wwPDB EM Validation Summary Report ⓘ

May 18, 2024 – 05:01 PM EDT

PDB ID	:	7M20
EMDB ID	:	EMD-23627
Title	:	18-mer HeLa-tubulin rings in complex with Cryptophycin 1
Authors	:	Eren, E.
Deposited on	:	2021-03-15
Resolution	:	3.84 Å(reported)
Based on initial model	:	6S8L

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

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

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

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

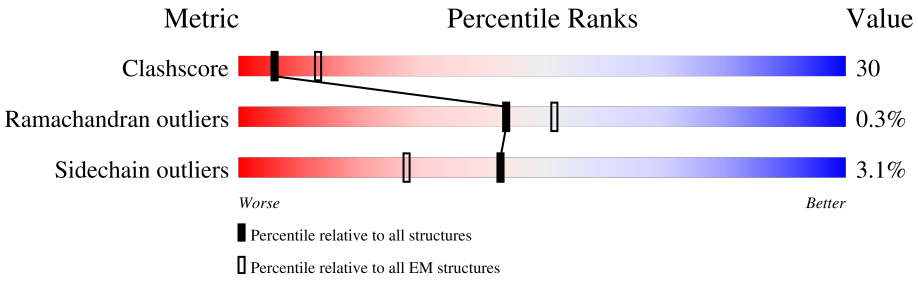
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	450	51% 43% • 5%
1	D	450	51% 43% • 5%
1	F	450	52% 42% • 5%
1	H	450	51% 43% • 5%
1	J	450	52% 43% • 5%
1	L	450	51% 44% • 5%
1	N	450	51% 43% • 5%
1	P	450	51% 43% • 5%

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Mol	Chain	Length	Quality of chain
1	R	450	51% 43% 5%
2	A	451	47% 48%
2	C	451	47% 48%
2	E	451	47% 48%
2	G	451	48% 48%
2	I	451	47% 48%
2	K	451	47% 48%
2	M	451	46% 49%
2	O	451	47% 49%
2	Q	451	47% 48%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GDP	B	1101	-	-	X	-
3	GDP	D	1101	-	-	X	-
3	GDP	F	1101	-	-	X	-
3	GDP	H	1101	-	-	X	-
3	GDP	J	1101	-	-	X	-
3	GDP	L	1101	-	-	X	-
3	GDP	N	1101	-	-	X	-
3	GDP	P	1101	-	-	X	-
3	GDP	R	1101	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 60705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin beta-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	D	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	F	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	H	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	J	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	L	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	N	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	P	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		
1	R	429	Total	C	N	O	S	0	0
			3314	2083	566	640	25		

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	C	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	E	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	G	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	I	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	K	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		

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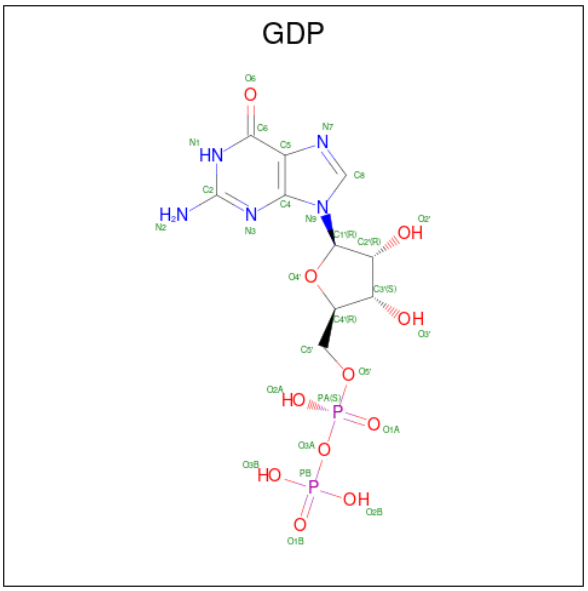
Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	O	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		
2	Q	436	Total	C	N	O	S	0	0
			3325	2109	564	632	20		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	D	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	H	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	J	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	L	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	N	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	P	1	Total	C	N	O	P	0
			28	10	5	11	2	

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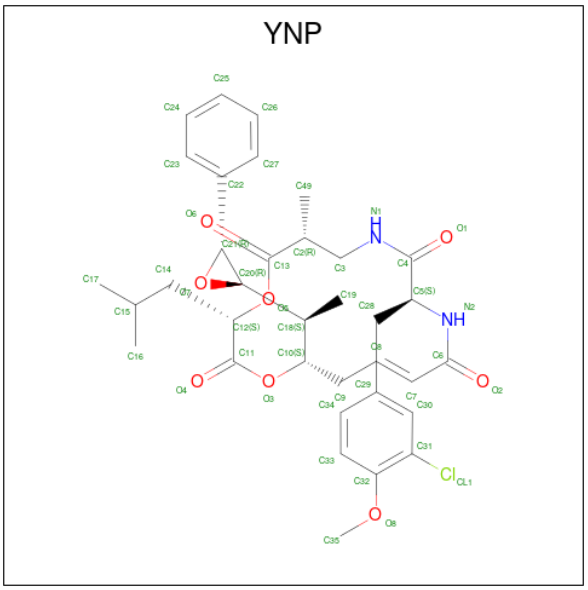
Mol	Chain	Residues	Atoms					AltConf
3	R	1	Total	C	N	O	P	0
			28	10	5	11	2	

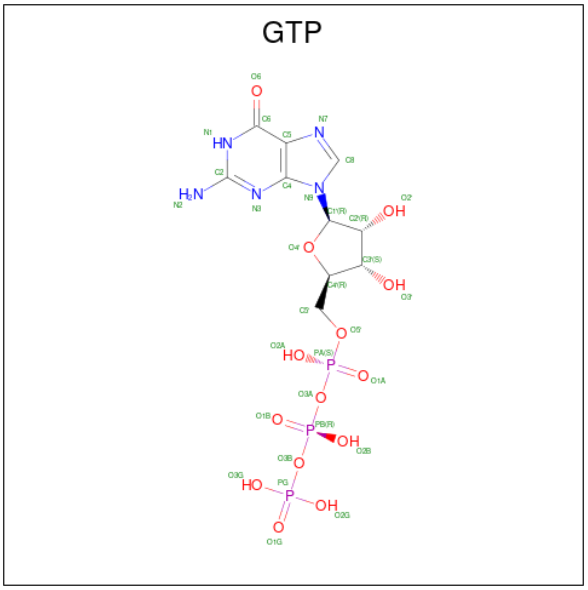
- Molecule 4 is Cryptophycin 1 (three-letter code: YNP) (formula: $C_{35}H_{43}ClN_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	C	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	E	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	G	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	I	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	K	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	M	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	O	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
4	Q	1	Total	C	Cl	N	O	0
			46	35	1	2	8	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

$C_{10}H_{16}N_5O_{14}P_3$).



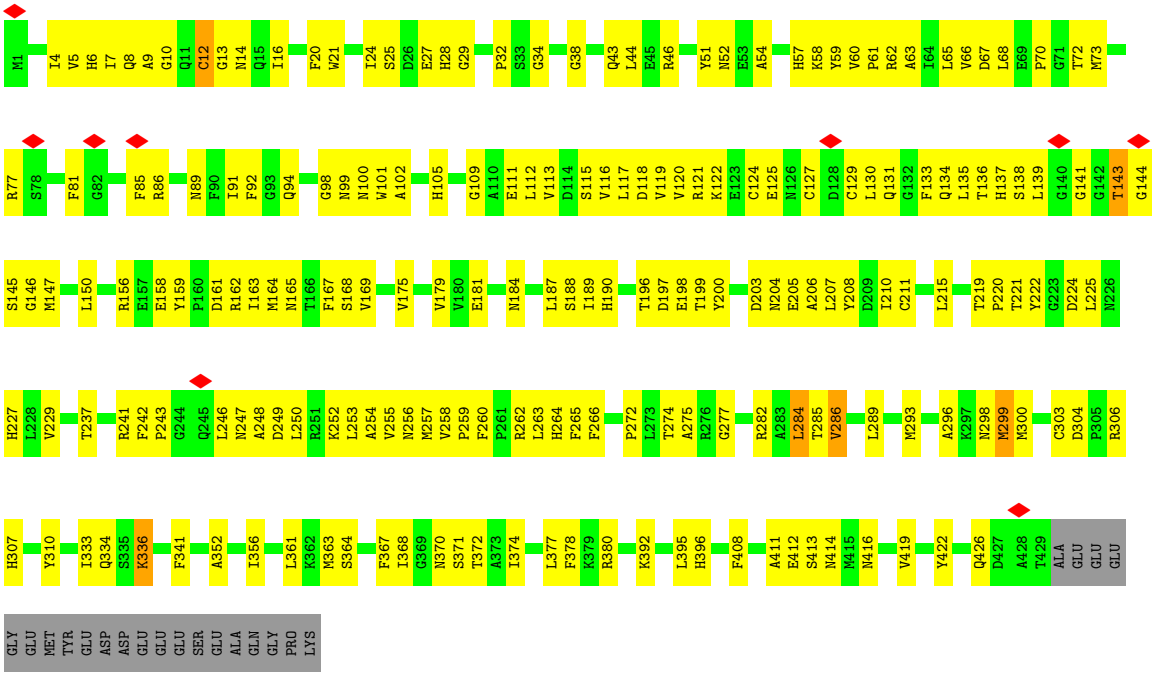
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots (i)

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

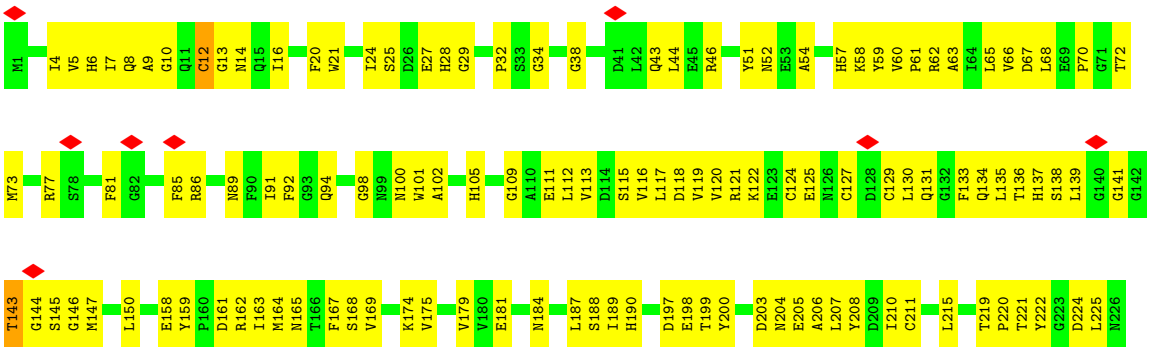
• Molecule 1: Tubulin beta-3 chain

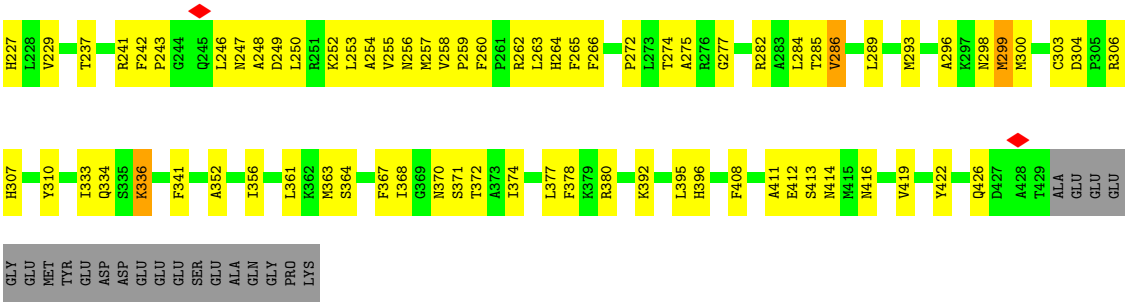
Chain B:



• Molecule 1: Tubulin beta-3 chain

Chain D:



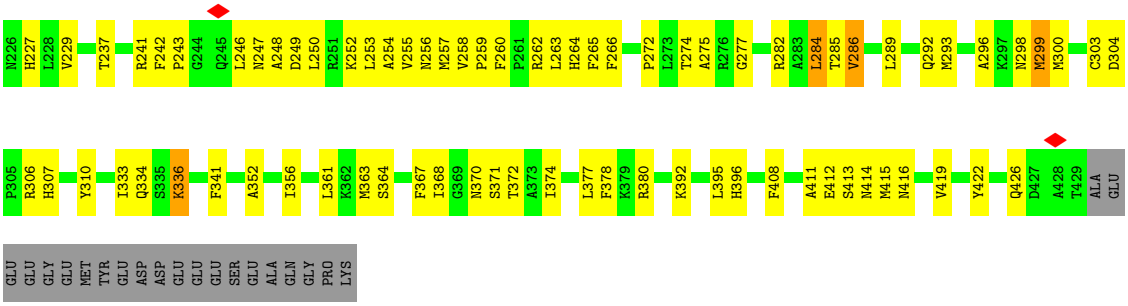


• Molecule 1: Tubulin beta-3 chain

Chain F:

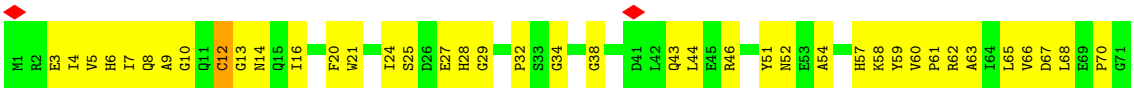
• Molecule 1: Tubulin beta-3 chain

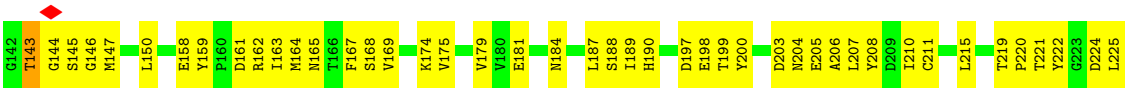
Chain H:

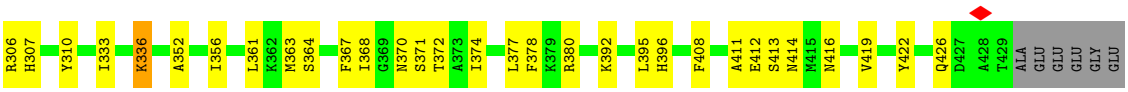


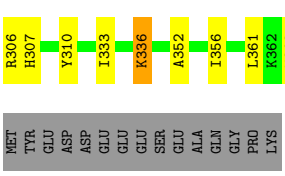
• Molecule 1: Tubulin beta-3 chain

Chain J:



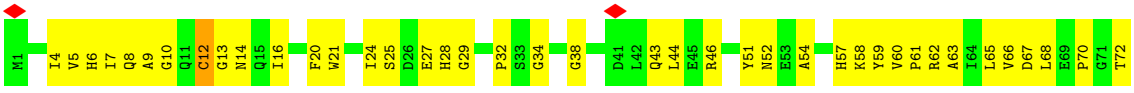


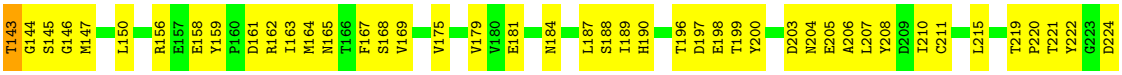




• Molecule 1: Tubulin beta-3 chain

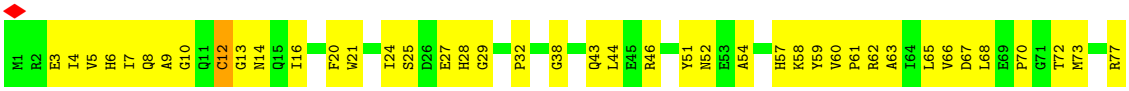
Chain L:

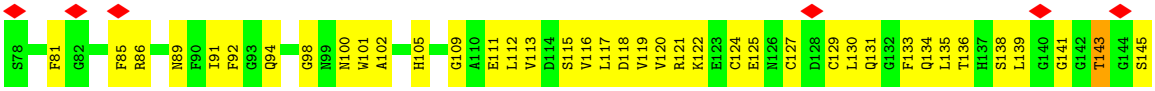


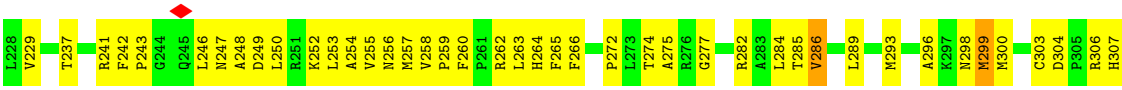


• Molecule 1: Tubulin beta-3 chain

Chain N:

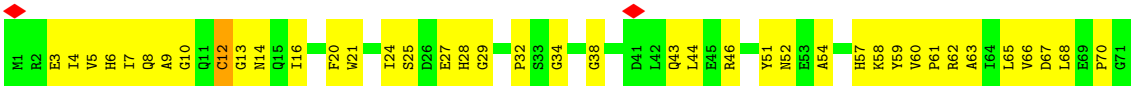


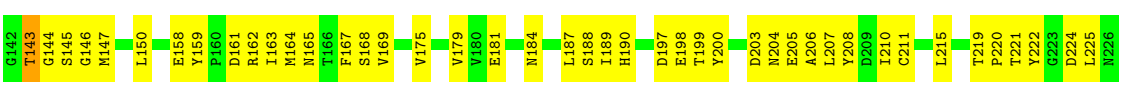


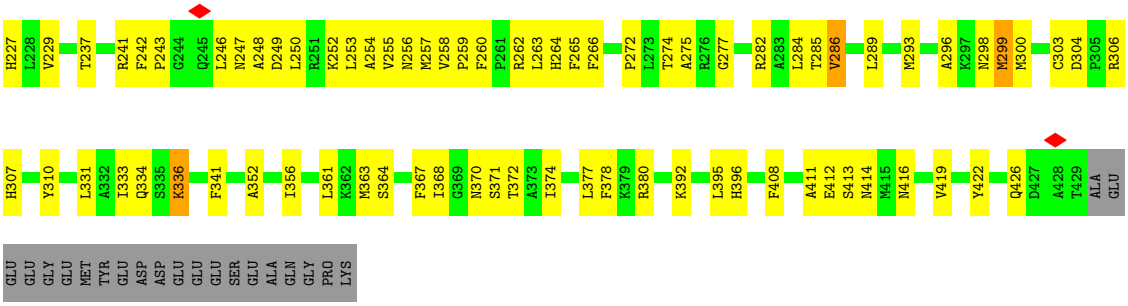


• Molecule 1: Tubulin beta-3 chain

Chain P:

