



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 10:24 PM JST

PDB ID : 8IXE / pdb_00008ixe
EMDB ID : EMD-35791
Title : GMPCPP-Alpha1C/Beta2A-microtubule decorated with kinesin 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

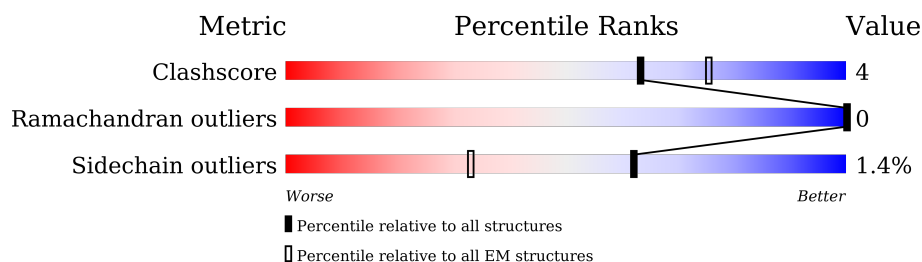
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	455	82% 12% 6%
1	H	455	82% 12% 6%
1	J	455	83% 11% 6%
1	K	455	83% 11% 6%
2	R	457	81% 12% 7%
2	W	457	82% 11% 7%
2	Z	457	82% 11% 7%
2	a	457	82% 11% 7%
3	h	372	79% 9% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	l	372	 76% 11% 13%
3	p	372	 78% 10% 13%
3	q	372	 79% 9% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37376 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-1C chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	427	Total	C	N	O	S	0	0
			3351	2124	570	636	21		
1	B	427	Total	C	N	O	S	0	0
			3351	2124	570	636	21		
1	J	427	Total	C	N	O	S	0	0
			3351	2124	570	636	21		
1	K	427	Total	C	N	O	S	0	0
			3351	2124	570	636	21		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	43	HIS	-	insertion	UNP P68373
H	44	HIS	-	insertion	UNP P68373
H	45	HIS	-	insertion	UNP P68373
H	46	HIS	-	insertion	UNP P68373
H	47	HIS	-	insertion	UNP P68373
H	48	HIS	-	insertion	UNP P68373
B	43	HIS	-	insertion	UNP P68373
B	44	HIS	-	insertion	UNP P68373
B	45	HIS	-	insertion	UNP P68373
B	46	HIS	-	insertion	UNP P68373
B	47	HIS	-	insertion	UNP P68373
B	48	HIS	-	insertion	UNP P68373
J	43	HIS	-	insertion	UNP P68373
J	44	HIS	-	insertion	UNP P68373
J	45	HIS	-	insertion	UNP P68373
J	46	HIS	-	insertion	UNP P68373
J	47	HIS	-	insertion	UNP P68373
J	48	HIS	-	insertion	UNP P68373
K	43	HIS	-	insertion	UNP P68373
K	44	HIS	-	insertion	UNP P68373
K	45	HIS	-	insertion	UNP P68373
K	46	HIS	-	insertion	UNP P68373

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	HIS	-	insertion	UNP P68373
K	48	HIS	-	insertion	UNP P68373

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
2	R	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
2	Z	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		
2	a	426	Total	C	N	O	S	0	0
			3354	2107	575	646	26		

There are 48 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	l	325	Total	C	N	O	S	0	0
			2544	1585	438	506	15		
3	h	325	Total	C	N	O	S	0	0
			2544	1585	438	506	15		
3	p	325	Total	C	N	O	S	0	0
			2544	1585	438	506	15		
3	q	325	Total	C	N	O	S	0	0
			2544	1585	438	506	15		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	-22	MET	-	initiating methionine	UNP P33176
l	-21	GLY	-	expression tag	UNP P33176

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

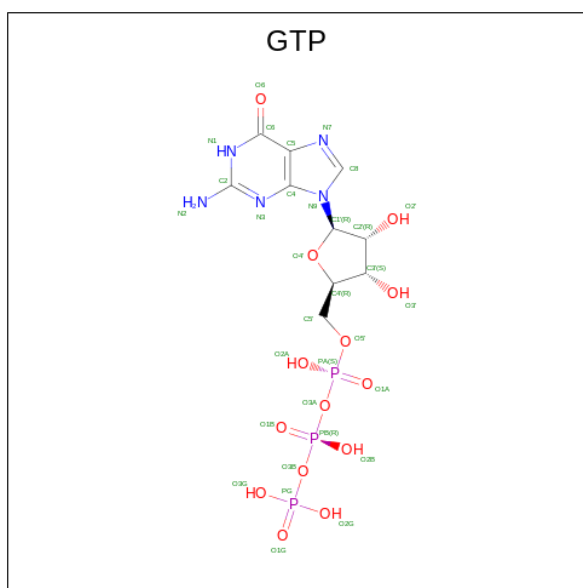
Chain	Residue	Modelled	Actual	Comment	Reference
h	-2	MET	-	expression tag	UNP P33176
h	-1	ALA	-	expression tag	UNP P33176
h	0	SER	-	expression tag	UNP P33176
h	236	ALA	GLU	conflict	UNP P33176
p	-22	MET	-	initiating methionine	UNP P33176
p	-21	GLY	-	expression tag	UNP P33176
p	-20	SER	-	expression tag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

Continued on next page...

Continued from previous page...

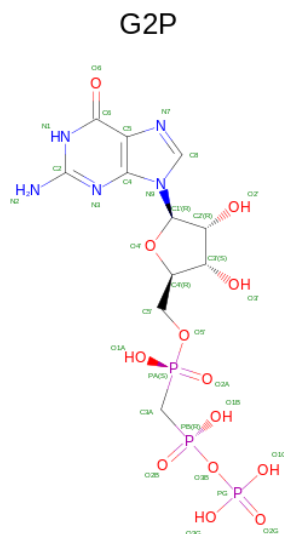
Chain	Residue	Modelled	Actual	Comment	Reference
q	-8	VAL	-	expression tag	UNP P33176
q	-7	PRO	-	expression tag	UNP P33176
q	-6	ARG	-	expression tag	UNP P33176
q	-5	GLY	-	expression tag	UNP P33176
q	-4	SER	-	expression tag	UNP P33176
q	-3	HIS	-	expression tag	UNP P33176
q	-2	MET	-	expression tag	UNP P33176
q	-1	ALA	-	expression tag	UNP P33176
q	0	SER	-	expression tag	UNP P33176
q	236	ALA	GLU	conflict	UNP P33176

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



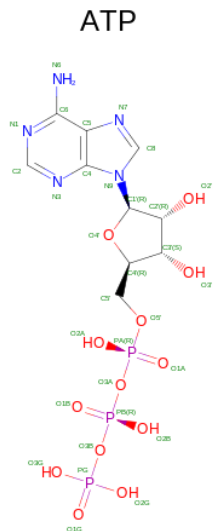
Mol	Chain	Residues	Atoms					AltConf
4	W	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	R	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	a	1	Total	C	N	O	P	0
			32	10	5	14	3	

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




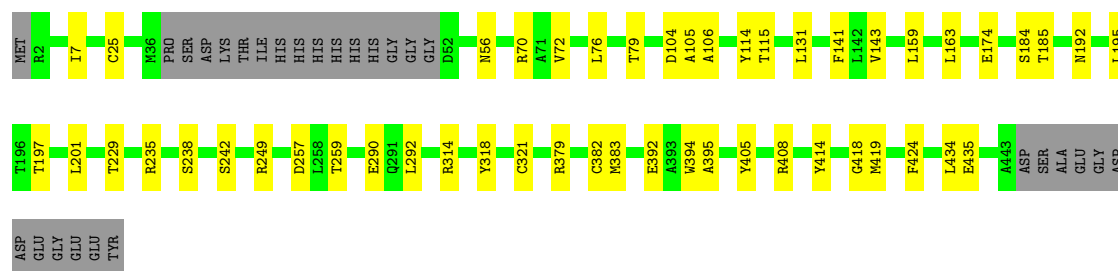
Mol	Chain	Residues	Atoms					AltConf
5	W	1	Total 32	C 11	N 5	O 13	P 3	0
5	R	1	Total 32	C 11	N 5	O 13	P 3	0
5	Z	1	Total 32	C 11	N 5	O 13	P 3	0
5	a	1	Total 32	C 11	N 5	O 13	P 3	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).




