



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 12:29 AM EDT

PDB ID : 8TEY / pdb_00008tey
EMDB ID : EMD-41209
Title : Avian Adeno-associated virus - empty capsid
Authors : Hsi, J.; Mietzsch, M.; Chipman, P.; Afione, S.; Zeher, A.; Huang, R.; Chiorini, J.; McKenna, R.
Deposited on : 2023-07-07
Resolution : 3.06 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

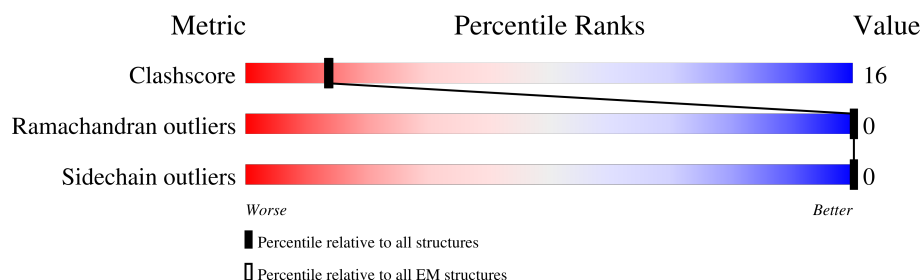
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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.
















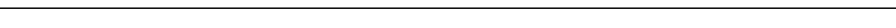











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	535	64% 33% .
1	2	535	65% 32% .
1	3	535	65% 32% .
1	4	535	65% 32% .
1	5	535	64% 33% .
1	6	535	64% 33% .
1	7	535	65% 32% .
1	8	535	64% 33% .














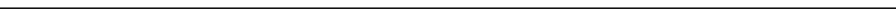











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Mol	Chain	Length	Quality of chain
1	A	535	 64% 33% .
1	B	535	 65% 32% .
1	C	535	 64% 33% .
1	D	535	 64% 33% .
1	E	535	 64% 33% .
1	F	535	 65% 32% .
1	G	535	 64% 33% .
1	H	535	 64% 33% .
1	I	535	 64% 33% .
1	J	535	 64% 33% .
1	K	535	 64% 33% .
1	L	535	 63% 34% .
1	M	535	 65% 32% .
1	N	535	 64% 33% .
1	O	535	 64% 33% .
1	P	535	 64% 33% .
1	Q	535	 64% 33% .
1	R	535	 64% 33% .
1	S	535	 64% 33% .
1	T	535	 64% 33% .
1	U	535	 65% 32% .
1	V	535	 64% 33% .
1	W	535	 64% 33% .
1	X	535	 64% 33% .
1	Y	535	 64% 33% .

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Mol	Chain	Length	Quality of chain
1	Z	535	 64% 33% .
1	a	535	 64% 33% .
1	b	535	 64% 33% .
1	c	535	 65% 32% .
1	d	535	 65% 32% .
1	e	535	 64% 33% .
1	f	535	 64% 33% .
1	g	535	 64% 33% .
1	h	535	 65% 32% .
1	i	535	 64% 33% .
1	j	535	 64% 33% .
1	k	535	 64% 33% .
1	l	535	 64% 33% .
1	m	535	 64% 33% .
1	n	535	 64% 33% .
1	o	535	 64% 33% .
1	p	535	 64% 33% .
1	q	535	 64% 33% .
1	r	535	 64% 33% .
1	s	535	 64% 33% .
1	t	535	 64% 33% .
1	u	535	 64% 33% .
1	v	535	 64% 33% .
1	w	535	 64% 33% .
1	x	535	 64% 33% .

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Mol	Chain	Length	Quality of chain
1	y	535	<div><div></div><div>65%</div><div>32%</div><div></div></div>
1	z	535	<div><div></div><div>63%</div><div>34%</div><div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 251280 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	B	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	C	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	D	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	E	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	F	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	G	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	H	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	I	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	J	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	K	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	L	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	M	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	N	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	O	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	P	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	Q	519	Total 4167	C 2642	N 725	O 786	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	S	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	T	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	U	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	V	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	W	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	X	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	Y	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	Z	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	a	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	b	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	c	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	d	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	e	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	f	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	g	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	h	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	i	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	j	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	k	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	l	519	Total 4167	C 2642	N 725	O 786	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	n	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	o	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	p	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	q	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	r	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	s	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	t	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	u	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	v	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	w	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	x	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	y	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	z	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	1	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	2	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	3	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	4	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	5	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	6	519	Total 4167	C 2642	N 725	O 786	S 14	0	0
1	7	519	Total 4167	C 2642	N 725	O 786	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	SER	PHE	conflict	UNP Q7TG43
A	339	ALA	GLY	conflict	UNP Q7TG43
A	621	LEU	PRO	conflict	UNP Q7TG43
A	622	GLN	THR	conflict	UNP Q7TG43
A	624	PRO	THR	conflict	UNP Q7TG43
A	625	ILE	HIS	conflict	UNP Q7TG43
A	626	TRP	LEU	conflict	UNP Q7TG43
A	644	GLY	ARG	conflict	UNP Q7TG43
B	334	SER	PHE	conflict	UNP Q7TG43
B	339	ALA	GLY	conflict	UNP Q7TG43
B	621	LEU	PRO	conflict	UNP Q7TG43
B	622	GLN	THR	conflict	UNP Q7TG43
B	624	PRO	THR	conflict	UNP Q7TG43
B	625	ILE	HIS	conflict	UNP Q7TG43
B	626	TRP	LEU	conflict	UNP Q7TG43
B	644	GLY	ARG	conflict	UNP Q7TG43
C	334	SER	PHE	conflict	UNP Q7TG43
C	339	ALA	GLY	conflict	UNP Q7TG43
C	621	LEU	PRO	conflict	UNP Q7TG43
C	622	GLN	THR	conflict	UNP Q7TG43
C	624	PRO	THR	conflict	UNP Q7TG43
C	625	ILE	HIS	conflict	UNP Q7TG43
C	626	TRP	LEU	conflict	UNP Q7TG43
C	644	GLY	ARG	conflict	UNP Q7TG43
D	334	SER	PHE	conflict	UNP Q7TG43
D	339	ALA	GLY	conflict	UNP Q7TG43
D	621	LEU	PRO	conflict	UNP Q7TG43
D	622	GLN	THR	conflict	UNP Q7TG43
D	624	PRO	THR	conflict	UNP Q7TG43
D	625	ILE	HIS	conflict	UNP Q7TG43
D	626	TRP	LEU	conflict	UNP Q7TG43
D	644	GLY	ARG	conflict	UNP Q7TG43
E	334	SER	PHE	conflict	UNP Q7TG43
E	339	ALA	GLY	conflict	UNP Q7TG43
E	621	LEU	PRO	conflict	UNP Q7TG43
E	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
E	624	PRO	THR	conflict	UNP Q7TG43
E	625	ILE	HIS	conflict	UNP Q7TG43
E	626	TRP	LEU	conflict	UNP Q7TG43
E	644	GLY	ARG	conflict	UNP Q7TG43
F	334	SER	PHE	conflict	UNP Q7TG43
F	339	ALA	GLY	conflict	UNP Q7TG43
F	621	LEU	PRO	conflict	UNP Q7TG43
F	622	GLN	THR	conflict	UNP Q7TG43
F	624	PRO	THR	conflict	UNP Q7TG43
F	625	ILE	HIS	conflict	UNP Q7TG43
F	626	TRP	LEU	conflict	UNP Q7TG43
F	644	GLY	ARG	conflict	UNP Q7TG43
G	334	SER	PHE	conflict	UNP Q7TG43
G	339	ALA	GLY	conflict	UNP Q7TG43
G	621	LEU	PRO	conflict	UNP Q7TG43
G	622	GLN	THR	conflict	UNP Q7TG43
G	624	PRO	THR	conflict	UNP Q7TG43
G	625	ILE	HIS	conflict	UNP Q7TG43
G	626	TRP	LEU	conflict	UNP Q7TG43
G	644	GLY	ARG	conflict	UNP Q7TG43
H	334	SER	PHE	conflict	UNP Q7TG43
H	339	ALA	GLY	conflict	UNP Q7TG43
H	621	LEU	PRO	conflict	UNP Q7TG43
H	622	GLN	THR	conflict	UNP Q7TG43
H	624	PRO	THR	conflict	UNP Q7TG43
H	625	ILE	HIS	conflict	UNP Q7TG43
H	626	TRP	LEU	conflict	UNP Q7TG43
H	644	GLY	ARG	conflict	UNP Q7TG43
I	334	SER	PHE	conflict	UNP Q7TG43
I	339	ALA	GLY	conflict	UNP Q7TG43
I	621	LEU	PRO	conflict	UNP Q7TG43
I	622	GLN	THR	conflict	UNP Q7TG43
I	624	PRO	THR	conflict	UNP Q7TG43
I	625	ILE	HIS	conflict	UNP Q7TG43
I	626	TRP	LEU	conflict	UNP Q7TG43
I	644	GLY	ARG	conflict	UNP Q7TG43
J	334	SER	PHE	conflict	UNP Q7TG43
J	339	ALA	GLY	conflict	UNP Q7TG43
J	621	LEU	PRO	conflict	UNP Q7TG43
J	622	GLN	THR	conflict	UNP Q7TG43
J	624	PRO	THR	conflict	UNP Q7TG43
J	625	ILE	HIS	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
J	626	TRP	LEU	conflict	UNP Q7TG43
J	644	GLY	ARG	conflict	UNP Q7TG43
K	334	SER	PHE	conflict	UNP Q7TG43
K	339	ALA	GLY	conflict	UNP Q7TG43
K	621	LEU	PRO	conflict	UNP Q7TG43
K	622	GLN	THR	conflict	UNP Q7TG43
K	624	PRO	THR	conflict	UNP Q7TG43
K	625	ILE	HIS	conflict	UNP Q7TG43
K	626	TRP	LEU	conflict	UNP Q7TG43
K	644	GLY	ARG	conflict	UNP Q7TG43
L	334	SER	PHE	conflict	UNP Q7TG43
L	339	ALA	GLY	conflict	UNP Q7TG43
L	621	LEU	PRO	conflict	UNP Q7TG43
L	622	GLN	THR	conflict	UNP Q7TG43
L	624	PRO	THR	conflict	UNP Q7TG43
L	625	ILE	HIS	conflict	UNP Q7TG43
L	626	TRP	LEU	conflict	UNP Q7TG43
L	644	GLY	ARG	conflict	UNP Q7TG43
M	334	SER	PHE	conflict	UNP Q7TG43
M	339	ALA	GLY	conflict	UNP Q7TG43
M	621	LEU	PRO	conflict	UNP Q7TG43
M	622	GLN	THR	conflict	UNP Q7TG43
M	624	PRO	THR	conflict	UNP Q7TG43
M	625	ILE	HIS	conflict	UNP Q7TG43
M	626	TRP	LEU	conflict	UNP Q7TG43
M	644	GLY	ARG	conflict	UNP Q7TG43
N	334	SER	PHE	conflict	UNP Q7TG43
N	339	ALA	GLY	conflict	UNP Q7TG43
N	621	LEU	PRO	conflict	UNP Q7TG43
N	622	GLN	THR	conflict	UNP Q7TG43
N	624	PRO	THR	conflict	UNP Q7TG43
N	625	ILE	HIS	conflict	UNP Q7TG43
N	626	TRP	LEU	conflict	UNP Q7TG43
N	644	GLY	ARG	conflict	UNP Q7TG43
O	334	SER	PHE	conflict	UNP Q7TG43
O	339	ALA	GLY	conflict	UNP Q7TG43
O	621	LEU	PRO	conflict	UNP Q7TG43
O	622	GLN	THR	conflict	UNP Q7TG43
O	624	PRO	THR	conflict	UNP Q7TG43
O	625	ILE	HIS	conflict	UNP Q7TG43
O	626	TRP	LEU	conflict	UNP Q7TG43
O	644	GLY	ARG	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
P	334	SER	PHE	conflict	UNP Q7TG43
P	339	ALA	GLY	conflict	UNP Q7TG43
P	621	LEU	PRO	conflict	UNP Q7TG43
P	622	GLN	THR	conflict	UNP Q7TG43
P	624	PRO	THR	conflict	UNP Q7TG43
P	625	ILE	HIS	conflict	UNP Q7TG43
P	626	TRP	LEU	conflict	UNP Q7TG43
P	644	GLY	ARG	conflict	UNP Q7TG43
Q	334	SER	PHE	conflict	UNP Q7TG43
Q	339	ALA	GLY	conflict	UNP Q7TG43
Q	621	LEU	PRO	conflict	UNP Q7TG43
Q	622	GLN	THR	conflict	UNP Q7TG43
Q	624	PRO	THR	conflict	UNP Q7TG43
Q	625	ILE	HIS	conflict	UNP Q7TG43
Q	626	TRP	LEU	conflict	UNP Q7TG43
Q	644	GLY	ARG	conflict	UNP Q7TG43
R	334	SER	PHE	conflict	UNP Q7TG43
R	339	ALA	GLY	conflict	UNP Q7TG43
R	621	LEU	PRO	conflict	UNP Q7TG43
R	622	GLN	THR	conflict	UNP Q7TG43
R	624	PRO	THR	conflict	UNP Q7TG43
R	625	ILE	HIS	conflict	UNP Q7TG43
R	626	TRP	LEU	conflict	UNP Q7TG43
R	644	GLY	ARG	conflict	UNP Q7TG43
S	334	SER	PHE	conflict	UNP Q7TG43
S	339	ALA	GLY	conflict	UNP Q7TG43
S	621	LEU	PRO	conflict	UNP Q7TG43
S	622	GLN	THR	conflict	UNP Q7TG43
S	624	PRO	THR	conflict	UNP Q7TG43
S	625	ILE	HIS	conflict	UNP Q7TG43
S	626	TRP	LEU	conflict	UNP Q7TG43
S	644	GLY	ARG	conflict	UNP Q7TG43
T	334	SER	PHE	conflict	UNP Q7TG43
T	339	ALA	GLY	conflict	UNP Q7TG43
T	621	LEU	PRO	conflict	UNP Q7TG43
T	622	GLN	THR	conflict	UNP Q7TG43
T	624	PRO	THR	conflict	UNP Q7TG43
T	625	ILE	HIS	conflict	UNP Q7TG43
T	626	TRP	LEU	conflict	UNP Q7TG43
T	644	GLY	ARG	conflict	UNP Q7TG43
U	334	SER	PHE	conflict	UNP Q7TG43
U	339	ALA	GLY	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
U	621	LEU	PRO	conflict	UNP Q7TG43
U	622	GLN	THR	conflict	UNP Q7TG43
U	624	PRO	THR	conflict	UNP Q7TG43
U	625	ILE	HIS	conflict	UNP Q7TG43
U	626	TRP	LEU	conflict	UNP Q7TG43
U	644	GLY	ARG	conflict	UNP Q7TG43
V	334	SER	PHE	conflict	UNP Q7TG43
V	339	ALA	GLY	conflict	UNP Q7TG43
V	621	LEU	PRO	conflict	UNP Q7TG43
V	622	GLN	THR	conflict	UNP Q7TG43
V	624	PRO	THR	conflict	UNP Q7TG43
V	625	ILE	HIS	conflict	UNP Q7TG43
V	626	TRP	LEU	conflict	UNP Q7TG43
V	644	GLY	ARG	conflict	UNP Q7TG43
W	334	SER	PHE	conflict	UNP Q7TG43
W	339	ALA	GLY	conflict	UNP Q7TG43
W	621	LEU	PRO	conflict	UNP Q7TG43
W	622	GLN	THR	conflict	UNP Q7TG43
W	624	PRO	THR	conflict	UNP Q7TG43
W	625	ILE	HIS	conflict	UNP Q7TG43
W	626	TRP	LEU	conflict	UNP Q7TG43
W	644	GLY	ARG	conflict	UNP Q7TG43
X	334	SER	PHE	conflict	UNP Q7TG43
X	339	ALA	GLY	conflict	UNP Q7TG43
X	621	LEU	PRO	conflict	UNP Q7TG43
X	622	GLN	THR	conflict	UNP Q7TG43
X	624	PRO	THR	conflict	UNP Q7TG43
X	625	ILE	HIS	conflict	UNP Q7TG43
X	626	TRP	LEU	conflict	UNP Q7TG43
X	644	GLY	ARG	conflict	UNP Q7TG43
Y	334	SER	PHE	conflict	UNP Q7TG43
Y	339	ALA	GLY	conflict	UNP Q7TG43
Y	621	LEU	PRO	conflict	UNP Q7TG43
Y	622	GLN	THR	conflict	UNP Q7TG43
Y	624	PRO	THR	conflict	UNP Q7TG43
Y	625	ILE	HIS	conflict	UNP Q7TG43
Y	626	TRP	LEU	conflict	UNP Q7TG43
Y	644	GLY	ARG	conflict	UNP Q7TG43
Z	334	SER	PHE	conflict	UNP Q7TG43
Z	339	ALA	GLY	conflict	UNP Q7TG43
Z	621	LEU	PRO	conflict	UNP Q7TG43
Z	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	624	PRO	THR	conflict	UNP Q7TG43
Z	625	ILE	HIS	conflict	UNP Q7TG43
Z	626	TRP	LEU	conflict	UNP Q7TG43
Z	644	GLY	ARG	conflict	UNP Q7TG43
a	334	SER	PHE	conflict	UNP Q7TG43
a	339	ALA	GLY	conflict	UNP Q7TG43
a	621	LEU	PRO	conflict	UNP Q7TG43
a	622	GLN	THR	conflict	UNP Q7TG43
a	624	PRO	THR	conflict	UNP Q7TG43
a	625	ILE	HIS	conflict	UNP Q7TG43
a	626	TRP	LEU	conflict	UNP Q7TG43
a	644	GLY	ARG	conflict	UNP Q7TG43
b	334	SER	PHE	conflict	UNP Q7TG43
b	339	ALA	GLY	conflict	UNP Q7TG43
b	621	LEU	PRO	conflict	UNP Q7TG43
b	622	GLN	THR	conflict	UNP Q7TG43
b	624	PRO	THR	conflict	UNP Q7TG43
b	625	ILE	HIS	conflict	UNP Q7TG43
b	626	TRP	LEU	conflict	UNP Q7TG43
b	644	GLY	ARG	conflict	UNP Q7TG43
c	334	SER	PHE	conflict	UNP Q7TG43
c	339	ALA	GLY	conflict	UNP Q7TG43
c	621	LEU	PRO	conflict	UNP Q7TG43
c	622	GLN	THR	conflict	UNP Q7TG43
c	624	PRO	THR	conflict	UNP Q7TG43
c	625	ILE	HIS	conflict	UNP Q7TG43
c	626	TRP	LEU	conflict	UNP Q7TG43
c	644	GLY	ARG	conflict	UNP Q7TG43
d	334	SER	PHE	conflict	UNP Q7TG43
d	339	ALA	GLY	conflict	UNP Q7TG43
d	621	LEU	PRO	conflict	UNP Q7TG43
d	622	GLN	THR	conflict	UNP Q7TG43
d	624	PRO	THR	conflict	UNP Q7TG43
d	625	ILE	HIS	conflict	UNP Q7TG43
d	626	TRP	LEU	conflict	UNP Q7TG43
d	644	GLY	ARG	conflict	UNP Q7TG43
e	334	SER	PHE	conflict	UNP Q7TG43
e	339	ALA	GLY	conflict	UNP Q7TG43
e	621	LEU	PRO	conflict	UNP Q7TG43
e	622	GLN	THR	conflict	UNP Q7TG43
e	624	PRO	THR	conflict	UNP Q7TG43
e	625	ILE	HIS	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
e	626	TRP	LEU	conflict	UNP Q7TG43
e	644	GLY	ARG	conflict	UNP Q7TG43
f	334	SER	PHE	conflict	UNP Q7TG43
f	339	ALA	GLY	conflict	UNP Q7TG43
f	621	LEU	PRO	conflict	UNP Q7TG43
f	622	GLN	THR	conflict	UNP Q7TG43
f	624	PRO	THR	conflict	UNP Q7TG43
f	625	ILE	HIS	conflict	UNP Q7TG43
f	626	TRP	LEU	conflict	UNP Q7TG43
f	644	GLY	ARG	conflict	UNP Q7TG43
g	334	SER	PHE	conflict	UNP Q7TG43
g	339	ALA	GLY	conflict	UNP Q7TG43
g	621	LEU	PRO	conflict	UNP Q7TG43
g	622	GLN	THR	conflict	UNP Q7TG43
g	624	PRO	THR	conflict	UNP Q7TG43
g	625	ILE	HIS	conflict	UNP Q7TG43
g	626	TRP	LEU	conflict	UNP Q7TG43
g	644	GLY	ARG	conflict	UNP Q7TG43
h	334	SER	PHE	conflict	UNP Q7TG43
h	339	ALA	GLY	conflict	UNP Q7TG43
h	621	LEU	PRO	conflict	UNP Q7TG43
h	622	GLN	THR	conflict	UNP Q7TG43
h	624	PRO	THR	conflict	UNP Q7TG43
h	625	ILE	HIS	conflict	UNP Q7TG43
h	626	TRP	LEU	conflict	UNP Q7TG43
h	644	GLY	ARG	conflict	UNP Q7TG43
i	334	SER	PHE	conflict	UNP Q7TG43
i	339	ALA	GLY	conflict	UNP Q7TG43
i	621	LEU	PRO	conflict	UNP Q7TG43
i	622	GLN	THR	conflict	UNP Q7TG43
i	624	PRO	THR	conflict	UNP Q7TG43
i	625	ILE	HIS	conflict	UNP Q7TG43
i	626	TRP	LEU	conflict	UNP Q7TG43
i	644	GLY	ARG	conflict	UNP Q7TG43
j	334	SER	PHE	conflict	UNP Q7TG43
j	339	ALA	GLY	conflict	UNP Q7TG43
j	621	LEU	PRO	conflict	UNP Q7TG43
j	622	GLN	THR	conflict	UNP Q7TG43
j	624	PRO	THR	conflict	UNP Q7TG43
j	625	ILE	HIS	conflict	UNP Q7TG43
j	626	TRP	LEU	conflict	UNP Q7TG43
j	644	GLY	ARG	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
k	334	SER	PHE	conflict	UNP Q7TG43
k	339	ALA	GLY	conflict	UNP Q7TG43
k	621	LEU	PRO	conflict	UNP Q7TG43
k	622	GLN	THR	conflict	UNP Q7TG43
k	624	PRO	THR	conflict	UNP Q7TG43
k	625	ILE	HIS	conflict	UNP Q7TG43
k	626	TRP	LEU	conflict	UNP Q7TG43
k	644	GLY	ARG	conflict	UNP Q7TG43
l	334	SER	PHE	conflict	UNP Q7TG43
l	339	ALA	GLY	conflict	UNP Q7TG43
l	621	LEU	PRO	conflict	UNP Q7TG43
l	622	GLN	THR	conflict	UNP Q7TG43
l	624	PRO	THR	conflict	UNP Q7TG43
l	625	ILE	HIS	conflict	UNP Q7TG43
l	626	TRP	LEU	conflict	UNP Q7TG43
l	644	GLY	ARG	conflict	UNP Q7TG43
m	334	SER	PHE	conflict	UNP Q7TG43
m	339	ALA	GLY	conflict	UNP Q7TG43
m	621	LEU	PRO	conflict	UNP Q7TG43
m	622	GLN	THR	conflict	UNP Q7TG43
m	624	PRO	THR	conflict	UNP Q7TG43
m	625	ILE	HIS	conflict	UNP Q7TG43
m	626	TRP	LEU	conflict	UNP Q7TG43
m	644	GLY	ARG	conflict	UNP Q7TG43
n	334	SER	PHE	conflict	UNP Q7TG43
n	339	ALA	GLY	conflict	UNP Q7TG43
n	621	LEU	PRO	conflict	UNP Q7TG43
n	622	GLN	THR	conflict	UNP Q7TG43
n	624	PRO	THR	conflict	UNP Q7TG43
n	625	ILE	HIS	conflict	UNP Q7TG43
n	626	TRP	LEU	conflict	UNP Q7TG43
n	644	GLY	ARG	conflict	UNP Q7TG43
o	334	SER	PHE	conflict	UNP Q7TG43
o	339	ALA	GLY	conflict	UNP Q7TG43
o	621	LEU	PRO	conflict	UNP Q7TG43
o	622	GLN	THR	conflict	UNP Q7TG43
o	624	PRO	THR	conflict	UNP Q7TG43
o	625	ILE	HIS	conflict	UNP Q7TG43
o	626	TRP	LEU	conflict	UNP Q7TG43
o	644	GLY	ARG	conflict	UNP Q7TG43
p	334	SER	PHE	conflict	UNP Q7TG43
p	339	ALA	GLY	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
p	621	LEU	PRO	conflict	UNP Q7TG43
p	622	GLN	THR	conflict	UNP Q7TG43
p	624	PRO	THR	conflict	UNP Q7TG43
p	625	ILE	HIS	conflict	UNP Q7TG43
p	626	TRP	LEU	conflict	UNP Q7TG43
p	644	GLY	ARG	conflict	UNP Q7TG43
q	334	SER	PHE	conflict	UNP Q7TG43
q	339	ALA	GLY	conflict	UNP Q7TG43
q	621	LEU	PRO	conflict	UNP Q7TG43
q	622	GLN	THR	conflict	UNP Q7TG43
q	624	PRO	THR	conflict	UNP Q7TG43
q	625	ILE	HIS	conflict	UNP Q7TG43
q	626	TRP	LEU	conflict	UNP Q7TG43
q	644	GLY	ARG	conflict	UNP Q7TG43
r	334	SER	PHE	conflict	UNP Q7TG43
r	339	ALA	GLY	conflict	UNP Q7TG43
r	621	LEU	PRO	conflict	UNP Q7TG43
r	622	GLN	THR	conflict	UNP Q7TG43
r	624	PRO	THR	conflict	UNP Q7TG43
r	625	ILE	HIS	conflict	UNP Q7TG43
r	626	TRP	LEU	conflict	UNP Q7TG43
r	644	GLY	ARG	conflict	UNP Q7TG43
s	334	SER	PHE	conflict	UNP Q7TG43
s	339	ALA	GLY	conflict	UNP Q7TG43
s	621	LEU	PRO	conflict	UNP Q7TG43
s	622	GLN	THR	conflict	UNP Q7TG43
s	624	PRO	THR	conflict	UNP Q7TG43
s	625	ILE	HIS	conflict	UNP Q7TG43
s	626	TRP	LEU	conflict	UNP Q7TG43
s	644	GLY	ARG	conflict	UNP Q7TG43
t	334	SER	PHE	conflict	UNP Q7TG43
t	339	ALA	GLY	conflict	UNP Q7TG43
t	621	LEU	PRO	conflict	UNP Q7TG43
t	622	GLN	THR	conflict	UNP Q7TG43
t	624	PRO	THR	conflict	UNP Q7TG43
t	625	ILE	HIS	conflict	UNP Q7TG43
t	626	TRP	LEU	conflict	UNP Q7TG43
t	644	GLY	ARG	conflict	UNP Q7TG43
u	334	SER	PHE	conflict	UNP Q7TG43
u	339	ALA	GLY	conflict	UNP Q7TG43
u	621	LEU	PRO	conflict	UNP Q7TG43
u	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
u	624	PRO	THR	conflict	UNP Q7TG43
u	625	ILE	HIS	conflict	UNP Q7TG43
u	626	TRP	LEU	conflict	UNP Q7TG43
u	644	GLY	ARG	conflict	UNP Q7TG43
v	334	SER	PHE	conflict	UNP Q7TG43
v	339	ALA	GLY	conflict	UNP Q7TG43
v	621	LEU	PRO	conflict	UNP Q7TG43
v	622	GLN	THR	conflict	UNP Q7TG43
v	624	PRO	THR	conflict	UNP Q7TG43
v	625	ILE	HIS	conflict	UNP Q7TG43
v	626	TRP	LEU	conflict	UNP Q7TG43
v	644	GLY	ARG	conflict	UNP Q7TG43
w	334	SER	PHE	conflict	UNP Q7TG43
w	339	ALA	GLY	conflict	UNP Q7TG43
w	621	LEU	PRO	conflict	UNP Q7TG43
w	622	GLN	THR	conflict	UNP Q7TG43
w	624	PRO	THR	conflict	UNP Q7TG43
w	625	ILE	HIS	conflict	UNP Q7TG43
w	626	TRP	LEU	conflict	UNP Q7TG43
w	644	GLY	ARG	conflict	UNP Q7TG43
x	334	SER	PHE	conflict	UNP Q7TG43
x	339	ALA	GLY	conflict	UNP Q7TG43
x	621	LEU	PRO	conflict	UNP Q7TG43
x	622	GLN	THR	conflict	UNP Q7TG43
x	624	PRO	THR	conflict	UNP Q7TG43
x	625	ILE	HIS	conflict	UNP Q7TG43
x	626	TRP	LEU	conflict	UNP Q7TG43
x	644	GLY	ARG	conflict	UNP Q7TG43
y	334	SER	PHE	conflict	UNP Q7TG43
y	339	ALA	GLY	conflict	UNP Q7TG43
y	621	LEU	PRO	conflict	UNP Q7TG43
y	622	GLN	THR	conflict	UNP Q7TG43
y	624	PRO	THR	conflict	UNP Q7TG43
y	625	ILE	HIS	conflict	UNP Q7TG43
y	626	TRP	LEU	conflict	UNP Q7TG43
y	644	GLY	ARG	conflict	UNP Q7TG43
z	334	SER	PHE	conflict	UNP Q7TG43
z	339	ALA	GLY	conflict	UNP Q7TG43
z	621	LEU	PRO	conflict	UNP Q7TG43
z	622	GLN	THR	conflict	UNP Q7TG43
z	624	PRO	THR	conflict	UNP Q7TG43
z	625	ILE	HIS	conflict	UNP Q7TG43

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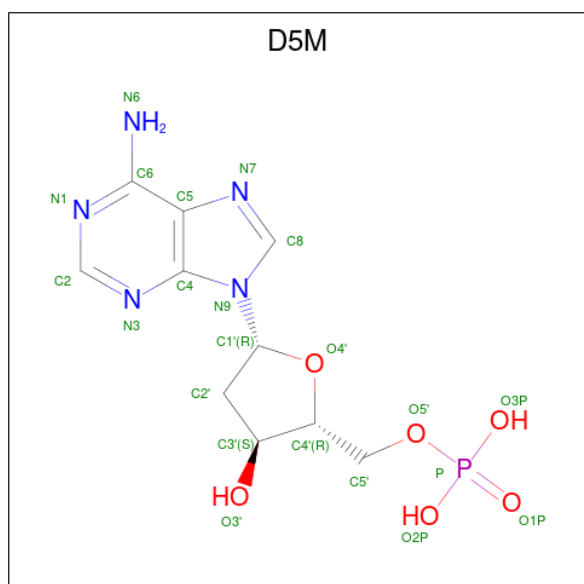
Chain	Residue	Modelled	Actual	Comment	Reference
z	626	TRP	LEU	conflict	UNP Q7TG43
z	644	GLY	ARG	conflict	UNP Q7TG43
1	334	SER	PHE	conflict	UNP Q7TG43
1	339	ALA	GLY	conflict	UNP Q7TG43
1	621	LEU	PRO	conflict	UNP Q7TG43
1	622	GLN	THR	conflict	UNP Q7TG43
1	624	PRO	THR	conflict	UNP Q7TG43
1	625	ILE	HIS	conflict	UNP Q7TG43
1	626	TRP	LEU	conflict	UNP Q7TG43
1	644	GLY	ARG	conflict	UNP Q7TG43
2	334	SER	PHE	conflict	UNP Q7TG43
2	339	ALA	GLY	conflict	UNP Q7TG43
2	621	LEU	PRO	conflict	UNP Q7TG43
2	622	GLN	THR	conflict	UNP Q7TG43
2	624	PRO	THR	conflict	UNP Q7TG43
2	625	ILE	HIS	conflict	UNP Q7TG43
2	626	TRP	LEU	conflict	UNP Q7TG43
2	644	GLY	ARG	conflict	UNP Q7TG43
3	334	SER	PHE	conflict	UNP Q7TG43
3	339	ALA	GLY	conflict	UNP Q7TG43
3	621	LEU	PRO	conflict	UNP Q7TG43
3	622	GLN	THR	conflict	UNP Q7TG43
3	624	PRO	THR	conflict	UNP Q7TG43
3	625	ILE	HIS	conflict	UNP Q7TG43
3	626	TRP	LEU	conflict	UNP Q7TG43
3	644	GLY	ARG	conflict	UNP Q7TG43
4	334	SER	PHE	conflict	UNP Q7TG43
4	339	ALA	GLY	conflict	UNP Q7TG43
4	621	LEU	PRO	conflict	UNP Q7TG43
4	622	GLN	THR	conflict	UNP Q7TG43
4	624	PRO	THR	conflict	UNP Q7TG43
4	625	ILE	HIS	conflict	UNP Q7TG43
4	626	TRP	LEU	conflict	UNP Q7TG43
4	644	GLY	ARG	conflict	UNP Q7TG43
5	334	SER	PHE	conflict	UNP Q7TG43
5	339	ALA	GLY	conflict	UNP Q7TG43
5	621	LEU	PRO	conflict	UNP Q7TG43
5	622	GLN	THR	conflict	UNP Q7TG43
5	624	PRO	THR	conflict	UNP Q7TG43
5	625	ILE	HIS	conflict	UNP Q7TG43
5	626	TRP	LEU	conflict	UNP Q7TG43
5	644	GLY	ARG	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
6	334	SER	PHE	conflict	UNP Q7TG43
6	339	ALA	GLY	conflict	UNP Q7TG43
6	621	LEU	PRO	conflict	UNP Q7TG43
6	622	GLN	THR	conflict	UNP Q7TG43
6	624	PRO	THR	conflict	UNP Q7TG43
6	625	ILE	HIS	conflict	UNP Q7TG43
6	626	TRP	LEU	conflict	UNP Q7TG43
6	644	GLY	ARG	conflict	UNP Q7TG43
7	334	SER	PHE	conflict	UNP Q7TG43
7	339	ALA	GLY	conflict	UNP Q7TG43
7	621	LEU	PRO	conflict	UNP Q7TG43
7	622	GLN	THR	conflict	UNP Q7TG43
7	624	PRO	THR	conflict	UNP Q7TG43
7	625	ILE	HIS	conflict	UNP Q7TG43
7	626	TRP	LEU	conflict	UNP Q7TG43
7	644	GLY	ARG	conflict	UNP Q7TG43
8	334	SER	PHE	conflict	UNP Q7TG43
8	339	ALA	GLY	conflict	UNP Q7TG43
8	621	LEU	PRO	conflict	UNP Q7TG43
8	622	GLN	THR	conflict	UNP Q7TG43
8	624	PRO	THR	conflict	UNP Q7TG43
8	625	ILE	HIS	conflict	UNP Q7TG43
8	626	TRP	LEU	conflict	UNP Q7TG43
8	644	GLY	ARG	conflict	UNP Q7TG43

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula: $C_{10}H_{14}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 21	C 10	N 5	O 5	P 1	0
2	B	1	Total 21	C 10	N 5	O 5	P 1	0
2	C	1	Total 21	C 10	N 5	O 5	P 1	0
2	D	1	Total 21	C 10	N 5	O 5	P 1	0
2	E	1	Total 21	C 10	N 5	O 5	P 1	0
2	F	1	Total 21	C 10	N 5	O 5	P 1	0
2	G	1	Total 21	C 10	N 5	O 5	P 1	0
2	H	1	Total 21	C 10	N 5	O 5	P 1	0
2	I	1	Total 21	C 10	N 5	O 5	P 1	0
2	J	1	Total 21	C 10	N 5	O 5	P 1	0
2	K	1	Total 21	C 10	N 5	O 5	P 1	0
2	L	1	Total 21	C 10	N 5	O 5	P 1	0
2	M	1	Total 21	C 10	N 5	O 5	P 1	0
2	N	1	Total 21	C 10	N 5	O 5	P 1	0
2	O	1	Total 21	C 10	N 5	O 5	P 1	0
2	P	1	Total 21	C 10	N 5	O 5	P 1	0
2	Q	1	Total 21	C 10	N 5	O 5	P 1	0
2	R	1	Total 21	C 10	N 5	O 5	P 1	0
2	S	1	Total 21	C 10	N 5	O 5	P 1	0
2	T	1	Total 21	C 10	N 5	O 5	P 1	0
2	U	1	Total 21	C 10	N 5	O 5	P 1	0
2	V	1	Total 21	C 10	N 5	O 5	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
2	W	1	Total 21	C 10	N 5	O 5	P 1	0
2	X	1	Total 21	C 10	N 5	O 5	P 1	0
2	Y	1	Total 21	C 10	N 5	O 5	P 1	0
2	Z	1	Total 21	C 10	N 5	O 5	P 1	0
2	a	1	Total 21	C 10	N 5	O 5	P 1	0
2	b	1	Total 21	C 10	N 5	O 5	P 1	0
2	c	1	Total 21	C 10	N 5	O 5	P 1	0
2	d	1	Total 21	C 10	N 5	O 5	P 1	0
2	e	1	Total 21	C 10	N 5	O 5	P 1	0
2	f	1	Total 21	C 10	N 5	O 5	P 1	0
2	g	1	Total 21	C 10	N 5	O 5	P 1	0
2	h	1	Total 21	C 10	N 5	O 5	P 1	0
2	i	1	Total 21	C 10	N 5	O 5	P 1	0
2	j	1	Total 21	C 10	N 5	O 5	P 1	0
2	k	1	Total 21	C 10	N 5	O 5	P 1	0
2	l	1	Total 21	C 10	N 5	O 5	P 1	0
2	m	1	Total 21	C 10	N 5	O 5	P 1	0
2	n	1	Total 21	C 10	N 5	O 5	P 1	0
2	o	1	Total 21	C 10	N 5	O 5	P 1	0
2	p	1	Total 21	C 10	N 5	O 5	P 1	0
2	q	1	Total 21	C 10	N 5	O 5	P 1	0

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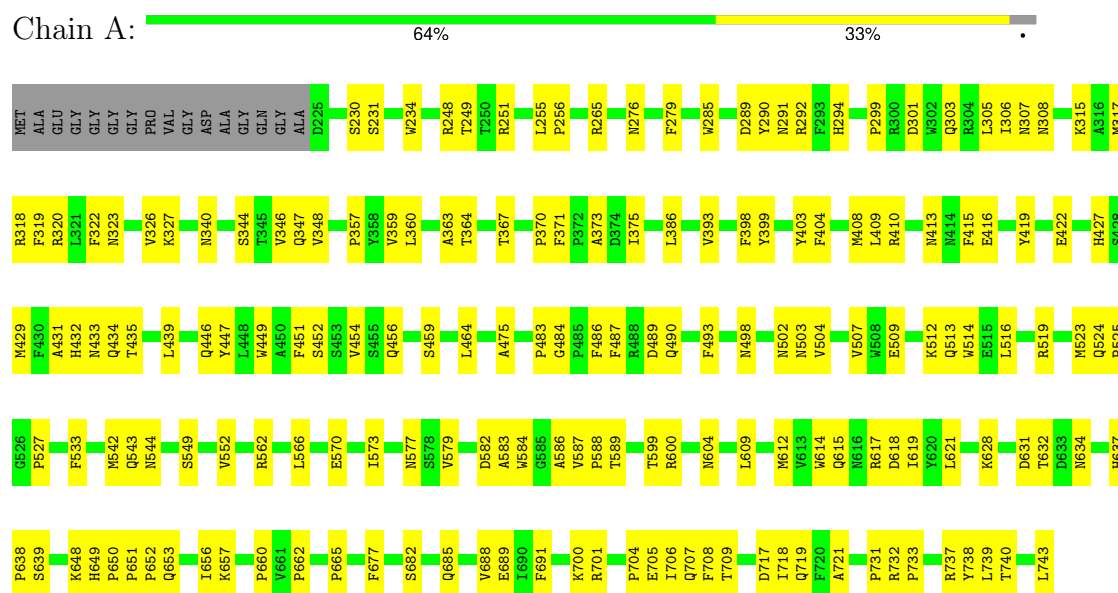
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Mol	Chain	Residues	Atoms					AltConf
2	r	1	Total 21	C 10	N 5	O 5	P 1	0
2	s	1	Total 21	C 10	N 5	O 5	P 1	0
2	t	1	Total 21	C 10	N 5	O 5	P 1	0
2	u	1	Total 21	C 10	N 5	O 5	P 1	0
2	v	1	Total 21	C 10	N 5	O 5	P 1	0
2	w	1	Total 21	C 10	N 5	O 5	P 1	0
2	x	1	Total 21	C 10	N 5	O 5	P 1	0
2	y	1	Total 21	C 10	N 5	O 5	P 1	0
2	z	1	Total 21	C 10	N 5	O 5	P 1	0
2	1	1	Total 21	C 10	N 5	O 5	P 1	0
2	2	1	Total 21	C 10	N 5	O 5	P 1	0
2	3	1	Total 21	C 10	N 5	O 5	P 1	0
2	4	1	Total 21	C 10	N 5	O 5	P 1	0
2	5	1	Total 21	C 10	N 5	O 5	P 1	0
2	6	1	Total 21	C 10	N 5	O 5	P 1	0
2	7	1	Total 21	C 10	N 5	O 5	P 1	0
2	8	1	Total 21	C 10	N 5	O 5	P 1	0