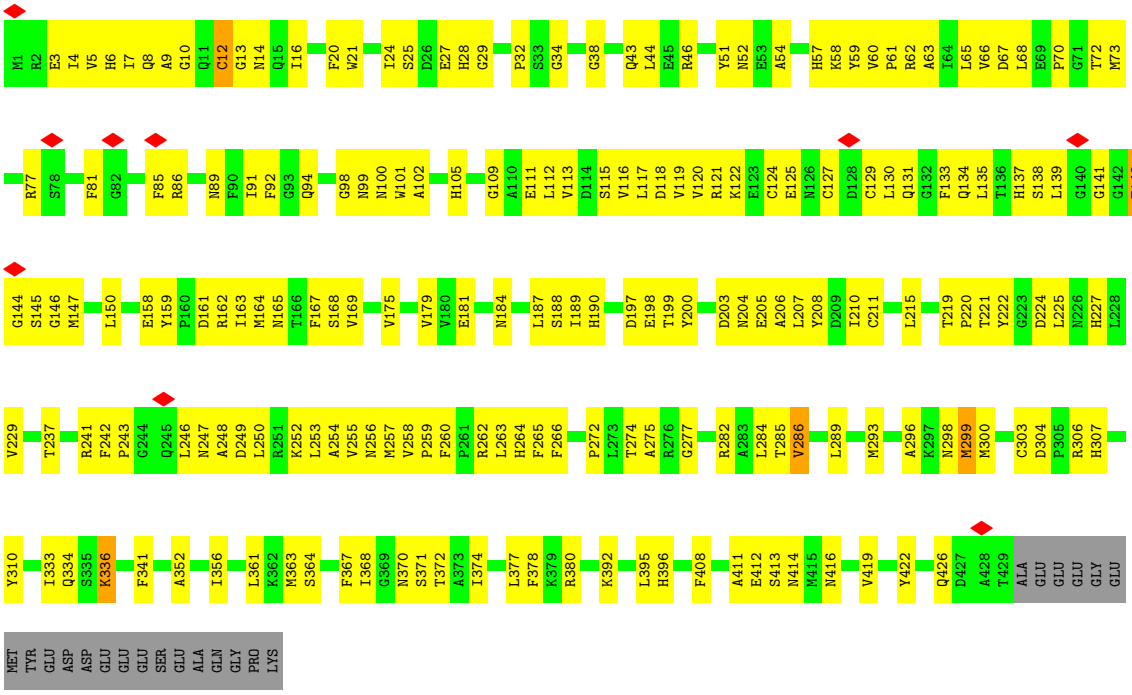






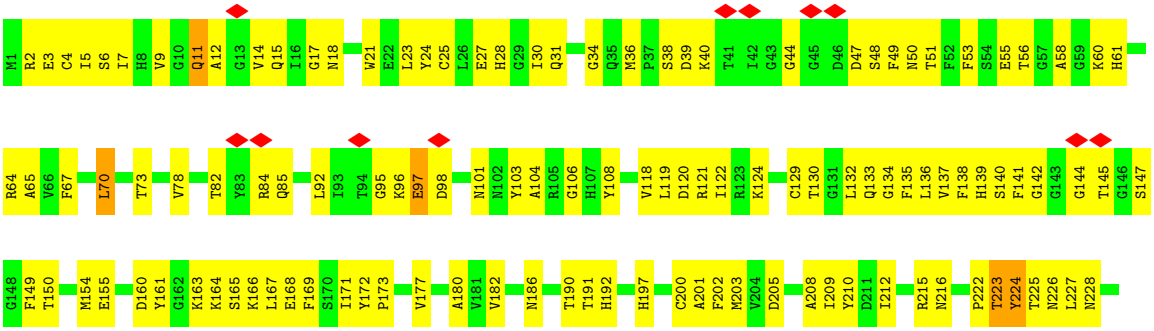
• Molecule 1: Tubulin beta-3 chain

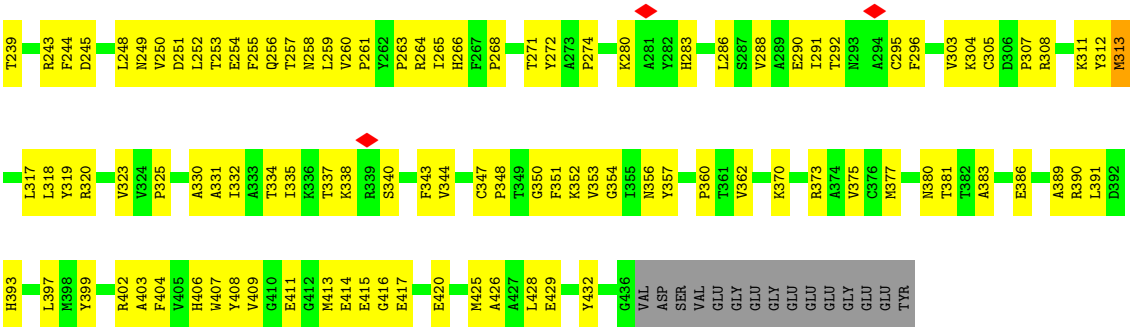
Chain R:



• Molecule 2: Tubulin alpha-1B chain

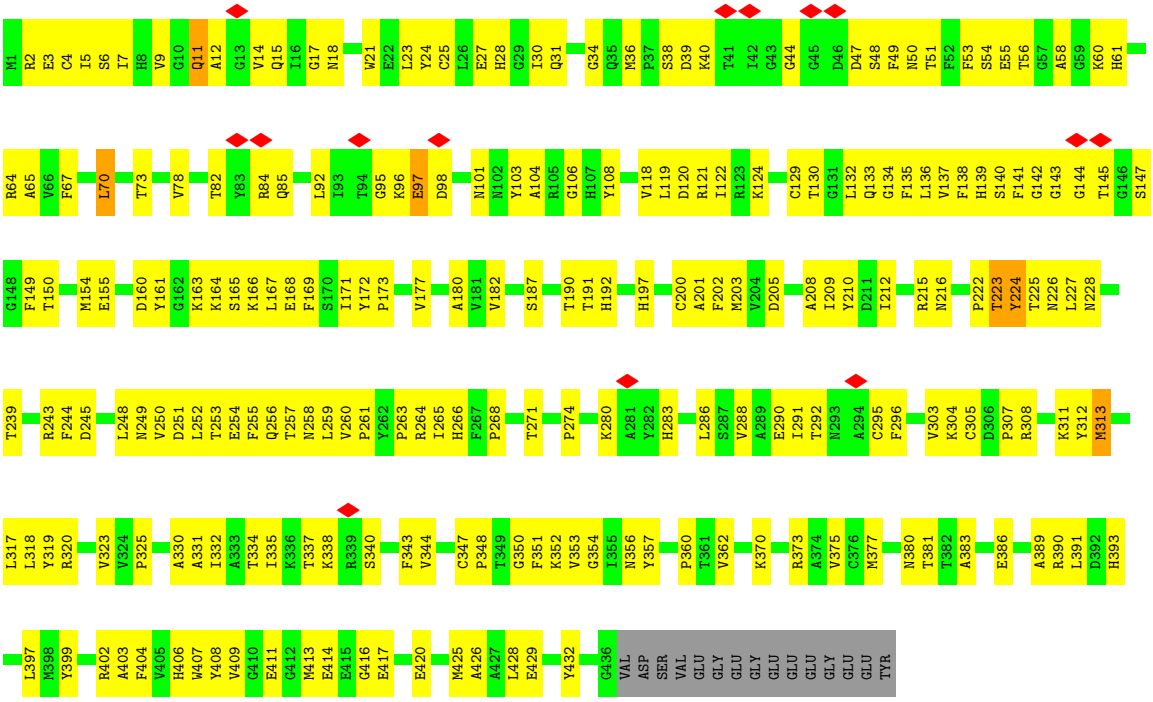
Chain A:





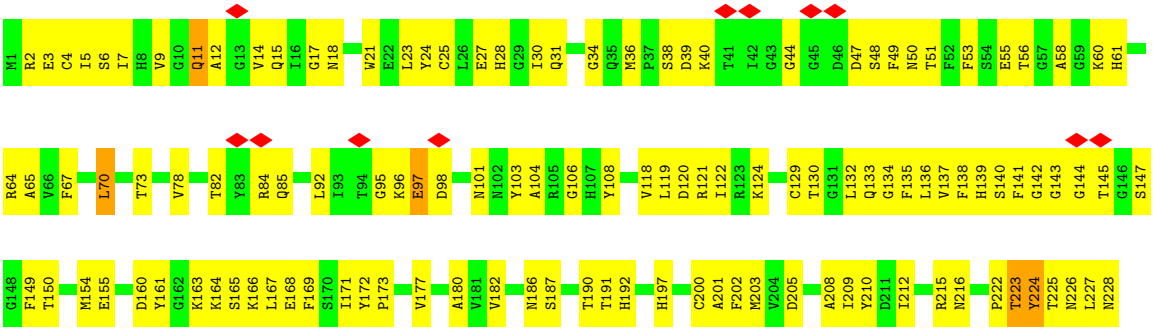
• Molecule 2: Tubulin alpha-1B chain

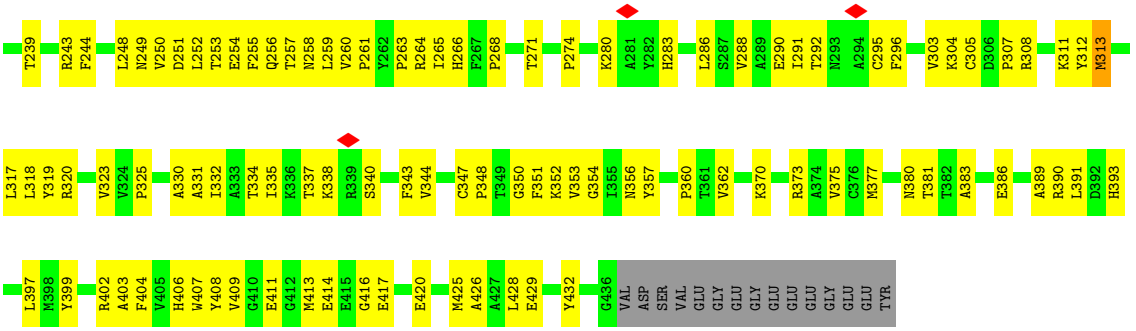
Chain C:



• Molecule 2: Tubulin alpha-1B chain

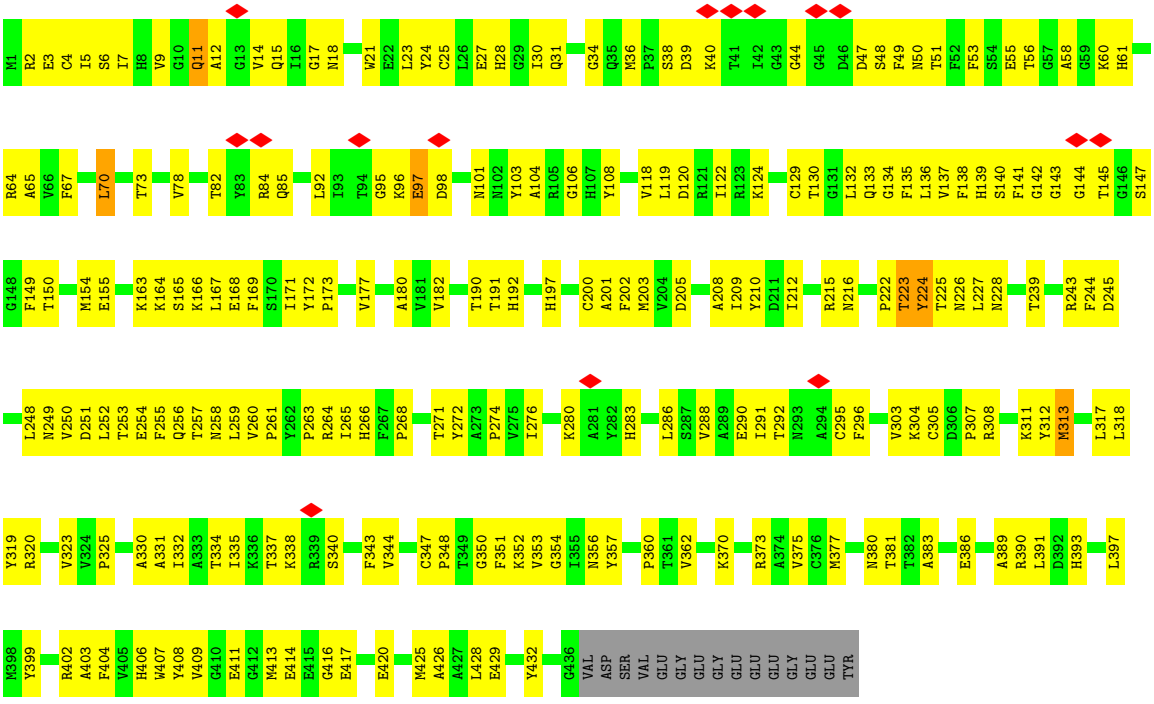
Chain E:





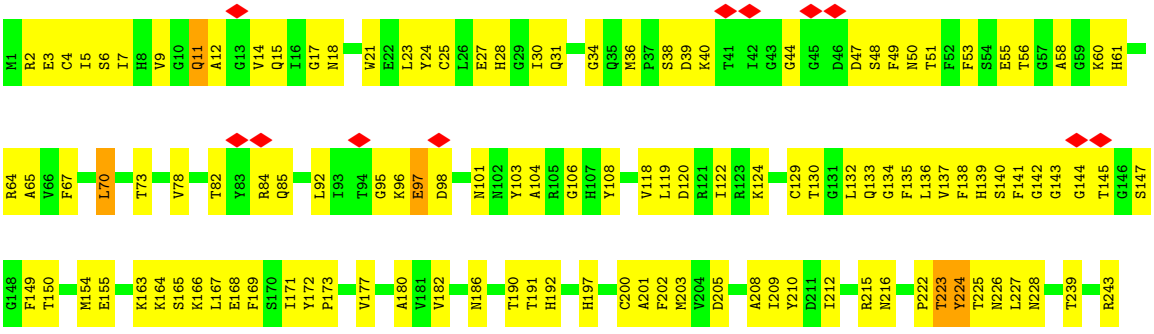
• Molecule 2: Tubulin alpha-1B chain

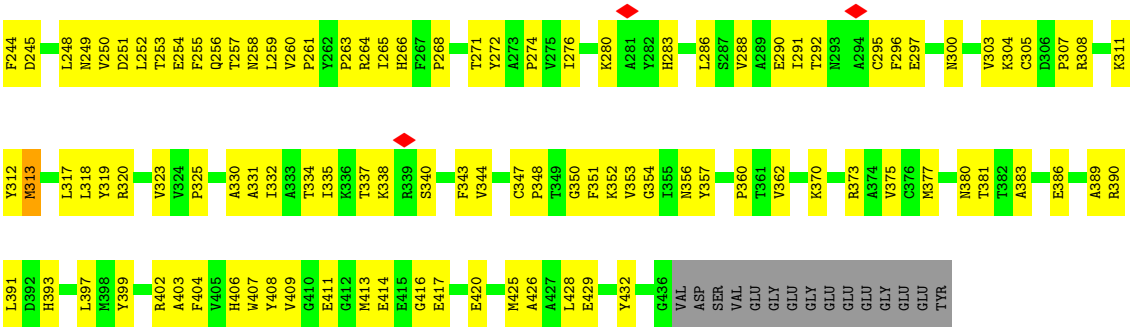
Chain G:



• Molecule 2: Tubulin alpha-1B chain

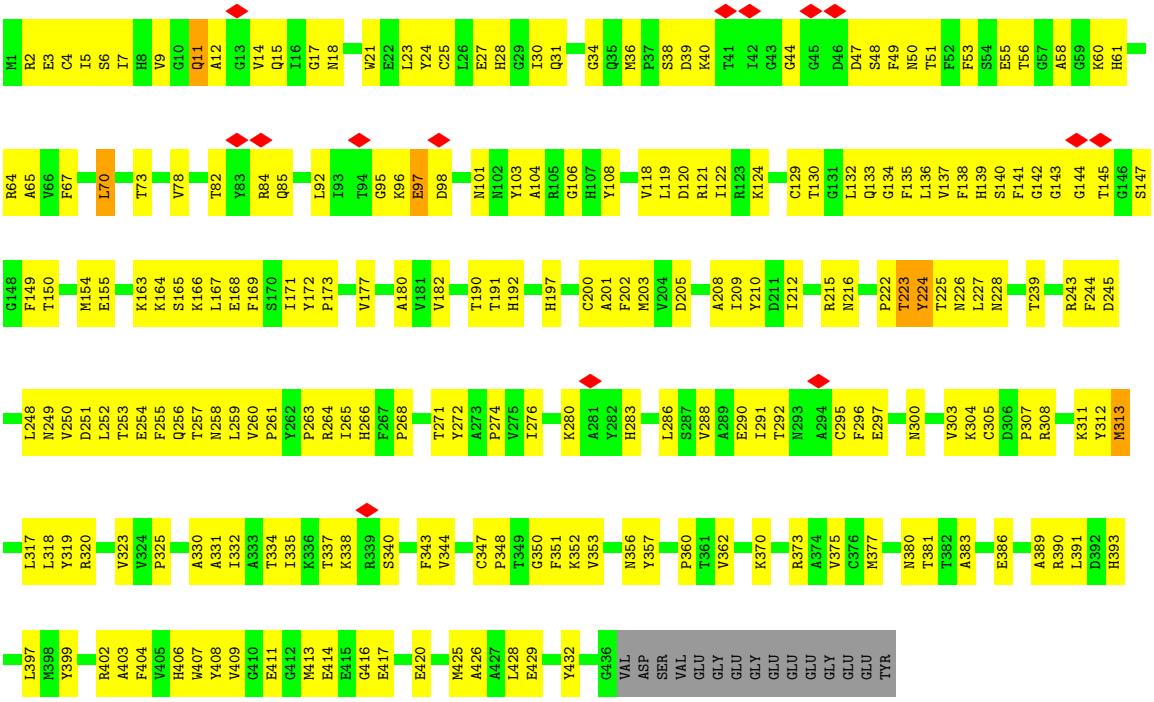
Chain I:





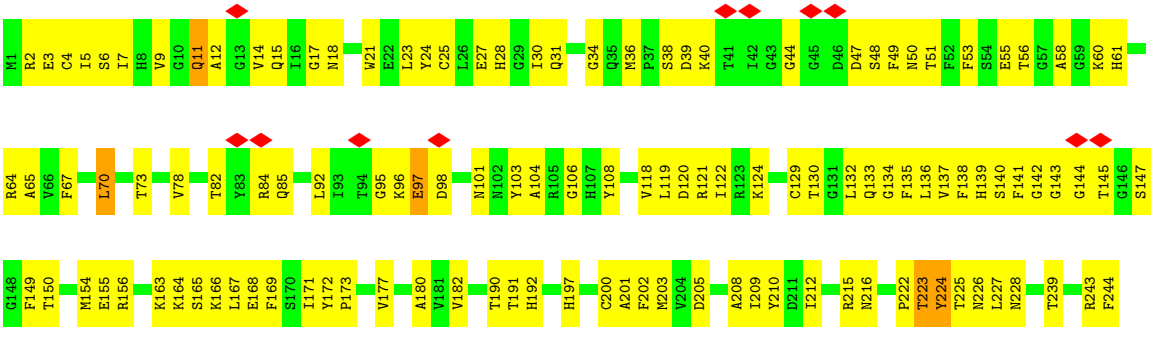
• Molecule 2: Tubulin alpha-1B chain

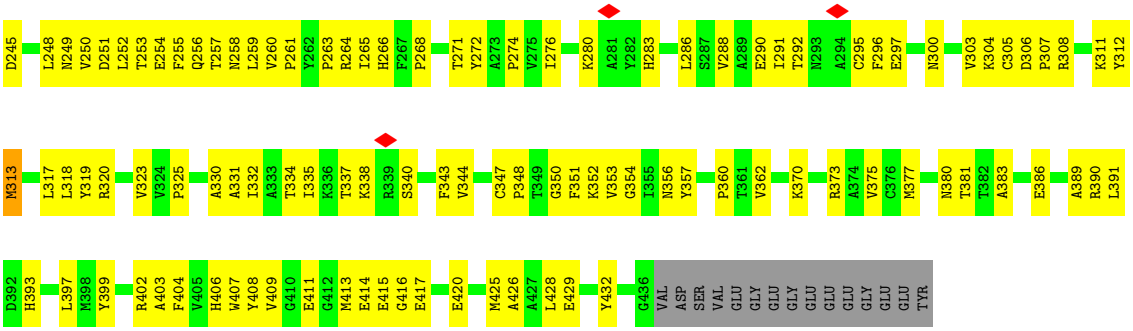
Chain K:



• Molecule 2: Tubulin alpha-1B chain

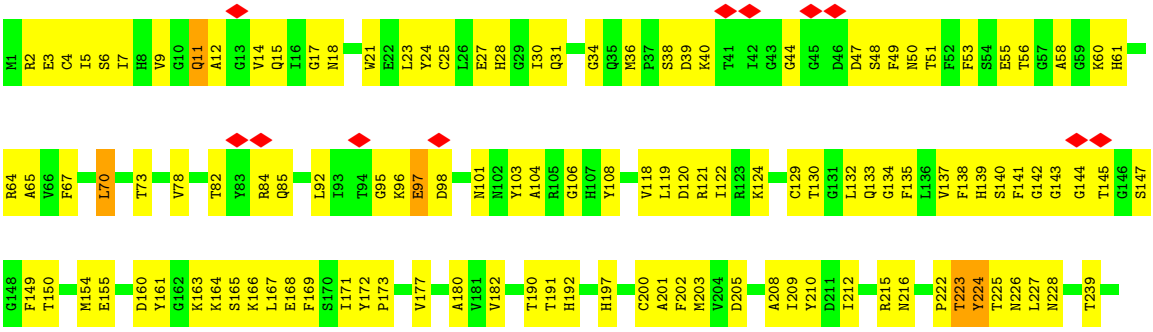
Chain M:





