



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:16 PM UTC

PDB ID : 7M18 / pdb_00007m18
EMDB ID : EMD-23615
Title : HeLa-tubulin in complex with cryptophycin 1
Authors : Eren, E.
Deposited on : 2021-03-12
Resolution : 3.38 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:

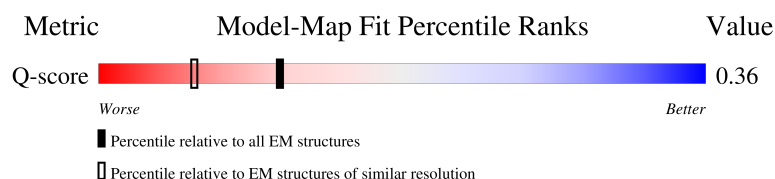
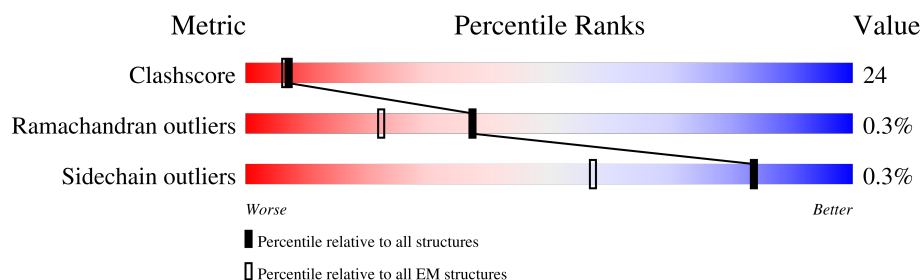
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.38 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.



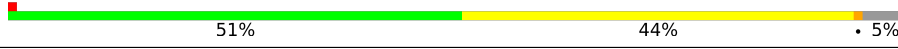
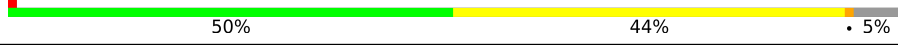
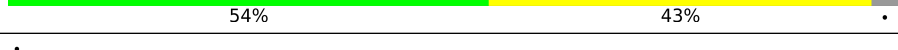
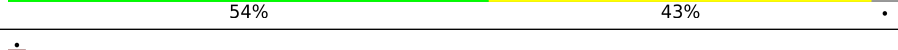
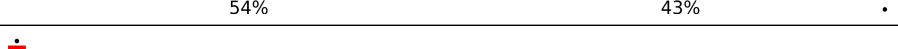
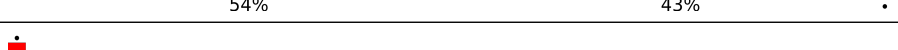
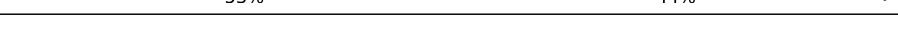
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14261 (2.88 - 3.88)

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 $\leq 5\%$. 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	
1	D	450	
1	F	450	
1	H	450	

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Mol	Chain	Length	Quality of chain
1	J	450	
1	L	450	
1	N	450	
1	P	450	
2	A	451	
2	C	451	
2	E	451	
2	G	451	
2	I	451	
2	K	451	
2	M	451	
2	O	451	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 54064 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	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	D	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	F	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	H	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	J	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	L	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	N	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		
1	P	427	Total	C	N	O	S	1	0
			3312	2084	568	635	25		

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

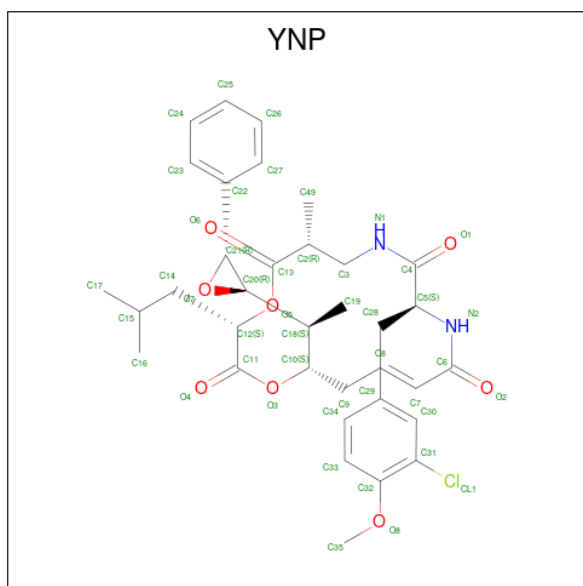
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	C	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	E	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	G	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	I	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	K	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		
2	M	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		

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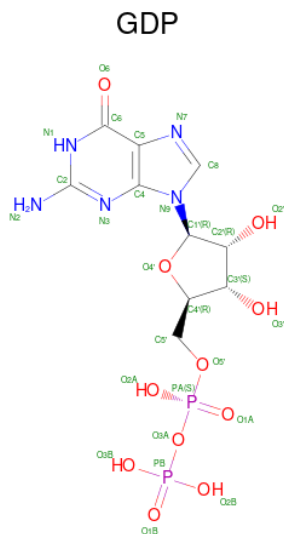
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	436	Total	C	N	O	S	0	0
			3340	2117	570	633	20		

- Molecule 3 is Cryptophycin 1 (CCD ID: YNP) (formula: $C_{35}H_{43}ClN_2O_8$).



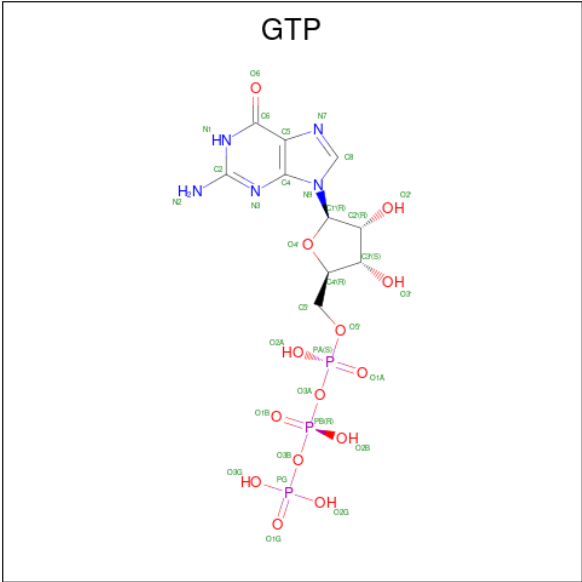
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	D	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	F	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	H	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	J	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	L	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	N	1	Total	C	Cl	N	O	0
			46	35	1	2	8	
3	P	1	Total	C	Cl	N	O	0
			46	35	1	2	8	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).

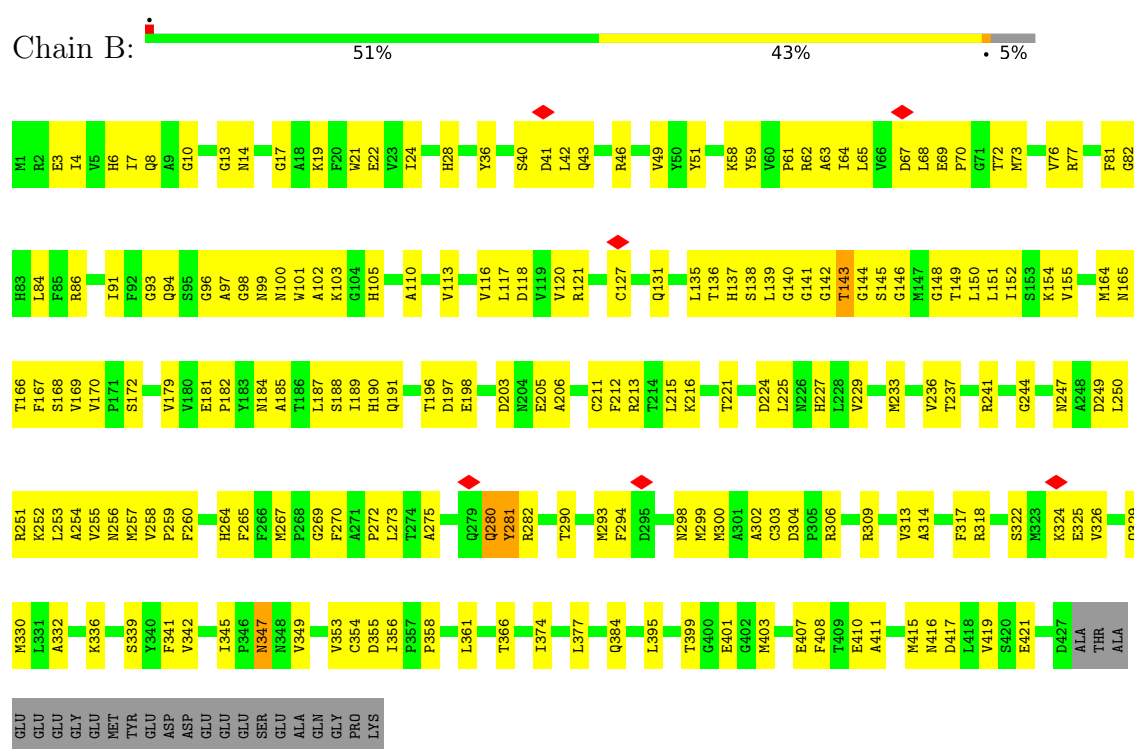


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	M	1	Total	C	N	O	P	0
			32	10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

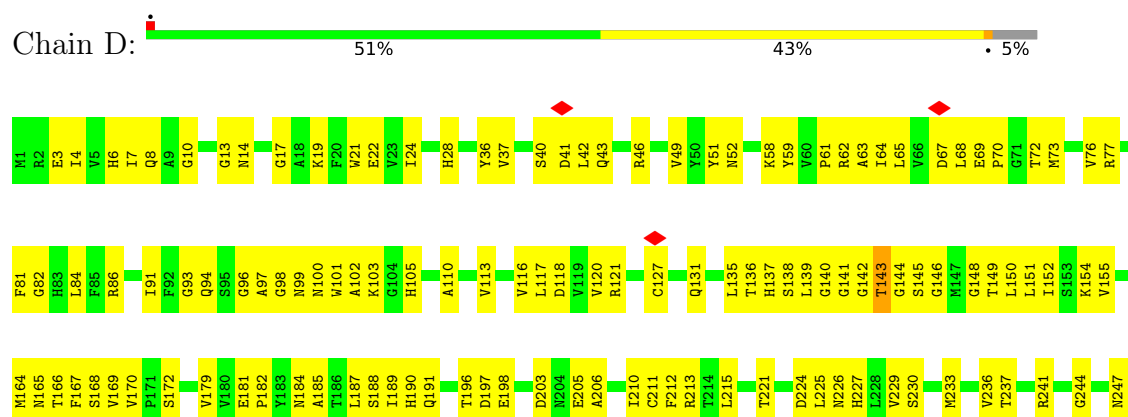
3 Residue-property plots

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.

