



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 04:22 PM UTC

PDB ID : 8IXF / pdb_00008ixf
EMDB ID : EMD-35792
Title : GMPCPP-Alpha4A/Beta2A-microtubule decorated with kinesin non-seam region
Authors : Zheng, W.; Zhao, Q.Y.; Diao, L.; Bao, L.; Cong, Y.
Deposited on : 2023-03-31
Resolution : 4.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

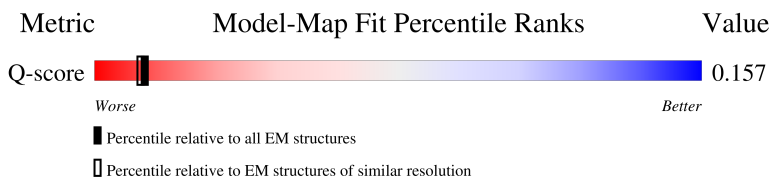
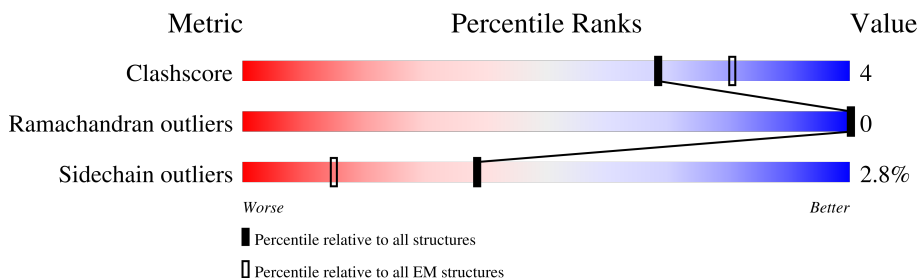
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	A	454	<div style="display: flex; justify-content: space-between;"> 24% 84% 10% 6% </div>
1	B	454	<div style="display: flex; justify-content: space-between;"> 25% 84% 10% 6% </div>
1	C	454	<div style="display: flex; justify-content: space-between;"> 24% 83% 10% 6% </div>
1	D	454	<div style="display: flex; justify-content: space-between;"> 20% 84% 10% 6% </div>

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Mol	Chain	Length	Quality of chain
1	E	454	24% 84% 10% 6%
1	F	454	22% 83% 10% 6%
1	G	454	19% 83% 10% 6%
1	H	454	25% 84% 10% 6%
1	I	454	21% 84% 10% 6%
2	J	457	19% 80% 13% 7%
2	K	457	21% 80% 13% 7%
2	L	457	20% 80% 13% 7%
2	M	457	17% 80% 13% 7%
2	N	457	19% 81% 12% 7%
2	O	457	20% 80% 13% 7%
2	P	457	17% 81% 12% 7%
2	Q	457	18% 80% 13% 7%
2	R	457	18% 81% 13% 7%
3	S	372	51% 78% 9% 13%
3	T	372	58% 78% 9% 13%
3	U	372	62% 78% 9% 13%
3	V	372	54% 78% 9% 13%
3	W	372	53% 78% 9% 13%
3	X	372	63% 79% 8% 13%
3	Y	372	52% 78% 9% 13%
3	Z	372	56% 79% 8% 13%
3	a	372	56% 78% 9% 13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 84087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	427	3350	2123	570	634	23	0	0
1	A	427	3350	2123	570	634	23	0	0
1	B	427	3350	2123	570	634	23	0	0
1	C	427	3350	2123	570	634	23	0	0
1	D	427	3350	2123	570	634	23	0	0
1	E	427	3350	2123	570	634	23	0	0
1	F	427	3350	2123	570	634	23	0	0
1	G	427	3350	2123	570	634	23	0	0
1	H	427	3350	2123	570	634	23	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	43	HIS	-	insertion	UNP P68368
I	44	HIS	-	insertion	UNP P68368
I	45	HIS	-	insertion	UNP P68368
I	46	HIS	-	insertion	UNP P68368
I	47	HIS	-	insertion	UNP P68368
I	48	HIS	-	insertion	UNP P68368
A	43	HIS	-	insertion	UNP P68368
A	44	HIS	-	insertion	UNP P68368
A	45	HIS	-	insertion	UNP P68368
A	46	HIS	-	insertion	UNP P68368
A	47	HIS	-	insertion	UNP P68368
A	48	HIS	-	insertion	UNP P68368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	43	HIS	-	insertion	UNP P68368
B	44	HIS	-	insertion	UNP P68368
B	45	HIS	-	insertion	UNP P68368
B	46	HIS	-	insertion	UNP P68368
B	47	HIS	-	insertion	UNP P68368
B	48	HIS	-	insertion	UNP P68368
C	43	HIS	-	insertion	UNP P68368
C	44	HIS	-	insertion	UNP P68368
C	45	HIS	-	insertion	UNP P68368
C	46	HIS	-	insertion	UNP P68368
C	47	HIS	-	insertion	UNP P68368
C	48	HIS	-	insertion	UNP P68368
D	43	HIS	-	insertion	UNP P68368
D	44	HIS	-	insertion	UNP P68368
D	45	HIS	-	insertion	UNP P68368
D	46	HIS	-	insertion	UNP P68368
D	47	HIS	-	insertion	UNP P68368
D	48	HIS	-	insertion	UNP P68368
E	43	HIS	-	insertion	UNP P68368
E	44	HIS	-	insertion	UNP P68368
E	45	HIS	-	insertion	UNP P68368
E	46	HIS	-	insertion	UNP P68368
E	47	HIS	-	insertion	UNP P68368
E	48	HIS	-	insertion	UNP P68368
F	43	HIS	-	insertion	UNP P68368
F	44	HIS	-	insertion	UNP P68368
F	45	HIS	-	insertion	UNP P68368
F	46	HIS	-	insertion	UNP P68368
F	47	HIS	-	insertion	UNP P68368
F	48	HIS	-	insertion	UNP P68368
G	43	HIS	-	insertion	UNP P68368
G	44	HIS	-	insertion	UNP P68368
G	45	HIS	-	insertion	UNP P68368
G	46	HIS	-	insertion	UNP P68368
G	47	HIS	-	insertion	UNP P68368
G	48	HIS	-	insertion	UNP P68368
H	43	HIS	-	insertion	UNP P68368
H	44	HIS	-	insertion	UNP P68368
H	45	HIS	-	insertion	UNP P68368
H	46	HIS	-	insertion	UNP P68368
H	47	HIS	-	insertion	UNP P68368
H	48	HIS	-	insertion	UNP P68368

- Molecule 2 is a protein called Tubulin beta-2A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Q	426	3354	2107	575	646	26	0	0
2	J	426	3354	2107	575	646	26	0	0
2	K	426	3354	2107	575	646	26	0	0
2	L	426	3354	2107	575	646	26	0	0
2	M	426	3354	2107	575	646	26	0	0
2	N	426	3354	2107	575	646	26	0	0
2	O	426	3354	2107	575	646	26	0	0
2	P	426	3354	2107	575	646	26	0	0
2	R	426	3354	2107	575	646	26	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	446	GLY	-	expression tag	UNP Q7TMM9
Q	447	GLY	-	expression tag	UNP Q7TMM9
Q	448	SER	-	expression tag	UNP Q7TMM9
Q	449	GLY	-	expression tag	UNP Q7TMM9
Q	450	GLY	-	expression tag	UNP Q7TMM9
Q	451	ASP	-	expression tag	UNP Q7TMM9
Q	452	TYR	-	expression tag	UNP Q7TMM9
Q	453	LYS	-	expression tag	UNP Q7TMM9
Q	454	ASP	-	expression tag	UNP Q7TMM9
Q	455	ASP	-	expression tag	UNP Q7TMM9
Q	456	ASP	-	expression tag	UNP Q7TMM9
Q	457	LYS	-	expression tag	UNP Q7TMM9
J	446	GLY	-	expression tag	UNP Q7TMM9
J	447	GLY	-	expression tag	UNP Q7TMM9
J	448	SER	-	expression tag	UNP Q7TMM9
J	449	GLY	-	expression tag	UNP Q7TMM9
J	450	GLY	-	expression tag	UNP Q7TMM9
J	451	ASP	-	expression tag	UNP Q7TMM9
J	452	TYR	-	expression tag	UNP Q7TMM9
J	453	LYS	-	expression tag	UNP Q7TMM9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	454	ASP	-	expression tag	UNP Q7TMM9
J	455	ASP	-	expression tag	UNP Q7TMM9
J	456	ASP	-	expression tag	UNP Q7TMM9
J	457	LYS	-	expression tag	UNP Q7TMM9
K	446	GLY	-	expression tag	UNP Q7TMM9
K	447	GLY	-	expression tag	UNP Q7TMM9
K	448	SER	-	expression tag	UNP Q7TMM9
K	449	GLY	-	expression tag	UNP Q7TMM9
K	450	GLY	-	expression tag	UNP Q7TMM9
K	451	ASP	-	expression tag	UNP Q7TMM9
K	452	TYR	-	expression tag	UNP Q7TMM9
K	453	LYS	-	expression tag	UNP Q7TMM9
K	454	ASP	-	expression tag	UNP Q7TMM9
K	455	ASP	-	expression tag	UNP Q7TMM9
K	456	ASP	-	expression tag	UNP Q7TMM9
K	457	LYS	-	expression tag	UNP Q7TMM9
L	446	GLY	-	expression tag	UNP Q7TMM9
L	447	GLY	-	expression tag	UNP Q7TMM9
L	448	SER	-	expression tag	UNP Q7TMM9
L	449	GLY	-	expression tag	UNP Q7TMM9
L	450	GLY	-	expression tag	UNP Q7TMM9
L	451	ASP	-	expression tag	UNP Q7TMM9
L	452	TYR	-	expression tag	UNP Q7TMM9
L	453	LYS	-	expression tag	UNP Q7TMM9
L	454	ASP	-	expression tag	UNP Q7TMM9
L	455	ASP	-	expression tag	UNP Q7TMM9
L	456	ASP	-	expression tag	UNP Q7TMM9
L	457	LYS	-	expression tag	UNP Q7TMM9
M	446	GLY	-	expression tag	UNP Q7TMM9
M	447	GLY	-	expression tag	UNP Q7TMM9
M	448	SER	-	expression tag	UNP Q7TMM9
M	449	GLY	-	expression tag	UNP Q7TMM9
M	450	GLY	-	expression tag	UNP Q7TMM9
M	451	ASP	-	expression tag	UNP Q7TMM9
M	452	TYR	-	expression tag	UNP Q7TMM9
M	453	LYS	-	expression tag	UNP Q7TMM9
M	454	ASP	-	expression tag	UNP Q7TMM9
M	455	ASP	-	expression tag	UNP Q7TMM9
M	456	ASP	-	expression tag	UNP Q7TMM9
M	457	LYS	-	expression tag	UNP Q7TMM9
N	446	GLY	-	expression tag	UNP Q7TMM9
N	447	GLY	-	expression tag	UNP Q7TMM9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	448	SER	-	expression tag	UNP Q7TMM9
N	449	GLY	-	expression tag	UNP Q7TMM9
N	450	GLY	-	expression tag	UNP Q7TMM9
N	451	ASP	-	expression tag	UNP Q7TMM9
N	452	TYR	-	expression tag	UNP Q7TMM9
N	453	LYS	-	expression tag	UNP Q7TMM9
N	454	ASP	-	expression tag	UNP Q7TMM9
N	455	ASP	-	expression tag	UNP Q7TMM9
N	456	ASP	-	expression tag	UNP Q7TMM9
N	457	LYS	-	expression tag	UNP Q7TMM9
O	446	GLY	-	expression tag	UNP Q7TMM9
O	447	GLY	-	expression tag	UNP Q7TMM9
O	448	SER	-	expression tag	UNP Q7TMM9
O	449	GLY	-	expression tag	UNP Q7TMM9
O	450	GLY	-	expression tag	UNP Q7TMM9
O	451	ASP	-	expression tag	UNP Q7TMM9
O	452	TYR	-	expression tag	UNP Q7TMM9
O	453	LYS	-	expression tag	UNP Q7TMM9
O	454	ASP	-	expression tag	UNP Q7TMM9
O	455	ASP	-	expression tag	UNP Q7TMM9
O	456	ASP	-	expression tag	UNP Q7TMM9
O	457	LYS	-	expression tag	UNP Q7TMM9
P	446	GLY	-	expression tag	UNP Q7TMM9
P	447	GLY	-	expression tag	UNP Q7TMM9
P	448	SER	-	expression tag	UNP Q7TMM9
P	449	GLY	-	expression tag	UNP Q7TMM9
P	450	GLY	-	expression tag	UNP Q7TMM9
P	451	ASP	-	expression tag	UNP Q7TMM9
P	452	TYR	-	expression tag	UNP Q7TMM9
P	453	LYS	-	expression tag	UNP Q7TMM9
P	454	ASP	-	expression tag	UNP Q7TMM9
P	455	ASP	-	expression tag	UNP Q7TMM9
P	456	ASP	-	expression tag	UNP Q7TMM9
P	457	LYS	-	expression tag	UNP Q7TMM9
R	446	GLY	-	expression tag	UNP Q7TMM9
R	447	GLY	-	expression tag	UNP Q7TMM9
R	448	SER	-	expression tag	UNP Q7TMM9
R	449	GLY	-	expression tag	UNP Q7TMM9
R	450	GLY	-	expression tag	UNP Q7TMM9
R	451	ASP	-	expression tag	UNP Q7TMM9
R	452	TYR	-	expression tag	UNP Q7TMM9
R	453	LYS	-	expression tag	UNP Q7TMM9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	454	ASP	-	expression tag	UNP Q7TMM9
R	455	ASP	-	expression tag	UNP Q7TMM9
R	456	ASP	-	expression tag	UNP Q7TMM9
R	457	LYS	-	expression tag	UNP Q7TMM9

- Molecule 3 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Y	325	2544	1585	438	506	15	0	0
3	S	325	2544	1585	438	506	15	0	0
3	T	325	2544	1585	438	506	15	0	0
3	U	325	2544	1585	438	506	15	0	0
3	V	325	2544	1585	438	506	15	0	0
3	W	325	2544	1585	438	506	15	0	0
3	X	325	2544	1585	438	506	15	0	0
3	Z	325	2544	1585	438	506	15	0	0
3	a	325	2544	1585	438	506	15	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-22	MET	-	initiating methionine	UNP P33176
Y	-21	GLY	-	expression tag	UNP P33176
Y	-20	SER	-	expression tag	UNP P33176
Y	-19	SER	-	expression tag	UNP P33176
Y	-18	HIS	-	expression tag	UNP P33176
Y	-17	HIS	-	expression tag	UNP P33176
Y	-16	HIS	-	expression tag	UNP P33176
Y	-15	HIS	-	expression tag	UNP P33176
Y	-14	HIS	-	expression tag	UNP P33176
Y	-13	HIS	-	expression tag	UNP P33176
Y	-12	SER	-	expression tag	UNP P33176
Y	-11	SER	-	expression tag	UNP P33176

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-10	GLY	-	expression tag	UNP P33176
Y	-9	LEU	-	expression tag	UNP P33176
Y	-8	VAL	-	expression tag	UNP P33176
Y	-7	PRO	-	expression tag	UNP P33176
Y	-6	ARG	-	expression tag	UNP P33176
Y	-5	GLY	-	expression tag	UNP P33176
Y	-4	SER	-	expression tag	UNP P33176
Y	-3	HIS	-	expression tag	UNP P33176
Y	-2	MET	-	expression tag	UNP P33176
Y	-1	ALA	-	expression tag	UNP P33176
Y	0	SER	-	expression tag	UNP P33176
Y	236	ALA	GLU	conflict	UNP P33176
S	-22	MET	-	initiating methionine	UNP P33176
S	-21	GLY	-	expression tag	UNP P33176
S	-20	SER	-	expression tag	UNP P33176
S	-19	SER	-	expression tag	UNP P33176
S	-18	HIS	-	expression tag	UNP P33176
S	-17	HIS	-	expression tag	UNP P33176
S	-16	HIS	-	expression tag	UNP P33176
S	-15	HIS	-	expression tag	UNP P33176
S	-14	HIS	-	expression tag	UNP P33176
S	-13	HIS	-	expression tag	UNP P33176
S	-12	SER	-	expression tag	UNP P33176
S	-11	SER	-	expression tag	UNP P33176
S	-10	GLY	-	expression tag	UNP P33176
S	-9	LEU	-	expression tag	UNP P33176
S	-8	VAL	-	expression tag	UNP P33176
S	-7	PRO	-	expression tag	UNP P33176
S	-6	ARG	-	expression tag	UNP P33176
S	-5	GLY	-	expression tag	UNP P33176
S	-4	SER	-	expression tag	UNP P33176
S	-3	HIS	-	expression tag	UNP P33176
S	-2	MET	-	expression tag	UNP P33176
S	-1	ALA	-	expression tag	UNP P33176
S	0	SER	-	expression tag	UNP P33176
S	236	ALA	GLU	conflict	UNP P33176
T	-22	MET	-	initiating methionine	UNP P33176
T	-21	GLY	-	expression tag	UNP P33176
T	-20	SER	-	expression tag	UNP P33176
T	-19	SER	-	expression tag	UNP P33176
T	-18	HIS	-	expression tag	UNP P33176
T	-17	HIS	-	expression tag	UNP P33176

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-16	HIS	-	expression tag	UNP P33176
T	-15	HIS	-	expression tag	UNP P33176
T	-14	HIS	-	expression tag	UNP P33176
T	-13	HIS	-	expression tag	UNP P33176
T	-12	SER	-	expression tag	UNP P33176
T	-11	SER	-	expression tag	UNP P33176
T	-10	GLY	-	expression tag	UNP P33176
T	-9	LEU	-	expression tag	UNP P33176
T	-8	VAL	-	expression tag	UNP P33176
T	-7	PRO	-	expression tag	UNP P33176
T	-6	ARG	-	expression tag	UNP P33176
T	-5	GLY	-	expression tag	UNP P33176
T	-4	SER	-	expression tag	UNP P33176
T	-3	HIS	-	expression tag	UNP P33176
T	-2	MET	-	expression tag	UNP P33176
T	-1	ALA	-	expression tag	UNP P33176
T	0	SER	-	expression tag	UNP P33176
T	236	ALA	GLU	conflict	UNP P33176
U	-22	MET	-	initiating methionine	UNP P33176
U	-21	GLY	-	expression tag	UNP P33176
U	-20	SER	-	expression tag	UNP P33176
U	-19	SER	-	expression tag	UNP P33176
U	-18	HIS	-	expression tag	UNP P33176
U	-17	HIS	-	expression tag	UNP P33176
U	-16	HIS	-	expression tag	UNP P33176
U	-15	HIS	-	expression tag	UNP P33176
U	-14	HIS	-	expression tag	UNP P33176
U	-13	HIS	-	expression tag	UNP P33176
U	-12	SER	-	expression tag	UNP P33176
U	-11	SER	-	expression tag	UNP P33176
U	-10	GLY	-	expression tag	UNP P33176
U	-9	LEU	-	expression tag	UNP P33176
U	-8	VAL	-	expression tag	UNP P33176
U	-7	PRO	-	expression tag	UNP P33176
U	-6	ARG	-	expression tag	UNP P33176
U	-5	GLY	-	expression tag	UNP P33176
U	-4	SER	-	expression tag	UNP P33176
U	-3	HIS	-	expression tag	UNP P33176
U	-2	MET	-	expression tag	UNP P33176
U	-1	ALA	-	expression tag	UNP P33176
U	0	SER	-	expression tag	UNP P33176
U	236	ALA	GLU	conflict	UNP P33176

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-22	MET	-	initiating methionine	UNP P33176
V	-21	GLY	-	expression tag	UNP P33176
V	-20	SER	-	expression tag	UNP P33176
V	-19	SER	-	expression tag	UNP P33176
V	-18	HIS	-	expression tag	UNP P33176
V	-17	HIS	-	expression tag	UNP P33176
V	-16	HIS	-	expression tag	UNP P33176
V	-15	HIS	-	expression tag	UNP P33176
V	-14	HIS	-	expression tag	UNP P33176
V	-13	HIS	-	expression tag	UNP P33176
V	-12	SER	-	expression tag	UNP P33176
V	-11	SER	-	expression tag	UNP P33176
V	-10	GLY	-	expression tag	UNP P33176
V	-9	LEU	-	expression tag	UNP P33176
V	-8	VAL	-	expression tag	UNP P33176
V	-7	PRO	-	expression tag	UNP P33176
V	-6	ARG	-	expression tag	UNP P33176
V	-5	GLY	-	expression tag	UNP P33176
V	-4	SER	-	expression tag	UNP P33176
V	-3	HIS	-	expression tag	UNP P33176
V	-2	MET	-	expression tag	UNP P33176
V	-1	ALA	-	expression tag	UNP P33176
V	0	SER	-	expression tag	UNP P33176
V	236	ALA	GLU	conflict	UNP P33176
W	-22	MET	-	initiating methionine	UNP P33176
W	-21	GLY	-	expression tag	UNP P33176
W	-20	SER	-	expression tag	UNP P33176
W	-19	SER	-	expression tag	UNP P33176
W	-18	HIS	-	expression tag	UNP P33176
W	-17	HIS	-	expression tag	UNP P33176
W	-16	HIS	-	expression tag	UNP P33176
W	-15	HIS	-	expression tag	UNP P33176
W	-14	HIS	-	expression tag	UNP P33176
W	-13	HIS	-	expression tag	UNP P33176
W	-12	SER	-	expression tag	UNP P33176
W	-11	SER	-	expression tag	UNP P33176
W	-10	GLY	-	expression tag	UNP P33176
W	-9	LEU	-	expression tag	UNP P33176
W	-8	VAL	-	expression tag	UNP P33176
W	-7	PRO	-	expression tag	UNP P33176
W	-6	ARG	-	expression tag	UNP P33176
W	-5	GLY	-	expression tag	UNP P33176

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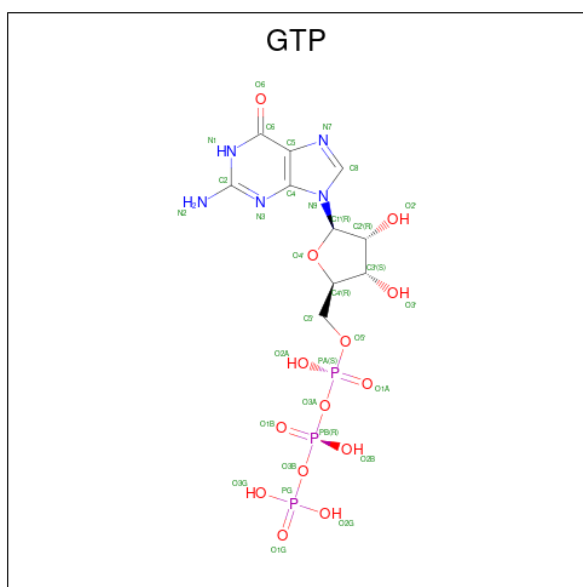
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W	-2	MET	-	expression tag	UNP P33176
W	-1	ALA	-	expression tag	UNP P33176
W	0	SER	-	expression tag	UNP P33176
W	236	ALA	GLU	conflict	UNP P33176
X	-22	MET	-	initiating methionine	UNP P33176
X	-21	GLY	-	expression tag	UNP P33176
X	-20	SER	-	expression tag	UNP P33176
X	-19	SER	-	expression tag	UNP P33176
X	-18	HIS	-	expression tag	UNP P33176
X	-17	HIS	-	expression tag	UNP P33176
X	-16	HIS	-	expression tag	UNP P33176
X	-15	HIS	-	expression tag	UNP P33176
X	-14	HIS	-	expression tag	UNP P33176
X	-13	HIS	-	expression tag	UNP P33176
X	-12	SER	-	expression tag	UNP P33176
X	-11	SER	-	expression tag	UNP P33176
X	-10	GLY	-	expression tag	UNP P33176
X	-9	LEU	-	expression tag	UNP P33176
X	-8	VAL	-	expression tag	UNP P33176
X	-7	PRO	-	expression tag	UNP P33176
X	-6	ARG	-	expression tag	UNP P33176
X	-5	GLY	-	expression tag	UNP P33176
X	-4	SER	-	expression tag	UNP P33176
X	-3	HIS	-	expression tag	UNP P33176
X	-2	MET	-	expression tag	UNP P33176
X	-1	ALA	-	expression tag	UNP P33176
X	0	SER	-	expression tag	UNP P33176
X	236	ALA	GLU	conflict	UNP P33176
Z	-22	MET	-	initiating methionine	UNP P33176
Z	-21	GLY	-	expression tag	UNP P33176
Z	-20	SER	-	expression tag	UNP P33176
Z	-19	SER	-	expression tag	UNP P33176
Z	-18	HIS	-	expression tag	UNP P33176
Z	-17	HIS	-	expression tag	UNP P33176
Z	-16	HIS	-	expression tag	UNP P33176
Z	-15	HIS	-	expression tag	UNP P33176
Z	-14	HIS	-	expression tag	UNP P33176
Z	-13	HIS	-	expression tag	UNP P33176
Z	-12	SER	-	expression tag	UNP P33176
Z	-11	SER	-	expression tag	UNP P33176

