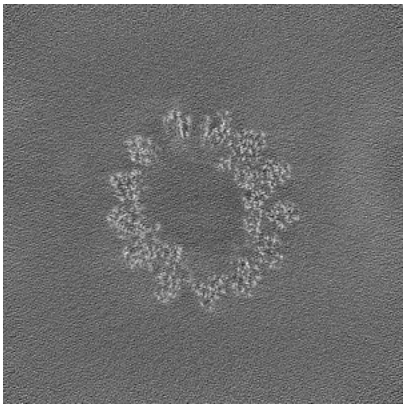
6.2.2 Raw map



X Index: 200



Y Index: 200

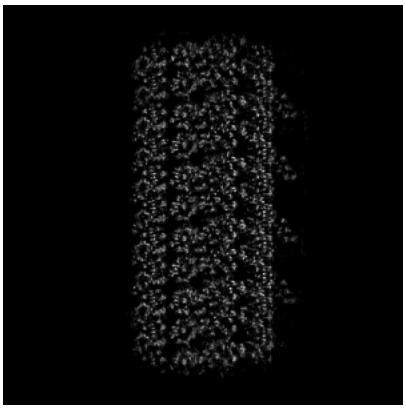


Z Index: 200

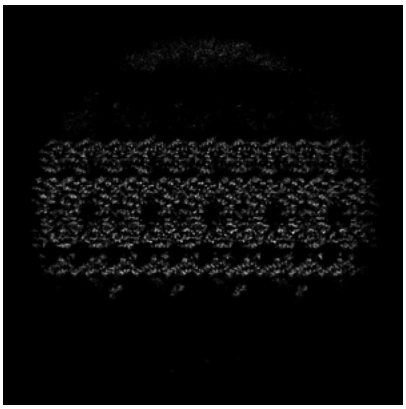
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

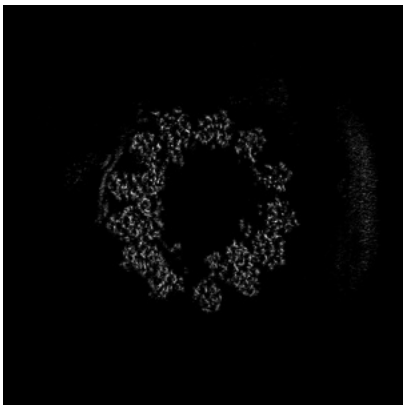
6.3.1 Primary map



X Index: 133

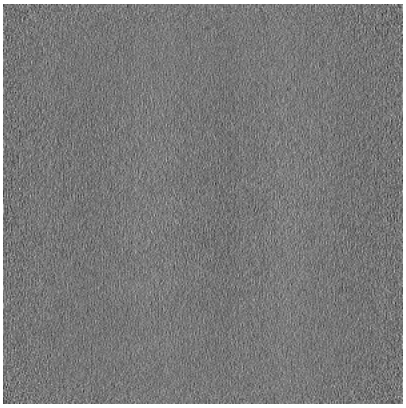


Y Index: 267

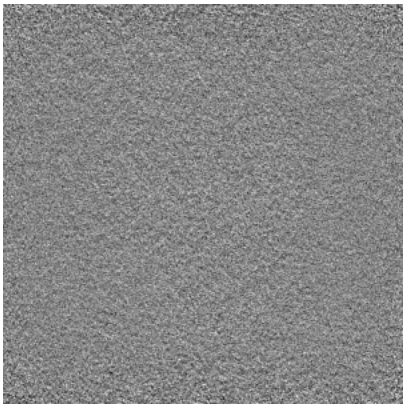


Z Index: 223

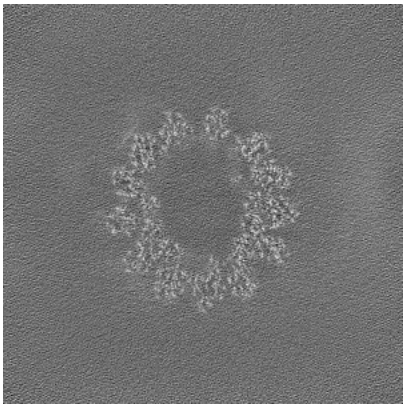
6.3.2 Raw map



X Index: 0



Y Index: 0

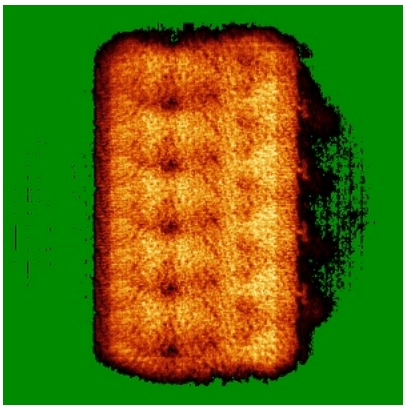


Z Index: 211

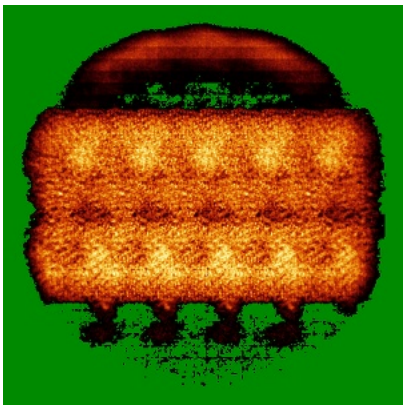
The images above show the largest variance slices of the map in three orthogonal directions.