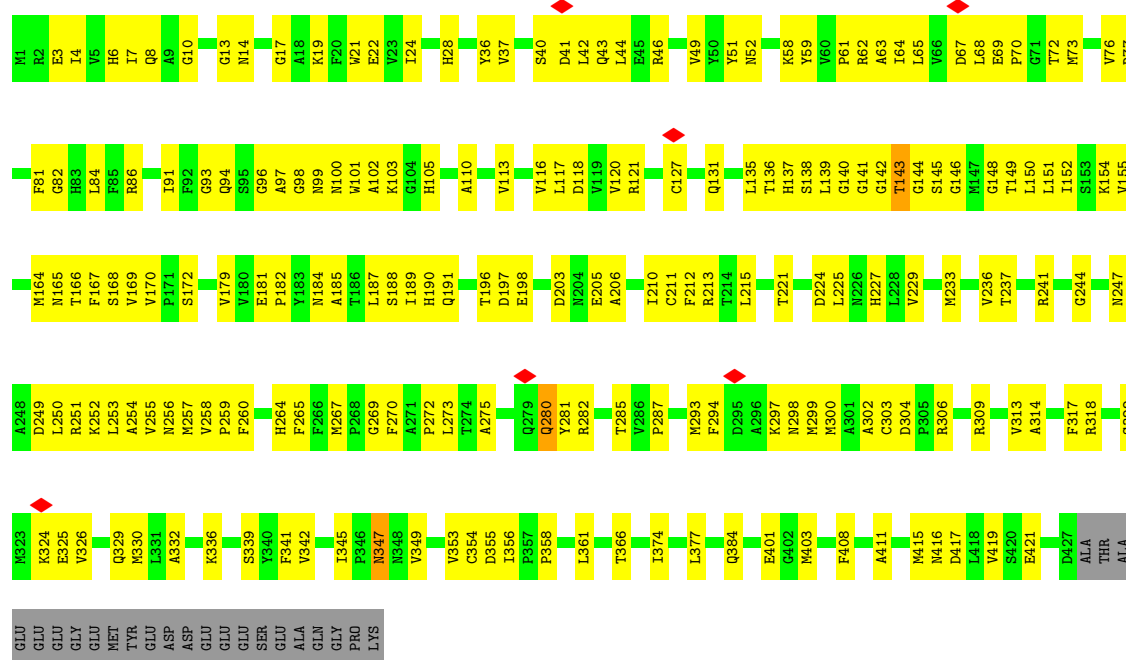
• Molecule 1: Tubulin beta-3 chain



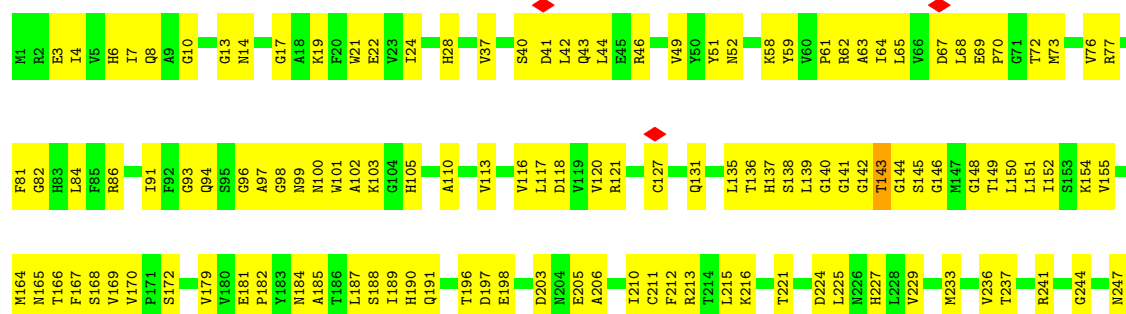
• Molecule 1: Tubulin beta-3 chain



- Molecule 1: Tubulin beta-3 chain



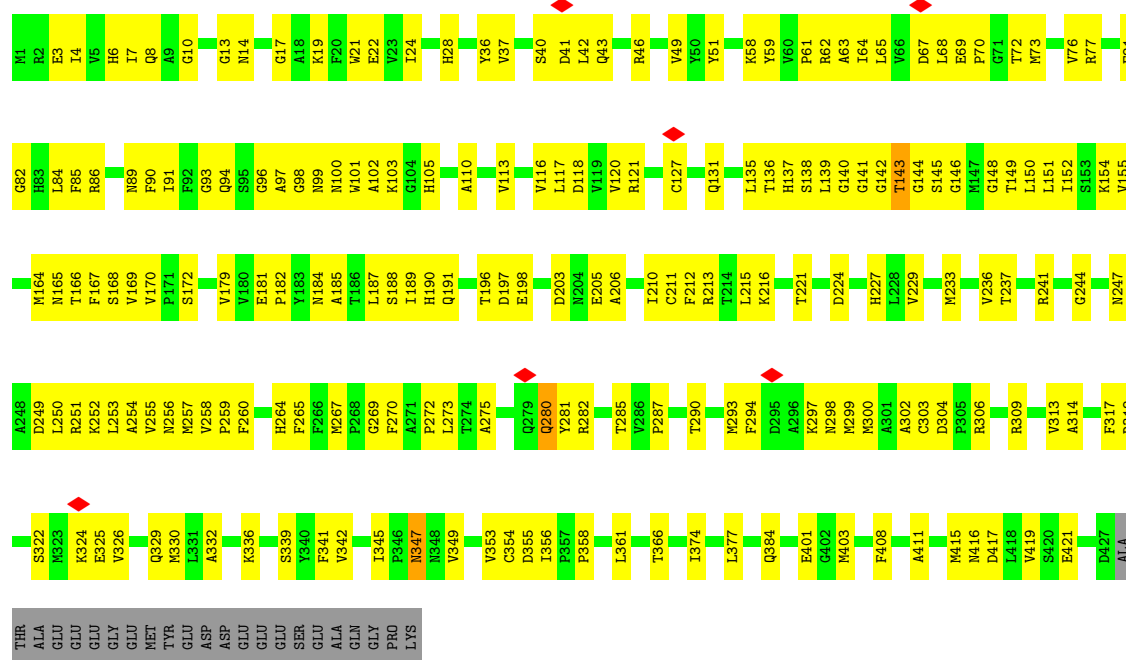
- Molecule 1: Tubulin beta-3 chain



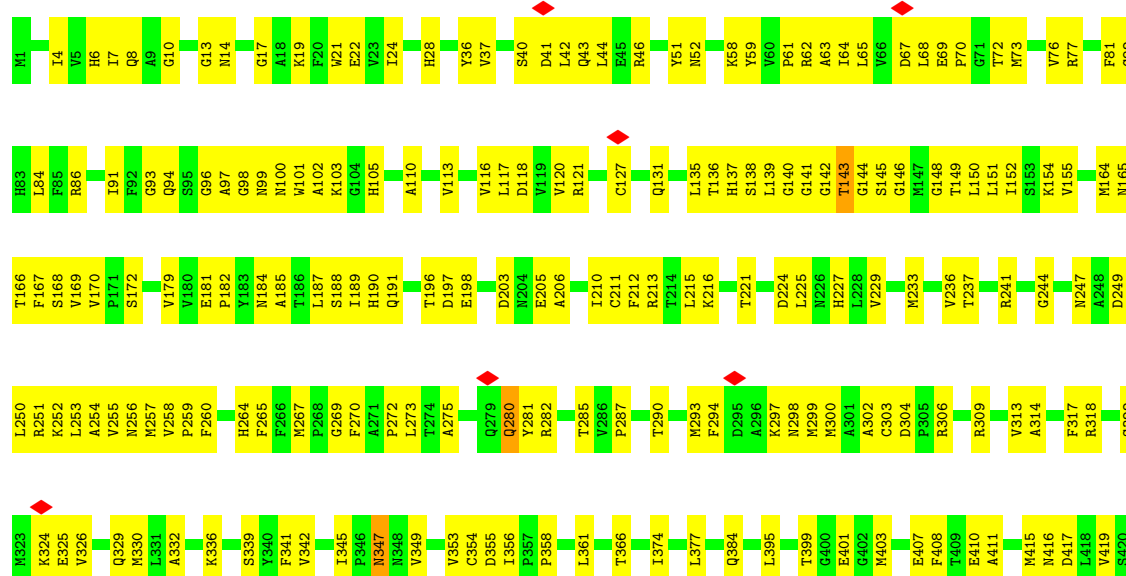


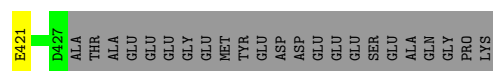


• Molecule 1: Tubulin beta-3 chain



• Molecule 1: Tubulin beta-3 chain





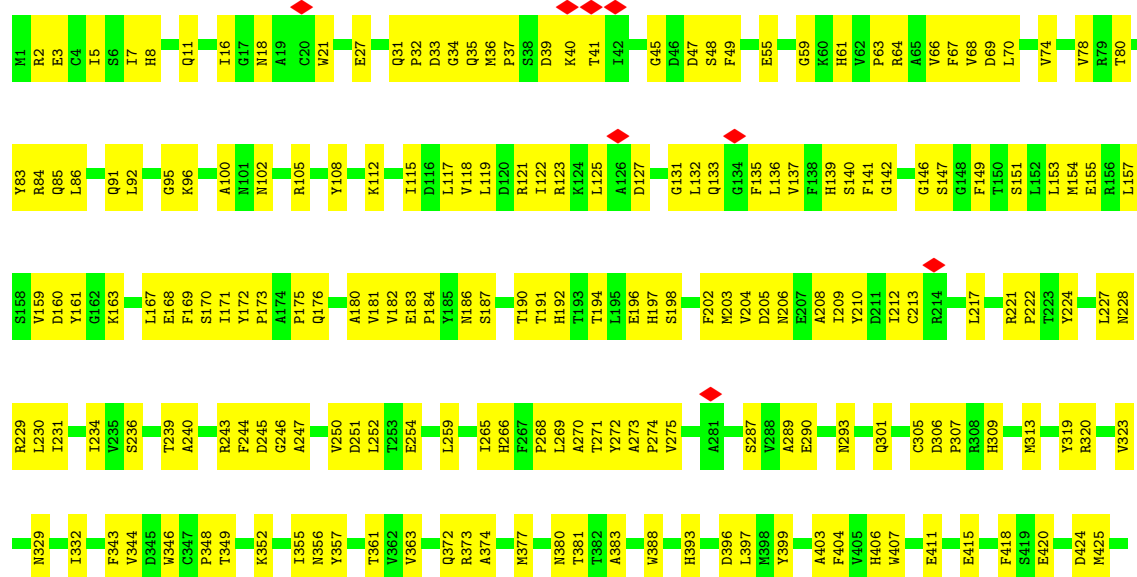
• Molecule 2: Tubulin alpha-1B chain

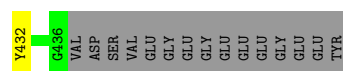
Chain A: 54% 43%



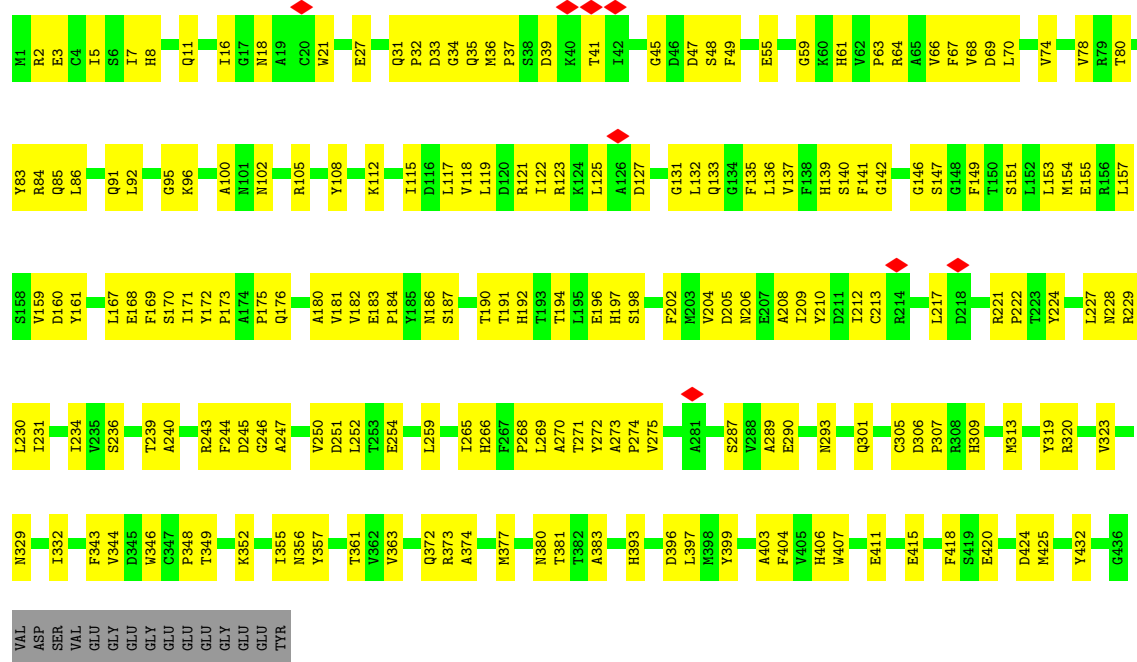
• Molecule 2: Tubulin alpha-1B chain

Chain C: 53% 43%

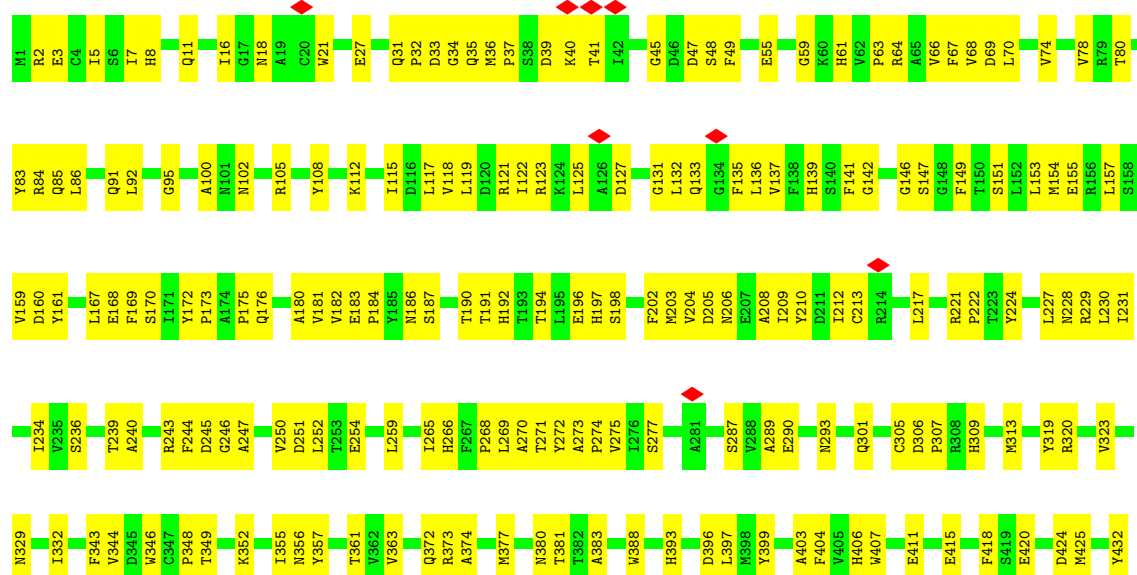


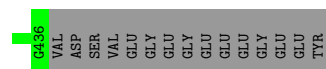


• Molecule 2: Tubulin alpha-1B chain



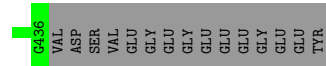
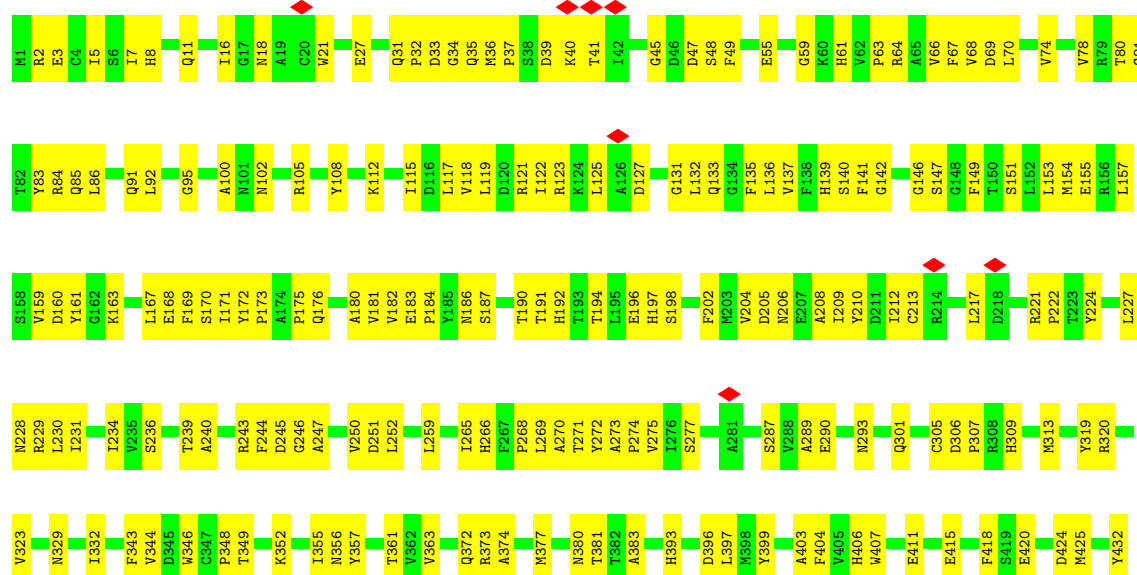
• Molecule 2: Tubulin alpha-1B chain





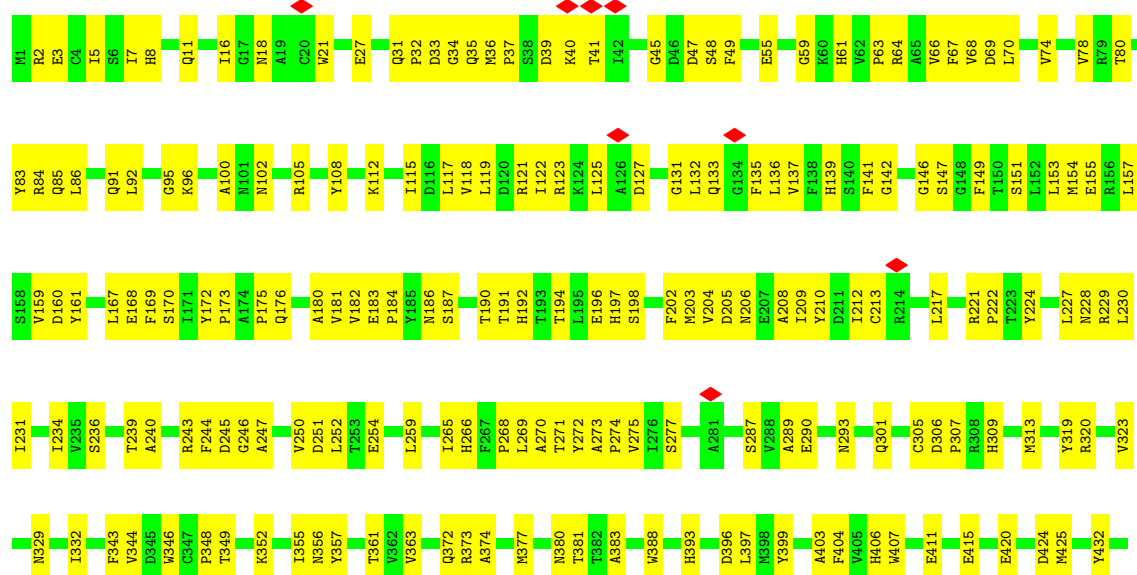
• Molecule 2: Tubulin alpha-1B chain

Chain I: 



• Molecule 2: Tubulin alpha-1B chain

Chain K: 



G436
VAL
ASP
SER
VAL
GLU
GLY
GLU
GLU
GLU
GLY
GLU
GLU
TYR

• Molecule 2: Tubulin alpha-1B chain

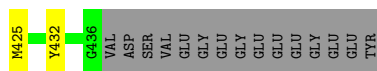
Chain M:  54% 43%

Y432	N329	T231	V159	H83	#1
G436	I332	L234	D160	R84	R2
VAL	I332	V235	Y161	Q85	E3
ASP	S236	S236	L167	L86	C4
SER	F343	T239	E168	Q91	I5
VAL	D344	A240	F169	L92	S6
GLU	V345	R243	S170	G95	I7
GLY	W346	G171	I171	G95	H8
GLU	C347	R243	Y172	G95	Q11
GLY	P348	F244	P173	A100	
GLU	T349	D245	A174	N101	I16
GLU	K352	G246	P175	H102	G17
GLY		A247	Q176	R105	N18
GLY	I355	V250	A180	Y108	A19
GLU	N356	D251	V181	Y108	C20
GLU	Y357	L252	H182		W21
TYR		T253	E183	K112	
	T361	E254	P184		E27
	V362		Y185	I115	
	V363	L259	N186	D116	Q31
			S187	L117	P32
				V118	D33
	Q372	I265		L119	C34
	R373	H266	T190	D120	Q35
	A374	F267	T191	R121	M36
	M377	P268	H192	I122	P37
		L269	T193	R123	S38
		A270	T194	R124	D39
	N380	T271	L195	K124	
	T381	Y272	E196	L125	F40
	T382	A273	H197	A126	T41
	A383	P274	S198	D127	I42
		V275			
	W388	I276	F202	G131	G45
		S277	M203	L132	D46
	H393		V204	Q133	D47
		A281	D205	G134	S48
	D396	S287	E206	F135	F49
	L397	V288	A208	L136	
	M398	A289	I209	V137	E55
	Y399	E290	Y210	F138	
	A403		D211	H139	G59
	F404		I212	S140	R60
	V405	W293	C213	F141	H61
	H406	Q301	R214	G142	V62
	W407				P63
		C305	L217	G146	R64
	E411	D306	D218	S147	A65
		P307		G148	V66
	E415	R308	R221	F149	F67
		H309	P222	T150	V68
	F418	M313	T223	S151	D69
	S419		Y224	L152	L70
	E420			L153	
		Y319	L227	M154	V74
	D424	R320	N228	E155	
	M425		R229	R156	V78
		V323	L230	L157	R79
				S158	T80

• Molecule 2: Tubulin alpha-1B chain

Chain O:  53% 44%

M1	R2	E3	C4	I5	S6	I7	H8	Q11	I16	G17	N18	A19	C20	W21	E27	Q31	P32	D33	G34	Q35	M36	P37	S38	D39	K40	T41	I42	G45	D46	D47	S48	F49	E55	G59	A60	H61	V62	P63	R64	A65	V66	F67	V68	D69	L70	V74	V78	R79	T80				
Y83	R84	Q85	L86	Q81	L92	Q95	A100	N101	N102	R105	Y108	K112	I115	D116	L117	V118	L119	D120	R121	I122	R123	K124	L125	A126	D127	G131	L132	Q133	G134	F135	L136	V137	F138	H139	S140	F141	G142	G146	S147	G148	F149	T150	S151	L152	L153	M154	E155	R156	L157	S158			
V159	D160	Y161	G162	K163	K166	L167	F168	F169	S170	I171	Y172	P173	A174	G175	Q176	A180	V181	V182	E183	P184	Y185	N186	S187	T190	T191	H192	I193	L194	L195	E196	H197	S198	F202	M203	V204	D205	N206	E207	A208	I209	Y210	D211	I212	C213	R214	L217	D218	R221	P222	T223	Y224	L227	N228
R229	L230	I231	I234	V235	S236	T239	A240	R243	F244	D245	G246	A247	V250	D251	L252	T253	E254	L259	I265	H266	F267	P268	L269	A270	T271	Y272	A273	P274	V275	S277	A281	S287	V288	A289	E290	N293	Q301	C305	D306	P307	R308	H309	M313	Y319	R320	D424							
V323	N329	I332	F343	V344	D345	W346	P348	T349	K352	I355	N356	Y357	T361	V362	V363	Q372	R373	A374	M377	N380	K381	T382	A383	W388	H393	D396	L397	M398	Y399	A403	F404	V405	H406	W407	E411	E415	F418	S419	E420	D424													



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of particles used	18899	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 ($e^-/\text{\AA}^2$)	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	35.696	Depositor
Minimum map value	-15.714	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.484	Depositor
Recommended contour level	4.5	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: GTP, YNP, 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	0.23	0/3389	0.52	2/4596 (0.0%)
1	D	0.23	0/3389	0.52	2/4596 (0.0%)
1	F	0.23	0/3389	0.52	2/4596 (0.0%)
1	H	0.23	0/3389	0.52	2/4596 (0.0%)
1	J	0.23	0/3389	0.52	2/4596 (0.0%)
1	L	0.23	0/3389	0.52	2/4596 (0.0%)
1	N	0.23	0/3389	0.52	2/4596 (0.0%)
1	P	0.23	0/3389	0.52	2/4596 (0.0%)
2	A	0.21	0/3417	0.51	3/4650 (0.1%)
2	C	0.21	0/3417	0.51	3/4650 (0.1%)
2	E	0.21	0/3417	0.51	3/4650 (0.1%)
2	G	0.21	0/3417	0.51	3/4650 (0.1%)
2	I	0.21	0/3417	0.51	3/4650 (0.1%)
2	K	0.21	0/3417	0.51	3/4650 (0.1%)
2	M	0.21	0/3417	0.51	3/4650 (0.1%)
2	O	0.21	0/3417	0.51	3/4650 (0.1%)
All	All	0.22	0/54448	0.51	40/73968 (0.1%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	181	VAL	N-CA-C	-6.98	106.33	113.10
2	G	181	VAL	N-CA-C	-6.98	106.33	113.10
2	K	181	VAL	N-CA-C	-6.98	106.33	113.10
2	O	181	VAL	N-CA-C	-6.98	106.33	113.10
2	A	181	VAL	N-CA-C	-6.96	106.35	113.10

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	3312	0	3174	179	0
1	D	3312	0	3174	182	0
1	F	3312	0	3174	181	0
1	H	3312	0	3174	185	0
1	J	3312	0	3174	182	0
1	L	3312	0	3174	185	0
1	N	3312	0	3174	183	0
1	P	3312	0	3174	181	0
2	A	3340	0	3212	150	0
2	C	3340	0	3212	151	0
2	E	3340	0	3212	149	0
2	G	3340	0	3212	150	0
2	I	3340	0	3212	150	0
2	K	3340	0	3212	151	0
2	M	3340	0	3212	149	0
2	O	3340	0	3212	152	0
3	B	46	0	0	1	0
3	D	46	0	0	1	0
3	F	46	0	0	1	0
3	H	46	0	0	1	0
3	J	46	0	0	1	0
3	L	46	0	0	1	0
3	N	46	0	0	1	0
3	P	46	0	0	1	0
4	B	28	0	12	4	0
4	D	28	0	12	4	0
4	F	28	0	12	4	0
4	H	28	0	12	4	0
4	J	28	0	12	3	0
4	L	28	0	12	4	0
4	N	28	0	12	3	0
4	P	28	0	12	4	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	E	32	0	12	0	0
5	G	32	0	12	0	0
5	I	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	32	0	12	0	0
5	M	32	0	12	0	0
5	O	32	0	12	0	0
All	All	54064	0	51280	2515	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 24.