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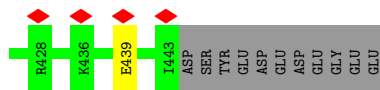
Chain	Residue	Modelled	Actual	Comment	Reference
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Z	-9	LEU	-	expression tag	UNP P33176
Z	-8	VAL	-	expression tag	UNP P33176
Z	-7	PRO	-	expression tag	UNP P33176
Z	-6	ARG	-	expression tag	UNP P33176
Z	-5	GLY	-	expression tag	UNP P33176
Z	-4	SER	-	expression tag	UNP P33176
Z	-3	HIS	-	expression tag	UNP P33176
Z	-2	MET	-	expression tag	UNP P33176
Z	-1	ALA	-	expression tag	UNP P33176
Z	0	SER	-	expression tag	UNP P33176
Z	236	ALA	GLU	conflict	UNP P33176
a	-22	MET	-	initiating methionine	UNP P33176
a	-21	GLY	-	expression tag	UNP P33176
a	-20	SER	-	expression tag	UNP P33176
a	-19	SER	-	expression tag	UNP P33176
a	-18	HIS	-	expression tag	UNP P33176
a	-17	HIS	-	expression tag	UNP P33176
a	-16	HIS	-	expression tag	UNP P33176
a	-15	HIS	-	expression tag	UNP P33176
a	-14	HIS	-	expression tag	UNP P33176
a	-13	HIS	-	expression tag	UNP P33176
a	-12	SER	-	expression tag	UNP P33176
a	-11	SER	-	expression tag	UNP P33176
a	-10	GLY	-	expression tag	UNP P33176
a	-9	LEU	-	expression tag	UNP P33176
a	-8	VAL	-	expression tag	UNP P33176
a	-7	PRO	-	expression tag	UNP P33176
a	-6	ARG	-	expression tag	UNP P33176
a	-5	GLY	-	expression tag	UNP P33176
a	-4	SER	-	expression tag	UNP P33176
a	-3	HIS	-	expression tag	UNP P33176
a	-2	MET	-	expression tag	UNP P33176
a	-1	ALA	-	expression tag	UNP P33176
a	0	SER	-	expression tag	UNP P33176
a	236	ALA	GLU	conflict	UNP P33176

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

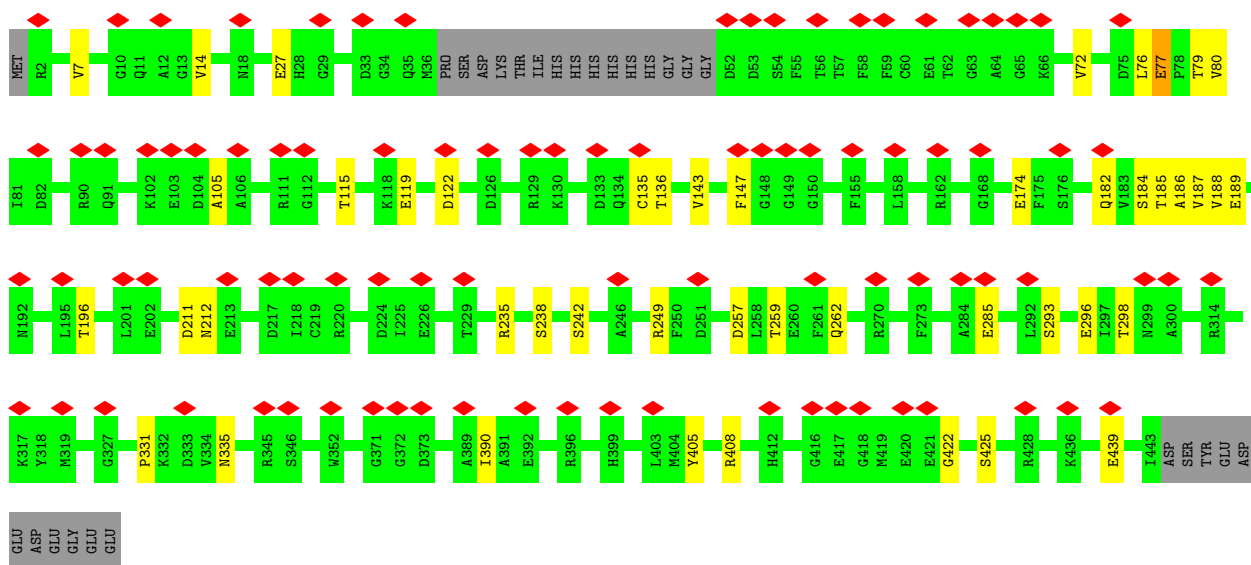
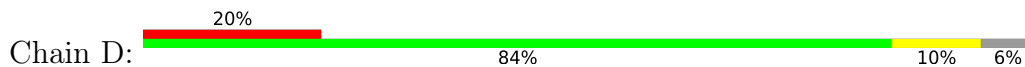


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	Q	1	Total 32	C 10	N 5	O 14	P 3	0
4	J	1	Total 32	C 10	N 5	O 14	P 3	0
4	K	1	Total 32	C 10	N 5	O 14	P 3	0
4	L	1	Total 32	C 10	N 5	O 14	P 3	0
4	M	1	Total 32	C 10	N 5	O 14	P 3	0
4	N	1	Total 32	C 10	N 5	O 14	P 3	0
4	O	1	Total 32	C 10	N 5	O 14	P 3	0
4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

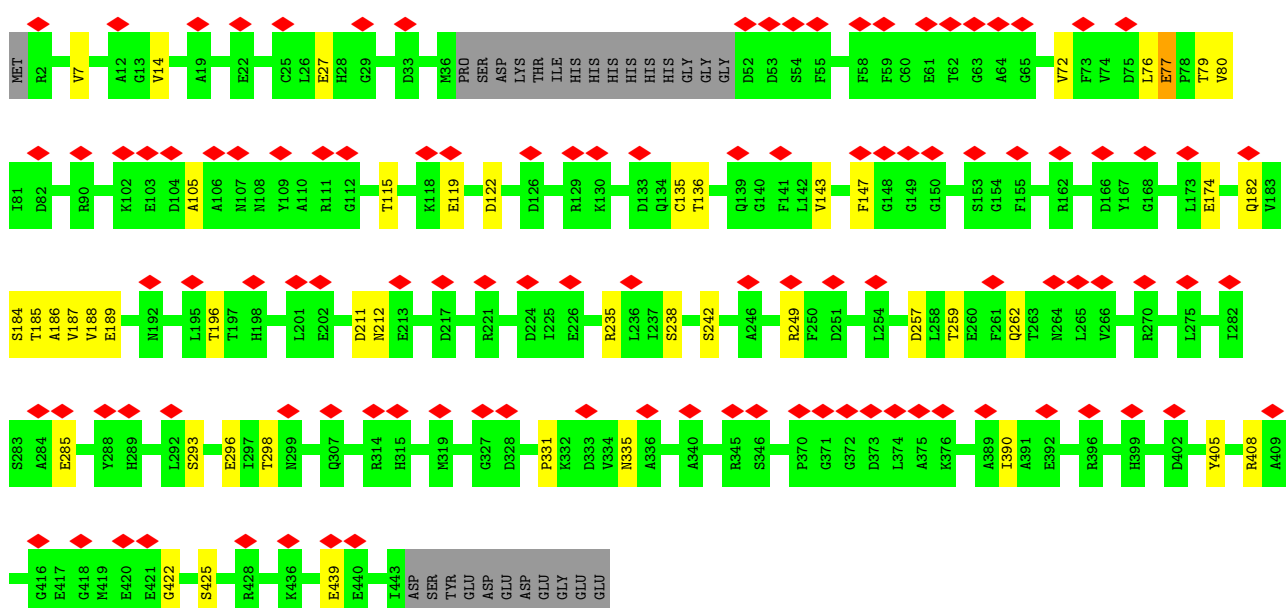
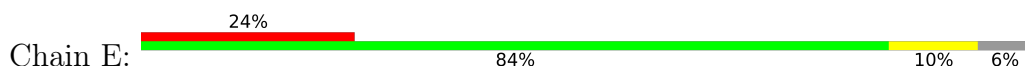
- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



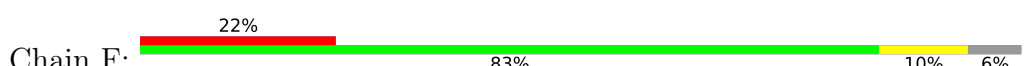
• Molecule 1: Tubulin alpha-4A chain

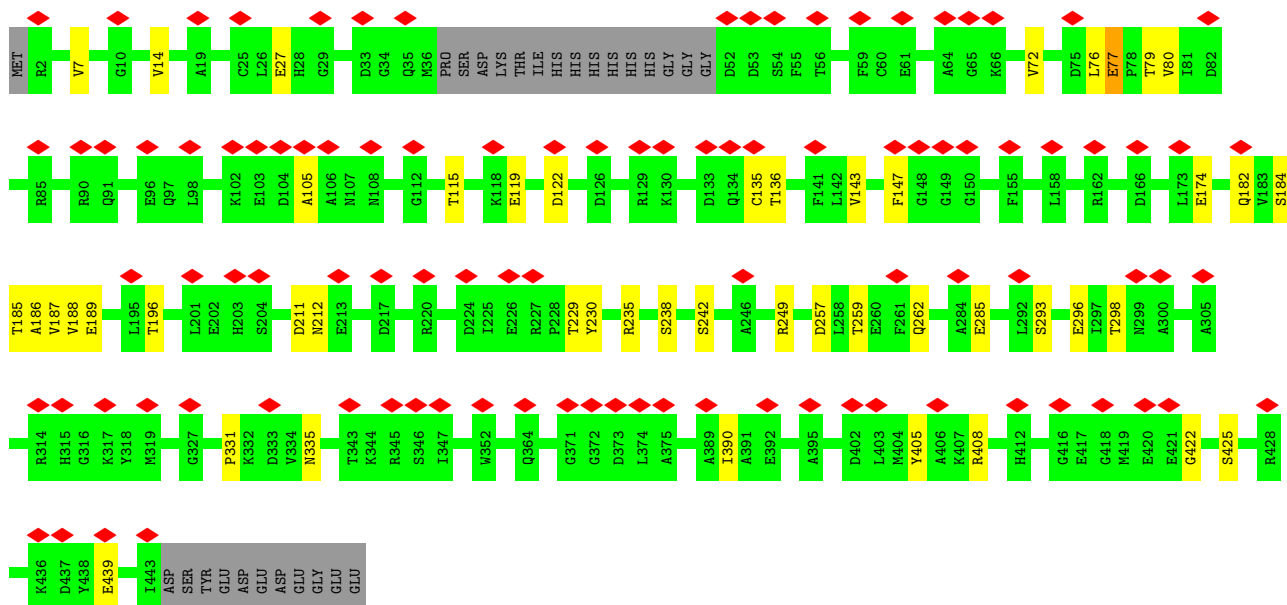


• Molecule 1: Tubulin alpha-4A chain

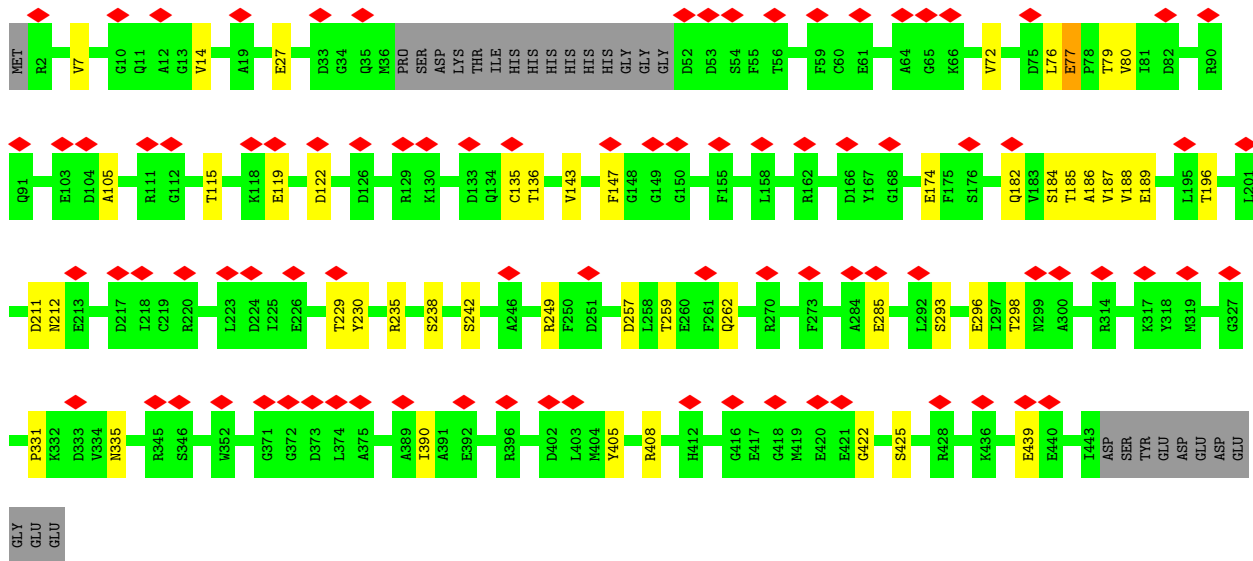
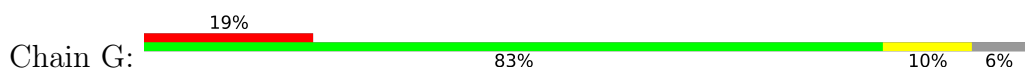


• Molecule 1: Tubulin alpha-4A chain

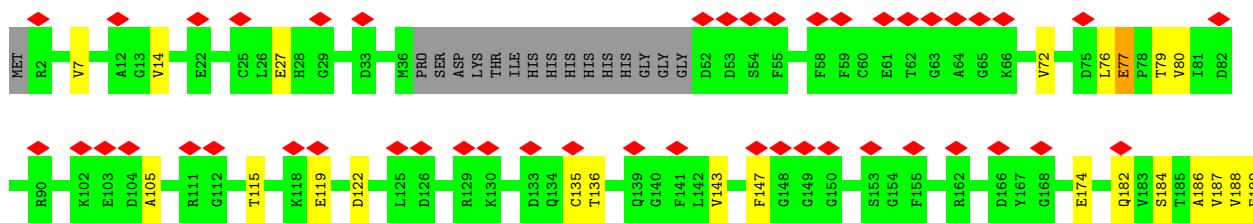
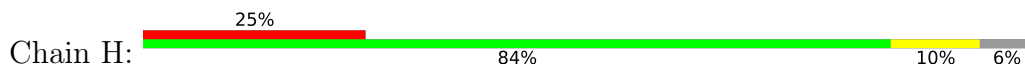


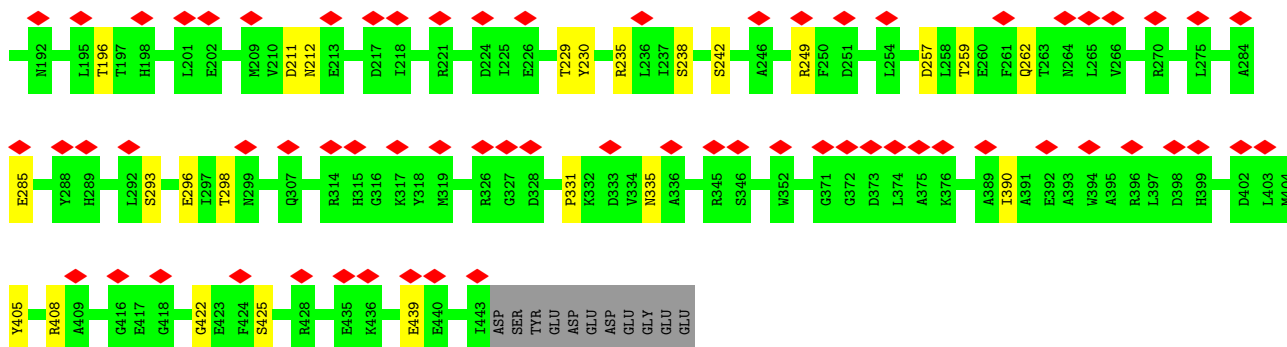


• Molecule 1: Tubulin alpha-4A chain

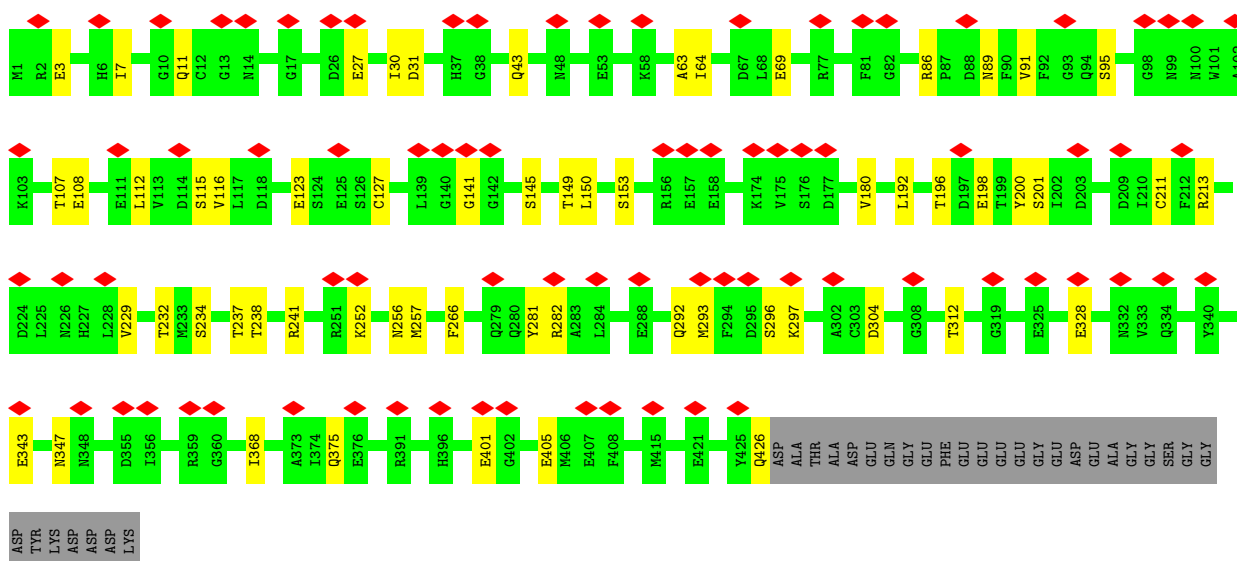
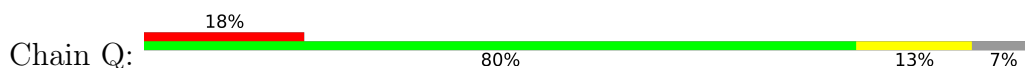


• Molecule 1: Tubulin alpha-4A chain

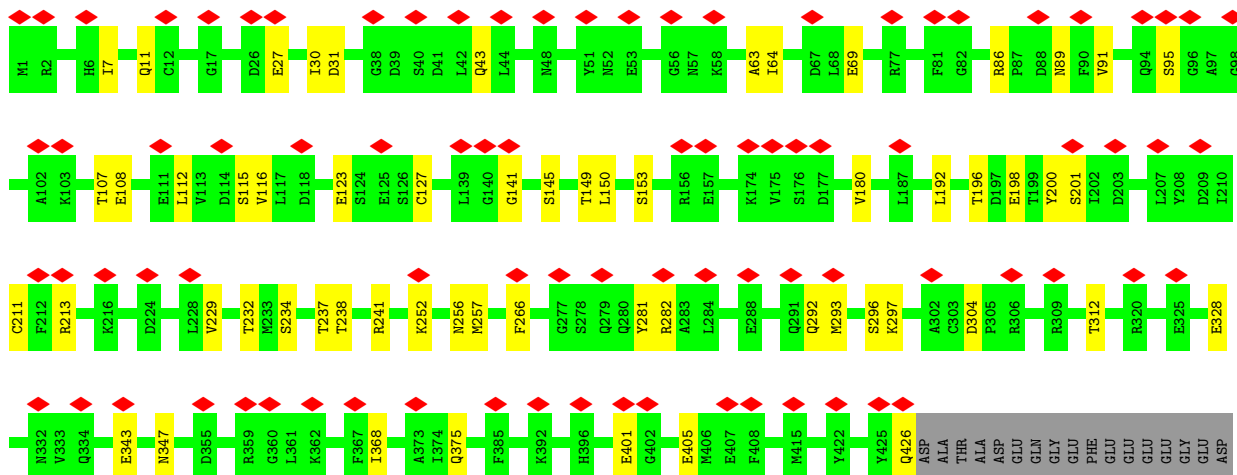




• Molecule 2: Tubulin beta-2A chain

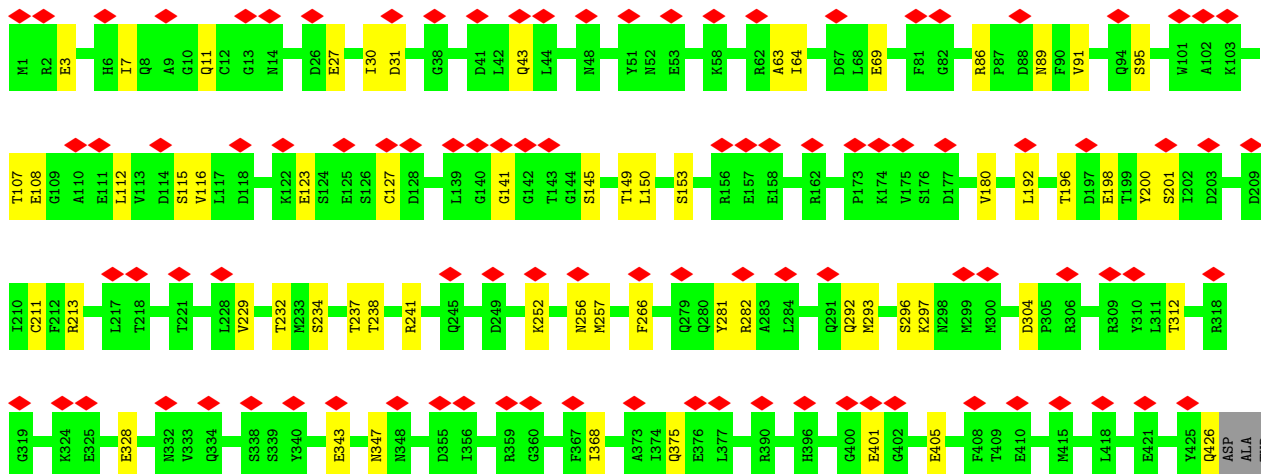
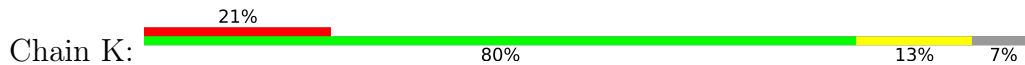