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

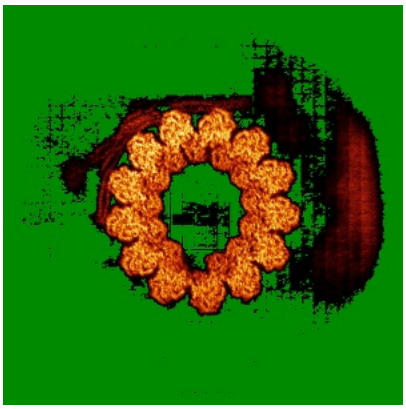
6.4.1 Primary map



X

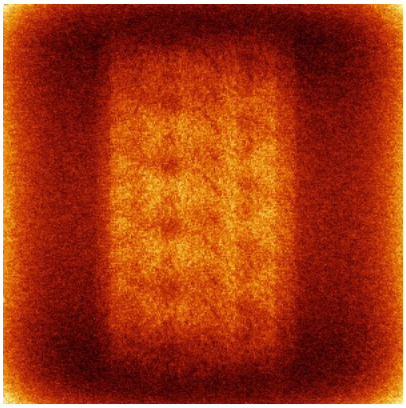


Y

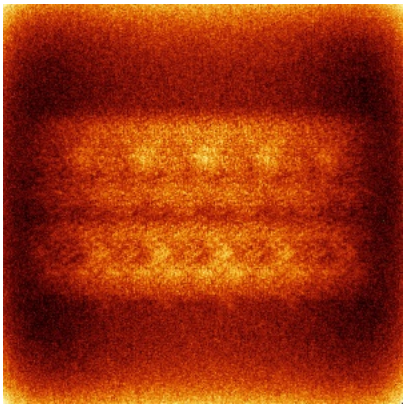


Z

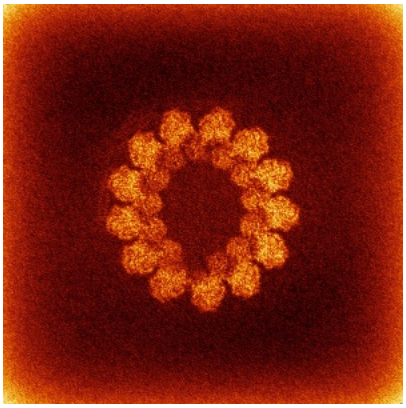
6.4.2 Raw map



X



Y

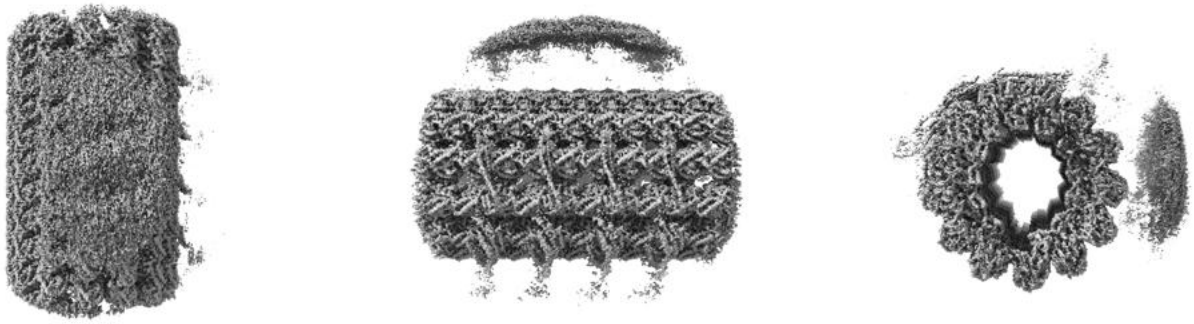


Z

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)

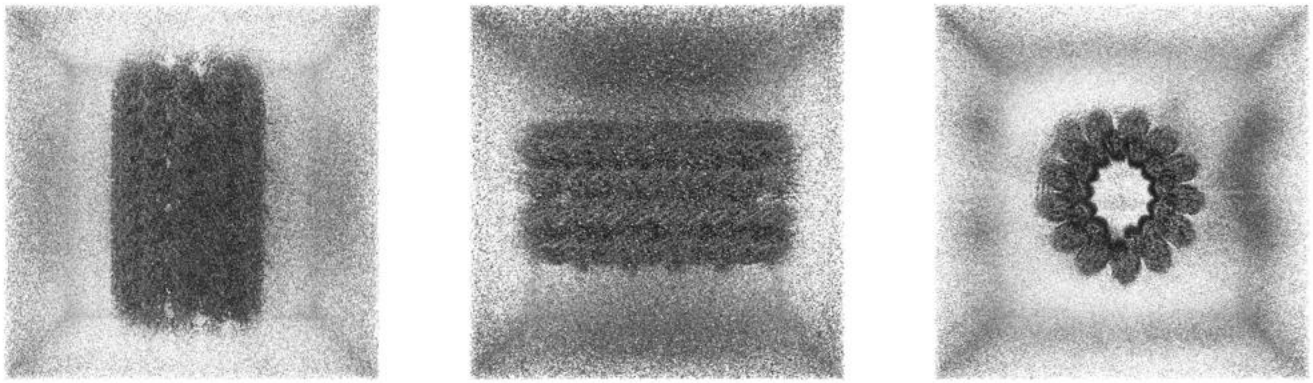
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