The worst 5 of 2515 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:B:259:PRO:O	2:O:406:HIS:CE1	1.73	1.42
2:A:406:HIS:CE1	1:D:259:PRO:O	1.73	1.42
2:E:406:HIS:CE1	1:H:259:PRO:O	1.73	1.41
2:C:406:HIS:CE1	1:F:259:PRO:O	1.73	1.40
2:G:406:HIS:CE1	1:J:259:PRO:O	1.73	1.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	D	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	F	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	H	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	J	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	L	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
1	N	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	426/450 (95%)	382 (90%)	42 (10%)	2 (0%)	24	53
2	A	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	C	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	E	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	G	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	I	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	K	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	M	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
2	O	434/451 (96%)	386 (89%)	47 (11%)	1 (0%)	43	70
All	All	6880/7208 (95%)	6144 (89%)	712 (10%)	24 (0%)	37	64

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	THR
2	A	37	PRO
1	D	143	THR
2	C	37	PRO
1	F	143	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	D	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	F	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	H	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	J	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	L	358/386 (93%)	356 (99%)	2 (1%)	78	80
1	N	358/386 (93%)	356 (99%)	2 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	358/386 (93%)	356 (99%)	2 (1%)	78	80
2	A	351/379 (93%)	351 (100%)	0	100	100
2	C	351/379 (93%)	351 (100%)	0	100	100
2	E	351/379 (93%)	351 (100%)	0	100	100
2	G	351/379 (93%)	351 (100%)	0	100	100
2	I	351/379 (93%)	351 (100%)	0	100	100
2	K	351/379 (93%)	351 (100%)	0	100	100
2	M	351/379 (93%)	351 (100%)	0	100	100
2	O	351/379 (93%)	351 (100%)	0	100	100
All	All	5672/6120 (93%)	5656 (100%)	16 (0%)	84	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	347	ASN
1	N	349	VAL
1	J	347	ASN
1	N	347	ASN
1	H	349	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	99	ASN
1	N	292	GLN
1	L	256	ASN
2	K	358	GLN
2	M	283	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
4	GDP	J	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
3	YNP	F	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.45	18 (30%)
3	YNP	N	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.45	18 (30%)
3	YNP	J	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.45	18 (30%)
4	GDP	L	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
4	GDP	F	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
3	YNP	D	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.44	18 (30%)
3	YNP	H	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.44	18 (30%)
3	YNP	L	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.44	18 (30%)
5	GTP	A	501	-	33,34,34	0.59	0	50,54,54	0.50	0
5	GTP	M	501	-	33,34,34	0.59	0	50,54,54	0.50	0
3	YNP	B	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.45	18 (30%)
5	GTP	O	501	-	33,34,34	0.59	0	50,54,54	0.50	0
4	GDP	H	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
5	GTP	K	501	-	33,34,34	0.59	0	50,54,54	0.50	0
5	GTP	G	501	-	33,34,34	0.59	0	50,54,54	0.50	0
4	GDP	N	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
3	YNP	P	501	-	49,49,49	2.75	14 (28%)	59,68,68	3.44	18 (30%)
4	GDP	P	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
5	GTP	I	501	-	33,34,34	0.59	0	50,54,54	0.50	0
4	GDP	B	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
4	GDP	D	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	5 (11%)
5	GTP	C	501	-	33,34,34	0.59	0	50,54,54	0.50	0
5	GTP	E	501	-	33,34,34	0.59	0	50,54,54	0.50	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
4	GDP	J	502	-	-	3/16/32/32	0/3/3/3
3	YNP	F	501	-	-	35/57/62/62	0/3/4/4
3	YNP	N	501	-	-	35/57/62/62	0/3/4/4
3	YNP	J	501	-	-	35/57/62/62	0/3/4/4
4	GDP	L	502	-	-	3/16/32/32	0/3/3/3
4	GDP	F	502	-	-	3/16/32/32	0/3/3/3
3	YNP	D	501	-	-	35/57/62/62	0/3/4/4
3	YNP	H	501	-	-	35/57/62/62	0/3/4/4
3	YNP	L	501	-	-	35/57/62/62	0/3/4/4
5	GTP	A	501	-	-	6/22/38/38	0/3/3/3
5	GTP	M	501	-	-	6/22/38/38	0/3/3/3
3	YNP	B	501	-	-	35/57/62/62	0/3/4/4
5	GTP	O	501	-	-	6/22/38/38	0/3/3/3
4	GDP	H	502	-	-	3/16/32/32	0/3/3/3
5	GTP	K	501	-	-	6/22/38/38	0/3/3/3
5	GTP	G	501	-	-	6/22/38/38	0/3/3/3
4	GDP	N	502	-	-	3/16/32/32	0/3/3/3
3	YNP	P	501	-	-	35/57/62/62	0/3/4/4
4	GDP	P	502	-	-	3/16/32/32	0/3/3/3
5	GTP	I	501	-	-	6/22/38/38	0/3/3/3
4	GDP	B	502	-	-	3/16/32/32	0/3/3/3
4	GDP	D	502	-	-	3/16/32/32	0/3/3/3
5	GTP	C	501	-	-	6/22/38/38	0/3/3/3
5	GTP	E	501	-	-	6/22/38/38	0/3/3/3

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	YNP	O1-C4	9.03	1.40	1.23
3	F	501	YNP	O1-C4	9.03	1.40	1.23
3	J	501	YNP	O1-C4	9.03	1.40	1.23
3	N	501	YNP	O1-C4	9.03	1.40	1.23
3	D	501	YNP	O1-C4	9.01	1.40	1.23

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	YNP	C20-O7-C21	14.85	71.20	60.82
3	F	501	YNP	C20-O7-C21	14.85	71.20	60.82
3	J	501	YNP	C20-O7-C21	14.85	71.20	60.82
3	N	501	YNP	C20-O7-C21	14.85	71.20	60.82
3	D	501	YNP	C20-O7-C21	14.82	71.18	60.82

There are no chirality outliers.

5 of 352 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	YNP	C5-C4-N1-C3
3	B	501	YNP	O1-C4-N1-C3
3	B	501	YNP	C13-C2-C3-N1
3	B	501	YNP	C28-C5-N2-C6
3	B	501	YNP	O2-C6-N2-C5

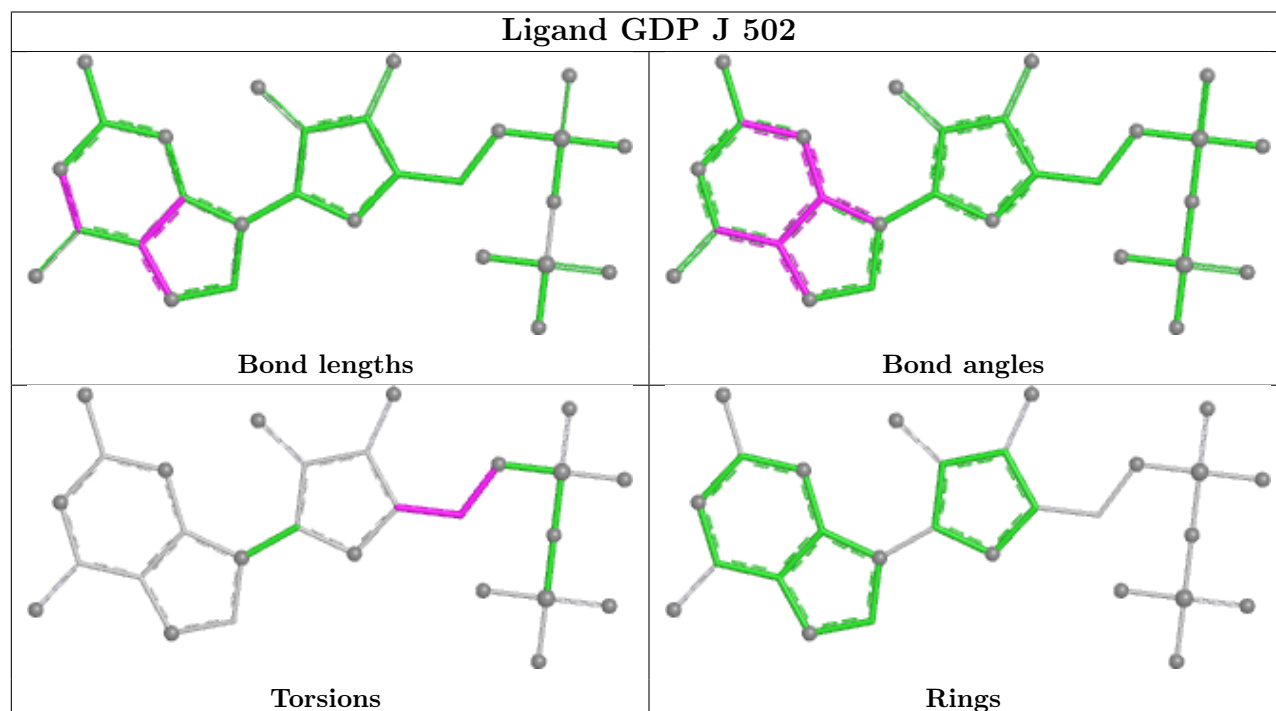
There are no ring outliers.

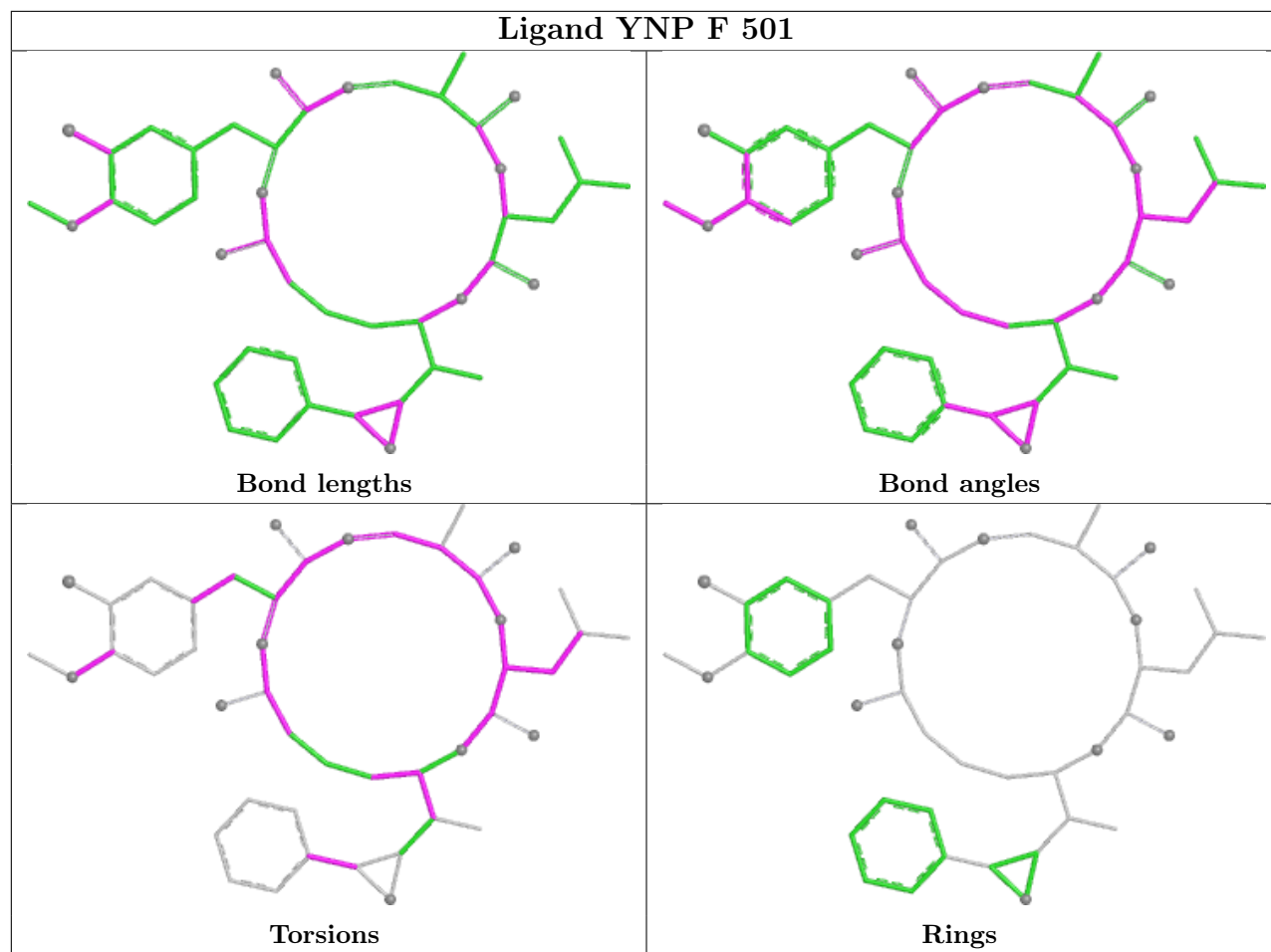
16 monomers are involved in 38 short contacts:

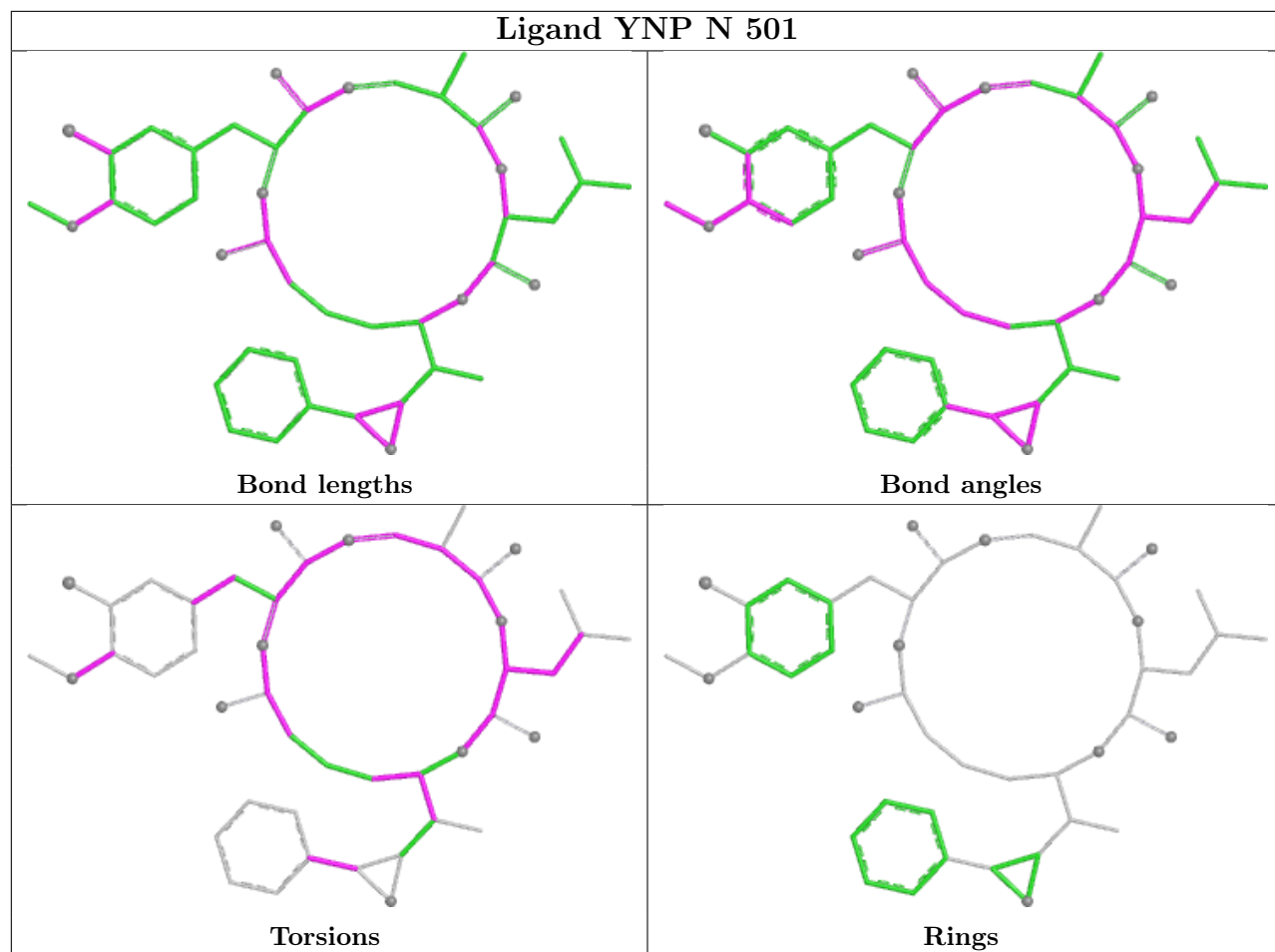
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	502	GDP	3	0
3	F	501	YNP	1	0
3	N	501	YNP	1	0
3	J	501	YNP	1	0
4	L	502	GDP	4	0
4	F	502	GDP	4	0
3	D	501	YNP	1	0
3	H	501	YNP	1	0
3	L	501	YNP	1	0
3	B	501	YNP	1	0
4	H	502	GDP	4	0
4	N	502	GDP	3	0
3	P	501	YNP	1	0
4	P	502	GDP	4	0
4	B	502	GDP	4	0
4	D	502	GDP	4	0