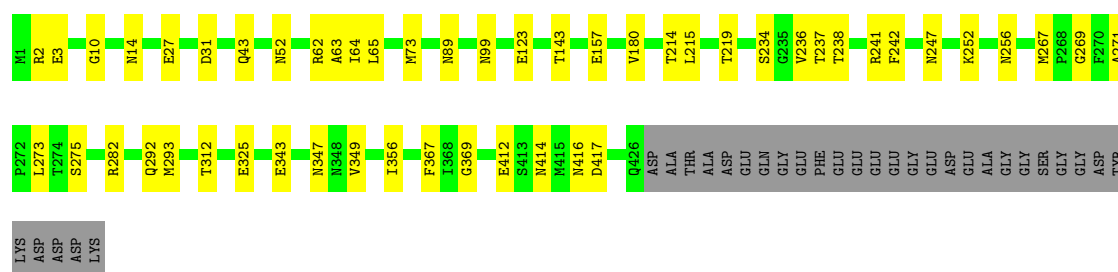
Mol	Chain	Residues	Atoms					AltConf
6	l	1	Total 31	C 10	N 5	O 13	P 3	0
6	h	1	Total 31	C 10	N 5	O 13	P 3	0
6	p	1	Total 31	C 10	N 5	O 13	P 3	0
6	q	1	Total 31	C 10	N 5	O 13	P 3	0

Chain K:  83% 11% 6%




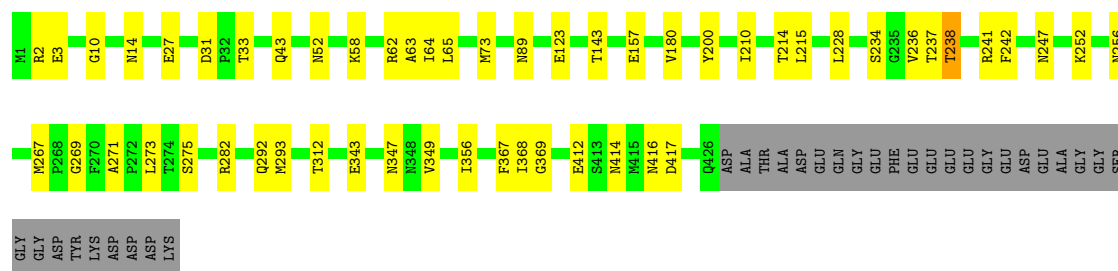
- Molecule 2: Tubulin beta-2A chain

Chain W:  82% 11% 7%




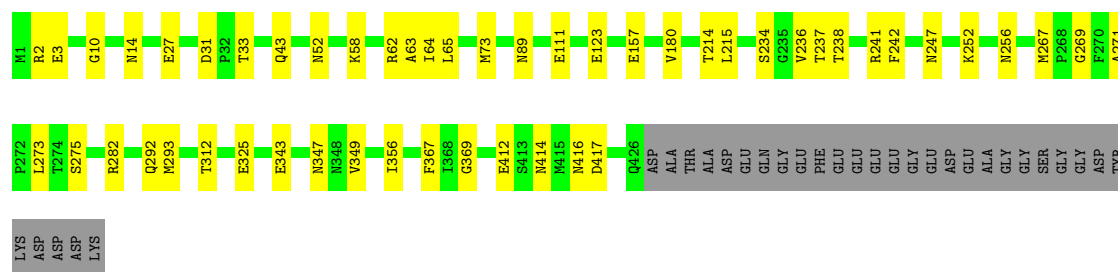
- Molecule 2: Tubulin beta-2A chain

Chain R:  81% 12% 7%



- Molecule 2: Tubulin beta-2A chain

Chain Z:  82% 11% 7%



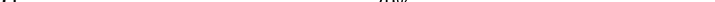
- Molecule 2: Tubulin beta-2A chain

TYR LYS ASP ASP ASP LYS	N256	R1
	LYS	R2
	ASP	E3
	ASP	G10
	ASP	M14
	LYS	E27
	Q280	D31
	R282	P32
	A283	T33
	L284	Q43
Q292	Q43	
M293	N52	
T312	R58	
E343	R62	
N347	A63	
N348	164	
V349	L65	
I368	M73	
A412	N89	
E413	E111	
N414	E123	
M415	T143	
N416	E157	
D417	V180	
Q426	Y200	
ASP	I210	
ALA	T214	
THR	L215	
ALA	L228	
ASP	S234	
GLU	G235	
GLN	V236	
GLY	T237	
PHE	T238	
GLU	R241	
GLU	N247	
GLU	K252	
GLU	ASP	

- | | | |
|-----|------|------|
| LYS | D140 | MET |
| TYR | | GLY |
| GLU | D158 | SER |
| LYS | | SER |
| GLU | V162 | HIS |
| LYS | | HIS |
| GLU | R190 | HIS |
| | | HIS |
| | S202 | HIS |
| | R203 | HIS |
| | S204 | SER |
| | H205 | SER |
| | S206 | GLY |
| | I207 | LEU |
| | F208 | VAL |
| | L209 | PRO |
| | I210 | ARG |
| | | GLY |
| | K213 | SER |
| | Q214 | HIS |
| | | MET |
| | Q218 | ALA |
| | | SER |
| | Y228 | MET |
| | L229 | ALA |
| | | ASP |
| | V238 | LEU |
| | | A5 |
| | N253 | |
| | S257 | V11 |
| | | R14 |
| | R278 | |
| | D279 | R25 |
| | S280 | G26 |
| | | D27 |
| | T283 | |
| | | Q58 |
| | S289 | |
| | C294 | T80 |
| | | F81 |
| | I298 | F82 |
| | | G90 |
| | N327 | |
| | T328 | H93 |
| | V329 | T94 |
| CYS | | H95 |
| VAL | | E96 |
| ASN | | |
| VAL | | I108 |
| GLU | | |
| LEU | | D123 |
| THR | | E124 |
| ALA | | |
| GLU | | Y134 |
| GLN | | F135 |
| TRP | | E136 |
| LYS | | I137 |

- | | | |
|------|-------|------|
| R190 | R1390 | MET |
| S202 | GLY | GLY |
| H205 | SER | SER |
| S206 | SER | SER |
| I207 | HIS | HIS |
| | HIS | HIS |
| Q218 | HIS | HIS |
| Y228 | SER | SER |
| L229 | GLY | GLY |
| V238 | LEU | LEU |
| | VAL | VAL |
| N253 | PRO | PRO |
| | ARG | ARG |
| S257 | GLY | GLY |
| R278 | SER | SER |
| D279 | HIS | HIS |
| S280 | MET | MET |
| | ALA | ALA |
| T283 | SER | SER |
| | MET | MET |
| | ALA | ALA |
| S289 | ASP | ASP |
| I298 | LEU | LEU |
| | | A5 |
| V329 | CYS | V11 |
| VAL | VAL | R14 |
| ASN | ASN | R25 |
| VAL | VAL | G26 |
| GLU | GLU | D27 |
| LEU | LEU | |
| THR | THR | T80 |
| ALA | ALA | I81 |
| GLU | GLU | F82 |
| GLN | GLN | |
| TRP | TRP | G90 |
| LYS | LYS | |
| LYS | LYS | T94 |
| LYS | LYS | M95 |
| TYR | TYR | E96 |
| GLU | GLU | |
| LYS | LYS | I108 |
| GLU | GLU | D123 |
| LYS | LYS | E124 |
| GLU | GLU | |
| | | V134 |
| | | F135 |
| | | |
| | | D140 |
| | | |
| | | D158 |
| | | |
| | | I167 |