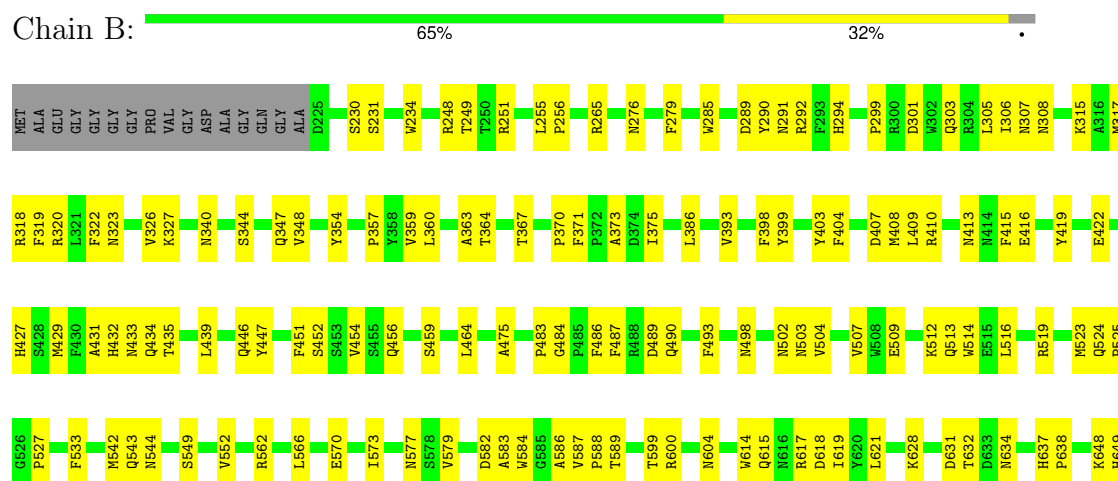
3 Residue-property plots

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

• Molecule 1: Capsid protein



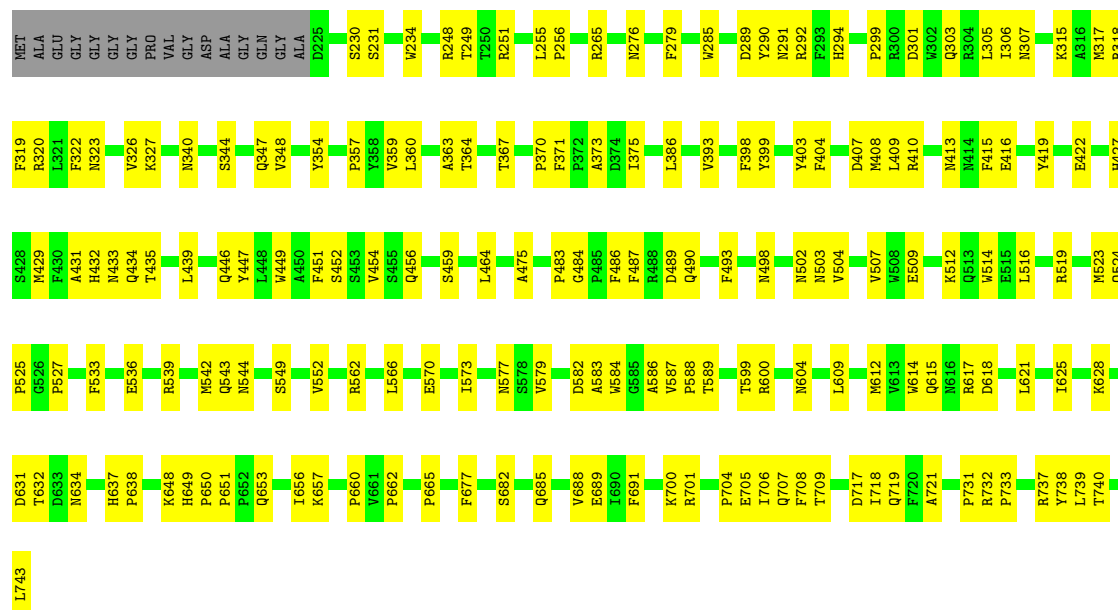
• Molecule 1: Capsid protein





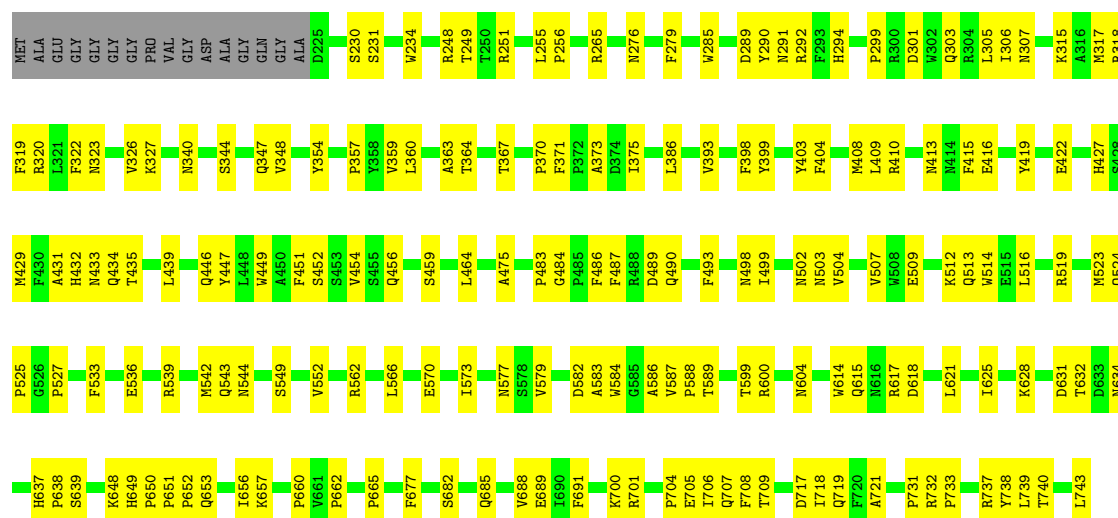
- Molecule 1: Capsid protein

Chain C: 64% 33%



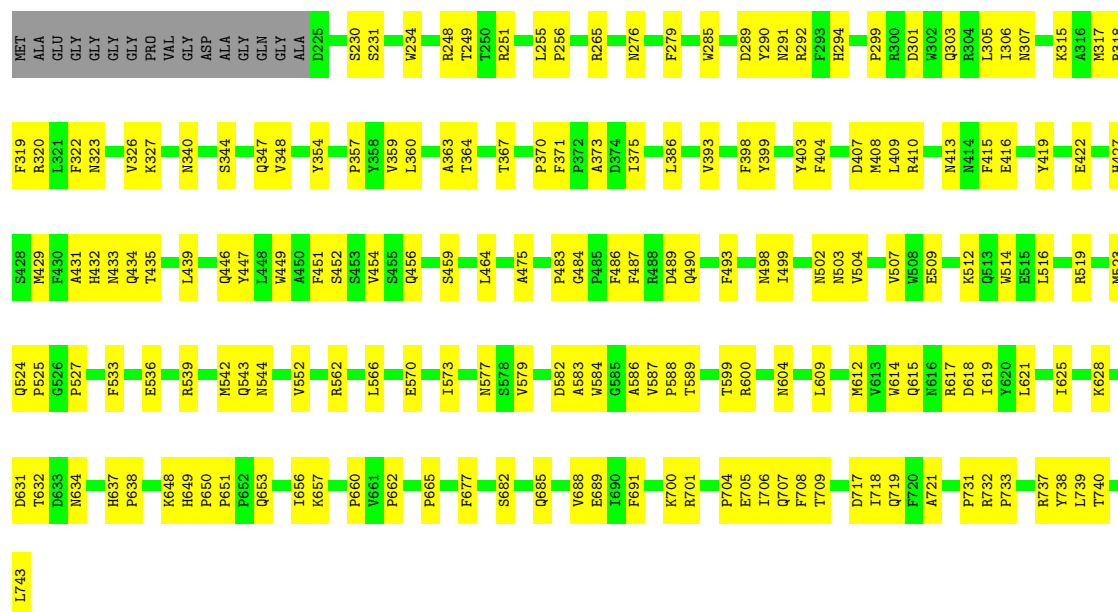
- Molecule 1: Capsid protein

Chain D: 64% 33%

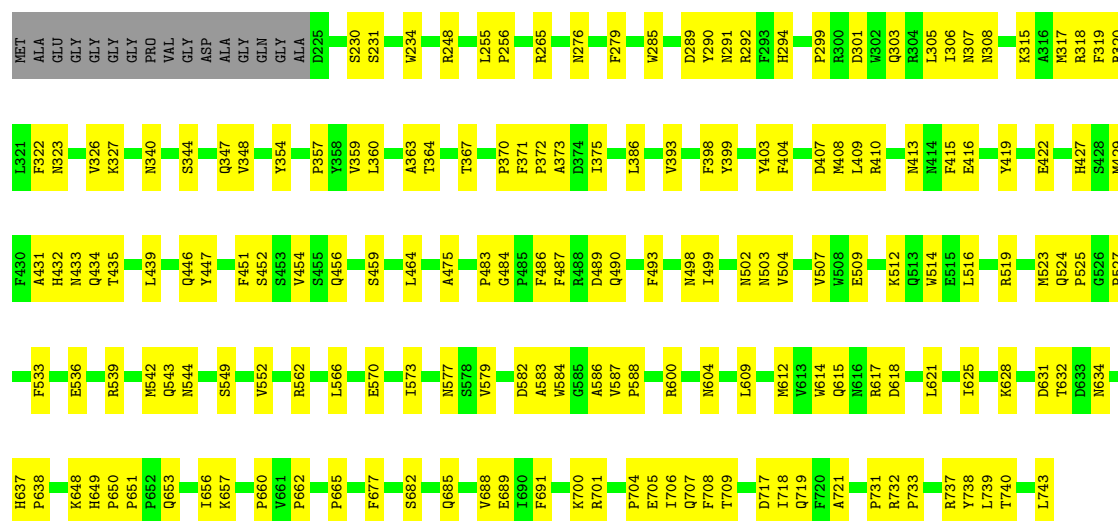


- Molecule 1: Capsid protein

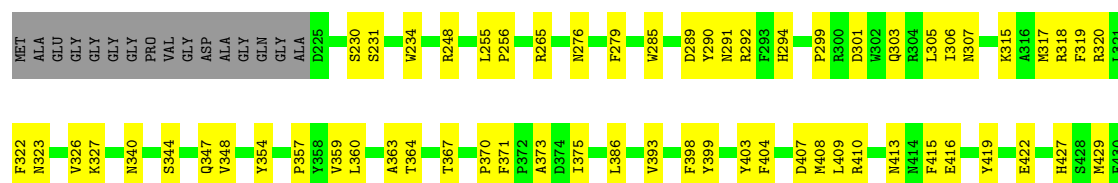
Chain E: 64% 33%

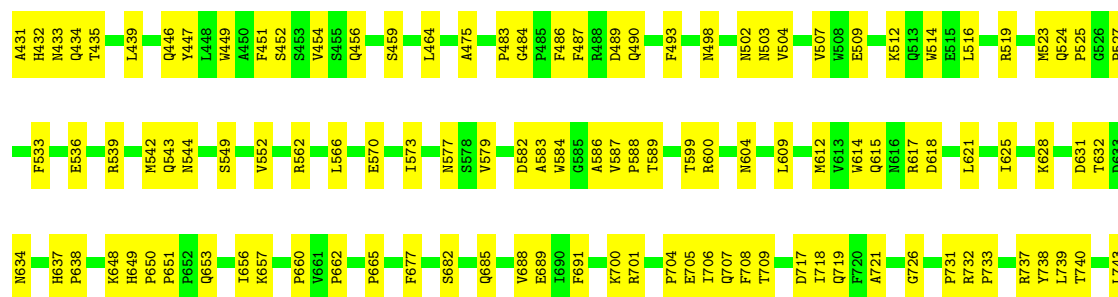


- Molecule 1: Capsid protein



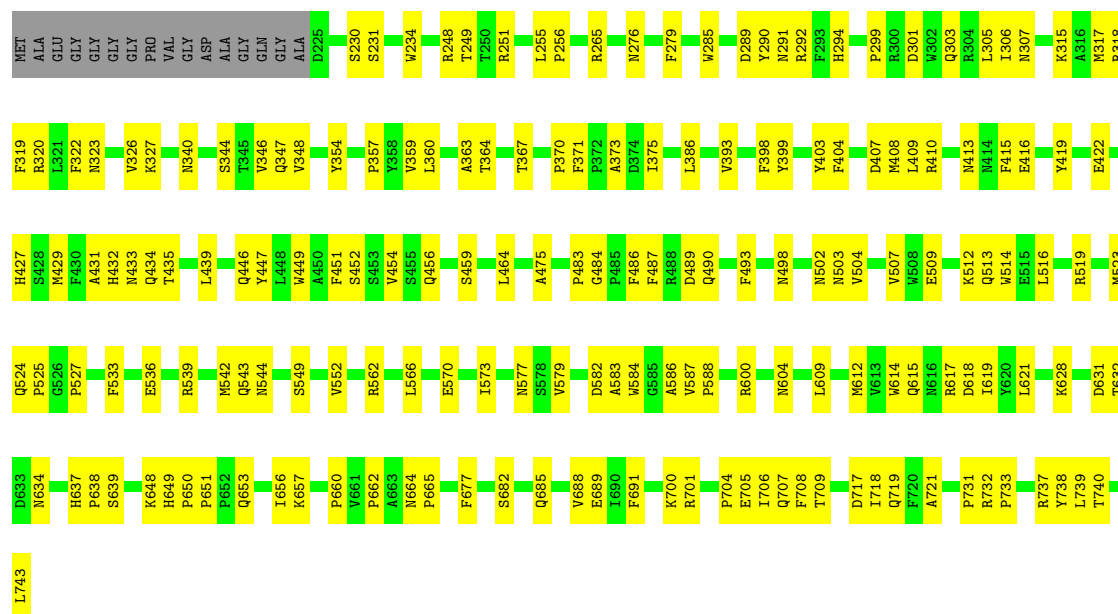
- Molecule 1: Capsid protein





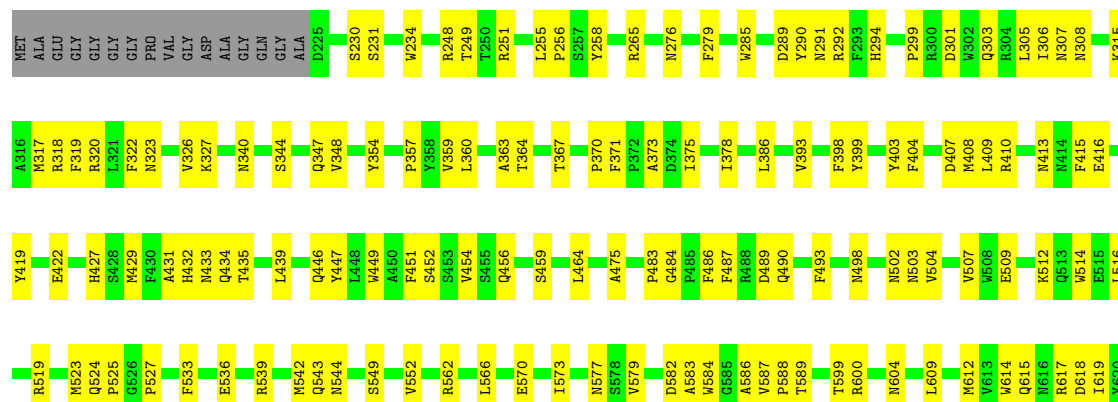
• Molecule 1: Capsid protein

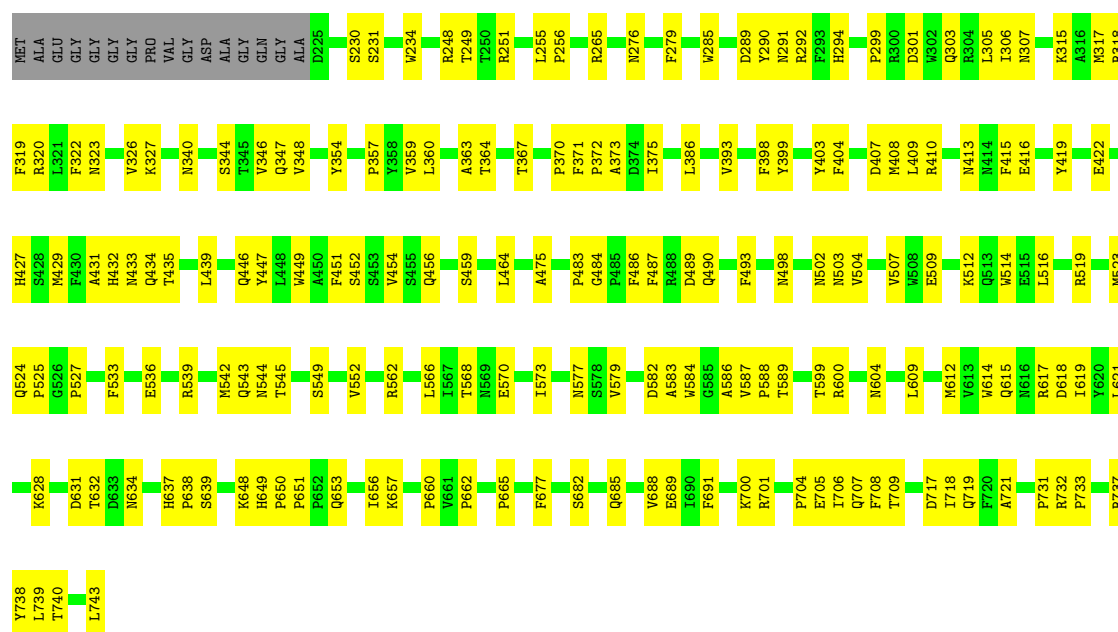
Chain H: 64% 33%



• Molecule 1: Capsid protein

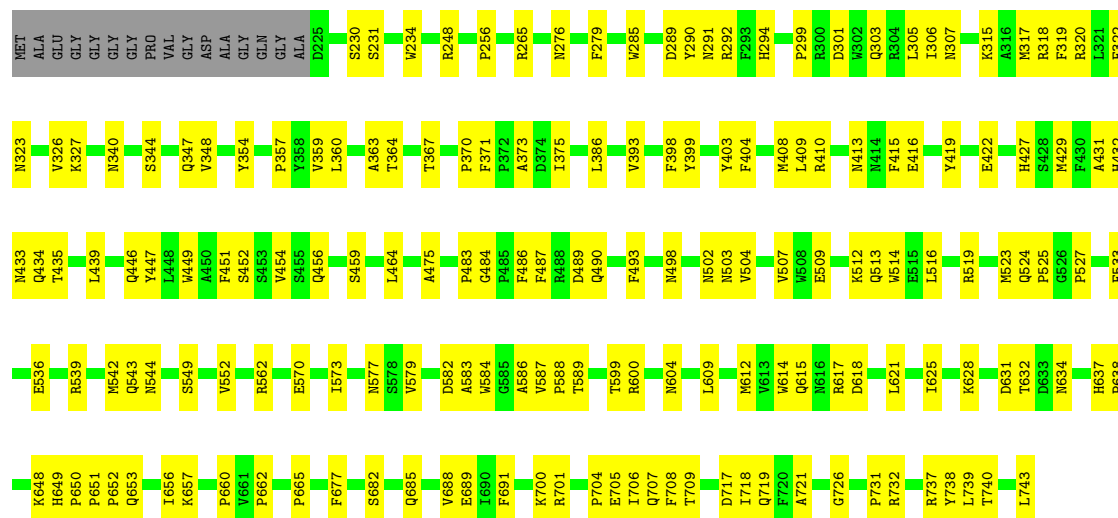
Chain I: 64% 33%





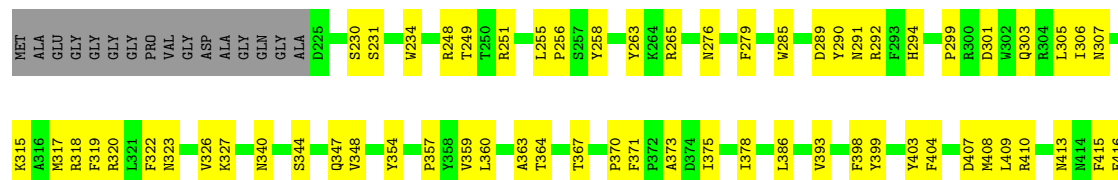
• Molecule 1: Capsid protein

Chain M: 65% 32%



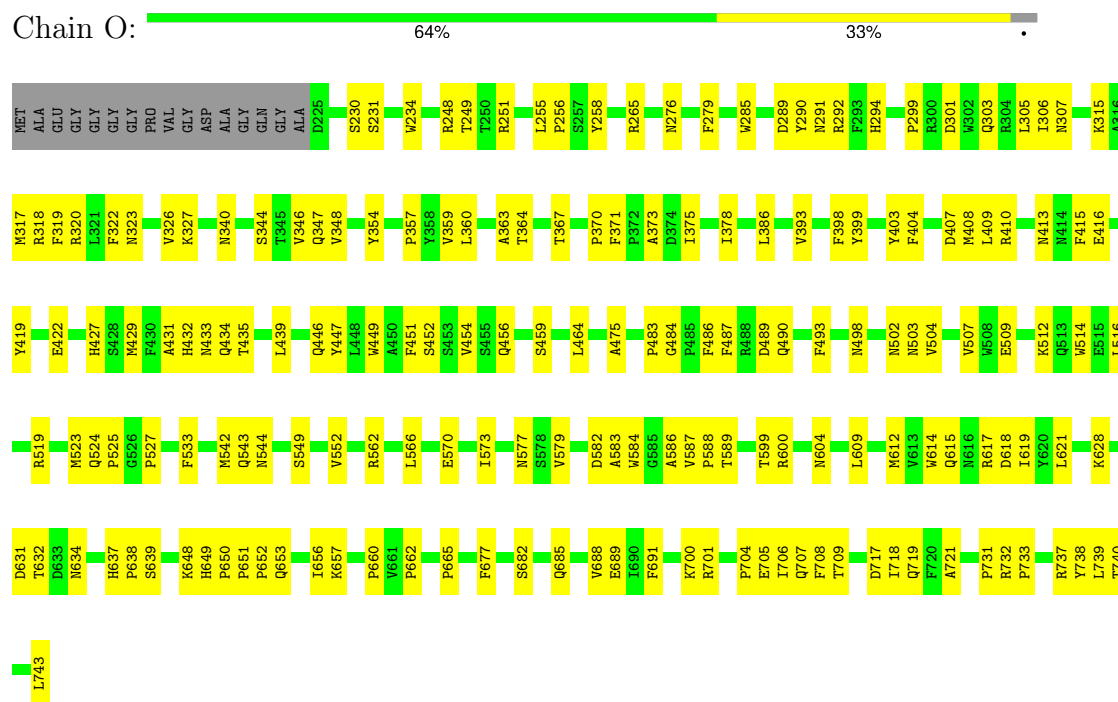
• Molecule 1: Capsid protein

Chain N: 64% 33%

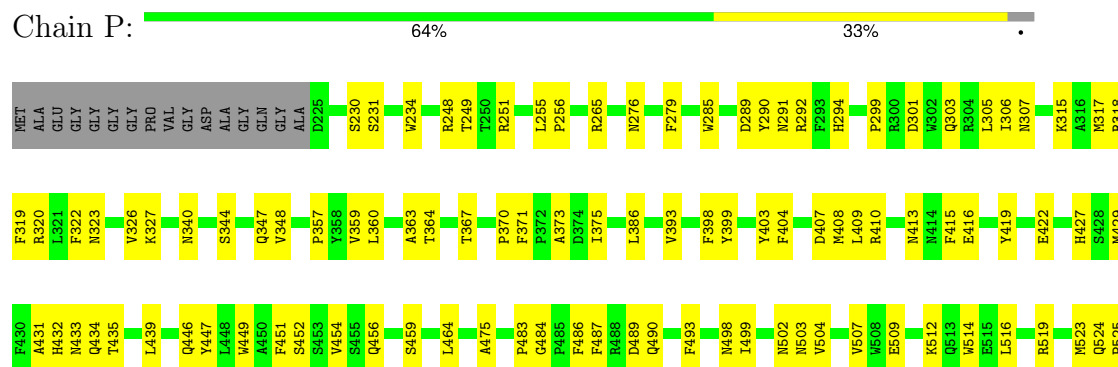


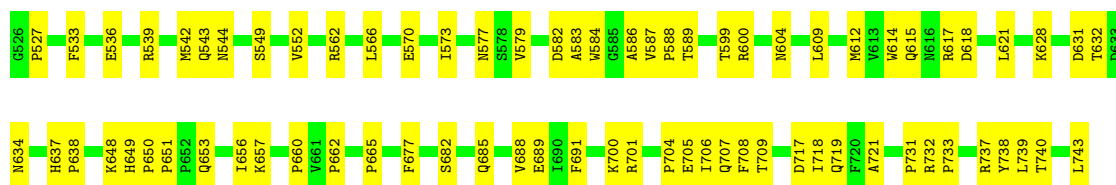


- Molecule 1: Capsid protein



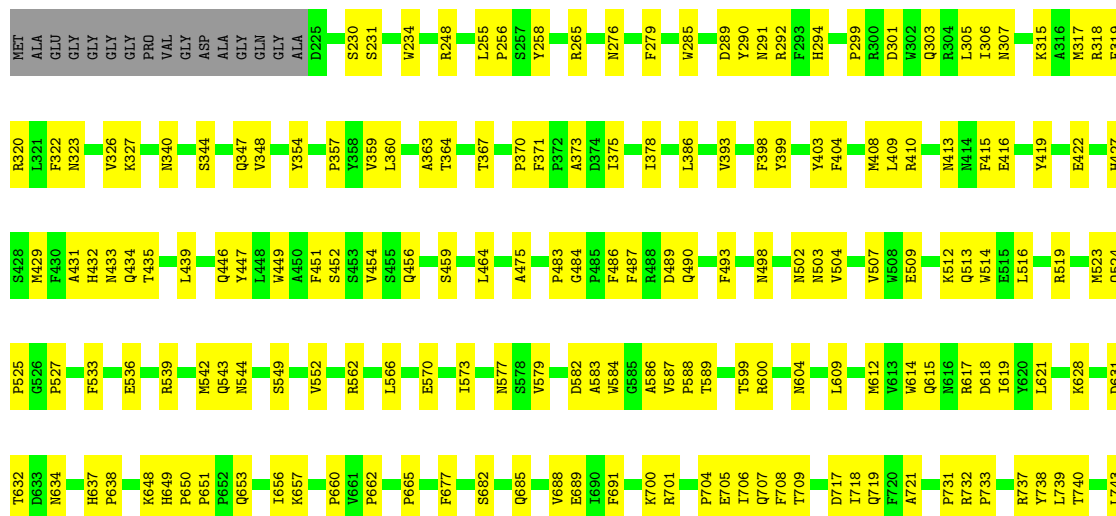
- Molecule 1: Capsid protein





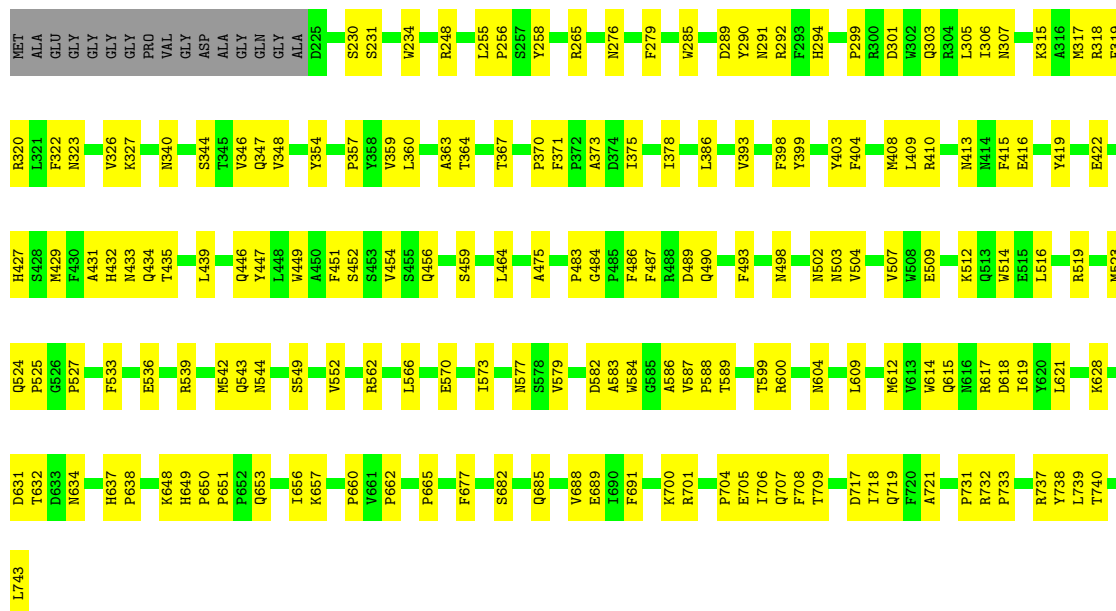
• Molecule 1: Capsid protein

Chain Q: 64% 33%



• Molecule 1: Capsid protein

Chain R: 64% 33%



• Molecule 1: Capsid protein

Chain S:  64% 33%

MET	ALA	GLU	GLY	GLY	GLY	PRO	VAL	GLY	ASP	ALA	GLY	GLN	GLY	ALA	D225	S230	S231	W234	R248	T249	T250	R251	P256	R265	N276	F279	W285	D289	Y290	N291	R292	F293	H294	P299	R300	D301	W302	Q303	R304	L305	T306	N307	K315	A316	R317	R318	F319
R320	L321	F322	N323	V326	K327		N340		S344		Q347	V348		Y354	P357	Y358	V359	L360	A363	T364		T367	P370	F371	F372	A373	D374	L375	L386		V393	F398	Y399	Y403	F404	D407	M408	L409	R410	N413	M414	Q415	E416	Y419	E422	H427	S428
M429	F430	A431	H432	Q434	T435	L439		Q446	Y447	W449	A450	F451	S452	S453	Y454	S455	Q456	S459		L464		A475	P483	Q484	F486	R487	R488	D489	Q490		F493	N498	I499	N502	N503	V504	V507	M508	E509	K512	Q513	W514	E515	L516	R519	M523	Q524
P525	S526	P527	F533	E536		R539		M542	Q543	N544	S549		V552	R562	L566	E570	I573	N577	S578	V579	D582	A583	W584	S585	V587	P588	T589	T599	R600	N604	L609	M612	V613	W614	O615	R616	R617	D618	L619	Y620	L621	K628	D631				
T632	D633	N634	H637	P638	K648	H649	P650	P651	P652	Q653	I656	K657	P660	V661	P662	P665	F677	S682	Q685	V688	E689	T690	F691	K700	R701	P704	E705	I706	Q707	F708	T709	D717	I718	Q719	F720	P721	P731	R732	P733	Y737	Y738	L739	T740	L743			

• Molecule 1: Capsid protein

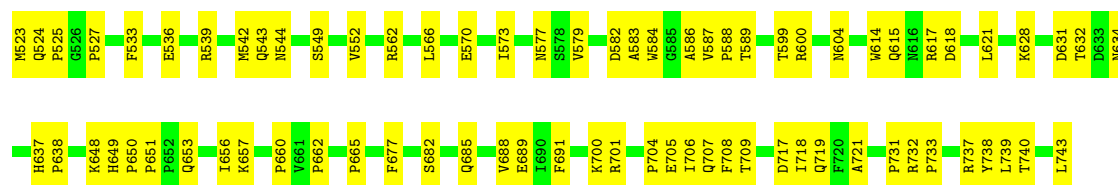
Chain T:  64% 33%

MET	ALA	GLU	GLY	GLY	GLY	PRO	VAL	GLY	ASP	ALA	GLY	GLN	GLY	ALA	D225	S230	S231	W234	R248	T249	T250	R251	P256	Y263	R265	N276	F279	W285	D289	Y290	N291	R292	F293	H294	P299	R300	D301	Q302	Q303	R304	L305	T306	N307	K315	A316	R317	M317																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	

• Molecule 1: Capsid protein

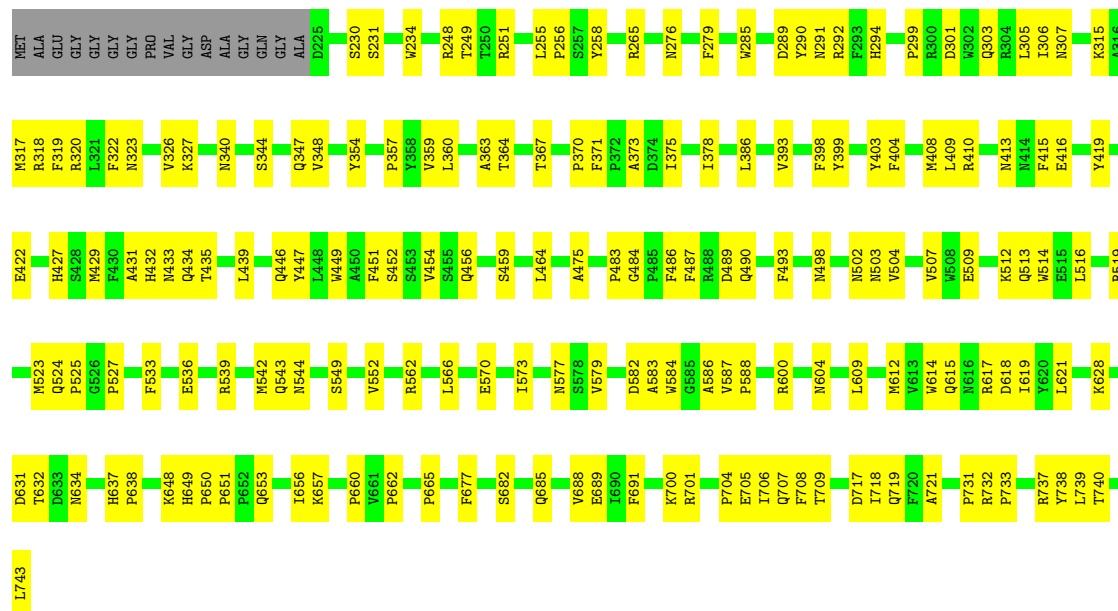
Chain U:  65% 32%

MET	ALA	GLU	GLY	GLY	GLY	PRO	VAL	GLY	ASP	ALA	GLY	GLN	GLY	ALA	D225	S230	S231	W234	R248	L255	P256	Y258	R265	N276	F279	W285	D289	Y290	N291	R292	F293	H294	P299	R300	D301	W302	Q303	R304	L305	T306	N307	K315	A316	R317	R318	F319
R320	L321	F322	N323	V326	K327	N340	S344	Q347	V348	Y354	P357	Y358	V359	L360	A363	T364	T367	P370	F371	F372	A373	R374	L375	L378	L386	V393	F398	Y399	Y403	F404	D407	M408	L409	R410	N413	M414	F415	E416	Y419	E422						
H427	S428	M429	F430	A431	H432	N433	Q434	T435	L439	Q446	Y447	W448	W449	A450	F451	S452	S453	S455	Q456	S459	L464	A475	P483	Q484	F486	R487	R488	D489	Q490	F493	N498	L499	N502	N503	V504	V507	W508	E509	K512	Q513	W514	E515	L516	R519		