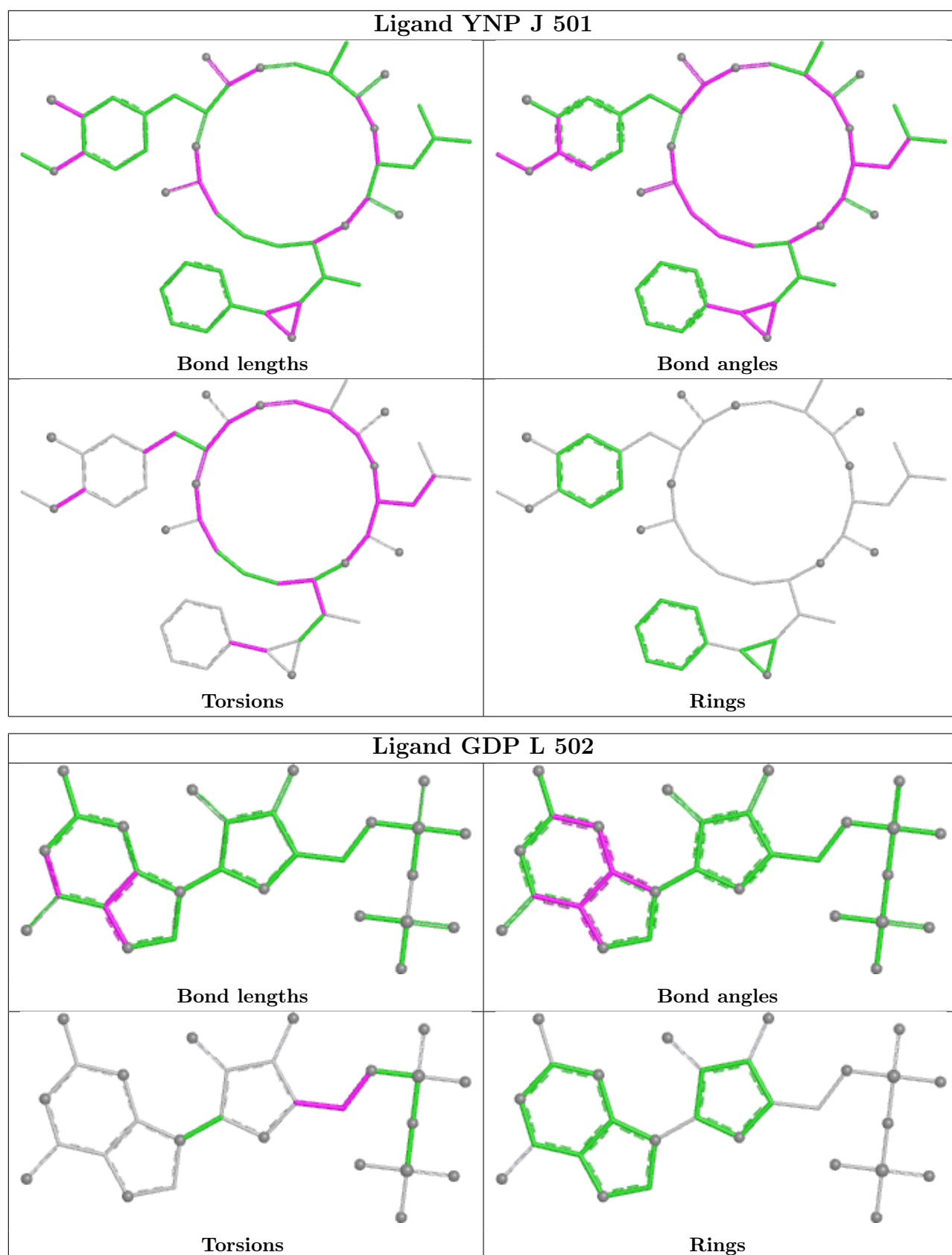
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

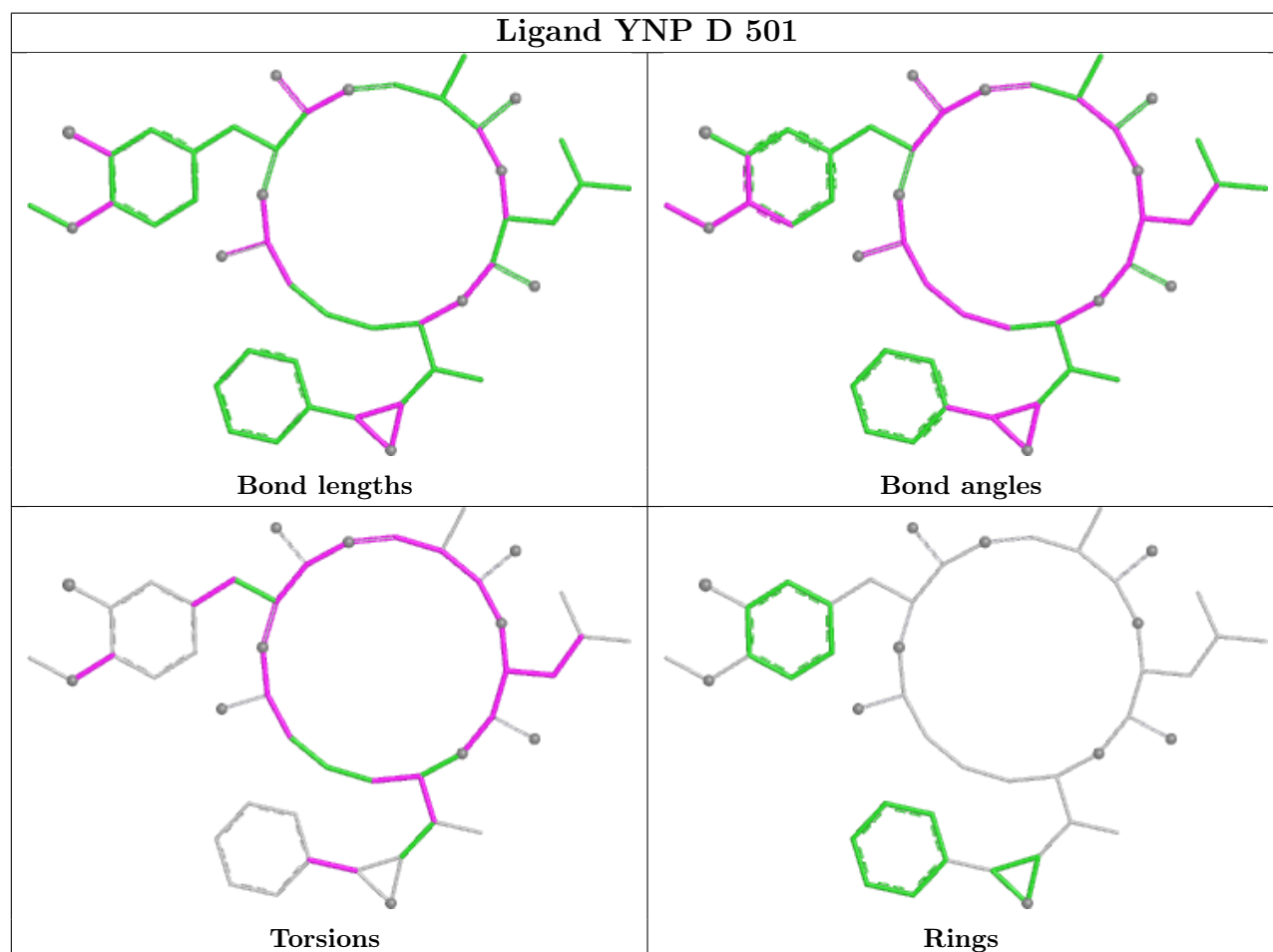
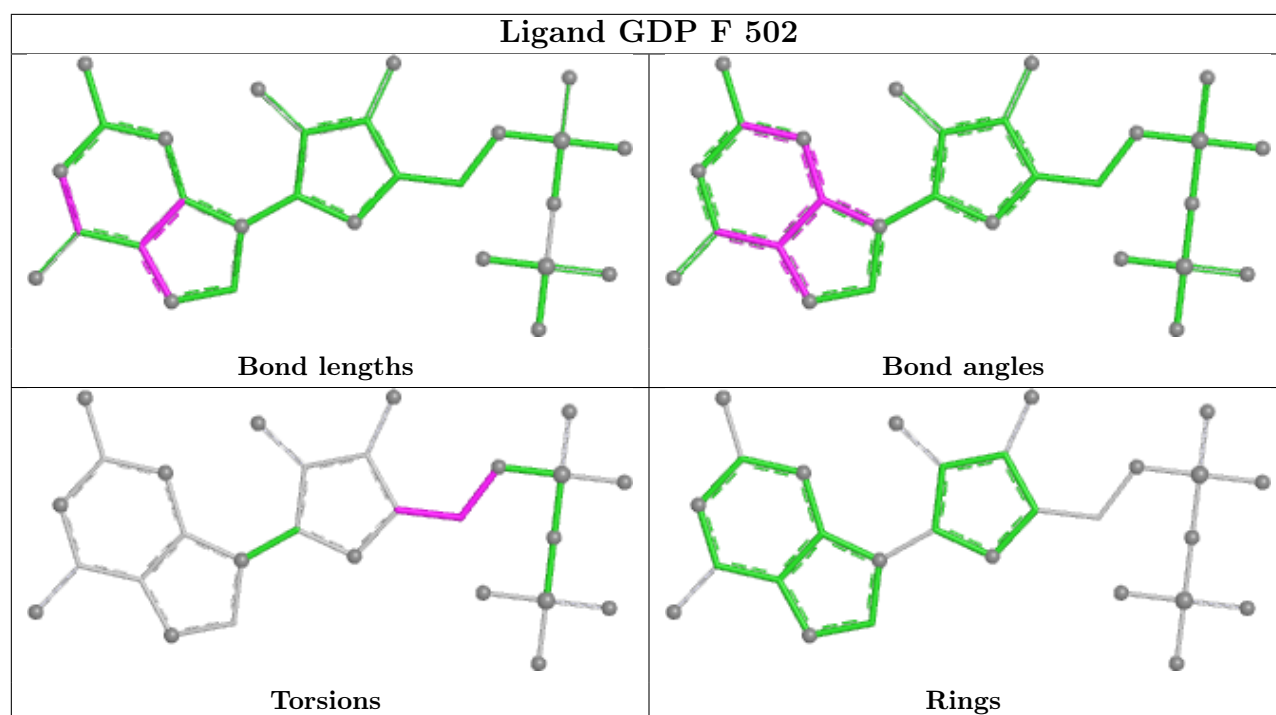
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