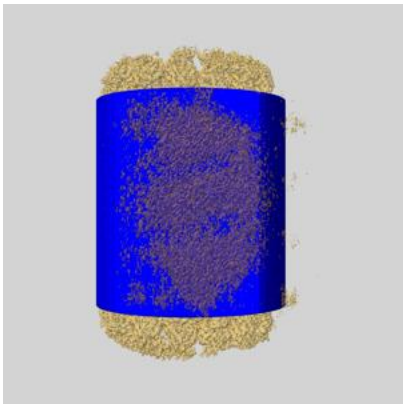
6.6 Mask visualisation (i)

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

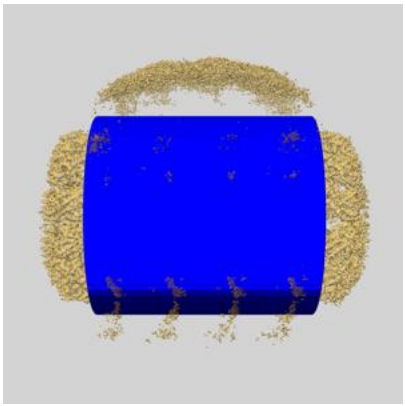
A mask typically either:

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

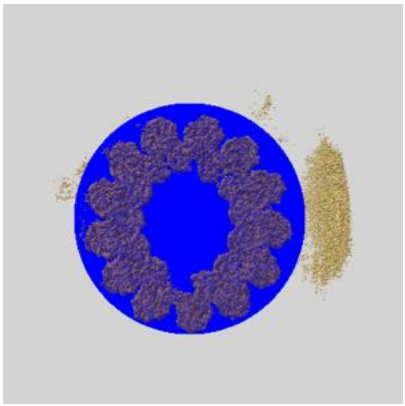
6.6.1 emd_72717_msk_1.map (i)