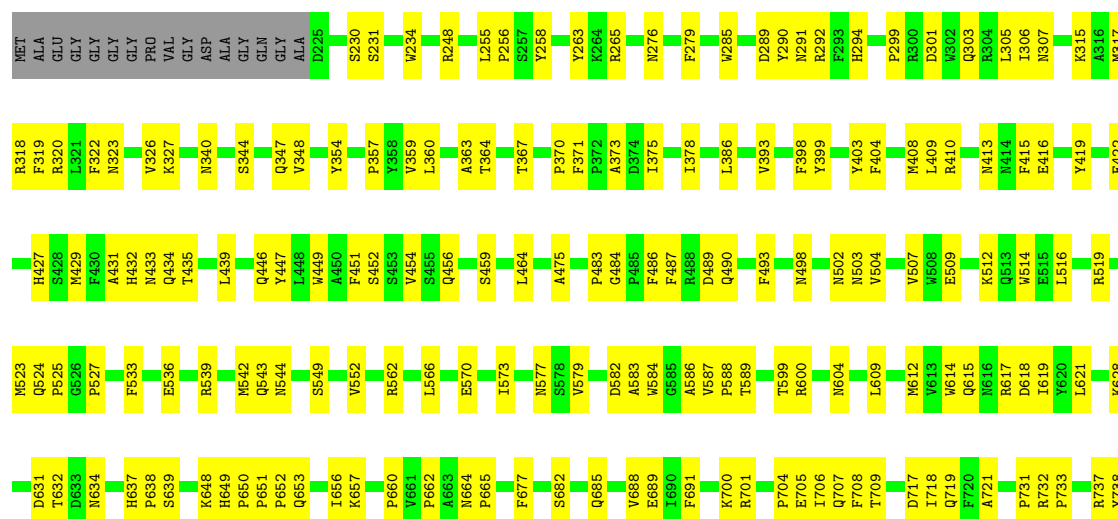
• Molecule 1: Capsid protein

Chain V: 64% 33%



• Molecule 1: Capsid protein

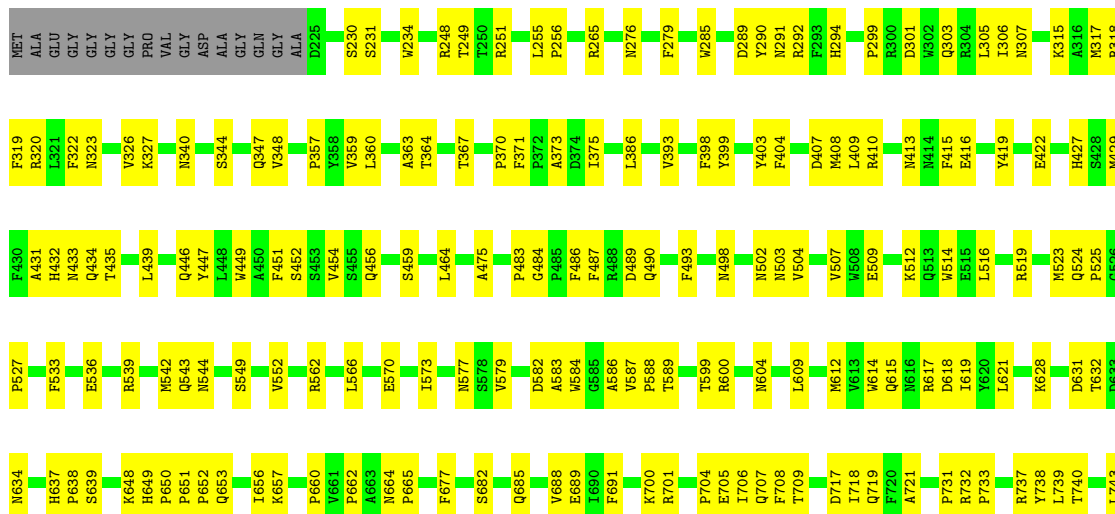
Chain W: 64% 33%



L739
T740
L743

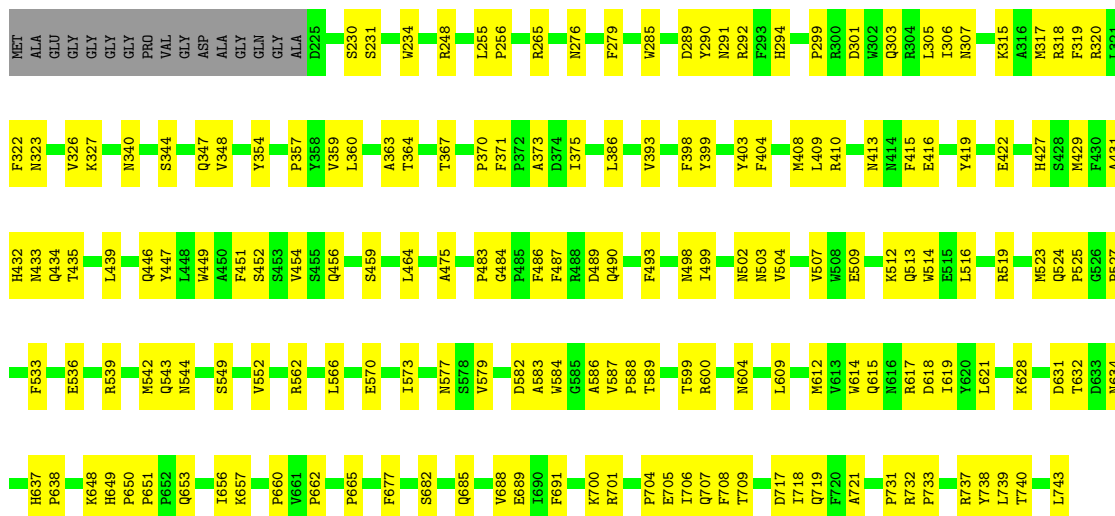
• Molecule 1: Capsid protein

Chain X:  64% 33%



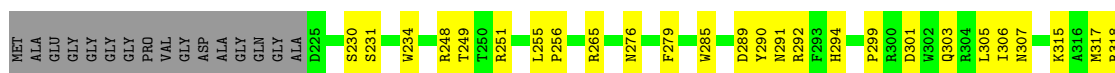
• Molecule 1: Capsid protein

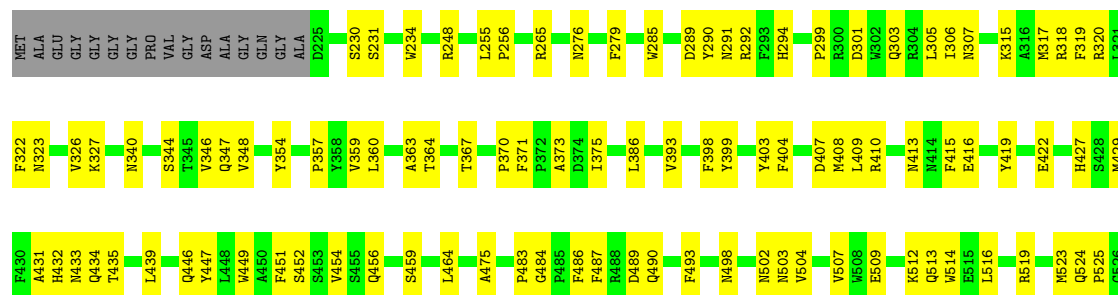
Chain Y:  64% 33%

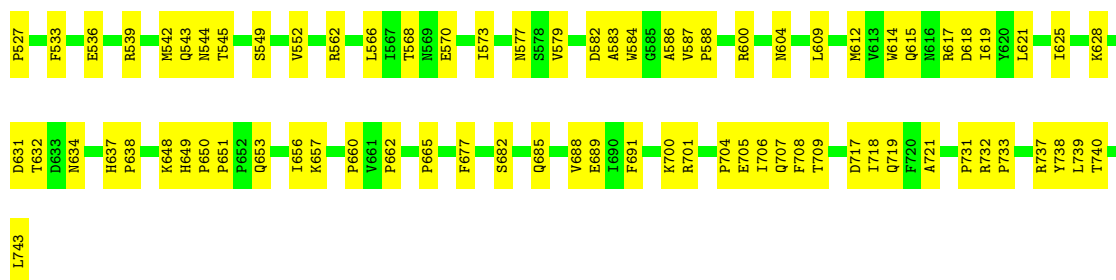


• Molecule 1: Capsid protein

Chain Z:  64% 33%

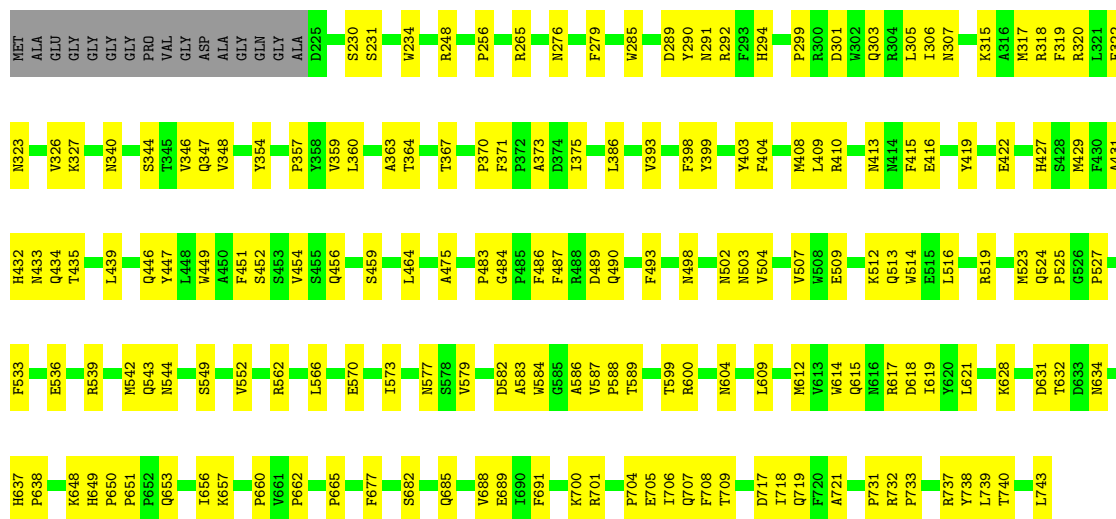






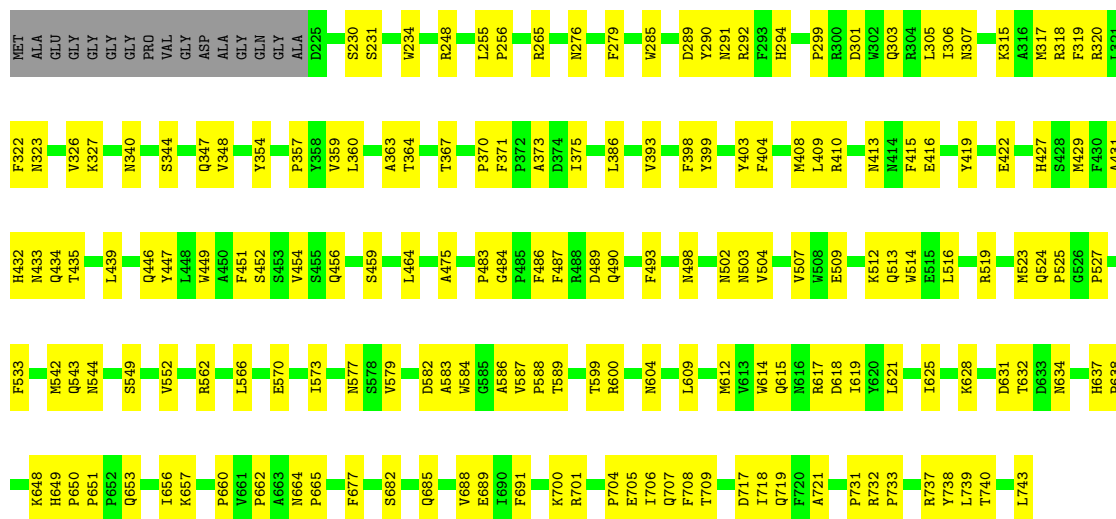
• Molecule 1: Capsid protein

Chain c: 65% 32% .



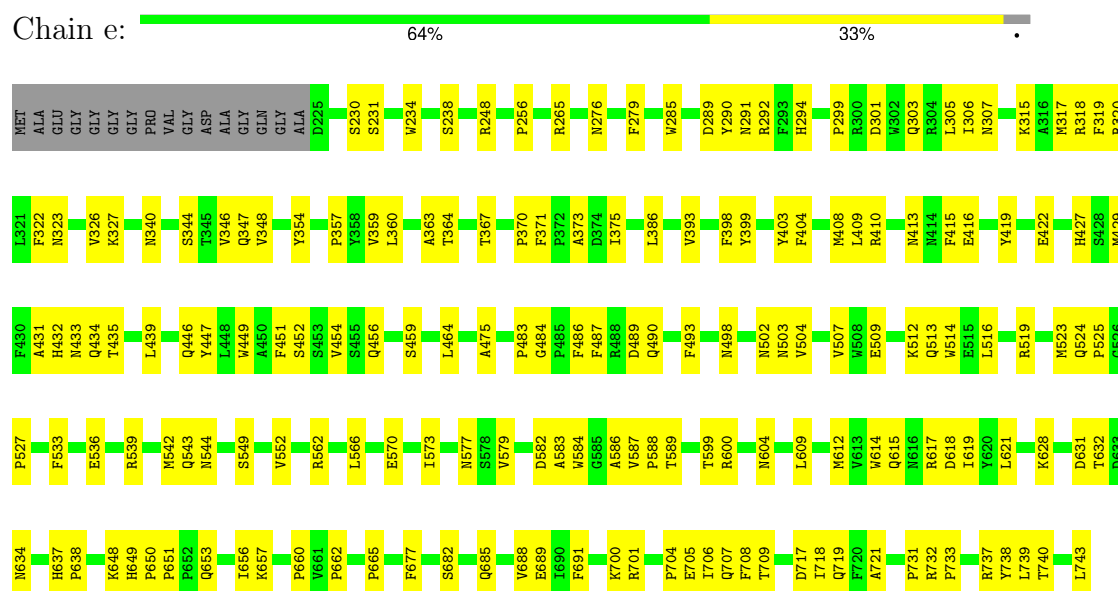
• Molecule 1: Capsid protein

Chain d: 65% 32% .



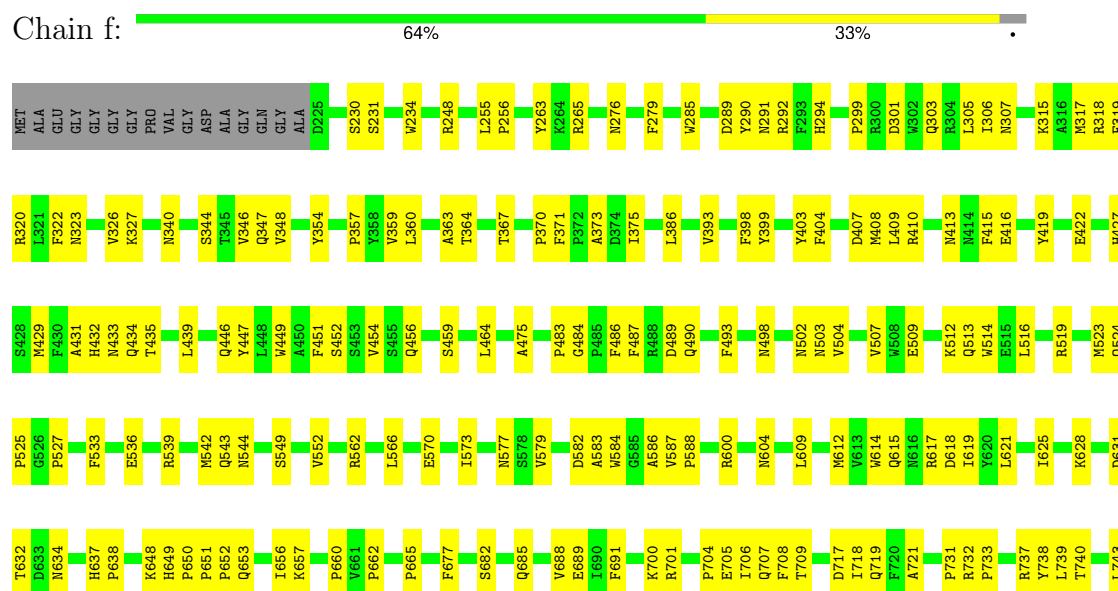
• Molecule 1: Capsid protein

Chain e:



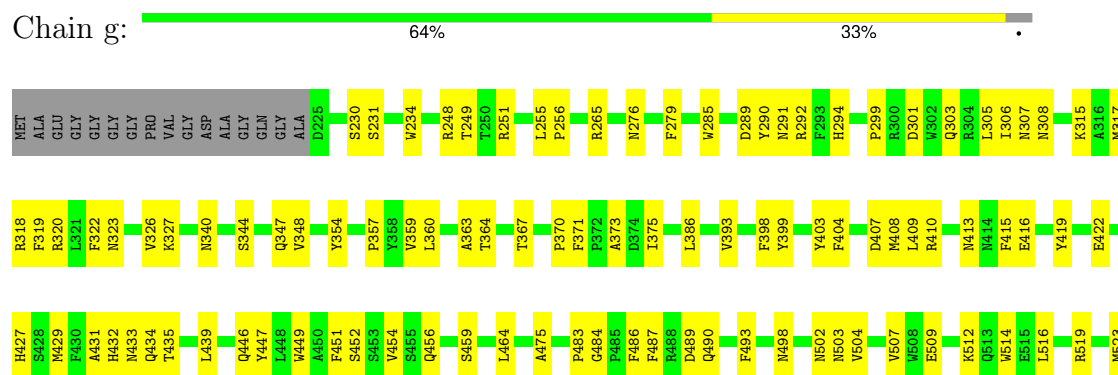
• Molecule 1: Capsid protein

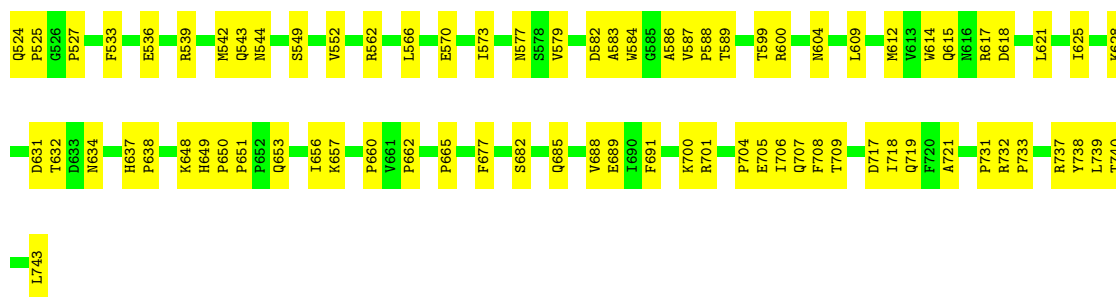
Chain f:



• Molecule 1: Capsid protein

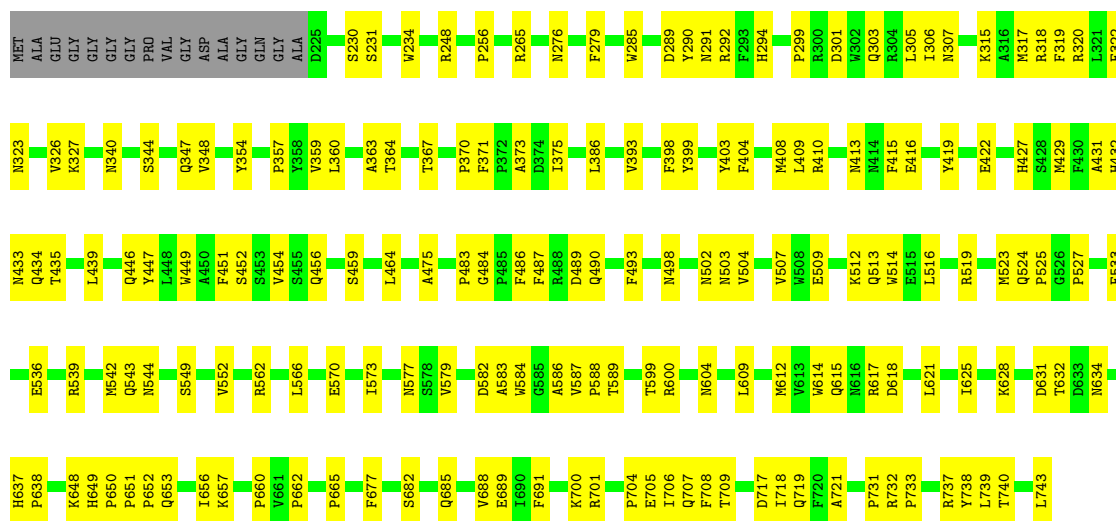
Chain g:





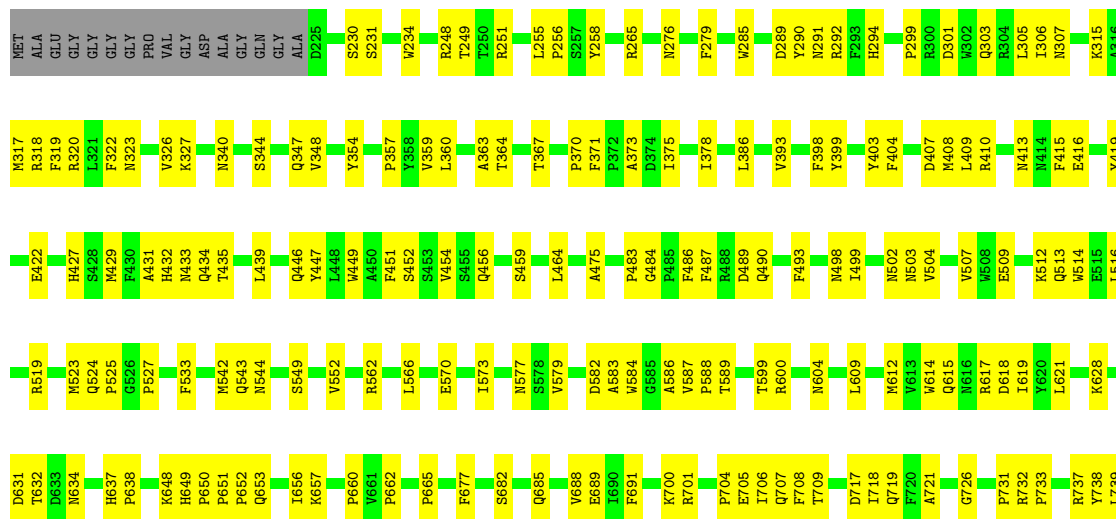
• Molecule 1: Capsid protein

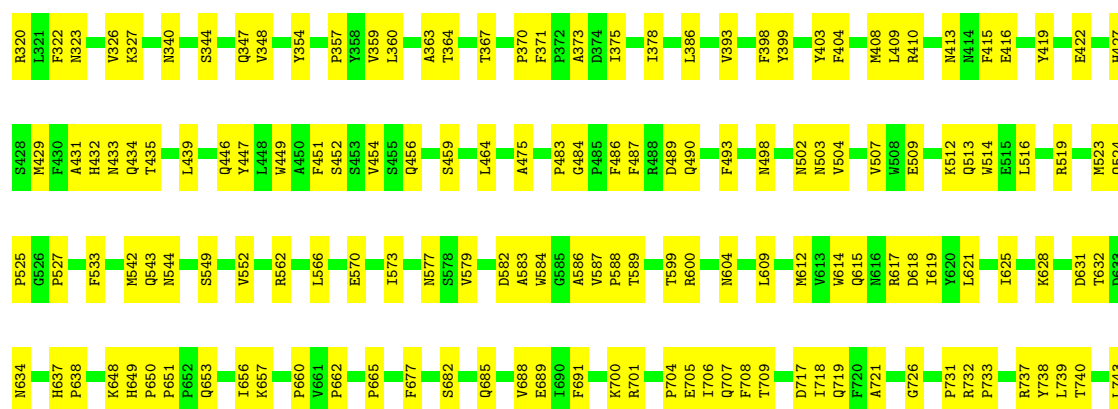
Chain h: 65% 32%



• Molecule 1: Capsid protein

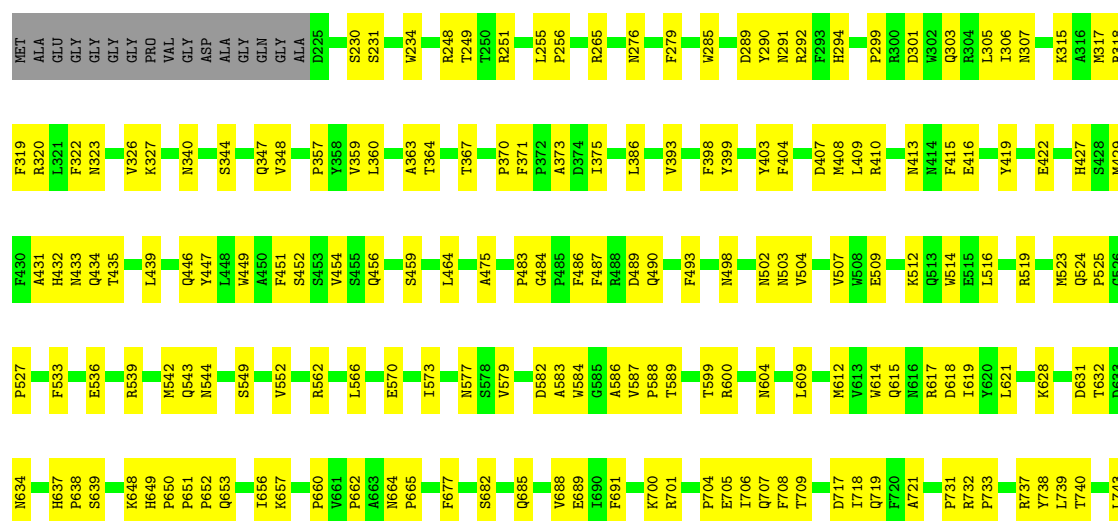
Chain i: 64% 33%





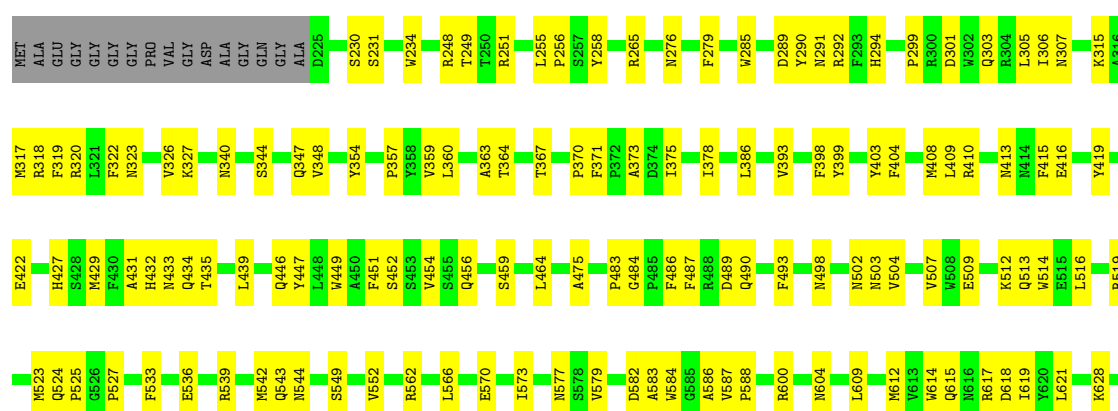
• Molecule 1: Capsid protein

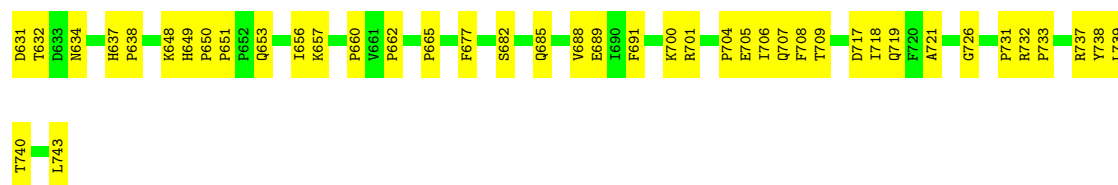
Chain o: 64% 33% •



• Molecule 1: Capsid protein

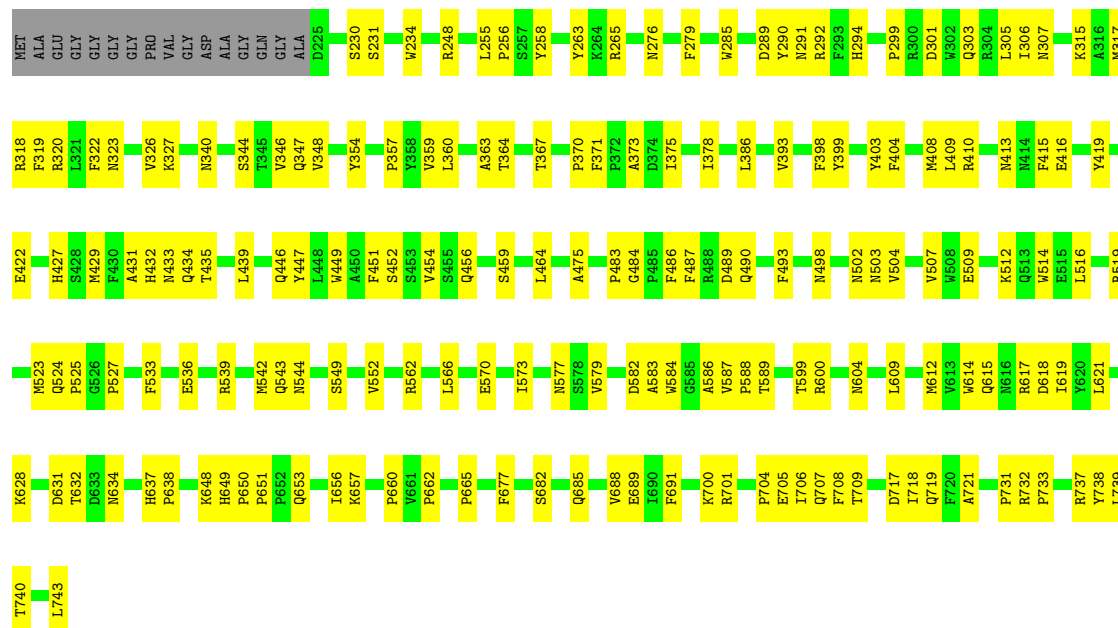
Chain p: 64% 33% •





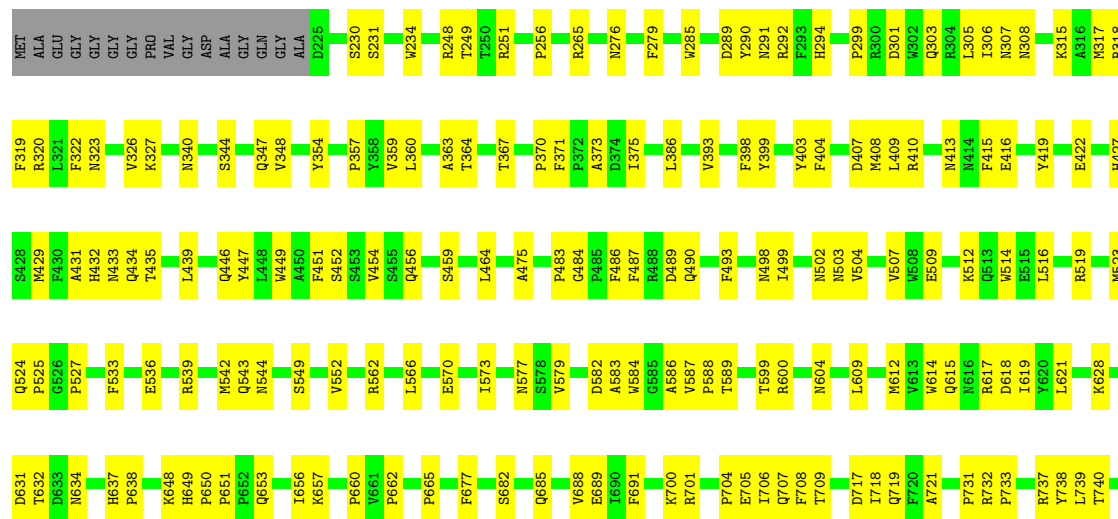
• Molecule 1: Capsid protein

Chain q: 64% 33%



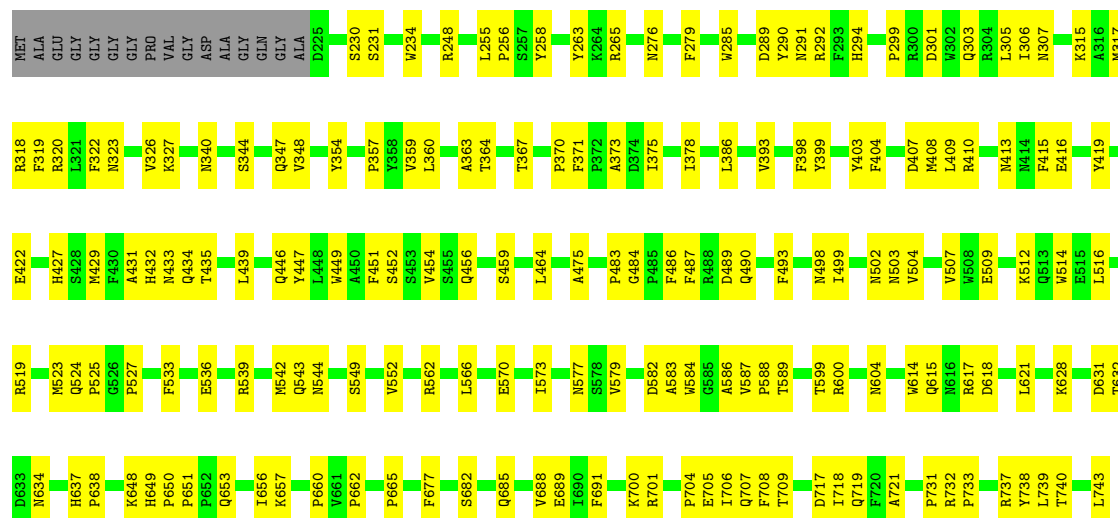
• Molecule 1: Capsid protein

Chain r: 64% 33%

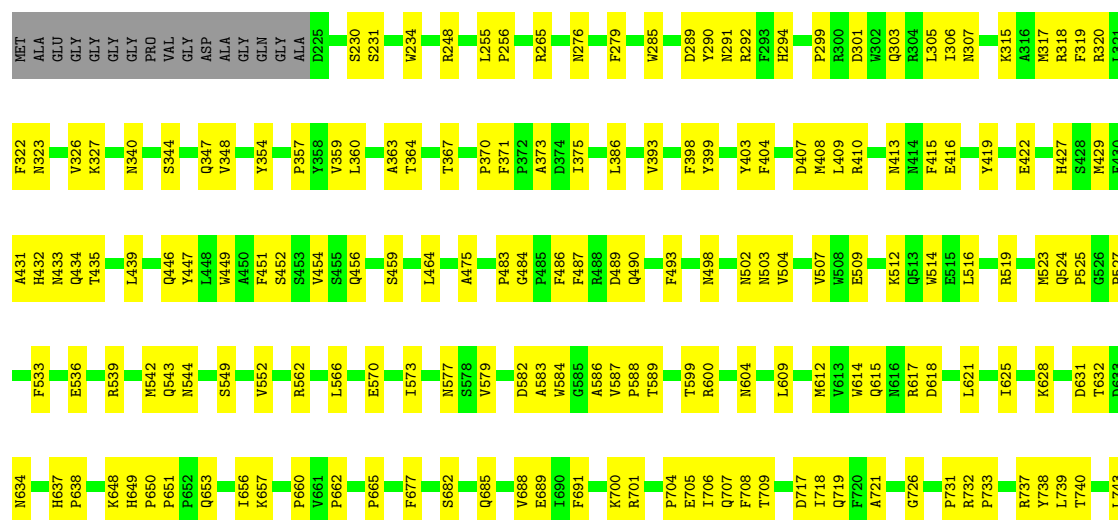


L743

- Molecule 1: Capsid protein

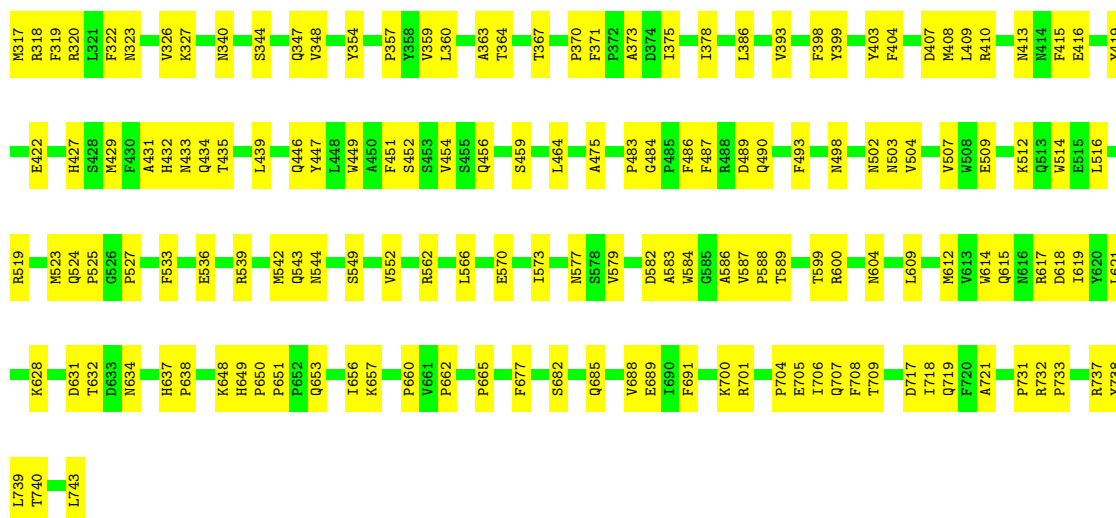
Chain s:  64% 33%

- Molecule 1: Capsid protein

Chain t:  64% 33%

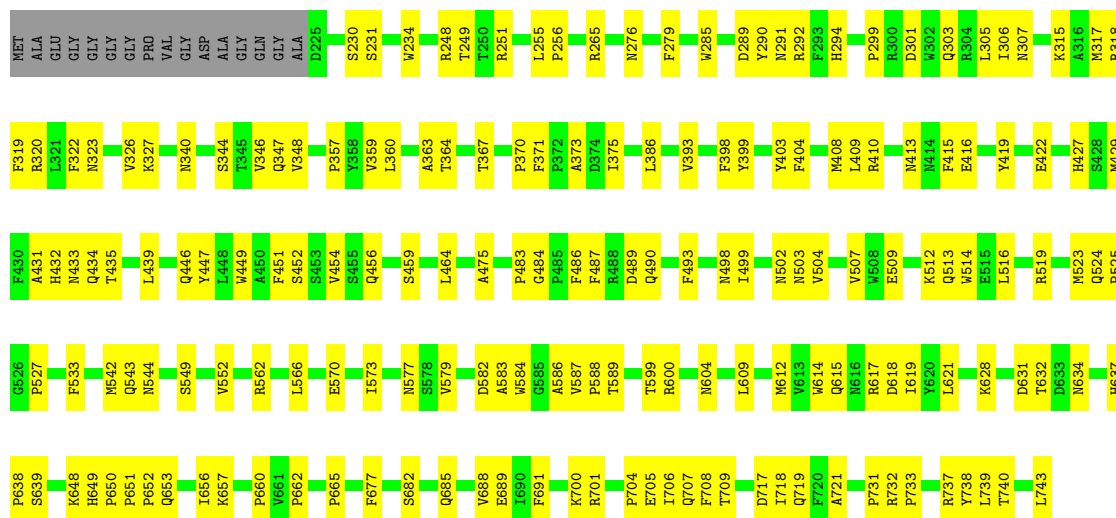
- Molecule 1: Capsid protein

Chain u:  64% 33%



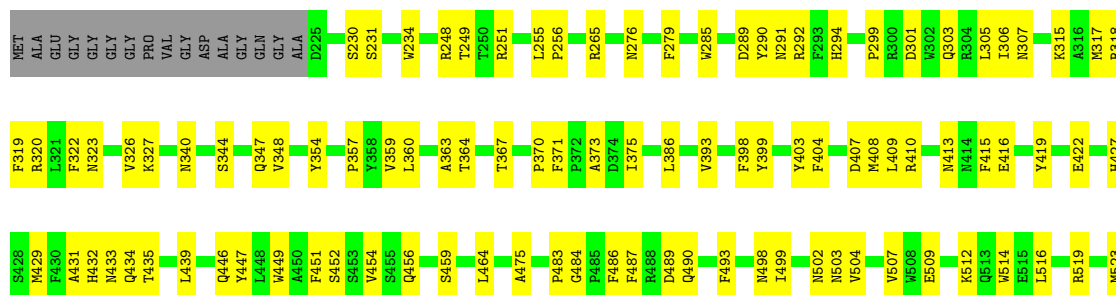
• Molecule 1: Capsid protein

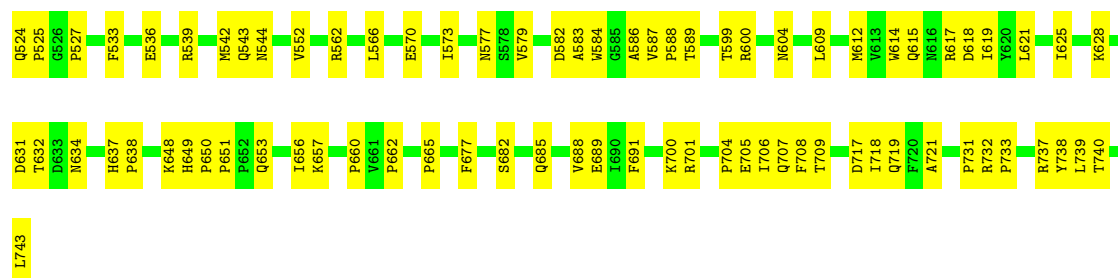
Chain v: 64% 33%



• Molecule 1: Capsid protein

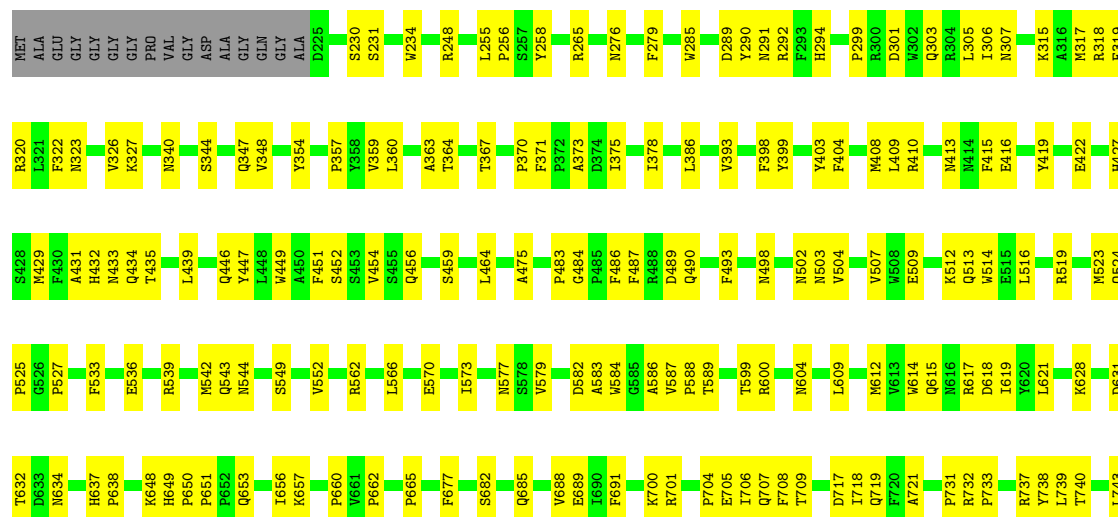
Chain w: 64% 33%





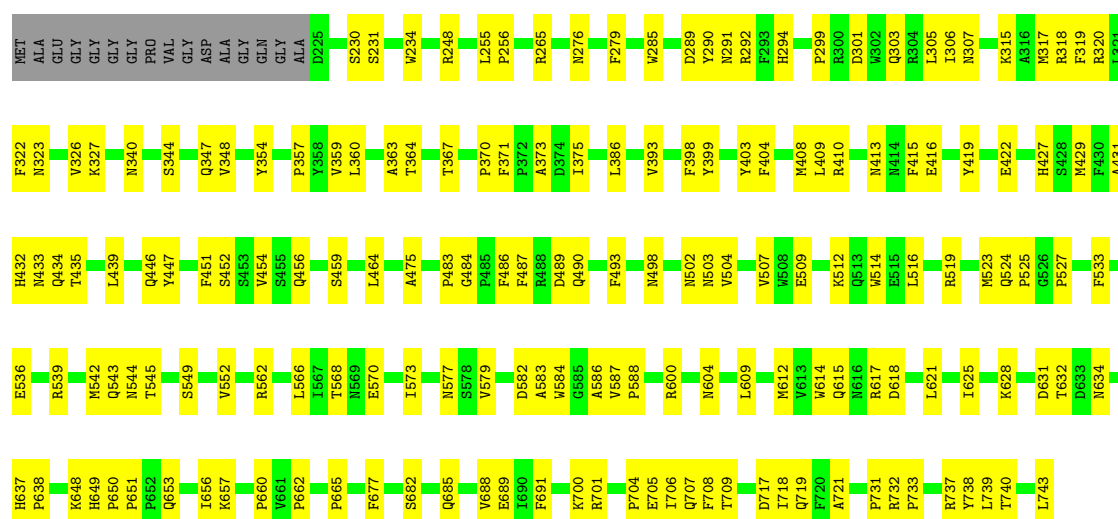
• Molecule 1: Capsid protein

Chain x: 64% 33%



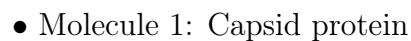
• Molecule 1: Capsid protein

Chain y: 65% 32%

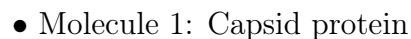


• Molecule 1: Capsid protein

Responsibility	Percentage
Current government	63%
Previous government	34%

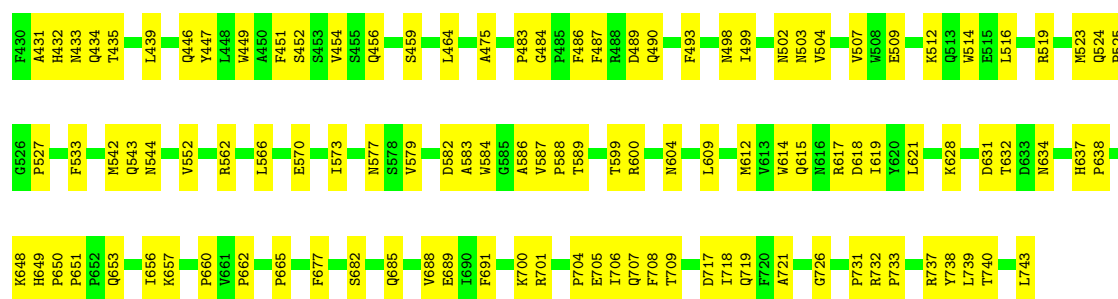


Response	Percentage
Yes, I have used a mobile app to book a flight	64%
No, I have not used a mobile app to book a flight	33%