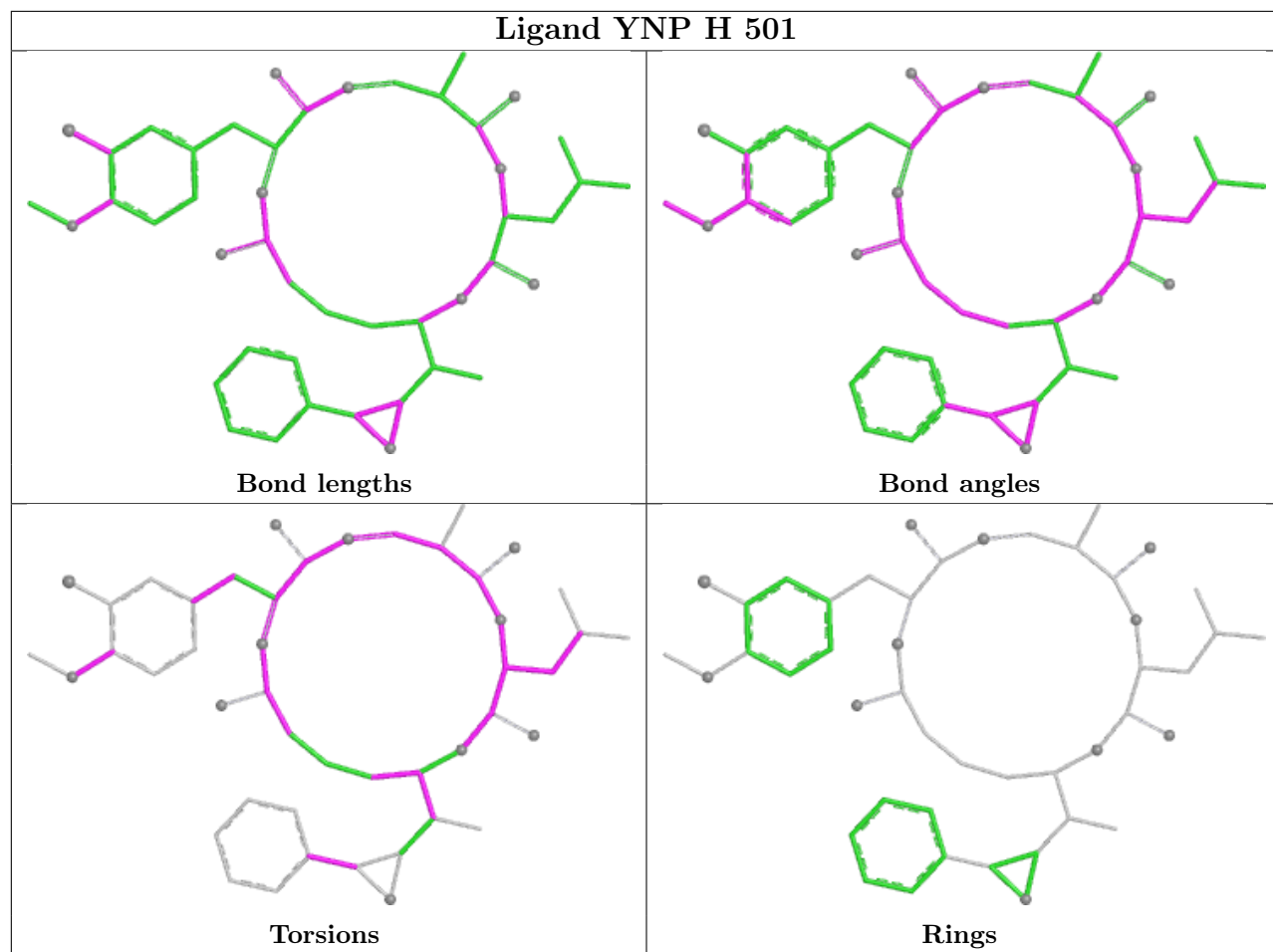


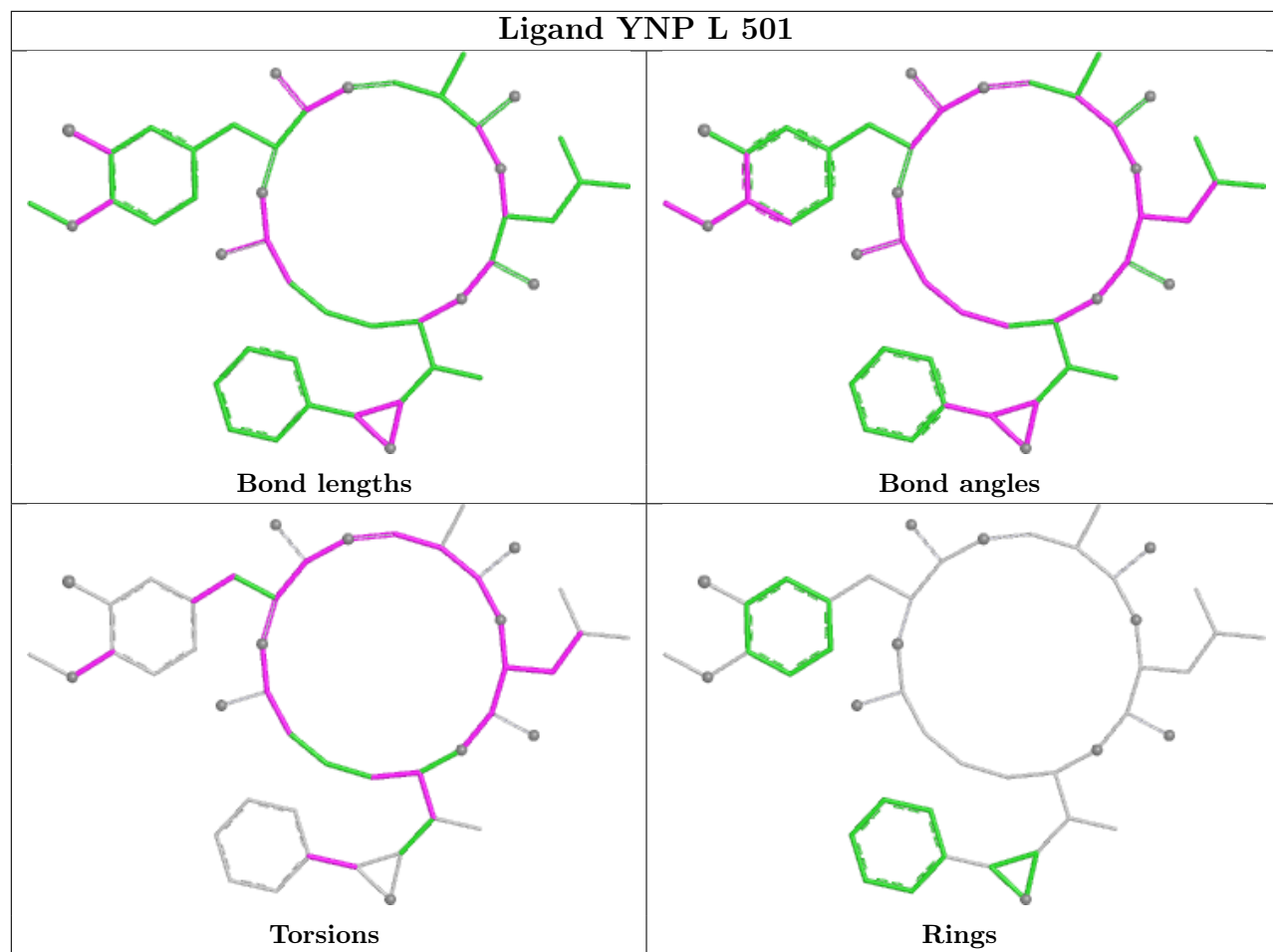


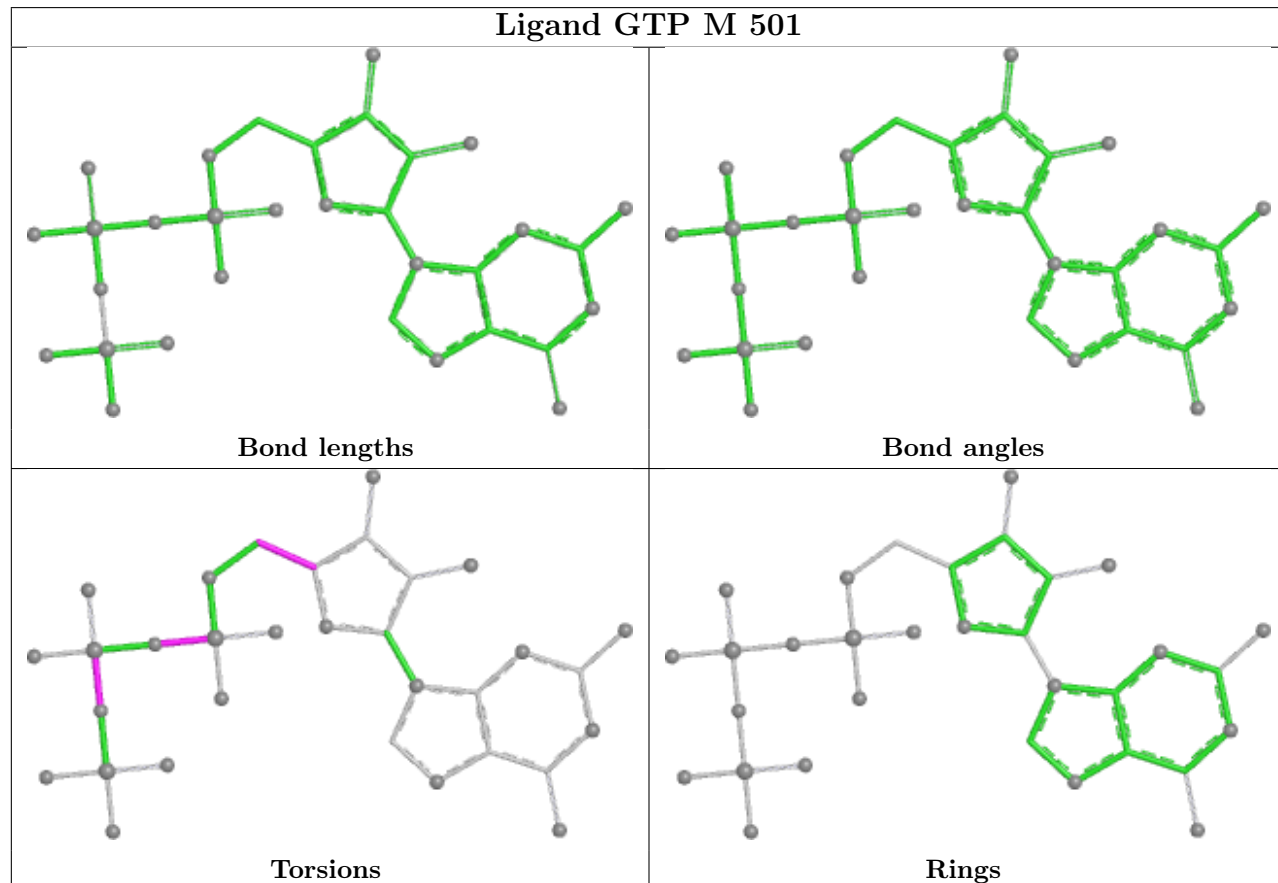
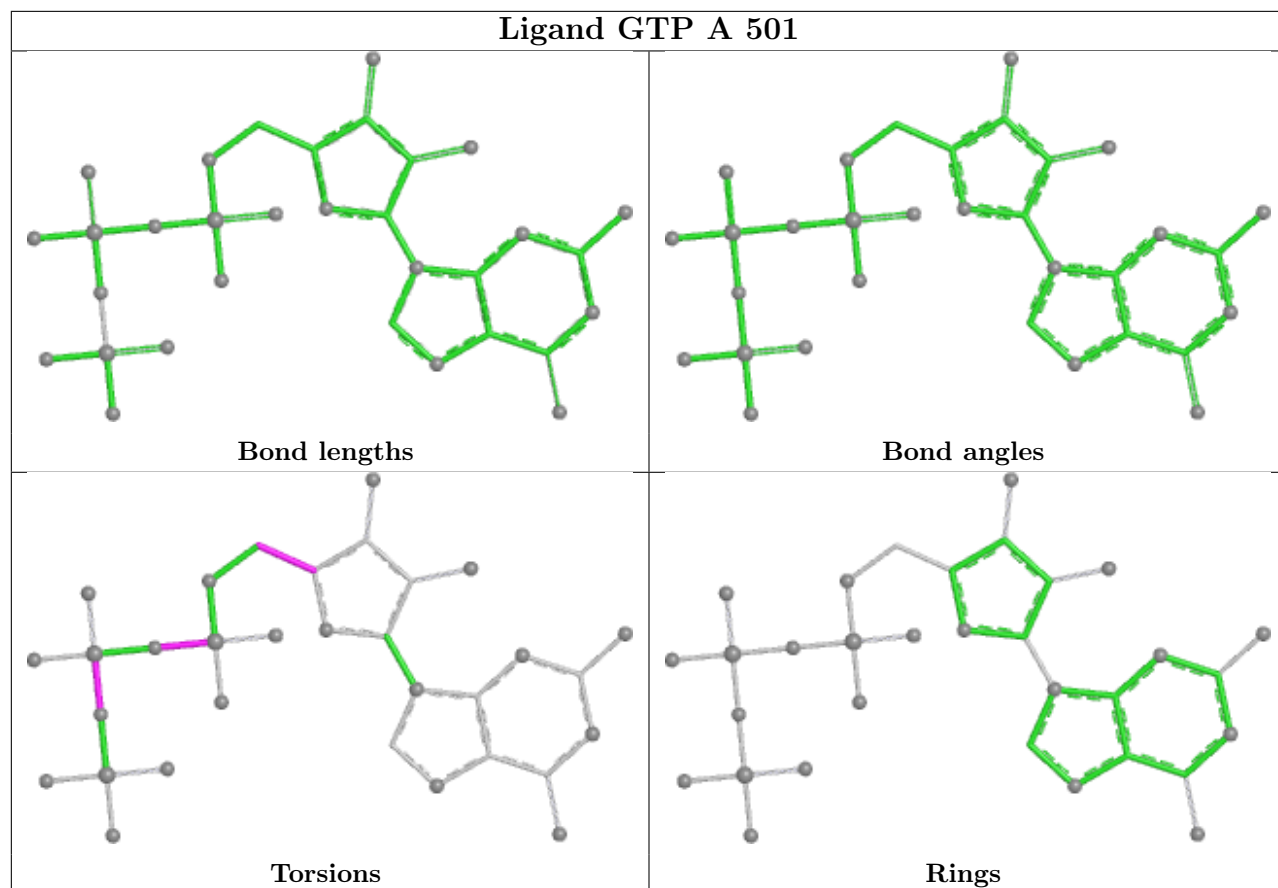


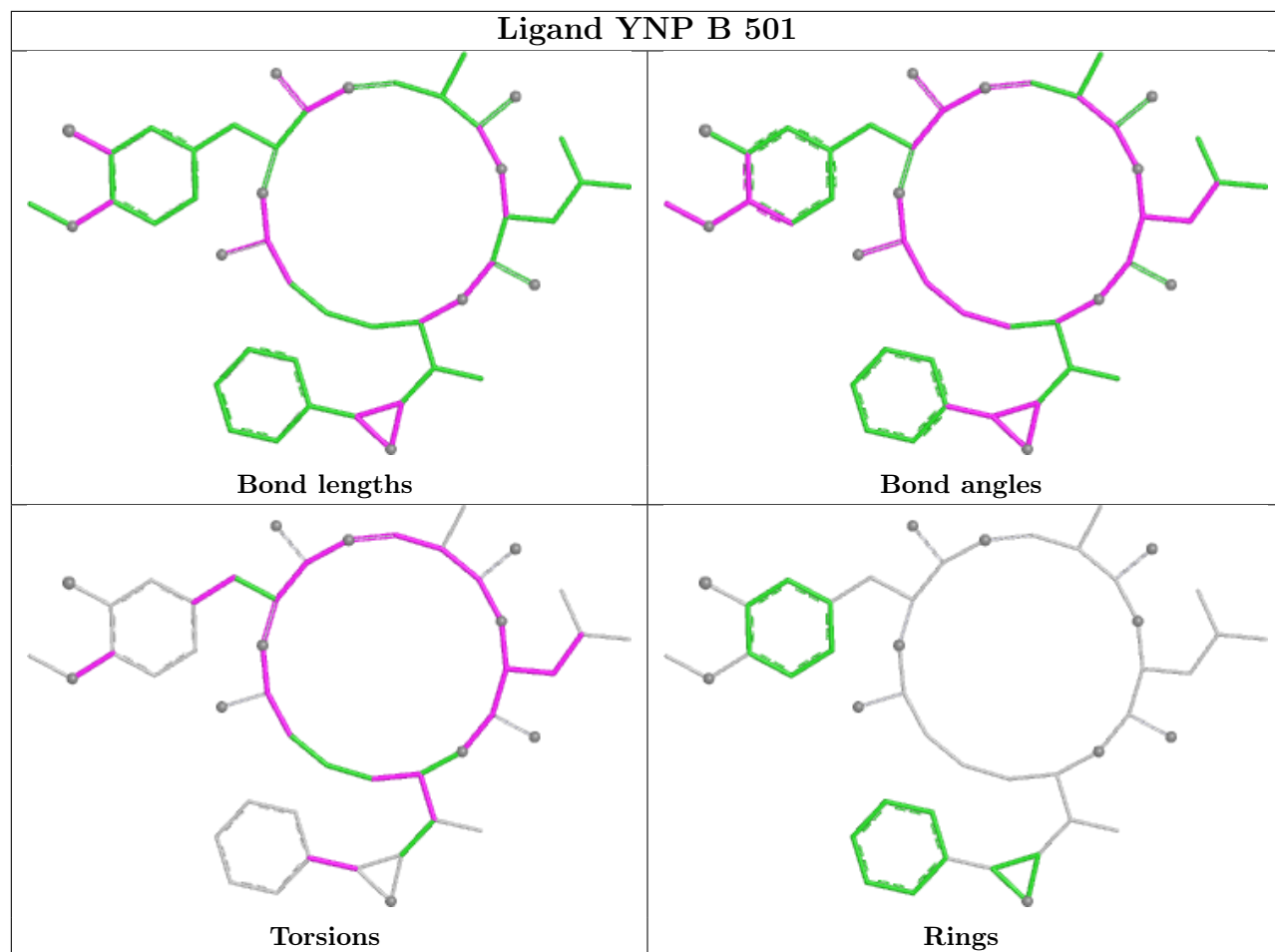


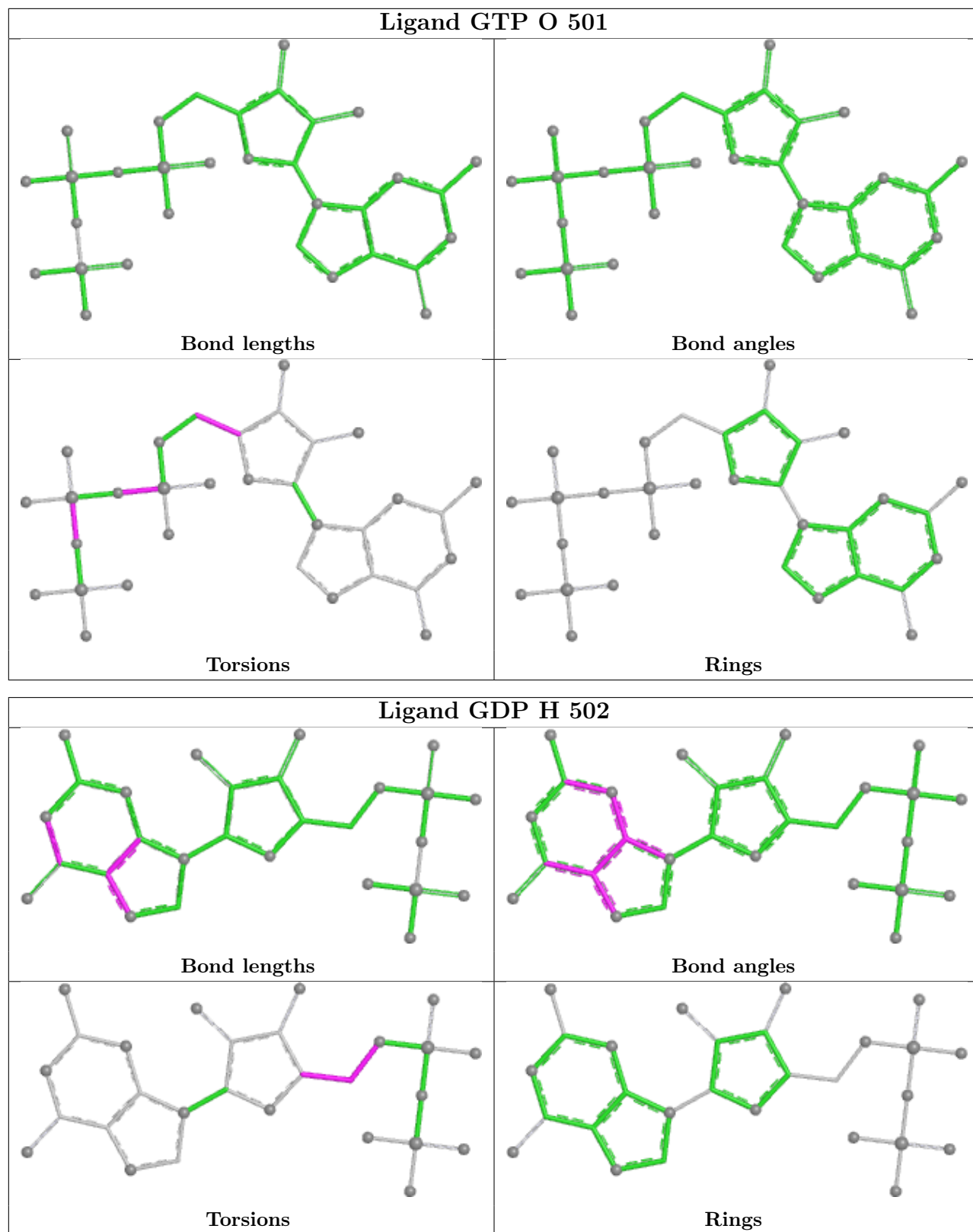


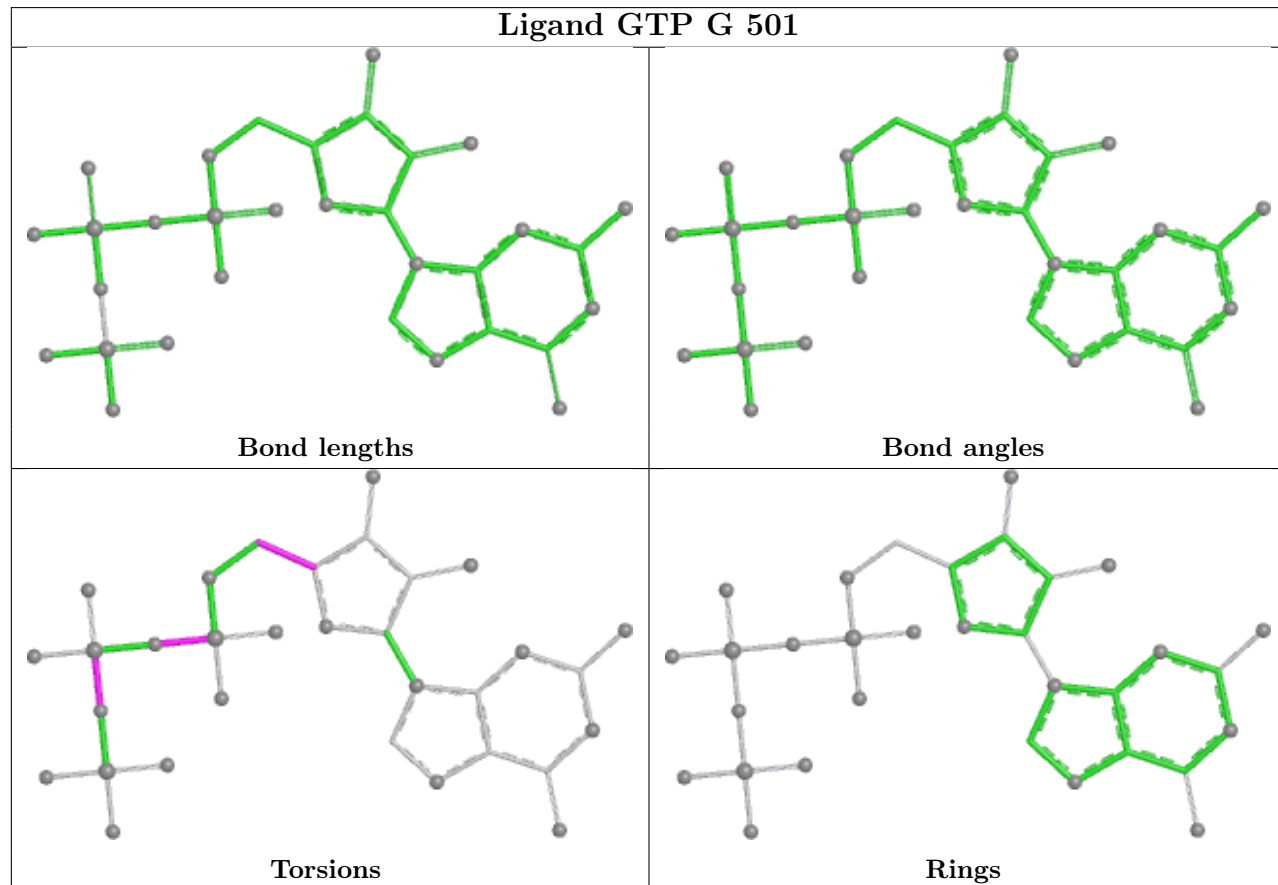
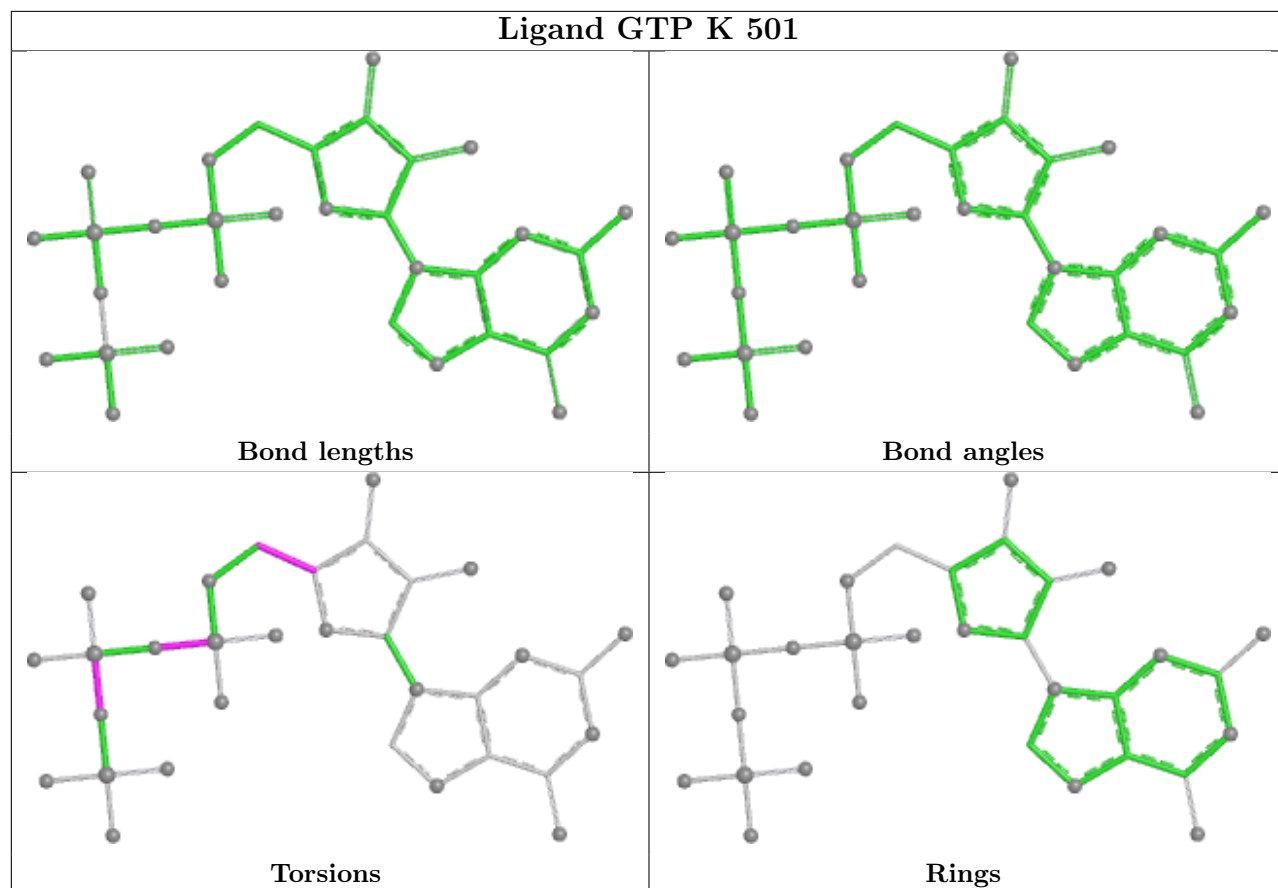