• Molecule 2: Tubulin beta-2A chain



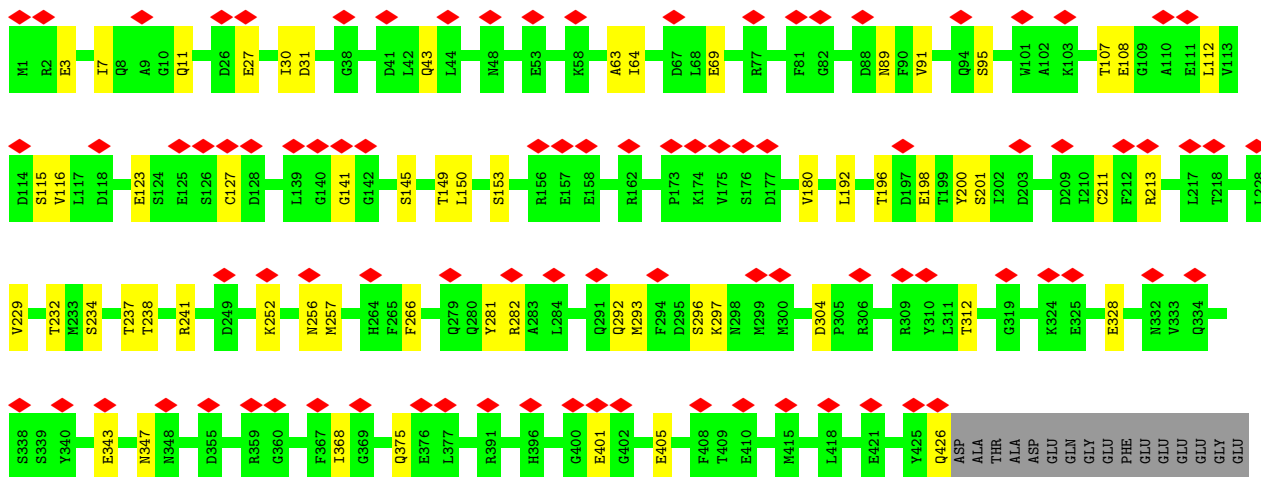
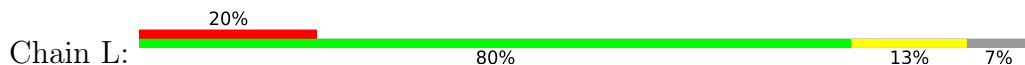
GLU
ALA
GLY
GLY
SER
GLY
GLY
ASP
TYR
LYS
ASP
ASP
ASP
LYS

• Molecule 2: Tubulin beta-2A chain



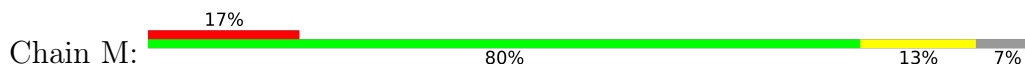
ALA
ASP
GLU
GLN
GLY
GLY
PHE
GLU
GLU
GLU
GLU
GLY
ASP
GLU
ALA
GLY
GLY
SER
GLY
TYR
LYS
ASP
ASP
ASP
LYS

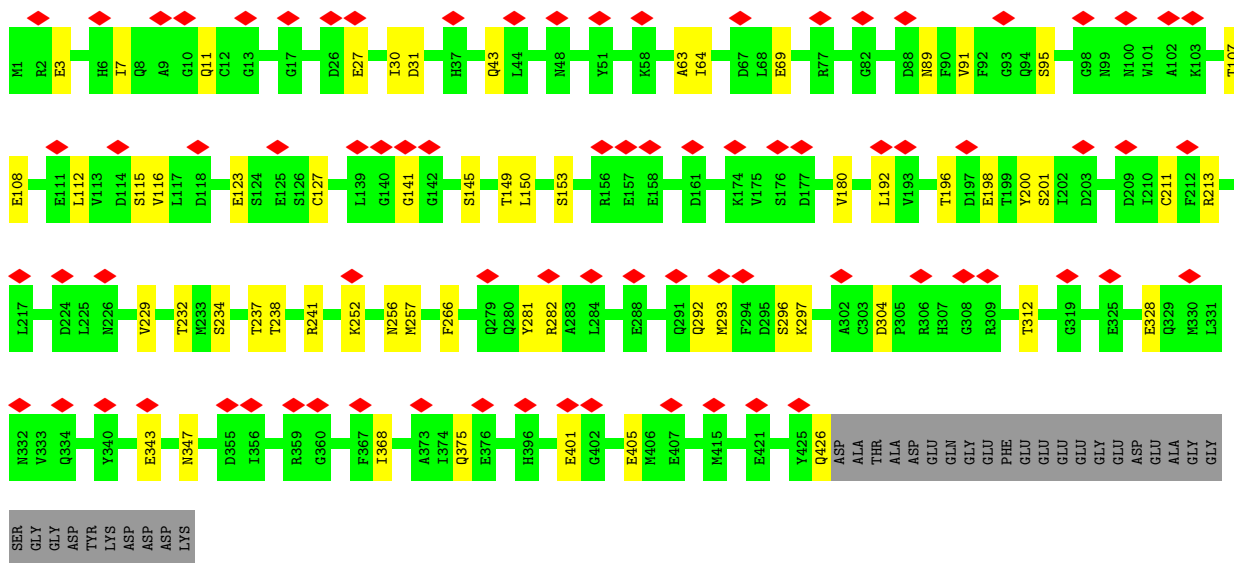
• Molecule 2: Tubulin beta-2A chain



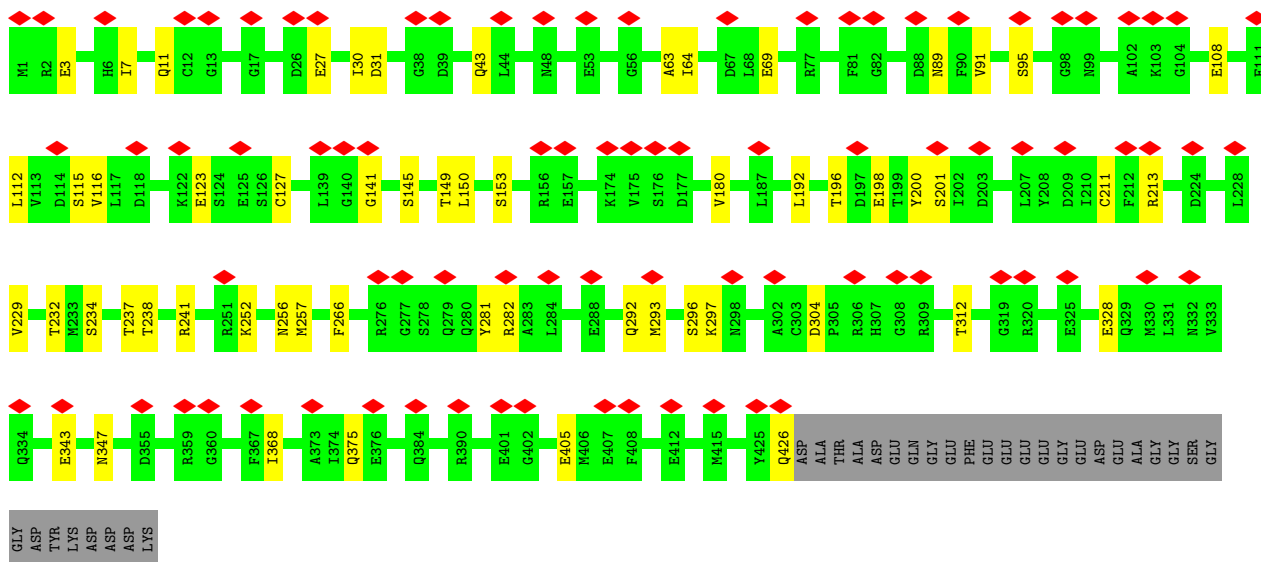
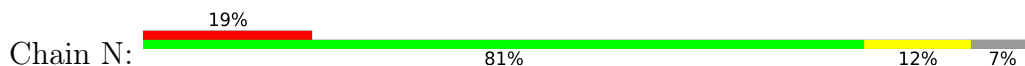
ASP
GLU
ALA
GLY
GLY
SER
GLY
GLY
ASP
LYS
ASP
ASP
ASP
LYS

• Molecule 2: Tubulin beta-2A chain

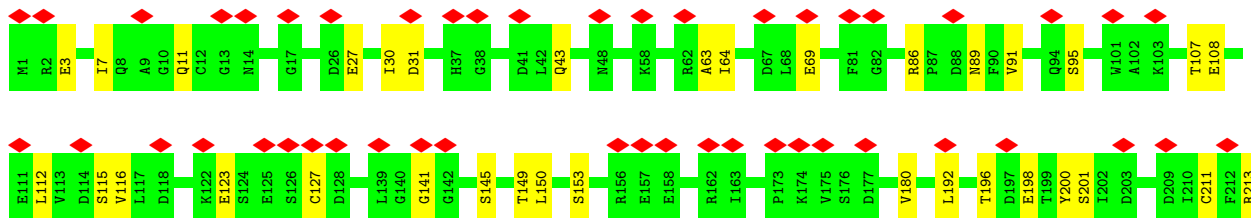
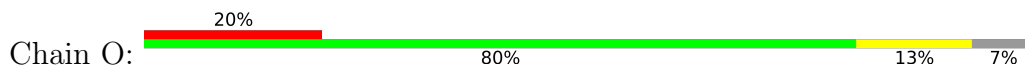


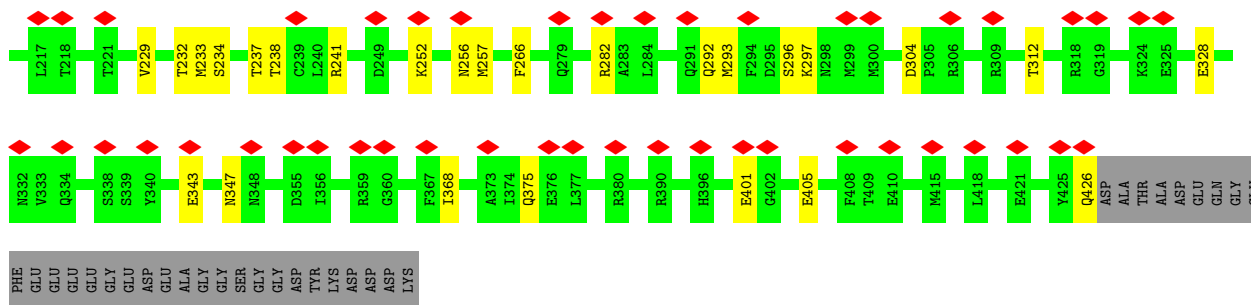


• Molecule 2: Tubulin beta-2A chain

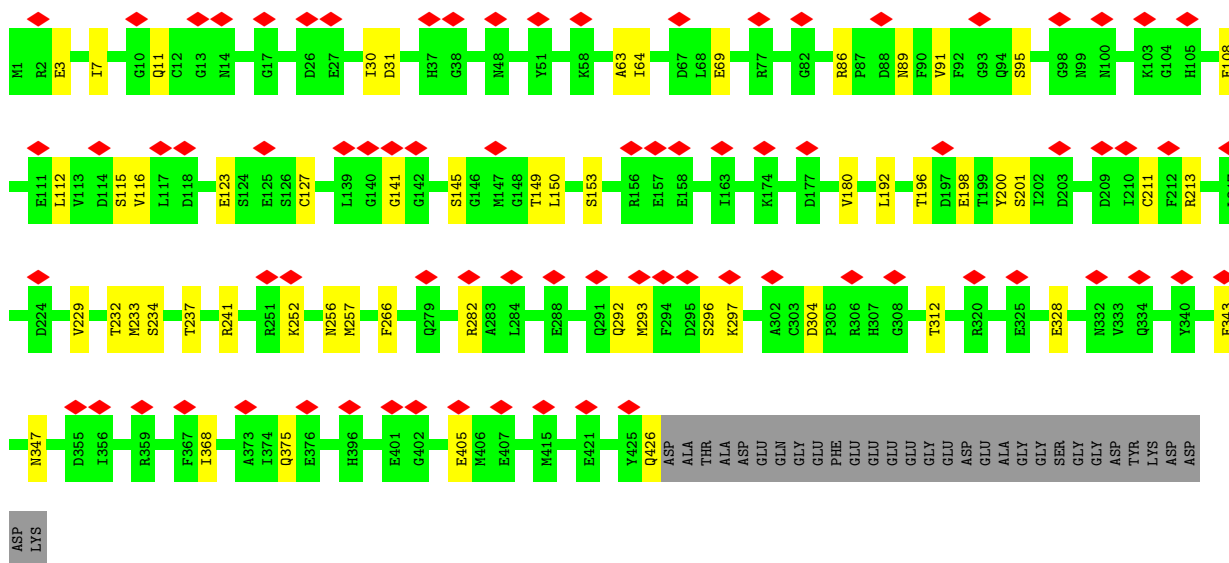
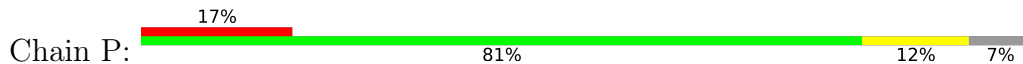


• Molecule 2: Tubulin beta-2A chain

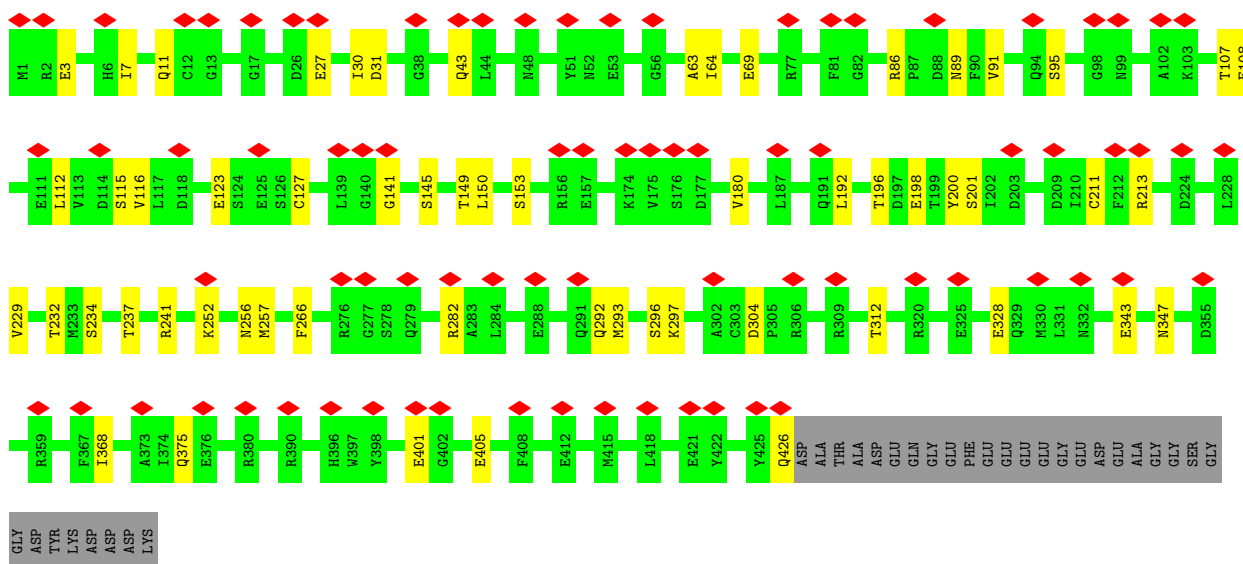
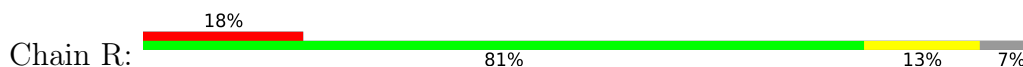




• Molecule 2: Tubulin beta-2A chain

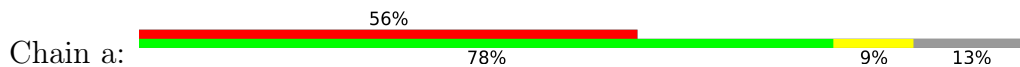


• Molecule 2: Tubulin beta-2A chain



T328
V329
CYS
VAL
ASN
GLU
LEU
THR
ALA
GLU
GLN
TRP
LYS
LYS
LYS
TYR
GLU
LYS
LYS
LYS
GLU

• Molecule 3: Kinesin-1 heavy chain



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	ALA	ALA	ASP	LEU	A5	E6	C7	N8	I9	K10	V11	M12	C13	R14	F15	R16	P17	L18	M19	E20	S21	E22	R25	G26	D27	K28	Y29	I30	Q34	D37	T38	V39	V40	I41				
A42	S43	K44	P45	Y46	A47	F48	D49	R50	V51	F52	S55	E59	Q60	V61	Y62	C65	A66	I69	V70	K71	D72	V73	L74	E75	G76	Y77	N78	F82	A83	Y84	G85	Q86	T87	S88	S89	G90	K91	T92	K150	T94	M95	E96	G97	K98	L99	H100	D101	P102	E103	G104	M105	G106	I107	I108				
P109	R110	I111	V112	Q113	D114	I115	F116	N117	Y118	I119	Y120	S121	M122	D123	E124	N125	L126	E127	F128	H129	I130	K131	V132	S133	Y134	F135	E136	I137	Y138	L139	D140	K141	I142	R143	D144	L145	L146	D147	V148	S149	K150	T151	N152	L153	V155	H156	E157	K159	N160	R161	V162	P163	K166	G167	T169			
E170	R171	F172	V173	C174	S175	T182	I183	D184	E185	S188	N189	R190	H191	V192	A193	V194	T195	N196	M197	N198	E199	H200	S201	S202	R203	S204	H205	F208	L209	I210	N211	V212	K213	Q214	E215	N216	T217	Q218	T219	E220	Q221	K222	L223	S224	G225	K226	L227	Y228	L229	V230	D231	L232	A233	S234	S235	A236		
K237	V238	S239	K240	T241	G242	A243	E244	G245	A246	V247	L248	D249	E250	N253	I254	L258	L261	G262	N263	A269	E270	G271	S272	T273	Y277	R278	D279	S280	K281	M282	T283	R284	S289	L290	G291	G292	N293	C294	R295	T296	T297	I298	V299	I300	C301	C302	S303	P304	S305	S306	E309	S310						
K313	L317	Q320	R321	A322	K323	T324	I325	K326	N327	T328	V329	CYS	VAL	ASN	VAL	GLU	LEU	THR	ALA	GLU	GLN	TRP	LYS	LYS	LYS	TYR	GLU	GLU	LYS	LYS	LYS	GLU	D279	S280	K281	M282	T283	R284	S289	L290	G291	G292	N293	C294	R295	T296	T297	I298	V299	I300	C301	C302	S303	P304	S305	S306	E309	S310

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.238	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.21	Depositor
Map size (\AA)	674.816, 674.816, 674.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.318, 1.318, 1.318	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, G2P, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/3428	0.44	0/4653
1	B	0.23	0/3428	0.44	0/4653
1	C	0.23	0/3428	0.44	0/4653
1	D	0.23	0/3428	0.44	0/4653
1	E	0.23	0/3428	0.44	0/4653
1	F	0.23	0/3428	0.44	0/4653
1	G	0.23	0/3428	0.44	0/4653
1	H	0.23	0/3428	0.44	0/4653
1	I	0.23	0/3428	0.44	0/4653
2	J	0.22	0/3429	0.44	0/4643
2	K	0.22	0/3429	0.44	0/4643
2	L	0.22	0/3429	0.44	0/4643
2	M	0.22	0/3429	0.44	0/4643
2	N	0.22	0/3429	0.44	0/4643
2	O	0.22	0/3429	0.44	0/4643
2	P	0.22	0/3429	0.44	0/4643
2	Q	0.22	0/3429	0.44	0/4643
2	R	0.22	0/3429	0.44	0/4643
3	S	0.22	0/2583	0.41	0/3482
3	T	0.22	0/2583	0.41	0/3482
3	U	0.22	0/2583	0.41	0/3482
3	V	0.22	0/2583	0.41	0/3482
3	W	0.22	0/2583	0.41	0/3482
3	X	0.22	0/2583	0.41	0/3482
3	Y	0.22	0/2583	0.41	0/3482
3	Z	0.22	0/2583	0.41	0/3482
3	a	0.22	0/2583	0.41	0/3482
All	All	0.22	0/84960	0.43	0/115002

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3256	21	0
1	B	3350	0	3256	21	0
1	C	3350	0	3256	22	0
1	D	3350	0	3256	21	0
1	E	3350	0	3256	21	0
1	F	3350	0	3256	22	0
1	G	3350	0	3256	22	0
1	H	3350	0	3256	21	0
1	I	3350	0	3256	21	0
2	J	3354	0	3239	30	0
2	K	3354	0	3239	31	0
2	L	3354	0	3239	30	0
2	M	3354	0	3239	30	0
2	N	3354	0	3239	29	0
2	O	3354	0	3239	31	0
2	P	3354	0	3239	28	0
2	Q	3354	0	3239	31	0
2	R	3354	0	3239	29	0
3	S	2544	0	2523	18	0
3	T	2544	0	2523	18	0
3	U	2544	0	2523	18	0
3	V	2544	0	2523	18	0
3	W	2544	0	2523	18	0
3	X	2544	0	2523	17	0
3	Y	2544	0	2523	18	0
3	Z	2544	0	2523	17	0
3	a	2544	0	2523	18	0
4	J	32	0	12	1	0
4	K	32	0	12	1	0
4	L	32	0	12	1	0
4	M	32	0	12	1	0
4	N	32	0	12	1	0
4	O	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	32	0	12	1	0
4	Q	32	0	12	1	0
4	R	32	0	12	0	0
5	J	32	0	14	4	0
5	K	32	0	14	4	0
5	L	32	0	14	4	0
5	M	32	0	14	4	0
5	N	32	0	14	4	0
5	O	32	0	14	4	0
5	P	32	0	14	4	0
5	Q	32	0	14	4	0
5	R	32	0	14	4	0
6	S	31	0	12	1	0
6	T	31	0	12	1	0
6	U	31	0	12	1	0
6	V	31	0	12	1	0
6	W	31	0	12	1	0
6	X	31	0	12	1	0
6	Y	31	0	12	1	0
6	Z	31	0	12	1	0
6	a	31	0	12	1	0
All	All	84087	0	81504	606	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 4.