X



Y

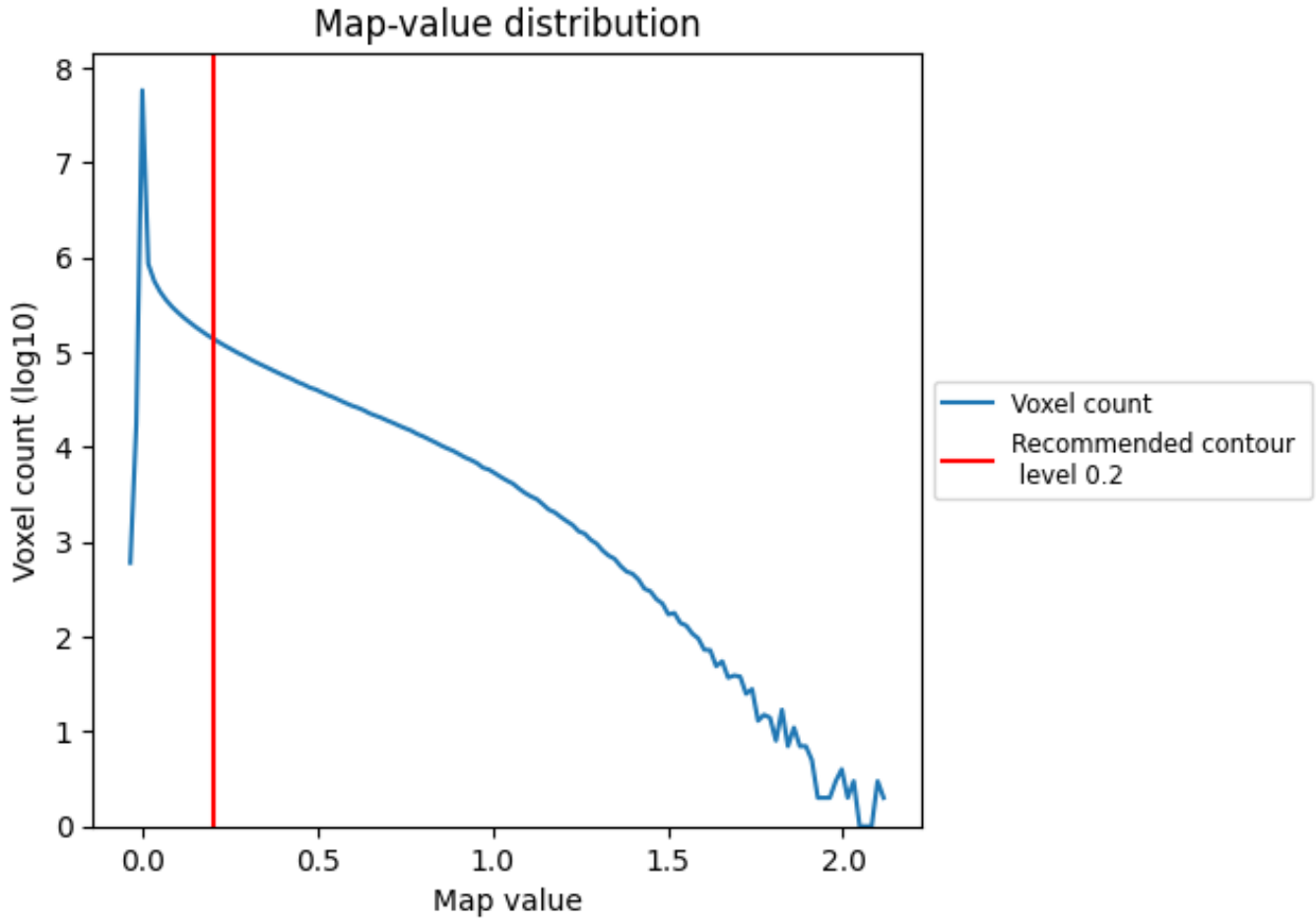


Z

7 Map analysis

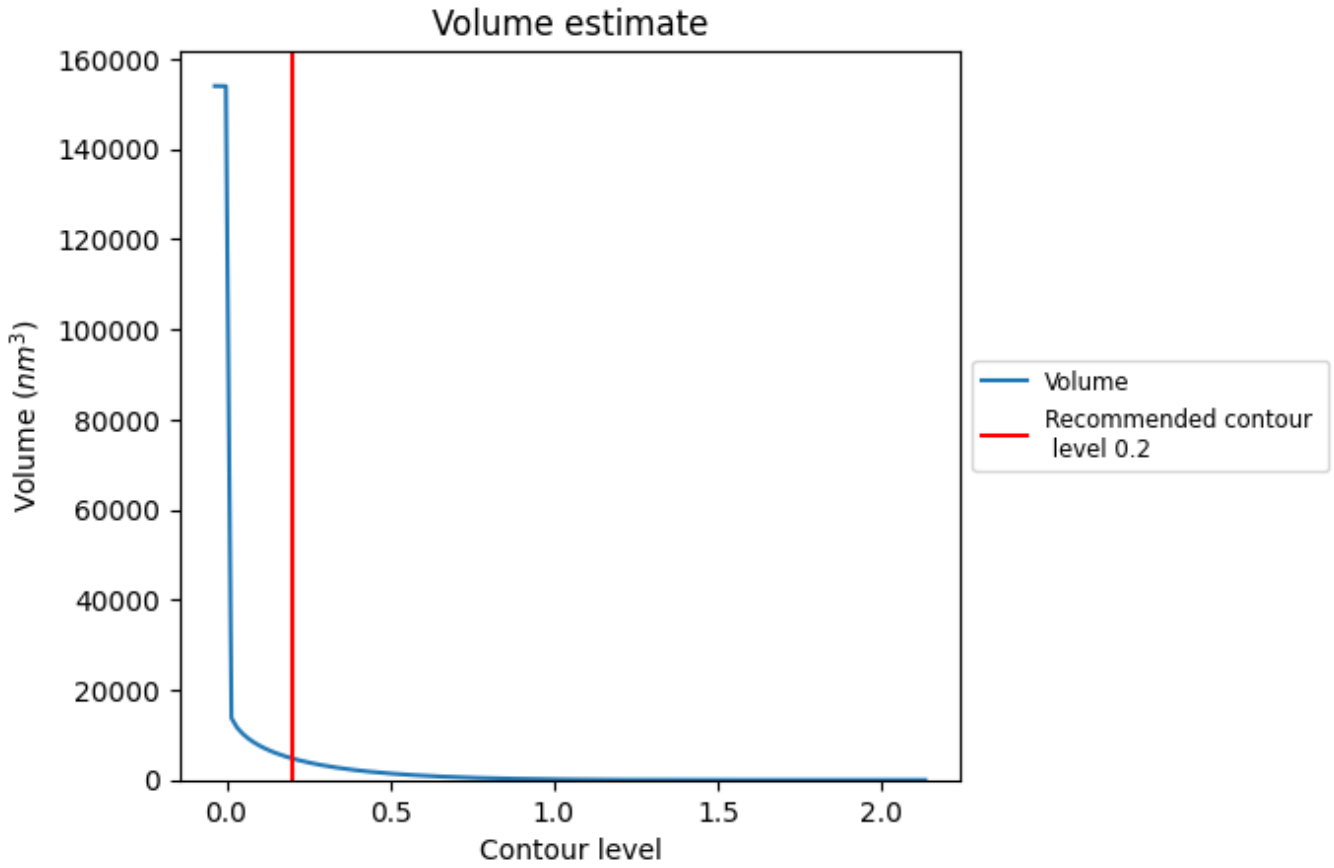
This section contains the results of statistical analysis of the map.