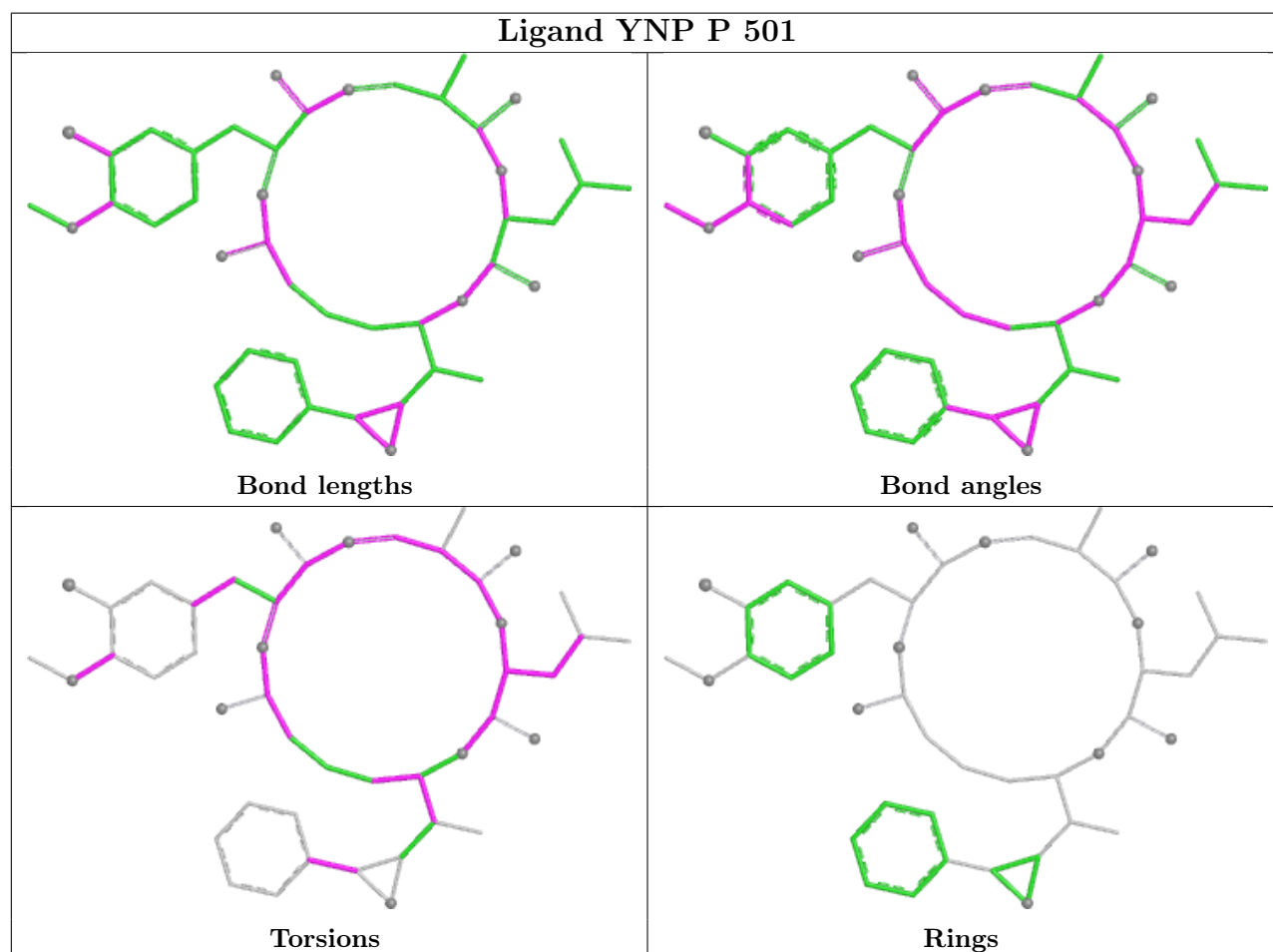
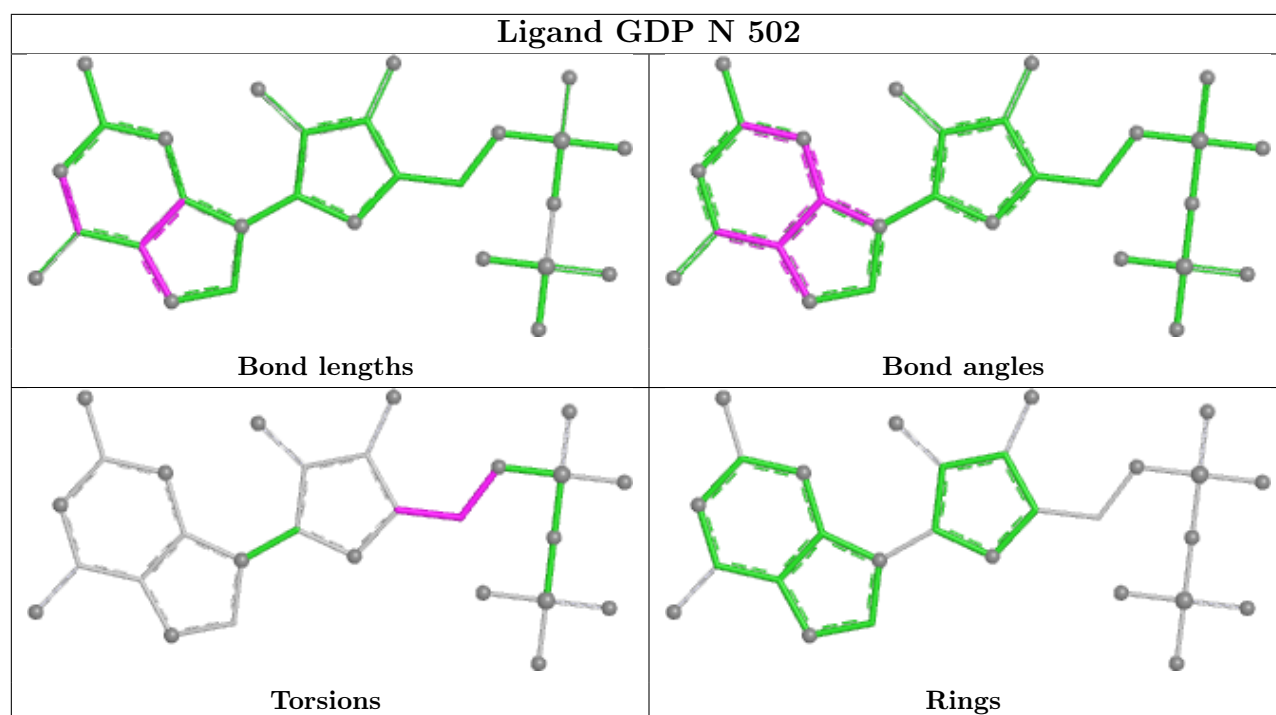


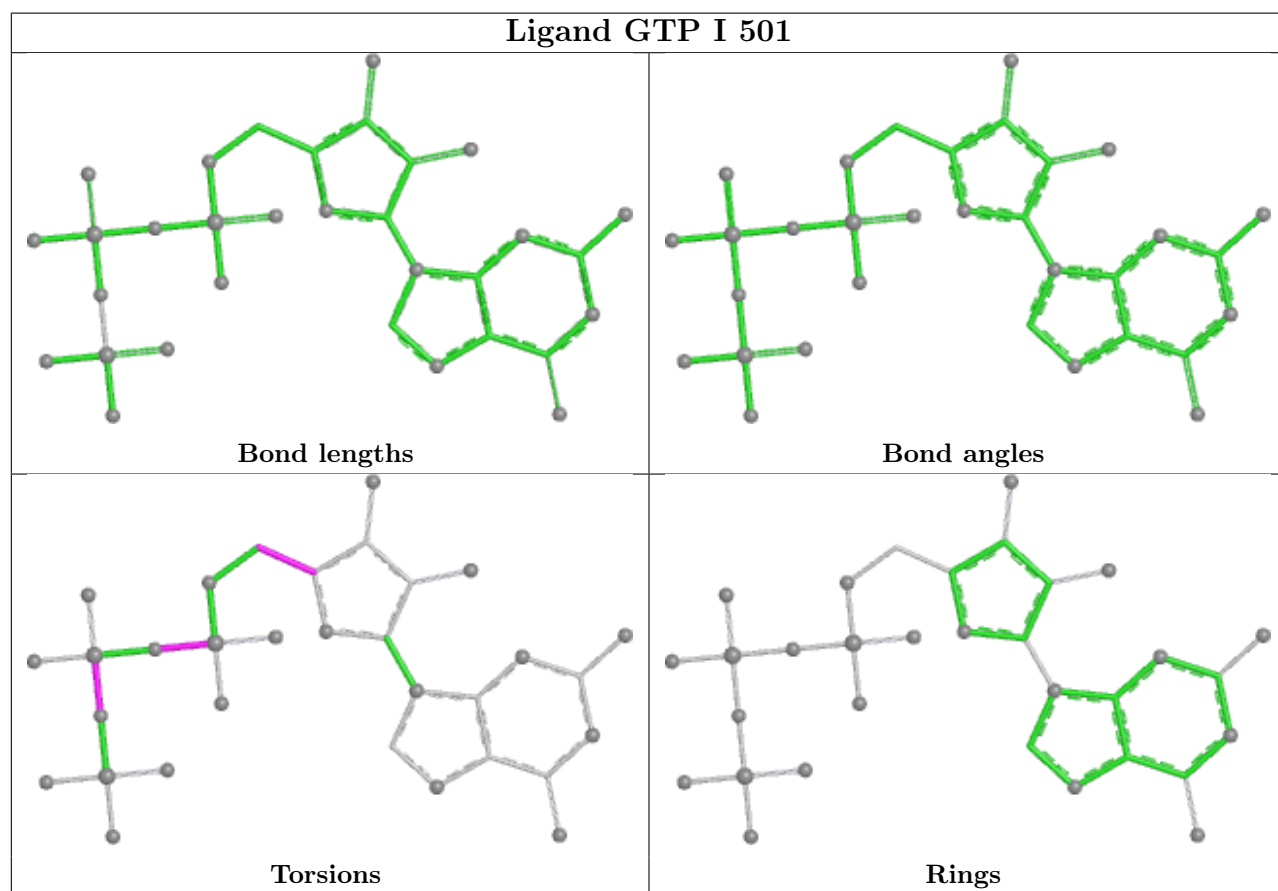
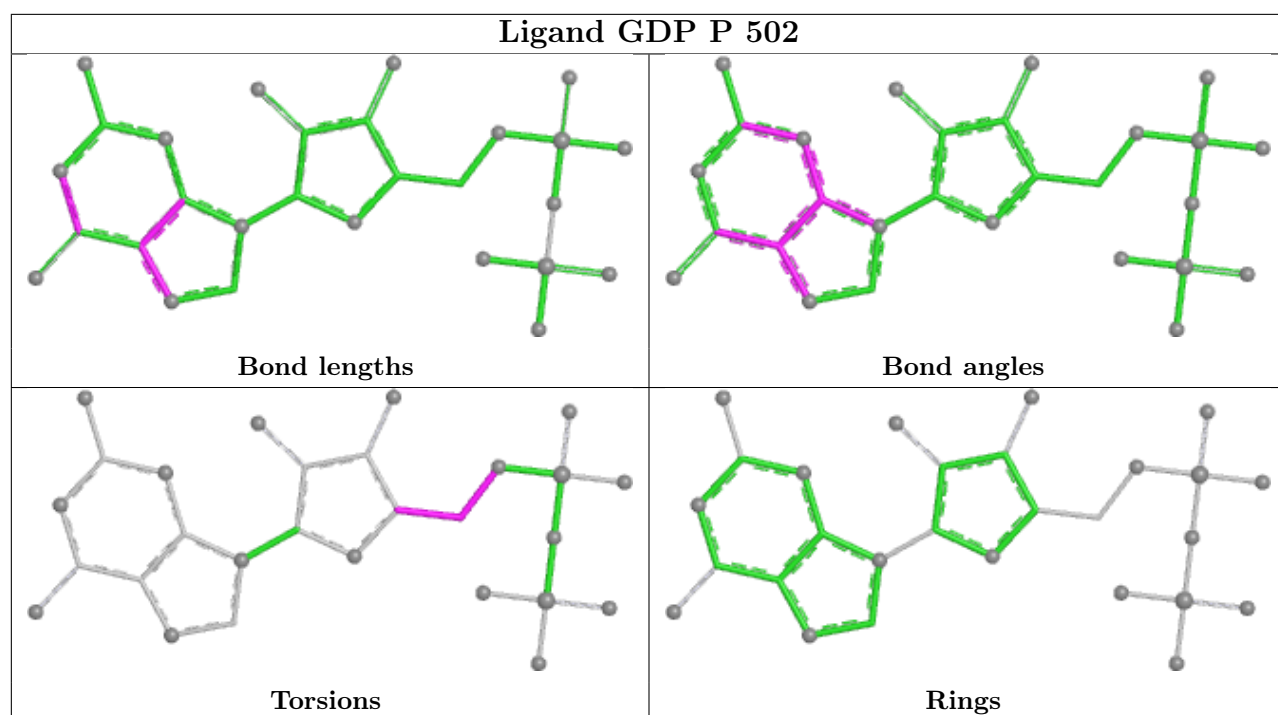


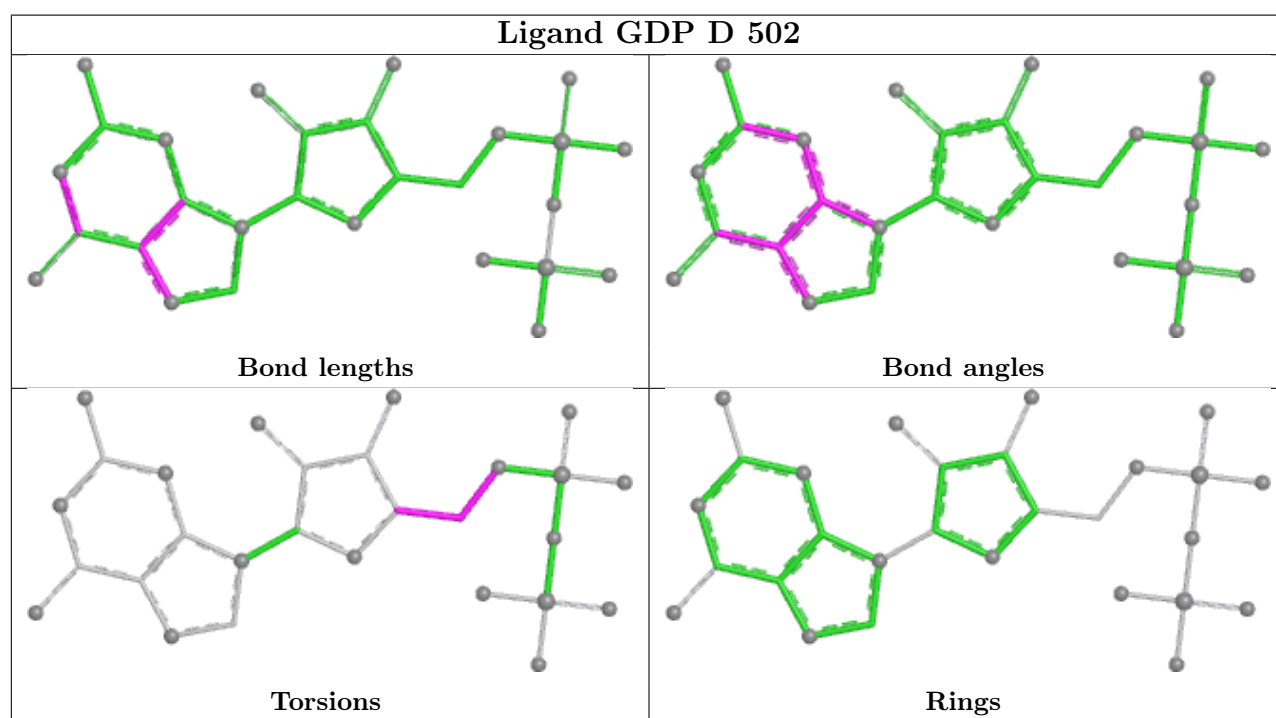
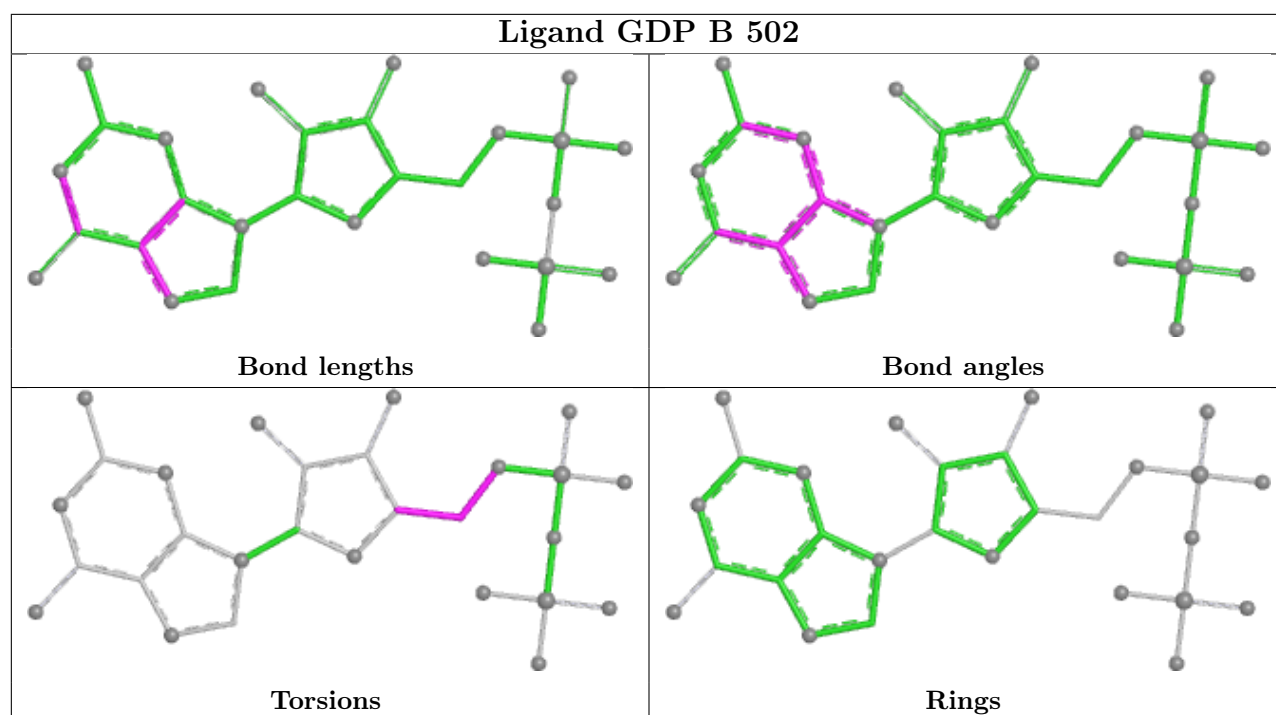