- | | |
|------|------|
| D140 | MET |
| R190 | GLY |
| S202 | SER |
| R303 | HIS |
| S204 | HIS |
| H205 | HIS |
| S206 | HIS |
| I207 | HIS |
| Q218 | SER |
| Y228 | SER |
| L229 | GLY |
| T238 | LEU |
| V238 | VAL |
| N253 | PRO |
| S257 | ARG |
| R278 | GLY |
| D279 | SER |
| S280 | HIS |
| T283 | HIS |
| S289 | ALA |
| C294 | ALA |
| I298 | SER |
| N327 | MET |
| T328 | ALA |
| S329 | ASP |
| CYS | LEU |
| VAL | A5 |
| ASN | V11 |
| VAL | R14 |
| GLU | R25 |
| THR | G26 |
| ALA | D27 |
| GLU | Q58 |
| THR | T80 |
| ALA | I81 |
| GLU | F82 |
| THR | G90 |
| GLU | H93 |
| GLN | T94 |
| TRP | H95 |
| LYS | E96 |
| LVS | I108 |
| TVR | D123 |
| LVS | E124 |
| GLU | Y134 |
| GLU | F135 |
| | E136 |
| | I137 |

- Chain q:  79% 9% 13%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	ALA	SER	MET	ALA	ASP	LEU	A5	V11	R14	R25	G26	D27	Q58	T80	I81	F82	G90	H93	T94	M95	E96	I108	D123	E124	Y134	F135	D140
R190	S202	H205	S206	I207	Q218	Y228	L229	V238	N253	S257	R278	D279	S280	T283	S289	I298	V329	CYS	VAL	ASN	VAL	GLU	LEU	THR	ALA	GLU	GLN	TRP	LYS	LYS	LYS	TYR	GLU	LYS	GLU	LYS	LYS	GLU	LYS	LYS	GLU	LYS	GLU			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21250	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

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: ATP, GTP, G2P

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	0/3427	0.48	0/4653
1	H	0.23	0/3427	0.49	0/4653
1	J	0.23	0/3427	0.48	0/4653
1	K	0.23	0/3427	0.48	0/4653
2	R	0.22	0/3429	0.46	0/4643
2	W	0.22	0/3429	0.46	0/4643
2	Z	0.22	0/3429	0.46	0/4643
2	a	0.22	0/3429	0.46	0/4643
3	h	0.24	0/2583	0.44	0/3482
3	l	0.24	0/2583	0.44	0/3482
3	p	0.23	0/2583	0.44	0/3482
3	q	0.23	0/2583	0.44	0/3482
All	All	0.23	0/37756	0.46	0/51112

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	B	3351	0	3262	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3351	0	3262	30	0
1	J	3351	0	3262	25	0
1	K	3351	0	3262	26	0
2	R	3354	0	3239	28	0
2	W	3354	0	3239	26	0
2	Z	3354	0	3239	25	0
2	a	3354	0	3239	26	0
3	h	2544	0	2523	22	0
3	l	2544	0	2523	27	0
3	p	2544	0	2523	24	0
3	q	2544	0	2523	22	0
4	R	32	0	12	2	0
4	W	32	0	12	3	0
4	Z	32	0	12	2	0
4	a	32	0	12	2	0
5	R	32	0	14	1	0
5	W	32	0	14	1	0
5	Z	32	0	14	0	0
5	a	32	0	14	1	0
6	h	31	0	12	1	0
6	l	31	0	12	1	0
6	p	31	0	12	1	0
6	q	31	0	12	1	0
All	All	37376	0	36248	293	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 293 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)
3:p:205:HIS:HE2	3:p:257:SER:HG	1.27	0.83
3:q:205:HIS:HE2	3:q:257:SER:HG	1.28	0.82
3:l:205:HIS:HE2	3:l:257:SER:HG	1.29	0.80
3:h:205:HIS:HE2	3:h:257:SER:HG	1.30	0.79
3:p:108:ILE:HG22	3:p:229:LEU:HD13	1.66	0.78

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	423/455 (93%)	412 (97%)	11 (3%)	0	100	100
1	H	423/455 (93%)	411 (97%)	12 (3%)	0	100	100
1	J	423/455 (93%)	412 (97%)	11 (3%)	0	100	100
1	K	423/455 (93%)	412 (97%)	11 (3%)	0	100	100
2	R	424/457 (93%)	416 (98%)	8 (2%)	0	100	100
2	W	424/457 (93%)	416 (98%)	8 (2%)	0	100	100
2	Z	424/457 (93%)	416 (98%)	8 (2%)	0	100	100
2	a	424/457 (93%)	417 (98%)	7 (2%)	0	100	100
3	h	323/372 (87%)	313 (97%)	10 (3%)	0	100	100
3	l	323/372 (87%)	313 (97%)	10 (3%)	0	100	100
3	p	323/372 (87%)	312 (97%)	11 (3%)	0	100	100
3	q	323/372 (87%)	312 (97%)	11 (3%)	0	100	100
All	All	4680/5136 (91%)	4562 (98%)	118 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	360/382 (94%)	354 (98%)	6 (2%)	56	72
1	H	360/382 (94%)	355 (99%)	5 (1%)	62	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	360/382 (94%)	351 (98%)	9 (2%)	42	62
1	K	360/382 (94%)	352 (98%)	8 (2%)	47	66
2	R	368/390 (94%)	362 (98%)	6 (2%)	58	74
2	W	368/390 (94%)	361 (98%)	7 (2%)	52	70
2	Z	368/390 (94%)	361 (98%)	7 (2%)	52	70
2	a	368/390 (94%)	360 (98%)	8 (2%)	47	66
3	h	289/330 (88%)	289 (100%)	0	100	100
3	l	289/330 (88%)	289 (100%)	0	100	100
3	p	289/330 (88%)	289 (100%)	0	100	100
3	q	289/330 (88%)	289 (100%)	0	100	100
All	All	4068/4408 (92%)	4012 (99%)	56 (1%)	62	76

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	143	VAL
2	a	343	GLU
2	Z	157	GLU
2	a	312	THR
2	a	111	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	56	ASN
2	a	105	HIS
1	K	335	ASN
2	a	375	GLN
3	h	19	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
6	ATP	p	401	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
6	ATP	q	401	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
5	G2P	W	502	-	27,34,34	6.06	12 (44%)	33,54,54	1.90	8 (24%)
5	G2P	R	502	-	27,34,34	6.06	12 (44%)	33,54,54	1.90	8 (24%)
5	G2P	a	502	-	27,34,34	6.05	12 (44%)	33,54,54	1.90	8 (24%)
6	ATP	l	401	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
6	ATP	h	401	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
4	GTP	Z	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.58	8 (25%)
4	GTP	W	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.58	8 (25%)
5	G2P	Z	502	-	27,34,34	6.06	12 (44%)	33,54,54	1.90	8 (24%)
4	GTP	R	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.58	8 (25%)
4	GTP	a	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.57	8 (25%)

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
6	ATP	p	401	-	-	6/18/38/38	0/3/3/3
6	ATP	q	401	-	-	5/18/38/38	0/3/3/3
5	G2P	W	502	-	-	8/15/38/38	0/3/3/3
5	G2P	R	502	-	-	8/15/38/38	0/3/3/3
5	G2P	a	502	-	-	8/15/38/38	0/3/3/3
6	ATP	l	401	-	-	6/18/38/38	0/3/3/3
6	ATP	h	401	-	-	6/18/38/38	0/3/3/3
4	GTP	Z	501	-	-	4/18/38/38	0/3/3/3
4	GTP	W	501	-	-	6/18/38/38	0/3/3/3
5	G2P	Z	502	-	-	8/15/38/38	0/3/3/3
4	GTP	R	501	-	-	5/18/38/38	0/3/3/3
4	GTP	a	501	-	-	5/18/38/38	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	502	G2P	C2'-C1'	-17.40	1.27	1.53
5	Z	502	G2P	C2'-C1'	-17.38	1.27	1.53
5	a	502	G2P	C2'-C1'	-17.38	1.27	1.53
5	R	502	G2P	C2'-C1'	-17.34	1.27	1.53
5	R	502	G2P	PB-O3B	14.88	1.75	1.58