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.

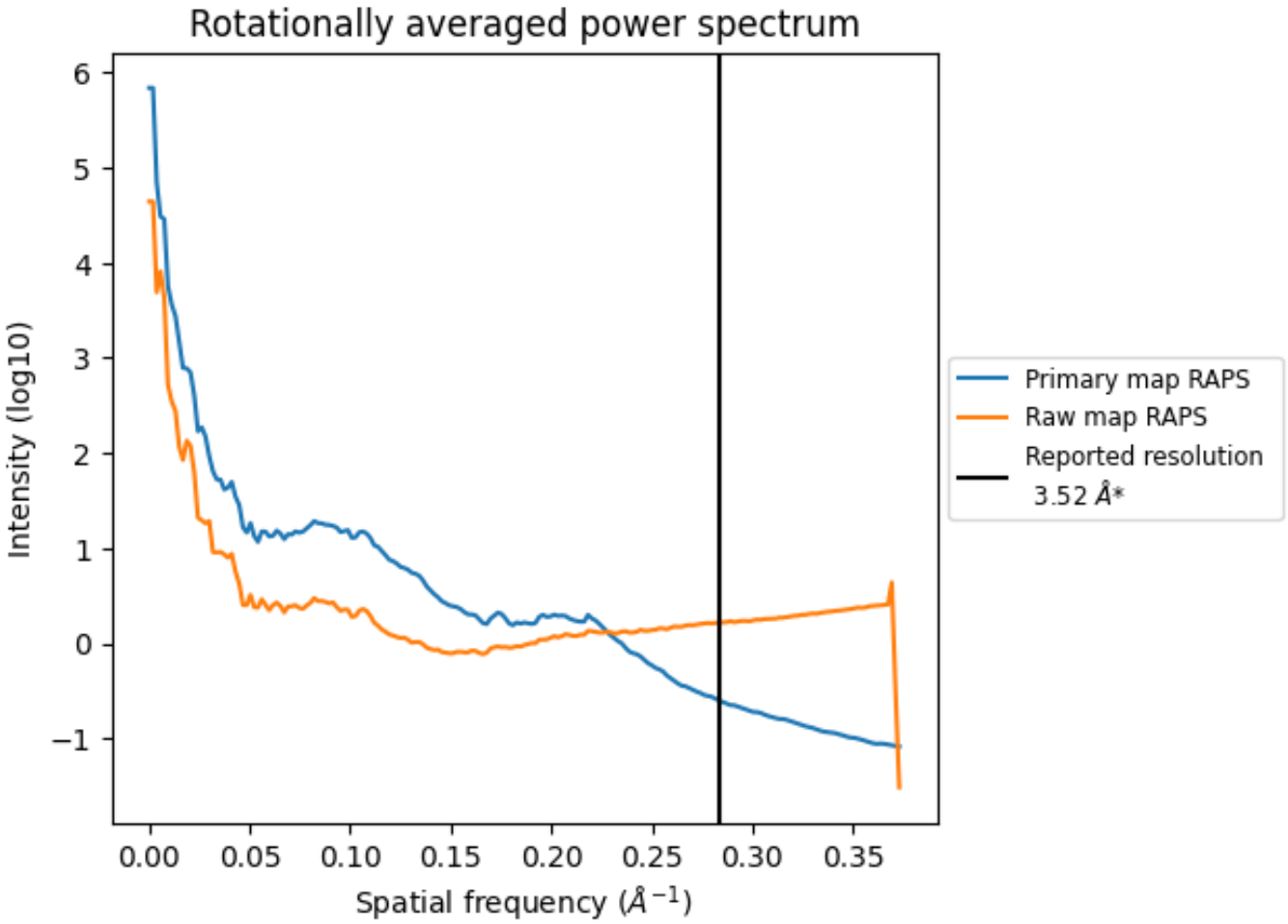
7.2 Volume estimate (i)



The volume at the recommended contour level is 4802 nm^3; this corresponds to an approximate mass of 4337 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)