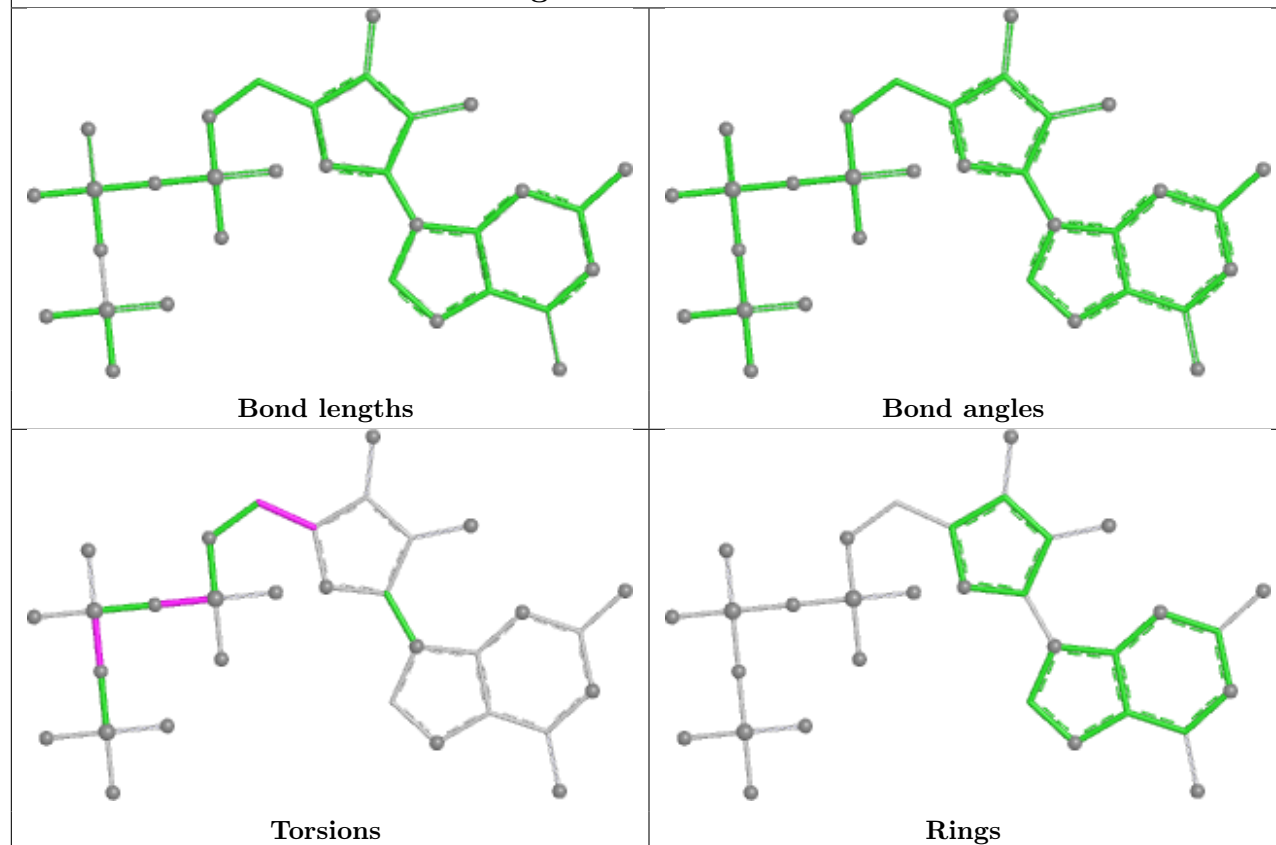




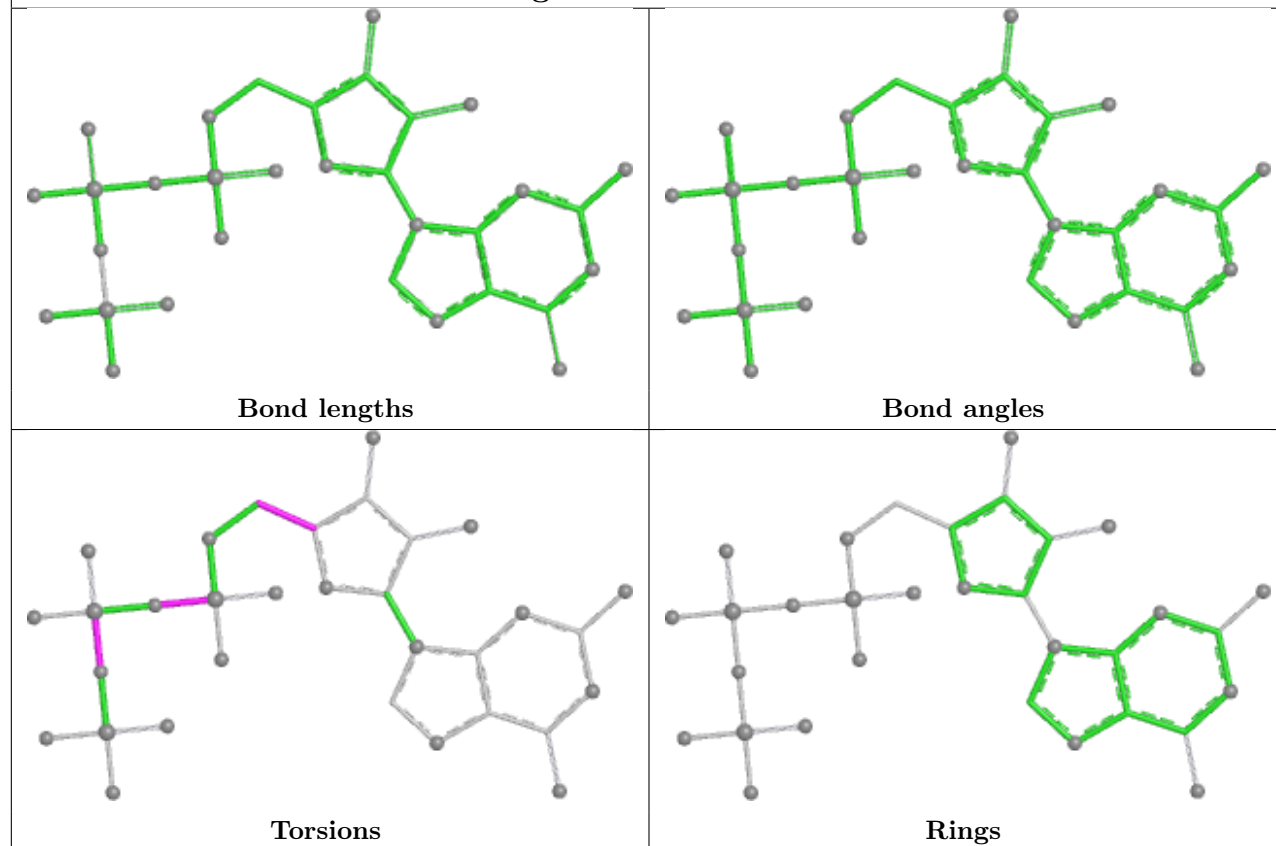




Ligand GTP C 501



Ligand GTP E 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 [i](#)

This section contains visualisations of the EMDB entry EMD-23615. These allow visual inspection of the internal detail of the map and identification of artifacts.

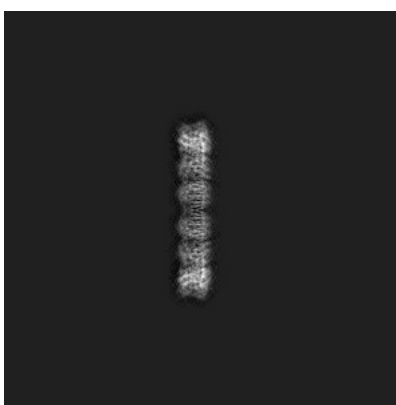
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

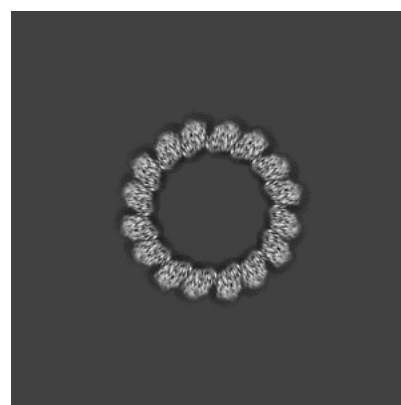
6.1.1 Primary map



X



Y

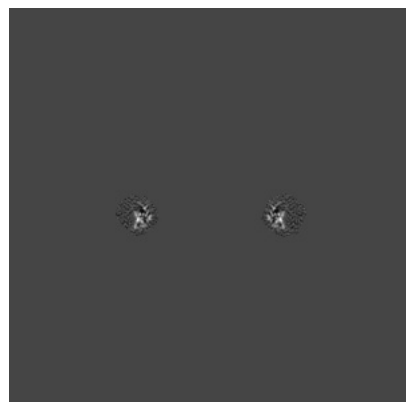


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 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: 398



Y Index: 398

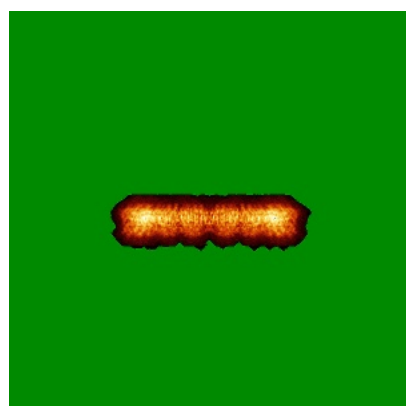


Z Index: 288

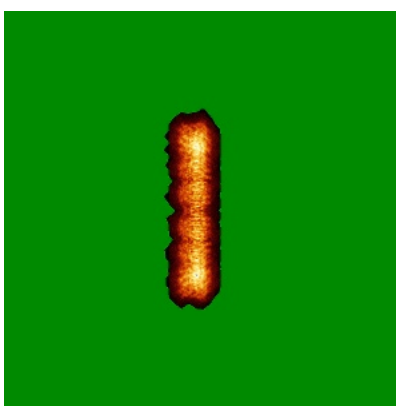
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

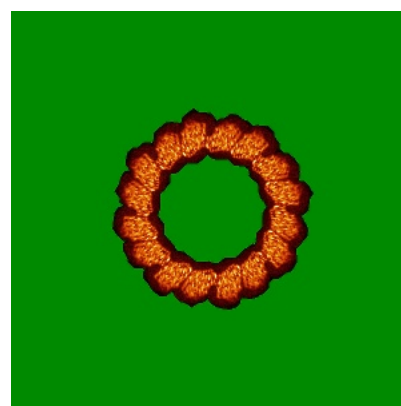
6.4.1 Primary map



X



Y

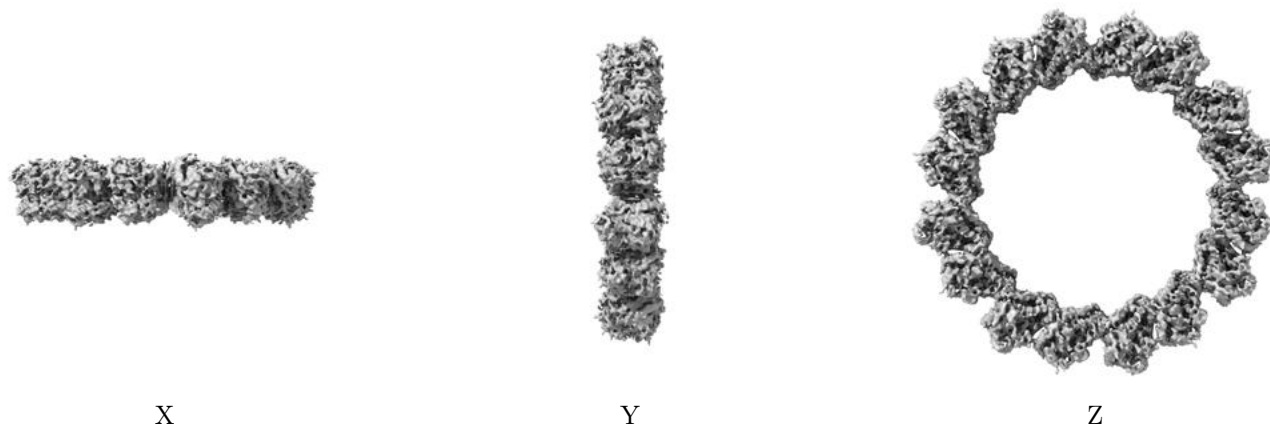


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

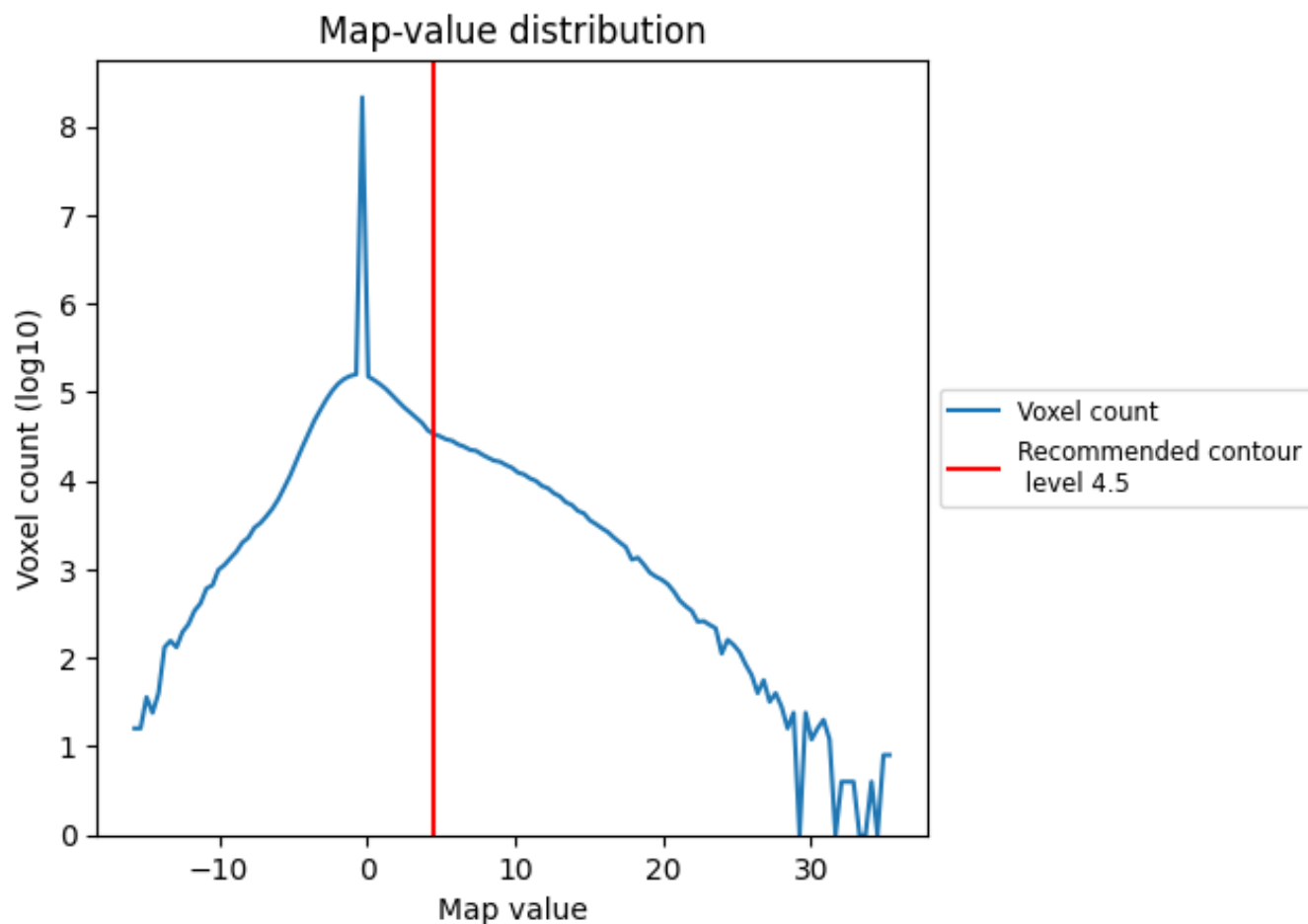
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

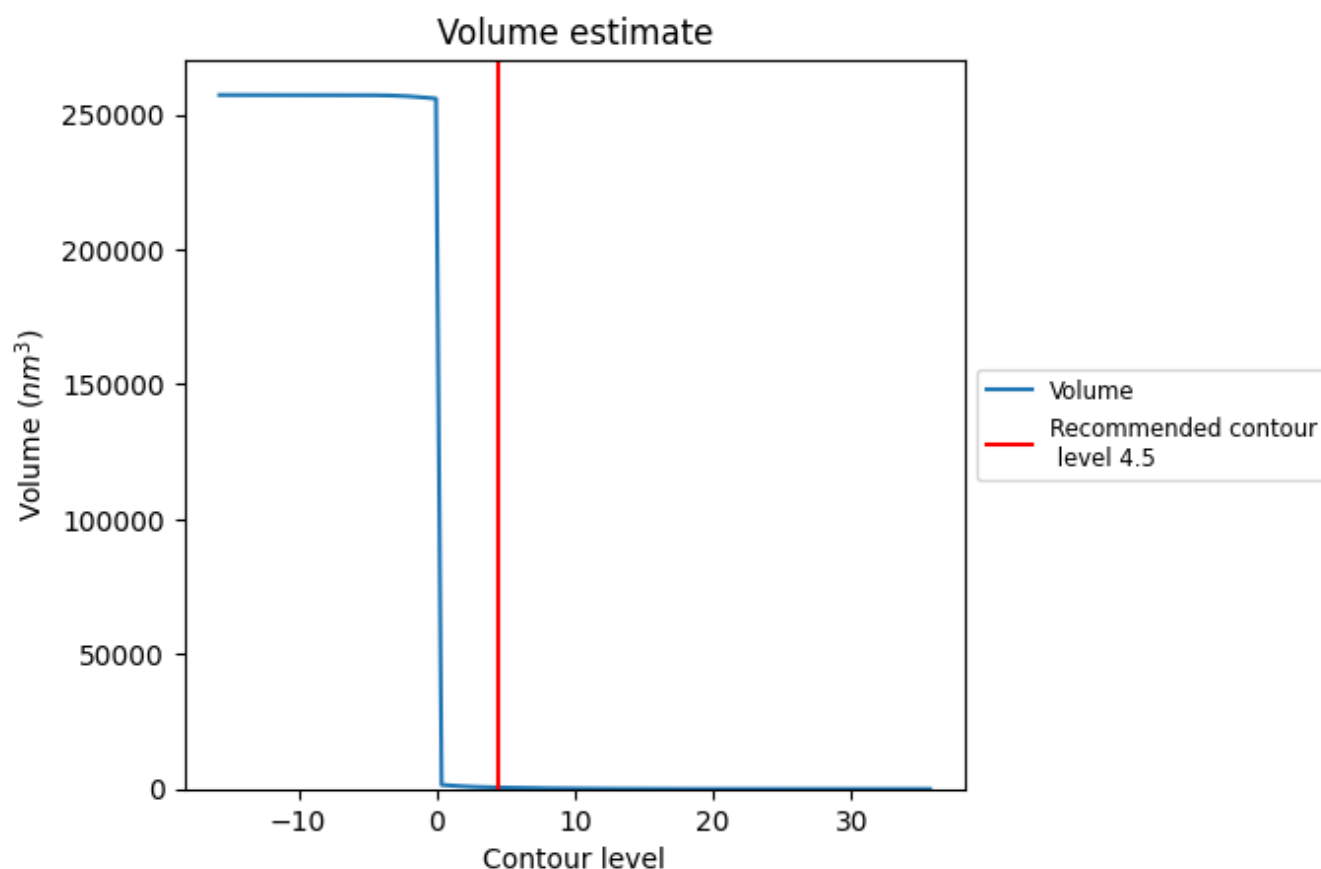
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