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	502	G2P	N3-C2-N1	-5.69	119.64	127.22
5	Z	502	G2P	N3-C2-N1	-5.68	119.65	127.22
5	R	502	G2P	N3-C2-N1	-5.67	119.66	127.22
5	W	502	G2P	N3-C2-N1	-5.66	119.67	127.22
5	a	502	G2P	C2-N3-C4	4.30	120.27	115.36

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

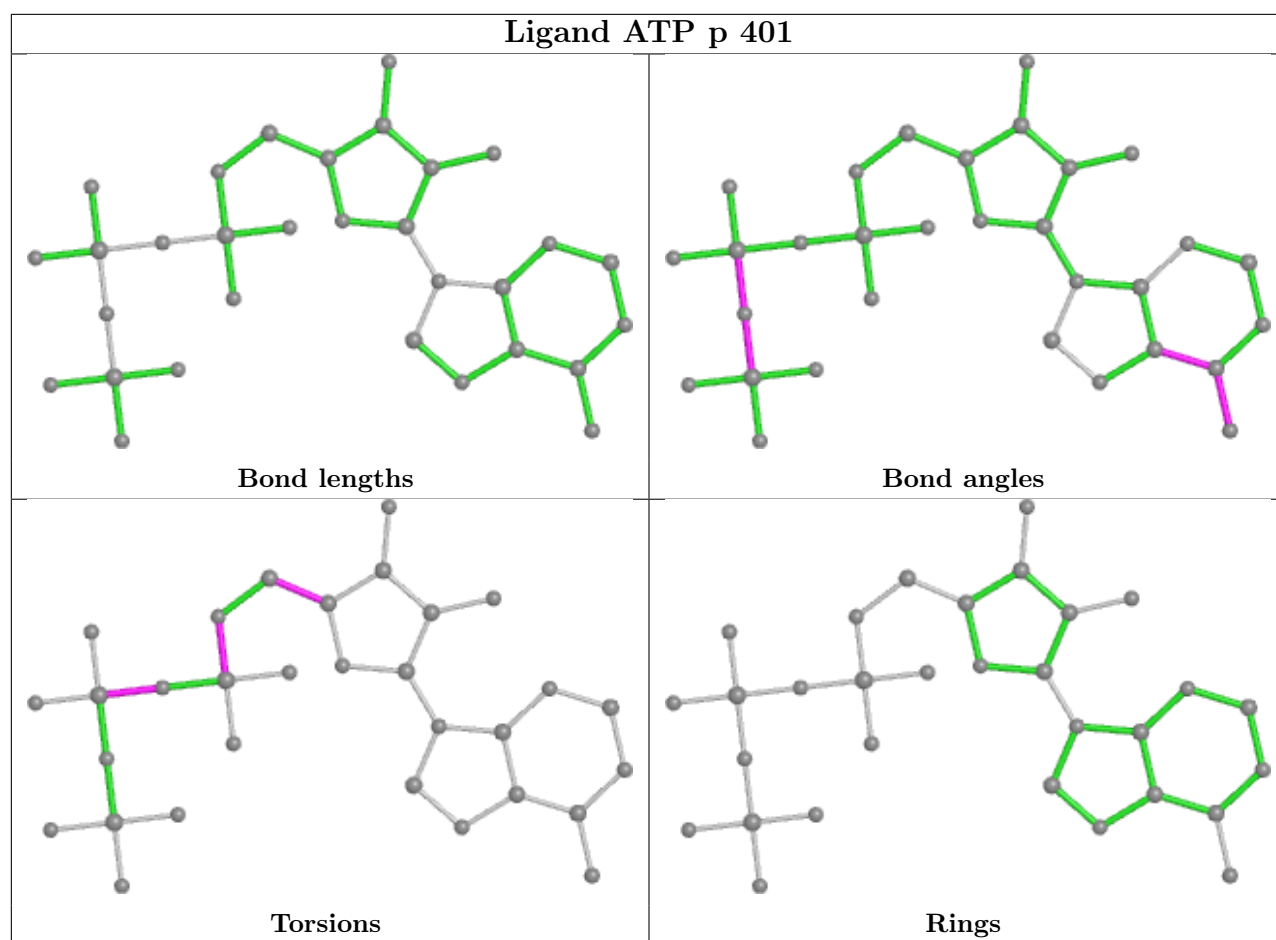
Mol	Chain	Res	Type	Atoms
4	W	501	GTP	C5'-O5'-PA-O3A
4	R	501	GTP	C5'-O5'-PA-O3A
4	a	501	GTP	C5'-O5'-PA-O3A
5	W	502	G2P	PB-O3B-PG-O3G
5	W	502	G2P	PB-C3A-PA-O1A

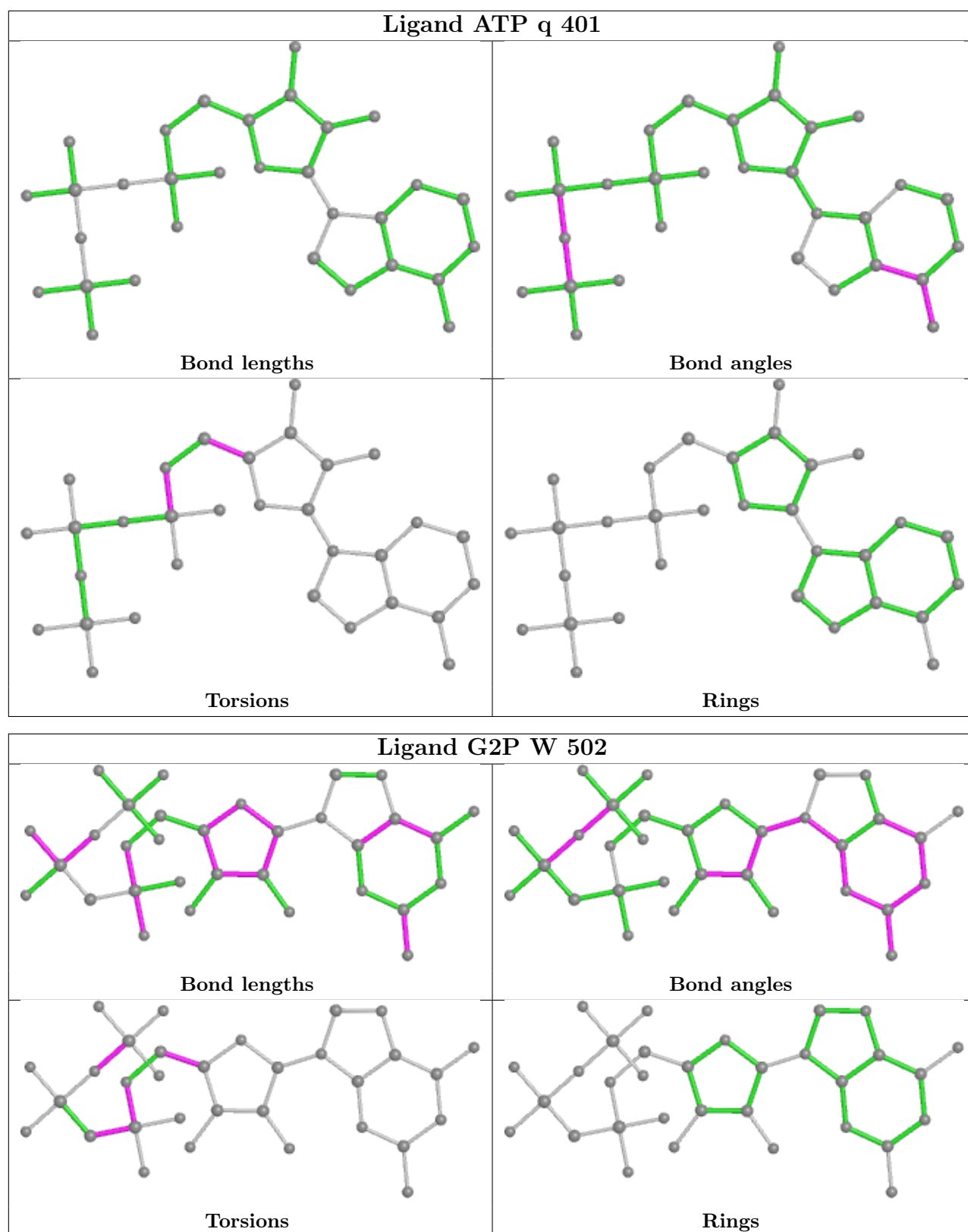
There are no ring outliers.