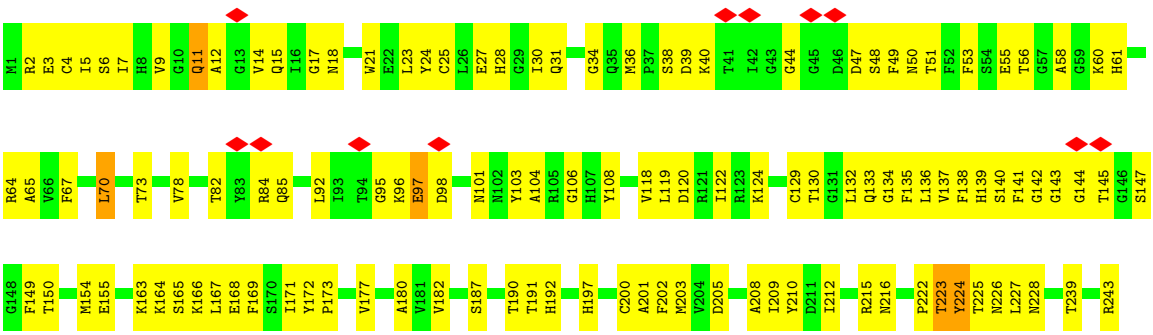
• Molecule 2: Tubulin alpha-1B chain

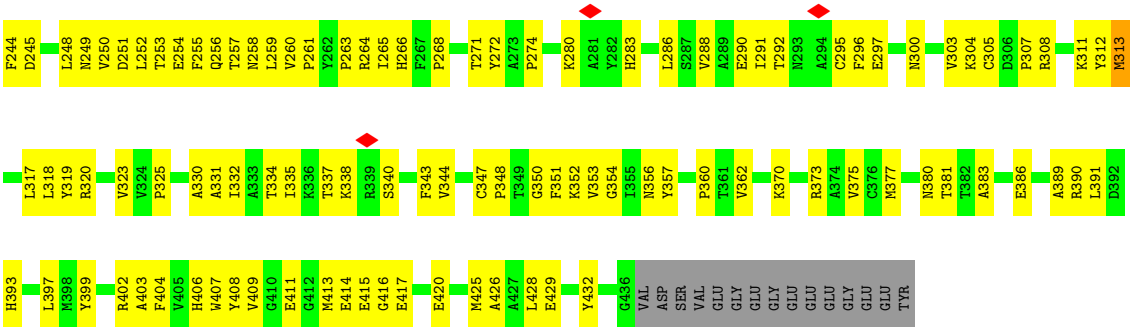
Chain O:



• Molecule 2: Tubulin alpha-1B chain

Chain Q:




F244 D245 L248 N249 V250 D251 L252 T253 E254 F255 Q256 T257 N258 L259 V260 P261 Y262 P263 R264 I265 H266 F267 P268 T271 Y272 A273 P274 K280 A281 Y282 H283 L286 S287 V288 A289 E290 I291 T292 N293 A294 C295 F296 E297 N300 V303 K304 C305 D306 P307 R308 K311 Y312 M313
L317 L318 Y319 R320 V323 V324 P325 A330 A331 I332 A333 T334 I335 K336 T337 K338 R339 S340 F343 V344 C347 P348 T349 G350 F351 K352 V353 G354 I355 N356 Y357 P360 T361 V362 K370 R373 A374 V375 C376 M377 N380 T381 T382 A383 E386 A389 R390 L391 D392
H393 L397 M398 Y399 R402 A403 F404 V405 H406 W407 Y408 V409 G410 E411 G412 M413 E414 E415 G416 E417 E420 M425 A426 A427 L428 E429 Y432 G436 VAL ASP SER VAL GLU GLY GLU GLY GLU GLU GLU GLY GLU TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	14468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	34.231	Depositor
Minimum map value	-17.498	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.504	Depositor
Recommended contour level	4.05	Depositor
Map size (Å)	635.99994, 635.99994, 635.99994	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.39	0/3386	0.57	0/4593
1	D	0.39	0/3386	0.57	0/4593
1	F	0.39	0/3386	0.57	0/4593
1	H	0.39	0/3386	0.57	0/4593
1	J	0.39	0/3386	0.57	0/4593
1	L	0.39	0/3386	0.57	0/4593
1	N	0.39	0/3386	0.57	0/4593
1	P	0.39	0/3386	0.57	0/4593
1	R	0.39	0/3386	0.57	0/4593
2	A	0.41	0/3401	0.58	0/4630
2	C	0.41	0/3401	0.58	0/4630
2	E	0.41	0/3401	0.58	0/4630
2	G	0.41	0/3401	0.58	0/4630
2	I	0.41	0/3401	0.58	0/4630
2	K	0.41	0/3401	0.58	0/4630
2	M	0.41	0/3401	0.58	0/4630
2	O	0.41	0/3401	0.58	0/4630
2	Q	0.41	0/3401	0.58	0/4630
All	All	0.40	0/61083	0.57	0/83007

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3314	0	3169	188	0
1	D	3314	0	3169	185	0
1	F	3314	0	3169	189	0
1	H	3314	0	3169	191	0
1	J	3314	0	3169	186	0
1	L	3314	0	3169	187	0
1	N	3314	0	3169	186	0
1	P	3314	0	3169	185	0
1	R	3314	0	3169	186	0
2	A	3325	0	3190	222	0
2	C	3325	0	3190	222	0
2	E	3325	0	3190	222	0
2	G	3325	0	3190	218	0
2	I	3325	0	3190	222	0
2	K	3325	0	3190	214	0
2	M	3325	0	3190	220	0
2	O	3325	0	3190	223	0
2	Q	3325	0	3190	220	0
3	B	28	0	12	9	0
3	D	28	0	12	9	0
3	F	28	0	12	9	0
3	H	28	0	12	9	0
3	J	28	0	12	9	0
3	L	28	0	12	9	0
3	N	28	0	12	9	0
3	P	28	0	12	9	0
3	R	28	0	12	9	0
4	A	46	0	0	3	0
4	C	46	0	0	3	0
4	E	46	0	0	3	0
4	G	46	0	0	3	0
4	I	46	0	0	3	0
4	K	46	0	0	3	0
4	M	46	0	0	3	0
4	O	46	0	0	2	0
4	Q	46	0	0	3	0
5	A	32	0	12	5	0
5	C	32	0	12	5	0
5	E	32	0	12	5	0
5	G	32	0	12	5	0
5	I	32	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	32	0	12	4	0
5	M	32	0	12	4	0
5	O	32	0	12	5	0
5	Q	32	0	12	5	0
All	All	60705	0	57447	3513	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 30.

The worst 5 of 3513 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:258:VAL:CG1	2:O:407:TRP:HE1	1.59	1.17
1:B:258:VAL:CG1	2:C:407:TRP:HE1	1.59	1.16
2:A:407:TRP:HE1	1:R:258:VAL:CG1	1.59	1.16
1:H:258:VAL:CG1	2:I:407:TRP:HE1	1.58	1.16
1:F:258:VAL:HG13	2:G:407:TRP:HE1	1.09	1.16

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	B	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47 78
1	D	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47 78
1	F	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47 78
1	H	427/450 (95%)	379 (89%)	47 (11%)	1 (0%)	47 78
1	J	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47 78
1	L	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	427/450 (95%)	379 (89%)	47 (11%)	1 (0%)	47	78
1	P	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47	78
1	R	427/450 (95%)	380 (89%)	46 (11%)	1 (0%)	47	78
2	A	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	C	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	E	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	G	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	I	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	K	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	M	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	O	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
2	Q	434/451 (96%)	383 (88%)	49 (11%)	2 (0%)	29	66
All	All	7749/8109 (96%)	6865 (89%)	857 (11%)	27 (0%)	44	74

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	224	TYR
2	C	224	TYR
2	E	224	TYR
2	G	224	TYR
2	I	224	TYR

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	B	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	D	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	F	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	H	357/386 (92%)	344 (96%)	13 (4%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	L	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	N	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	P	357/386 (92%)	344 (96%)	13 (4%)	35	62
1	R	357/386 (92%)	344 (96%)	13 (4%)	35	62
2	A	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	C	348/379 (92%)	340 (98%)	8 (2%)	50	71
2	E	348/379 (92%)	340 (98%)	8 (2%)	50	71
2	G	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	I	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	K	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	M	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	O	348/379 (92%)	339 (97%)	9 (3%)	46	69
2	Q	348/379 (92%)	339 (97%)	9 (3%)	46	69
All	All	6345/6885 (92%)	6149 (97%)	196 (3%)	43	65

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	298	ASN
2	M	11	GLN
1	L	336	LYS
1	N	12	CYS
2	M	272	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	414	ASN
2	O	197	HIS
2	M	15	GLN
1	P	292	GLN
1	R	414	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GDP	B	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
3	GDP	R	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.27	3 (10%)
4	YNP	O	501	-	49,49,49	2.77	14 (28%)	59,68,68	4.47	17 (28%)
5	GTP	C	502	-	26,34,34	0.97	2 (7%)	32,54,54	0.83	0
5	GTP	G	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
5	GTP	M	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
4	YNP	G	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.46	15 (25%)
4	YNP	M	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.47	16 (27%)
4	YNP	Q	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.46	16 (27%)
5	GTP	K	502	-	26,34,34	0.97	2 (7%)	32,54,54	0.83	0
3	GDP	J	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
4	YNP	I	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.46	17 (28%)
3	GDP	D	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
3	GDP	N	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	YNP	A	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.46	16 (27%)
5	GTP	Q	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
4	YNP	C	501	-	49,49,49	2.77	14 (28%)	59,68,68	4.45	16 (27%)
5	GTP	O	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
3	GDP	L	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
4	YNP	E	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.46	16 (27%)
5	GTP	I	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
3	GDP	F	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
4	YNP	K	501	-	49,49,49	2.76	14 (28%)	59,68,68	4.45	17 (28%)
3	GDP	P	1101	-	24,30,30	1.09	2 (8%)	30,47,47	1.26	3 (10%)
5	GTP	E	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0
3	GDP	H	1101	-	24,30,30	1.10	2 (8%)	30,47,47	1.26	3 (10%)
5	GTP	A	502	-	26,34,34	0.98	2 (7%)	32,54,54	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	B	1101	-	-	4/12/32/32	0/3/3/3
3	GDP	R	1101	-	-	4/12/32/32	0/3/3/3
4	YNP	O	501	-	-	30/57/62/62	0/3/4/4
5	GTP	C	502	-	-	4/18/38/38	0/3/3/3
5	GTP	G	502	-	-	4/18/38/38	0/3/3/3
5	GTP	M	502	-	-	4/18/38/38	0/3/3/3
4	YNP	G	501	-	-	30/57/62/62	0/3/4/4
4	YNP	M	501	-	-	32/57/62/62	0/3/4/4
4	YNP	Q	501	-	-	33/57/62/62	0/3/4/4
5	GTP	K	502	-	-	4/18/38/38	0/3/3/3
3	GDP	J	1101	-	-	4/12/32/32	0/3/3/3
4	YNP	I	501	-	-	31/57/62/62	0/3/4/4
3	GDP	D	1101	-	-	4/12/32/32	0/3/3/3
3	GDP	N	1101	-	-	4/12/32/32	0/3/3/3
4	YNP	A	501	-	-	31/57/62/62	0/3/4/4
5	GTP	Q	502	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YNP	C	501	-	-	32/57/62/62	0/3/4/4
5	GTP	O	502	-	-	4/18/38/38	0/3/3/3
3	GDP	L	1101	-	-	4/12/32/32	0/3/3/3
4	YNP	E	501	-	-	32/57/62/62	0/3/4/4
5	GTP	I	502	-	-	4/18/38/38	0/3/3/3
3	GDP	F	1101	-	-	4/12/32/32	0/3/3/3
4	YNP	K	501	-	-	30/57/62/62	0/3/4/4
3	GDP	P	1101	-	-	4/12/32/32	0/3/3/3
5	GTP	E	502	-	-	4/18/38/38	0/3/3/3
3	GDP	H	1101	-	-	4/12/32/32	0/3/3/3
5	GTP	A	502	-	-	4/18/38/38	0/3/3/3

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	YNP	O1-C4	8.66	1.40	1.23
4	Q	501	YNP	O1-C4	8.66	1.40	1.23
4	K	501	YNP	O1-C4	8.65	1.40	1.23
4	A	501	YNP	O1-C4	8.64	1.40	1.23
4	O	501	YNP	O1-C4	8.64	1.40	1.23

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	501	YNP	C3-N1-C4	25.02	170.45	122.67
4	C	501	YNP	C3-N1-C4	24.94	170.28	122.67
4	G	501	YNP	C3-N1-C4	24.91	170.24	122.67
4	E	501	YNP	C3-N1-C4	24.91	170.22	122.67
4	M	501	YNP	C3-N1-C4	24.91	170.22	122.67

There are no chirality outliers.

5 of 353 torsion outliers are listed below:

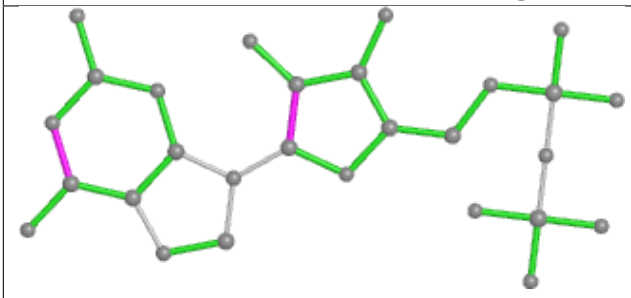
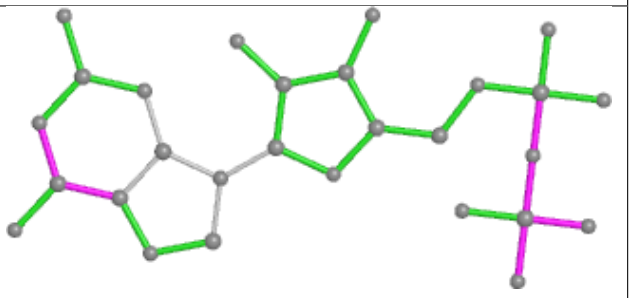
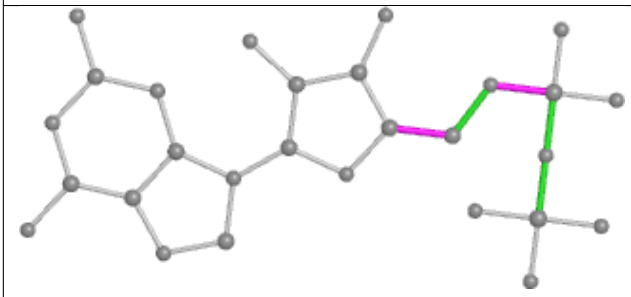
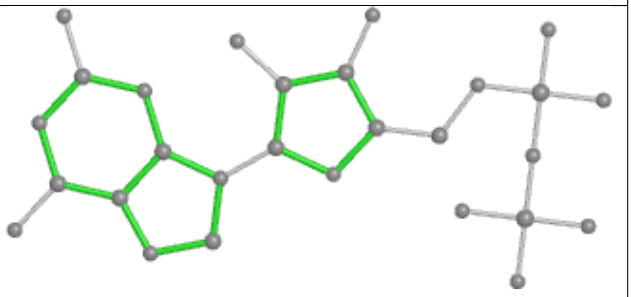
Mol	Chain	Res	Type	Atoms
3	B	1101	GDP	C5'-O5'-PA-O3A
3	B	1101	GDP	C5'-O5'-PA-O2A
3	B	1101	GDP	C3'-C4'-C5'-O5'
3	D	1101	GDP	C5'-O5'-PA-O3A
3	D	1101	GDP	C5'-O5'-PA-O2A

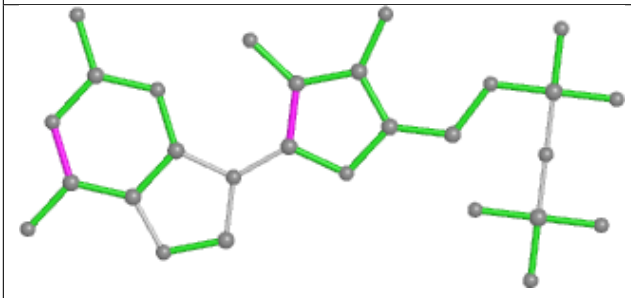
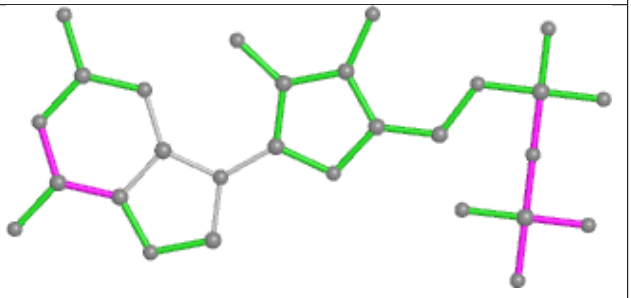
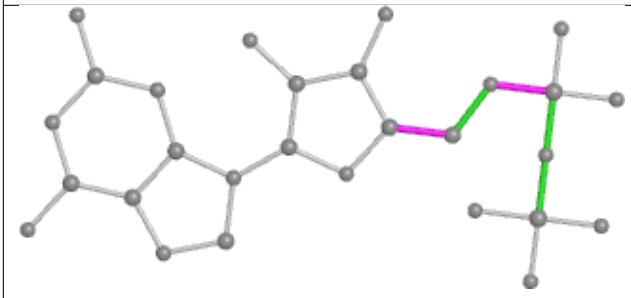
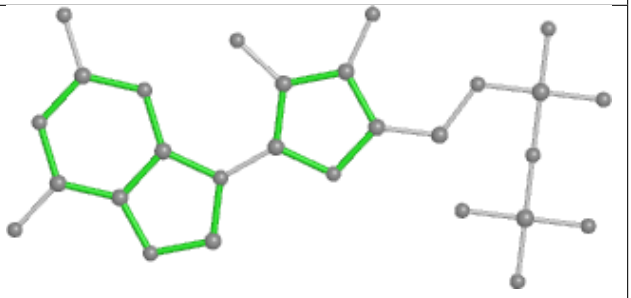
There are no ring outliers.

27 monomers are involved in 150 short contacts:

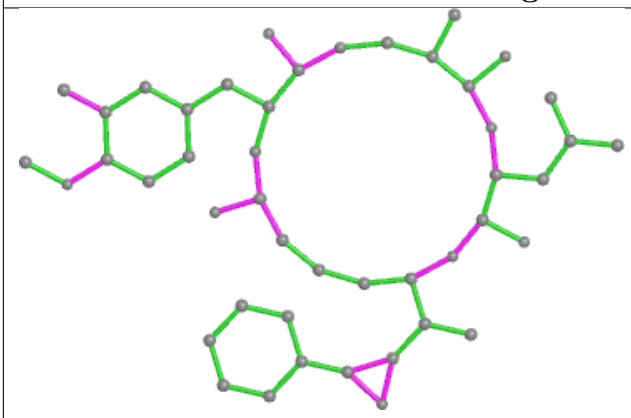
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1101	GDP	9	0
3	R	1101	GDP	9	0
4	O	501	YNP	2	0
5	C	502	GTP	5	0
5	G	502	GTP	5	0
5	M	502	GTP	4	0
4	G	501	YNP	3	0
4	M	501	YNP	3	0
4	Q	501	YNP	3	0
5	K	502	GTP	4	0
3	J	1101	GDP	9	0
4	I	501	YNP	3	0
3	D	1101	GDP	9	0
3	N	1101	GDP	9	0
4	A	501	YNP	3	0
5	Q	502	GTP	5	0
4	C	501	YNP	3	0
5	O	502	GTP	5	0
3	L	1101	GDP	9	0
4	E	501	YNP	3	0
5	I	502	GTP	5	0
3	F	1101	GDP	9	0
4	K	501	YNP	3	0
3	P	1101	GDP	9	0
5	E	502	GTP	5	0
3	H	1101	GDP	9	0
5	A	502	GTP	5	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 GDP B 1101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP R 1101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand YNP O 501



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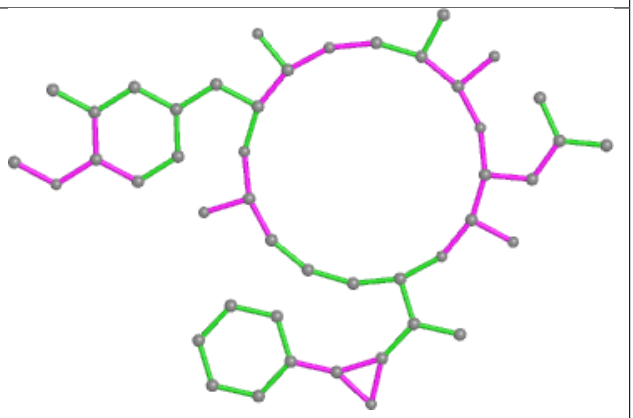