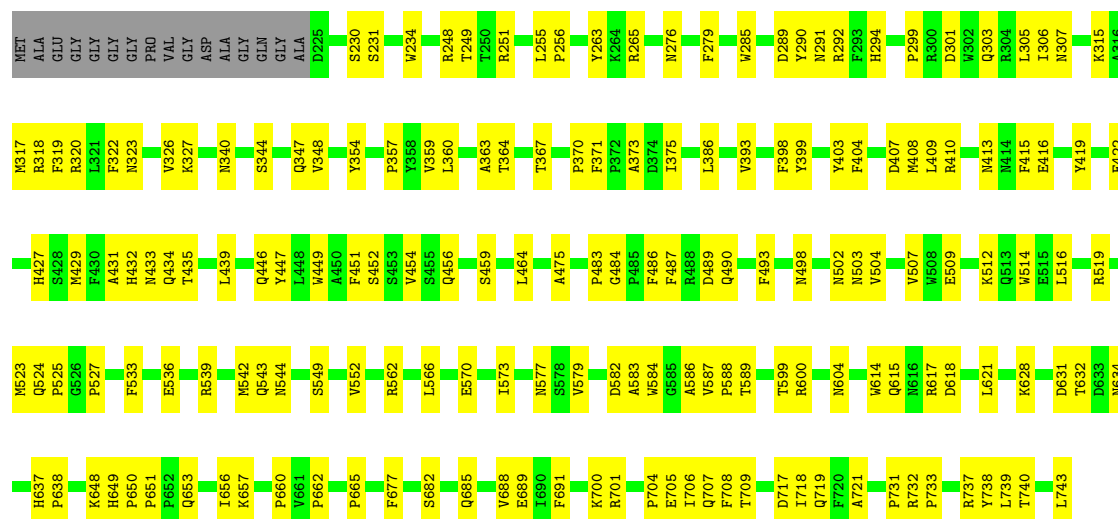


Opinion	Percentage
Doing a good job	65%
Doing a bad job	32%

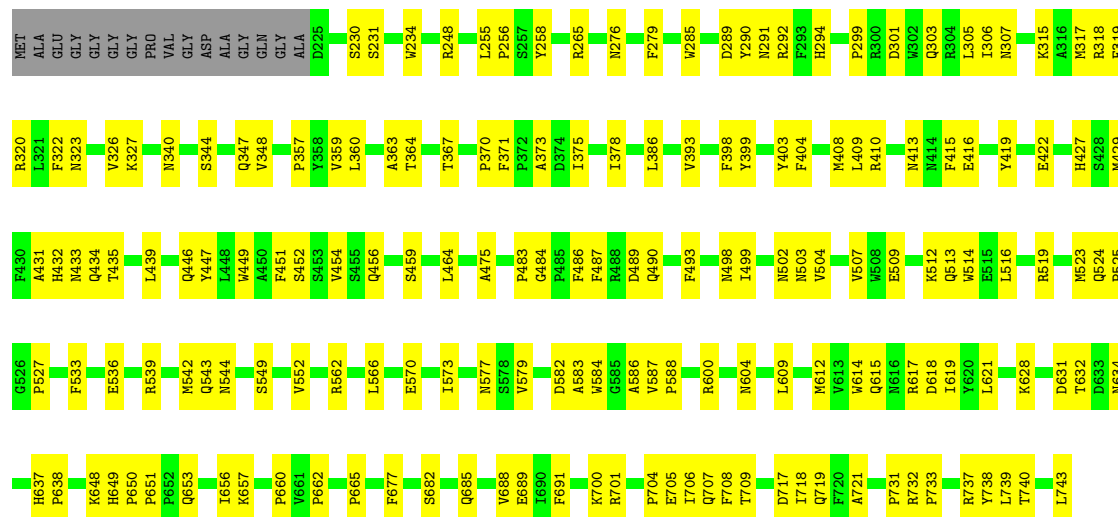




- Molecule 1: Capsid protein

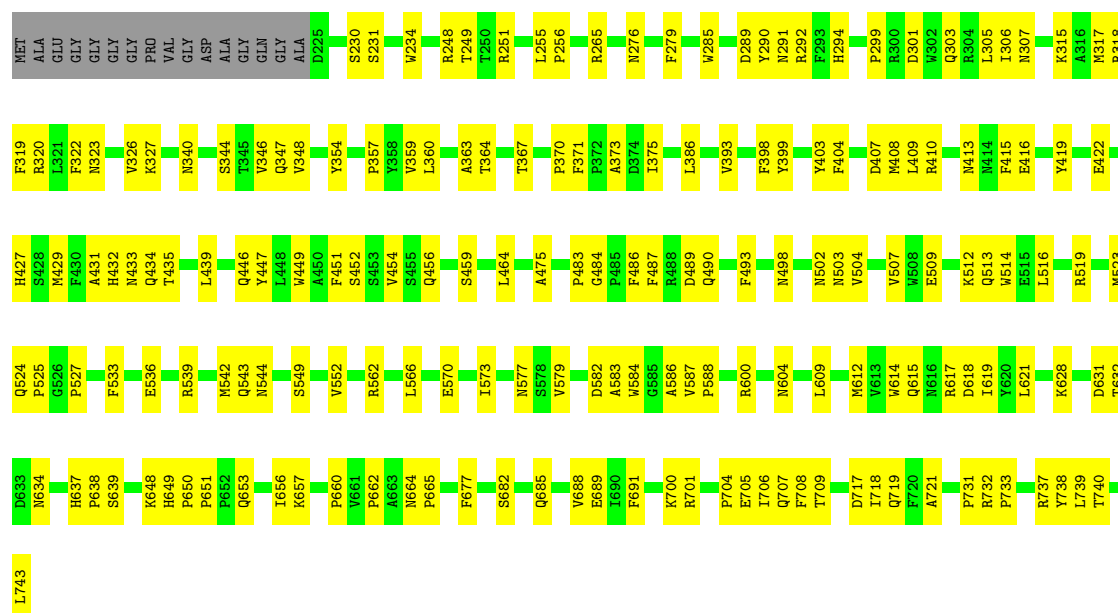


- Molecule 1: Capsid protein



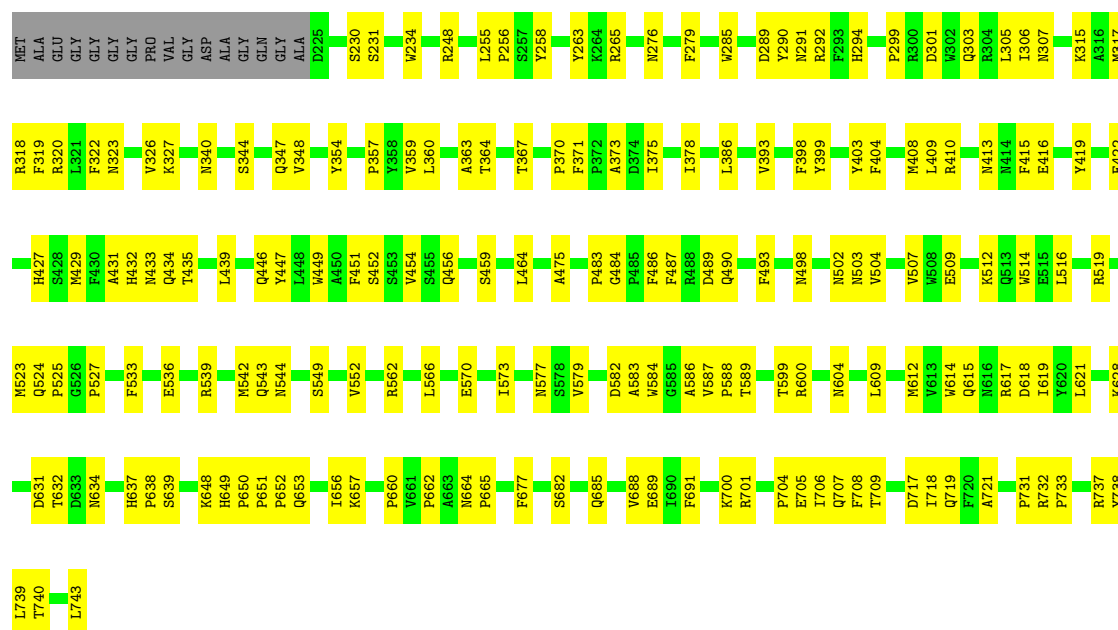
- Molecule 1: Capsid protein

Chain 5:  64% 33%



• Molecule 1: Capsid protein

Chain 6:  64% 33%



• Molecule 1: Capsid protein

Chain 7:  65% 32%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	16.894	Depositor
Minimum map value	-12.547	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (\AA)	443.09998, 443.09998, 443.09998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.42	0/4297	0.52	0/5867
1	2	0.42	0/4297	0.52	0/5867
1	3	0.42	0/4297	0.52	0/5867
1	4	0.42	0/4297	0.52	0/5867
1	5	0.42	0/4297	0.52	0/5867
1	6	0.42	0/4297	0.52	0/5867
1	7	0.42	0/4297	0.52	0/5867
1	8	0.42	0/4297	0.52	0/5867
1	A	0.42	0/4297	0.52	0/5867
1	B	0.42	0/4297	0.52	0/5867
1	C	0.42	0/4297	0.52	0/5867
1	D	0.42	0/4297	0.52	0/5867
1	E	0.42	0/4297	0.52	0/5867
1	F	0.42	0/4297	0.52	0/5867
1	G	0.42	0/4297	0.52	0/5867
1	H	0.42	0/4297	0.52	0/5867
1	I	0.42	0/4297	0.52	0/5867
1	J	0.42	0/4297	0.52	0/5867
1	K	0.42	0/4297	0.52	0/5867
1	L	0.42	0/4297	0.52	0/5867
1	M	0.42	0/4297	0.52	0/5867
1	N	0.42	0/4297	0.52	0/5867
1	O	0.42	0/4297	0.52	0/5867
1	P	0.42	0/4297	0.52	0/5867
1	Q	0.42	0/4297	0.52	0/5867
1	R	0.42	0/4297	0.52	0/5867
1	S	0.42	0/4297	0.52	0/5867
1	T	0.42	0/4297	0.52	0/5867
1	U	0.42	0/4297	0.52	0/5867
1	V	0.42	0/4297	0.52	0/5867
1	W	0.42	0/4297	0.52	0/5867
1	X	0.42	0/4297	0.52	0/5867

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.42	0/4297	0.52	0/5867
1	Z	0.42	0/4297	0.52	0/5867
1	a	0.42	0/4297	0.52	0/5867
1	b	0.42	0/4297	0.52	0/5867
1	c	0.42	0/4297	0.52	0/5867
1	d	0.42	0/4297	0.52	0/5867
1	e	0.42	0/4297	0.52	0/5867
1	f	0.42	0/4297	0.52	0/5867
1	g	0.42	0/4297	0.52	0/5867
1	h	0.42	0/4297	0.52	0/5867
1	i	0.42	0/4297	0.52	0/5867
1	j	0.42	0/4297	0.52	0/5867
1	k	0.42	0/4297	0.52	0/5867
1	l	0.42	0/4297	0.52	0/5867
1	m	0.42	0/4297	0.52	0/5867
1	n	0.42	0/4297	0.52	0/5867
1	o	0.42	0/4297	0.52	0/5867
1	p	0.42	0/4297	0.52	0/5867
1	q	0.42	0/4297	0.52	0/5867
1	r	0.42	0/4297	0.52	0/5867
1	s	0.42	0/4297	0.52	0/5867
1	t	0.42	0/4297	0.52	0/5867
1	u	0.42	0/4297	0.52	0/5867
1	v	0.42	0/4297	0.52	0/5867
1	w	0.42	0/4297	0.52	0/5867
1	x	0.42	0/4297	0.52	0/5867
1	y	0.42	0/4297	0.52	0/5867
1	z	0.42	0/4297	0.52	0/5867
All	All	0.42	0/257820	0.52	0/352020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4167	0	3925	162	0
1	2	4167	0	3925	159	0
1	3	4167	0	3925	160	0
1	4	4167	0	3925	161	0
1	5	4167	0	3925	160	0
1	6	4167	0	3925	161	0
1	7	4167	0	3925	157	0
1	8	4167	0	3925	167	0
1	A	4167	0	3925	163	0
1	B	4167	0	3925	160	0
1	C	4167	0	3925	160	0
1	D	4167	0	3925	165	0
1	E	4167	0	3925	163	0
1	F	4167	0	3925	162	0
1	G	4167	0	3925	164	0
1	H	4167	0	3925	159	0
1	I	4167	0	3925	164	0
1	J	4167	0	3925	161	0
1	K	4167	0	3925	160	0
1	L	4167	0	3925	162	0
1	M	4167	0	3925	160	0
1	N	4167	0	3925	167	0
1	O	4167	0	3925	167	0
1	P	4167	0	3925	163	0
1	Q	4167	0	3925	160	0
1	R	4167	0	3925	163	0
1	S	4167	0	3925	162	0
1	T	4167	0	3925	160	0
1	U	4167	0	3925	159	0
1	V	4167	0	3925	162	0
1	W	4167	0	3925	163	0
1	X	4167	0	3925	163	0
1	Y	4167	0	3925	159	0
1	Z	4167	0	3925	164	0
1	a	4167	0	3925	161	0
1	b	4167	0	3925	165	0
1	c	4167	0	3925	162	0
1	d	4167	0	3925	158	0
1	e	4167	0	3925	162	0
1	f	4167	0	3925	163	0
1	g	4167	0	3925	161	0
1	h	4167	0	3925	160	0
1	i	4167	0	3925	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4167	0	3925	163	0
1	k	4167	0	3925	164	0
1	l	4167	0	3925	168	0
1	m	4167	0	3925	163	0
1	n	4167	0	3925	162	0
1	o	4167	0	3925	165	0
1	p	4167	0	3925	165	0
1	q	4167	0	3925	163	0
1	r	4167	0	3925	163	0
1	s	4167	0	3925	161	0
1	t	4167	0	3925	163	0
1	u	4167	0	3925	165	0
1	v	4167	0	3925	164	0
1	w	4167	0	3925	160	0
1	x	4167	0	3925	159	0
1	y	4167	0	3925	158	0
1	z	4167	0	3925	164	0
2	1	21	0	12	3	0
2	2	21	0	12	3	0
2	3	21	0	12	3	0
2	4	21	0	12	3	0
2	5	21	0	12	3	0
2	6	21	0	12	3	0
2	7	21	0	12	3	0
2	8	21	0	12	3	0
2	A	21	0	12	3	0
2	B	21	0	12	3	0
2	C	21	0	12	3	0
2	D	21	0	12	3	0
2	E	21	0	12	3	0
2	F	21	0	12	3	0
2	G	21	0	12	3	0
2	H	21	0	12	3	0
2	I	21	0	12	3	0
2	J	21	0	12	3	0
2	K	21	0	12	3	0
2	L	21	0	12	3	0
2	M	21	0	12	3	0
2	N	21	0	12	3	0
2	O	21	0	12	4	0
2	P	21	0	12	3	0
2	Q	21	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	21	0	12	3	0
2	S	21	0	12	3	0
2	T	21	0	12	3	0
2	U	21	0	12	3	0
2	V	21	0	12	3	0
2	W	21	0	12	3	0
2	X	21	0	12	3	0
2	Y	21	0	12	3	0
2	Z	21	0	12	3	0
2	a	21	0	12	3	0
2	b	21	0	12	4	0
2	c	21	0	12	3	0
2	d	21	0	12	3	0
2	e	21	0	12	3	0
2	f	21	0	12	4	0
2	g	21	0	12	4	0
2	h	21	0	12	3	0
2	i	21	0	12	3	0
2	j	21	0	12	3	0
2	k	21	0	12	3	0
2	l	21	0	12	4	0
2	m	21	0	12	3	0
2	n	21	0	12	3	0
2	o	21	0	12	3	0
2	p	21	0	12	3	0
2	q	21	0	12	3	0
2	r	21	0	12	3	0
2	s	21	0	12	3	0
2	t	21	0	12	3	0
2	u	21	0	12	3	0
2	v	21	0	12	3	0
2	w	21	0	12	3	0
2	x	21	0	12	3	0
2	y	21	0	12	3	0
2	z	21	0	12	3	0
All	All	251280	0	236220	7633	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 16.

The worst 5 of 7633 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:493:PHE:H	1:u:502:ASN:HD21	1.20	0.90
1:I:493:PHE:H	1:I:502:ASN:HD21	1.20	0.90
1:K:493:PHE:H	1:K:502:ASN:HD21	1.20	0.90
1:4:493:PHE:H	1:4:502:ASN:HD21	1.20	0.90
1:e:493:PHE:H	1:e:502:ASN:HD21	1.20	0.89

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	1	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	2	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	3	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	4	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	5	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	6	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	7	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	8	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	A	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	B	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	C	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	D	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	E	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	F	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	G	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	H	517/535 (97%)	505 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	J	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	K	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	L	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	M	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	N	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	O	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	P	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	Q	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	R	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	S	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	T	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	U	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	V	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	W	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	X	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	Y	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	Z	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	a	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	b	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	c	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	d	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	e	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	f	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	g	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	h	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	i	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	j	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	k	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	l	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	m	517/535 (97%)	505 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	o	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	p	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	q	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	r	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	s	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	t	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	u	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	v	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	w	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	x	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	y	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
1	z	517/535 (97%)	505 (98%)	12 (2%)	0	100	100
All	All	31020/32100 (97%)	30300 (98%)	720 (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	1	452/458 (99%)	452 (100%)	0	100	100
1	2	452/458 (99%)	452 (100%)	0	100	100
1	3	452/458 (99%)	452 (100%)	0	100	100
1	4	452/458 (99%)	452 (100%)	0	100	100
1	5	452/458 (99%)	452 (100%)	0	100	100
1	6	452/458 (99%)	452 (100%)	0	100	100
1	7	452/458 (99%)	452 (100%)	0	100	100
1	8	452/458 (99%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/458 (99%)	452 (100%)	0	100	100
1	B	452/458 (99%)	452 (100%)	0	100	100
1	C	452/458 (99%)	452 (100%)	0	100	100
1	D	452/458 (99%)	452 (100%)	0	100	100
1	E	452/458 (99%)	452 (100%)	0	100	100
1	F	452/458 (99%)	452 (100%)	0	100	100
1	G	452/458 (99%)	452 (100%)	0	100	100
1	H	452/458 (99%)	452 (100%)	0	100	100
1	I	452/458 (99%)	452 (100%)	0	100	100
1	J	452/458 (99%)	452 (100%)	0	100	100
1	K	452/458 (99%)	452 (100%)	0	100	100
1	L	452/458 (99%)	452 (100%)	0	100	100
1	M	452/458 (99%)	452 (100%)	0	100	100
1	N	452/458 (99%)	452 (100%)	0	100	100
1	O	452/458 (99%)	452 (100%)	0	100	100
1	P	452/458 (99%)	452 (100%)	0	100	100
1	Q	452/458 (99%)	452 (100%)	0	100	100
1	R	452/458 (99%)	452 (100%)	0	100	100
1	S	452/458 (99%)	452 (100%)	0	100	100
1	T	452/458 (99%)	452 (100%)	0	100	100
1	U	452/458 (99%)	452 (100%)	0	100	100
1	V	452/458 (99%)	452 (100%)	0	100	100
1	W	452/458 (99%)	452 (100%)	0	100	100
1	X	452/458 (99%)	452 (100%)	0	100	100
1	Y	452/458 (99%)	452 (100%)	0	100	100
1	Z	452/458 (99%)	452 (100%)	0	100	100
1	a	452/458 (99%)	452 (100%)	0	100	100
1	b	452/458 (99%)	452 (100%)	0	100	100
1	c	452/458 (99%)	452 (100%)	0	100	100
1	d	452/458 (99%)	452 (100%)	0	100	100
1	e	452/458 (99%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	452/458 (99%)	452 (100%)	0	100	100
1	g	452/458 (99%)	452 (100%)	0	100	100
1	h	452/458 (99%)	452 (100%)	0	100	100
1	i	452/458 (99%)	452 (100%)	0	100	100
1	j	452/458 (99%)	452 (100%)	0	100	100
1	k	452/458 (99%)	452 (100%)	0	100	100
1	l	452/458 (99%)	452 (100%)	0	100	100
1	m	452/458 (99%)	452 (100%)	0	100	100
1	n	452/458 (99%)	452 (100%)	0	100	100
1	o	452/458 (99%)	452 (100%)	0	100	100
1	p	452/458 (99%)	452 (100%)	0	100	100
1	q	452/458 (99%)	452 (100%)	0	100	100
1	r	452/458 (99%)	452 (100%)	0	100	100
1	s	452/458 (99%)	452 (100%)	0	100	100
1	t	452/458 (99%)	452 (100%)	0	100	100
1	u	452/458 (99%)	452 (100%)	0	100	100
1	v	452/458 (99%)	452 (100%)	0	100	100
1	w	452/458 (99%)	452 (100%)	0	100	100
1	x	452/458 (99%)	452 (100%)	0	100	100
1	y	452/458 (99%)	452 (100%)	0	100	100
1	z	452/458 (99%)	452 (100%)	0	100	100
All	All	27120/27480 (99%)	27120 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1132 such sidechains are listed below:

Mol	Chain	Res	Type
1	x	323	ASN
1	y	521	ASN
1	x	276	ASN
1	4	413	ASN
1	U	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

60 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	$\# Z > 2$
2	D5M	S	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	O	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	N	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	h	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	u	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	c	801	-	17,23,24	0.83	0	17,33,36	0.75	0
2	D5M	m	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	L	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	r	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	U	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	B	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	f	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	s	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	D	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	g	801	-	17,23,24	0.83	0	17,33,36	0.75	0
2	D5M	l	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	C	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	Q	801	-	17,23,24	0.82	0	17,33,36	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D5M	b	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	W	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	K	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	A	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	5	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	j	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	e	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	q	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	t	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	X	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	n	801	-	17,23,24	0.81	0	17,33,36	0.75	0
2	D5M	G	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	v	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	l	801	-	17,23,24	0.81	0	17,33,36	0.75	0
2	D5M	d	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	i	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	8	801	-	17,23,24	0.84	0	17,33,36	0.75	0
2	D5M	o	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	7	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	Z	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	6	801	-	17,23,24	0.82	0	17,33,36	0.74	0
2	D5M	3	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	p	801	-	17,23,24	0.81	0	17,33,36	0.76	0
2	D5M	w	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	J	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	Y	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	y	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	E	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	P	801	-	17,23,24	0.83	0	17,33,36	0.74	0
2	D5M	T	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	F	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	I	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	k	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	2	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	H	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	V	801	-	17,23,24	0.82	0	17,33,36	0.75	0
2	D5M	x	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	4	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	R	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	a	801	-	17,23,24	0.83	0	17,33,36	0.76	0
2	D5M	z	801	-	17,23,24	0.82	0	17,33,36	0.76	0
2	D5M	M	801	-	17,23,24	0.82	0	17,33,36	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	S	801	-	-	2/3/21/22	0/3/3/3
2	D5M	O	801	-	-	2/3/21/22	0/3/3/3
2	D5M	N	801	-	-	2/3/21/22	0/3/3/3
2	D5M	h	801	-	-	2/3/21/22	0/3/3/3
2	D5M	u	801	-	-	2/3/21/22	0/3/3/3
2	D5M	c	801	-	-	2/3/21/22	0/3/3/3
2	D5M	m	801	-	-	2/3/21/22	0/3/3/3
2	D5M	L	801	-	-	2/3/21/22	0/3/3/3
2	D5M	r	801	-	-	2/3/21/22	0/3/3/3
2	D5M	U	801	-	-	2/3/21/22	0/3/3/3
2	D5M	B	801	-	-	2/3/21/22	0/3/3/3
2	D5M	f	801	-	-	2/3/21/22	0/3/3/3
2	D5M	s	801	-	-	2/3/21/22	0/3/3/3
2	D5M	D	801	-	-	2/3/21/22	0/3/3/3
2	D5M	g	801	-	-	2/3/21/22	0/3/3/3
2	D5M	l	801	-	-	2/3/21/22	0/3/3/3
2	D5M	C	801	-	-	2/3/21/22	0/3/3/3
2	D5M	Q	801	-	-	2/3/21/22	0/3/3/3
2	D5M	b	801	-	-	2/3/21/22	0/3/3/3
2	D5M	W	801	-	-	2/3/21/22	0/3/3/3
2	D5M	K	801	-	-	2/3/21/22	0/3/3/3
2	D5M	A	801	-	-	2/3/21/22	0/3/3/3
2	D5M	5	801	-	-	2/3/21/22	0/3/3/3
2	D5M	j	801	-	-	2/3/21/22	0/3/3/3
2	D5M	e	801	-	-	2/3/21/22	0/3/3/3
2	D5M	q	801	-	-	2/3/21/22	0/3/3/3
2	D5M	t	801	-	-	2/3/21/22	0/3/3/3
2	D5M	X	801	-	-	2/3/21/22	0/3/3/3
2	D5M	n	801	-	-	2/3/21/22	0/3/3/3
2	D5M	G	801	-	-	2/3/21/22	0/3/3/3
2	D5M	v	801	-	-	2/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	l	801	-	-	2/3/21/22	0/3/3/3
2	D5M	d	801	-	-	2/3/21/22	0/3/3/3
2	D5M	i	801	-	-	2/3/21/22	0/3/3/3
2	D5M	8	801	-	-	2/3/21/22	0/3/3/3
2	D5M	o	801	-	-	2/3/21/22	0/3/3/3
2	D5M	7	801	-	-	2/3/21/22	0/3/3/3
2	D5M	Z	801	-	-	2/3/21/22	0/3/3/3
2	D5M	6	801	-	-	2/3/21/22	0/3/3/3
2	D5M	3	801	-	-	2/3/21/22	0/3/3/3
2	D5M	p	801	-	-	2/3/21/22	0/3/3/3
2	D5M	w	801	-	-	2/3/21/22	0/3/3/3
2	D5M	J	801	-	-	2/3/21/22	0/3/3/3
2	D5M	Y	801	-	-	2/3/21/22	0/3/3/3
2	D5M	y	801	-	-	2/3/21/22	0/3/3/3
2	D5M	E	801	-	-	2/3/21/22	0/3/3/3
2	D5M	P	801	-	-	2/3/21/22	0/3/3/3
2	D5M	T	801	-	-	2/3/21/22	0/3/3/3
2	D5M	F	801	-	-	2/3/21/22	0/3/3/3
2	D5M	I	801	-	-	2/3/21/22	0/3/3/3
2	D5M	k	801	-	-	2/3/21/22	0/3/3/3
2	D5M	2	801	-	-	2/3/21/22	0/3/3/3
2	D5M	H	801	-	-	2/3/21/22	0/3/3/3
2	D5M	V	801	-	-	2/3/21/22	0/3/3/3
2	D5M	x	801	-	-	2/3/21/22	0/3/3/3
2	D5M	4	801	-	-	2/3/21/22	0/3/3/3
2	D5M	R	801	-	-	2/3/21/22	0/3/3/3
2	D5M	a	801	-	-	2/3/21/22	0/3/3/3
2	D5M	z	801	-	-	2/3/21/22	0/3/3/3
2	D5M	M	801	-	-	2/3/21/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	D5M	C4'-C5'-O5'-P
2	B	801	D5M	C4'-C5'-O5'-P
2	C	801	D5M	C4'-C5'-O5'-P
2	D	801	D5M	C4'-C5'-O5'-P
2	E	801	D5M	C4'-C5'-O5'-P

There are no ring outliers.

60 monomers are involved in 185 short contacts:

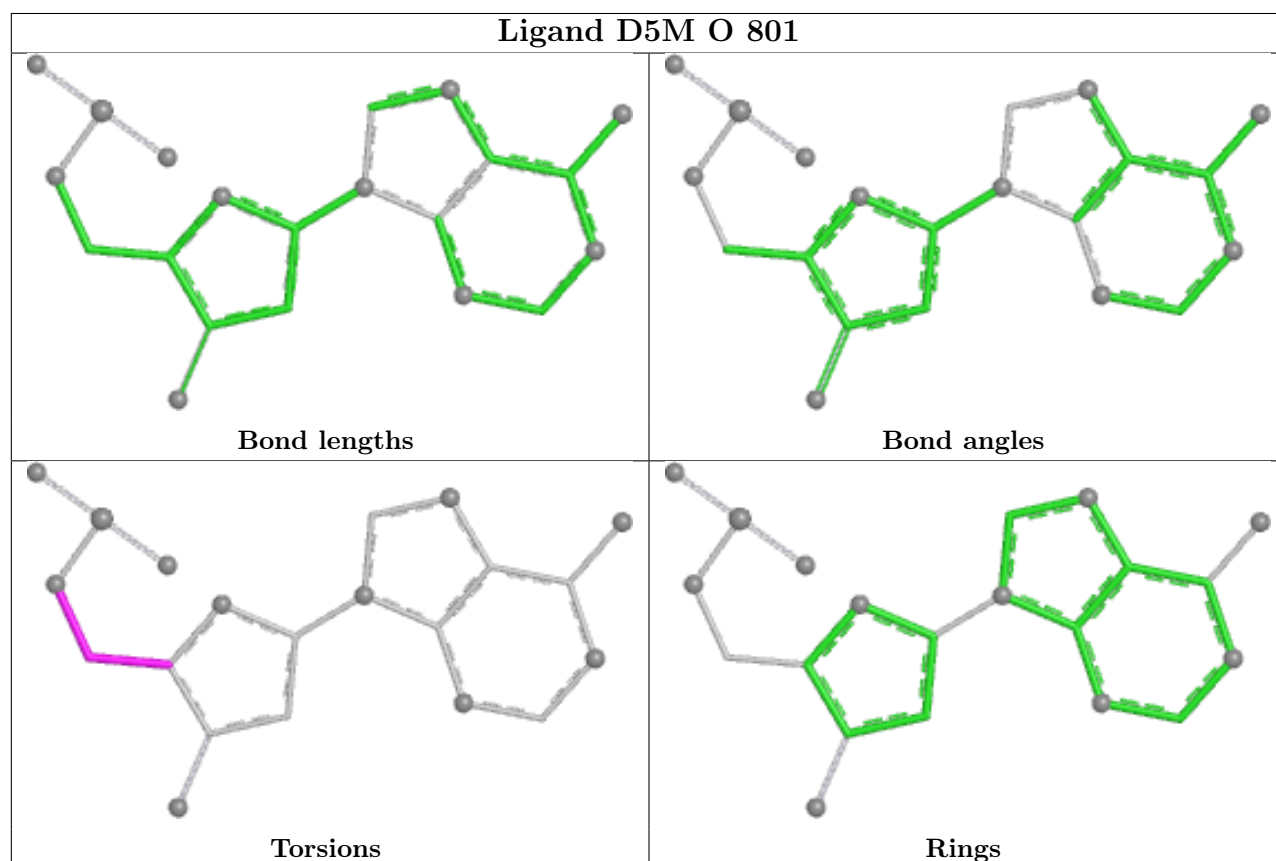
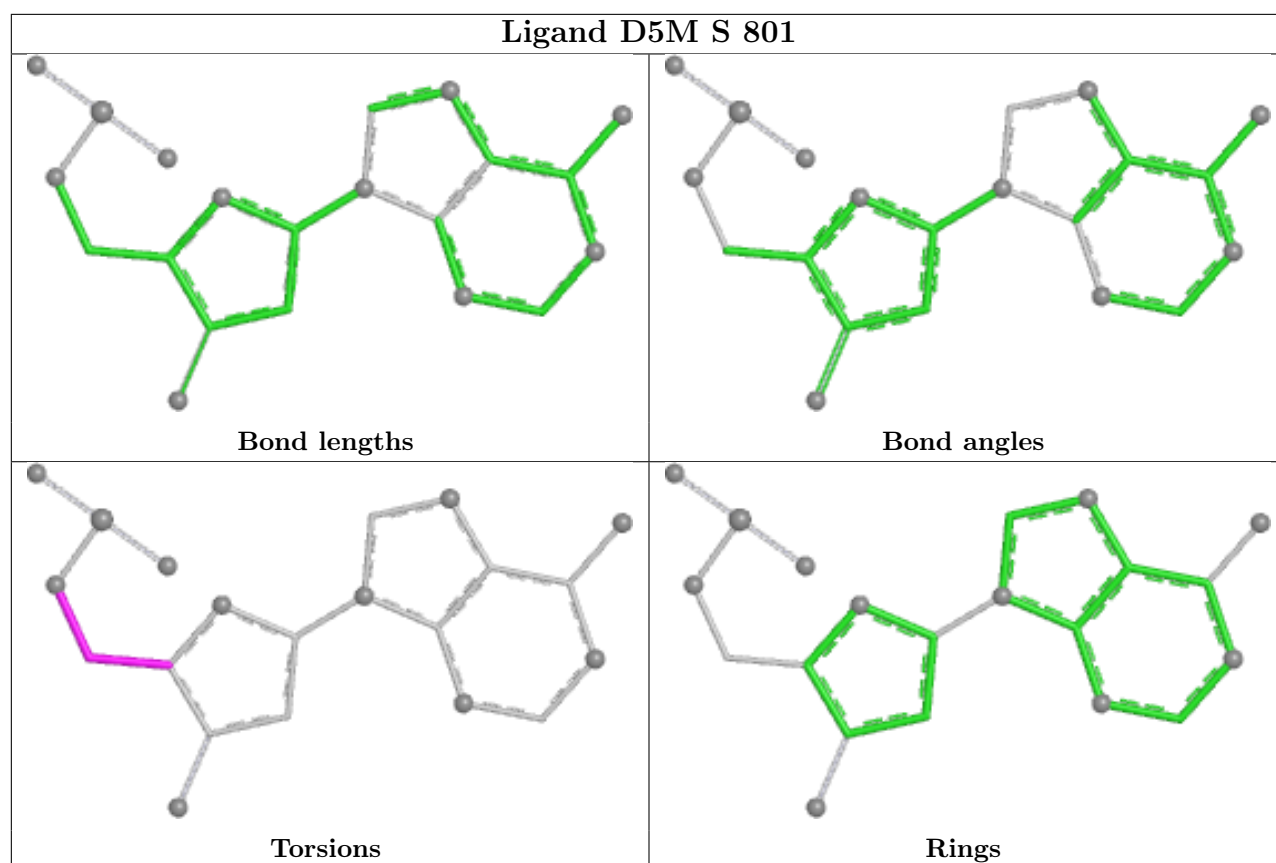
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	801	D5M	3	0
2	O	801	D5M	4	0
2	N	801	D5M	3	0
2	h	801	D5M	3	0
2	u	801	D5M	3	0
2	c	801	D5M	3	0
2	m	801	D5M	3	0
2	L	801	D5M	3	0
2	r	801	D5M	3	0
2	U	801	D5M	3	0
2	B	801	D5M	3	0
2	f	801	D5M	4	0
2	s	801	D5M	3	0
2	D	801	D5M	3	0
2	g	801	D5M	4	0
2	l	801	D5M	3	0
2	C	801	D5M	3	0
2	Q	801	D5M	3	0
2	b	801	D5M	4	0
2	W	801	D5M	3	0
2	K	801	D5M	3	0
2	A	801	D5M	3	0
2	5	801	D5M	3	0
2	j	801	D5M	3	0
2	e	801	D5M	3	0
2	q	801	D5M	3	0
2	t	801	D5M	3	0
2	X	801	D5M	3	0
2	n	801	D5M	3	0
2	G	801	D5M	3	0
2	v	801	D5M	3	0
2	l	801	D5M	4	0
2	d	801	D5M	3	0