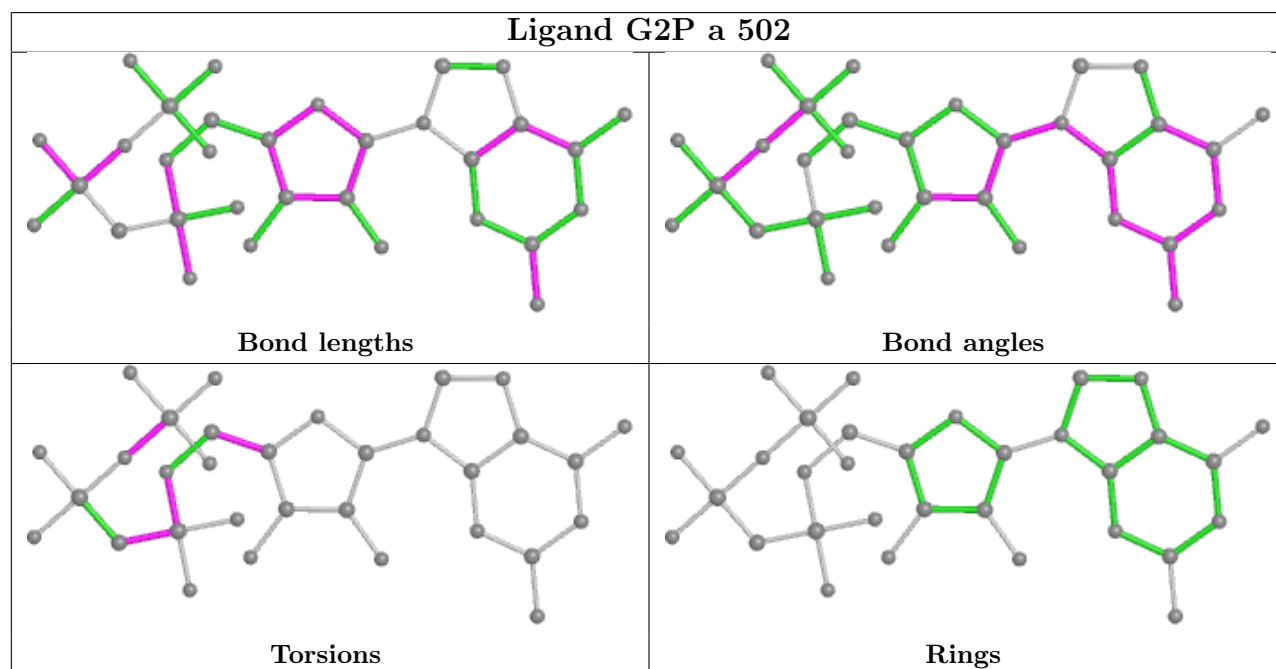
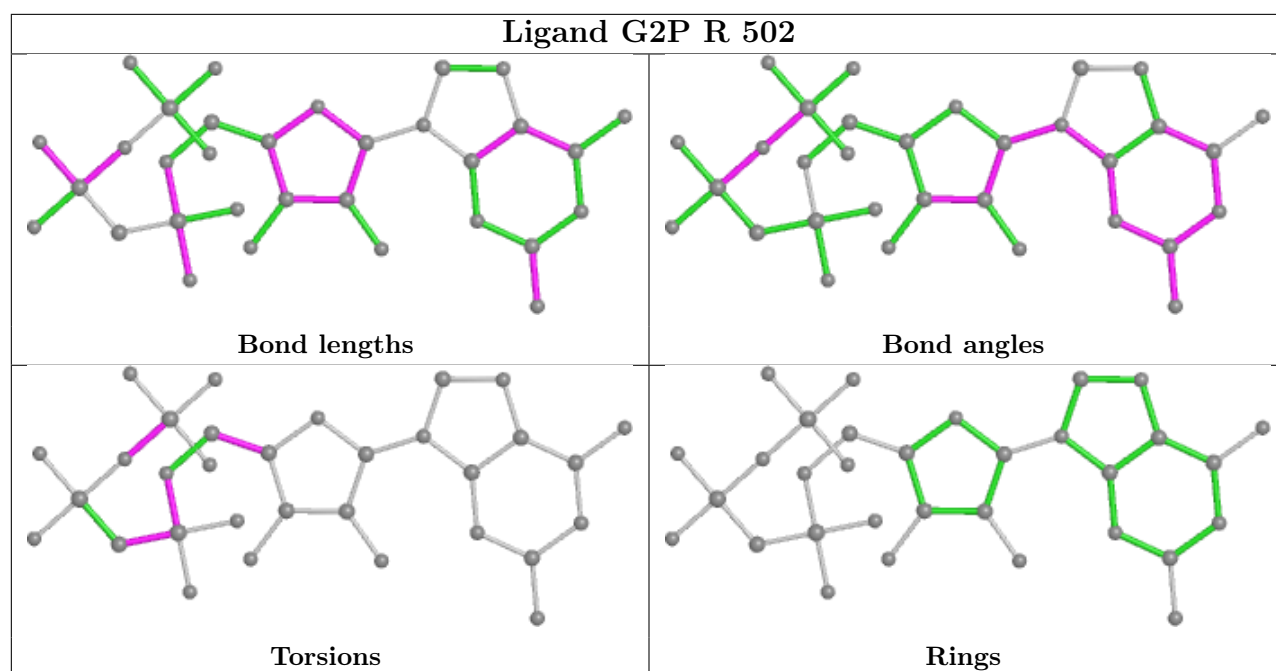
11 monomers are involved in 16 short contacts:

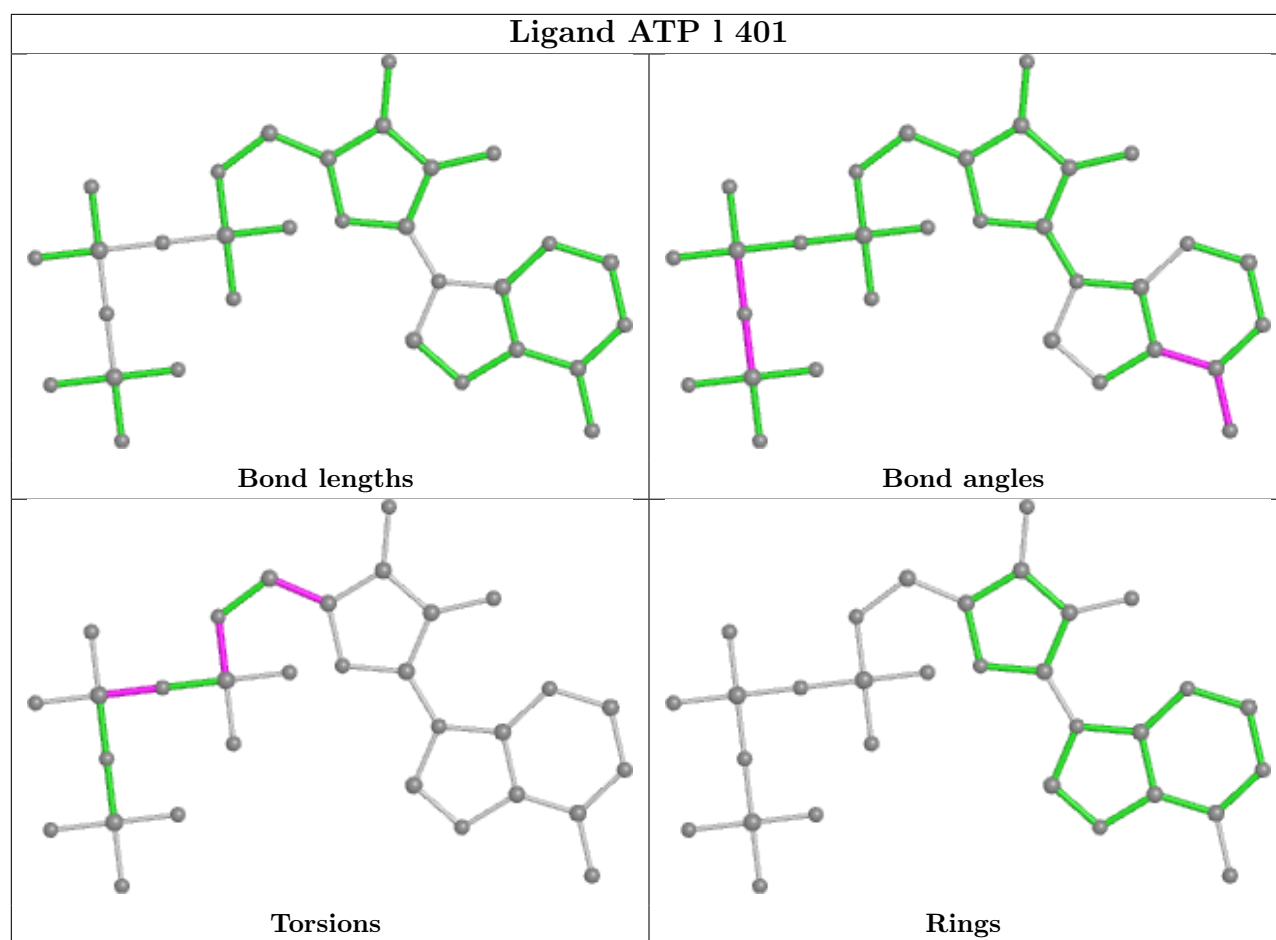
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	p	401	ATP	1	0
6	q	401	ATP	1	0
5	W	502	G2P	1	0
5	R	502	G2P	1	0
5	a	502	G2P	1	0
6	l	401	ATP	1	0
6	h	401	ATP	1	0
4	Z	501	GTP	2	0
4	W	501	GTP	3	0
4	R	501	GTP	2	0
4	a	501	GTP	2	0

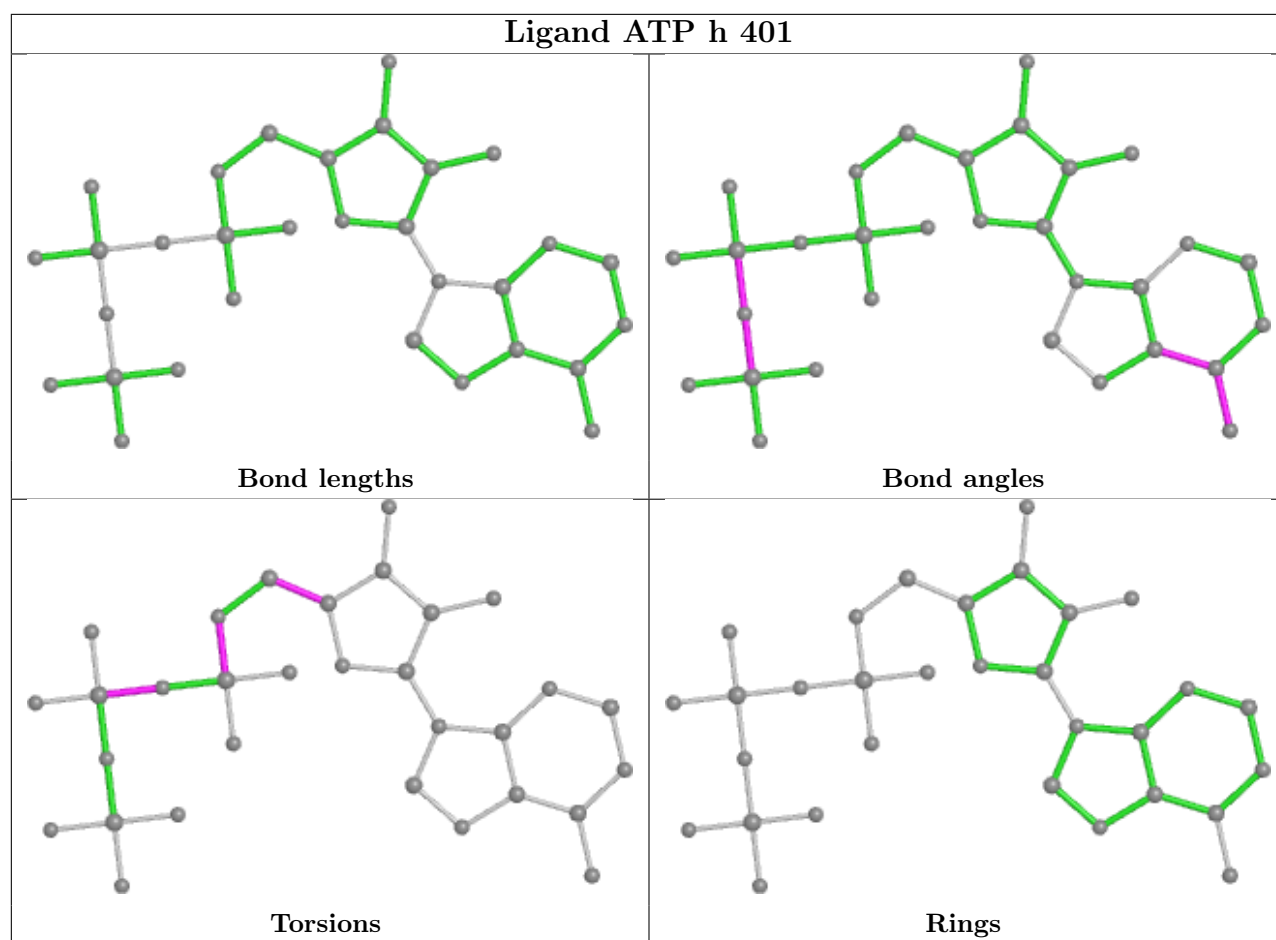
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