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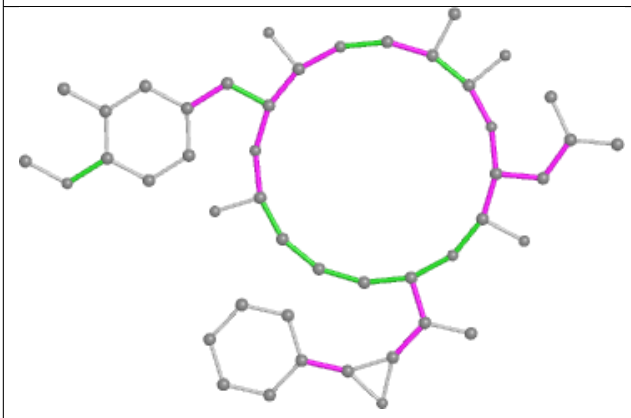

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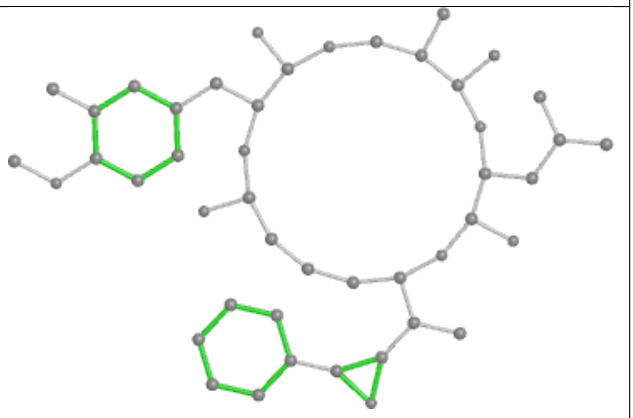
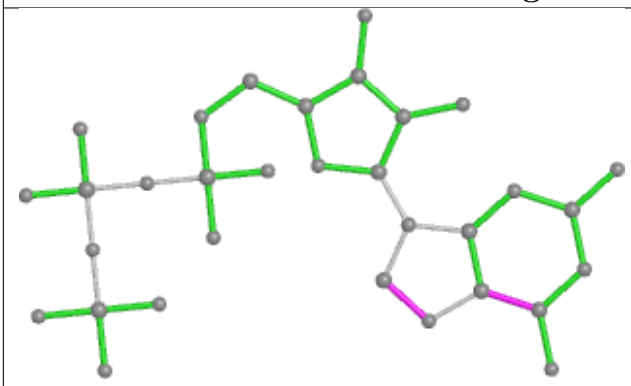


Rings

Ligand GTP C 502



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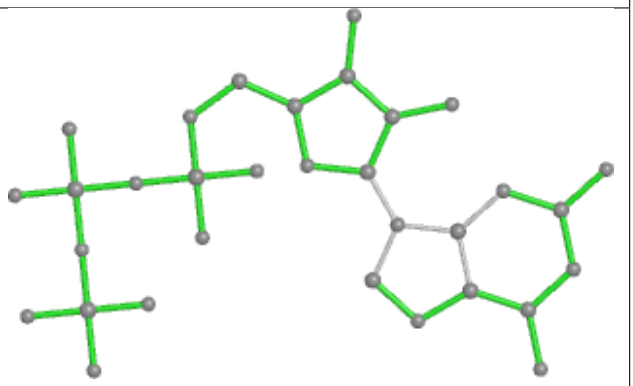

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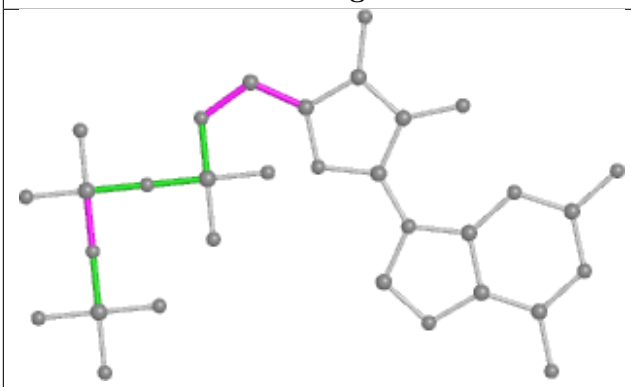

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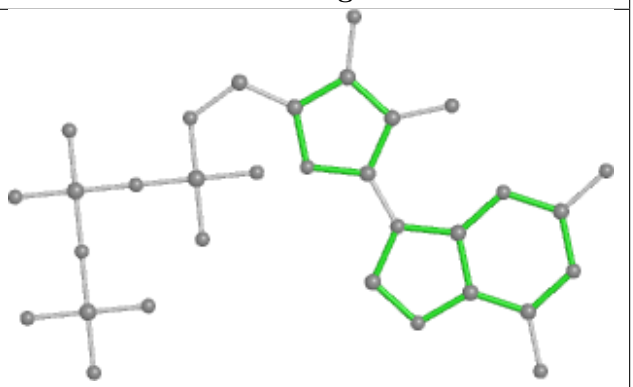

Rings

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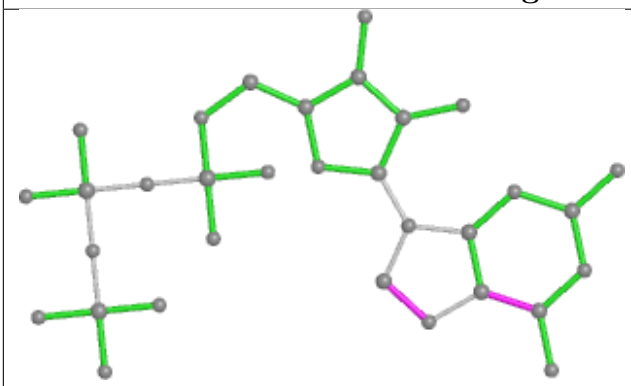

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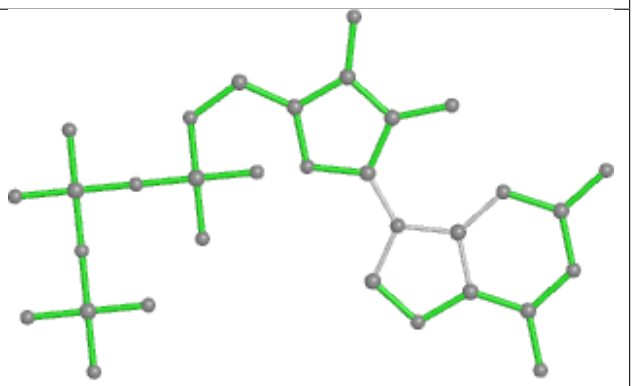

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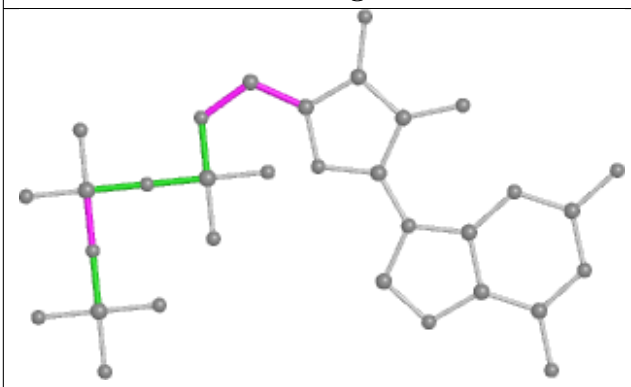

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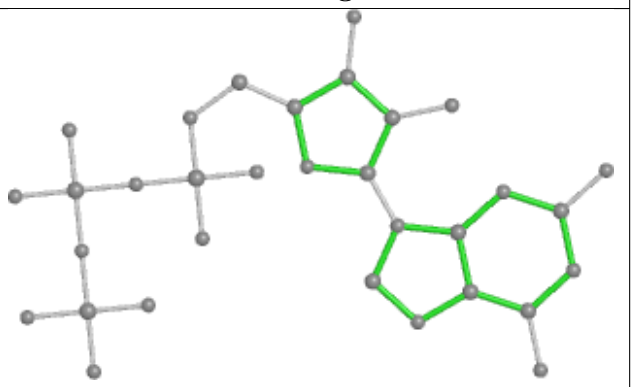
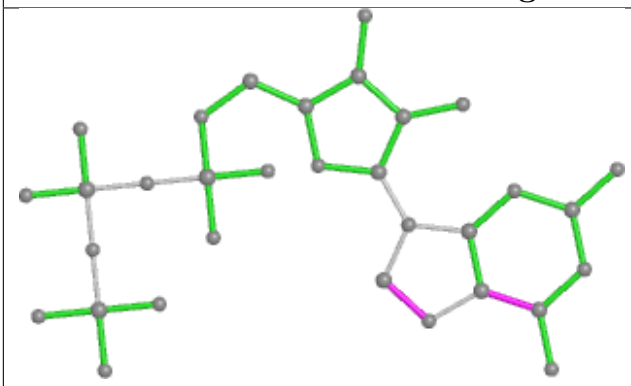


Rings

Ligand GTP M 502



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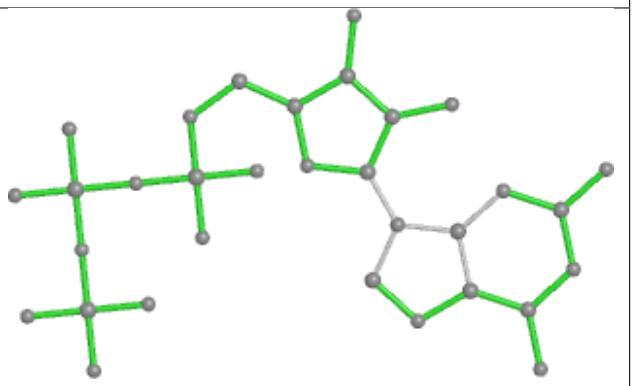

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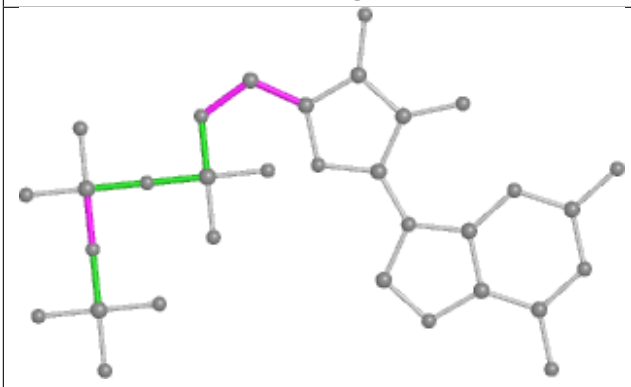

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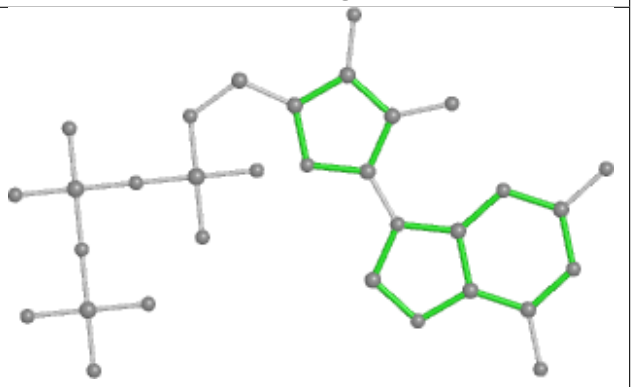
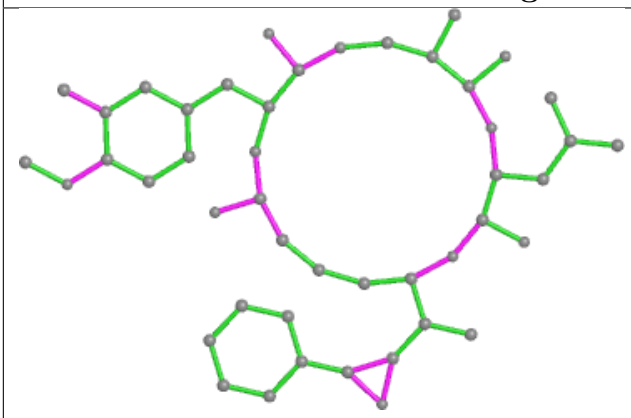


Rings

Ligand YNP G 501



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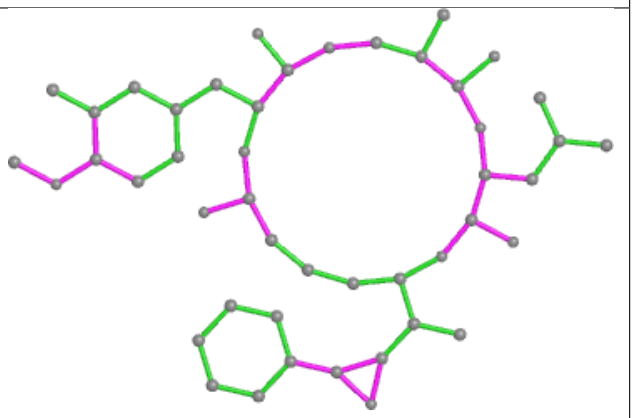

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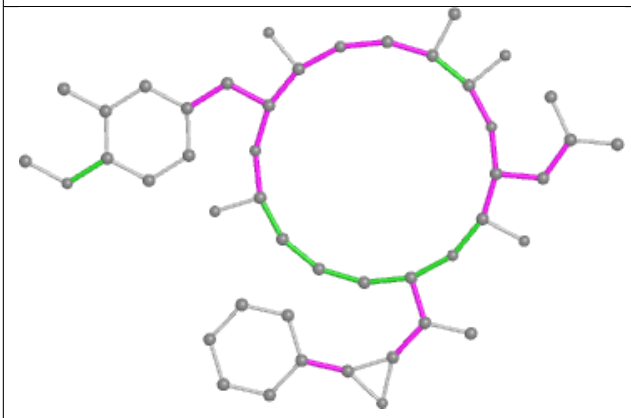

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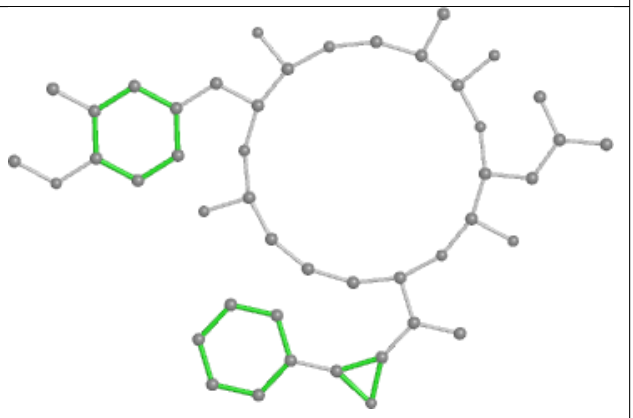
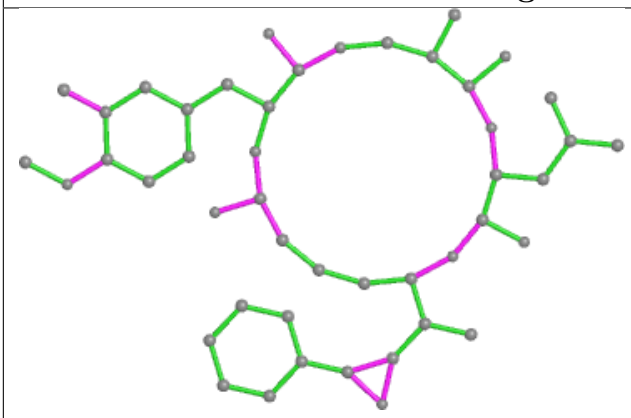


Rings

Ligand YNP M 501



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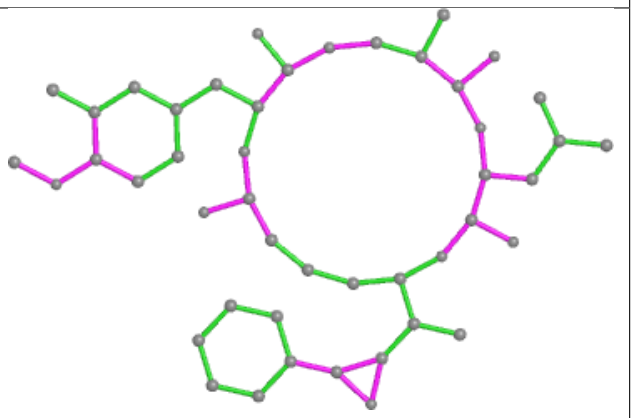

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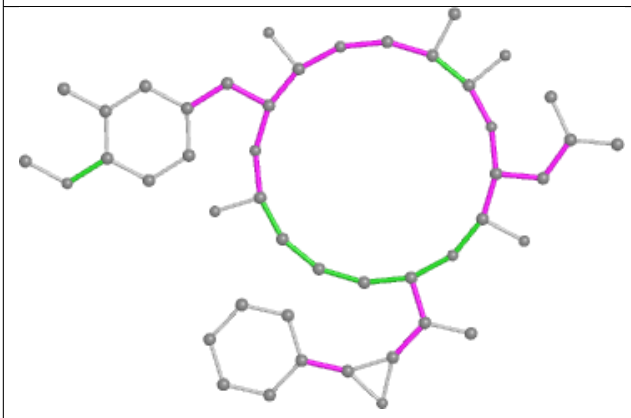

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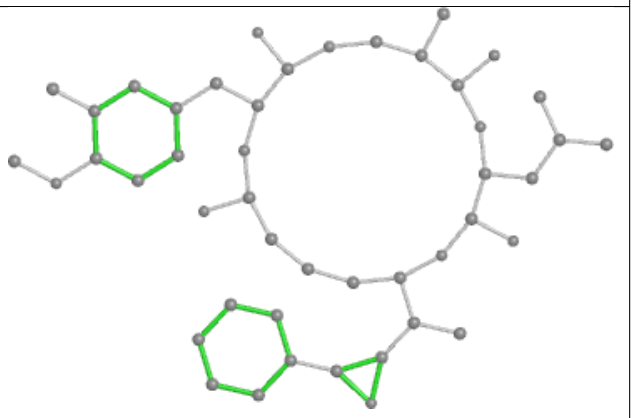
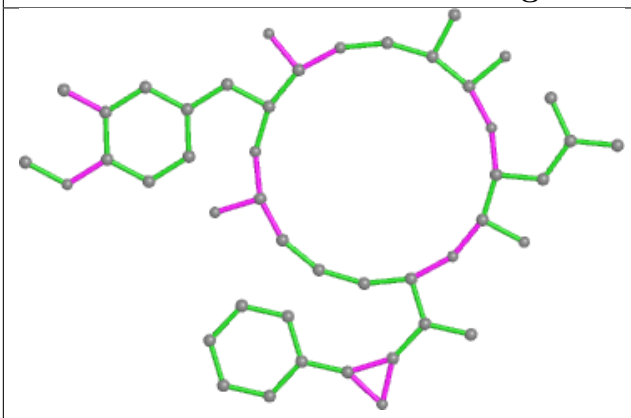


Rings

Ligand YNP Q 501



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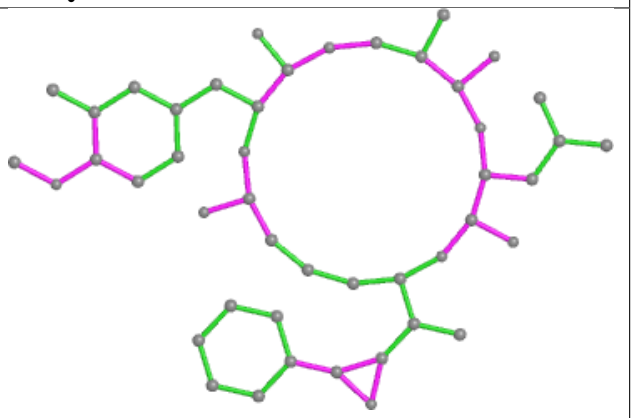

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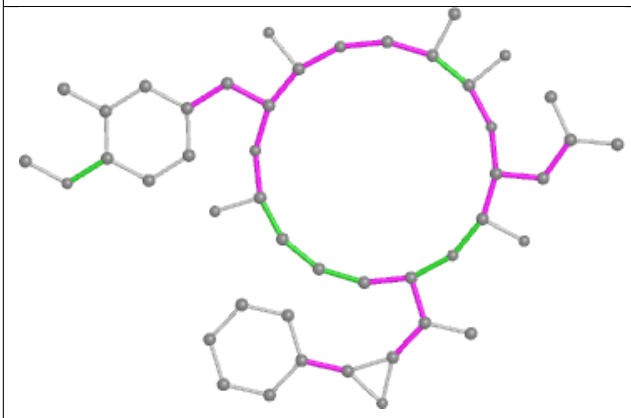