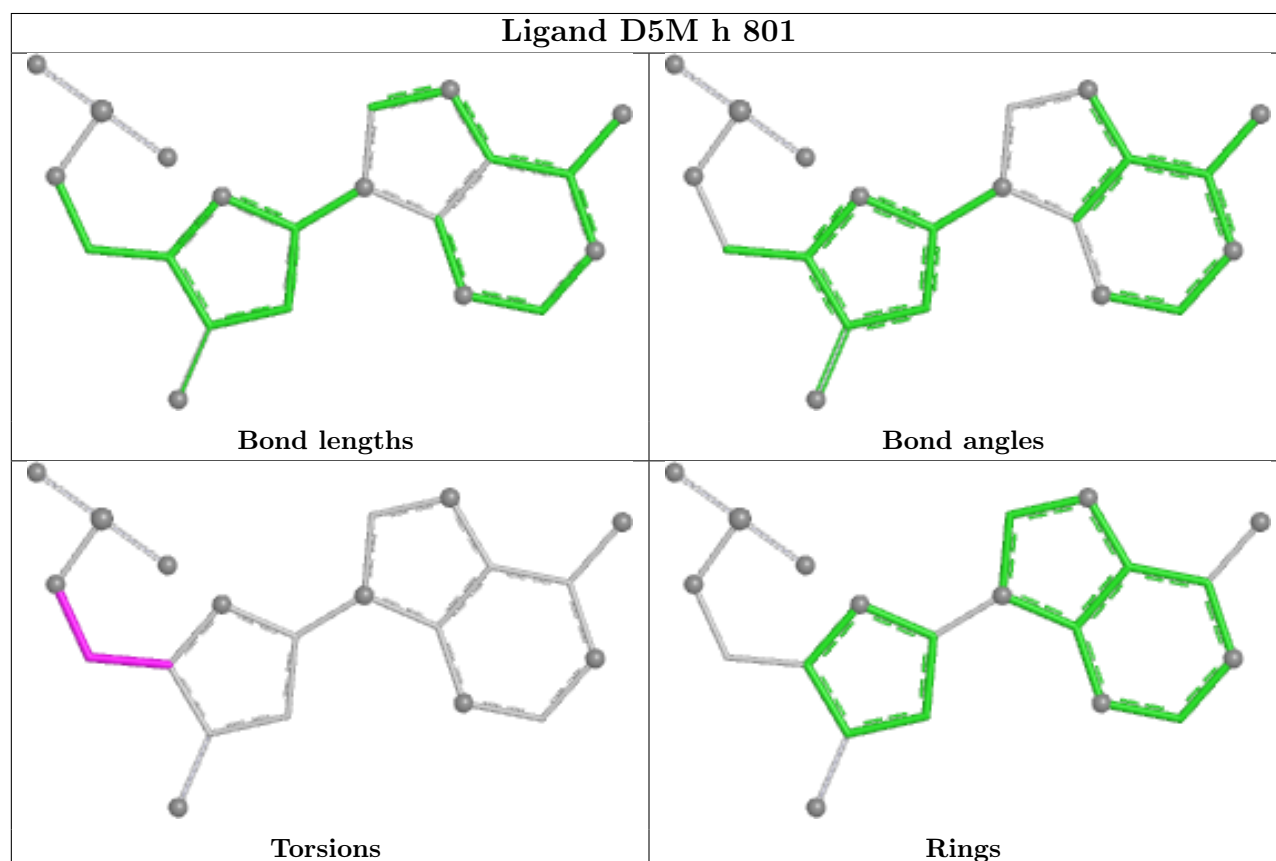
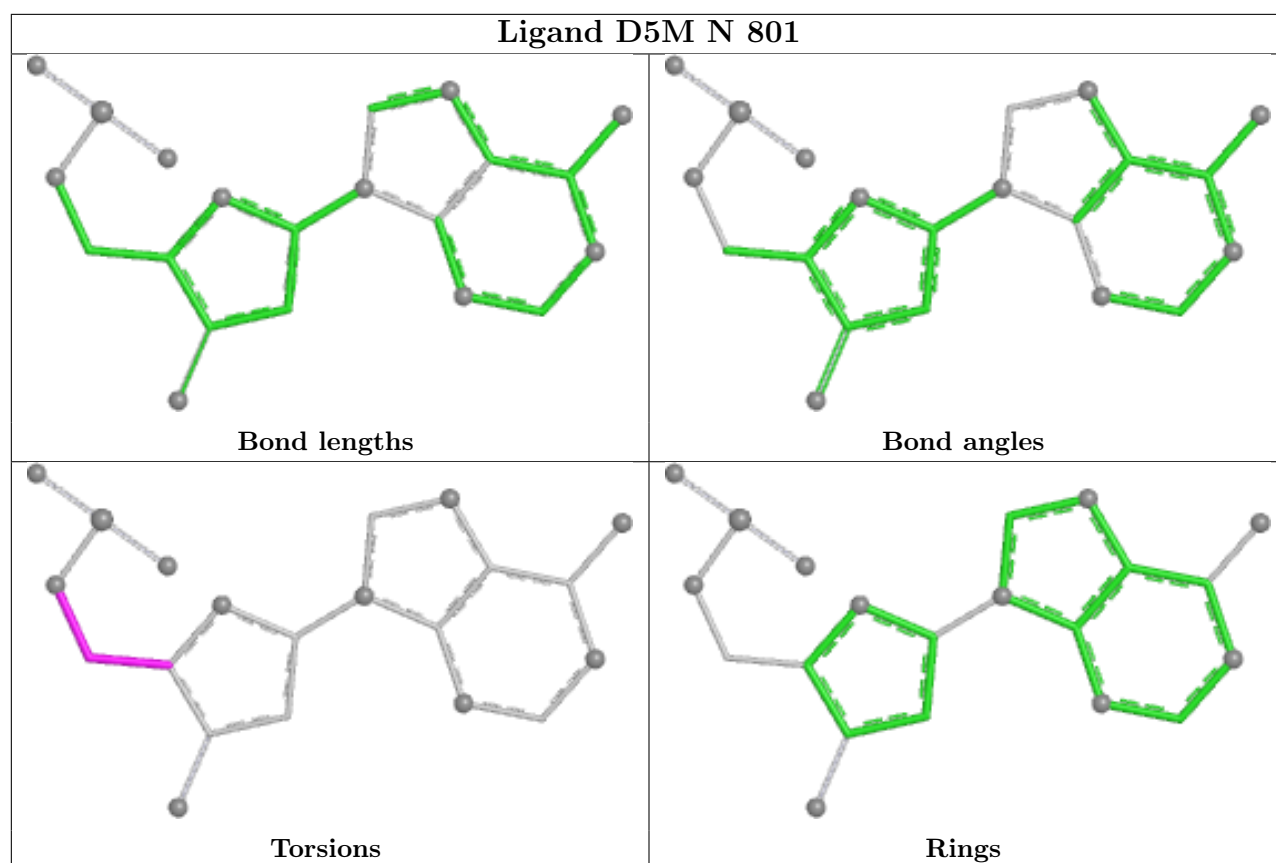
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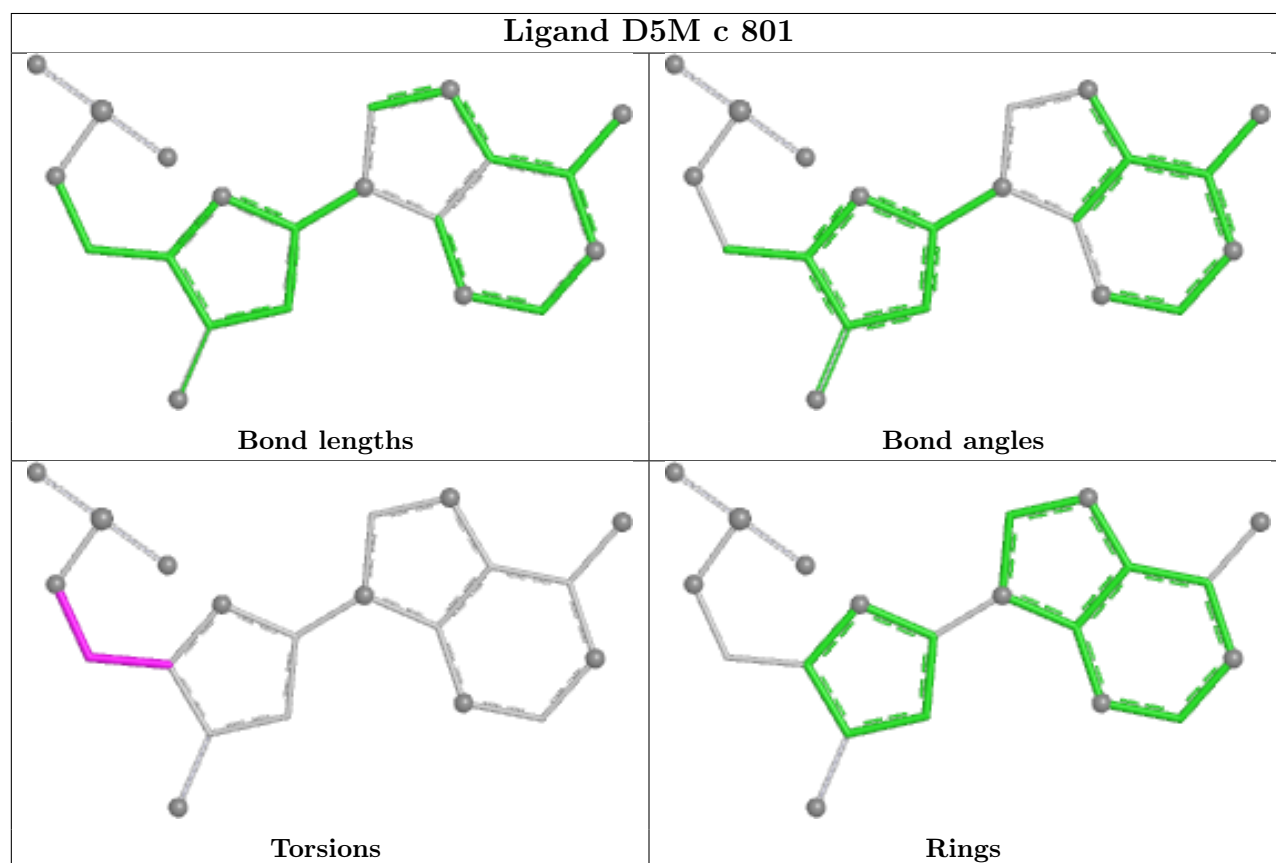
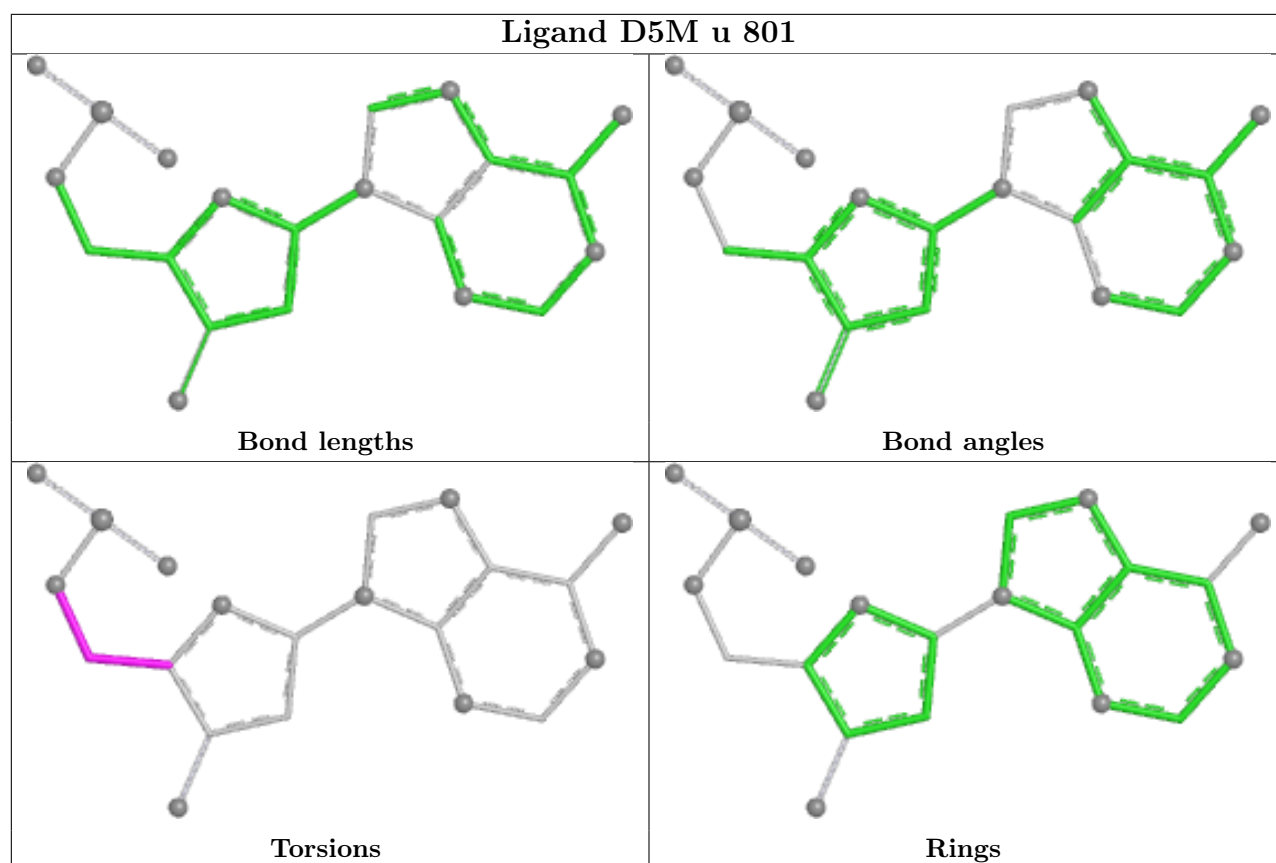
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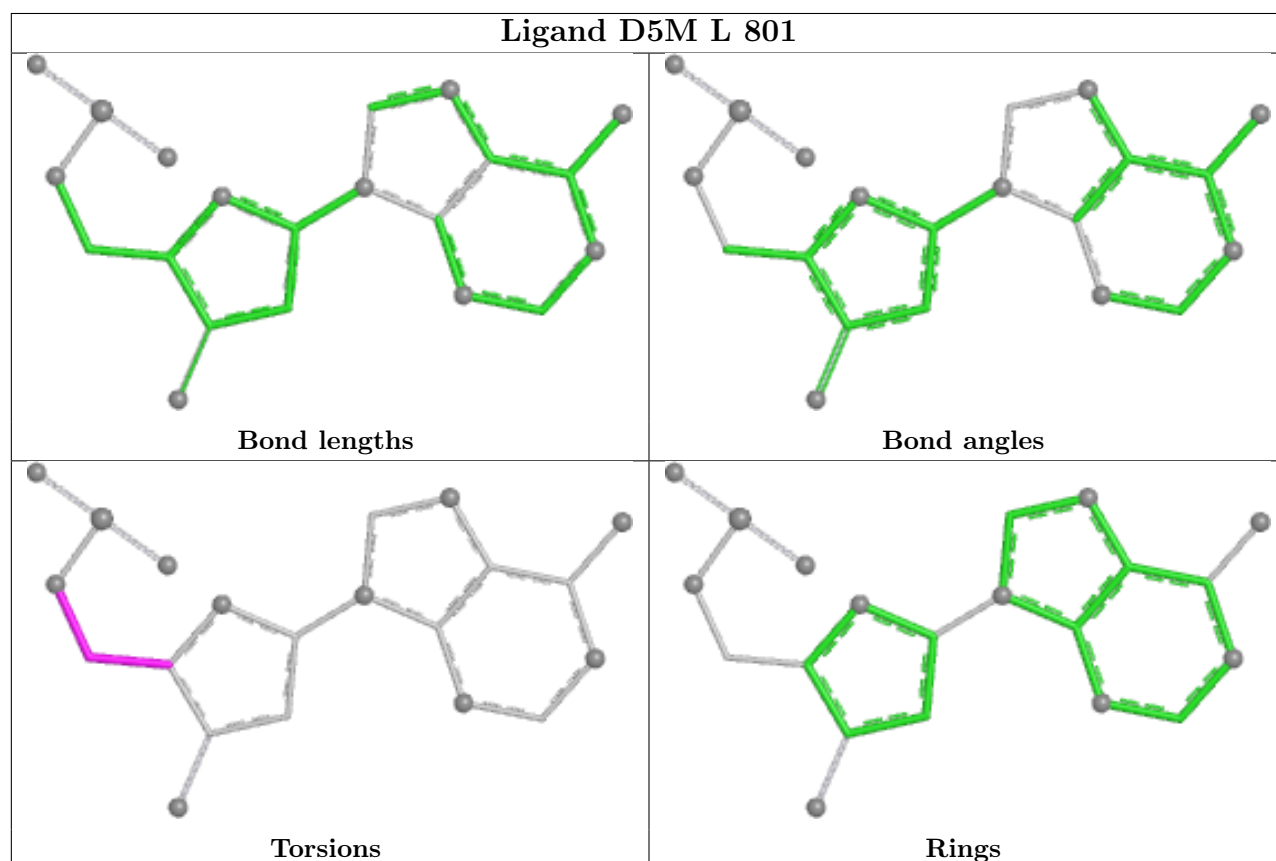
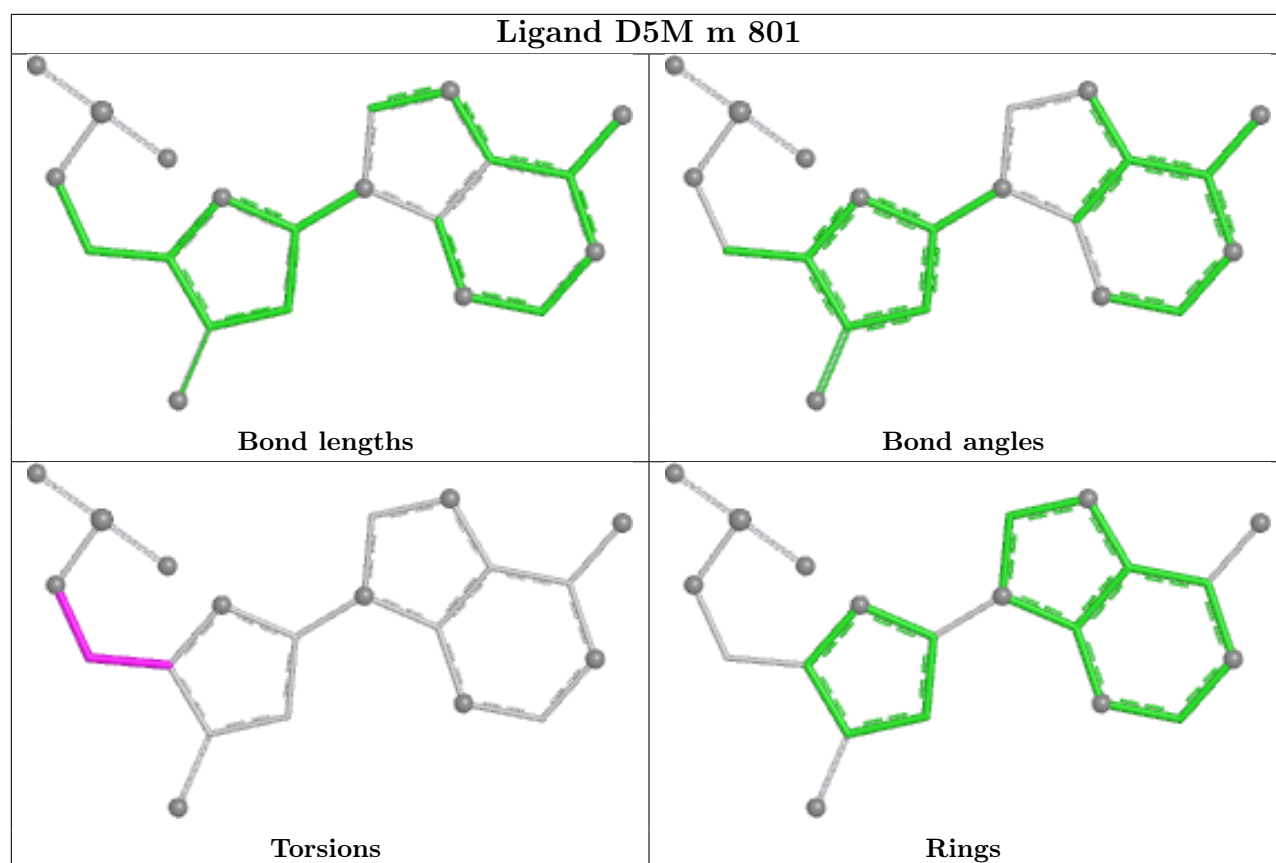
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	i	801	D5M	3	0
2	8	801	D5M	3	0
2	o	801	D5M	3	0
2	7	801	D5M	3	0
2	Z	801	D5M	3	0
2	6	801	D5M	3	0
2	3	801	D5M	3	0
2	p	801	D5M	3	0
2	w	801	D5M	3	0
2	J	801	D5M	3	0
2	Y	801	D5M	3	0
2	y	801	D5M	3	0
2	E	801	D5M	3	0
2	P	801	D5M	3	0
2	T	801	D5M	3	0
2	F	801	D5M	3	0
2	I	801	D5M	3	0
2	k	801	D5M	3	0
2	2	801	D5M	3	0
2	H	801	D5M	3	0
2	V	801	D5M	3	0
2	x	801	D5M	3	0
2	4	801	D5M	3	0
2	R	801	D5M	3	0
2	a	801	D5M	3	0
2	z	801	D5M	3	0
2	M	801	D5M	3	0

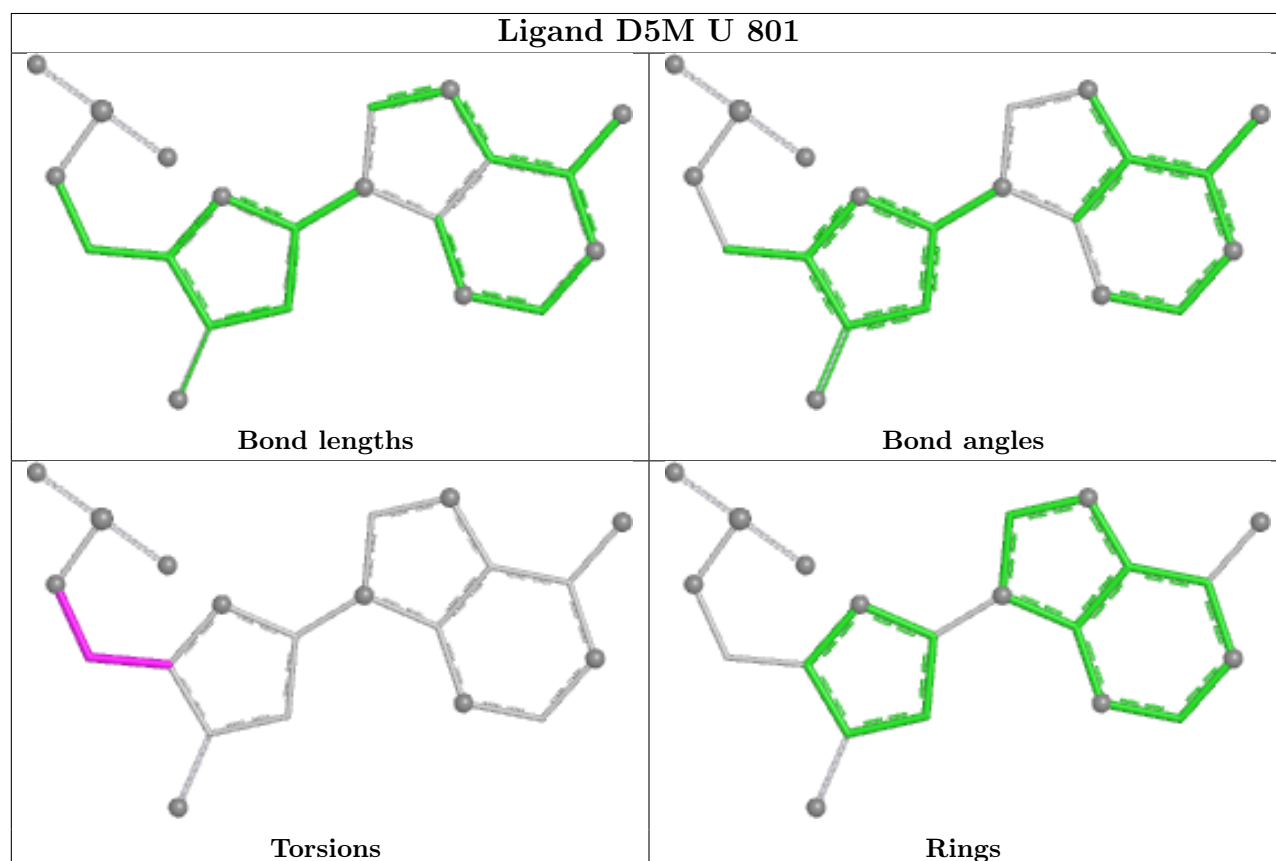
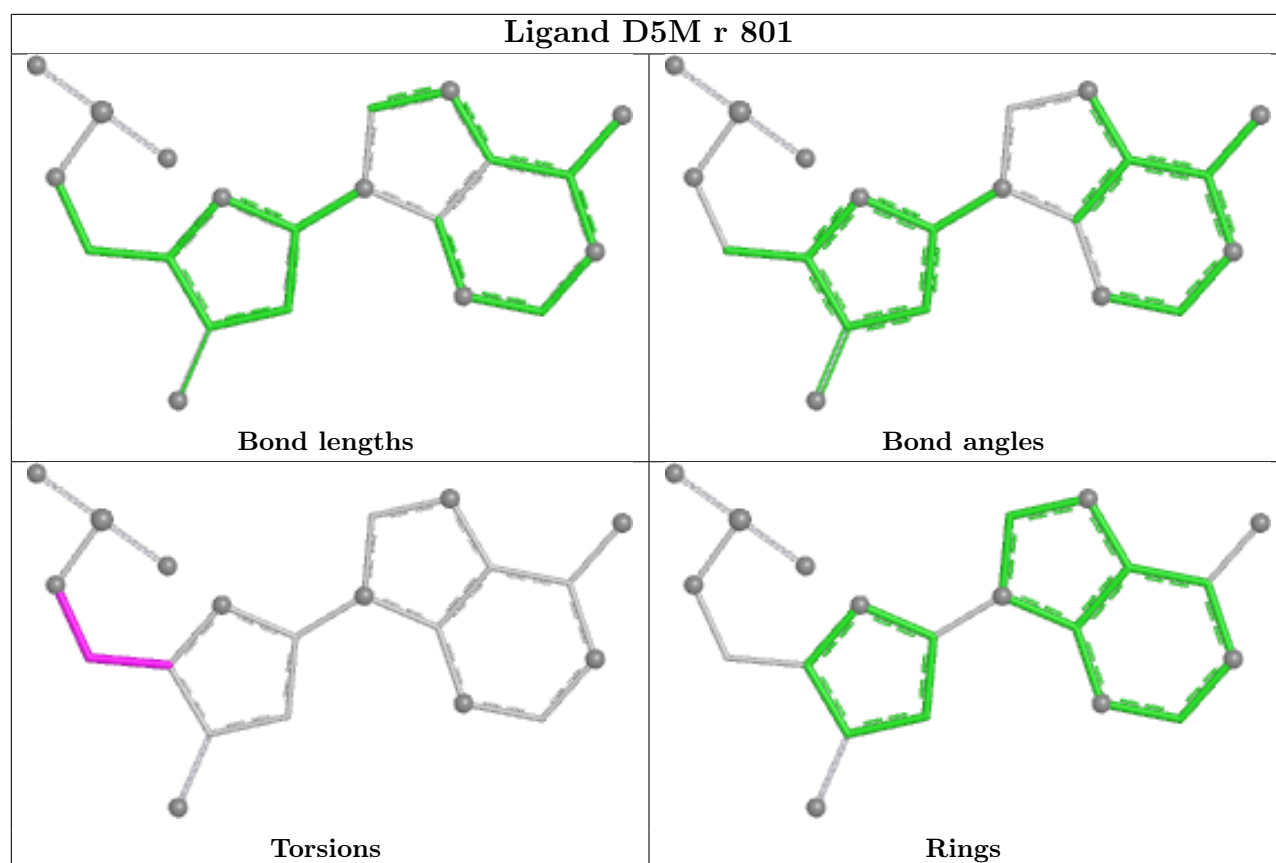
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

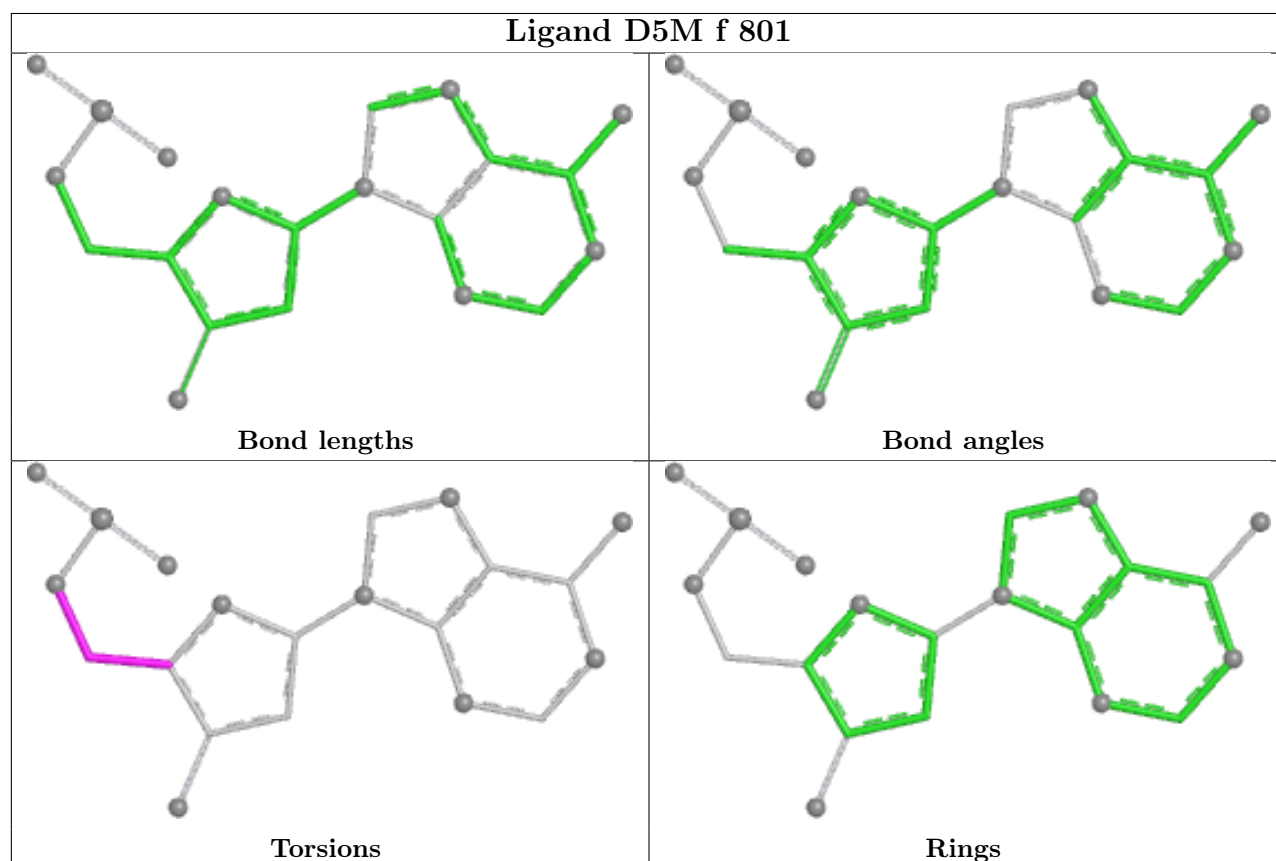
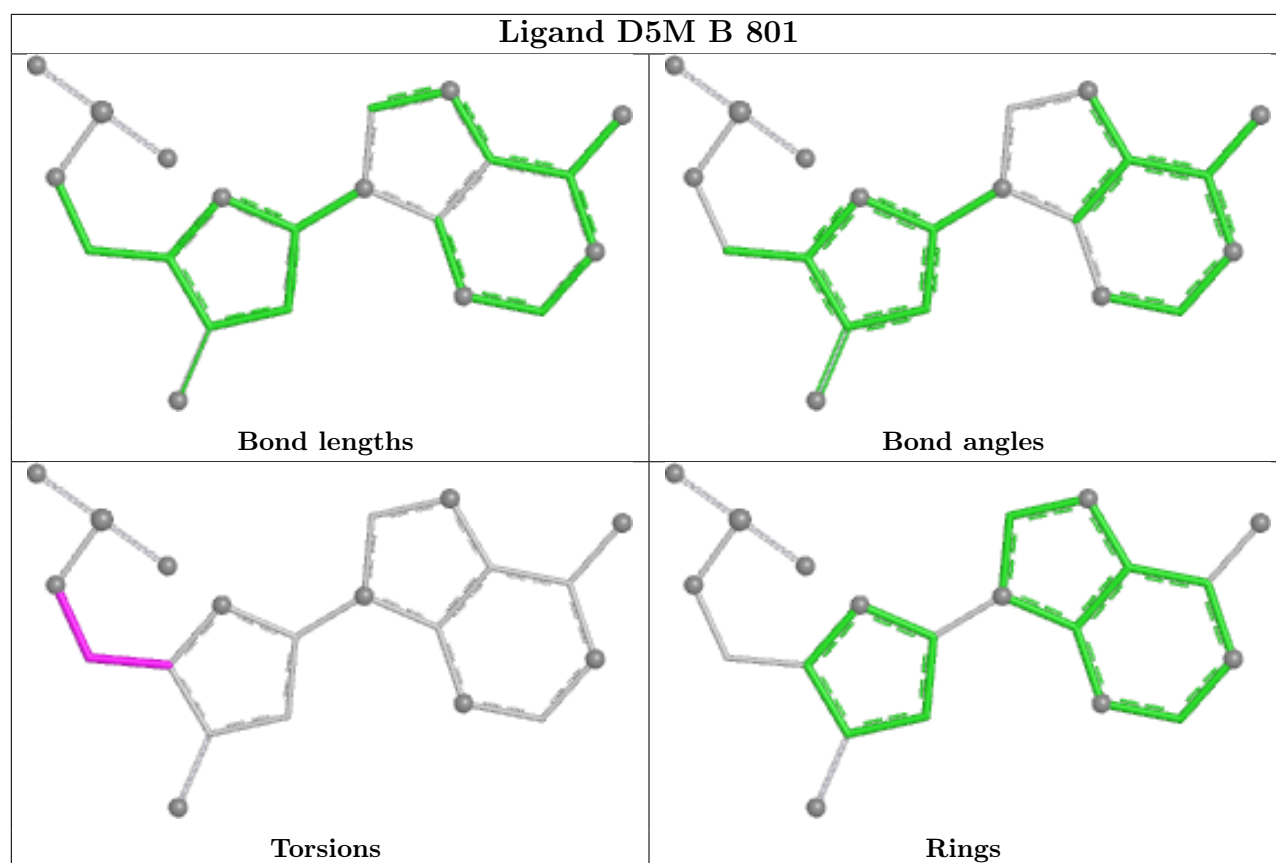


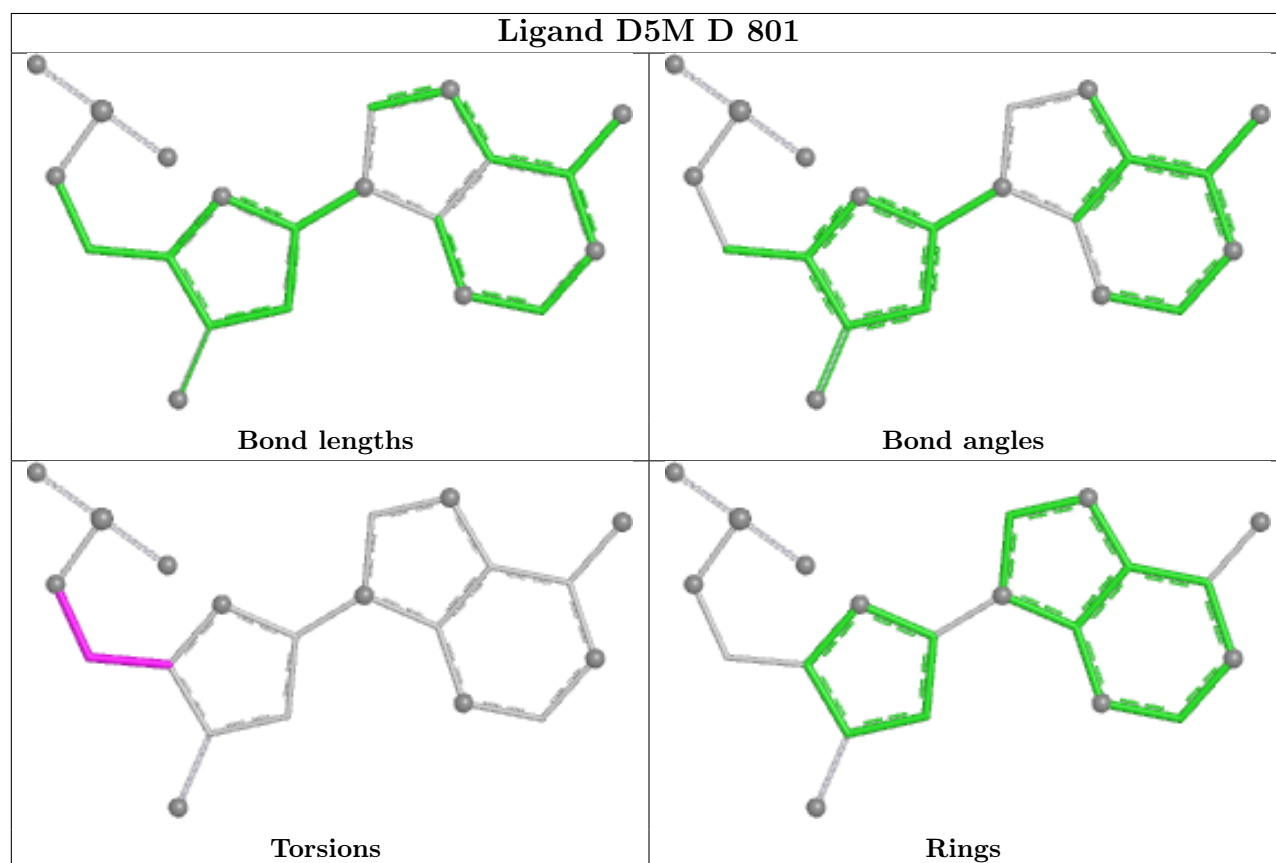
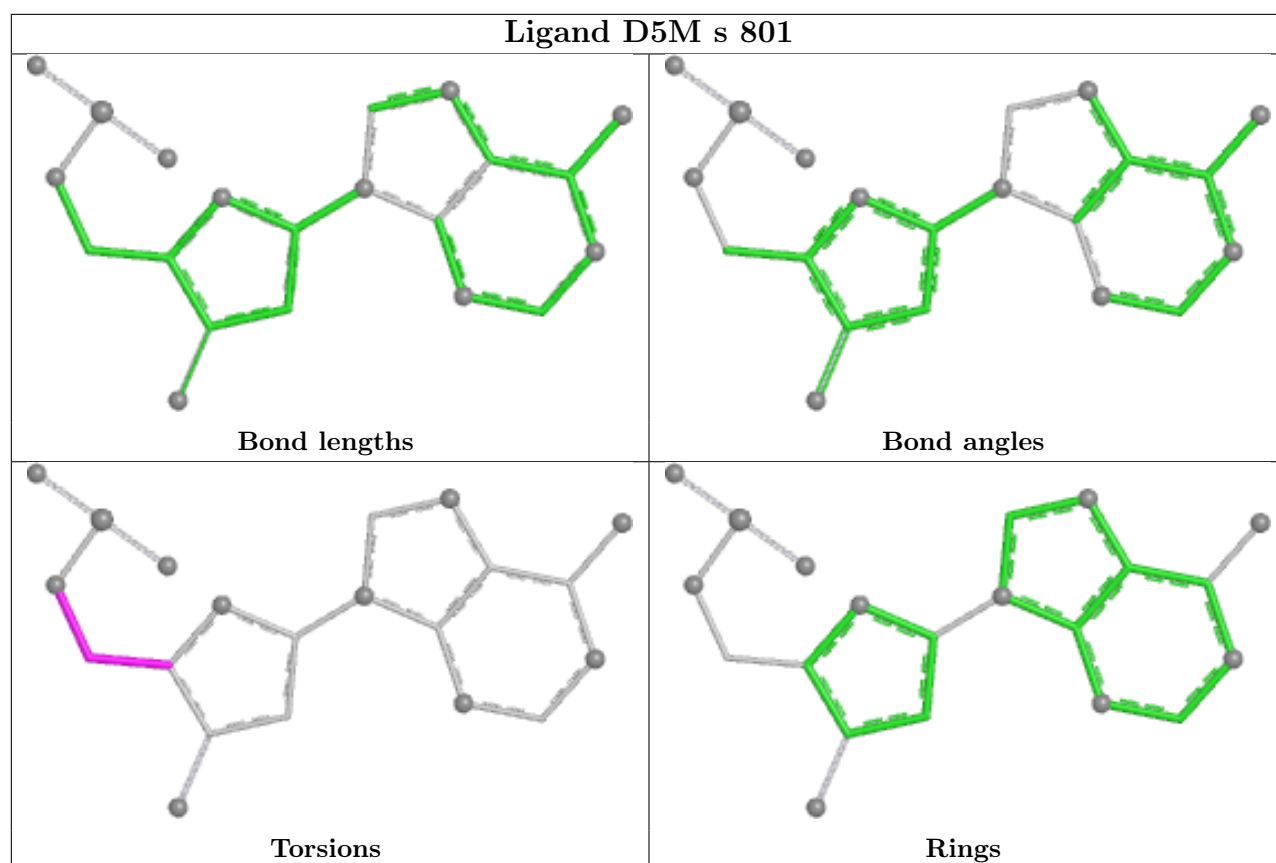