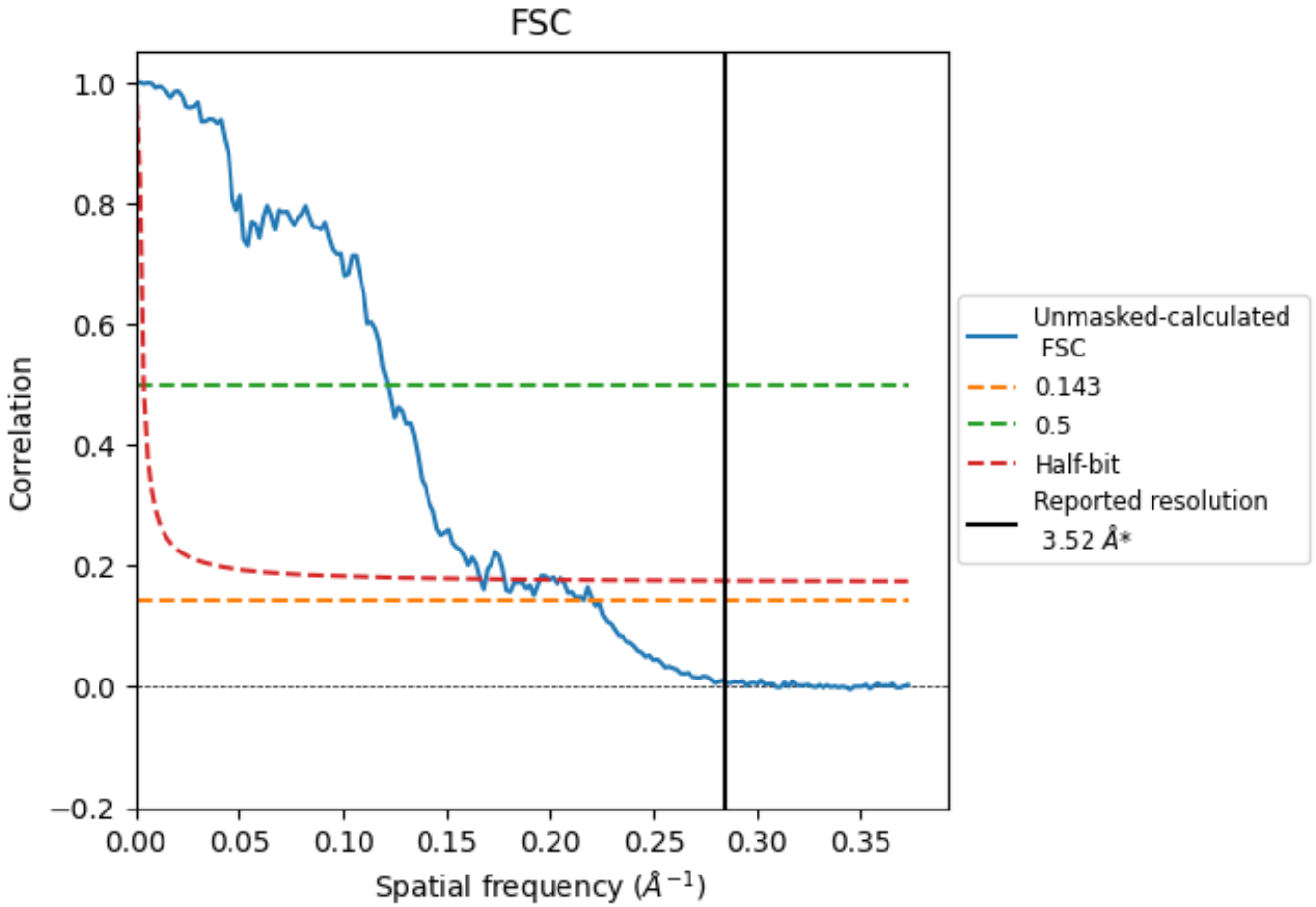


*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

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 0.284 Å^{-1}

8.2 Resolution estimates (i)

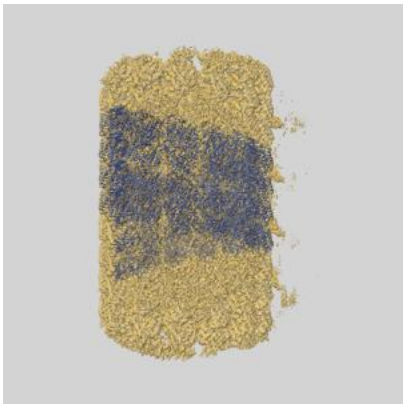
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.53	8.22	6.01

*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 4.53 differs from the reported value 3.52 by more than 10 %

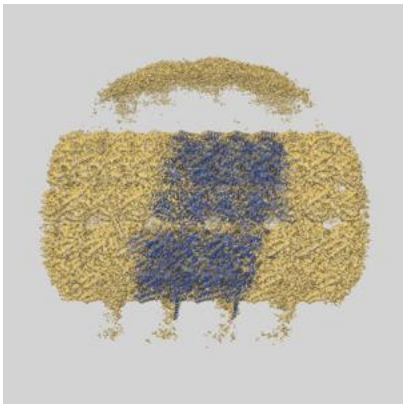
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72717 and PDB model 9YA1. Per-residue inclusion information can be found in section 3 on page 19.