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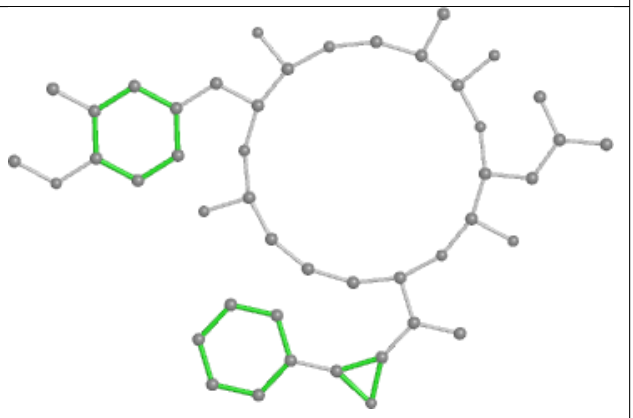
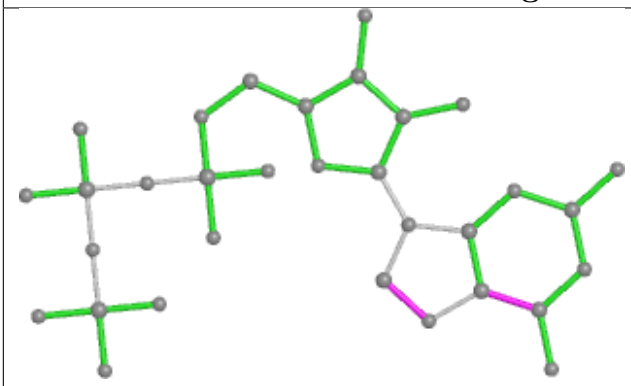


Rings

Ligand GTP K 502



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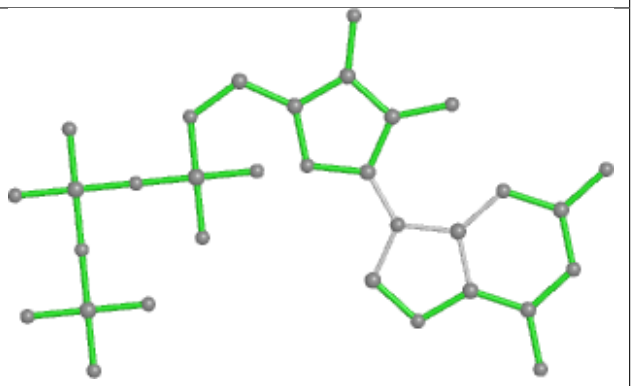

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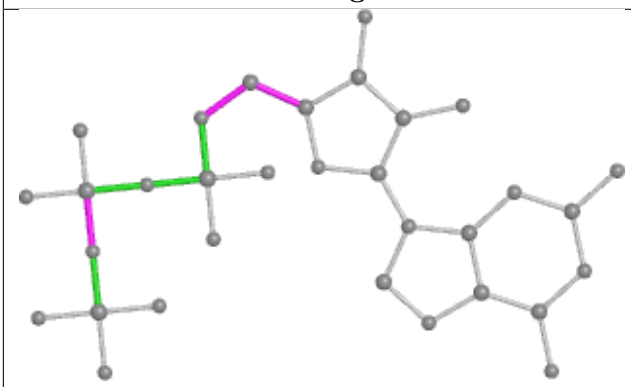

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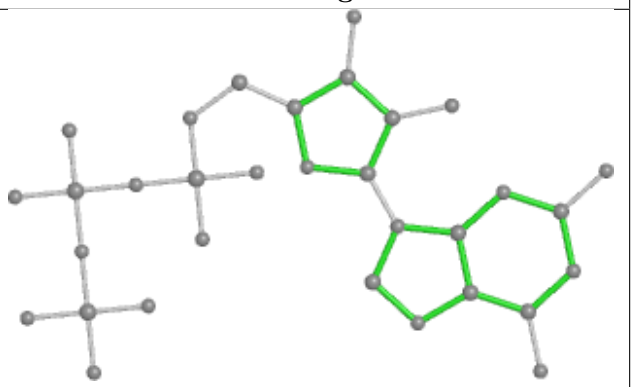
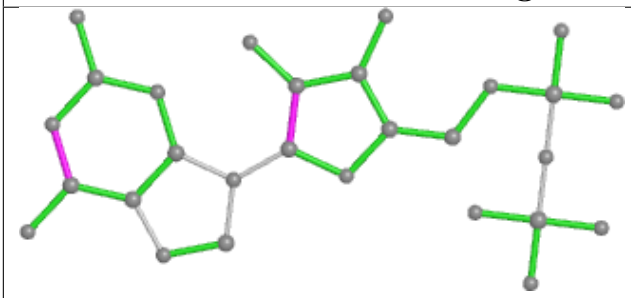


Rings

Ligand GDP J 1101



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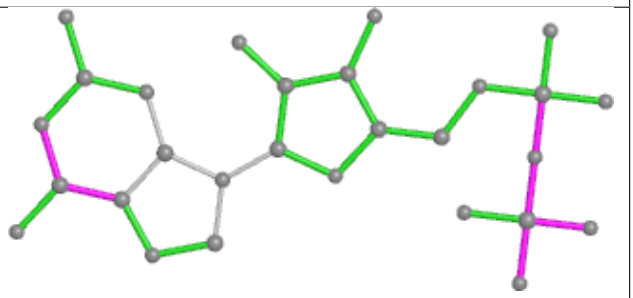

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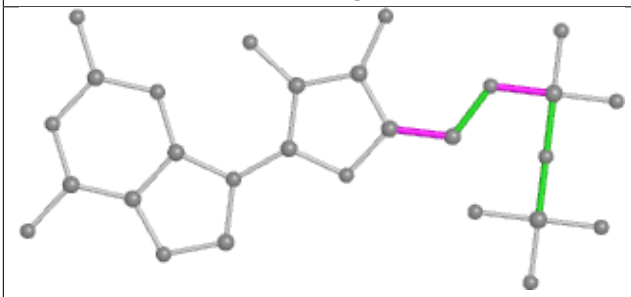

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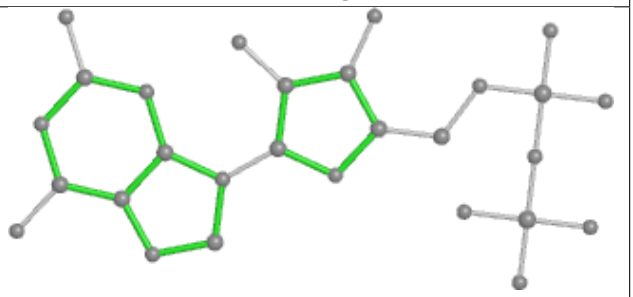
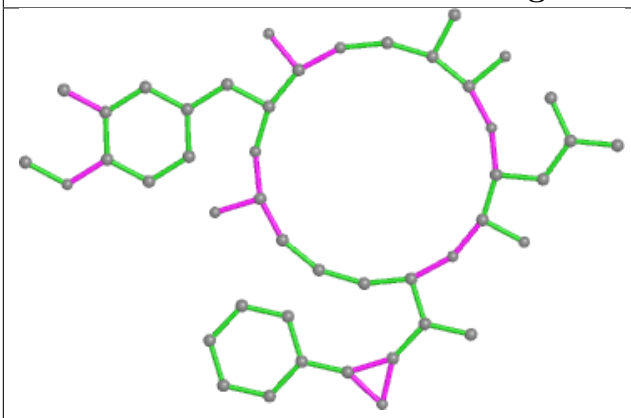


Rings

Ligand YNP I 501



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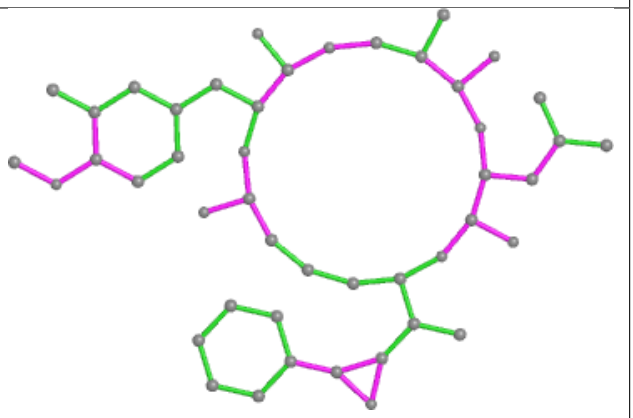

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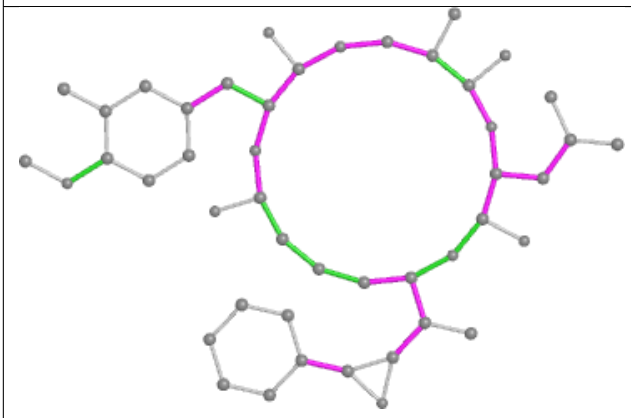

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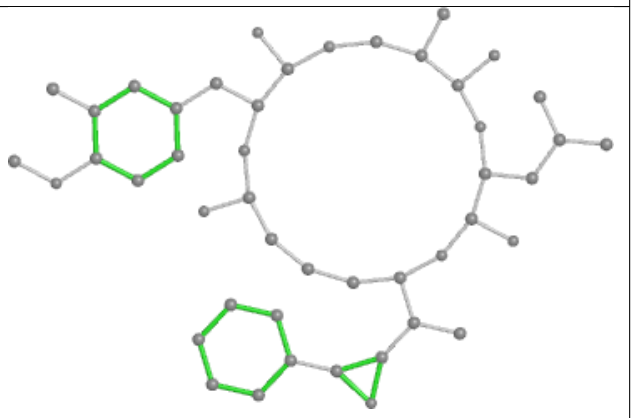
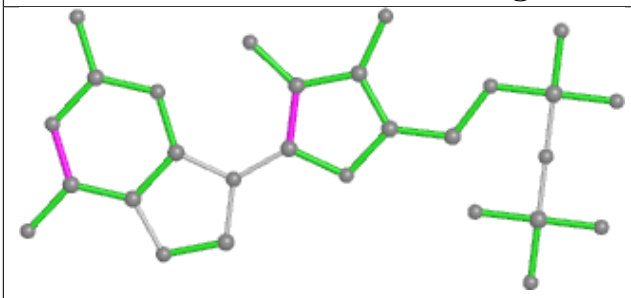


Rings

Ligand GDP D 1101



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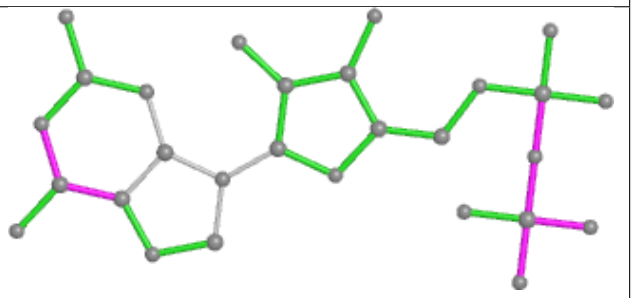

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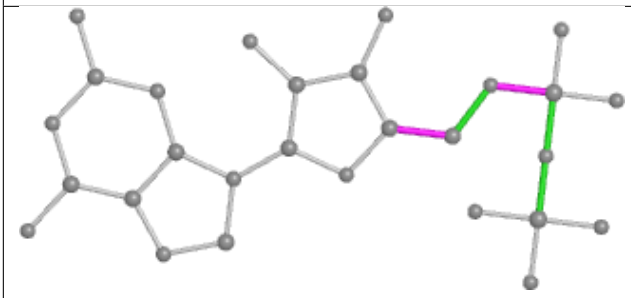

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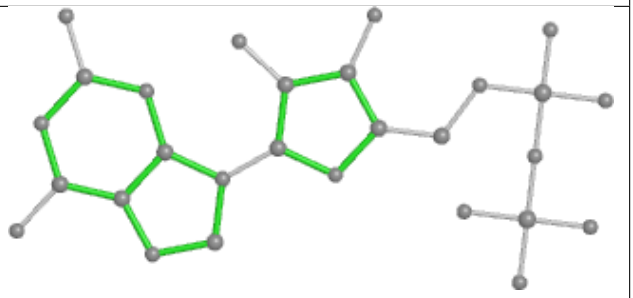
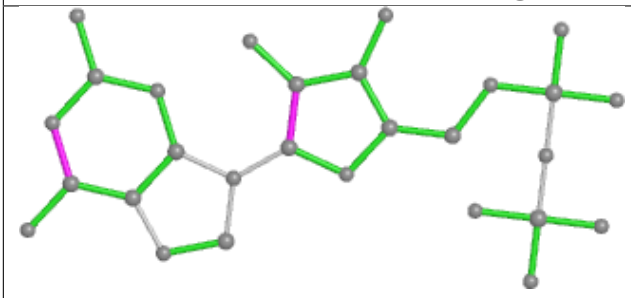


Rings

Ligand GDP N 1101



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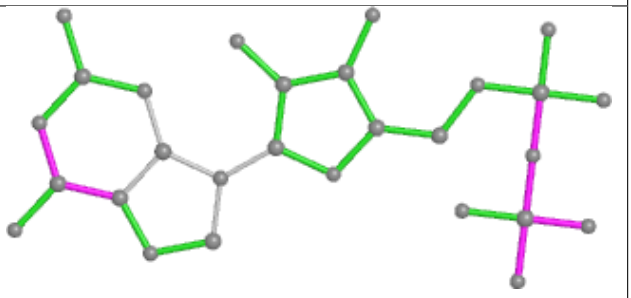

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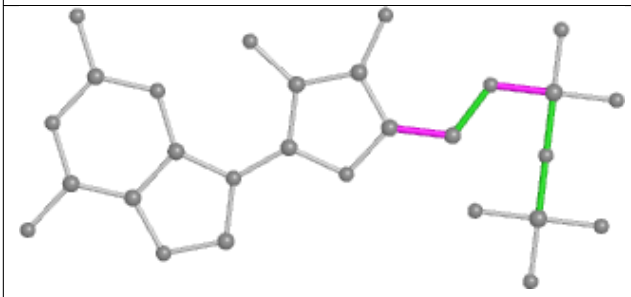

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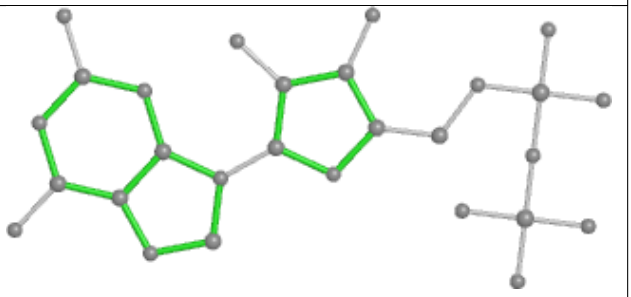
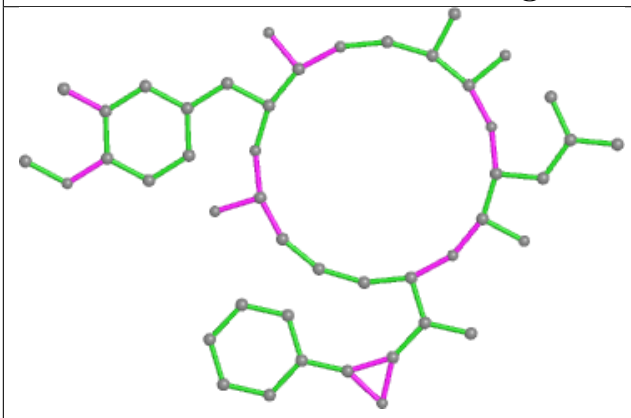


Rings

Ligand YNP A 501



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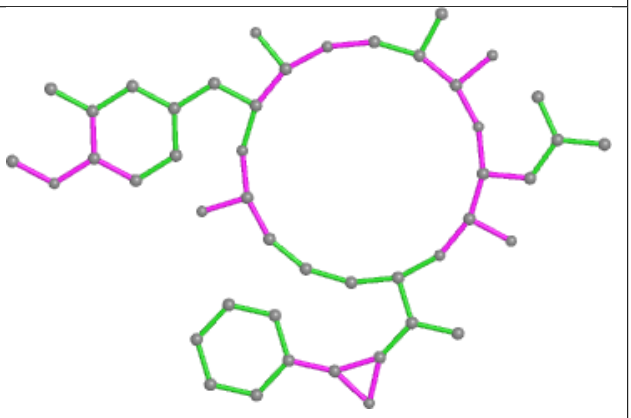
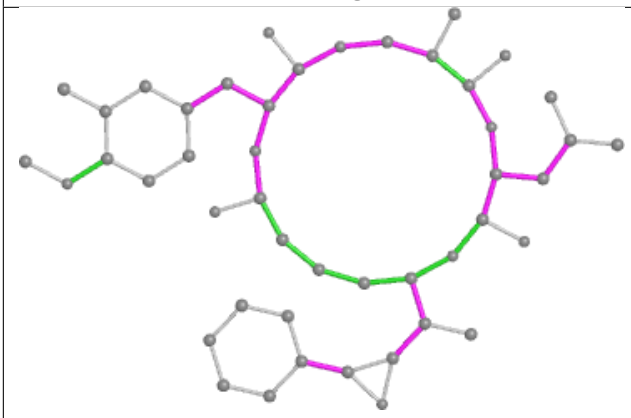


Bond angles



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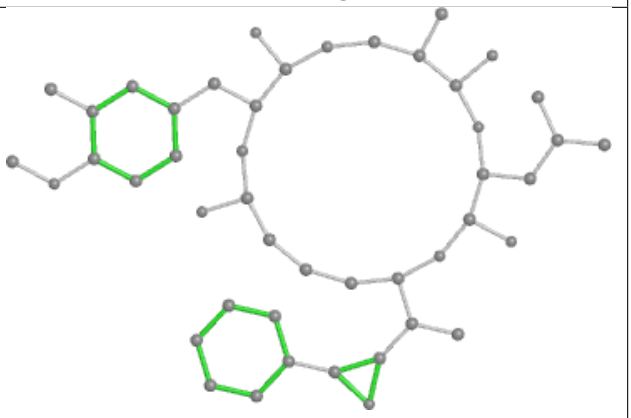
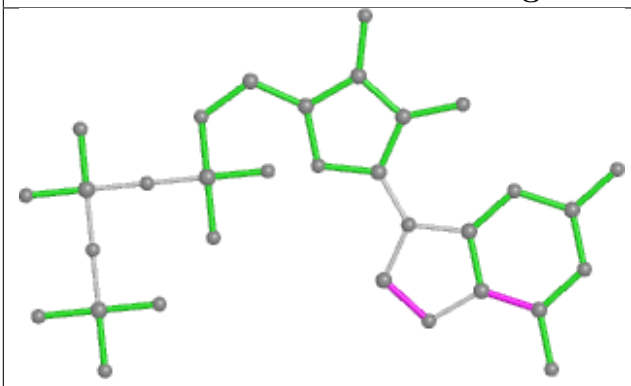
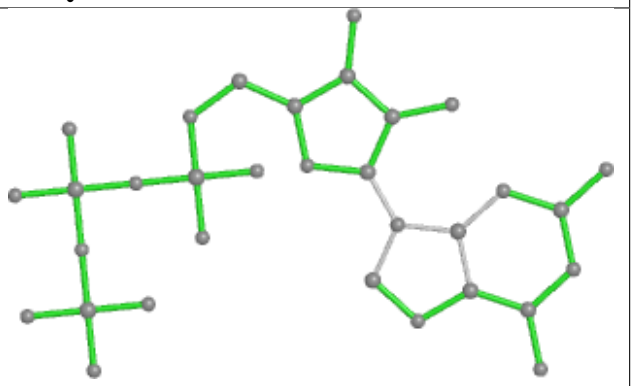