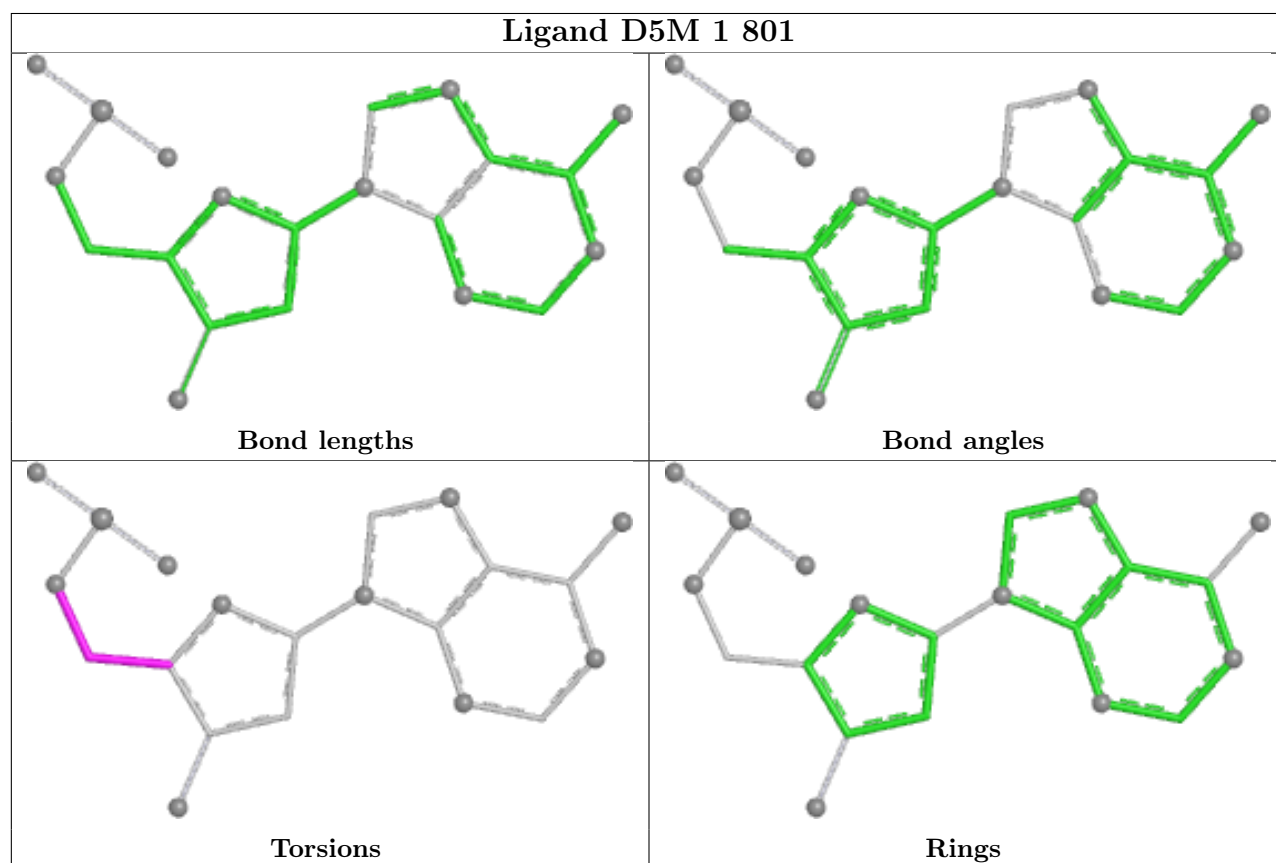
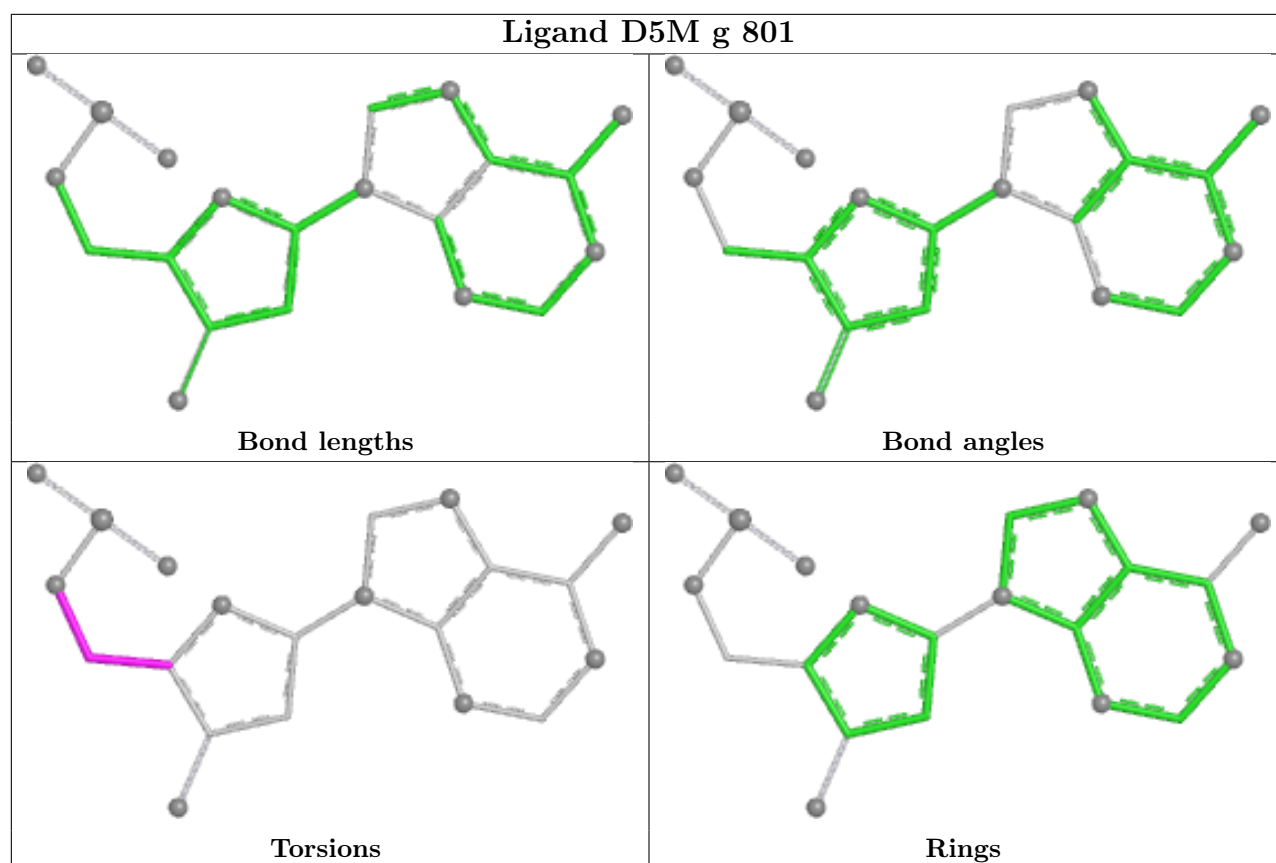


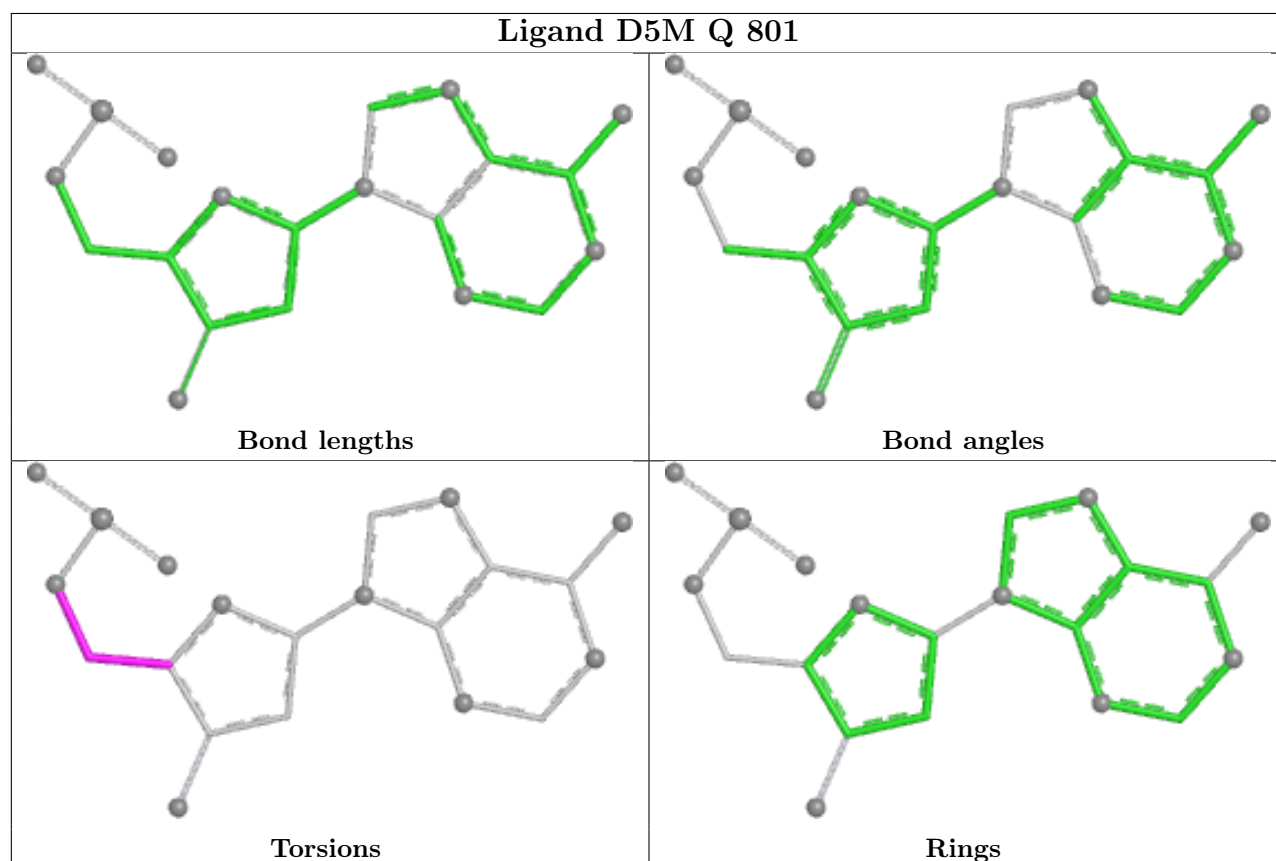
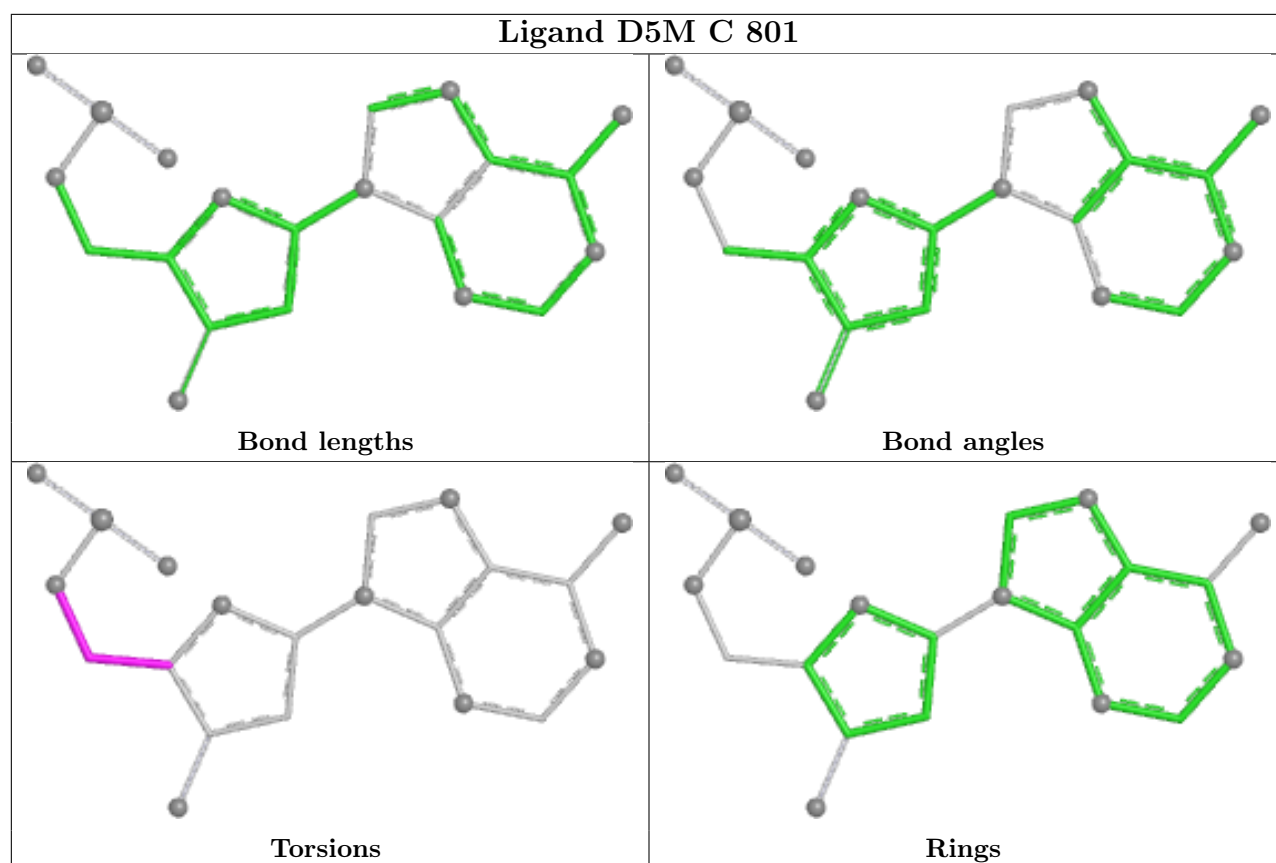


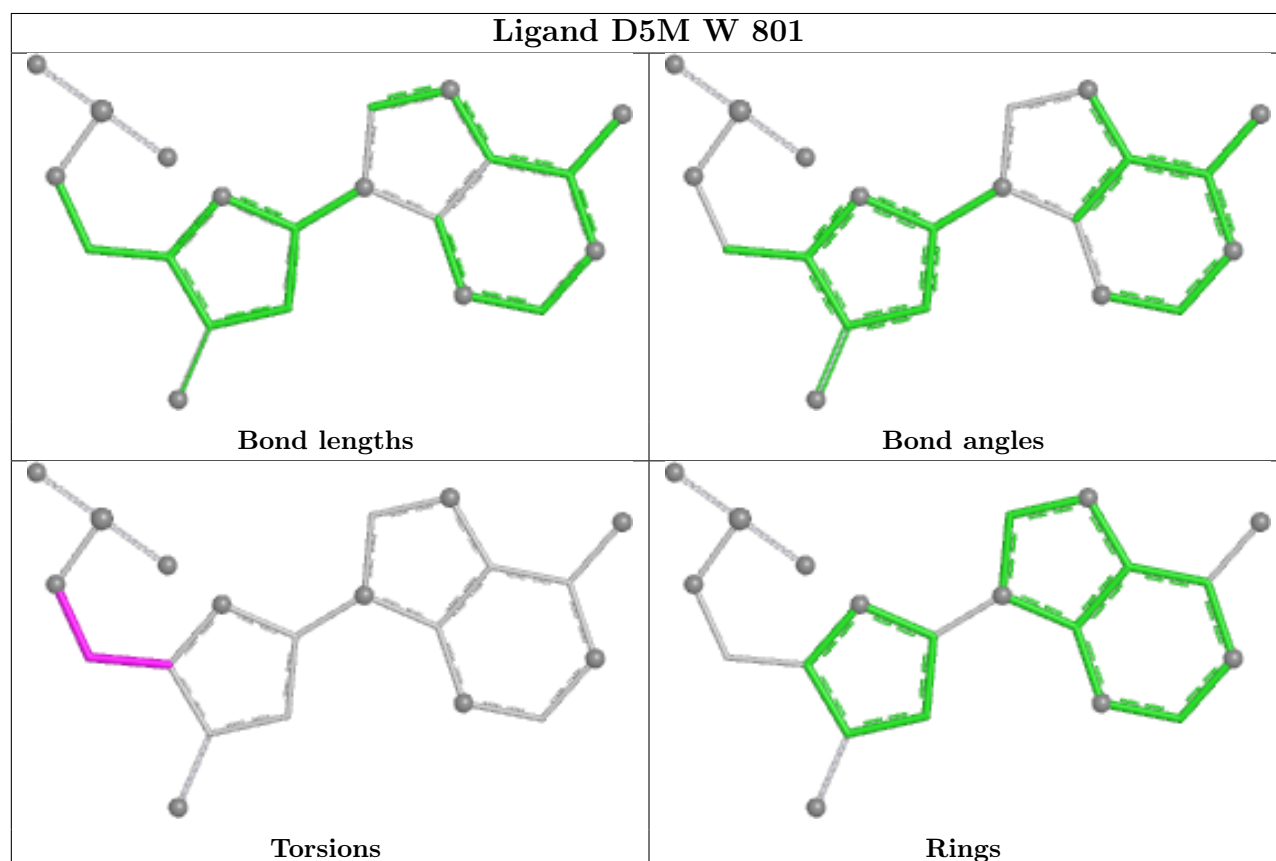
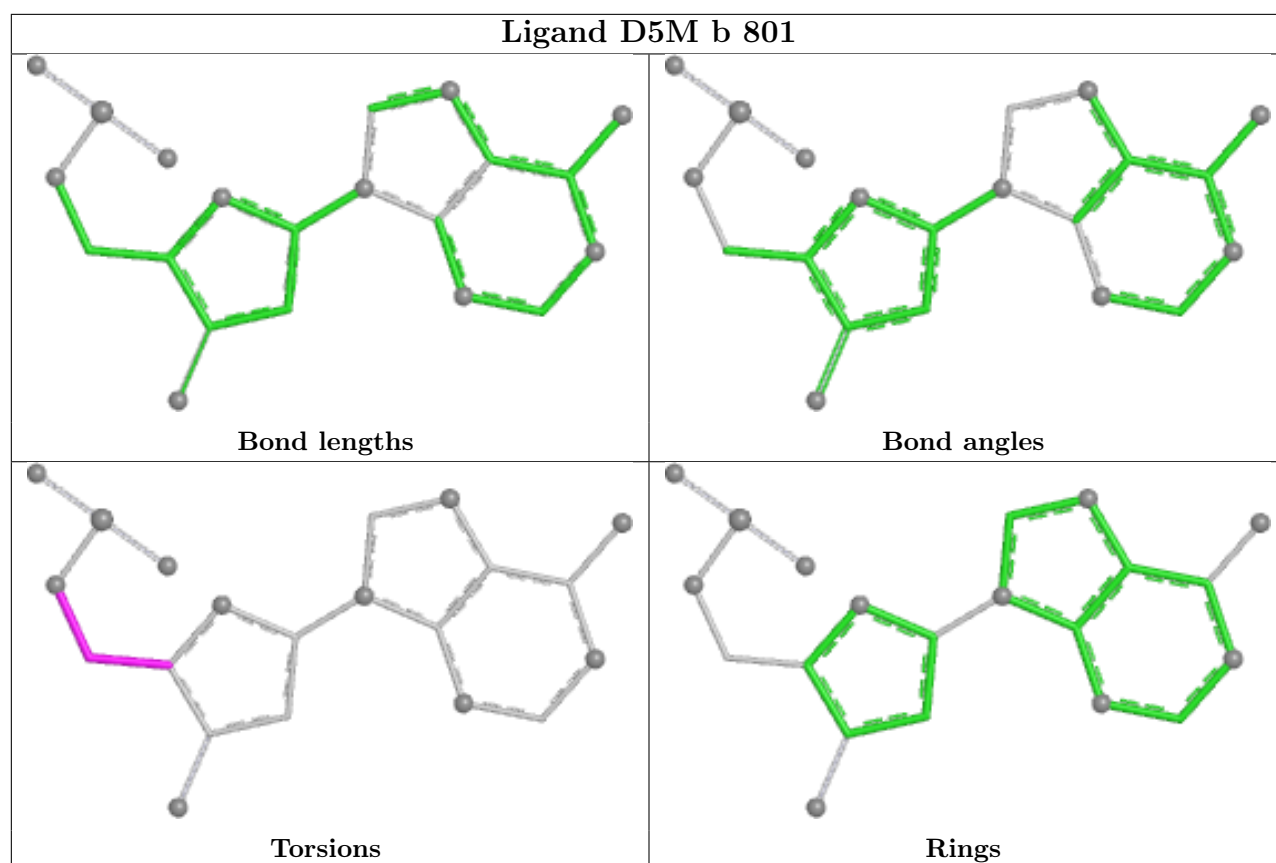


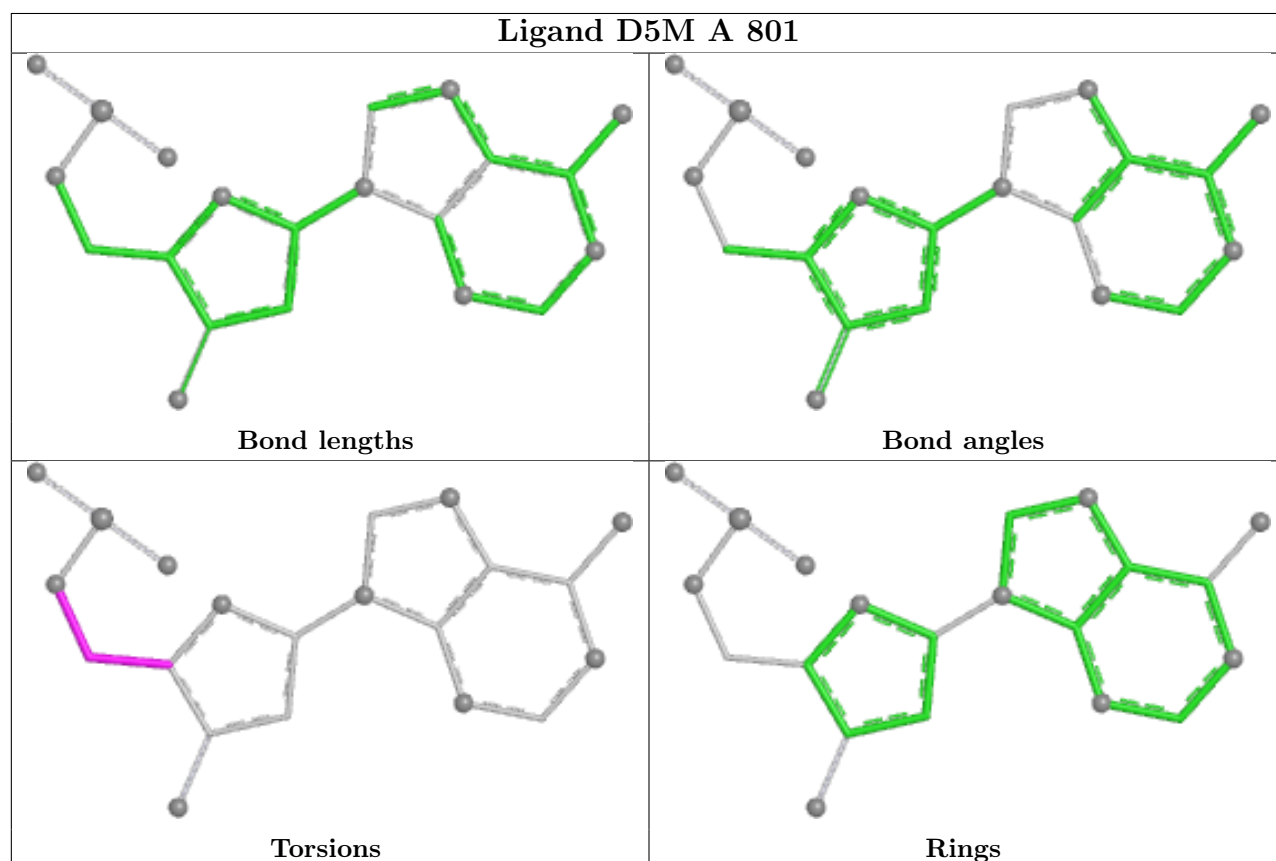
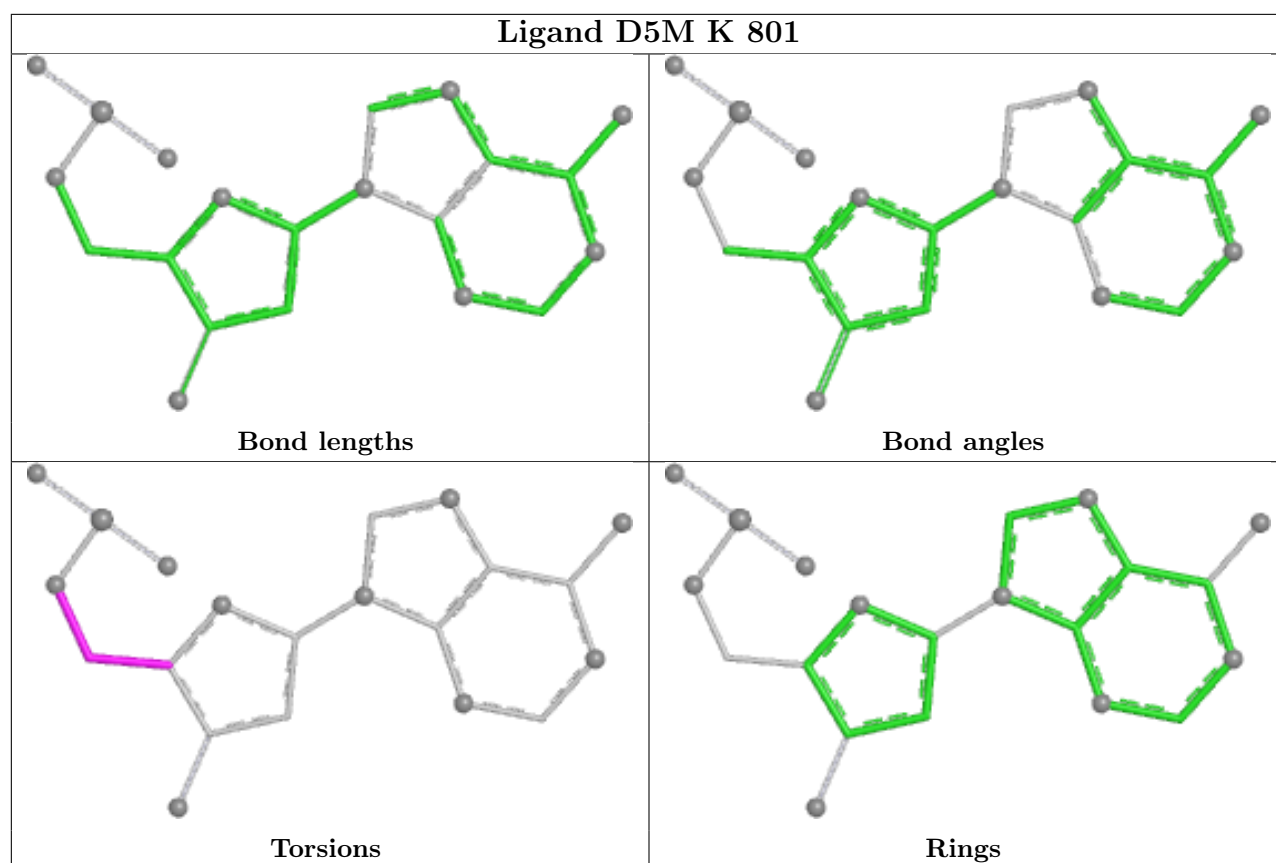


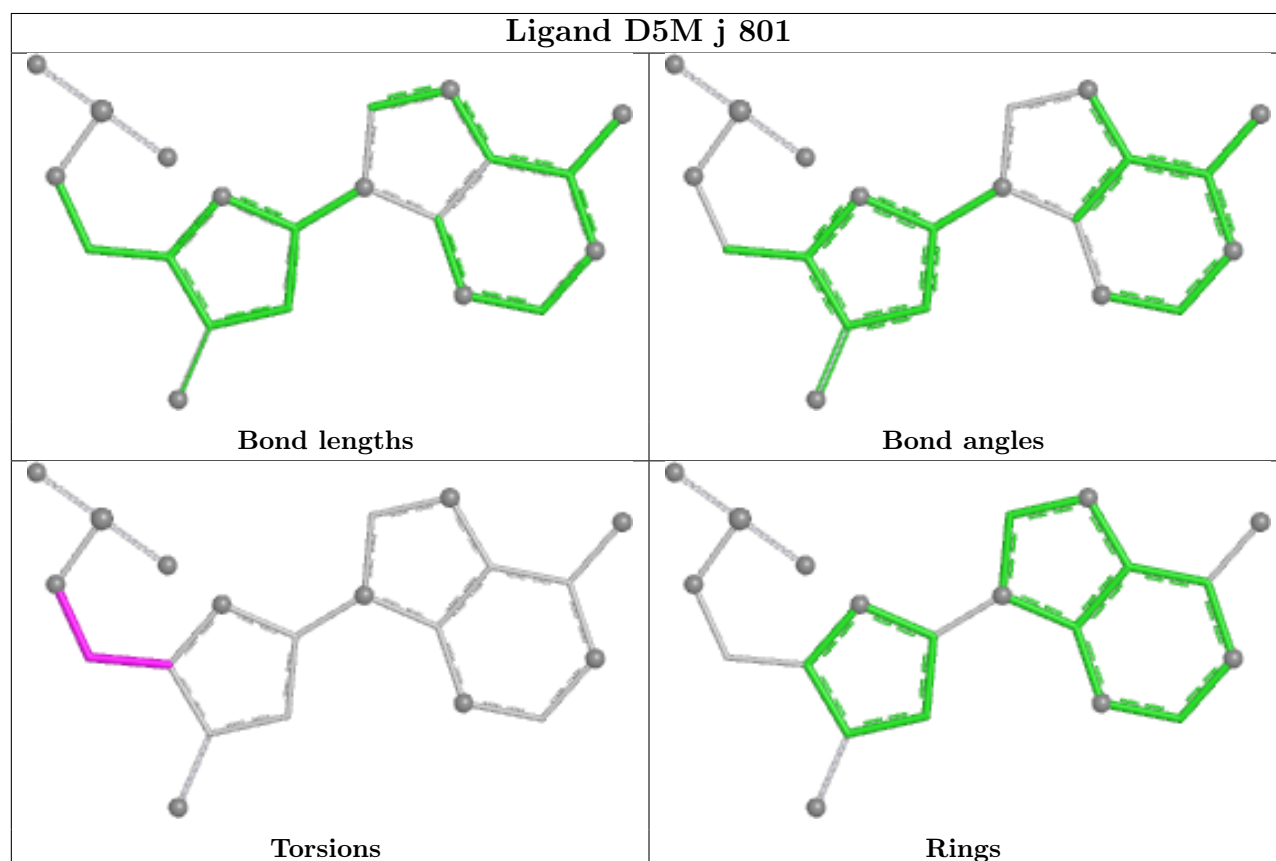
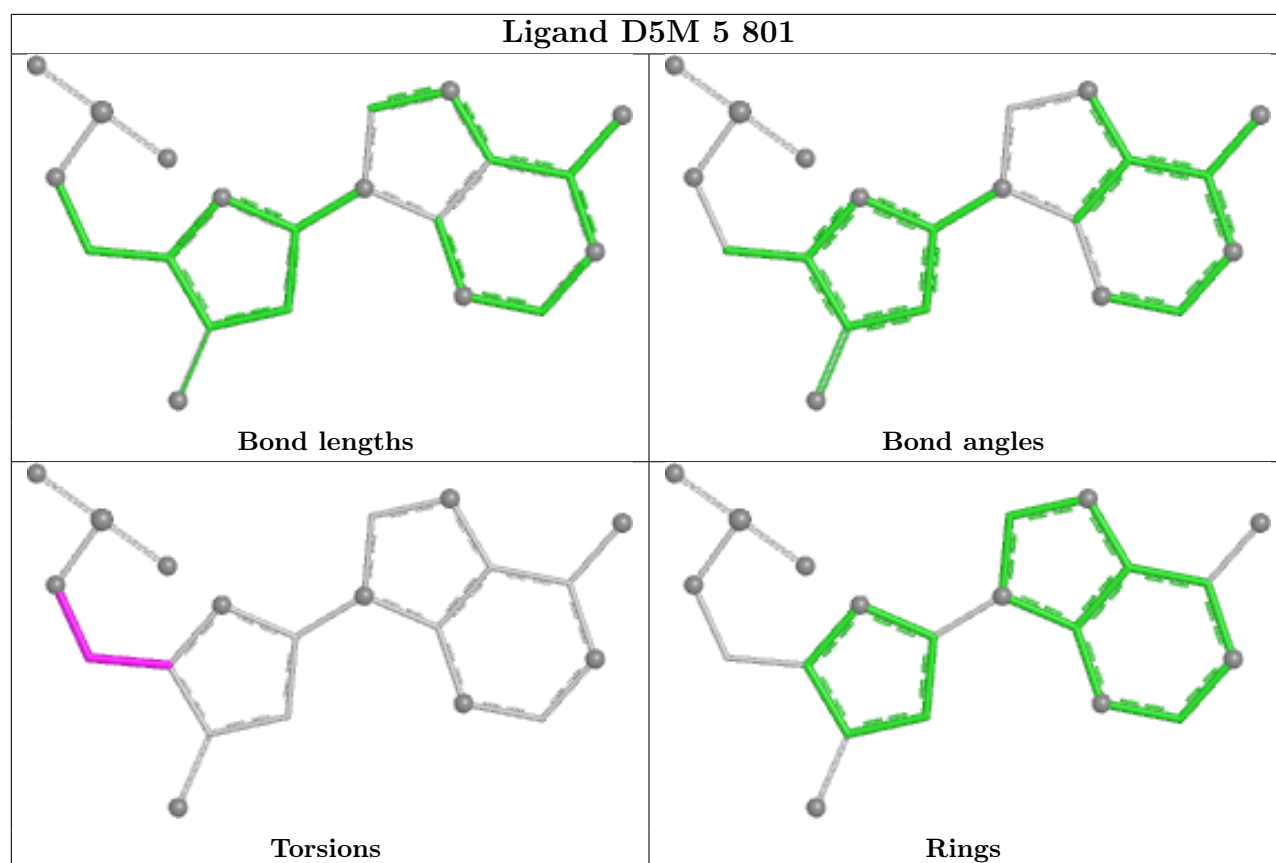


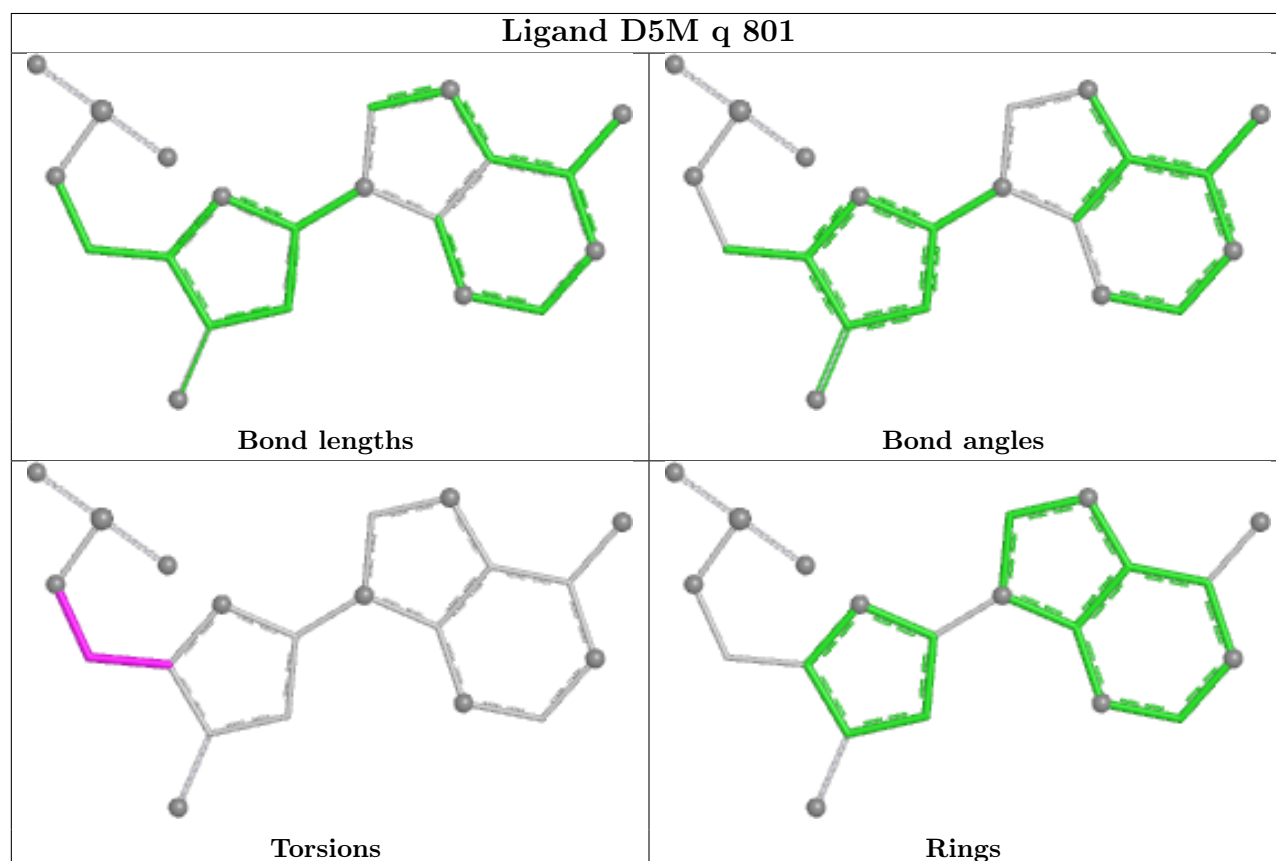
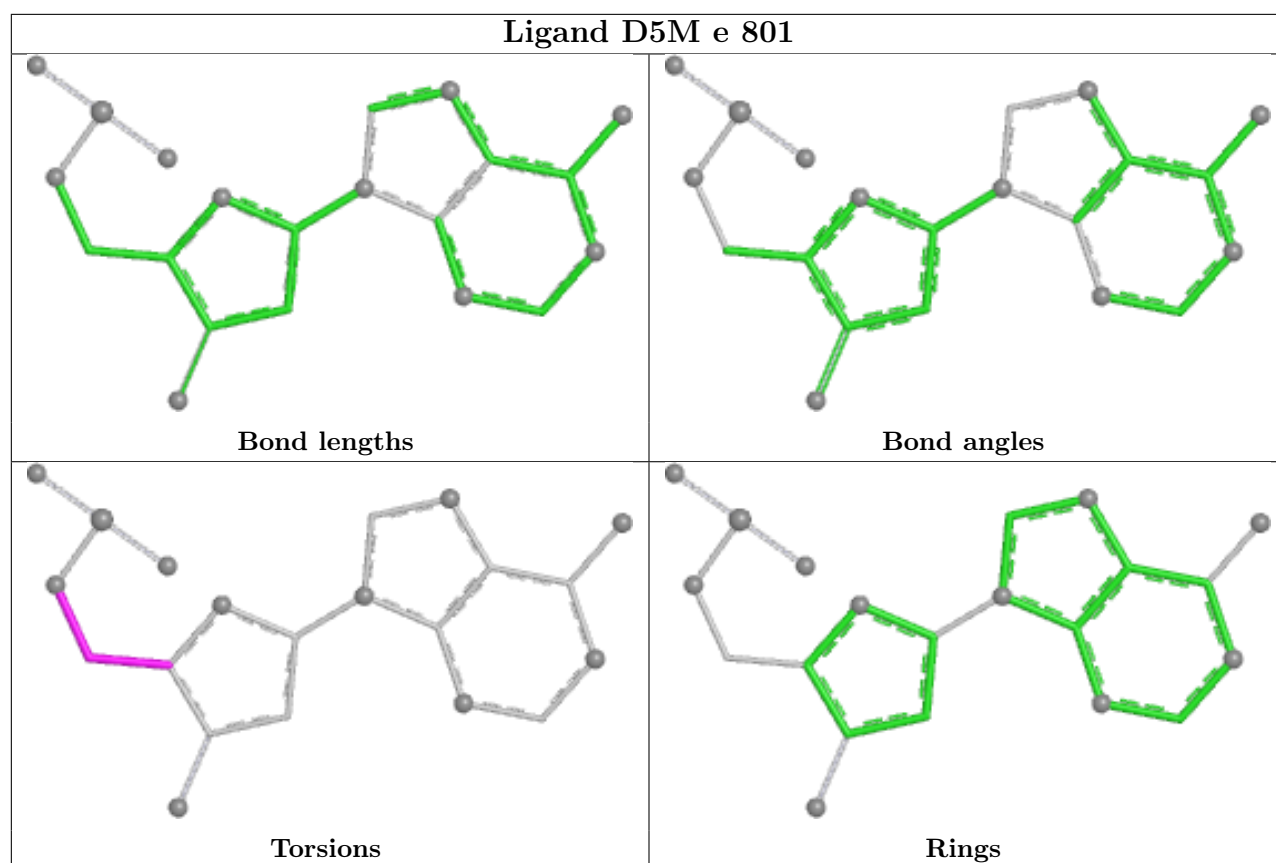