The worst 5 of 606 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:11:GLN:HB3	5:O:502:G2P:O1A	1.68	0.93
2:K:11:GLN:HB3	5:K:502:G2P:O1A	1.68	0.92
2:Q:11:GLN:HB3	5:Q:502:G2P:O1A	1.68	0.92
2:L:11:GLN:HB3	5:L:502:G2P:O1A	1.68	0.92
2:P:11:GLN:HB3	5:P:502:G2P:O1A	1.68	0.92

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	A	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	B	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	C	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	D	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	E	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	F	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	G	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	H	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	I	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
2	J	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	K	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	L	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	M	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	N	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	O	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	P	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	Q	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
2	R	424/457 (93%)	419 (99%)	5 (1%)	0	100	100
3	S	323/372 (87%)	316 (98%)	7 (2%)	0	100	100
3	T	323/372 (87%)	315 (98%)	8 (2%)	0	100	100
3	U	323/372 (87%)	316 (98%)	7 (2%)	0	100	100
3	V	323/372 (87%)	316 (98%)	7 (2%)	0	100	100
3	W	323/372 (87%)	315 (98%)	8 (2%)	0	100	100
3	X	323/372 (87%)	316 (98%)	7 (2%)	0	100	100
3	Y	323/372 (87%)	316 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Z	323/372 (87%)	316 (98%)	7 (2%)	0	100	100
3	a	323/372 (87%)	315 (98%)	8 (2%)	0	100	100
All	All	10530/11547 (91%)	10311 (98%)	219 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	B	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	C	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	D	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	E	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	F	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	G	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	H	361/384 (94%)	351 (97%)	10 (3%)	38	59
1	I	361/384 (94%)	351 (97%)	10 (3%)	38	59
2	J	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	K	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	L	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	M	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	N	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	O	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	P	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	Q	368/390 (94%)	355 (96%)	13 (4%)	32	53
2	R	368/390 (94%)	355 (96%)	13 (4%)	32	53
3	S	289/330 (88%)	284 (98%)	5 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	U	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	V	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	W	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	X	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	Y	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	Z	289/330 (88%)	284 (98%)	5 (2%)	53	67
3	a	289/330 (88%)	284 (98%)	5 (2%)	53	67
All	All	9162/9936 (92%)	8910 (97%)	252 (3%)	38	59

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	119	GLU
3	Z	137	ILE
1	E	119	GLU
3	Z	20	GLU
2	R	31	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	264	ASN
1	G	335	ASN
1	H	335	ASN
1	C	234	ASN
2	K	11	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	GTP	M	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.59	8 (16%)
6	ATP	S	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.81	10 (20%)
6	ATP	a	401	-	32,33,33	1.42	5 (15%)	48,52,52	1.81	10 (20%)
6	ATP	U	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.80	10 (20%)
4	GTP	J	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
5	G2P	M	502	-	30,34,34	4.52	11 (36%)	46,54,54	1.77	12 (26%)
6	ATP	X	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.81	10 (20%)
6	ATP	W	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.81	10 (20%)
6	ATP	T	401	-	32,33,33	1.42	5 (15%)	48,52,52	1.81	10 (20%)
5	G2P	K	502	-	30,34,34	4.51	11 (36%)	46,54,54	1.77	12 (26%)
4	GTP	K	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
5	G2P	N	502	-	30,34,34	4.53	11 (36%)	46,54,54	1.77	12 (26%)
5	G2P	P	502	-	30,34,34	4.52	11 (36%)	46,54,54	1.76	12 (26%)
4	GTP	R	501	-	33,34,34	0.96	2 (6%)	50,54,54	1.59	8 (16%)
5	G2P	J	502	-	30,34,34	4.51	11 (36%)	46,54,54	1.77	12 (26%)
4	GTP	Q	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
5	G2P	Q	502	-	30,34,34	4.52	11 (36%)	46,54,54	1.77	12 (26%)
4	GTP	N	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
4	GTP	O	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.59	8 (16%)
4	GTP	L	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
5	G2P	L	502	-	30,34,34	4.51	11 (36%)	46,54,54	1.77	13 (28%)
6	ATP	V	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.80	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	Z	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.82	10 (20%)
4	GTP	P	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
5	G2P	R	502	-	30,34,34	4.52	11 (36%)	46,54,54	1.77	12 (26%)
6	ATP	Y	401	-	32,33,33	1.42	4 (12%)	48,52,52	1.81	10 (20%)
5	G2P	O	502	-	30,34,34	4.52	11 (36%)	46,54,54	1.77	12 (26%)

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	GTP	M	501	-	-	3/22/38/38	0/3/3/3
6	ATP	S	401	-	-	4/22/38/38	0/3/3/3
6	ATP	a	401	-	-	4/22/38/38	0/3/3/3
6	ATP	U	401	-	-	4/22/38/38	0/3/3/3
4	GTP	J	501	-	-	3/22/38/38	0/3/3/3
5	G2P	M	502	-	-	8/19/38/38	0/3/3/3
6	ATP	X	401	-	-	4/22/38/38	0/3/3/3
6	ATP	W	401	-	-	4/22/38/38	0/3/3/3
6	ATP	T	401	-	-	4/22/38/38	0/3/3/3
5	G2P	K	502	-	-	8/19/38/38	0/3/3/3
4	GTP	K	501	-	-	3/22/38/38	0/3/3/3
5	G2P	N	502	-	-	8/19/38/38	0/3/3/3
5	G2P	P	502	-	-	8/19/38/38	0/3/3/3
4	GTP	R	501	-	-	3/22/38/38	0/3/3/3
5	G2P	J	502	-	-	8/19/38/38	0/3/3/3
4	GTP	Q	501	-	-	3/22/38/38	0/3/3/3
5	G2P	Q	502	-	-	8/19/38/38	0/3/3/3
4	GTP	N	501	-	-	3/22/38/38	0/3/3/3
4	GTP	O	501	-	-	3/22/38/38	0/3/3/3
4	GTP	L	501	-	-	3/22/38/38	0/3/3/3
5	G2P	L	502	-	-	8/19/38/38	0/3/3/3
6	ATP	V	401	-	-	4/22/38/38	0/3/3/3
6	ATP	Z	401	-	-	4/22/38/38	0/3/3/3
4	GTP	P	501	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G2P	R	502	-	-	8/19/38/38	0/3/3/3
6	ATP	Y	401	-	-	4/22/38/38	0/3/3/3
5	G2P	O	502	-	-	8/19/38/38	0/3/3/3

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	502	G2P	PB-O3B	14.92	1.75	1.58
5	R	502	G2P	PB-O3B	14.87	1.74	1.58
5	P	502	G2P	PB-O3B	14.85	1.74	1.58
5	M	502	G2P	PB-O3B	14.84	1.74	1.58
5	Q	502	G2P	PB-O3B	14.82	1.74	1.58

The worst 5 of 272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	401	ATP	C5-C4-N3	-5.91	118.57	126.72
6	T	401	ATP	C5-C4-N3	-5.89	118.60	126.72
6	a	401	ATP	C5-C4-N3	-5.88	118.61	126.72
6	S	401	ATP	C5-C4-N3	-5.88	118.62	126.72
6	Y	401	ATP	C5-C4-N3	-5.88	118.62	126.72

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	502	G2P	PB-O3B-PG-O3G
5	Q	502	G2P	PB-C3A-PA-O1A
5	Q	502	G2P	PB-C3A-PA-O2A
5	Q	502	G2P	PB-C3A-PA-O5'
5	Q	502	G2P	C5'-O5'-PA-C3A

There are no ring outliers.

26 monomers are involved in 53 short contacts:

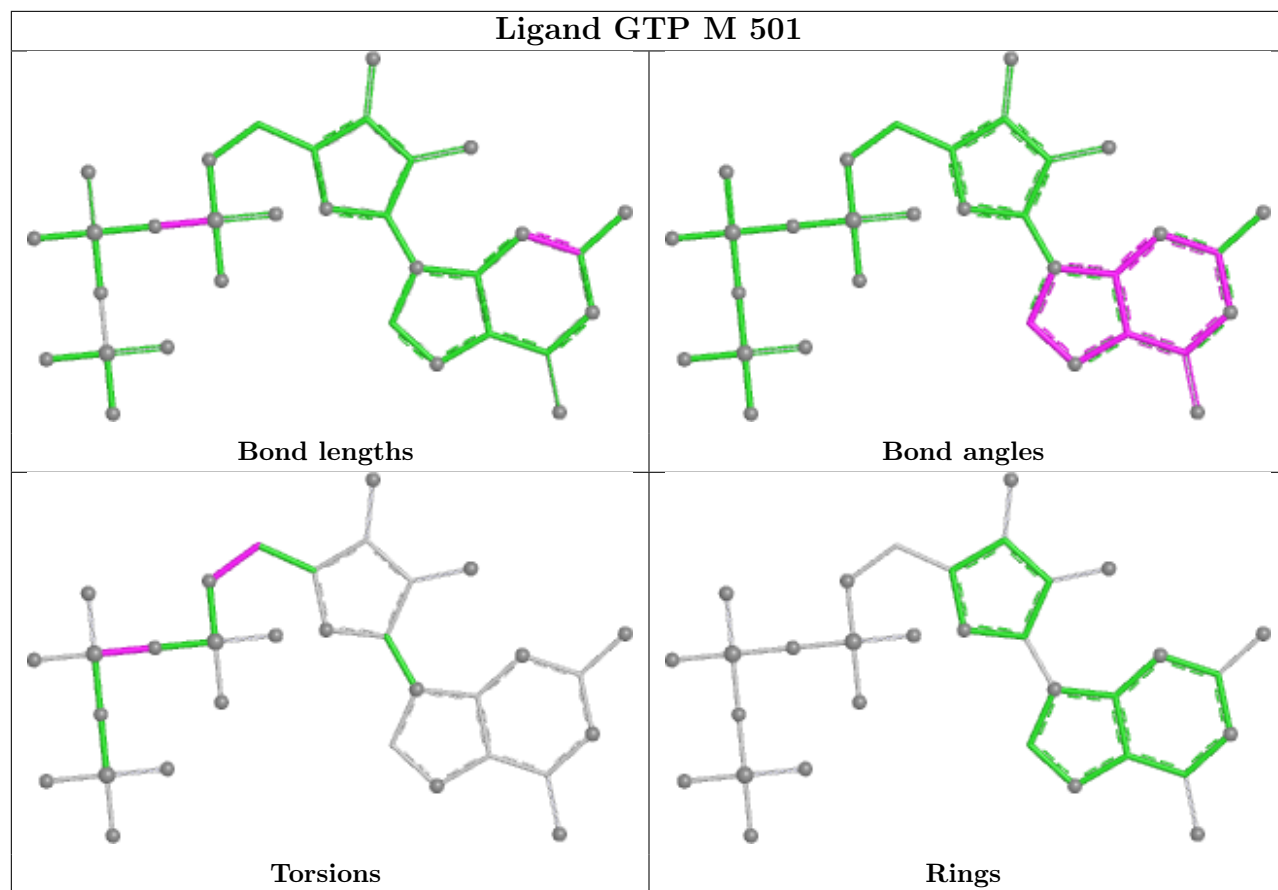
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	501	GTP	1	0
6	S	401	ATP	1	0
6	a	401	ATP	1	0
6	U	401	ATP	1	0

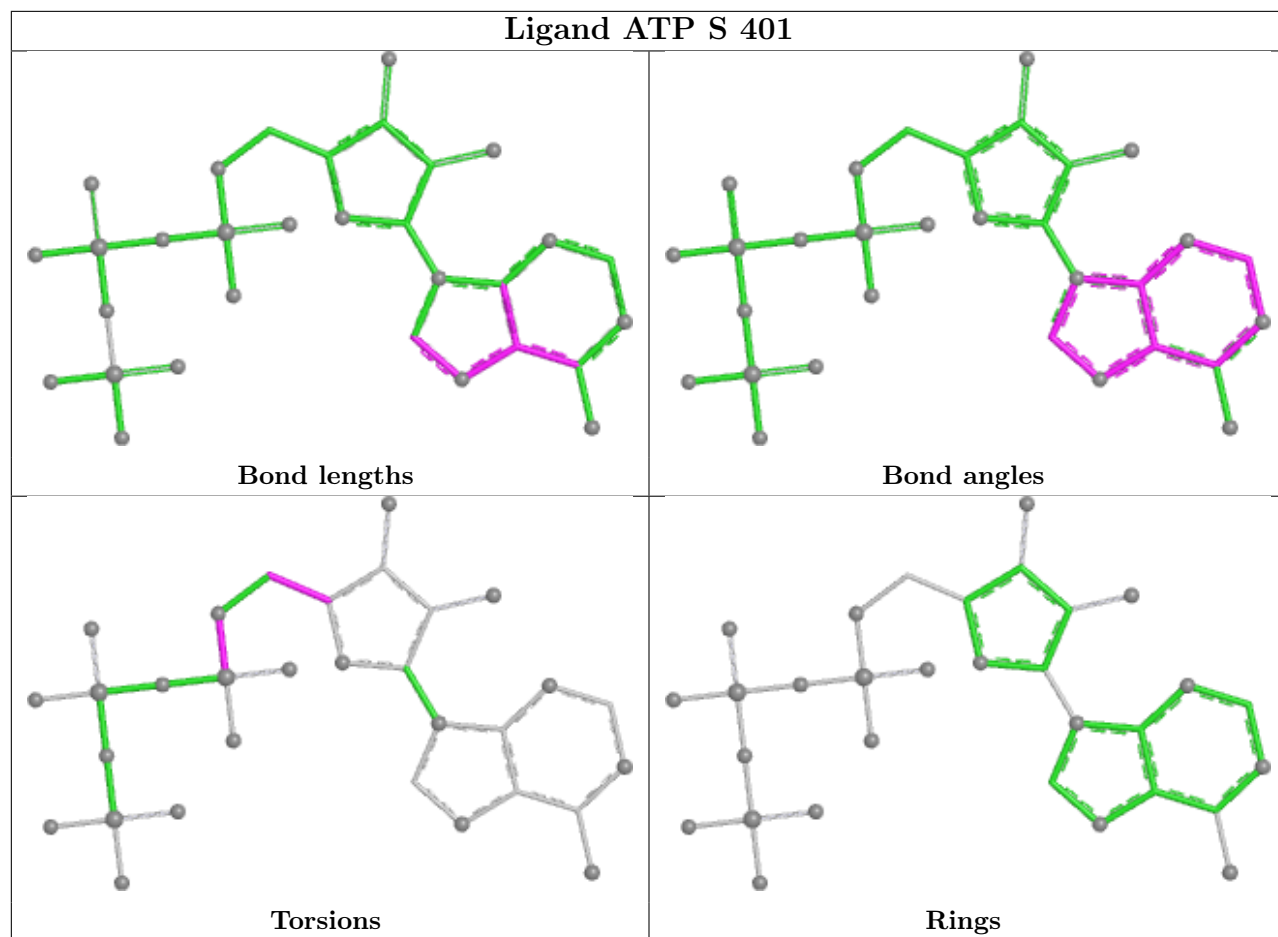
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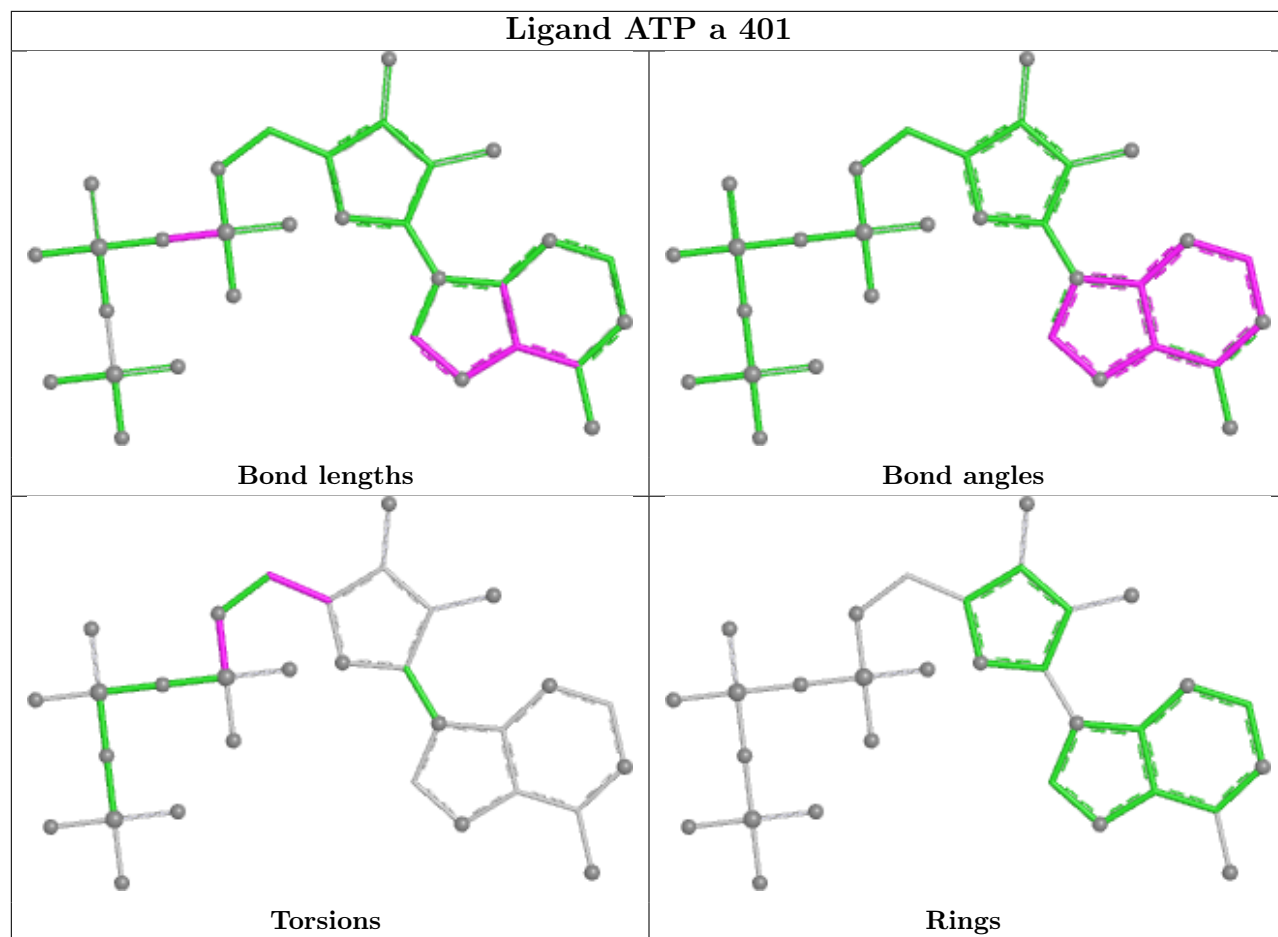
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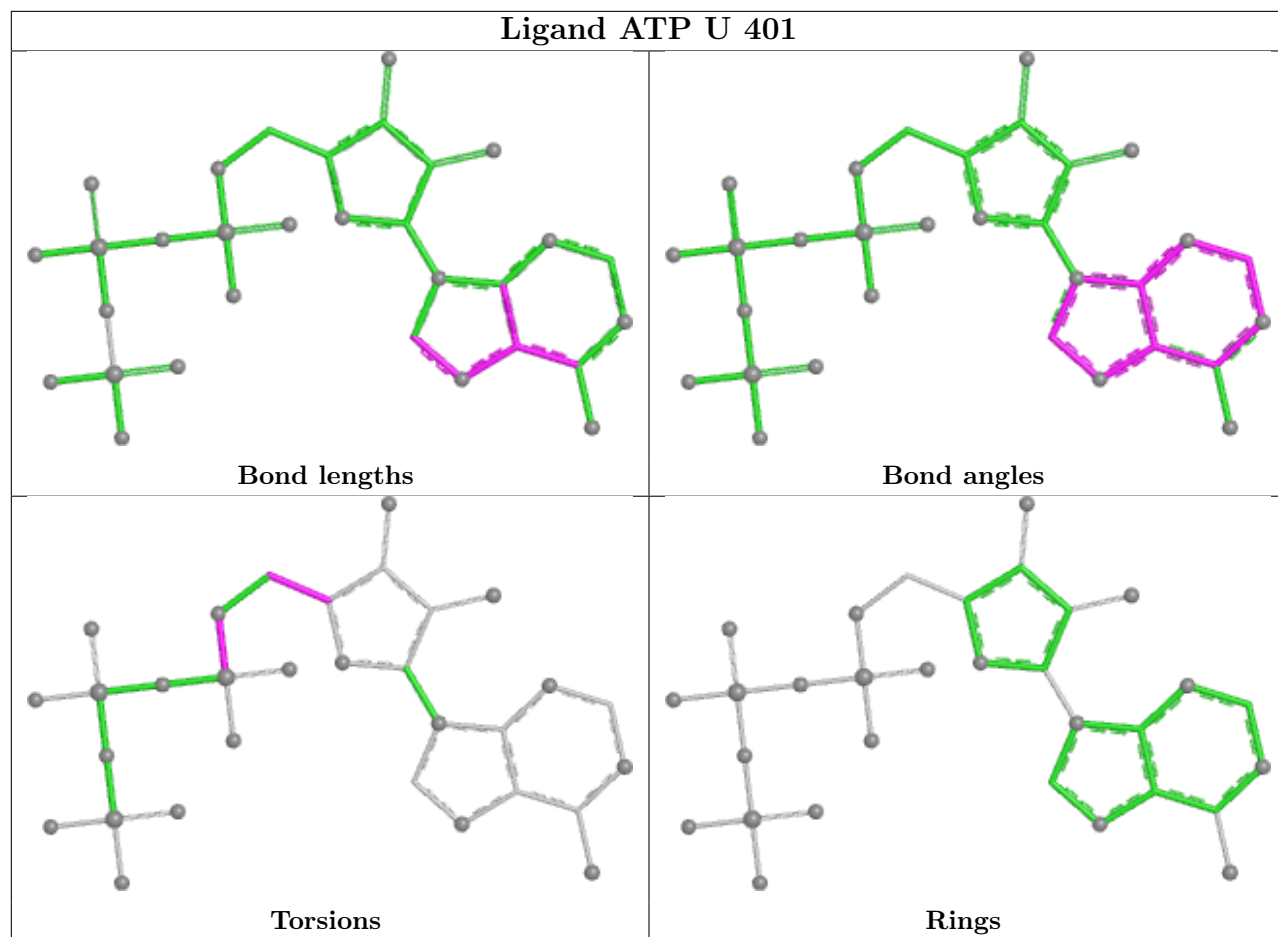
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	501	GTP	1	0
5	M	502	G2P	4	0
6	X	401	ATP	1	0
6	W	401	ATP	1	0
6	T	401	ATP	1	0
5	K	502	G2P	4	0
4	K	501	GTP	1	0
5	N	502	G2P	4	0
5	P	502	G2P	4	0
5	J	502	G2P	4	0
4	Q	501	GTP	1	0
5	Q	502	G2P	4	0
4	N	501	GTP	1	0
4	O	501	GTP	1	0
4	L	501	GTP	1	0
5	L	502	G2P	4	0
6	V	401	ATP	1	0
6	Z	401	ATP	1	0
4	P	501	GTP	1	0
5	R	502	G2P	4	0
6	Y	401	ATP	1	0
5	O	502	G2P	4	0

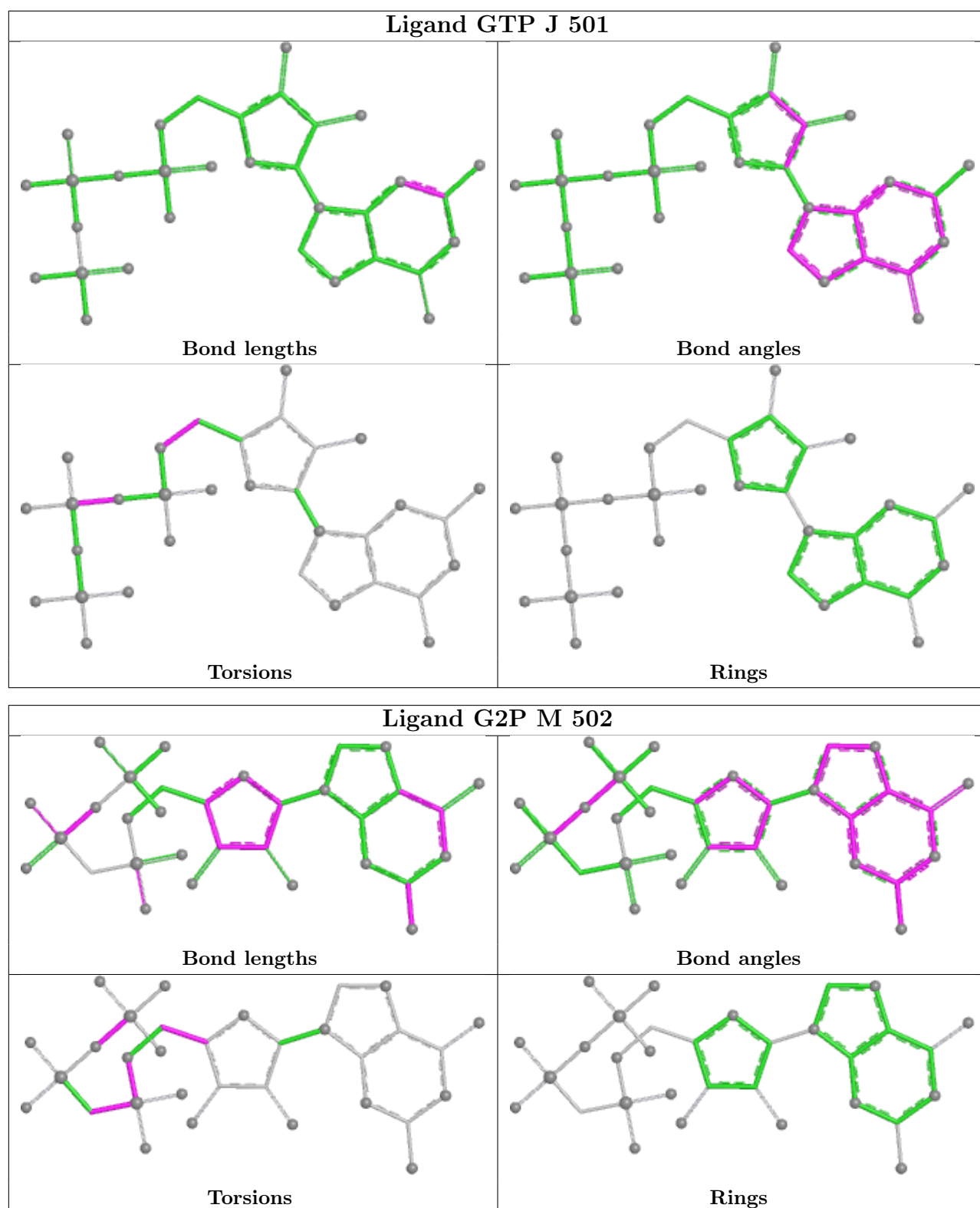
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