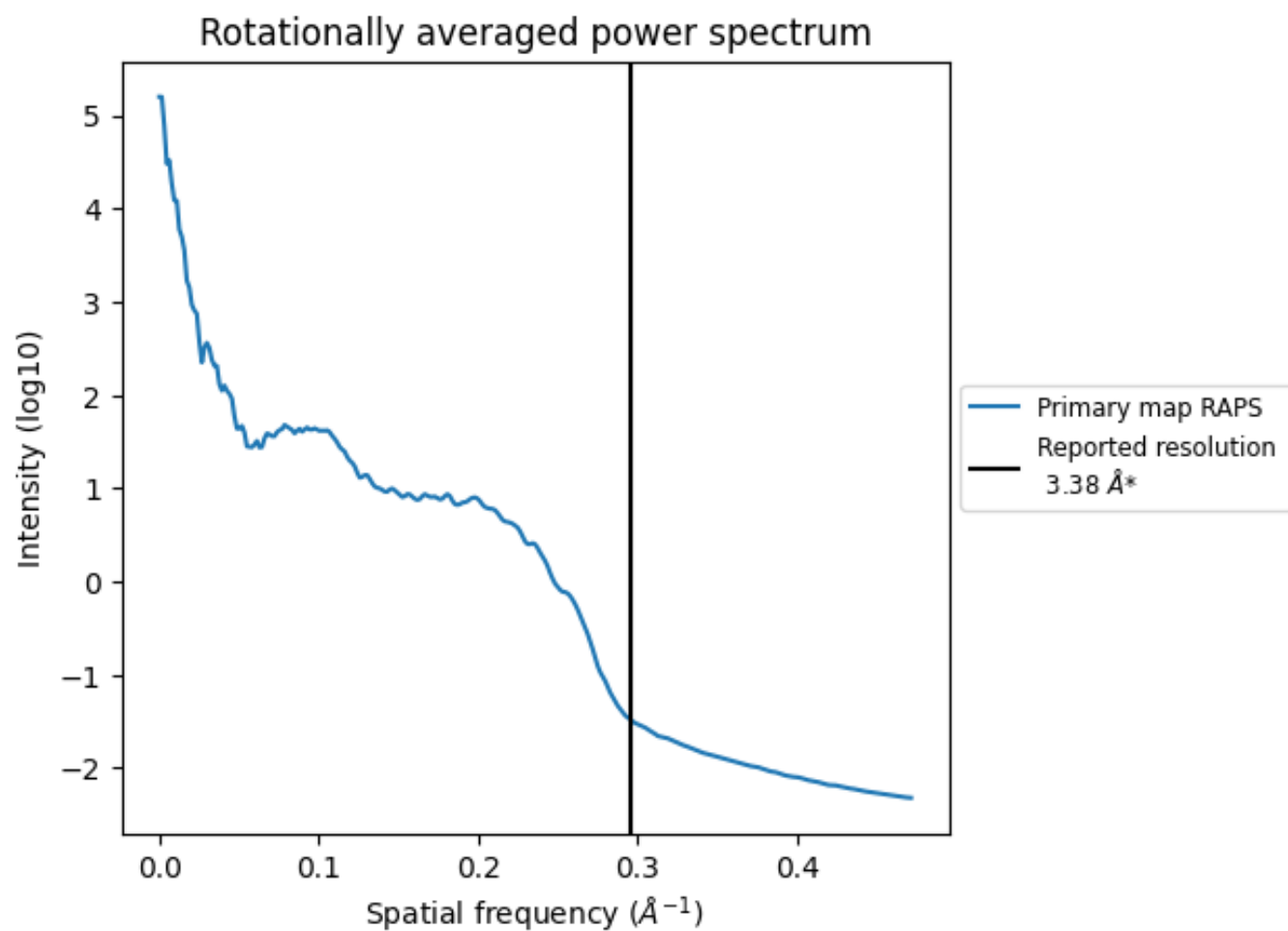
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 530 nm^3 ; this corresponds to an approximate mass of 479 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 ⓘ

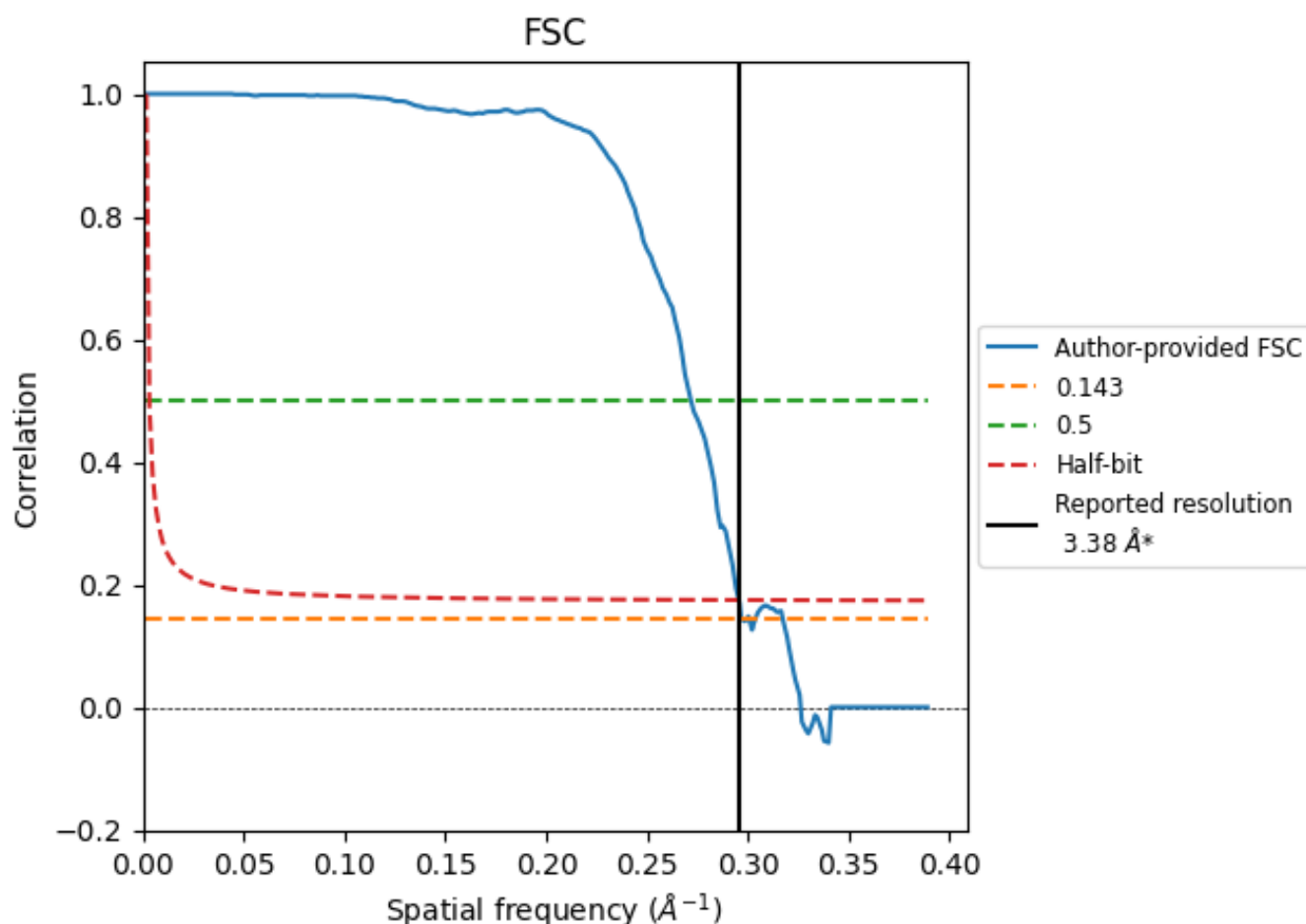


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

8.2 Resolution estimates [i](#)

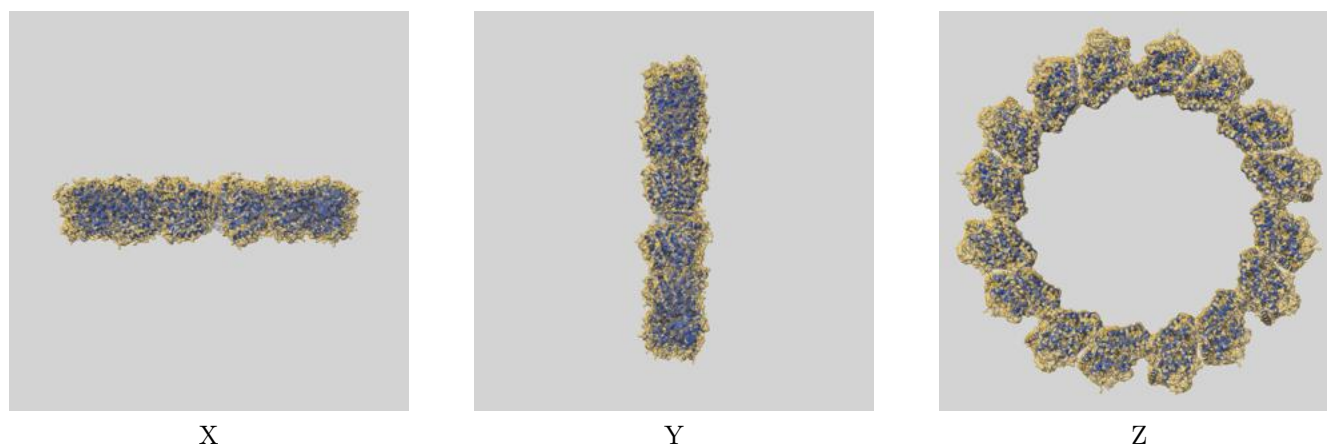
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.36	3.68	3.38
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

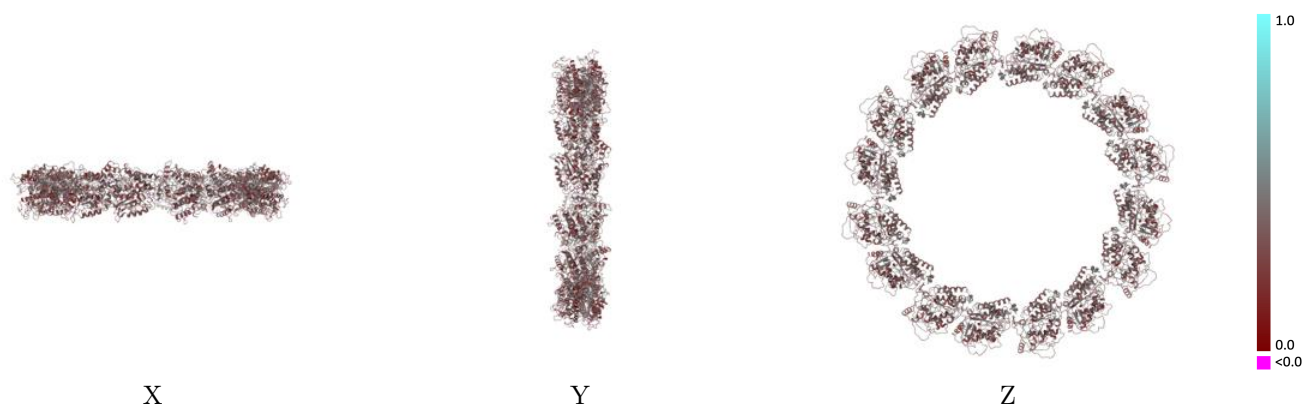
This section contains information regarding the fit between EMDB map EMD-23615 and PDB model 7M18. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



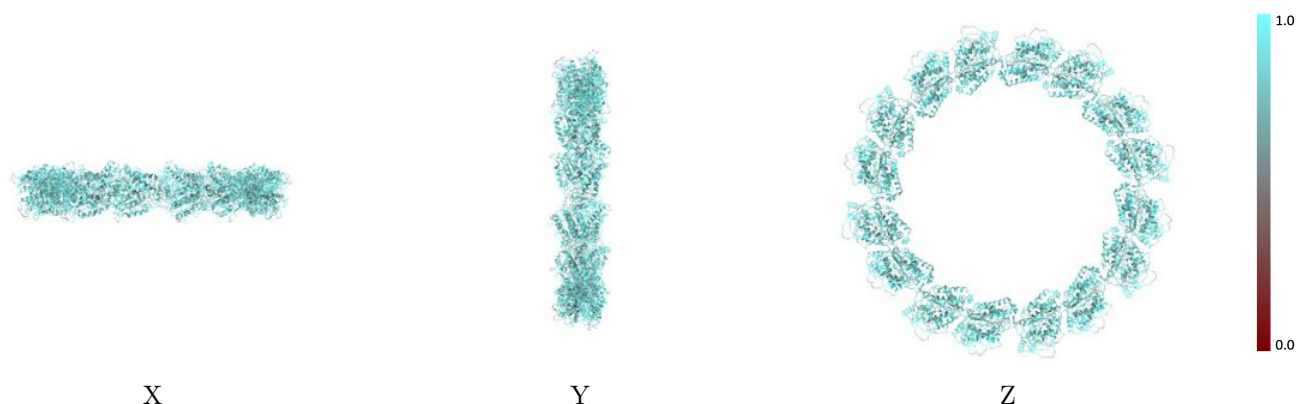
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



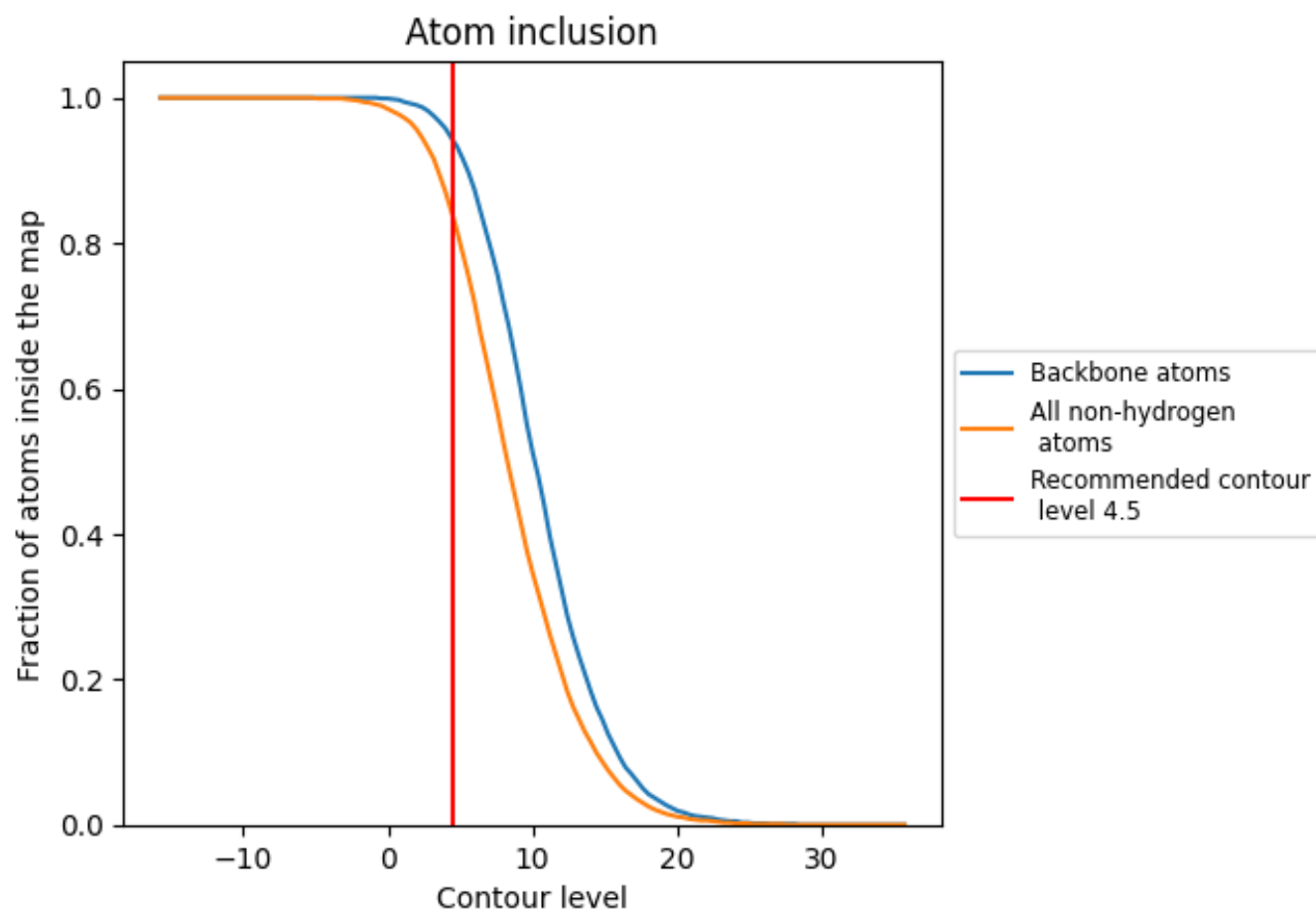
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.3600
A	0.8390	0.3640
B	0.8340	0.3560
C	0.8350	0.3620
D	0.8360	0.3560
E	0.8390	0.3660
F	0.8340	0.3580
G	0.8350	0.3630
H	0.8350	0.3570
I	0.8390	0.3640
J	0.8340	0.3580
K	0.8350	0.3630
L	0.8360	0.3560
M	0.8390	0.3650
N	0.8340	0.3580
O	0.8350	0.3620
P	0.8350	0.3560

1.0

0.0

<0.0