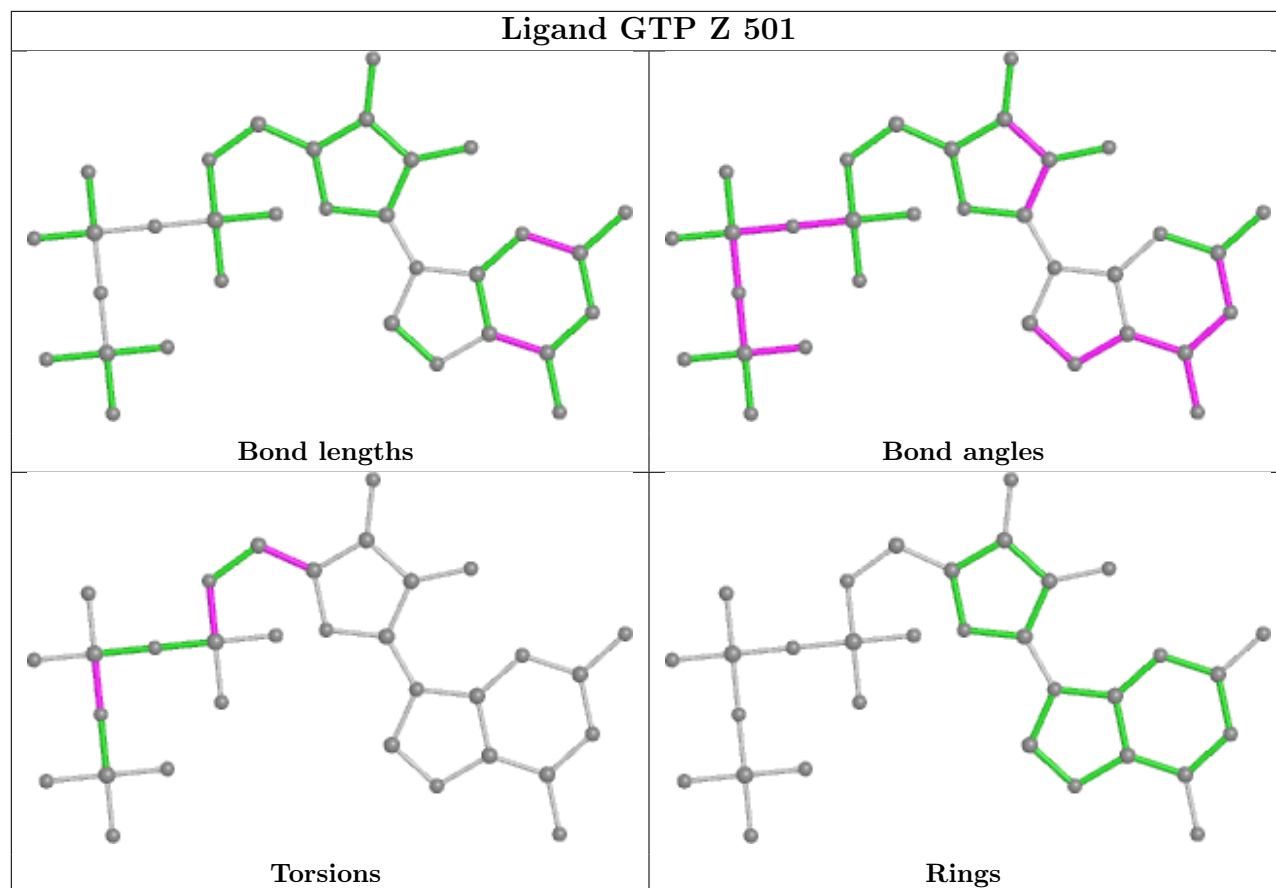




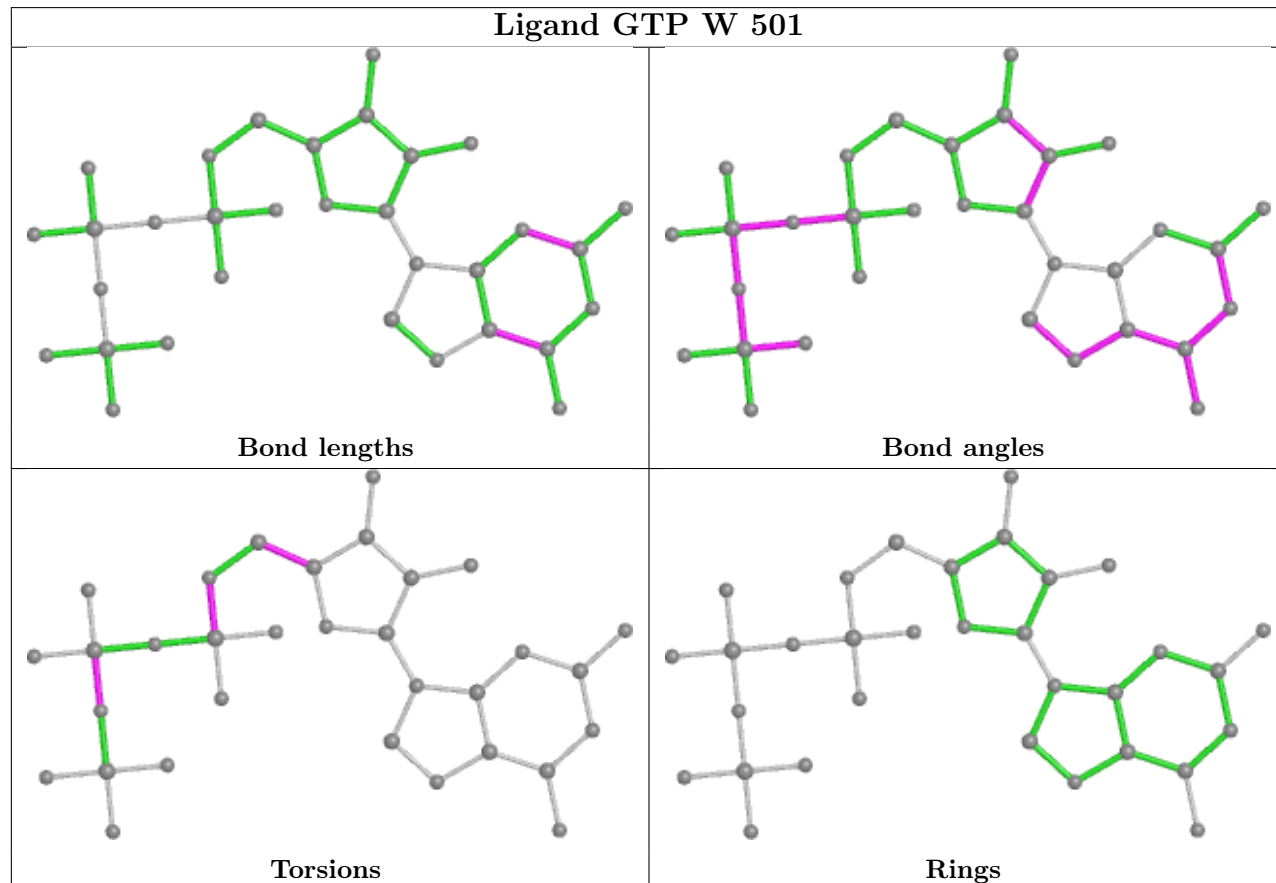


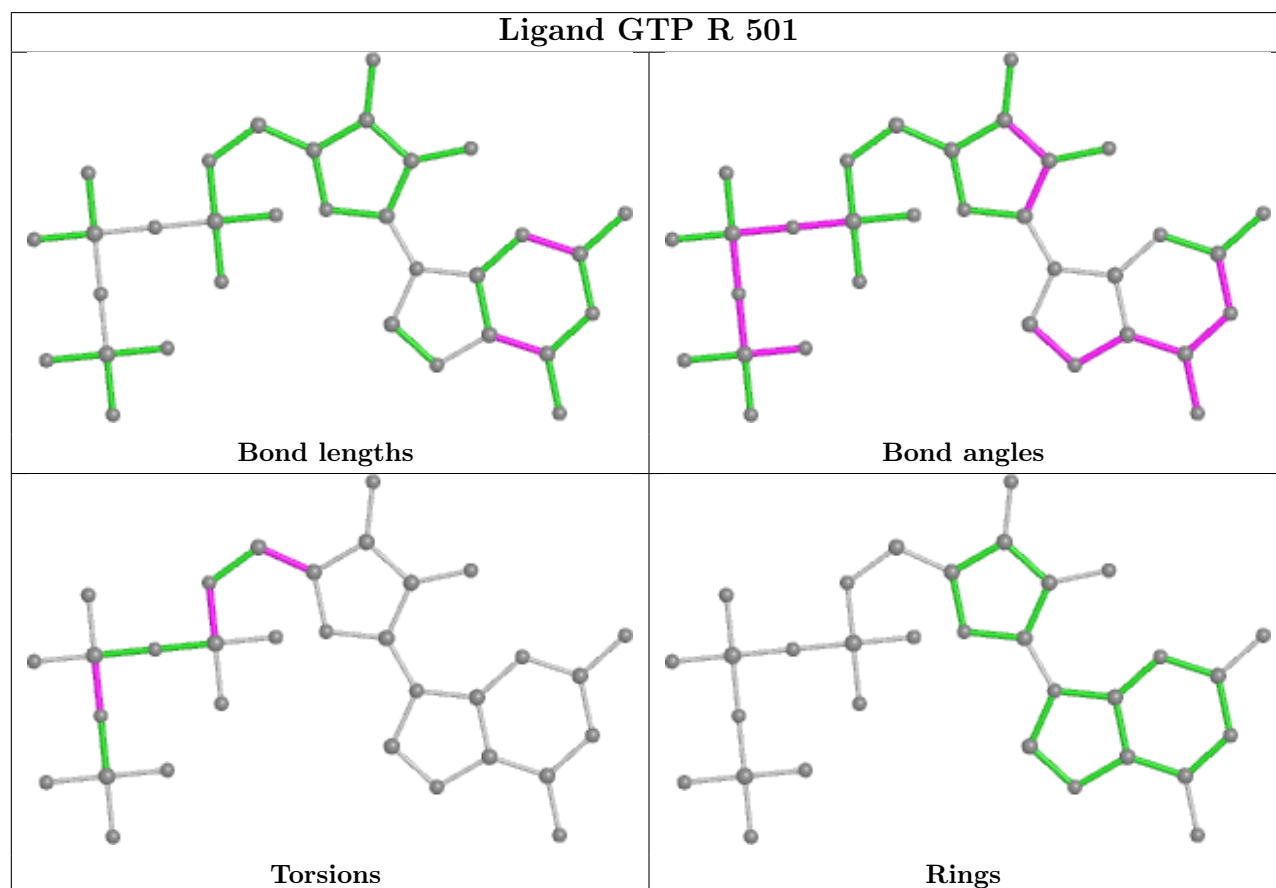