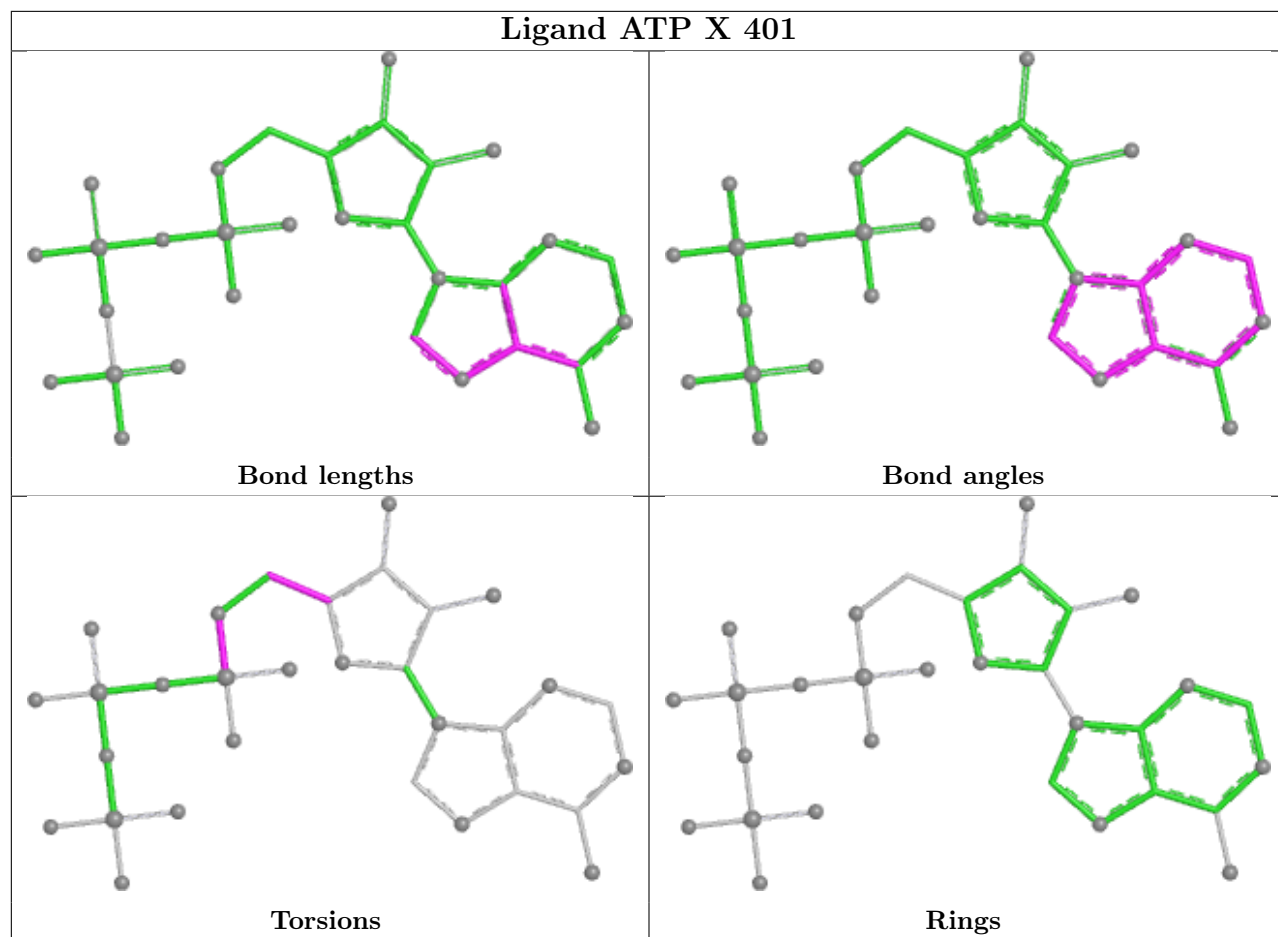


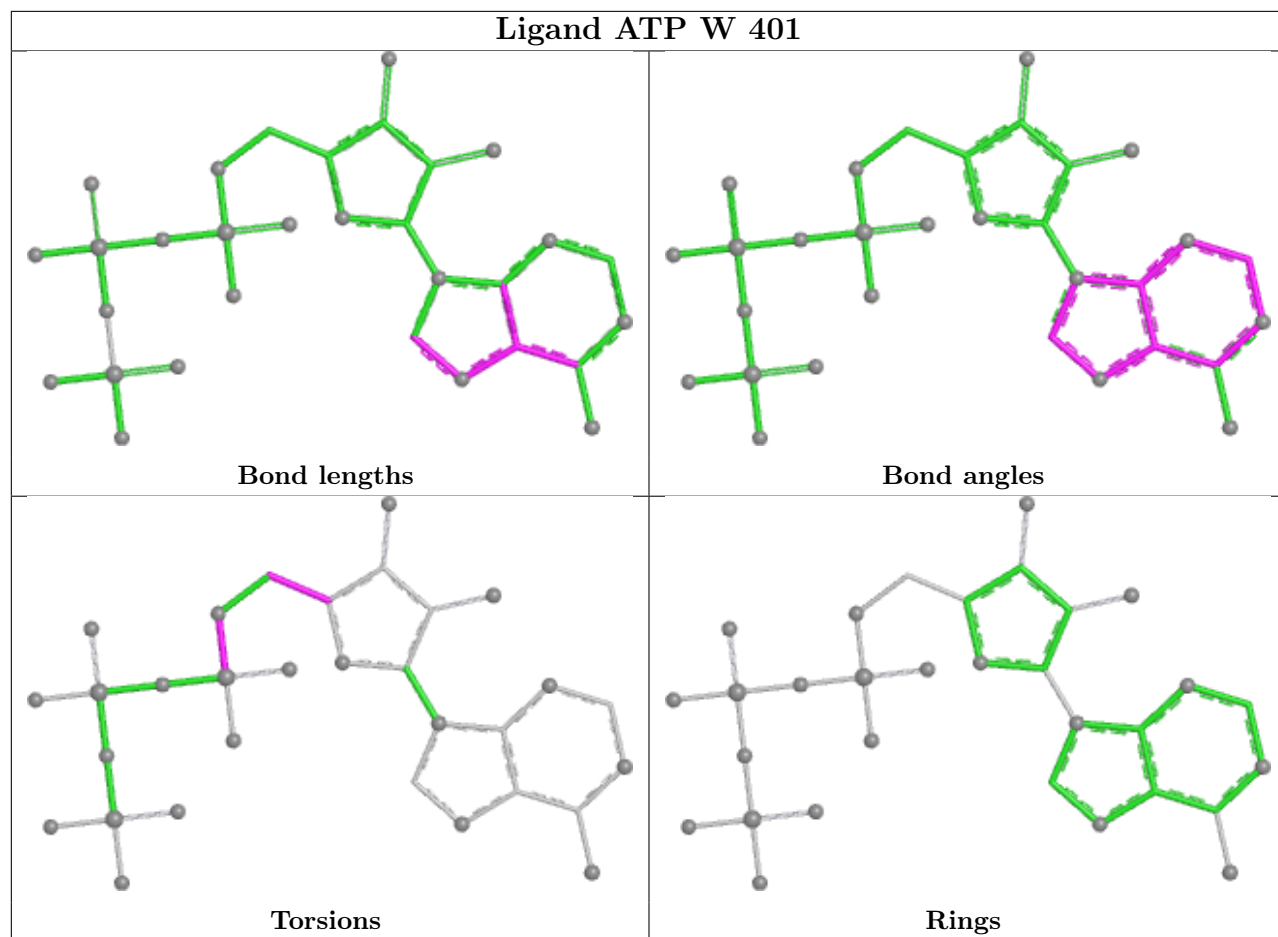


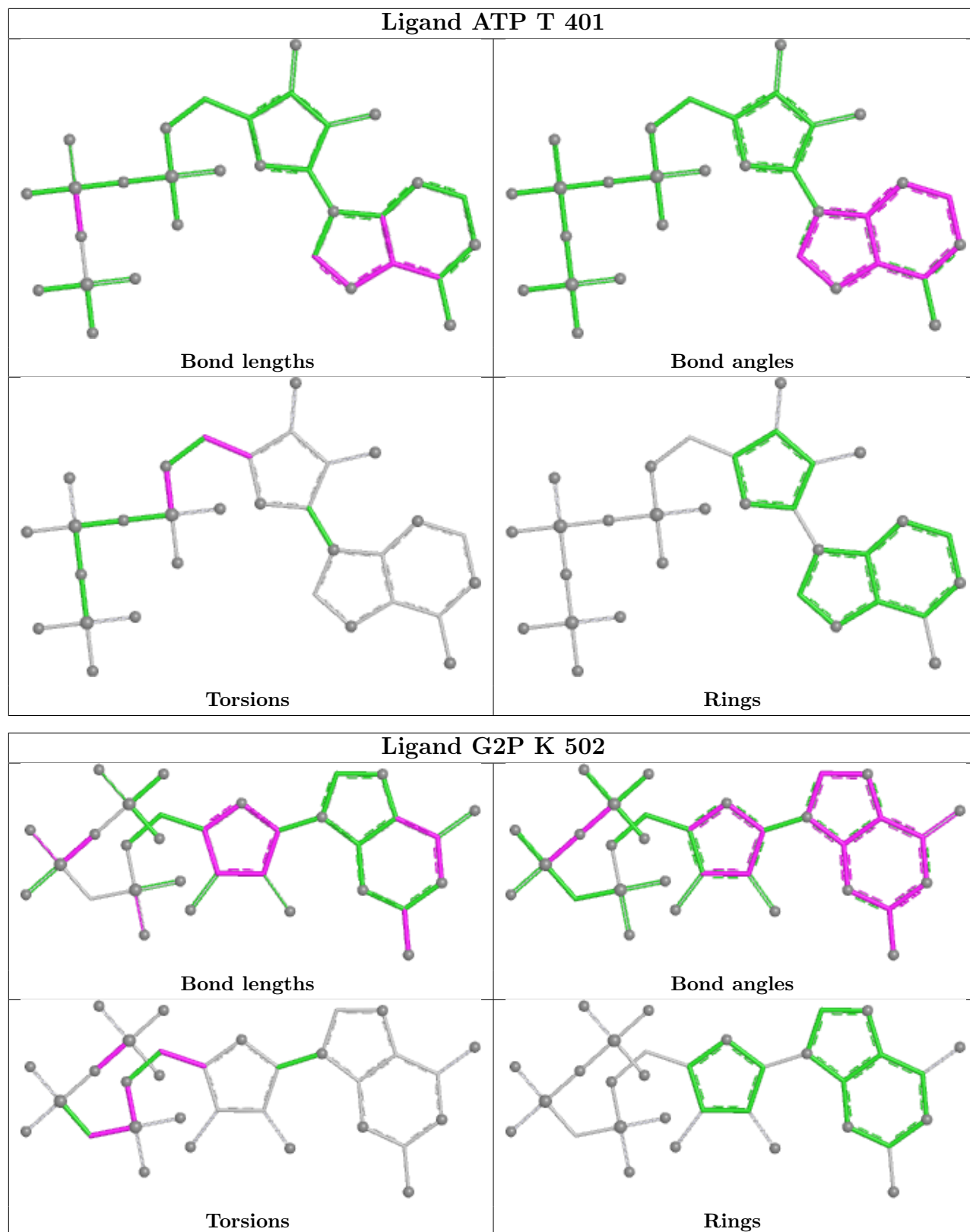


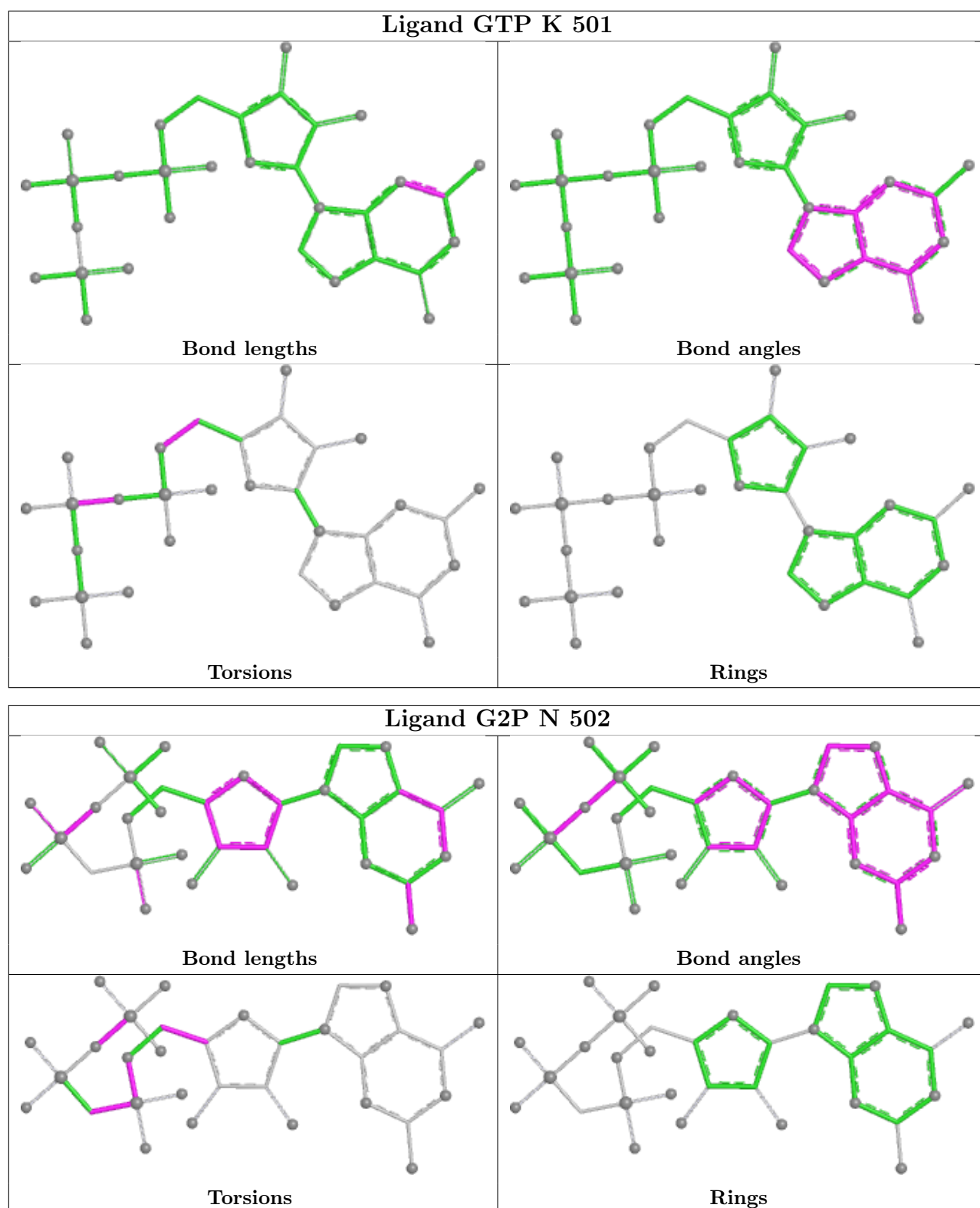


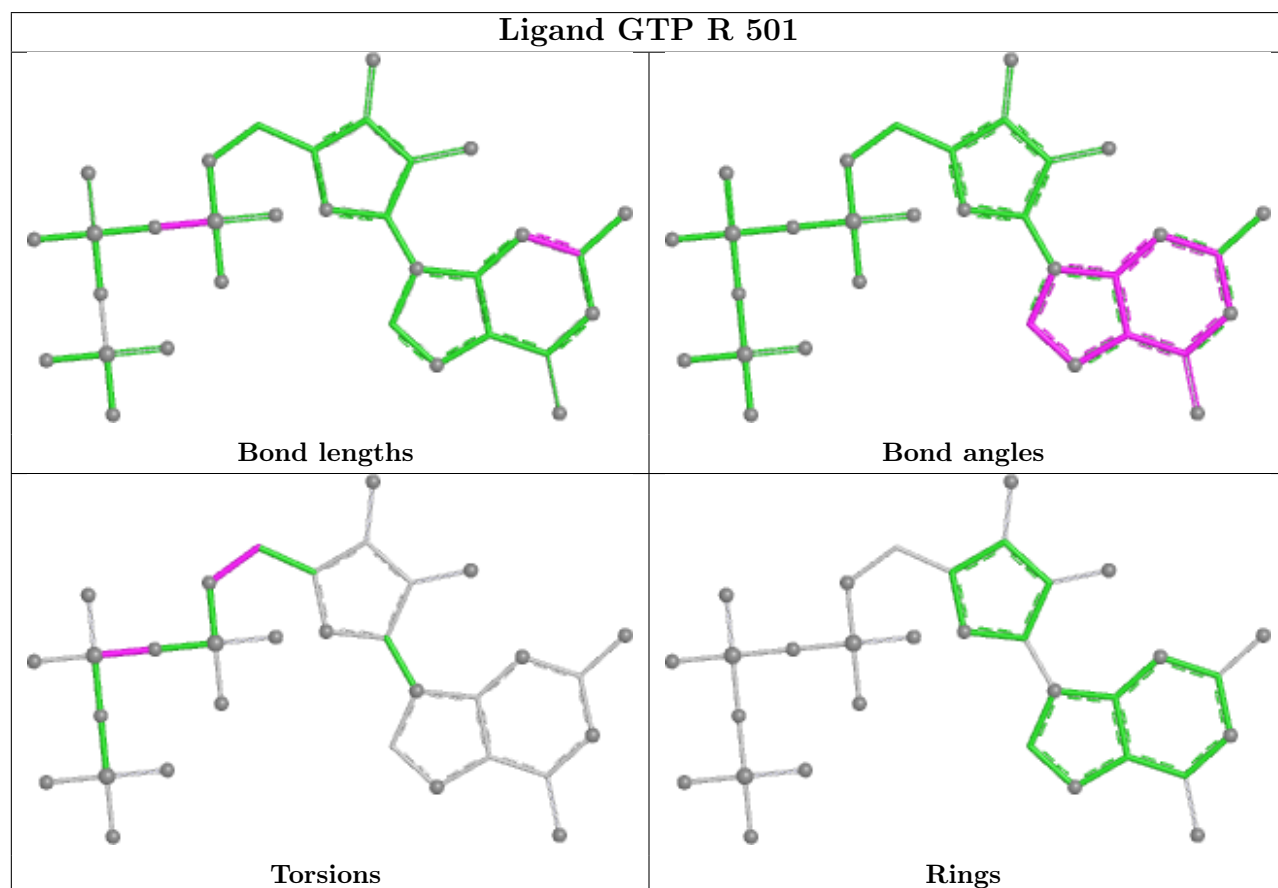
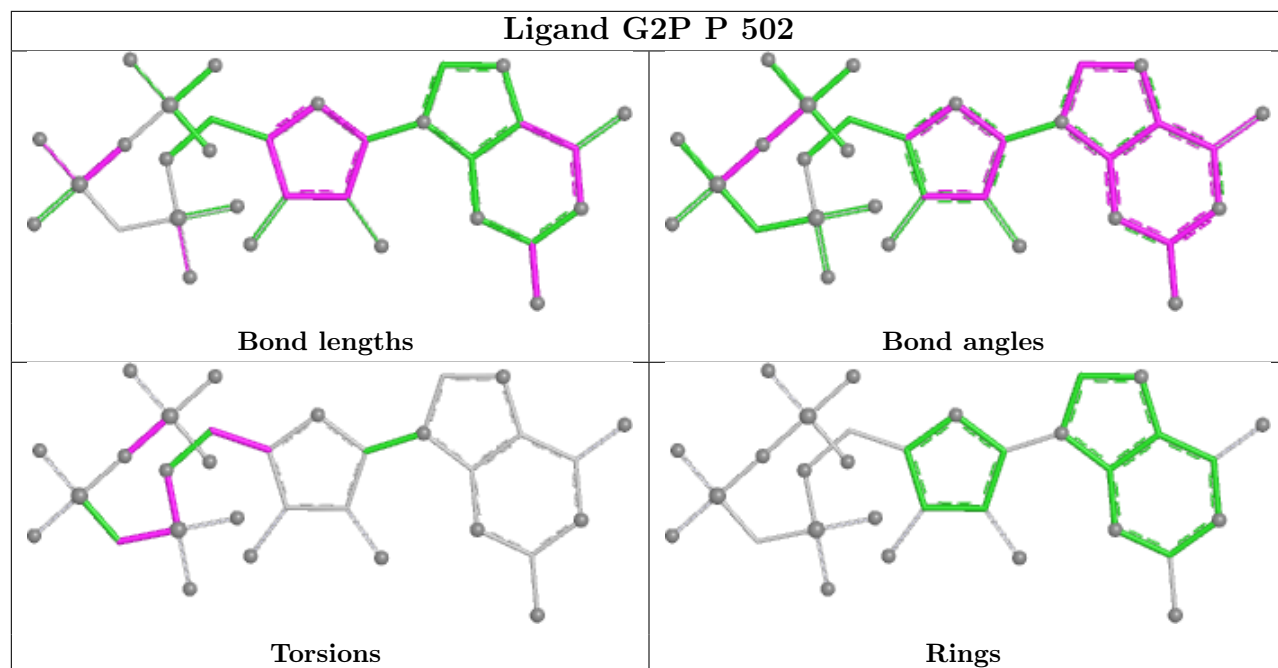