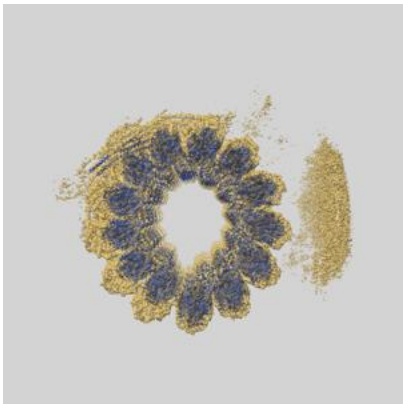
9.1 Map-model overlay



X



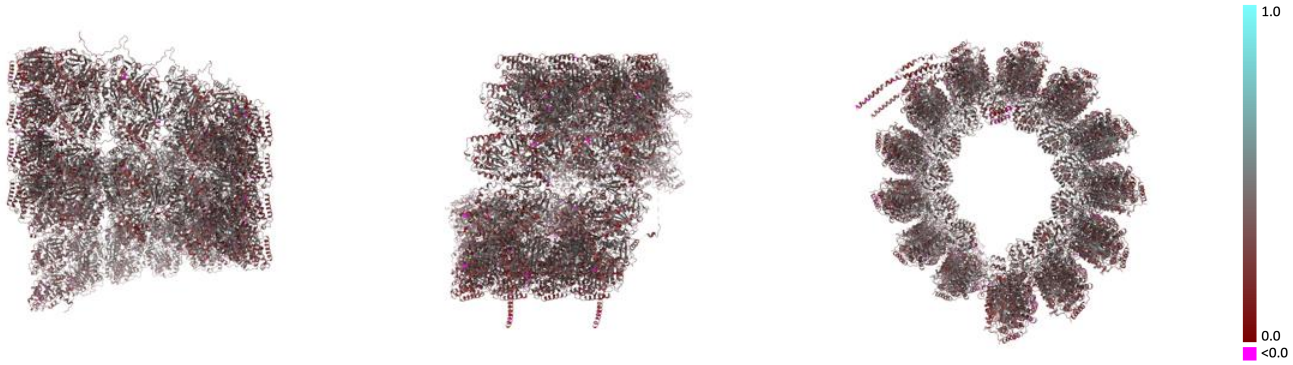
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

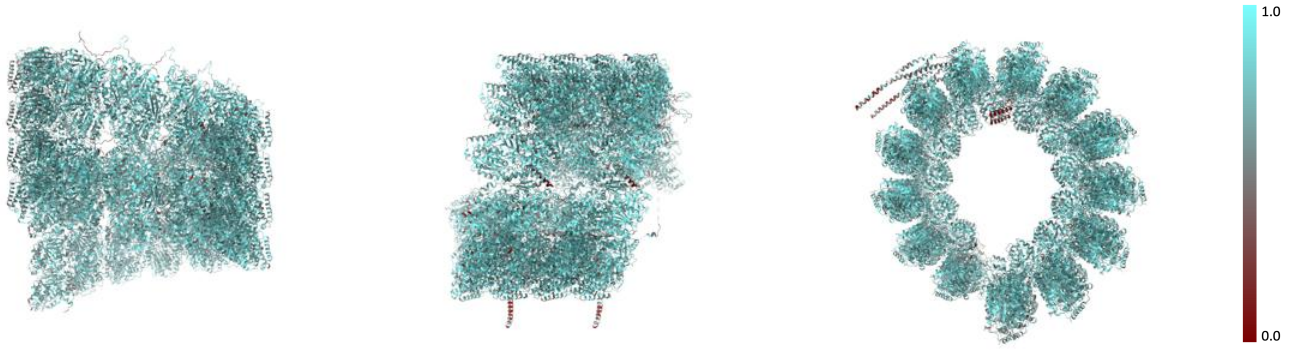
9.2 Q-score mapped to coordinate model



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.