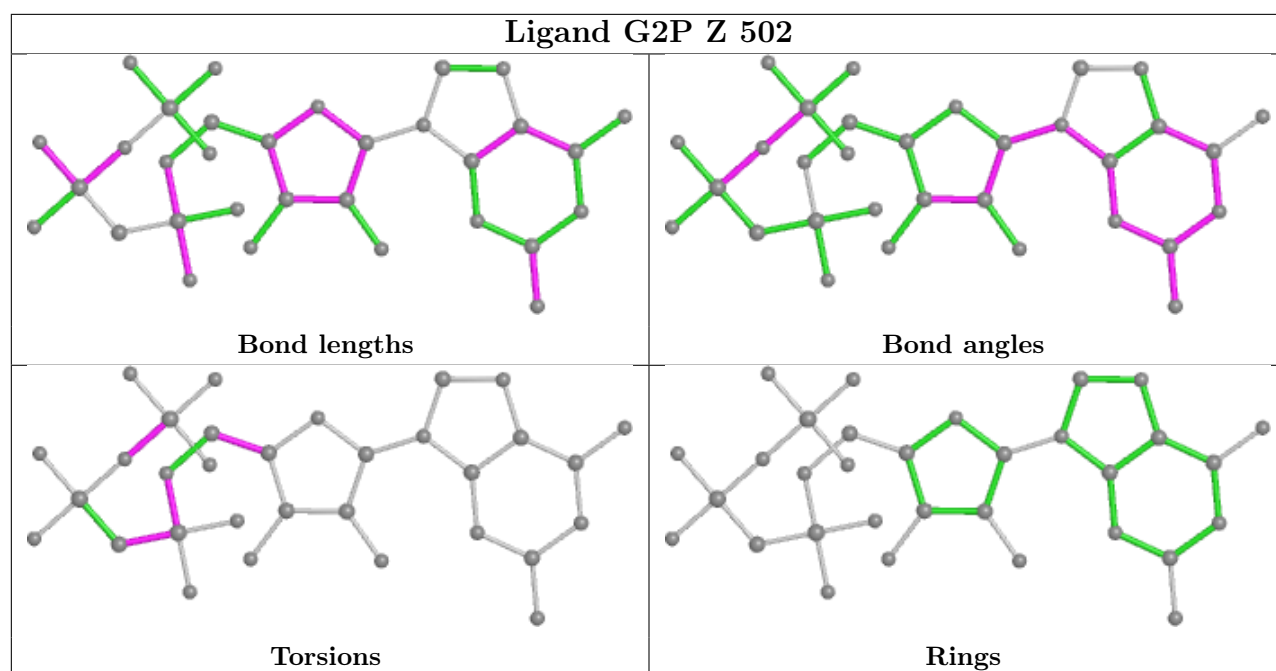


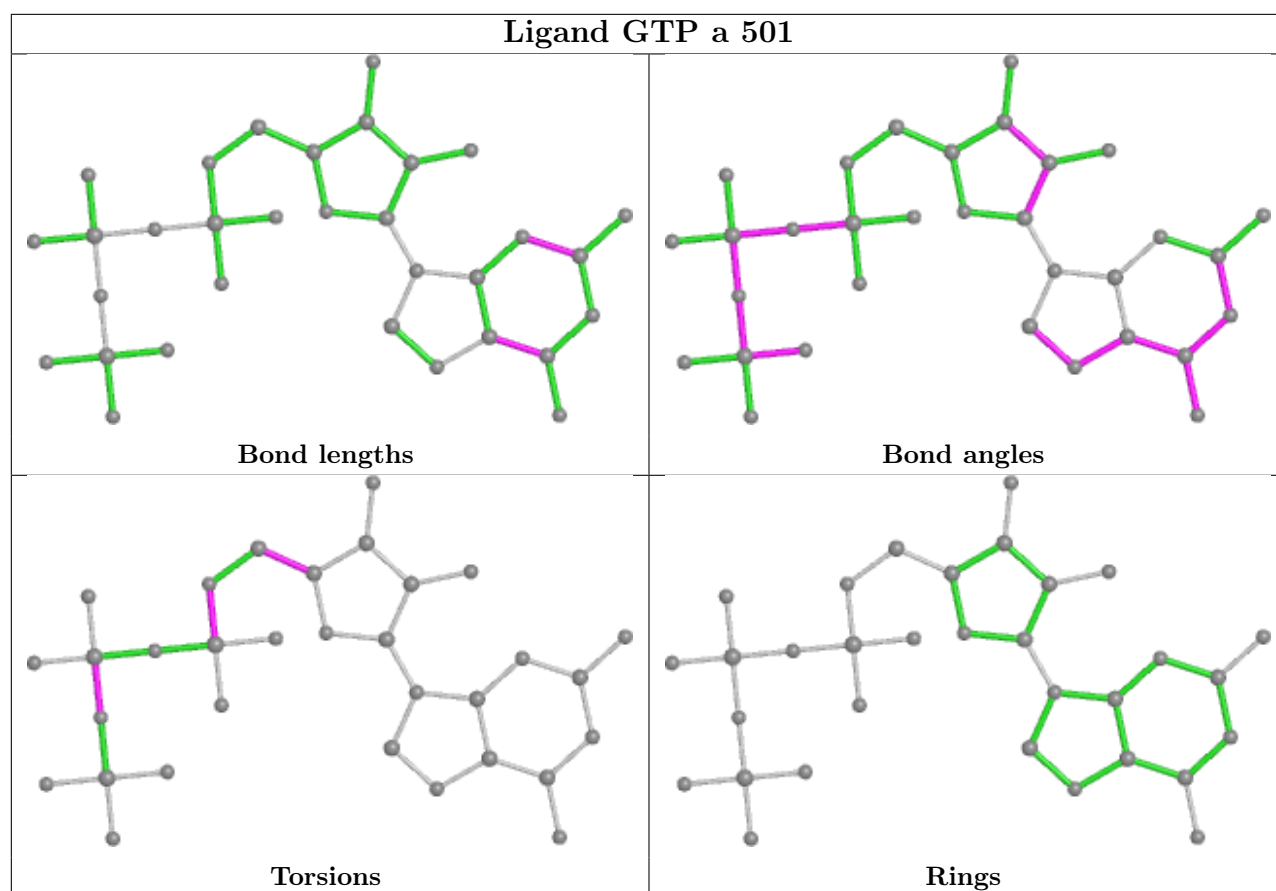
Ligand GTP Z 501



Ligand GTP W 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.