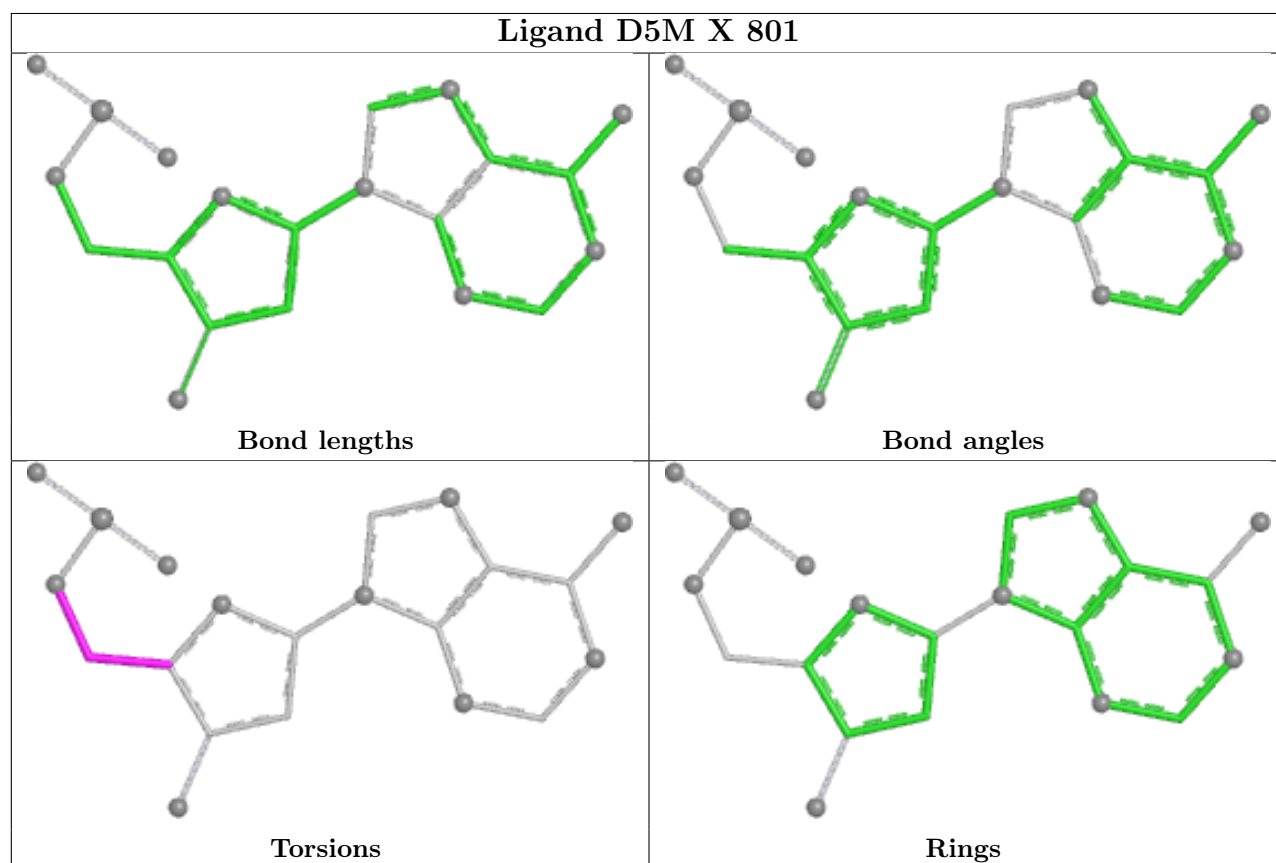
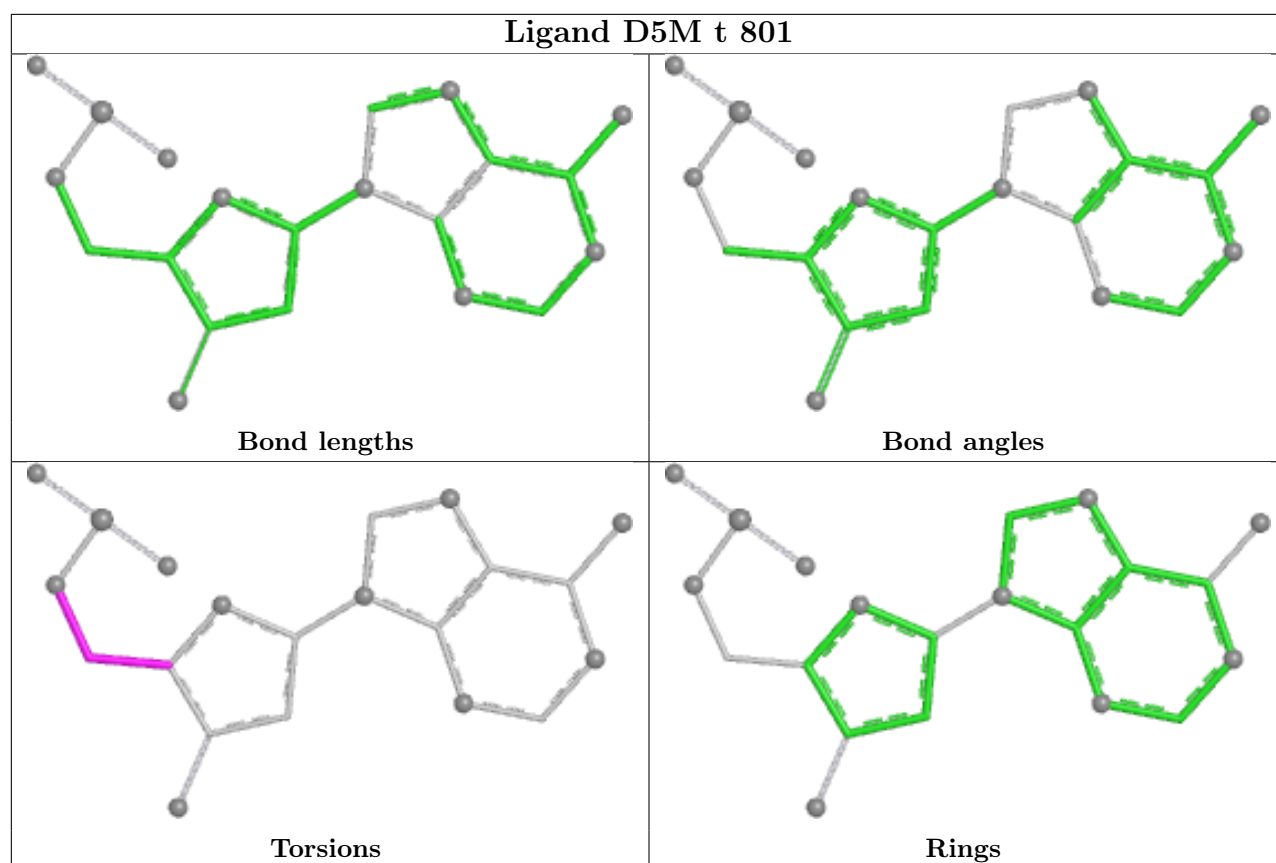


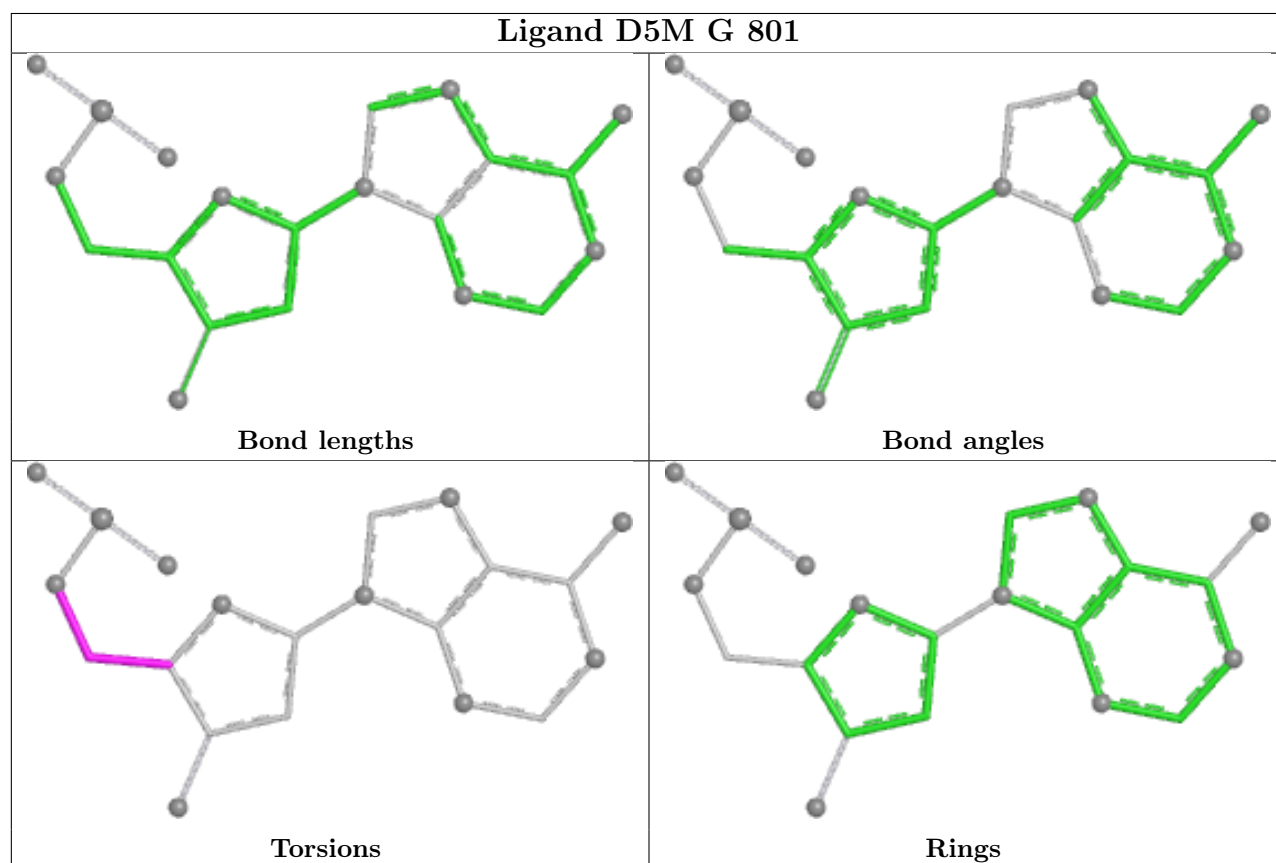
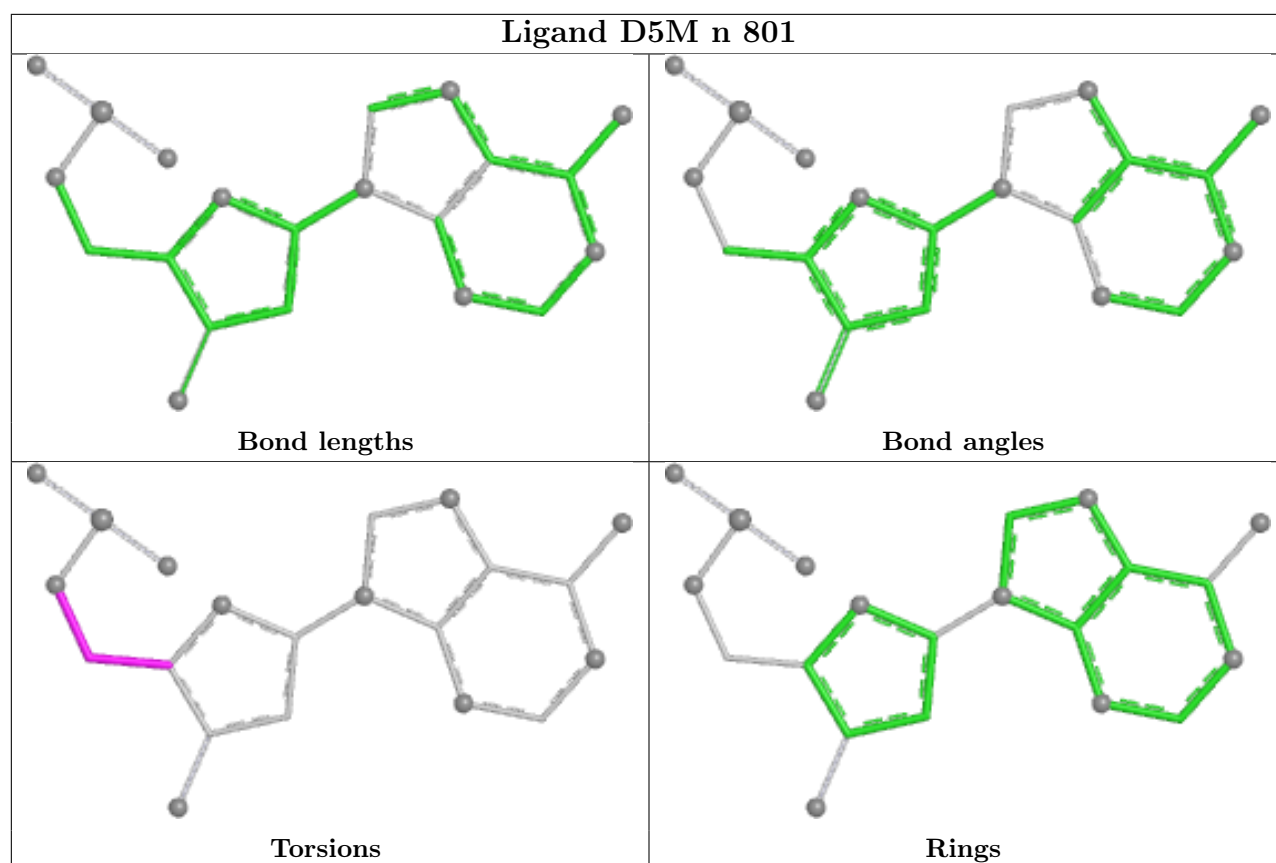


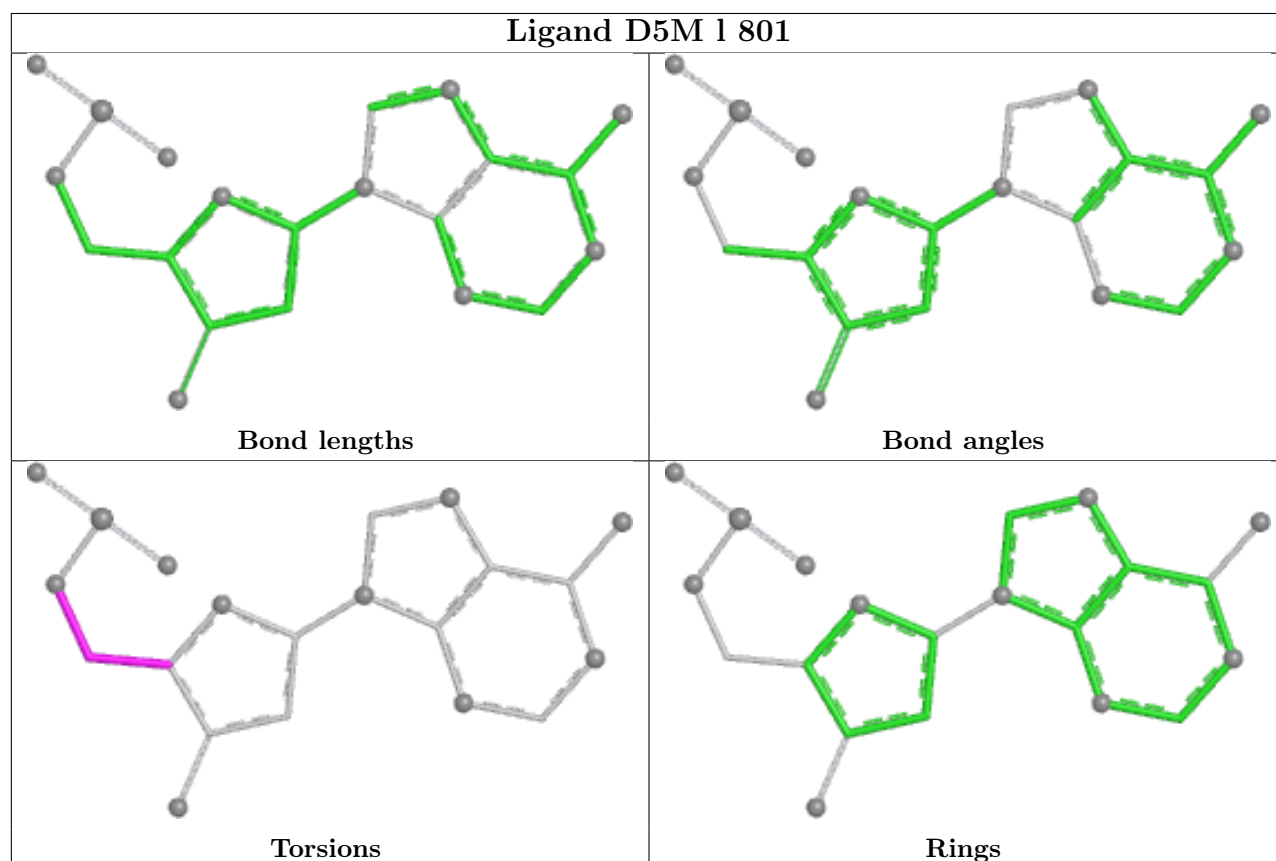
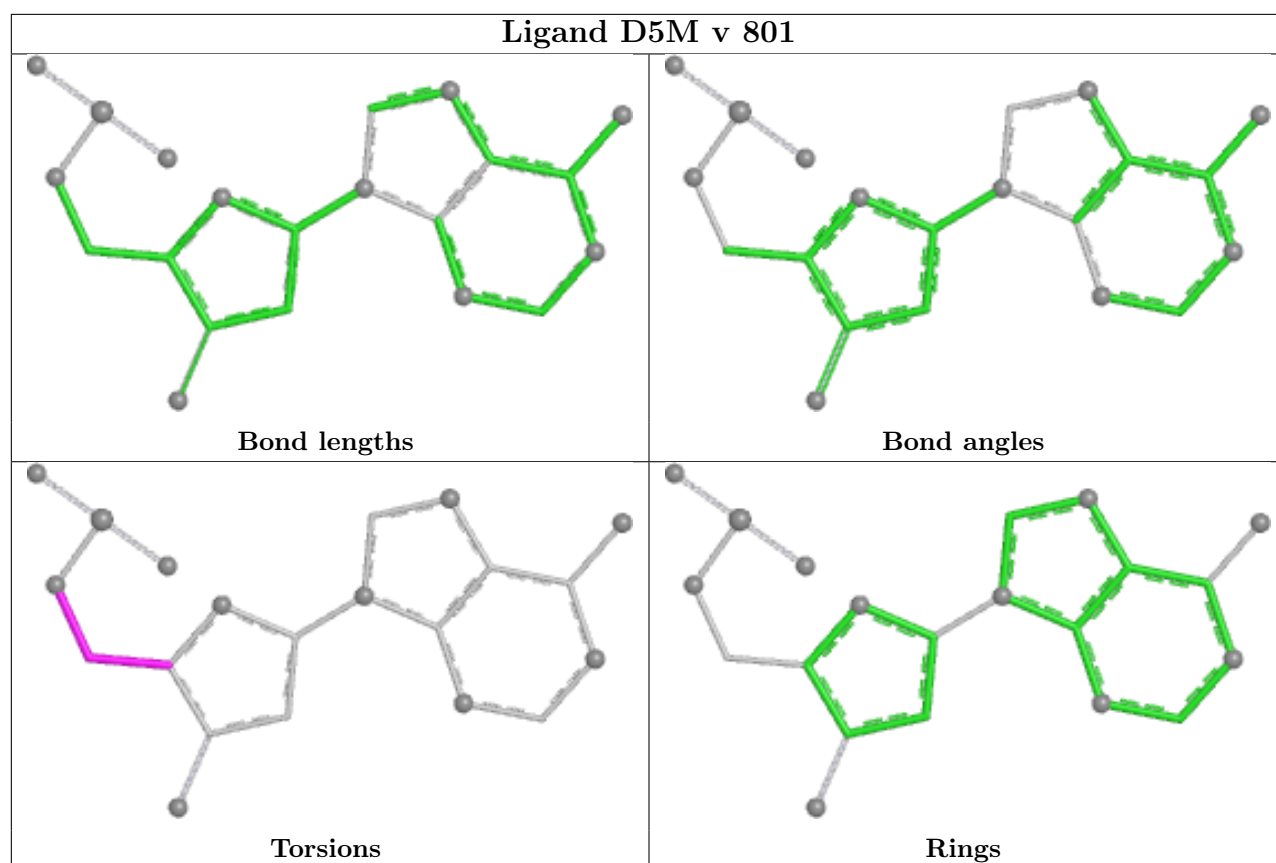


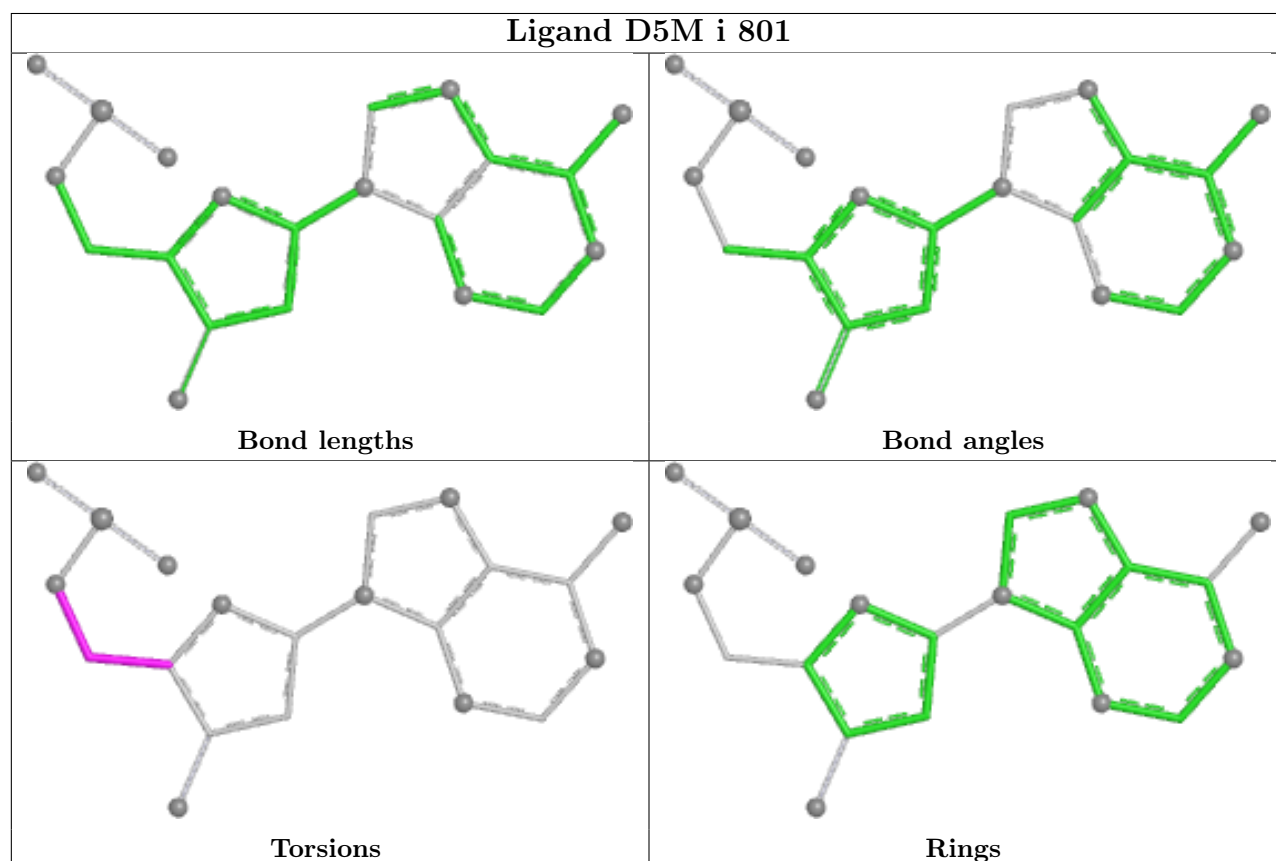
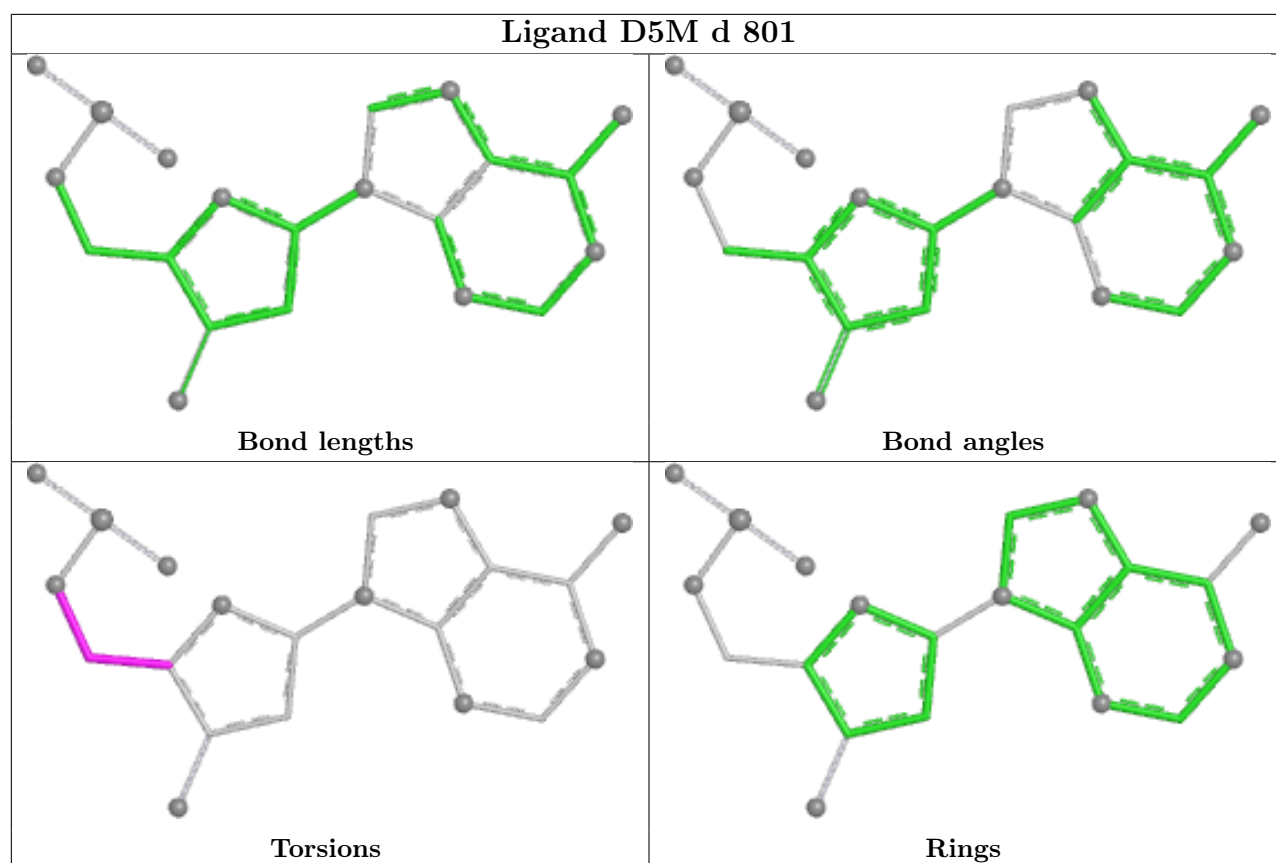


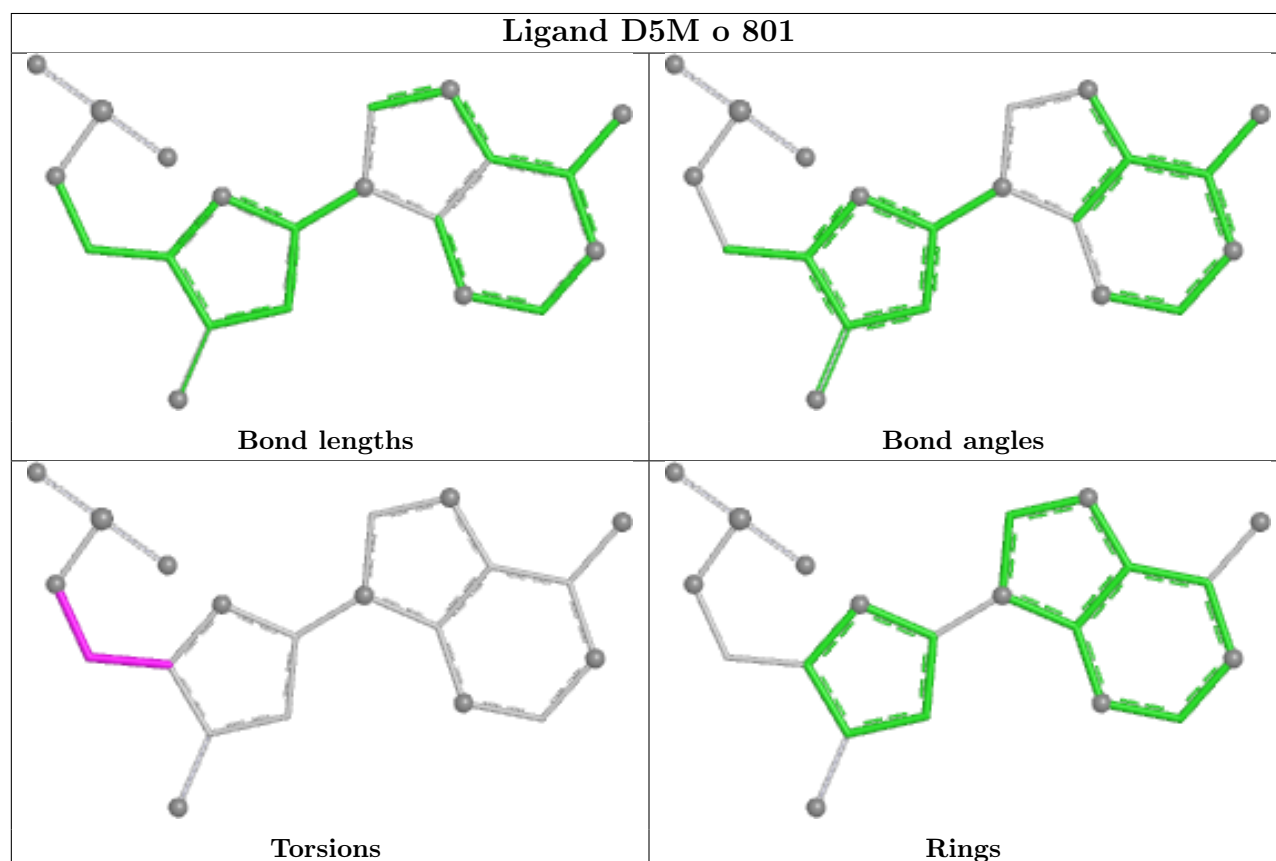
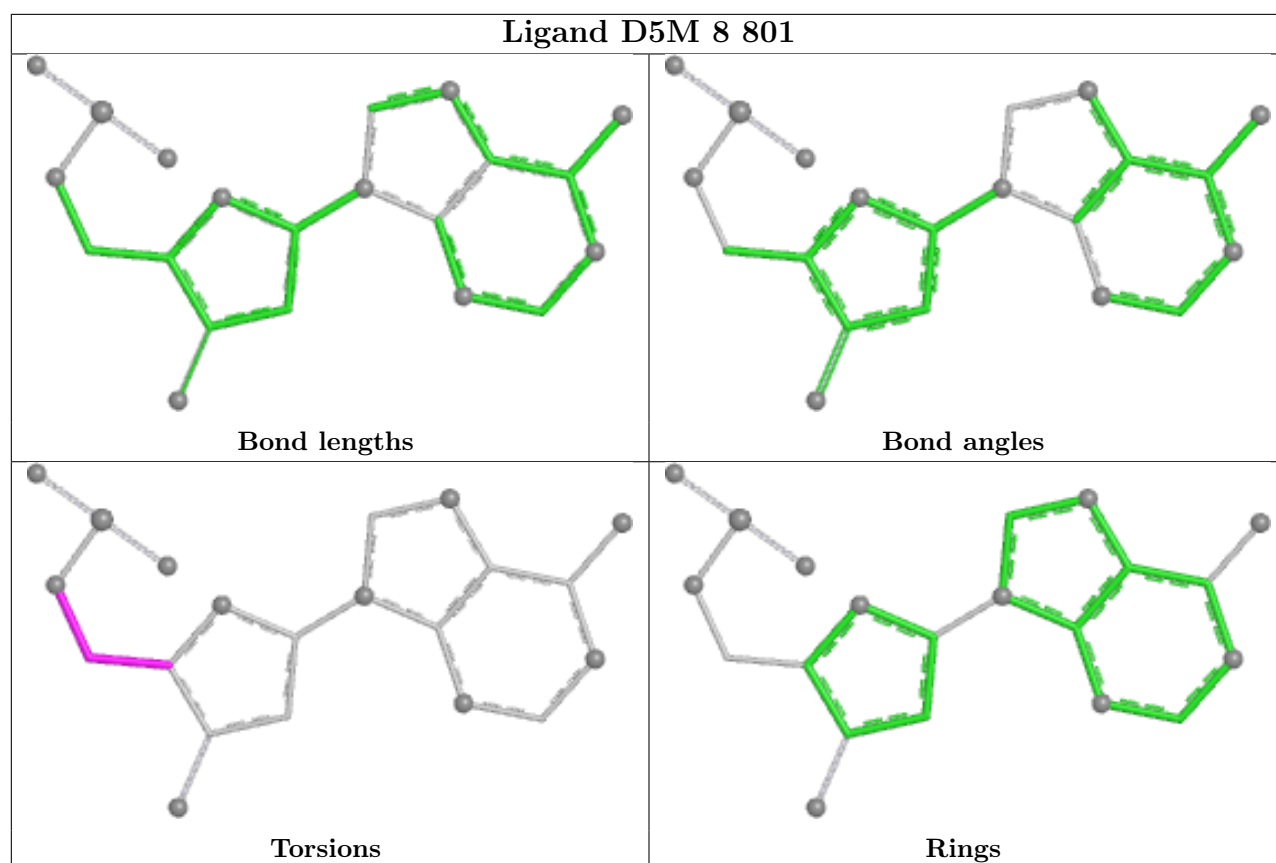


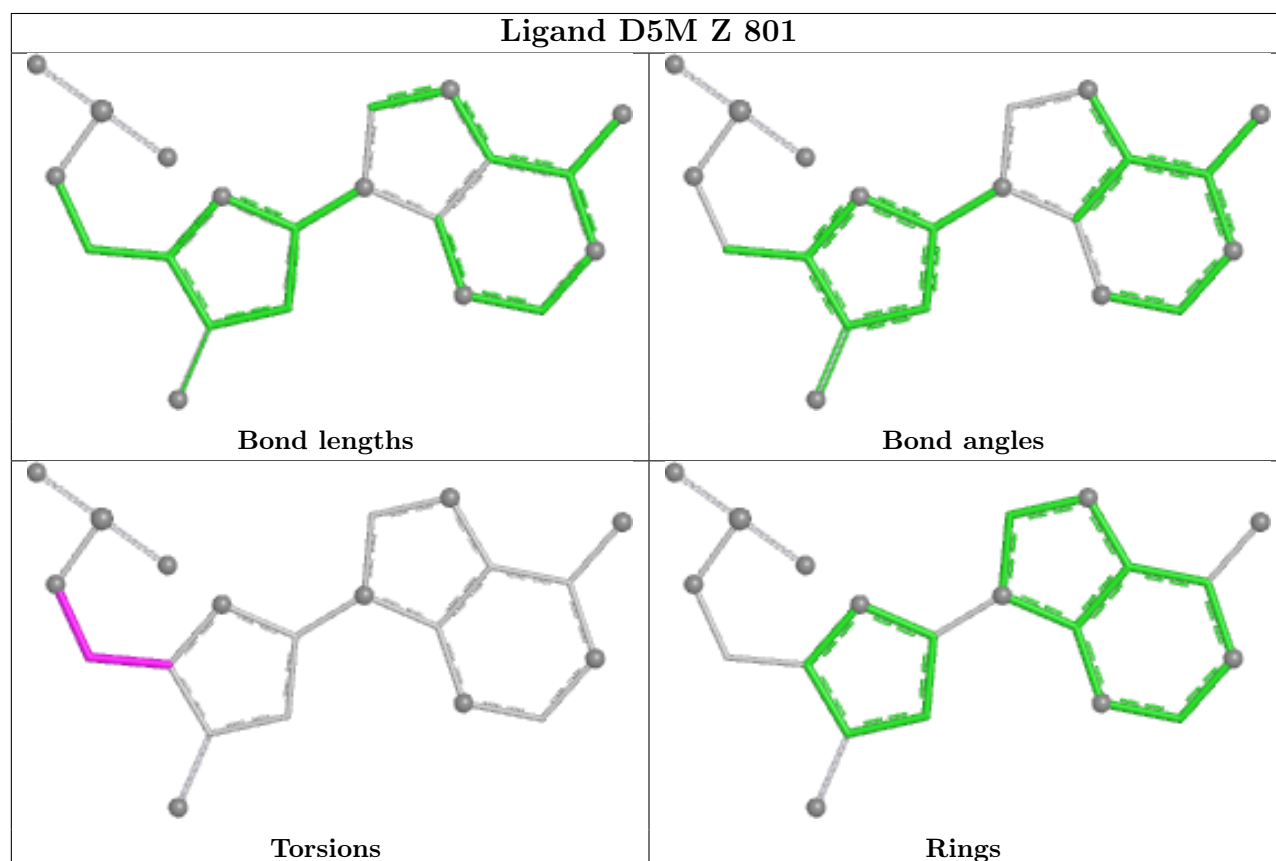
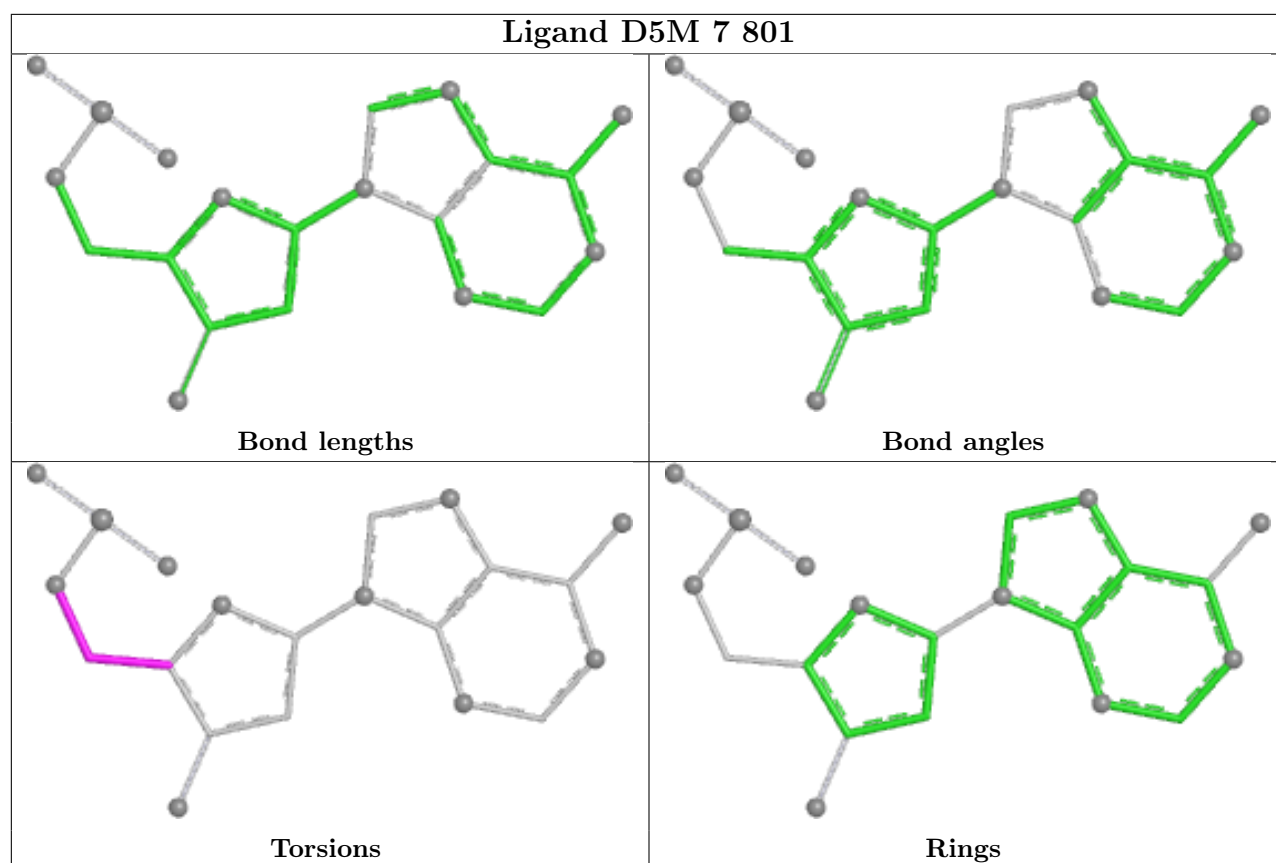