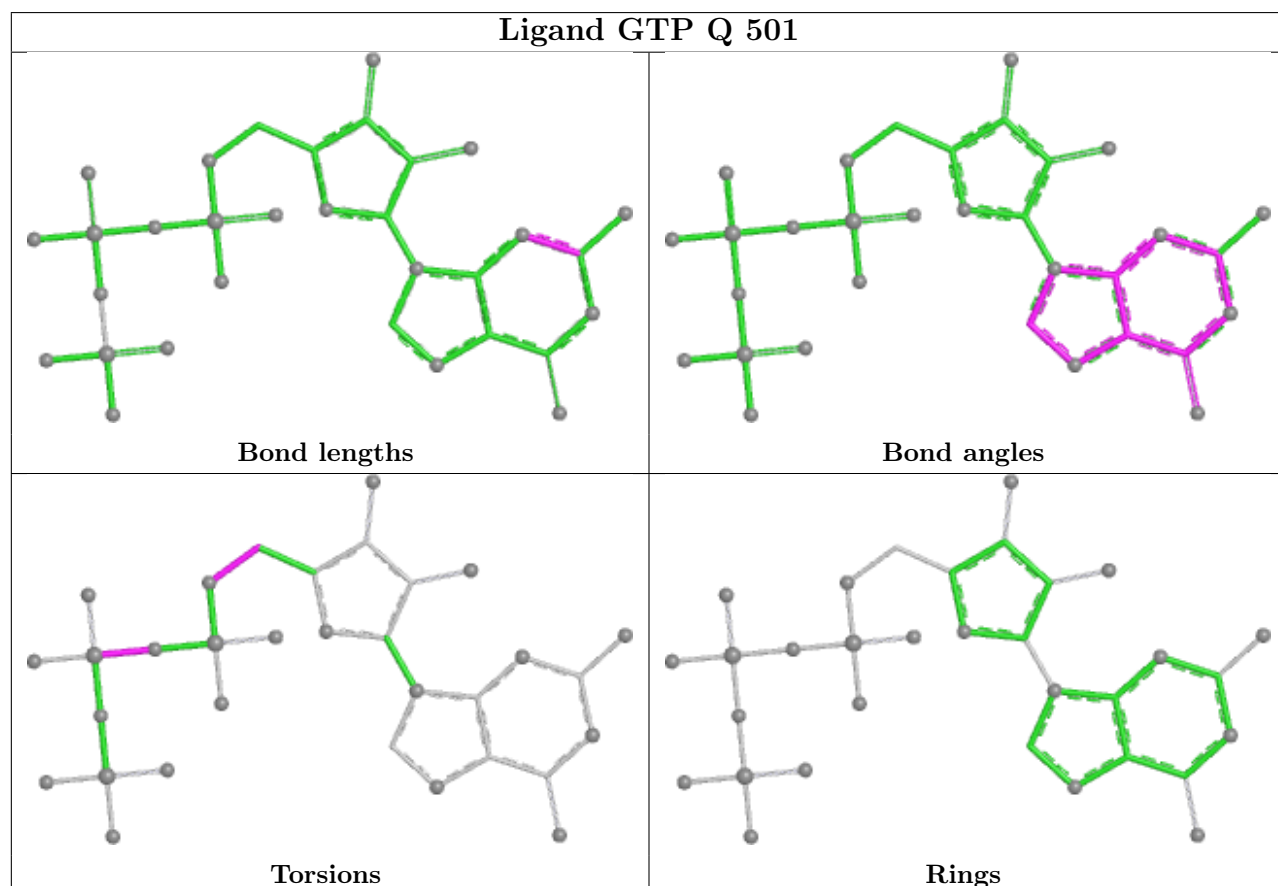
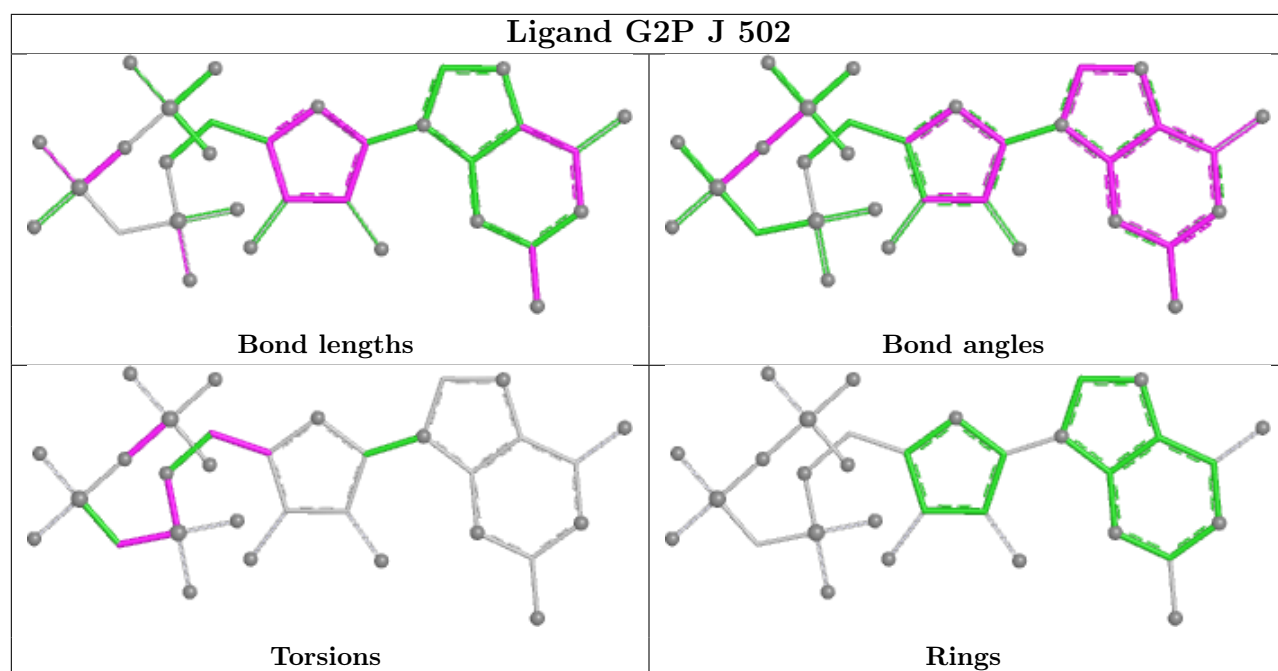


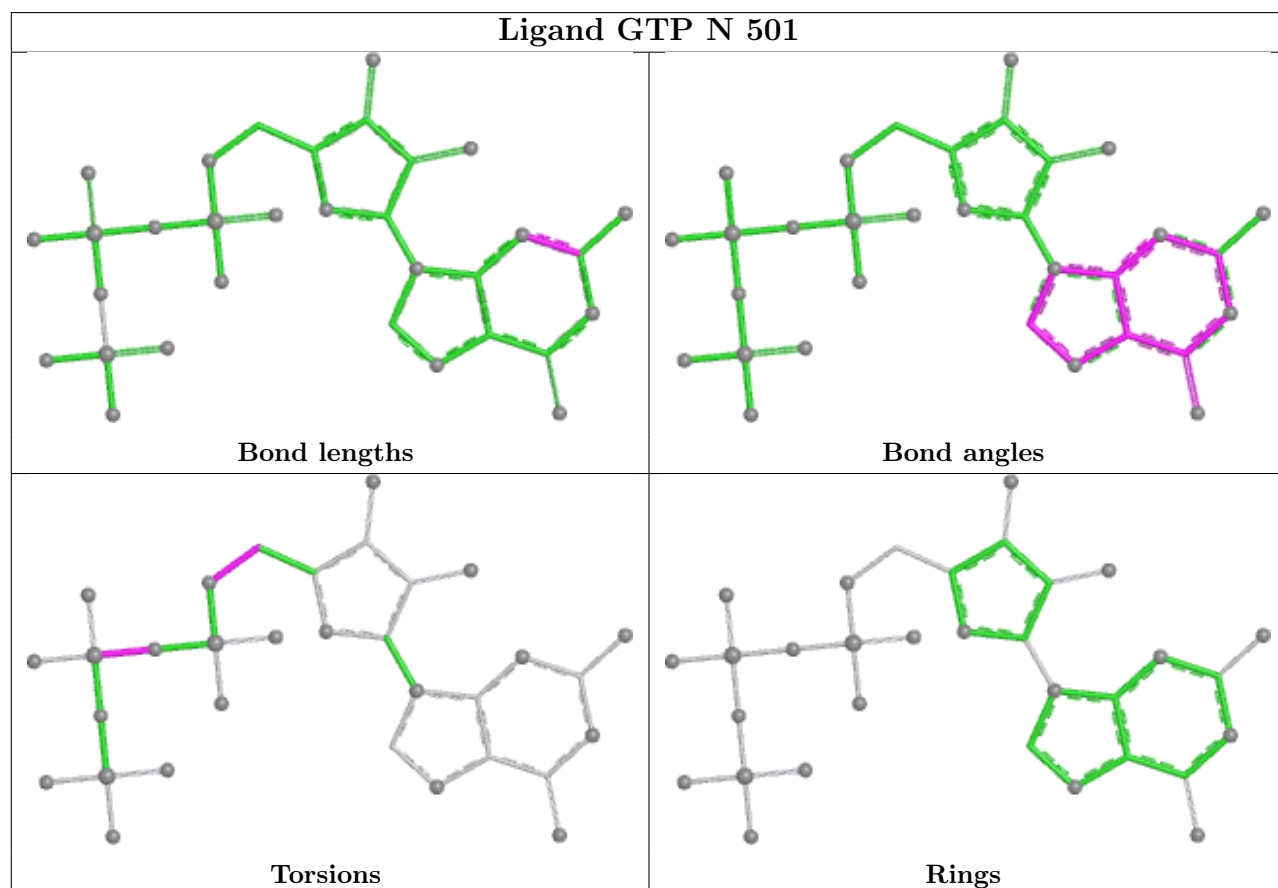
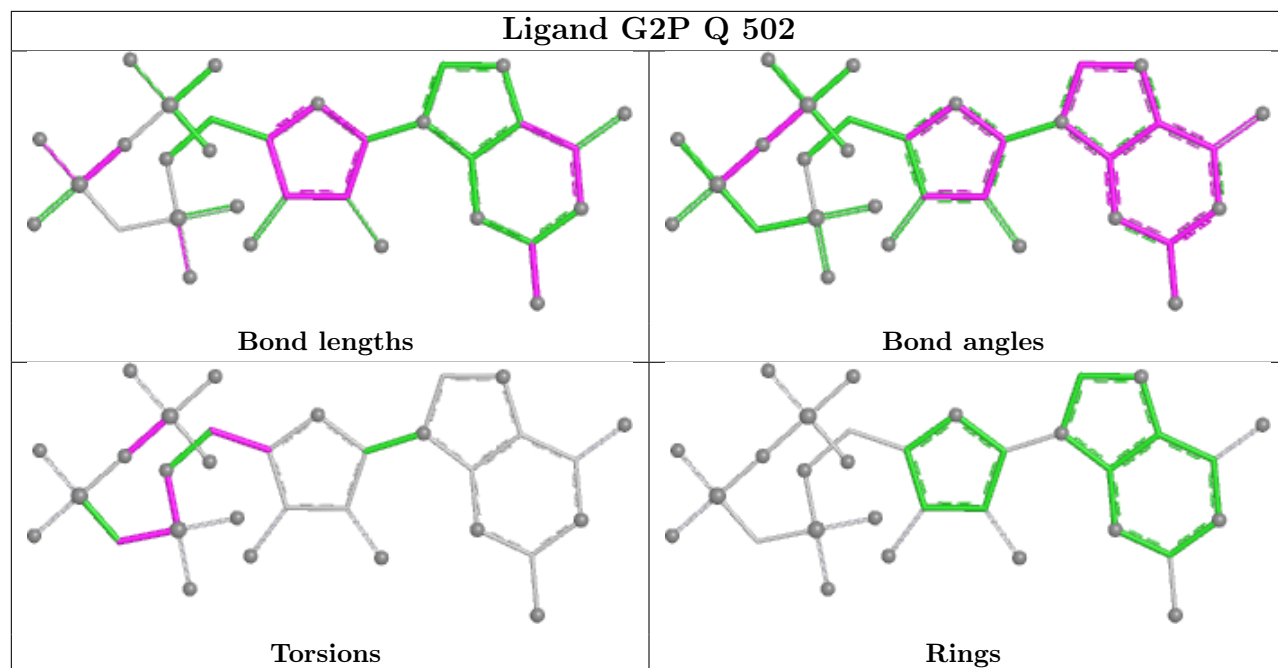


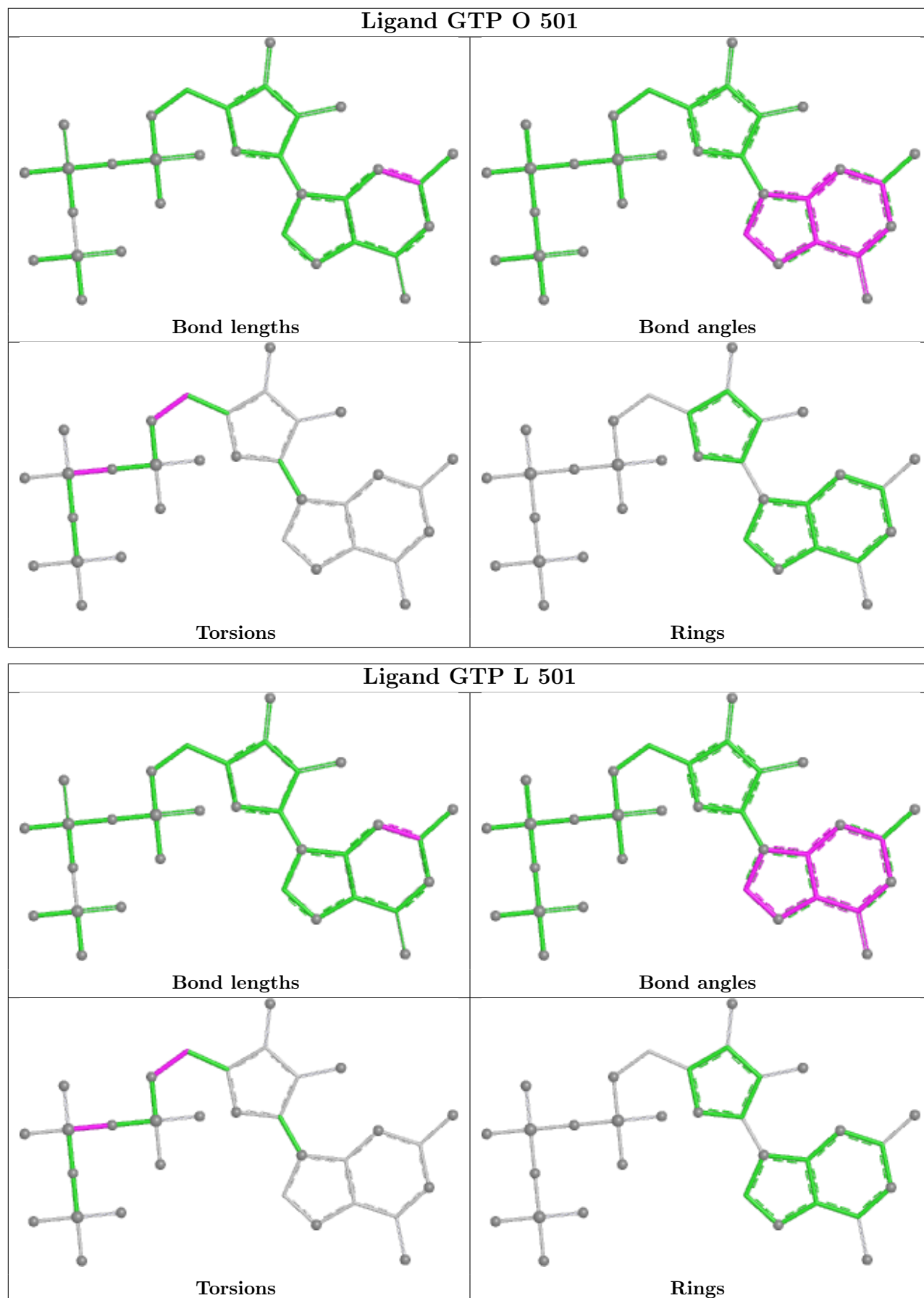


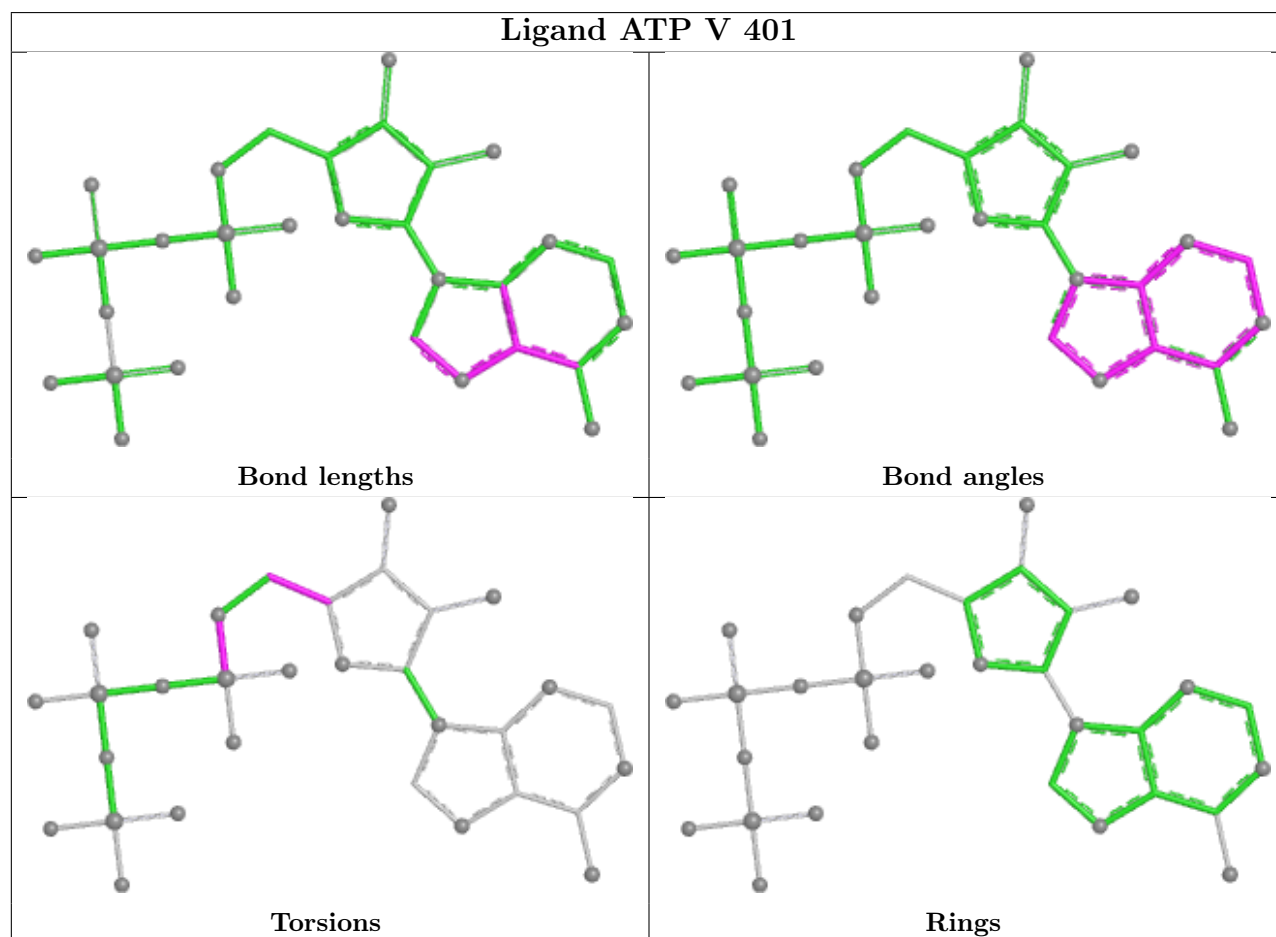
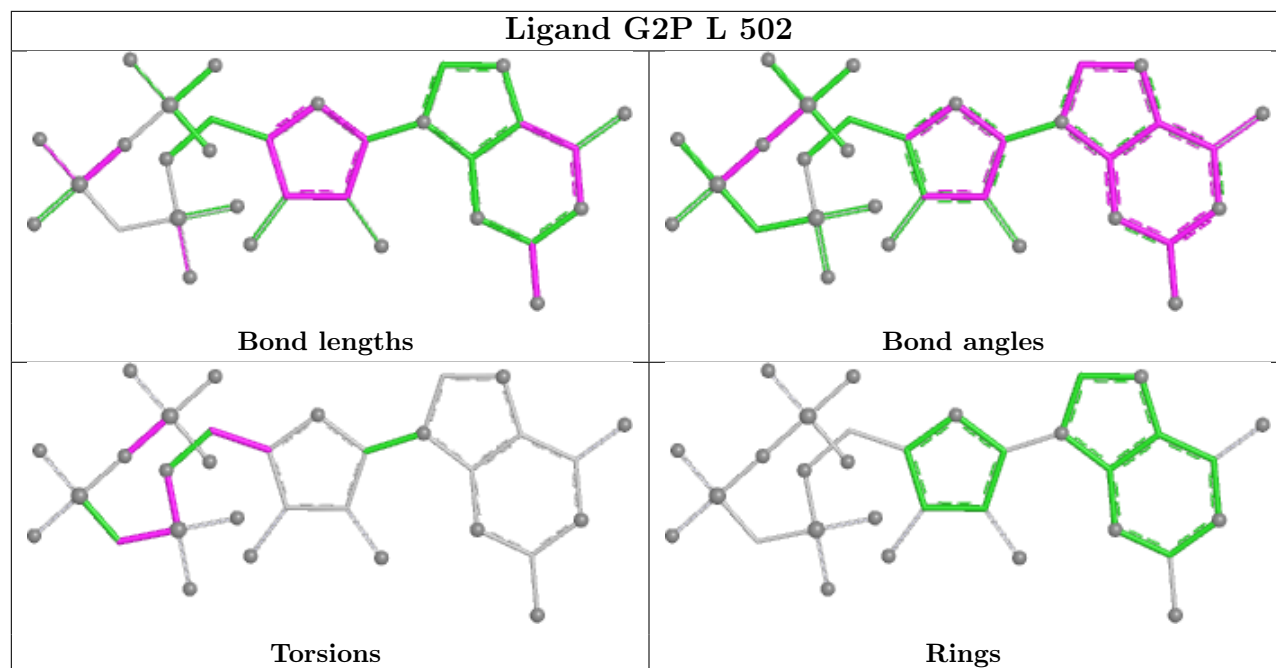