Rings

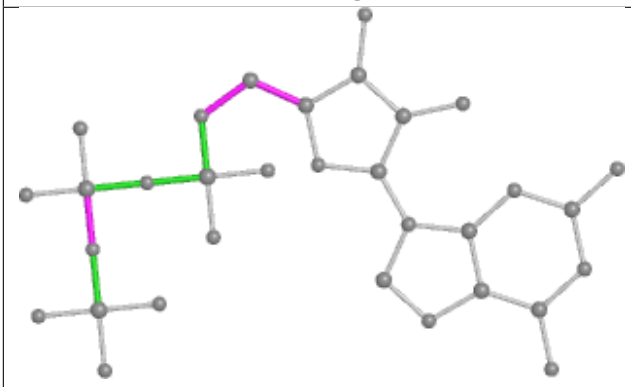
Ligand GTP Q 502



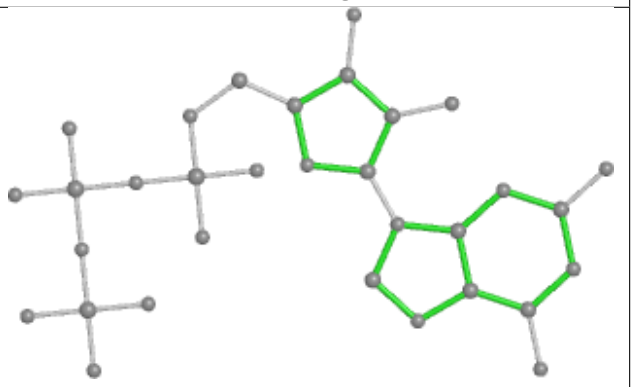
Bond lengths



Bond angles

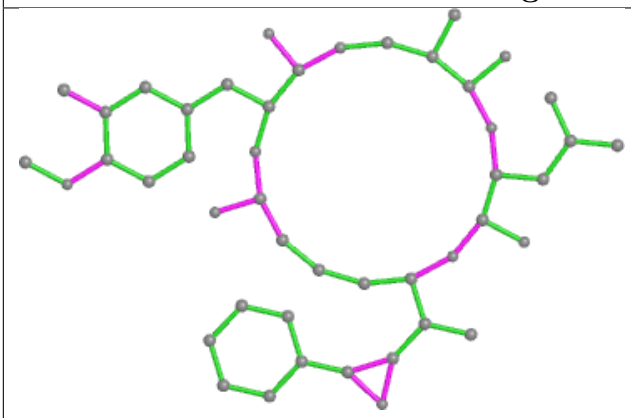


Torsions



Rings

Ligand YNP C 501



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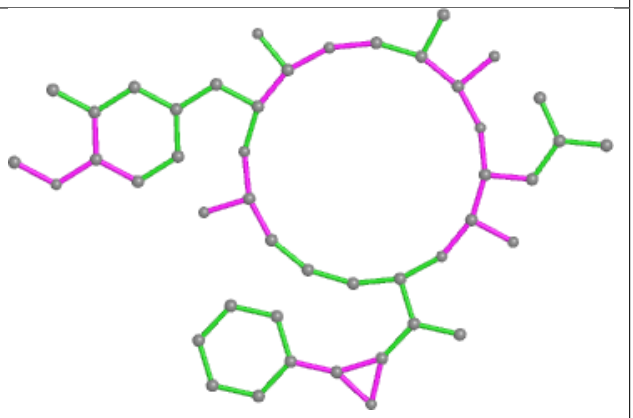

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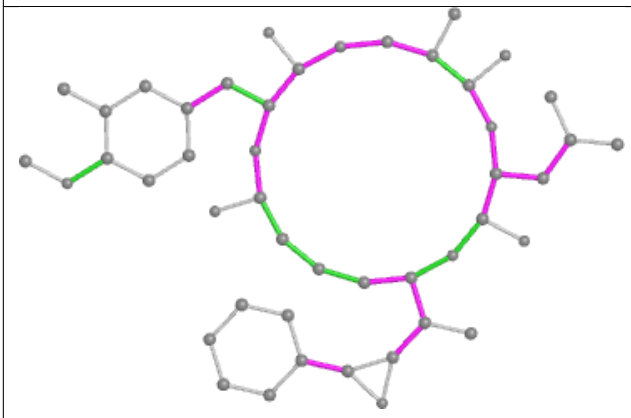

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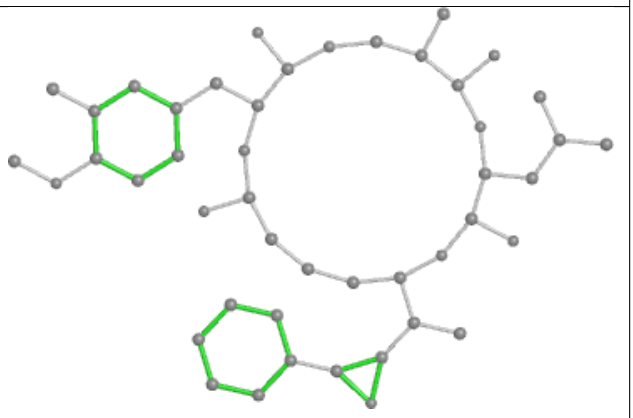
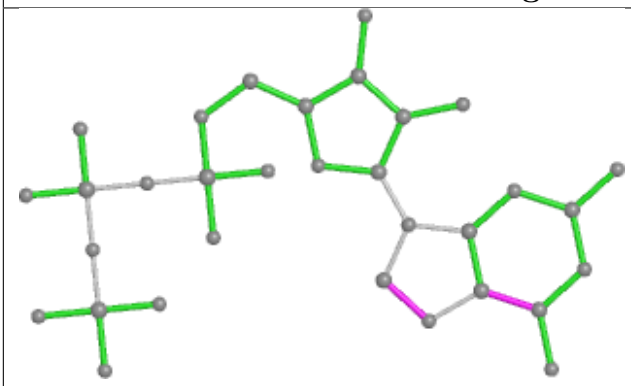


Rings

Ligand GTP O 502



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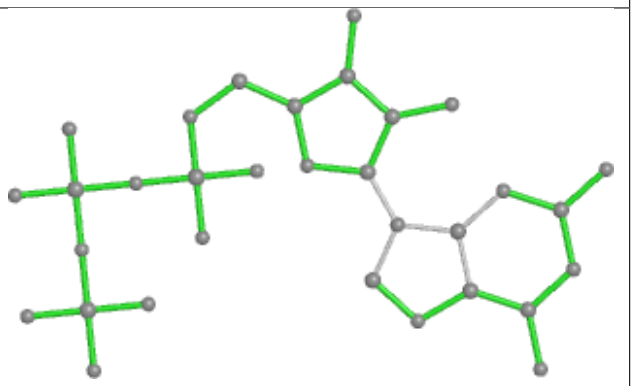
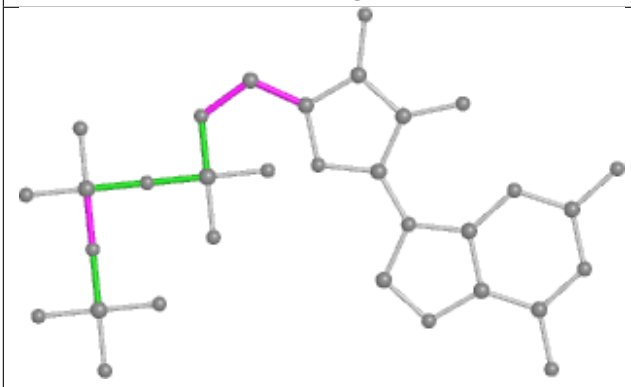
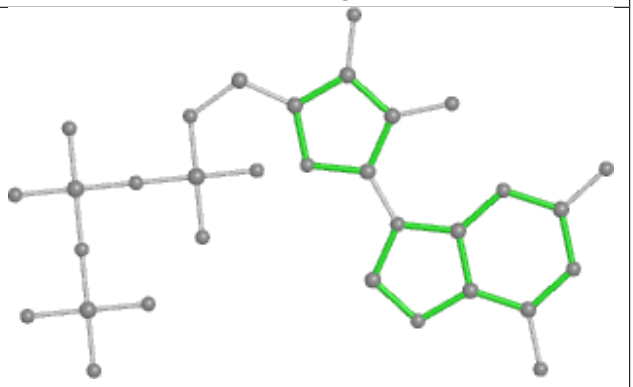


Bond angles

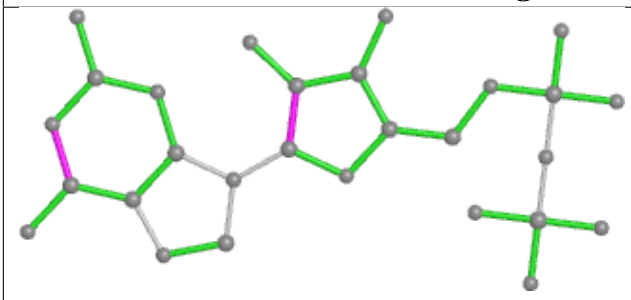


Torsions

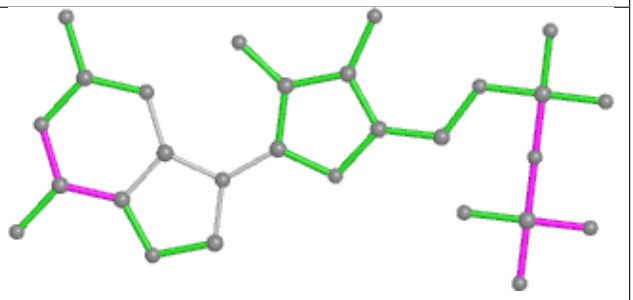


Rings

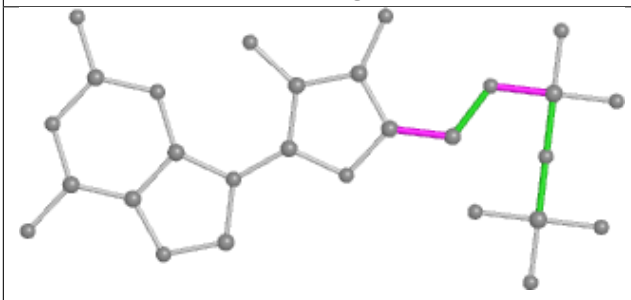
Ligand GDP L 1101



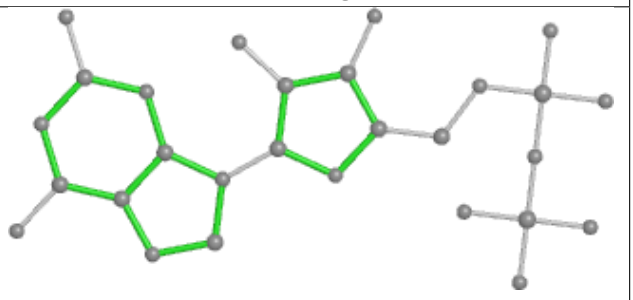
Bond lengths



Bond angles

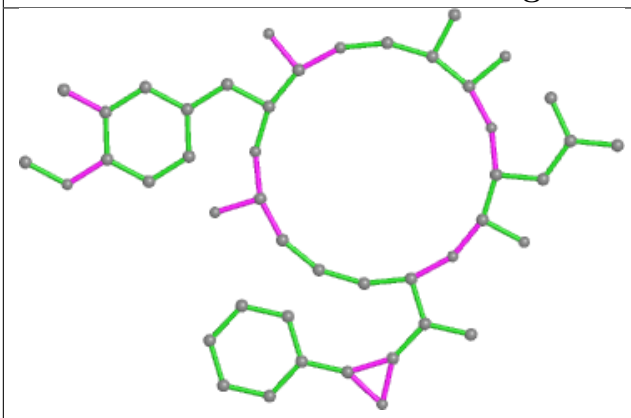


Torsions



Rings

Ligand YNP E 501



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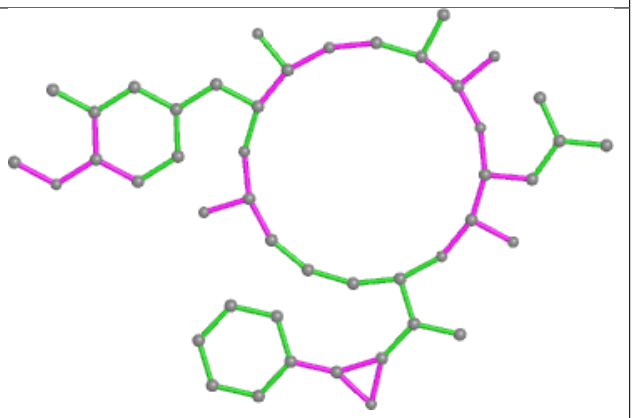
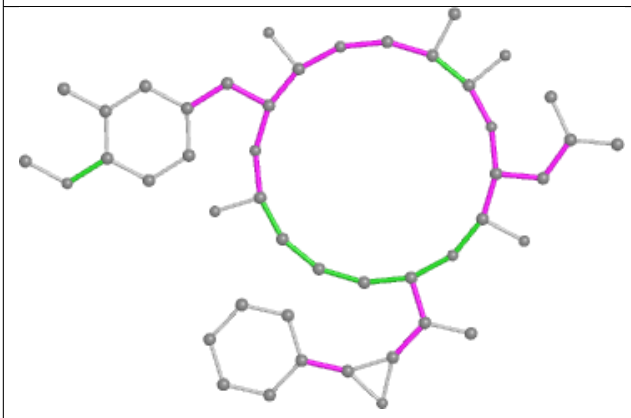


Bond angles



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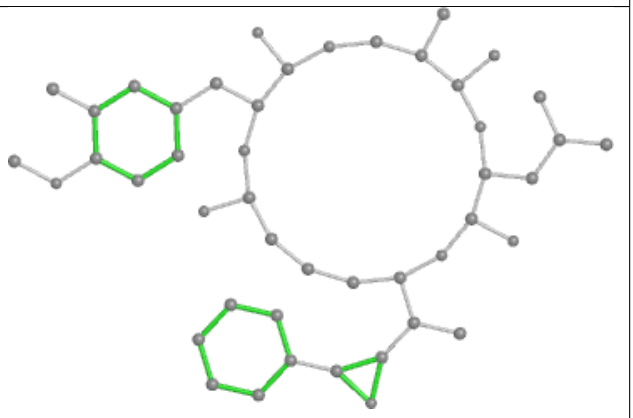
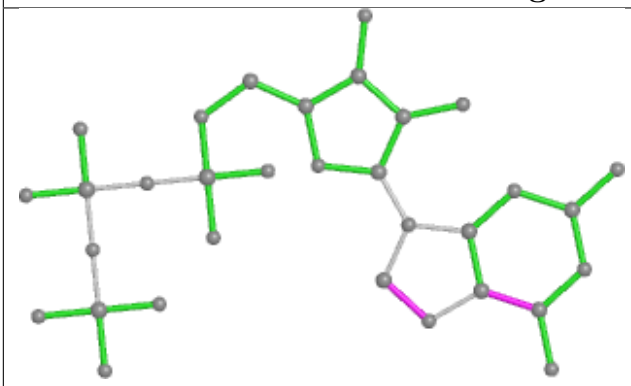
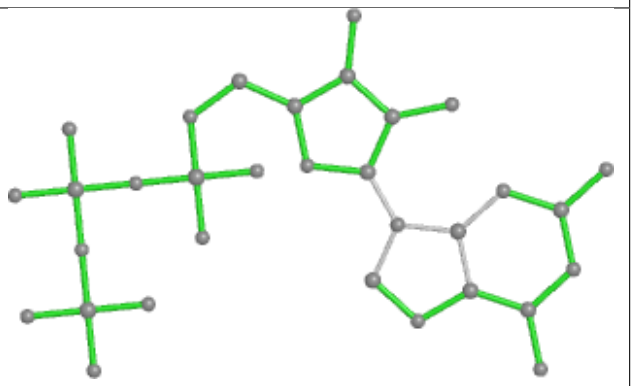


Rings

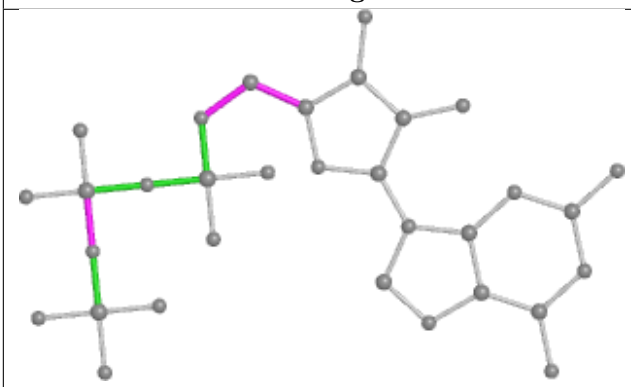
Ligand GTP I 502



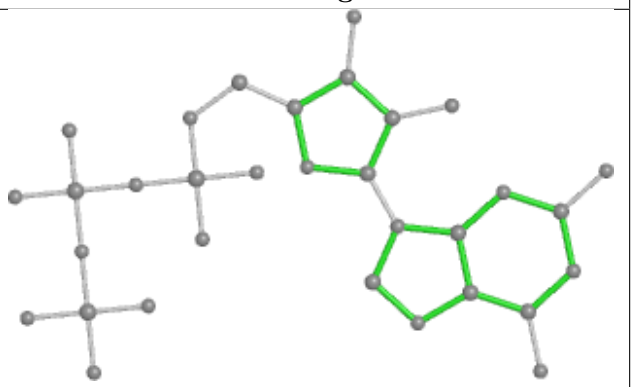
Bond lengths



Bond angles

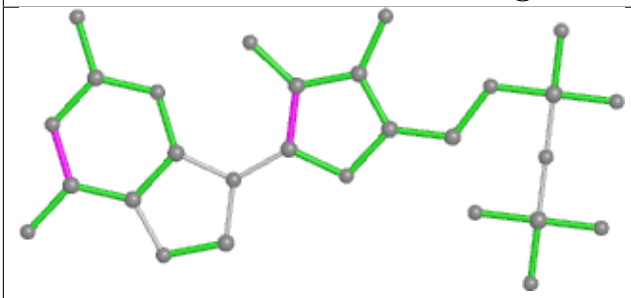


Torsions

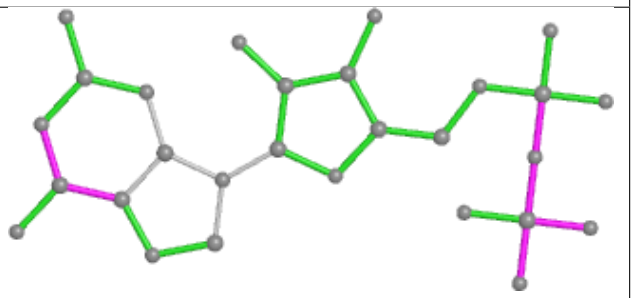


Rings

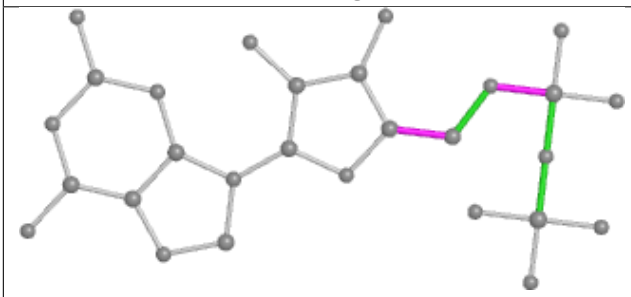
Ligand GDP F 1101



Bond lengths



Bond angles



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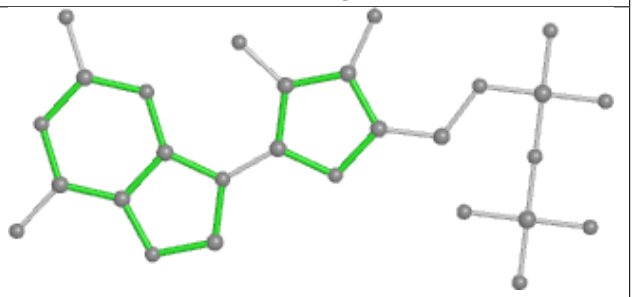
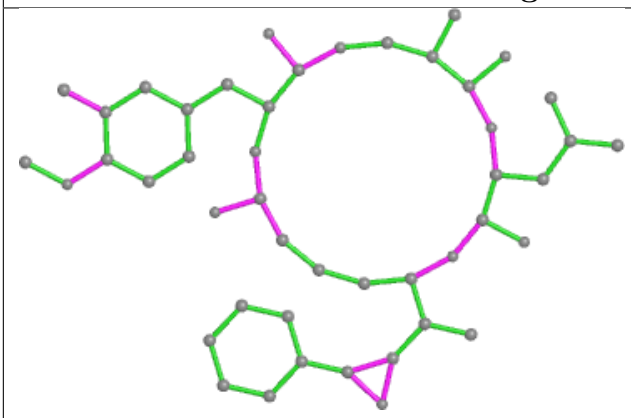