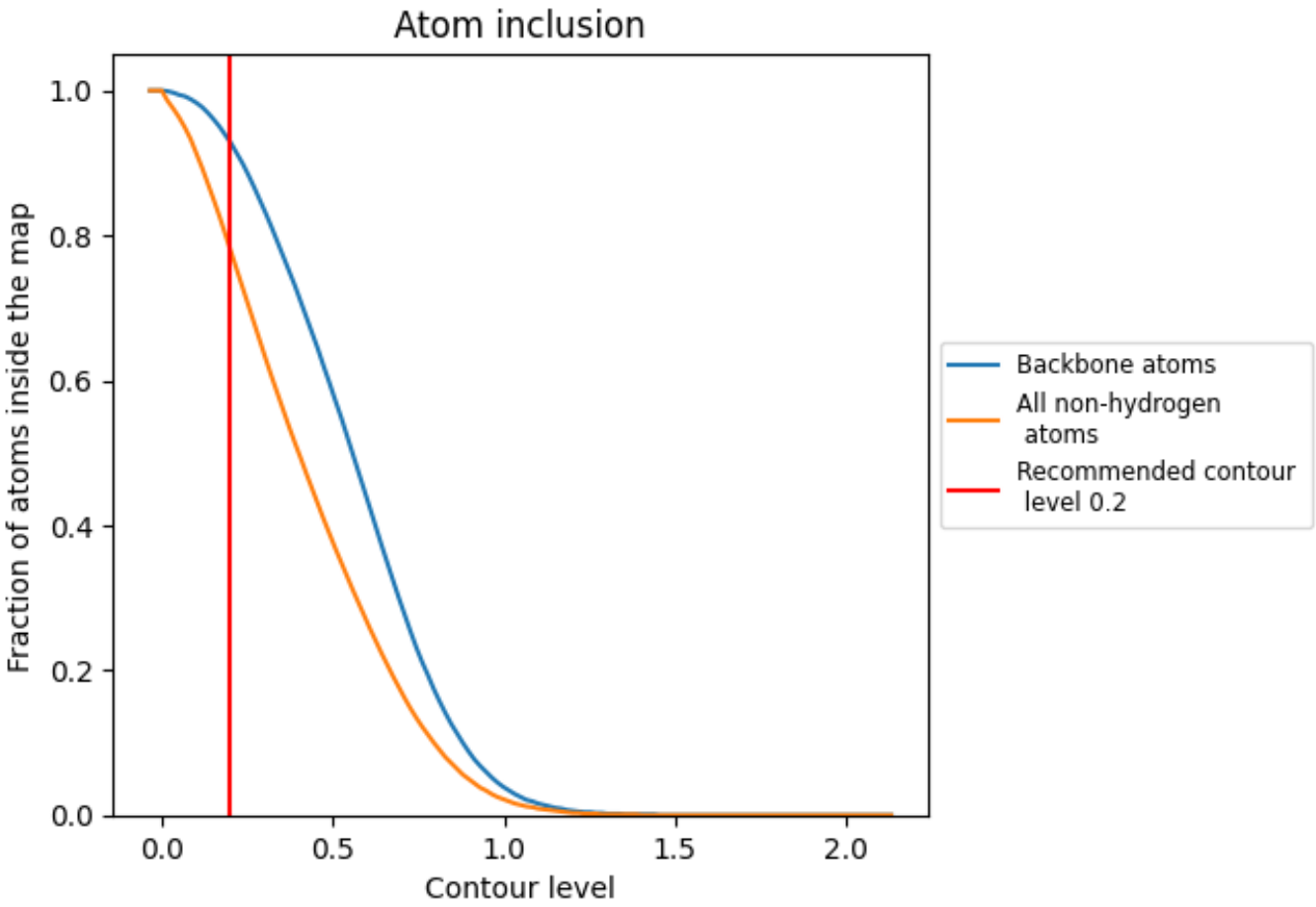
9.3 Atom inclusion mapped to coordinate model



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.3490
1	0.5160	0.2480
2	0.4690	0.2140
A	0.6640	0.3540
A0	0.7760	0.3430
A1	0.7730	0.3460
A2	0.7630	0.3250
A3	0.7330	0.3260
A4	0.8020	0.3530
A5	0.7760	0.3470
A6	0.7980	0.3510
A7	0.7720	0.3460
A8	0.8170	0.3360
A9	0.7900	0.3400
B	0.7450	0.3720
B0	0.8010	0.3340
B1	0.7910	0.3340
B2	0.8310	0.3570
B3	0.8060	0.3460
B4	0.8200	0.3400
B5	0.7920	0.3270
B6	0.8320	0.3670
B7	0.8190	0.3670
B8	0.8290	0.3650
B9	0.7980	0.3470
C	0.7460	0.3350
C0	0.8260	0.3490
C1	0.8000	0.3460
C2	0.8250	0.3580
C3	0.8080	0.3490
C4	0.8210	0.3410
C5	0.7950	0.3380
C6	0.8260	0.3460
C7	0.8060	0.3480
C8	0.7980	0.3480

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
C9	0.7910	0.3630
D	0.6730	0.3600
D0	0.8050	0.3650
D1	0.7830	0.3650
D2	0.8140	0.3730
D3	0.7950	0.3870
D4	0.8190	0.3830
D5	0.7910	0.3790
D6	0.8030	0.3620
D7	0.7910	0.3720
D8	0.8210	0.3740
D9	0.7980	0.3770
E	0.6780	0.3690
E0	0.7750	0.3450
E1	0.7770	0.3620
E2	0.8150	0.3750
E3	0.7840	0.3710
E4	0.7420	0.3370
E5	0.7360	0.3420
E6	0.7680	0.3600
E7	0.7700	0.3730
E8	0.6790	0.3060
E9	0.7150	0.3240
F	0.6980	0.3550
F0	0.7410	0.3520
F1	0.7440	0.3470
G	0.5790	0.3380
H	0.7110	0.3730
I	0.7620	0.3640
J	0.7860	0.3710
K	0.6800	0.3570
O	0.5930	0.2810
P	0.6190	0.2860
R	0.6260	0.3020
U	0.5900	0.2840
V	0.6420	0.2780
W	0.6330	0.2740
X	0.6840	0.3020
a	0.8030	0.3610
b	0.7900	0.3490
c	0.8130	0.3450
d	0.8310	0.3650

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.8350	0.3530
f	0.8410	0.3540
g	0.8220	0.3500
h	0.8190	0.3440
i	0.8000	0.3550
j	0.7950	0.3530
k	0.7580	0.3250
l	0.7600	0.3170
m	0.6250	0.2830
n	0.6190	0.2840
o	0.8130	0.3750
p	0.7980	0.3770
q	0.8200	0.3920
r	0.8380	0.4010
s	0.8290	0.3750
t	0.8380	0.3930
u	0.8060	0.3520
v	0.8120	0.3620
w	0.7480	0.3360
x	0.7610	0.3450