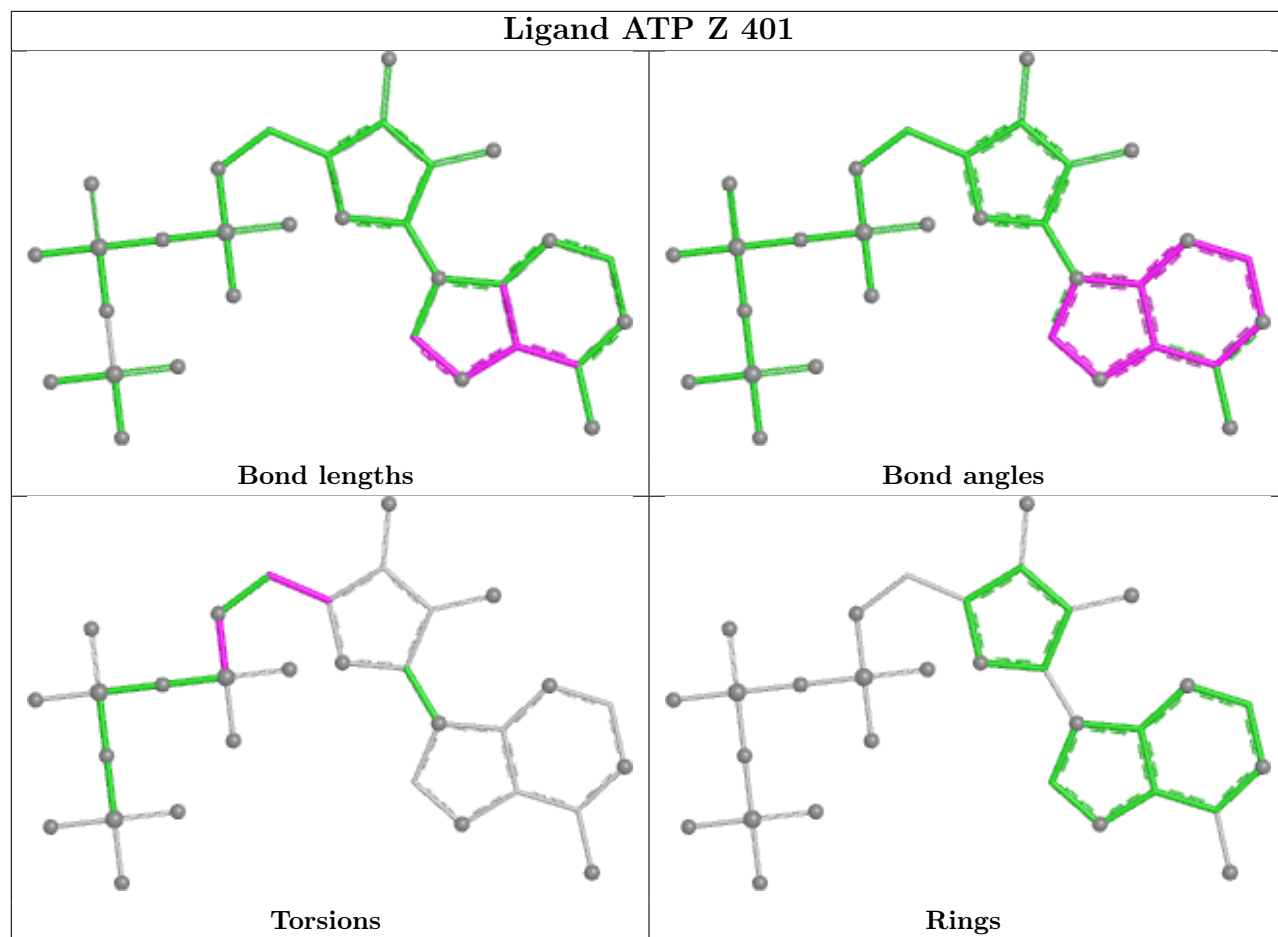


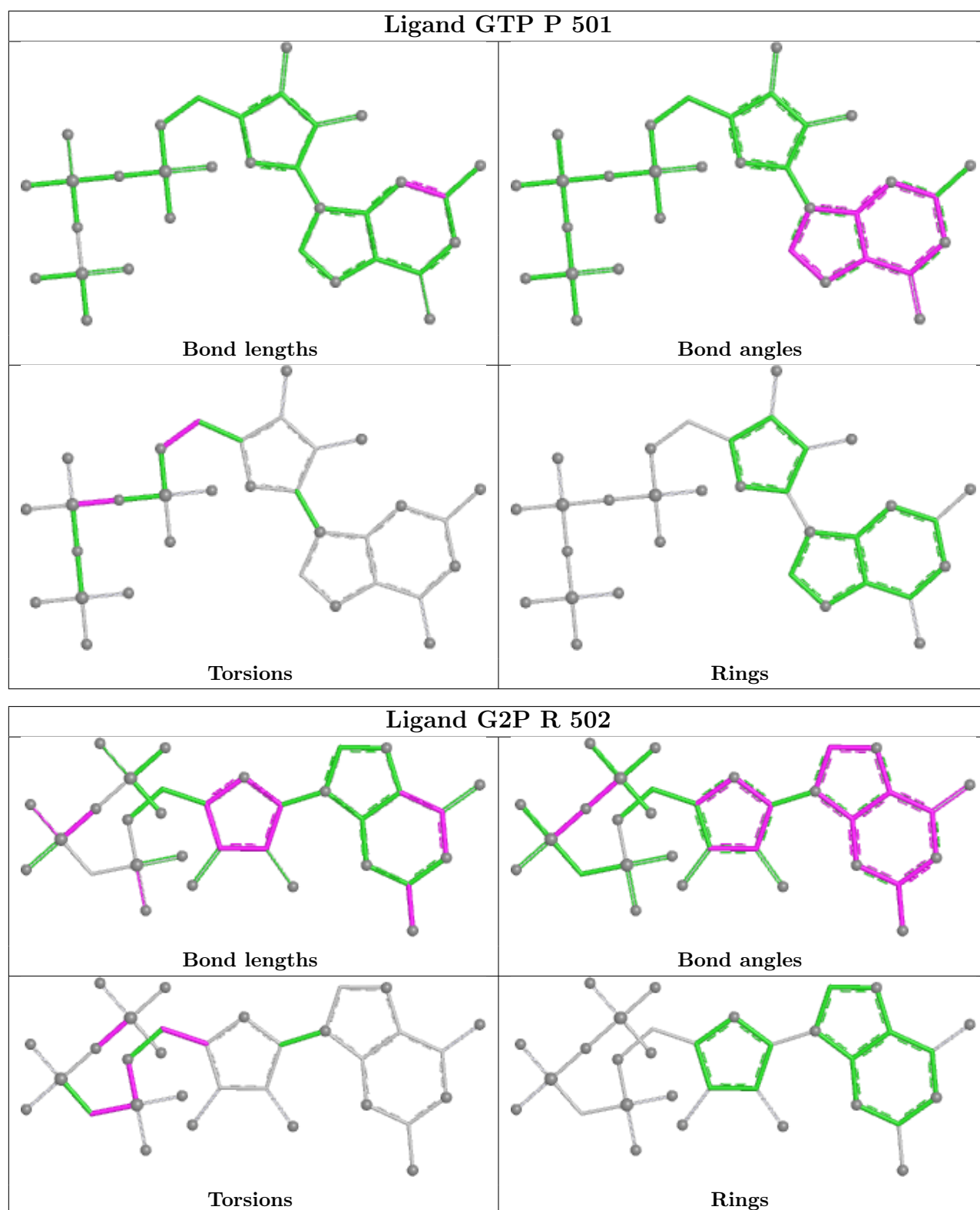


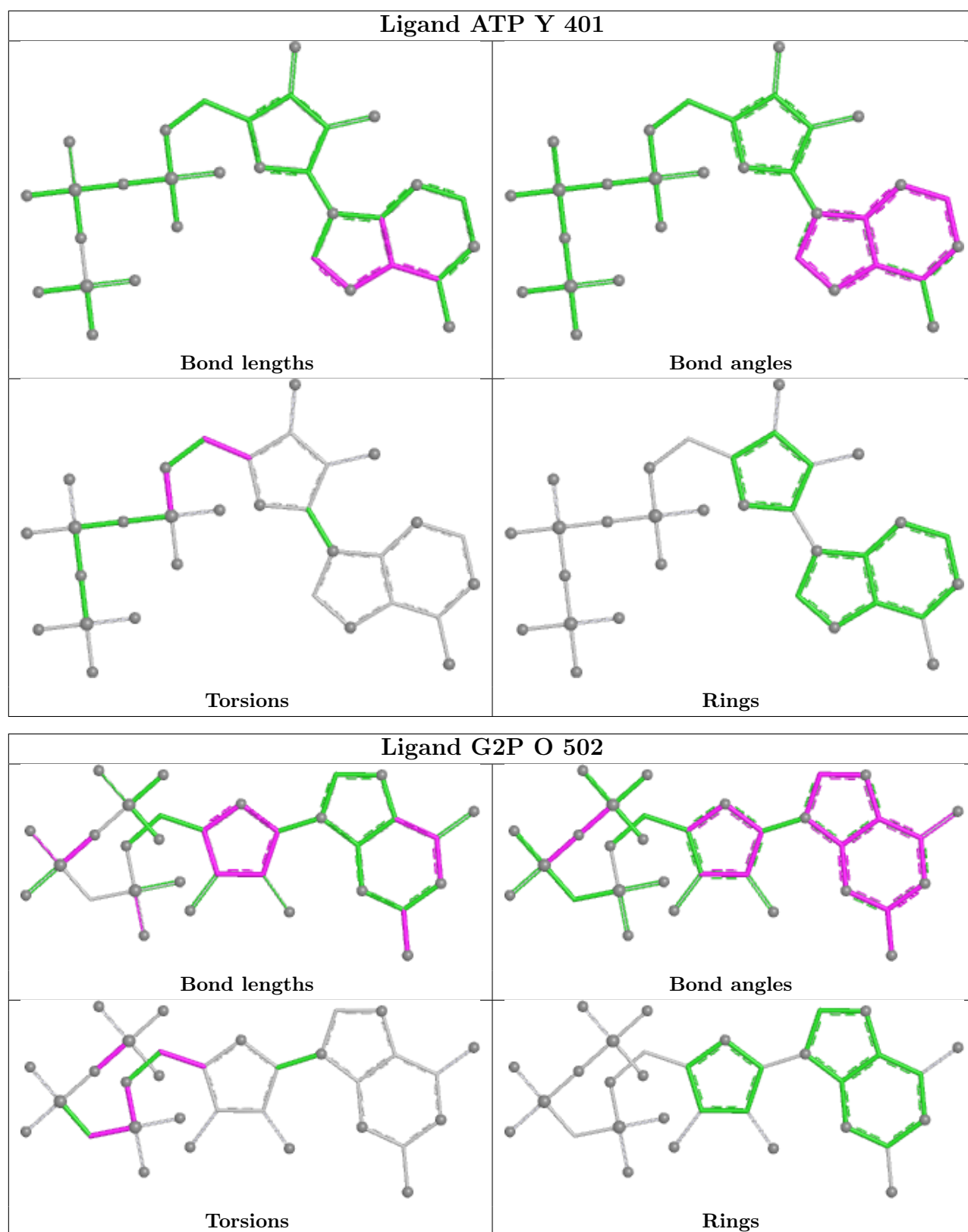












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

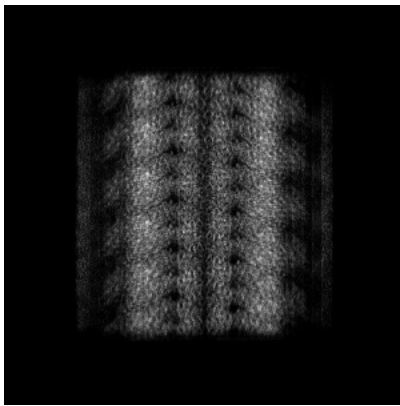
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35792. These allow visual inspection of the internal detail of the map and identification of artifacts.

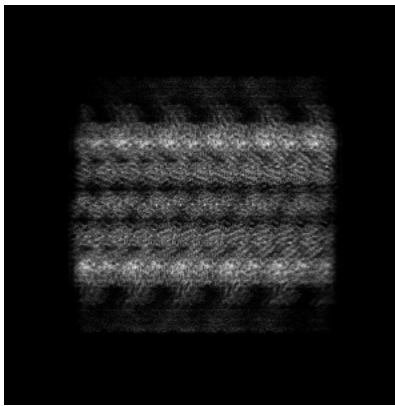
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

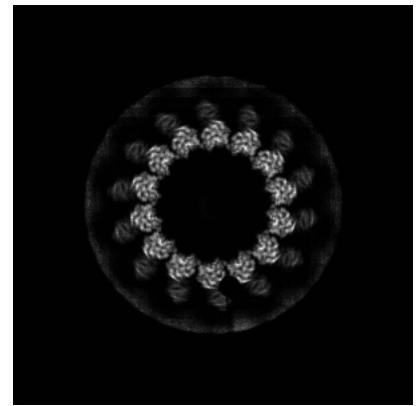
6.1.1 Primary map



X

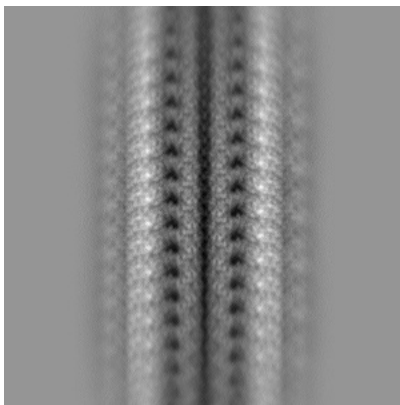


Y

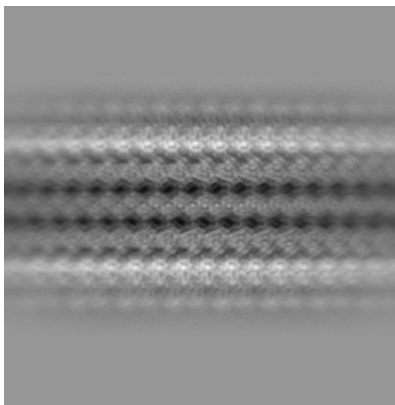


Z

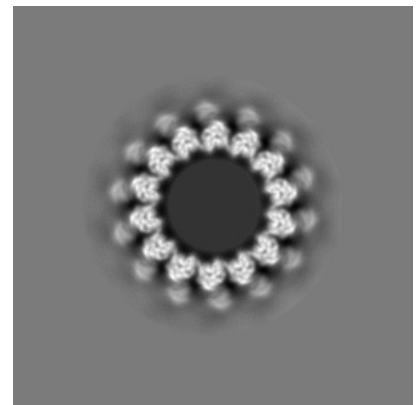
6.1.2 Raw map



X



Y

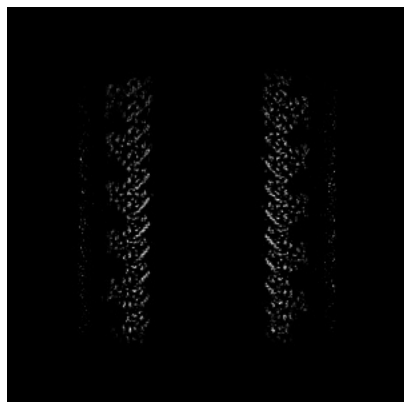


Z

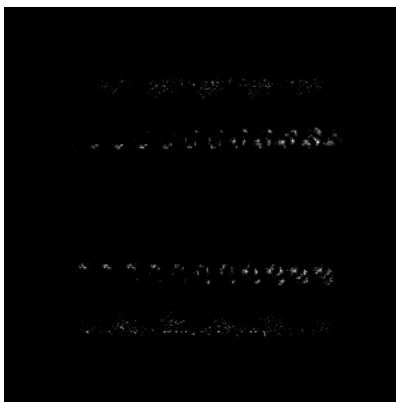
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

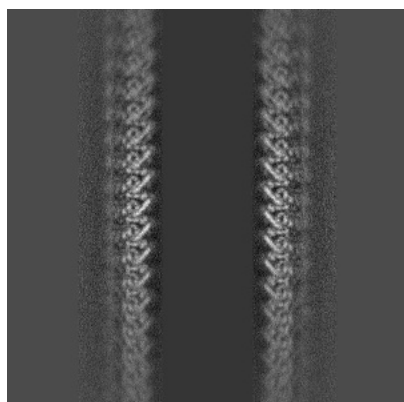


Y Index: 256

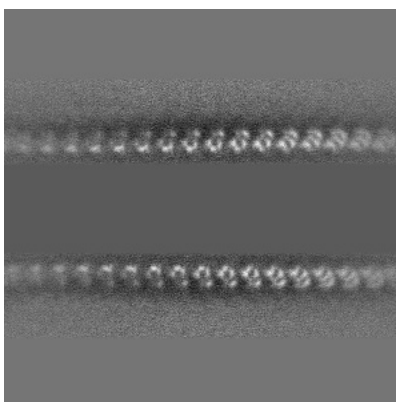


Z Index: 256

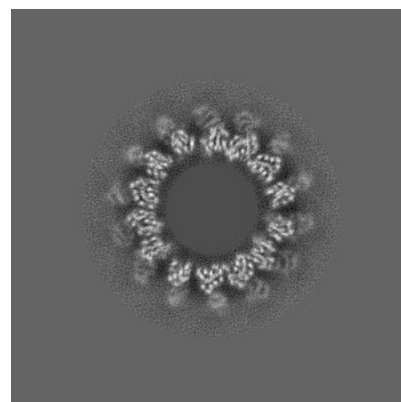
6.2.2 Raw map



X Index: 256



Y Index: 256

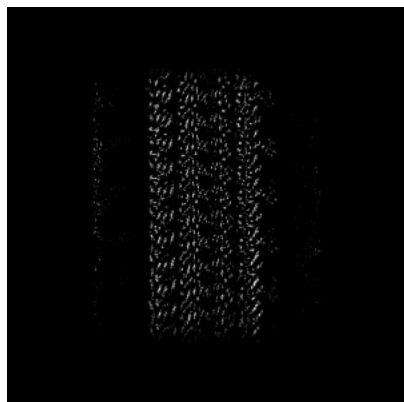


Z Index: 256

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

6.3 Largest variance slices [i](#)

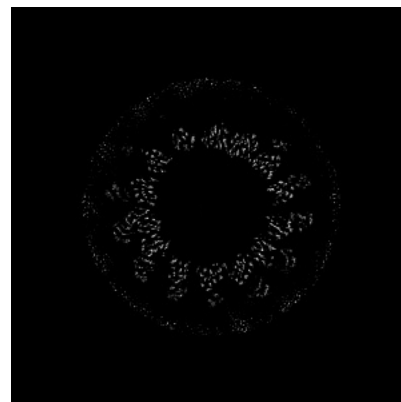
6.3.1 Primary map



X Index: 334

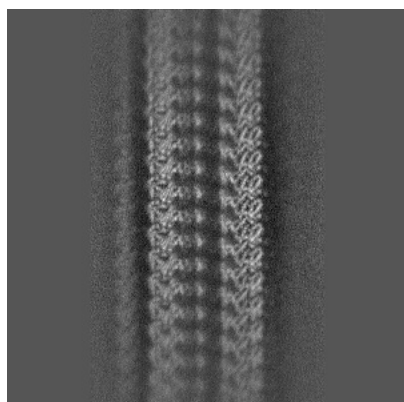


Y Index: 339

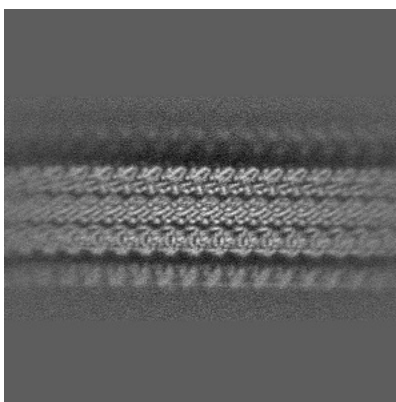


Z Index: 286

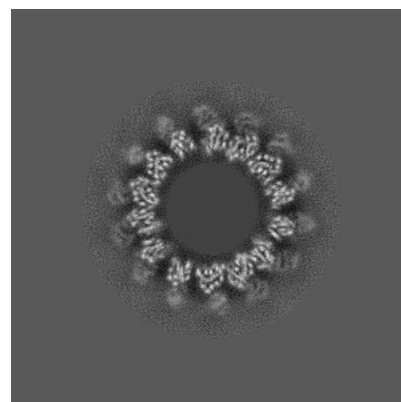
6.3.2 Raw map



X Index: 326



Y Index: 173

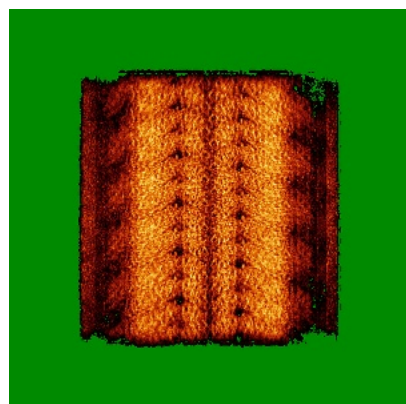


Z Index: 258

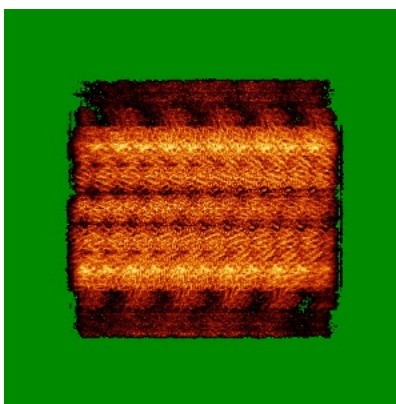
The images above show the largest variance slices of the map in three orthogonal directions.

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

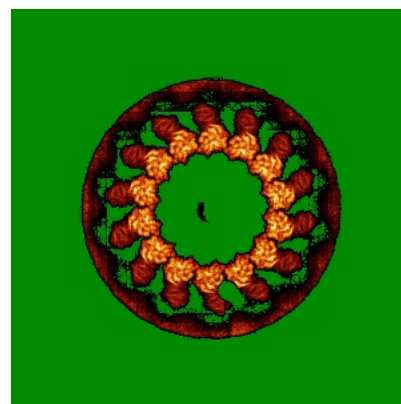
6.4.1 Primary map



X

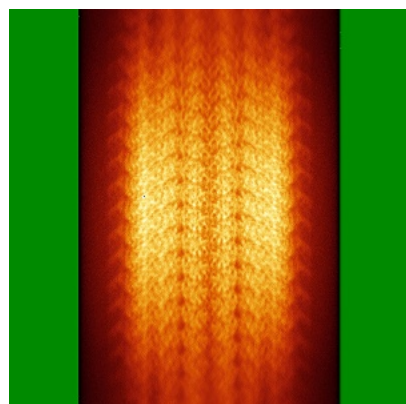


Y

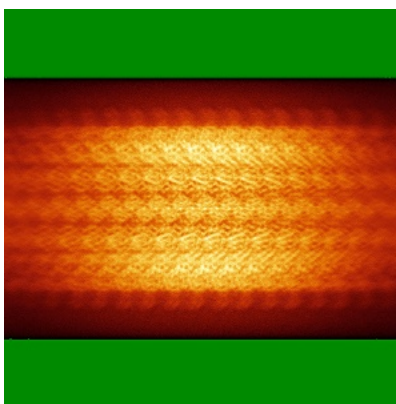


Z

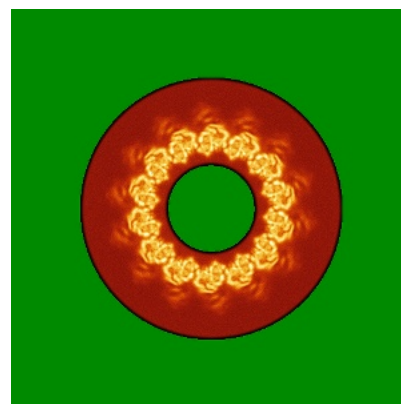
6.4.2 Raw map



X



Y

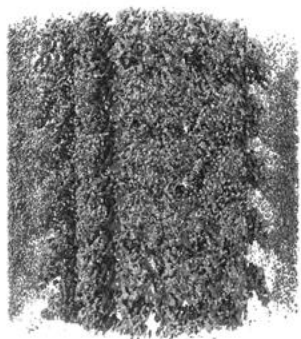


Z

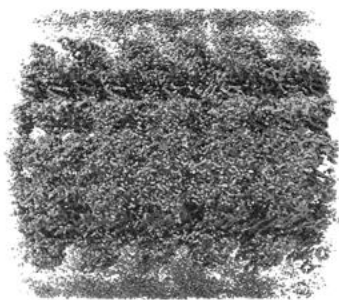
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