Rings

Ligand YNP K 501



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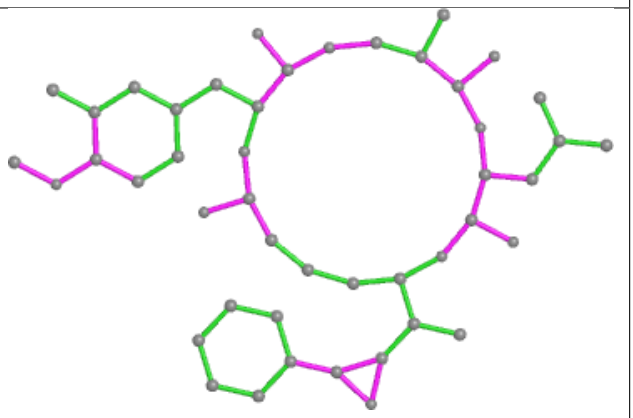
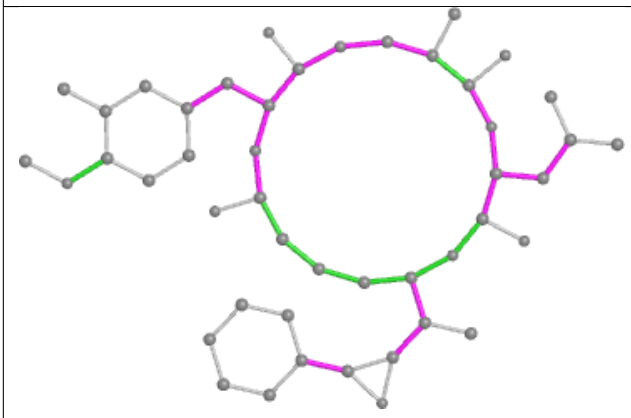
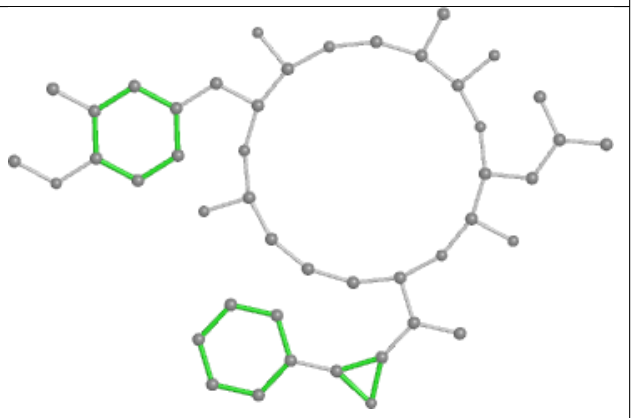


Bond angles

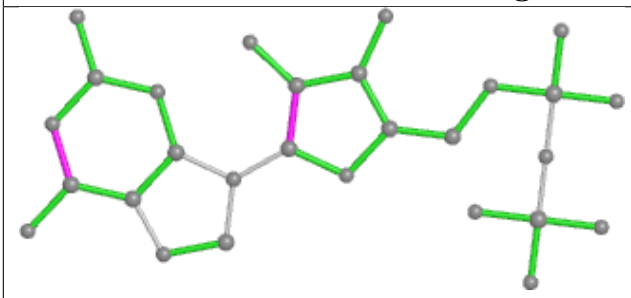


Torsions

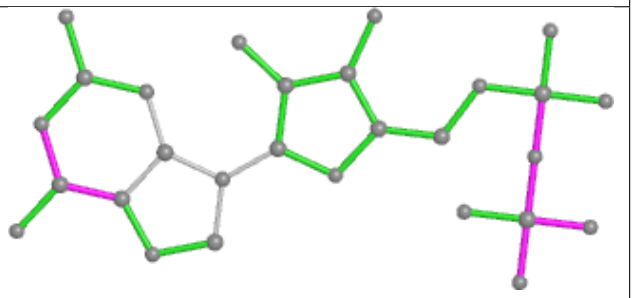


Rings

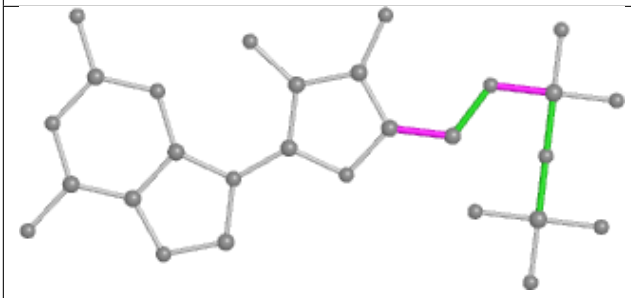
Ligand GDP P 1101



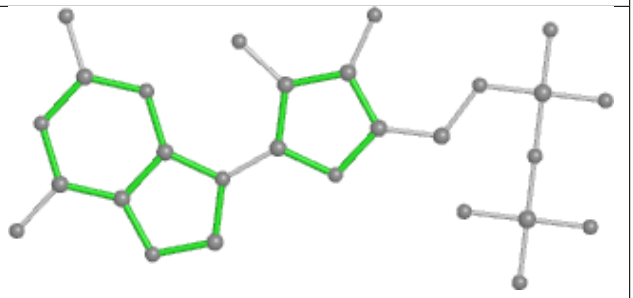
Bond lengths



Bond angles

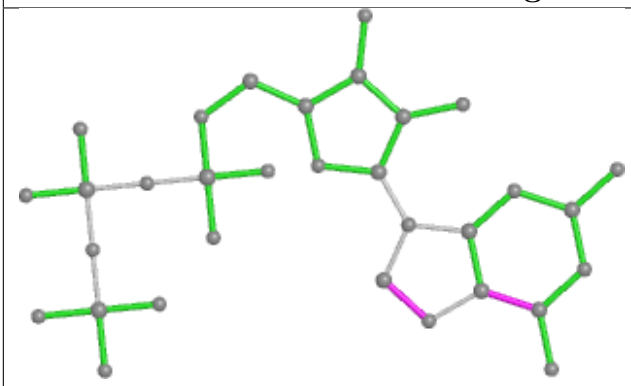


Torsions



Rings

Ligand GTP E 502



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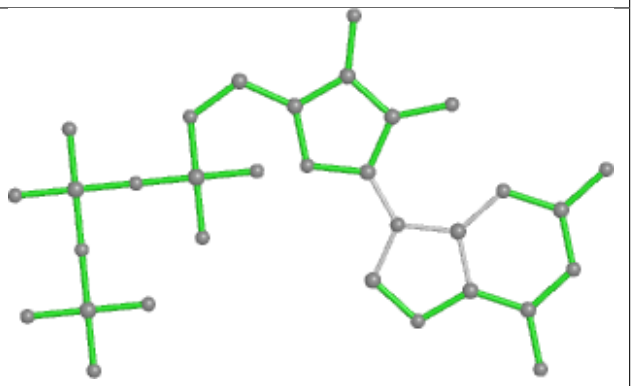
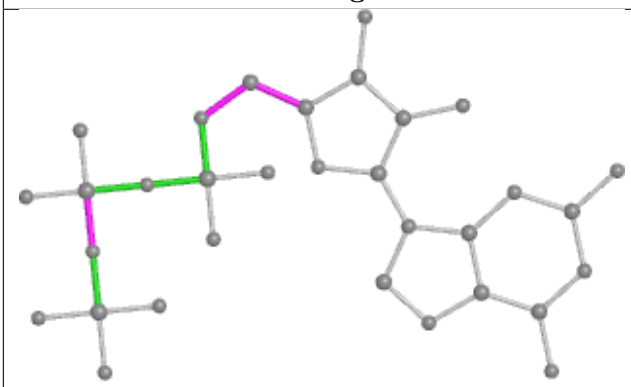
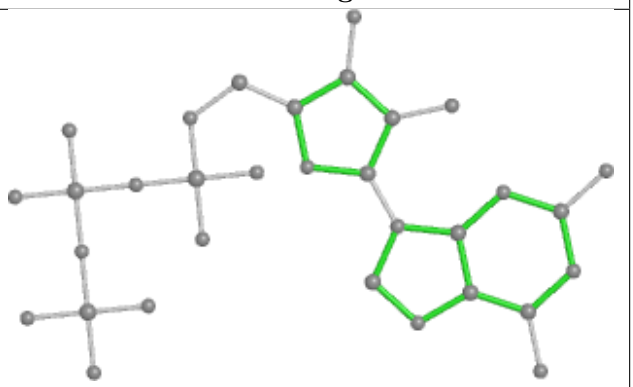


Bond angles

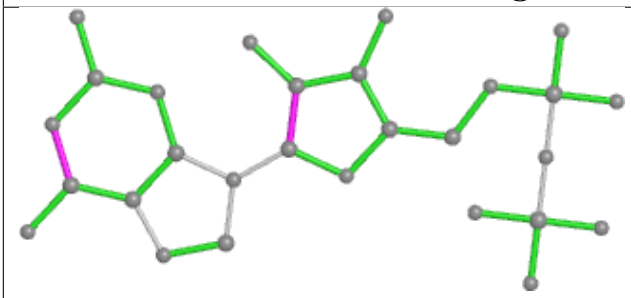


Torsions



Rings

Ligand GDP H 1101



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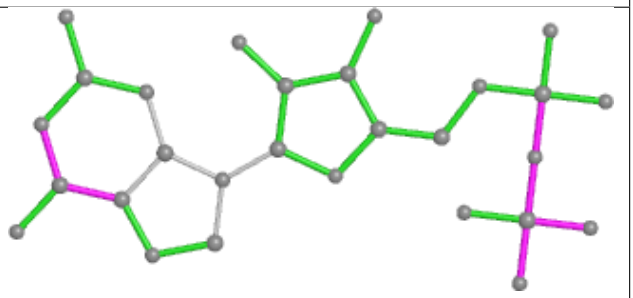
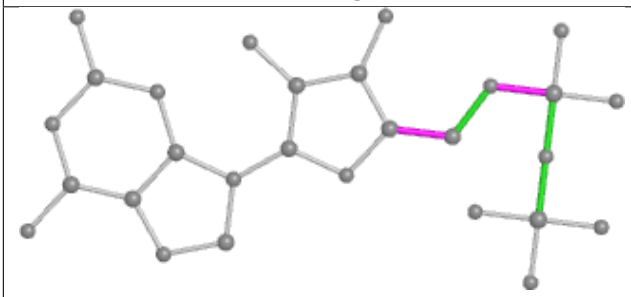
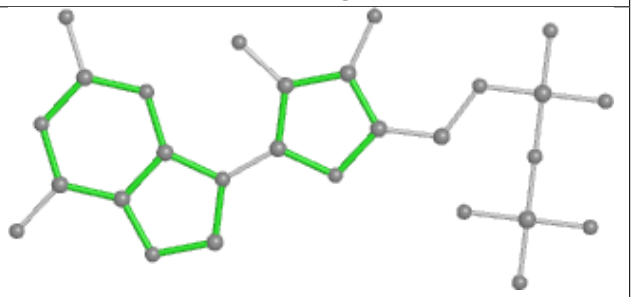


Bond angles

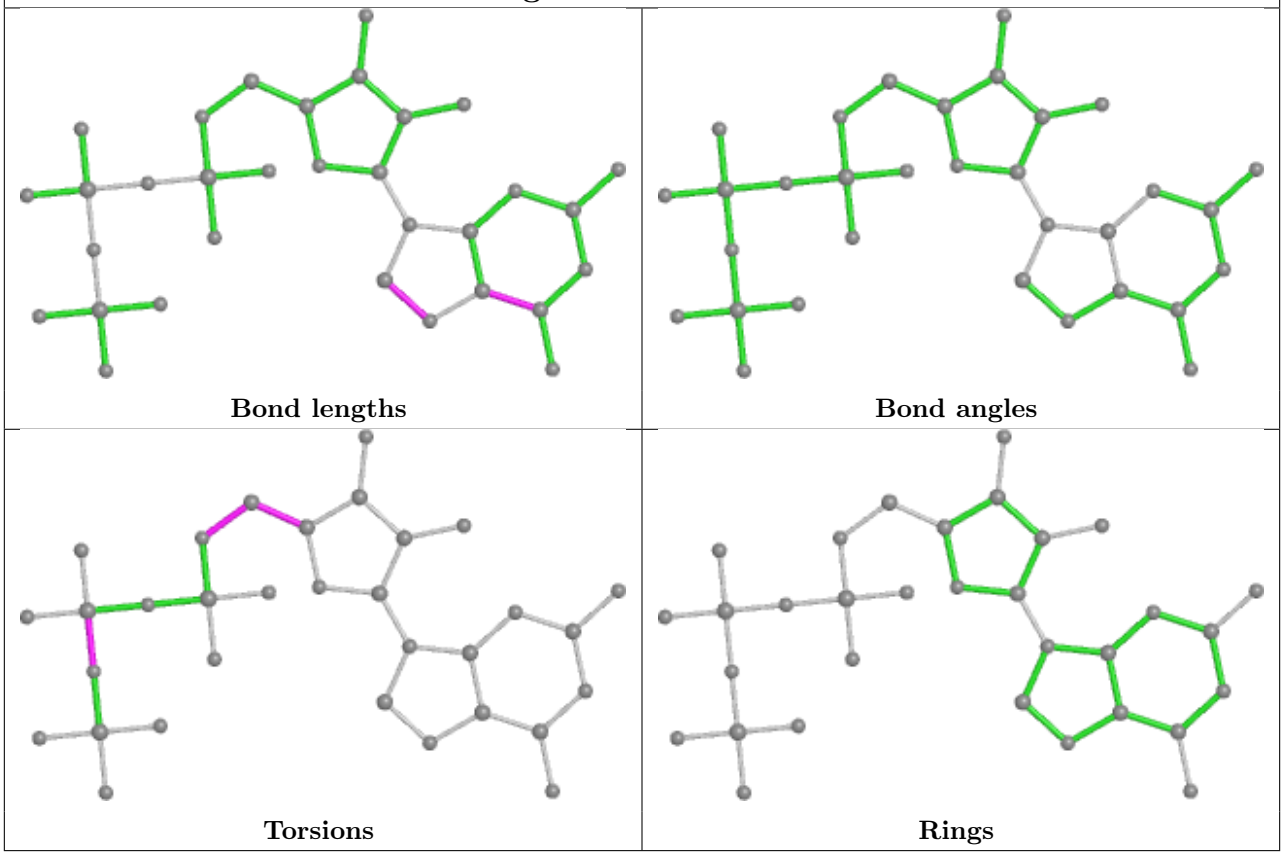


Torsions



Rings

Ligand GTP A 502



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-23627. These allow visual inspection of the internal detail of the map and identification of artifacts.

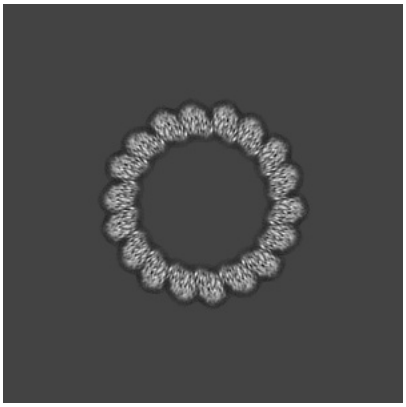
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X

Y



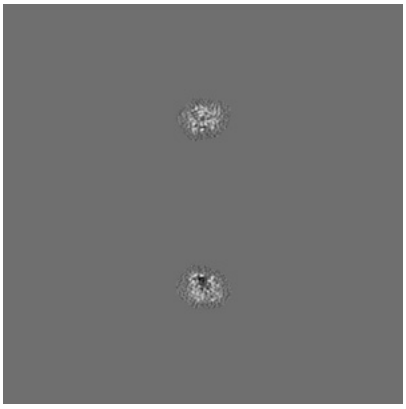
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 300



Y Index: 300

Z Index: 300

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: 410

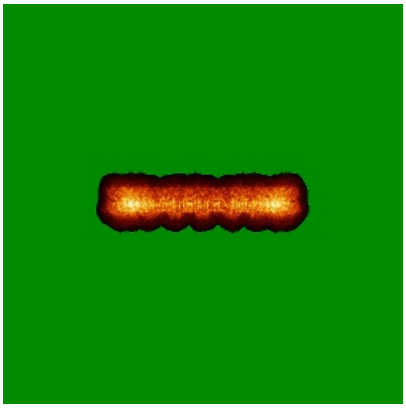
Y Index: 193

Z Index: 300

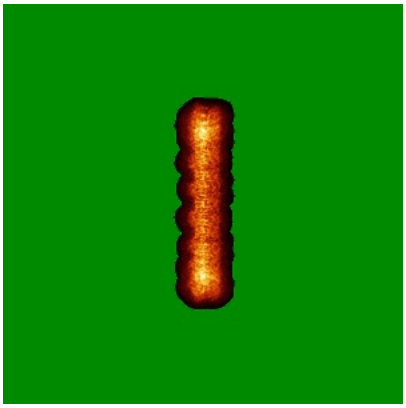
The images above show the largest variance slices of the map in three orthogonal directions.

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

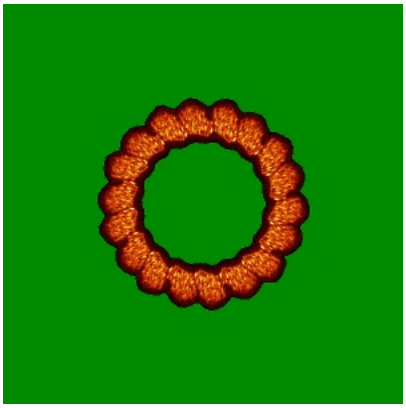
6.4.1 Primary map



X



Y



Z

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 4.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

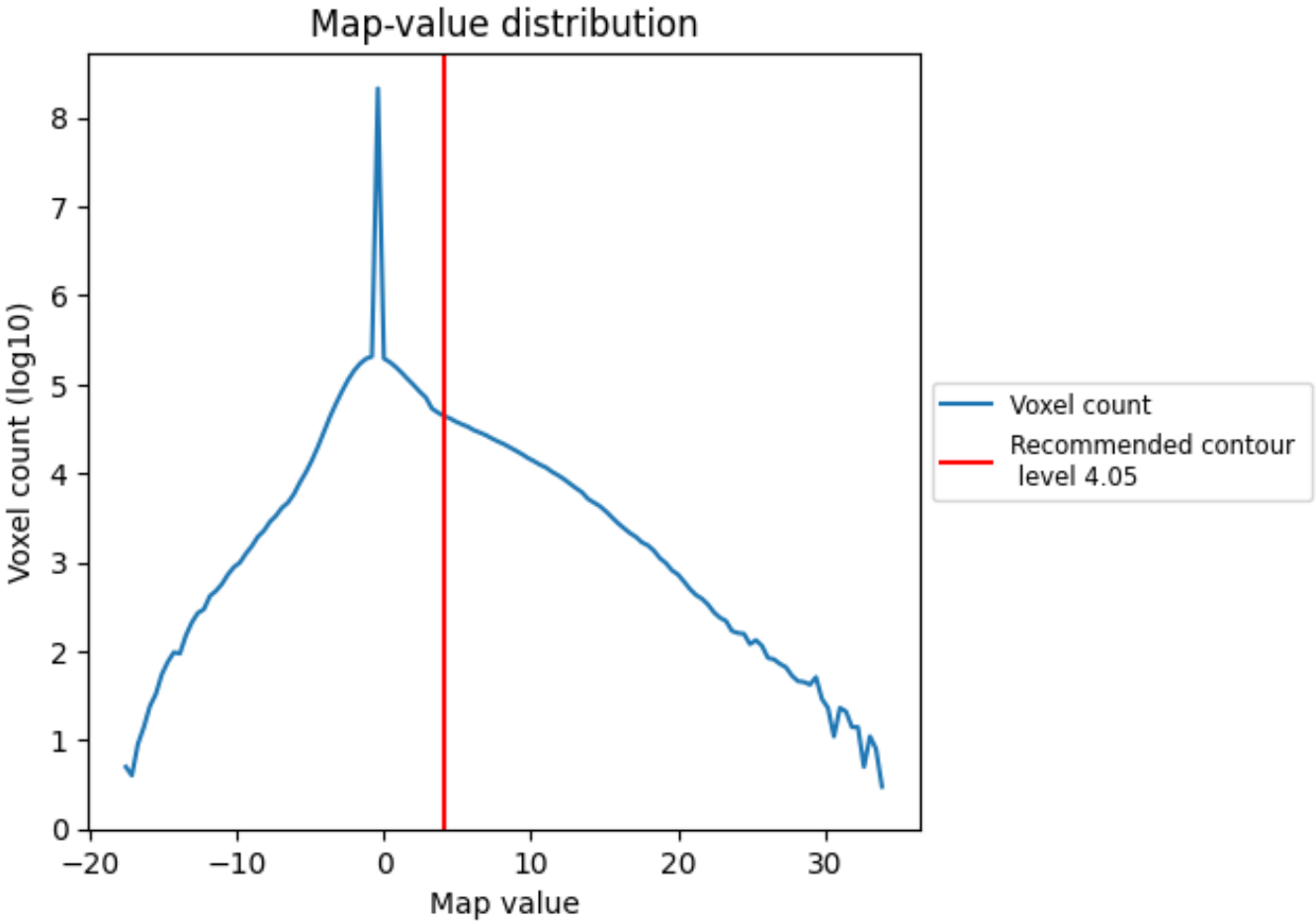
6.6 Mask visualisation (i)

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

7 Map analysis

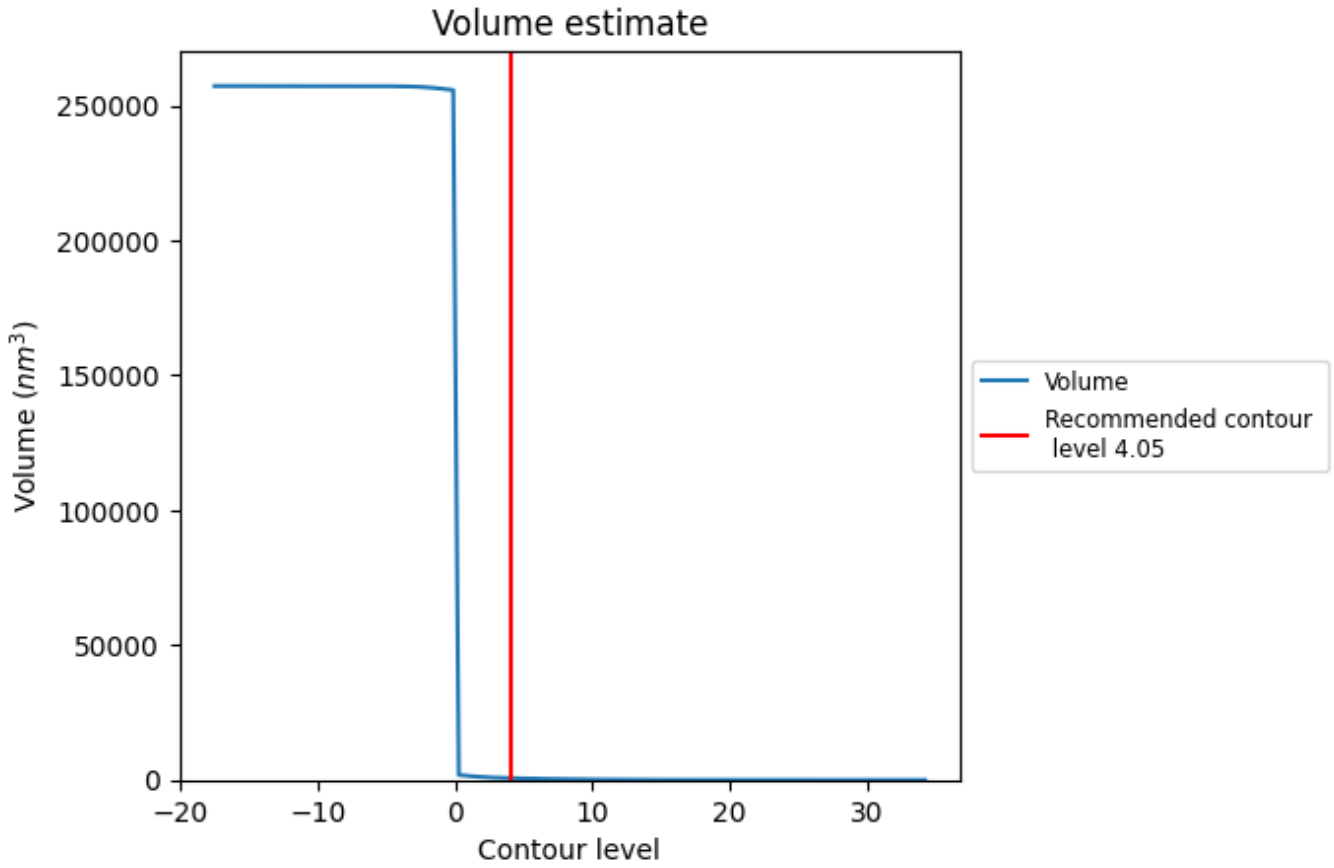
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

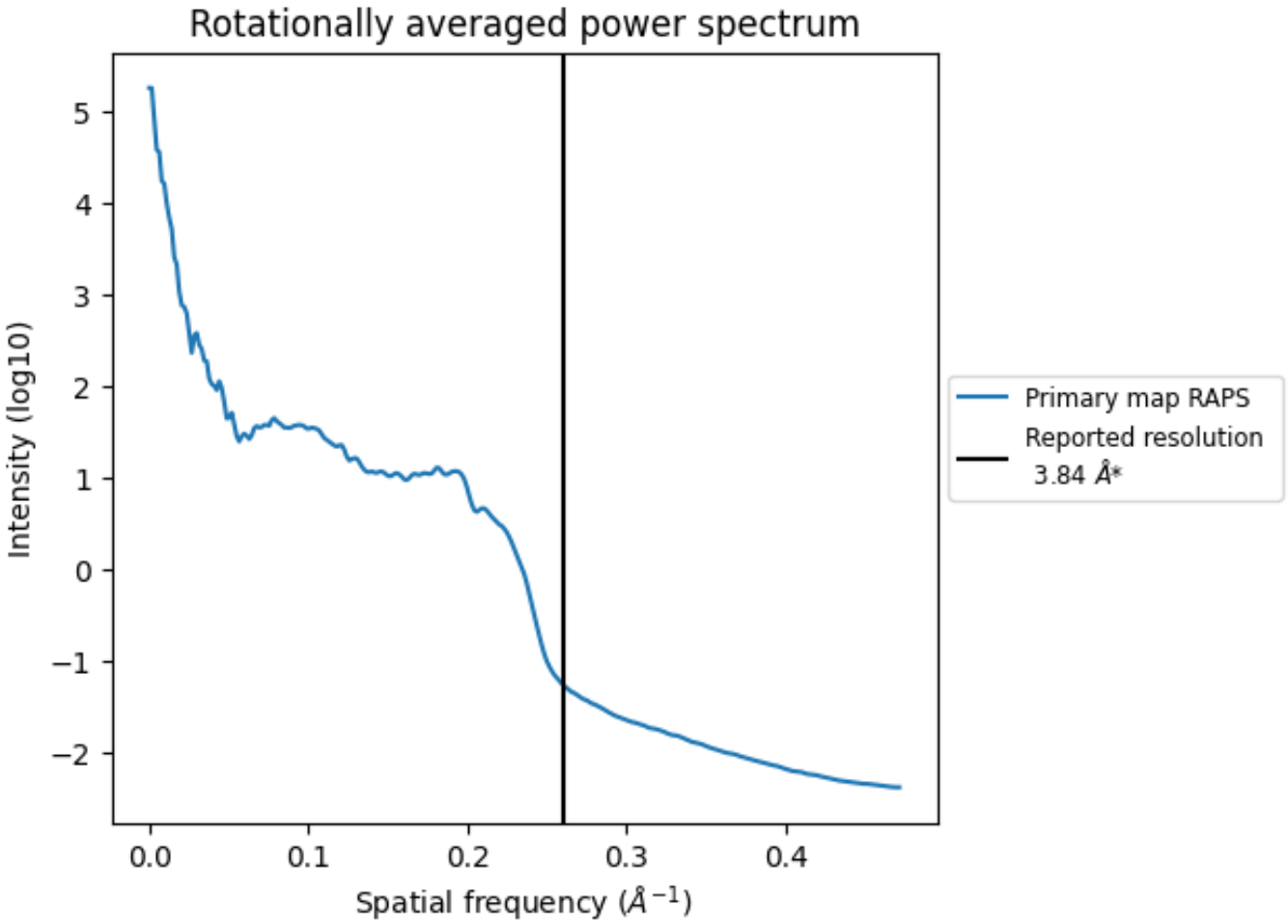
7.2 Volume estimate (i)



The volume at the recommended contour level is 658 nm^3; this corresponds to an approximate mass of 594 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)

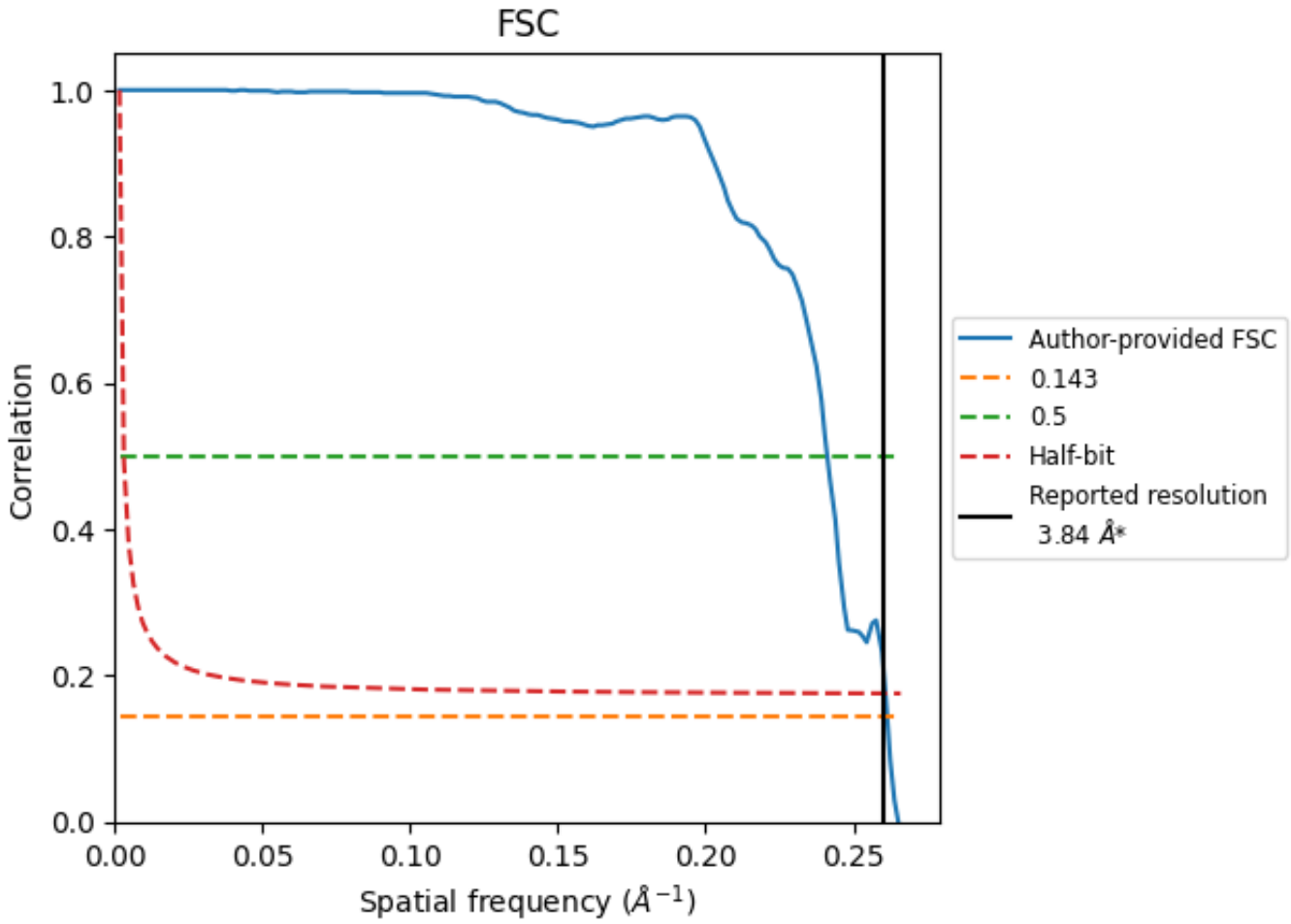


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

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 0.260 Å^{-1}

8.2 Resolution estimates (i)

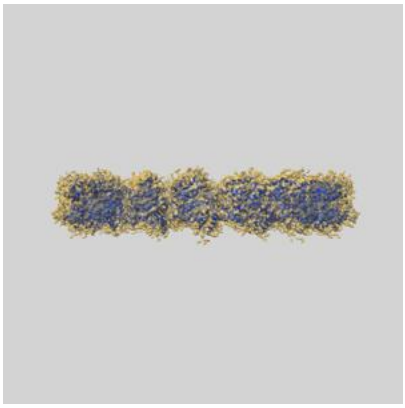
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.82	4.15	3.83
Unmasked-calculated*	-	-	-

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

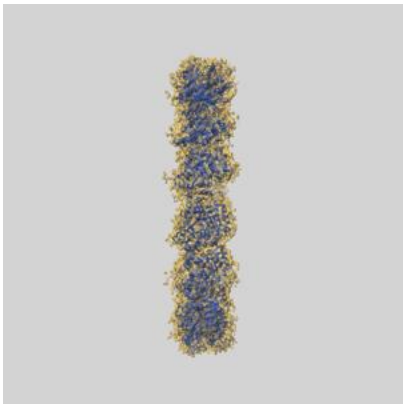
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23627 and PDB model 7M20. Per-residue inclusion information can be found in section 3 on page 8.

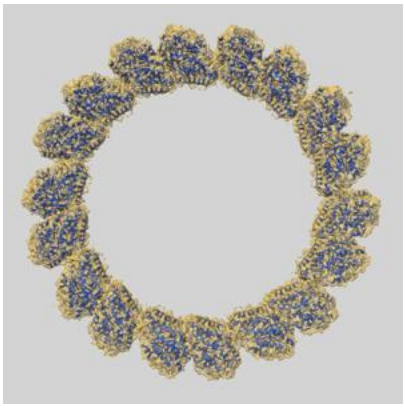
9.1 Map-model overlay



X



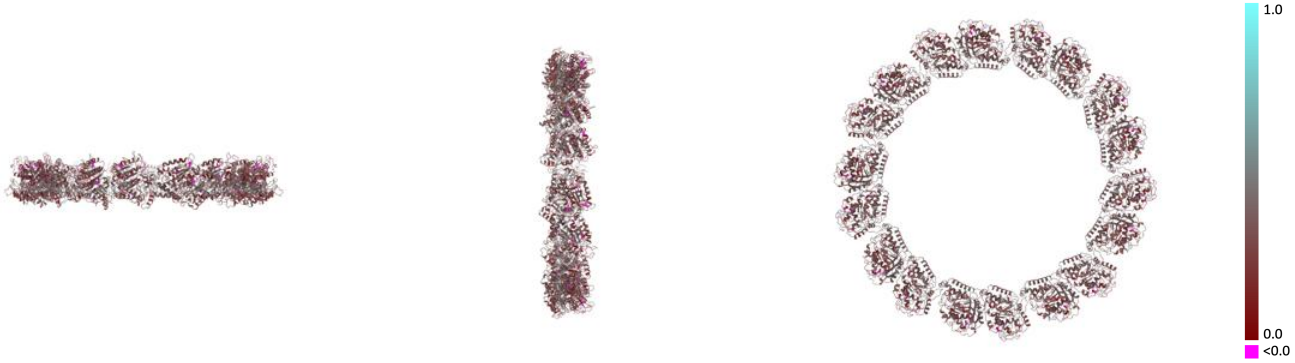
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.05 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.

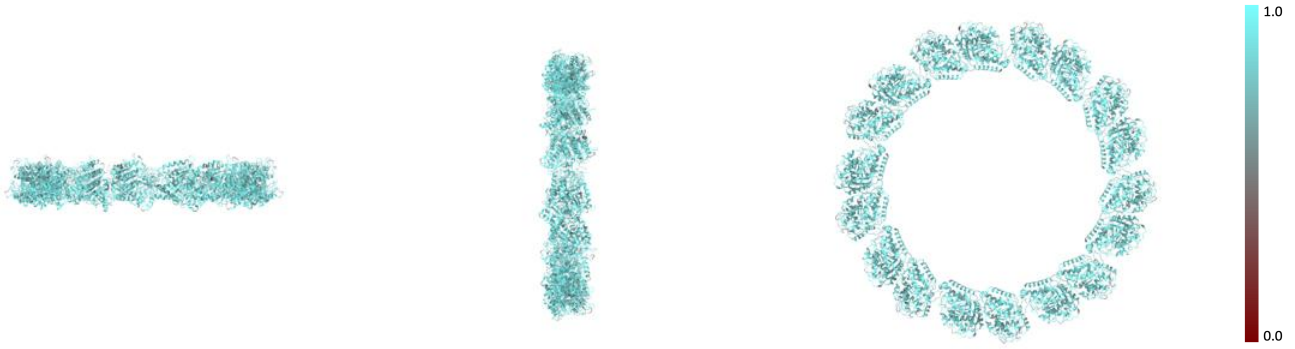
9.2 Q-score mapped to coordinate model



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.

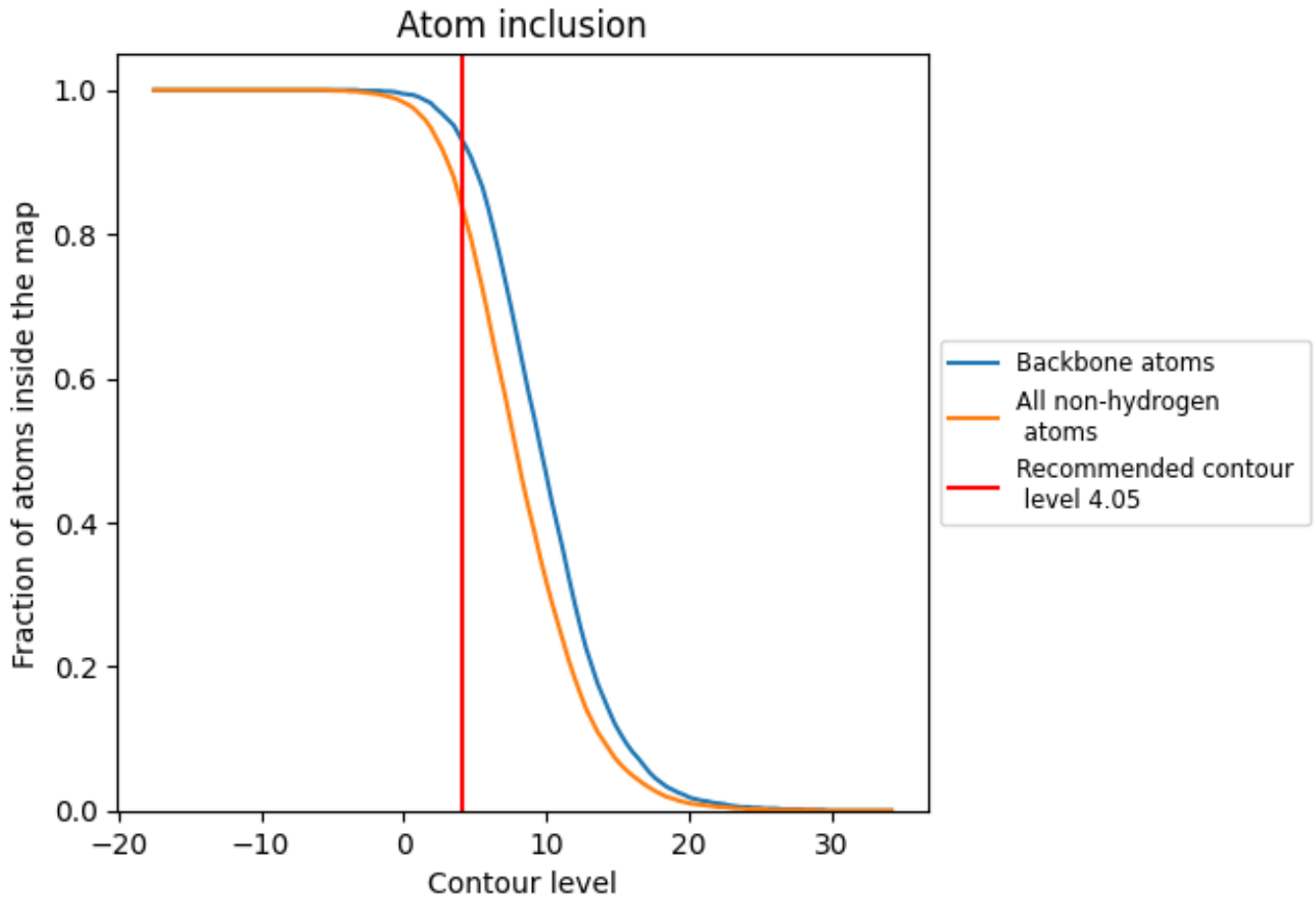
9.3 Atom inclusion mapped to coordinate model



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 (4.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 84% 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 (4.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.3380
A	0.8460	0.3350
B	0.8400	0.3420
C	0.8410	0.3350
D	0.8400	0.3400
E	0.8420	0.3330
F	0.8400	0.3410
G	0.8420	0.3340
H	0.8440	0.3410
I	0.8430	0.3350
J	0.8400	0.3400
K	0.8430	0.3350
L	0.8420	0.3410
M	0.8440	0.3350
N	0.8400	0.3410
O	0.8430	0.3350
P	0.8400	0.3400
Q	0.8440	0.3340
R	0.8410	0.3400