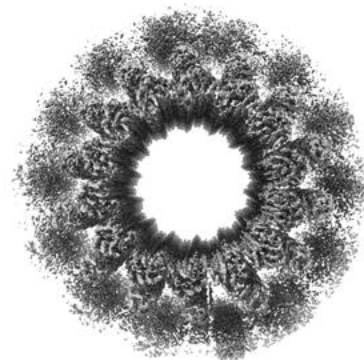
6.5.1 Primary map



X



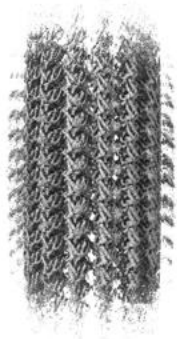
Y



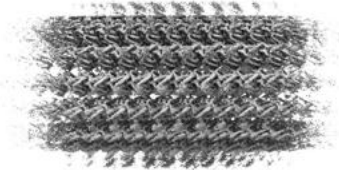
Z

The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

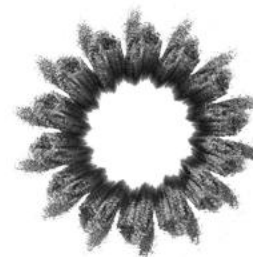
6.5.2 Raw map



X



Y



Z

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

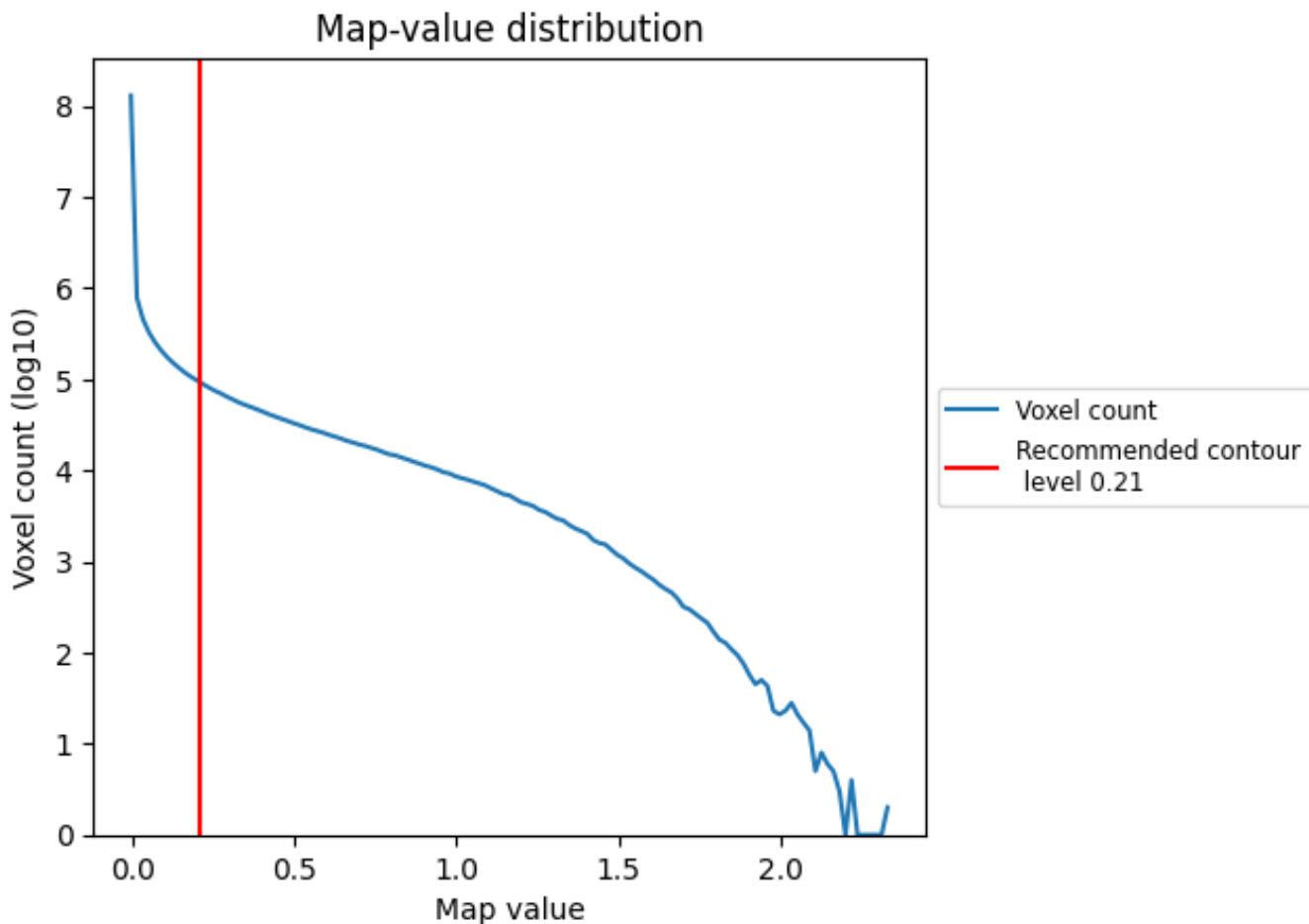
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

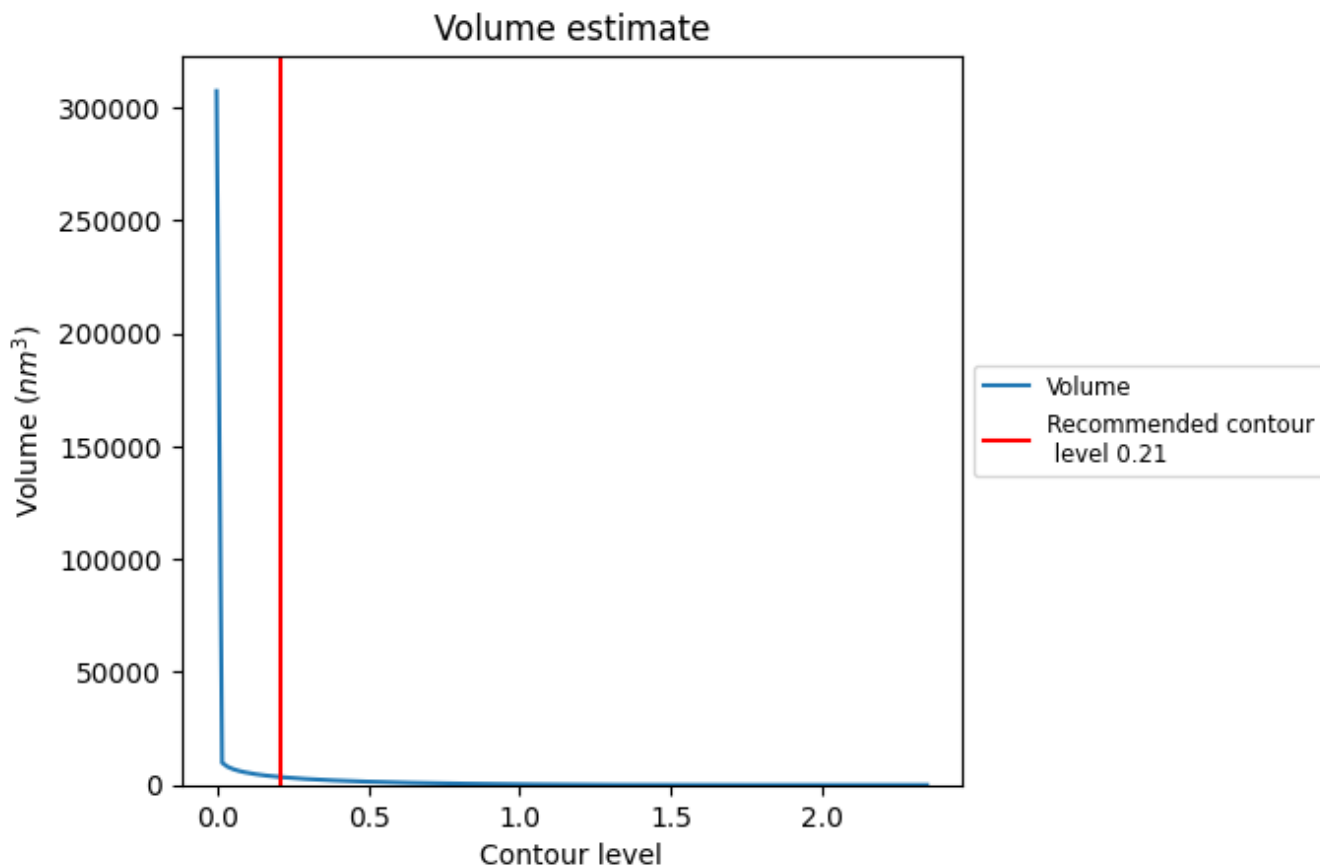
This section contains the results of statistical analysis of the map.

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.

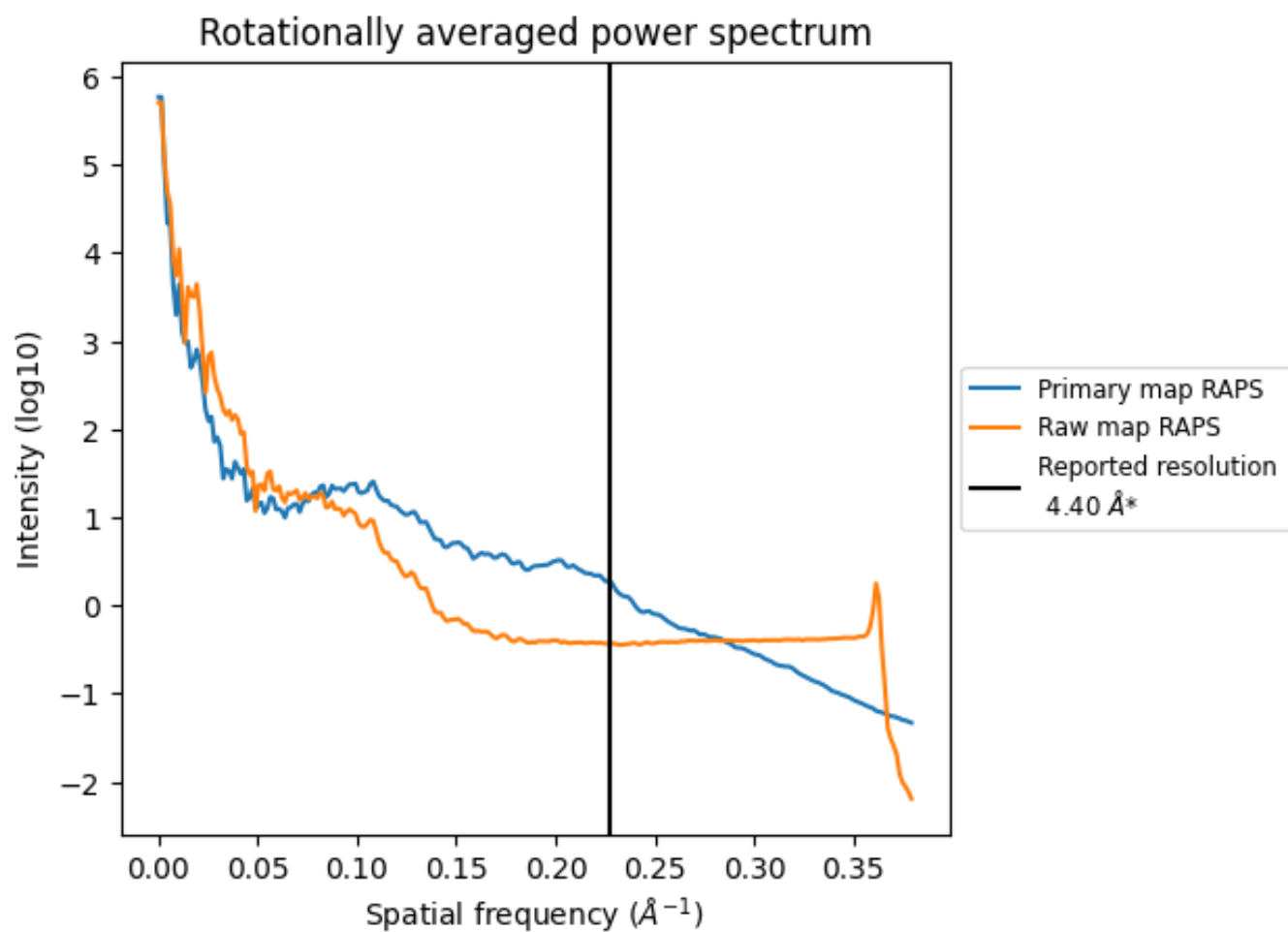
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3473 nm³; this corresponds to an approximate mass of 3137 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

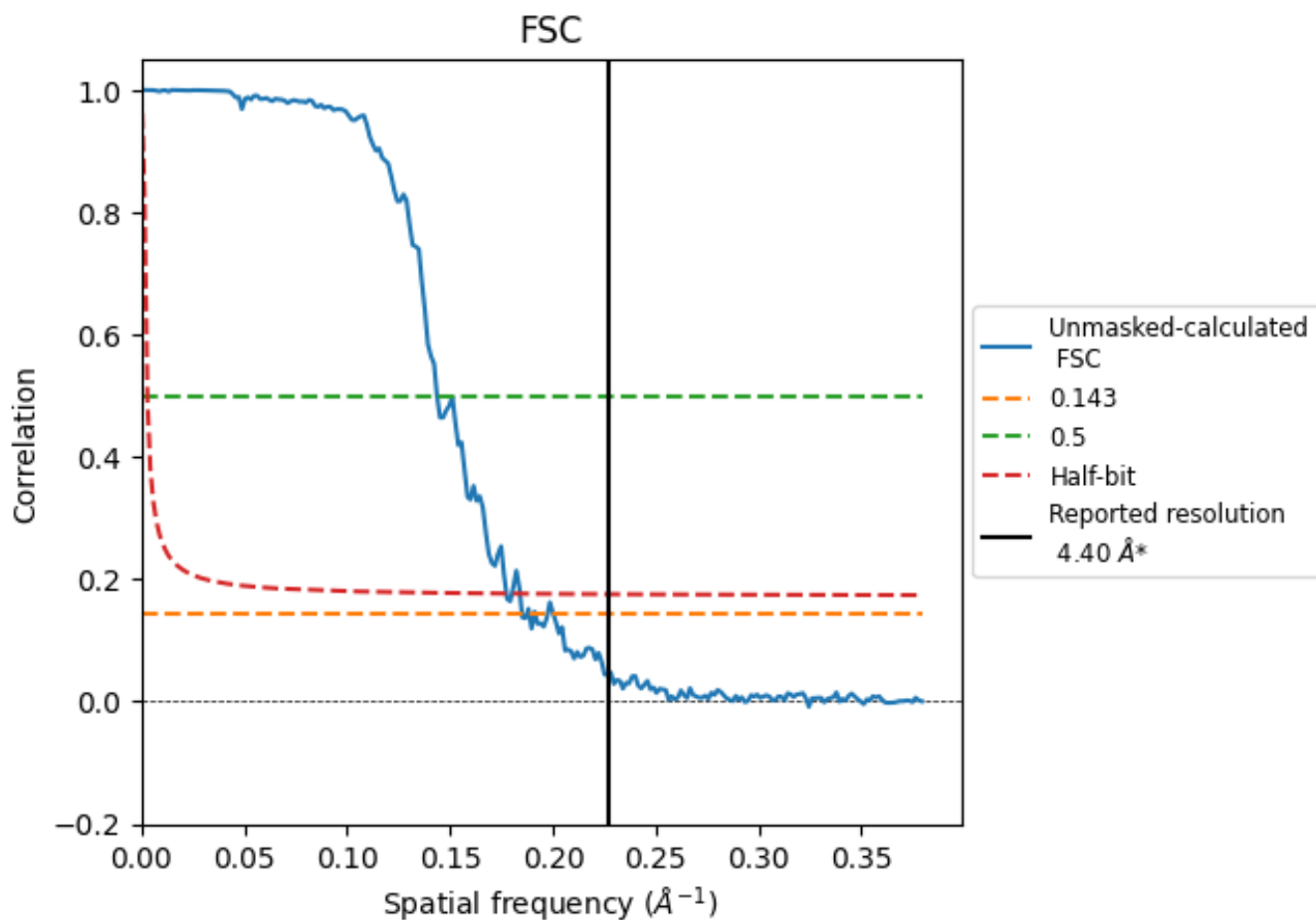


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

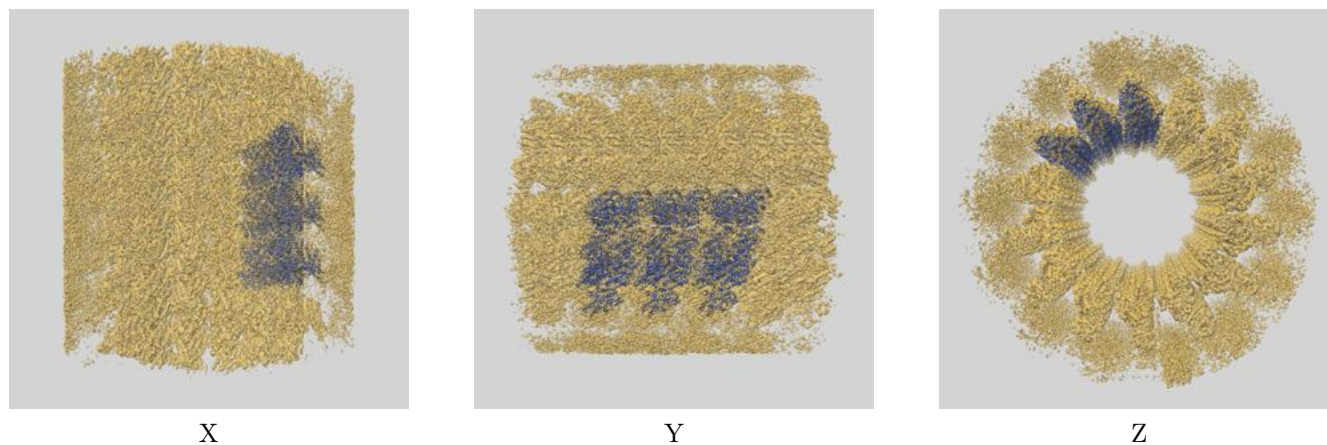
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.40	6.95	5.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.40 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

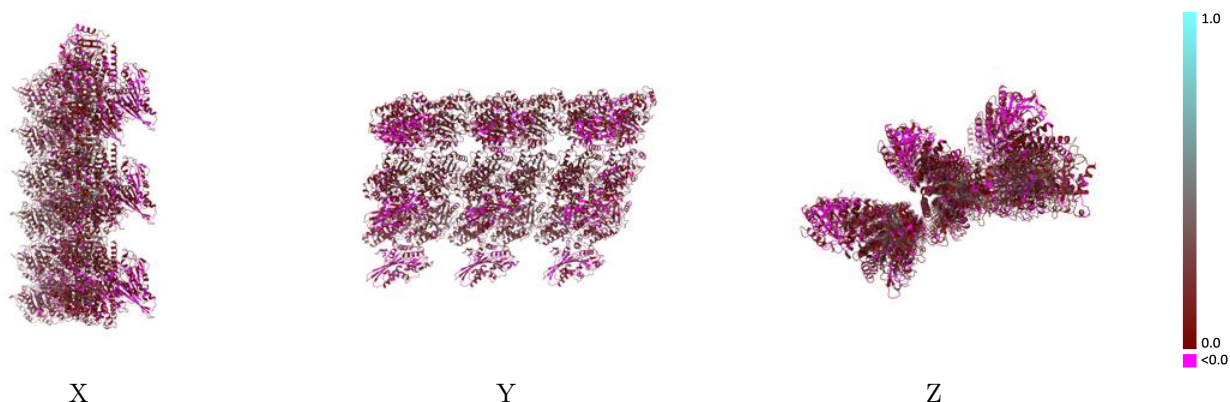
This section contains information regarding the fit between EMDB map EMD-35792 and PDB model 8IXF. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



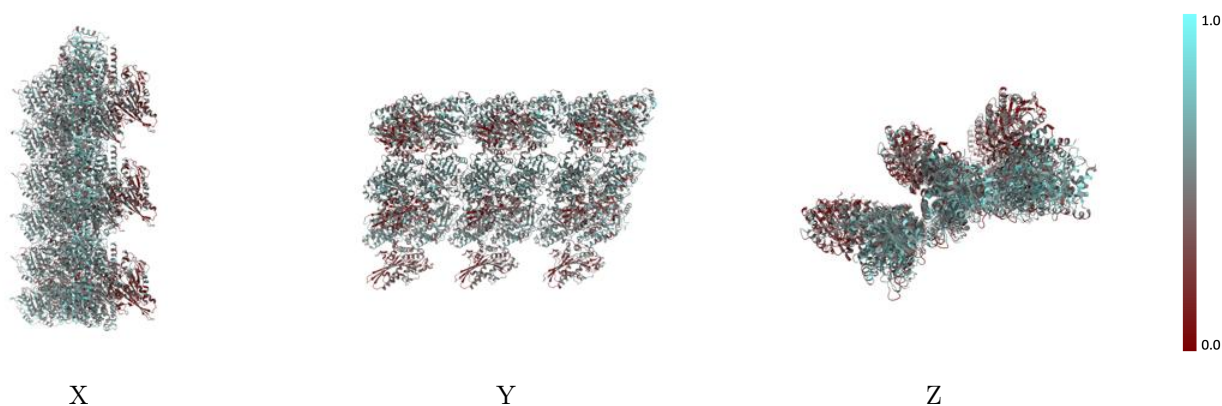
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



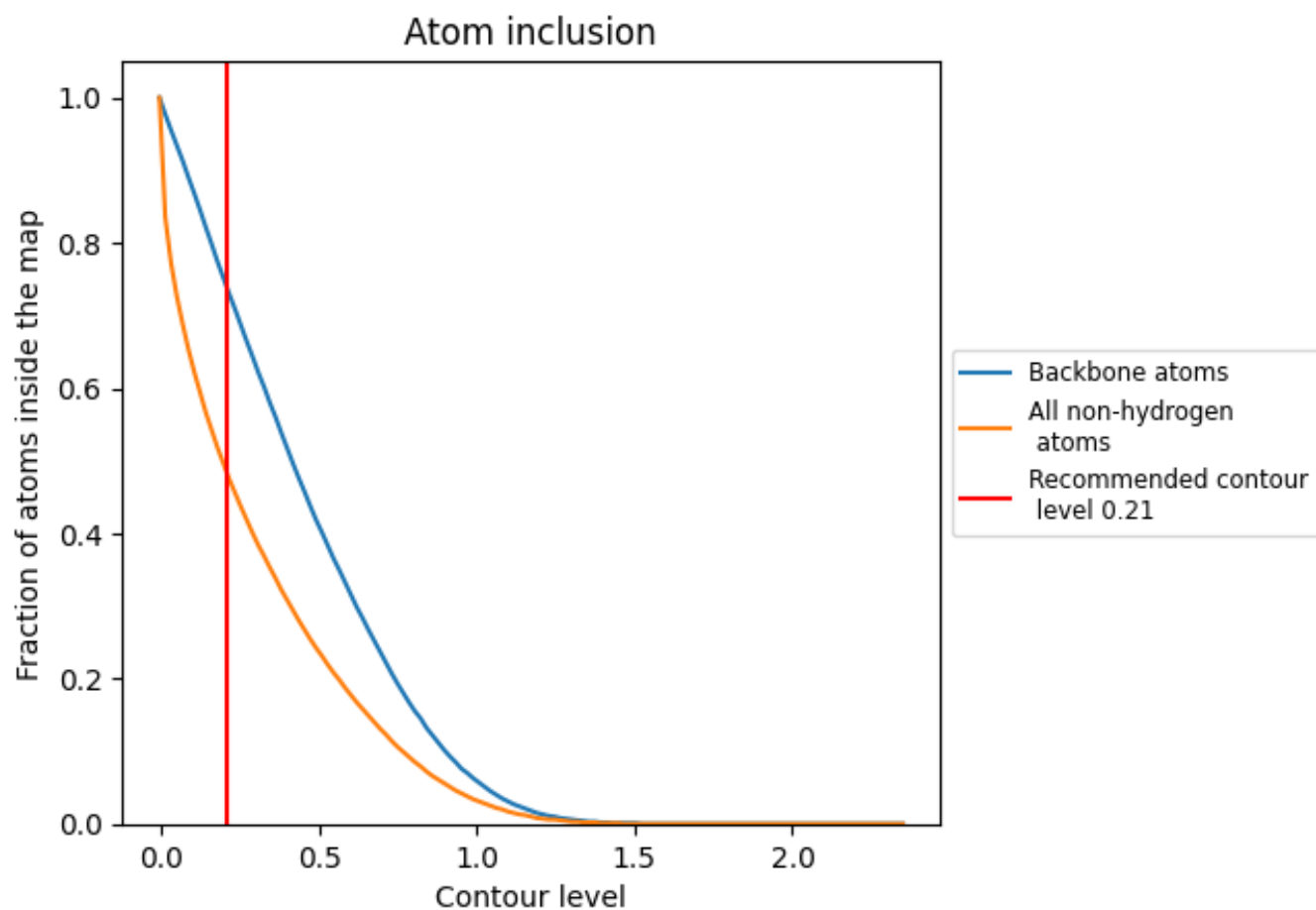
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4820	 0.1570
A	 0.5250	 0.1580
B	 0.5260	 0.1840
C	 0.5330	 0.1840
D	 0.5520	 0.2080
E	 0.5240	 0.1560
F	 0.5440	 0.1960
G	 0.5670	 0.2230
H	 0.5340	 0.1630
I	 0.5500	 0.2120
J	 0.5420	 0.1840
K	 0.5380	 0.1720
L	 0.5430	 0.1720
M	 0.5610	 0.2080
N	 0.5510	 0.1840
O	 0.5480	 0.1850
P	 0.5670	 0.2240
Q	 0.5570	 0.2150
R	 0.5590	 0.1940
S	 0.3400	 0.0690
T	 0.3120	 0.0580
U	 0.2860	 0.0520
V	 0.3290	 0.0930
W	 0.3180	 0.0650
X	 0.2770	 0.0530
Y	 0.3440	 0.0960
Z	 0.3160	 0.0900
a	 0.3110	 0.0610