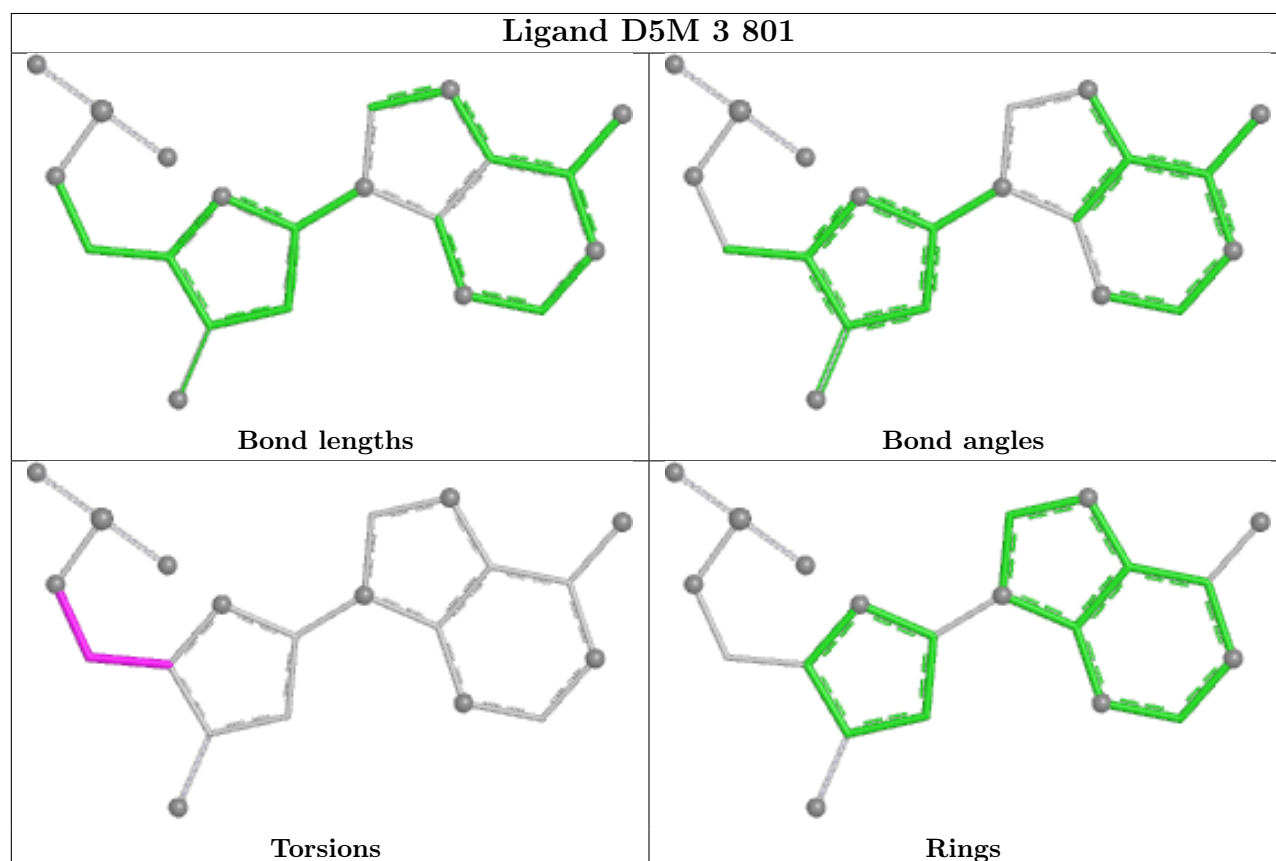
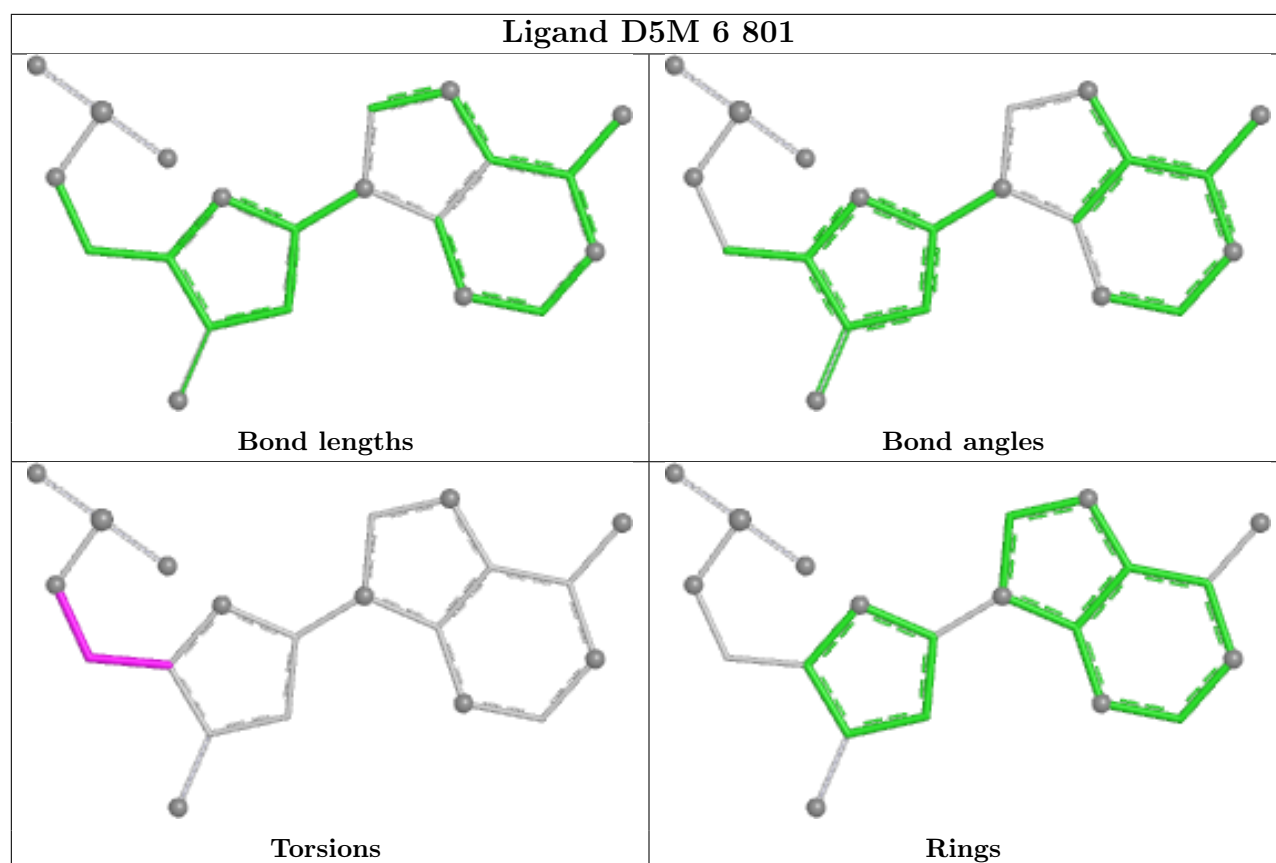


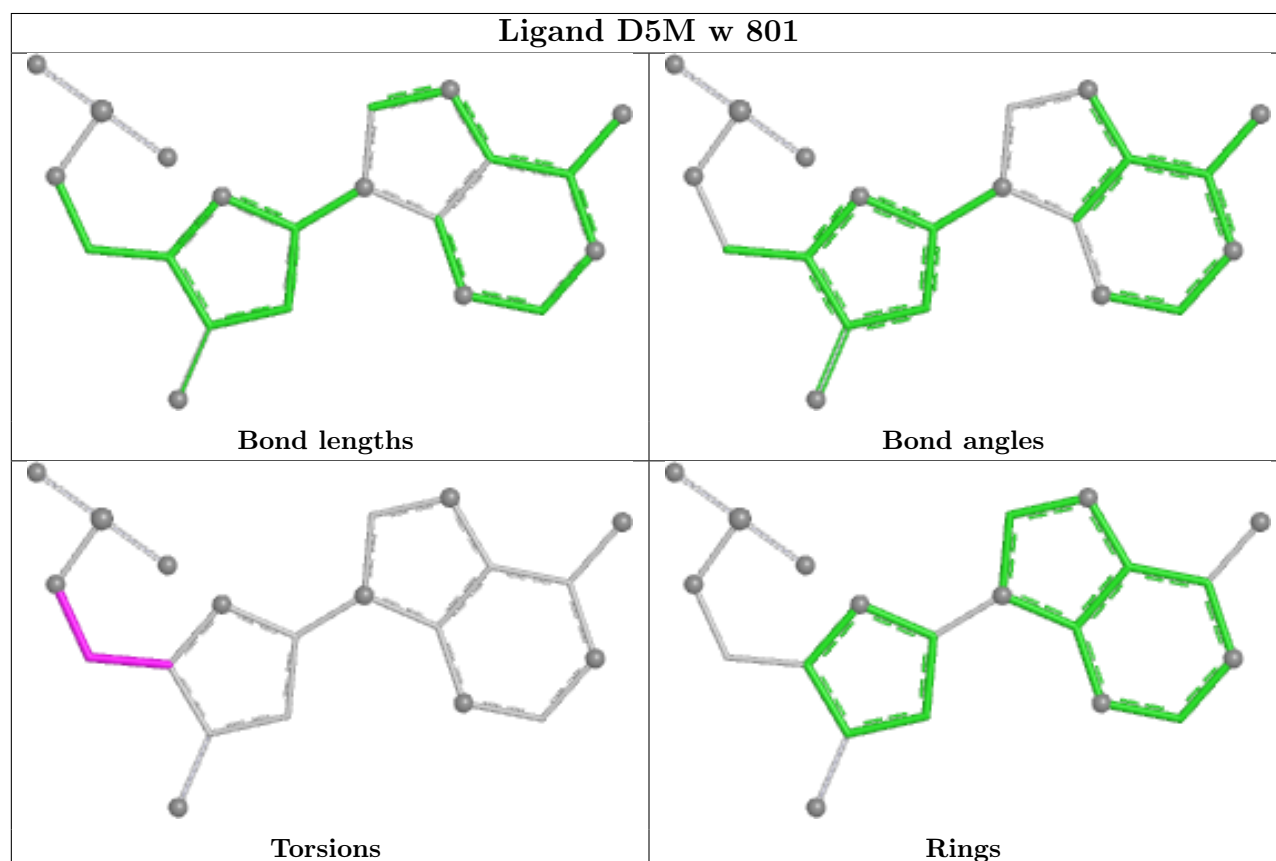
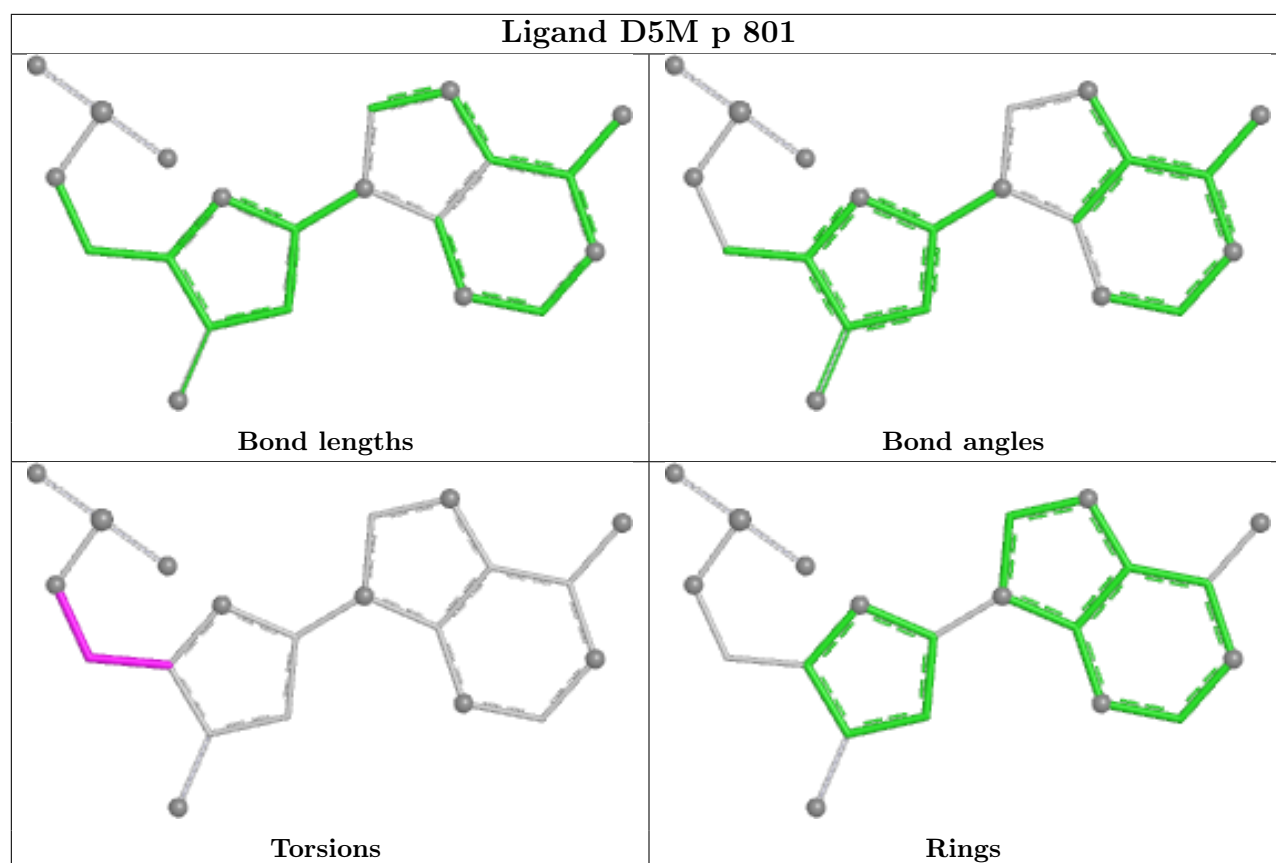


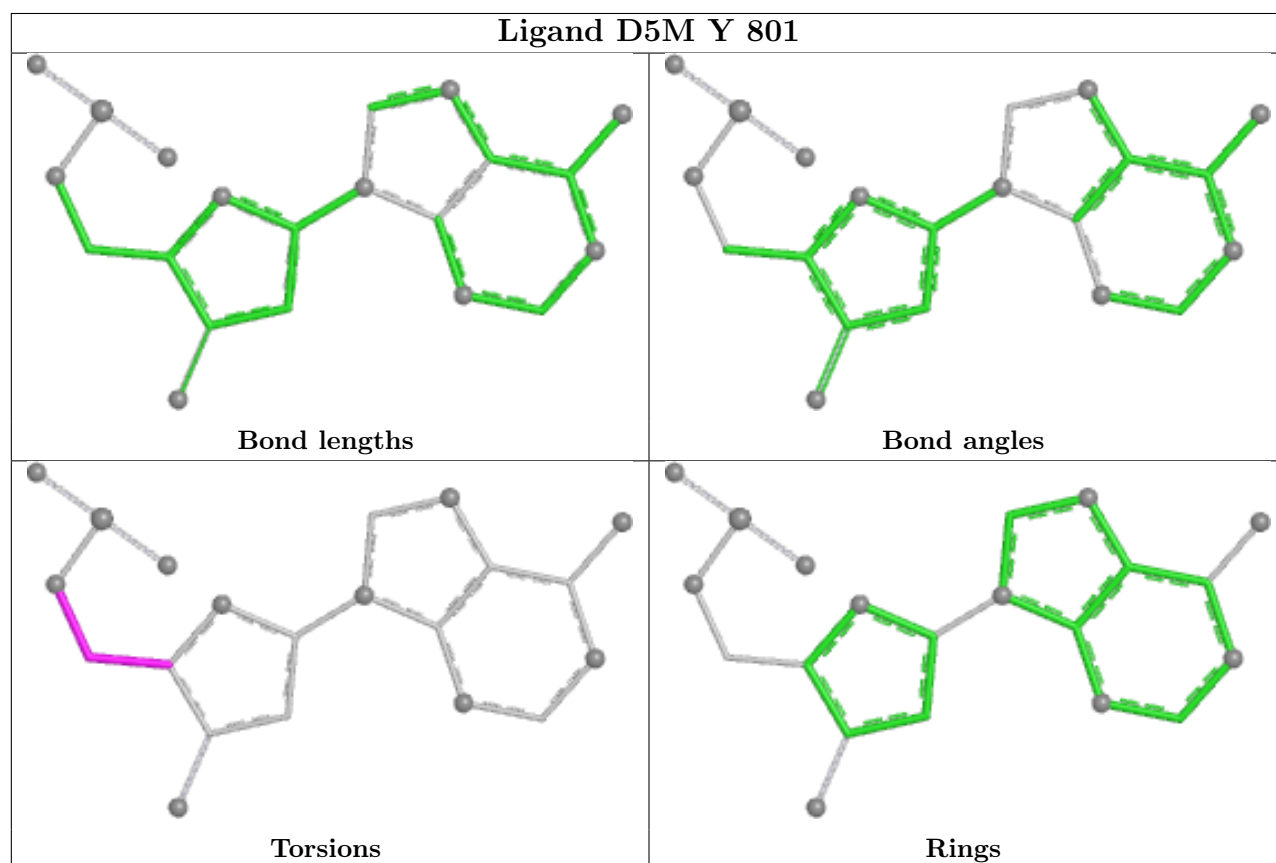
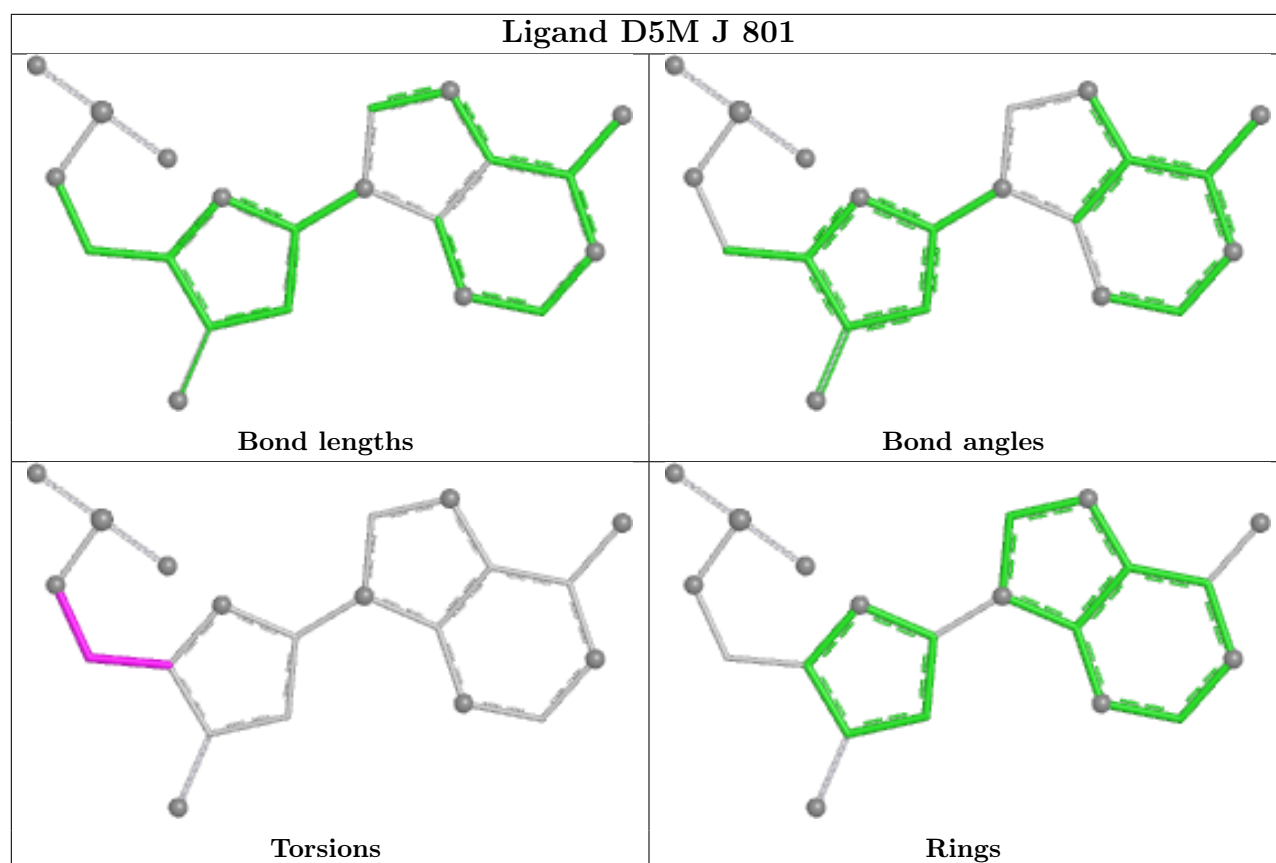


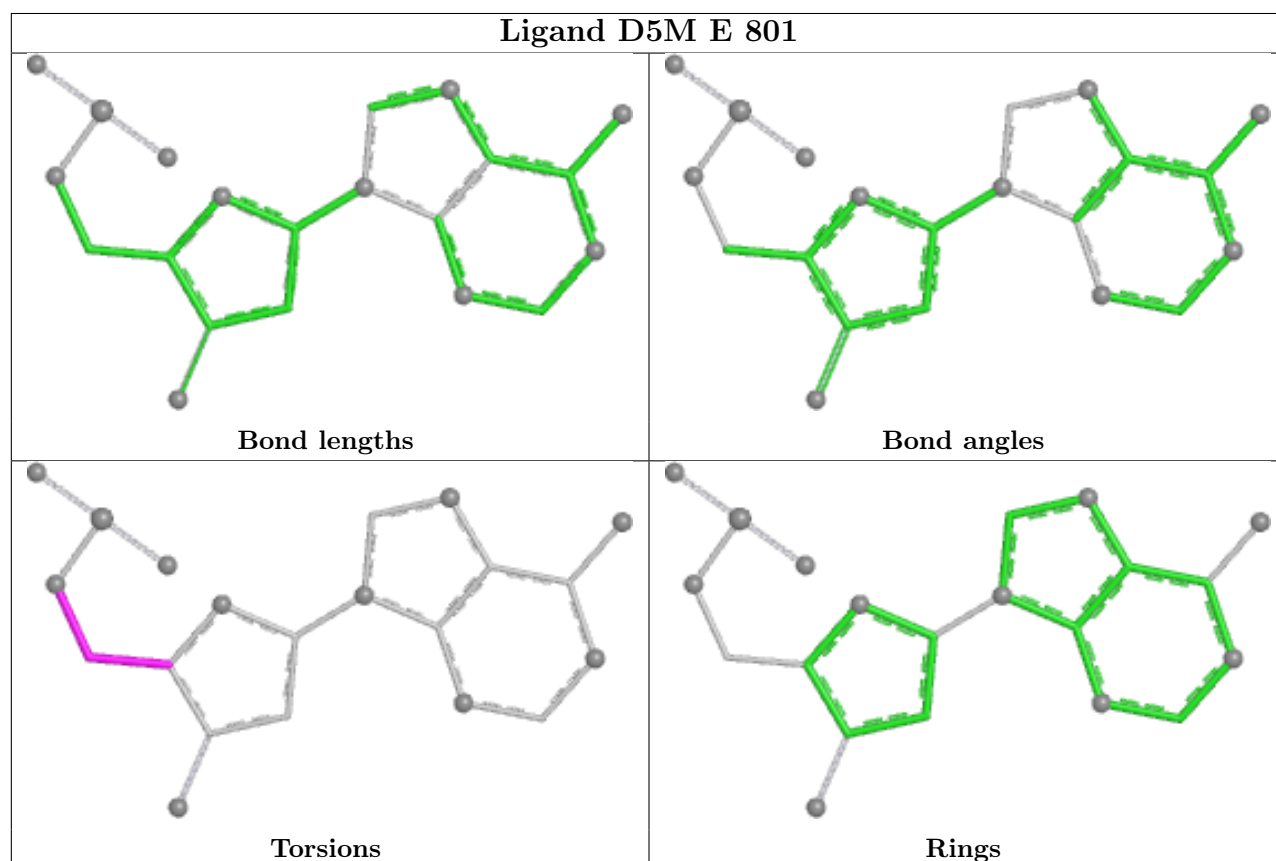
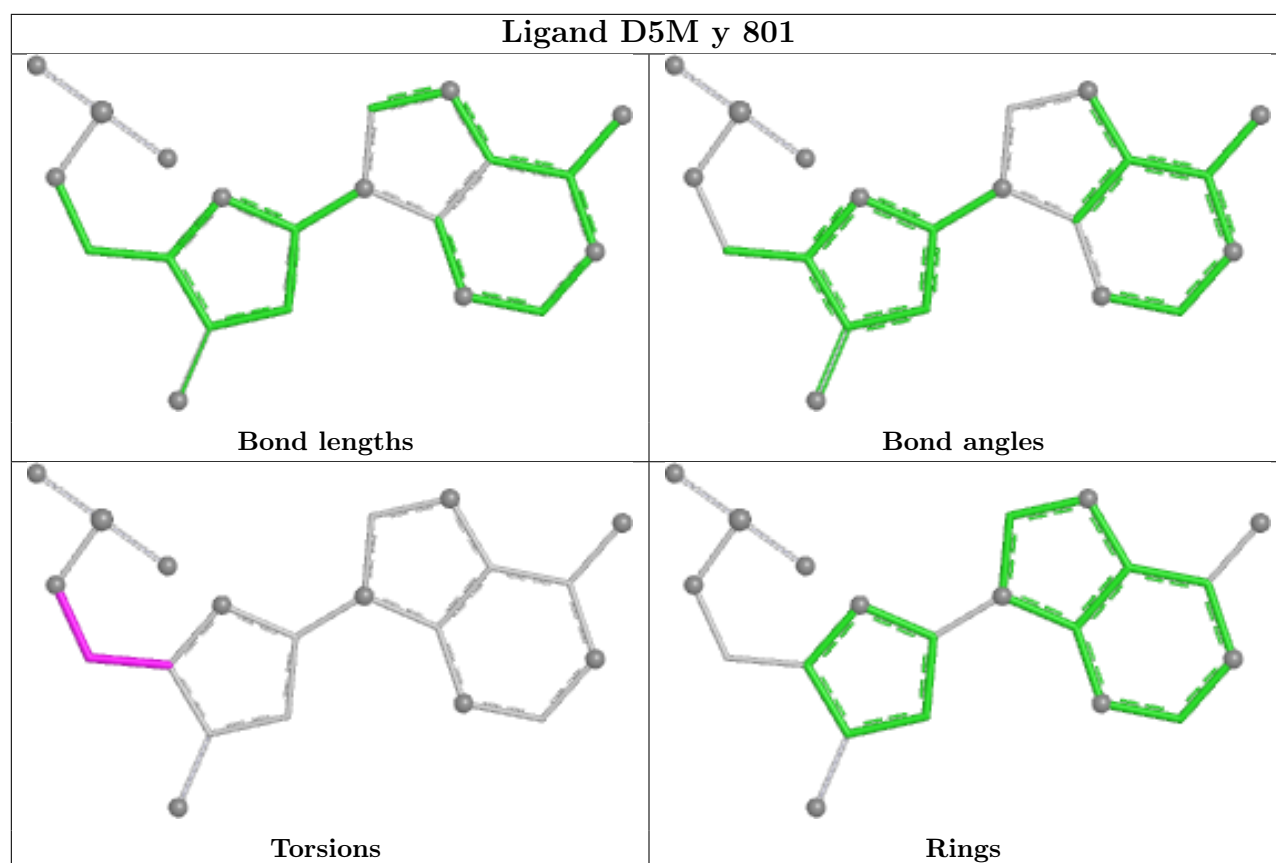


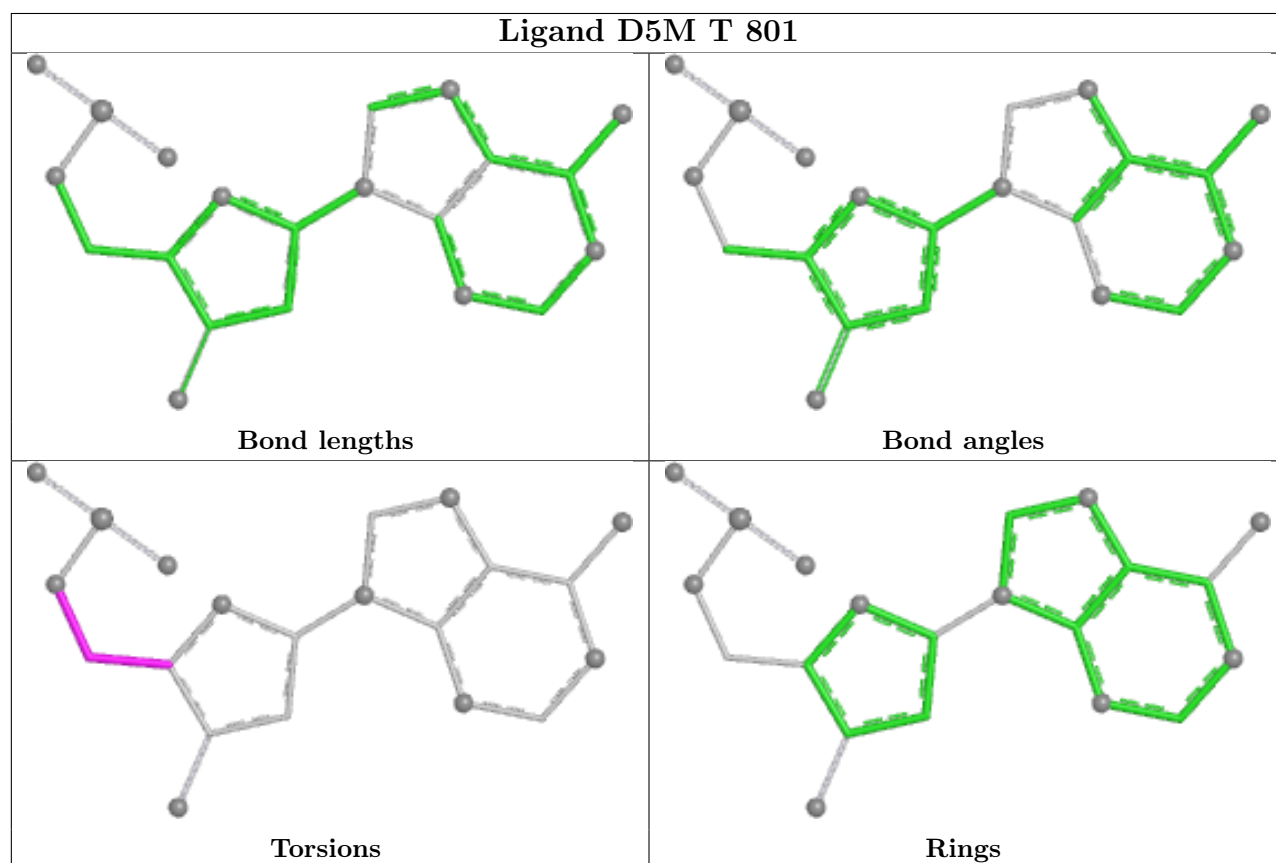
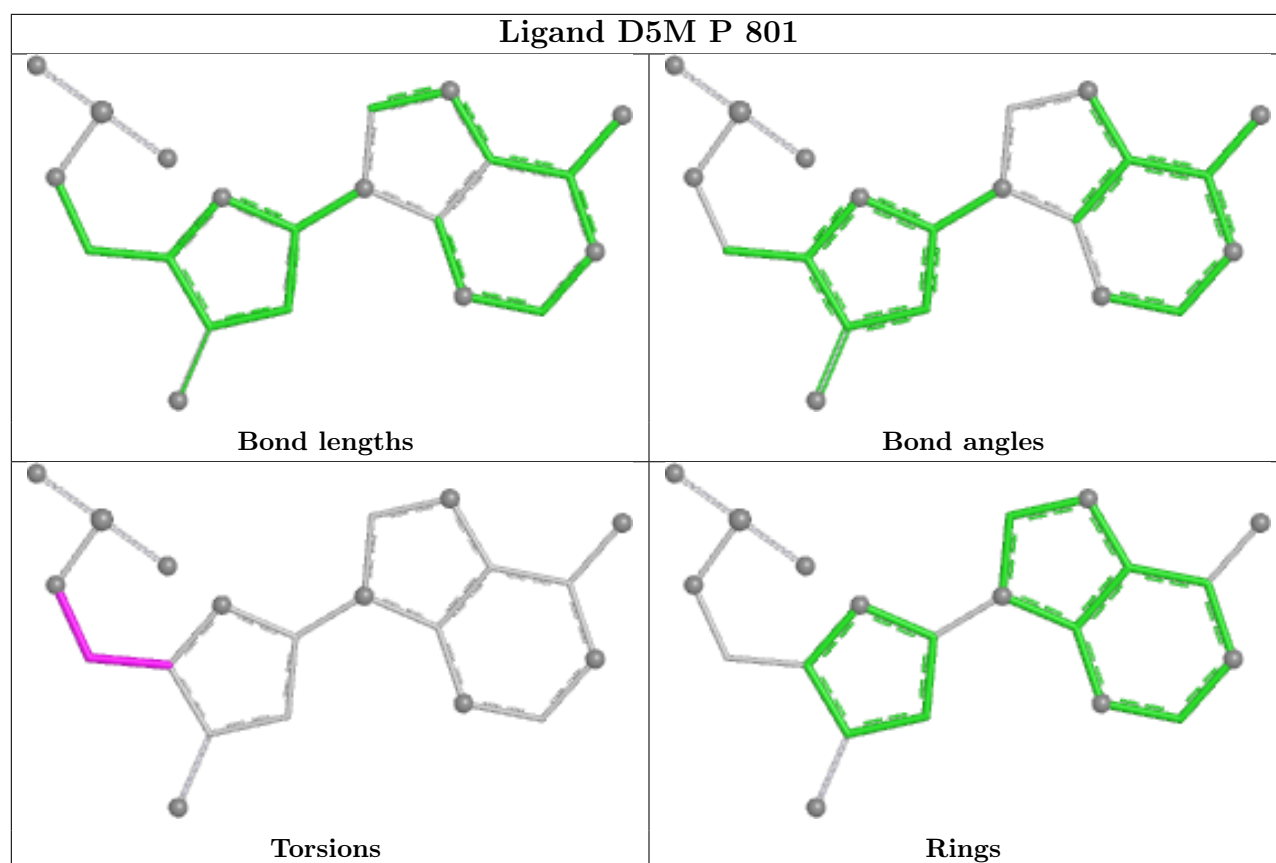


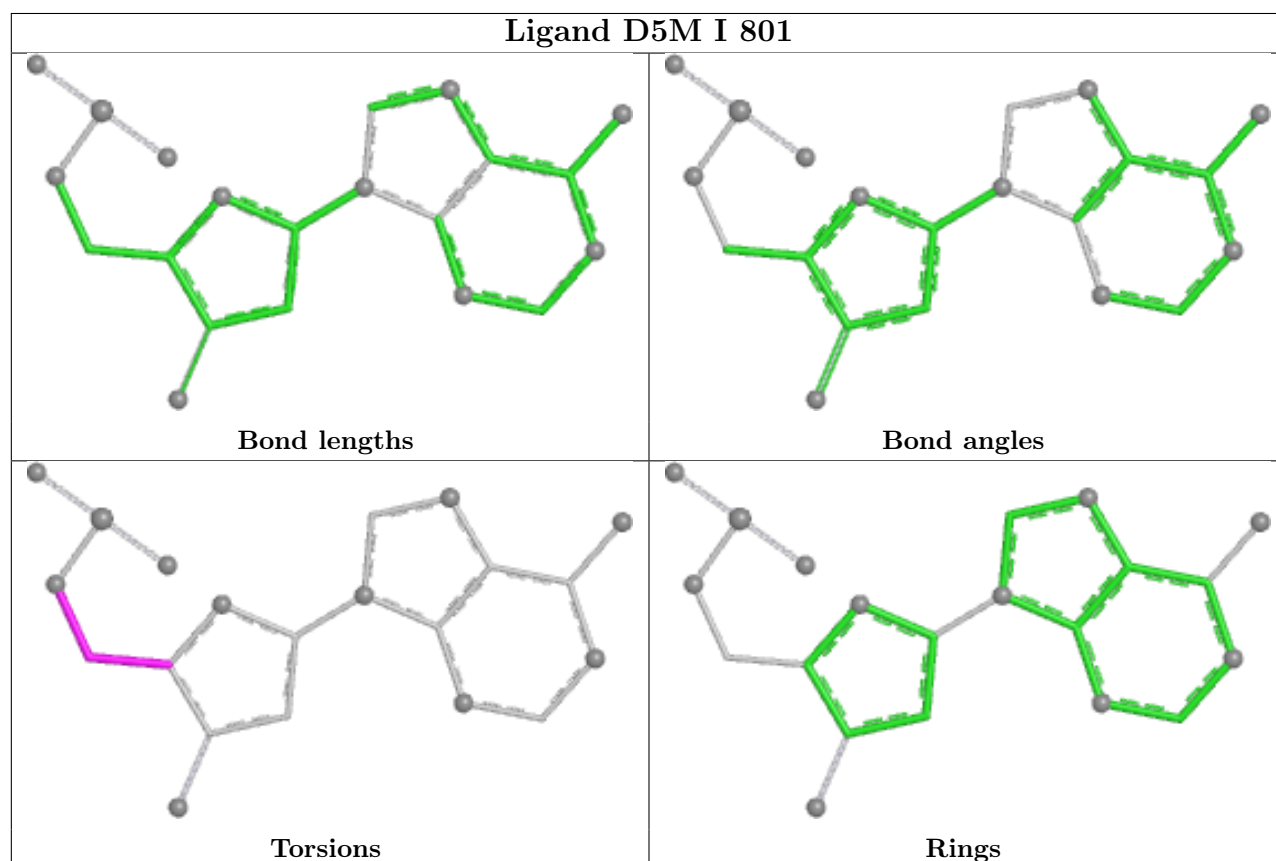
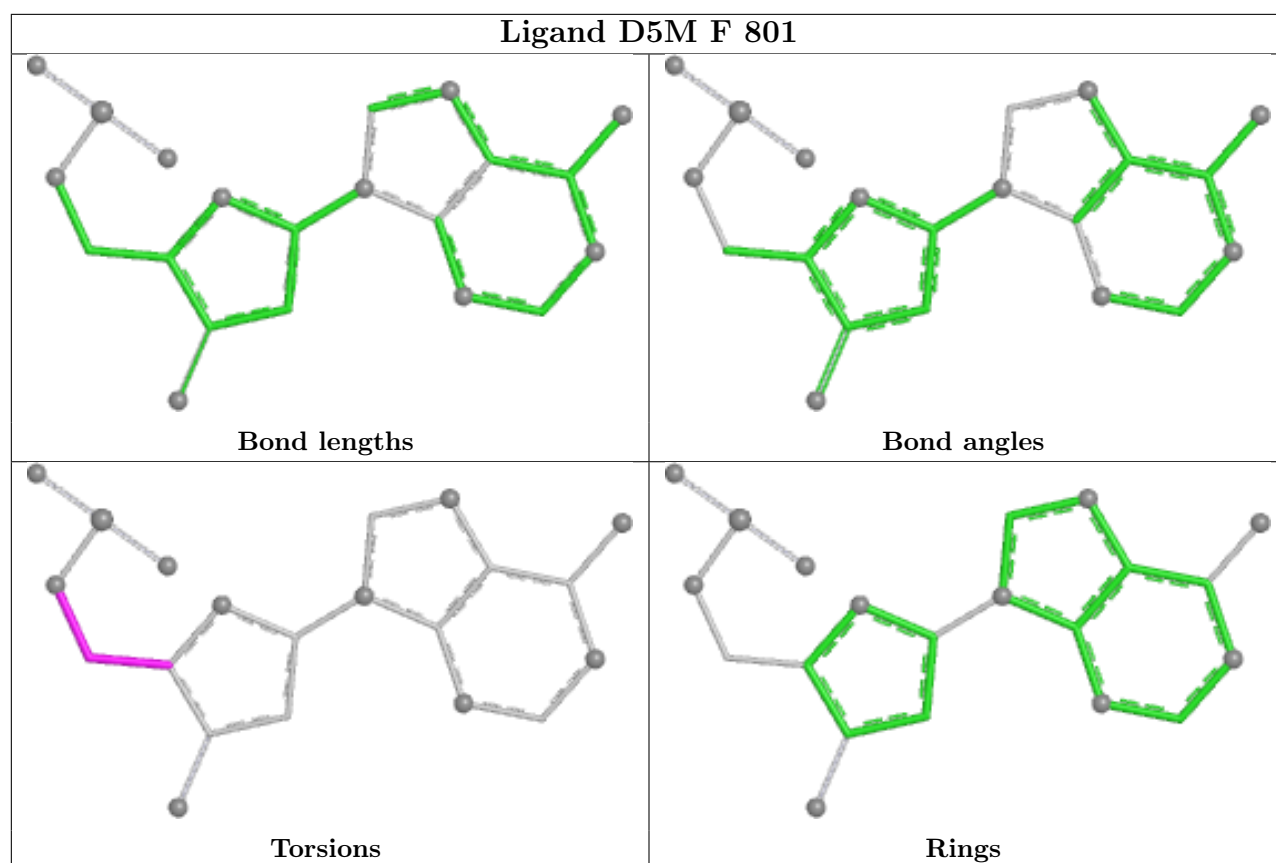


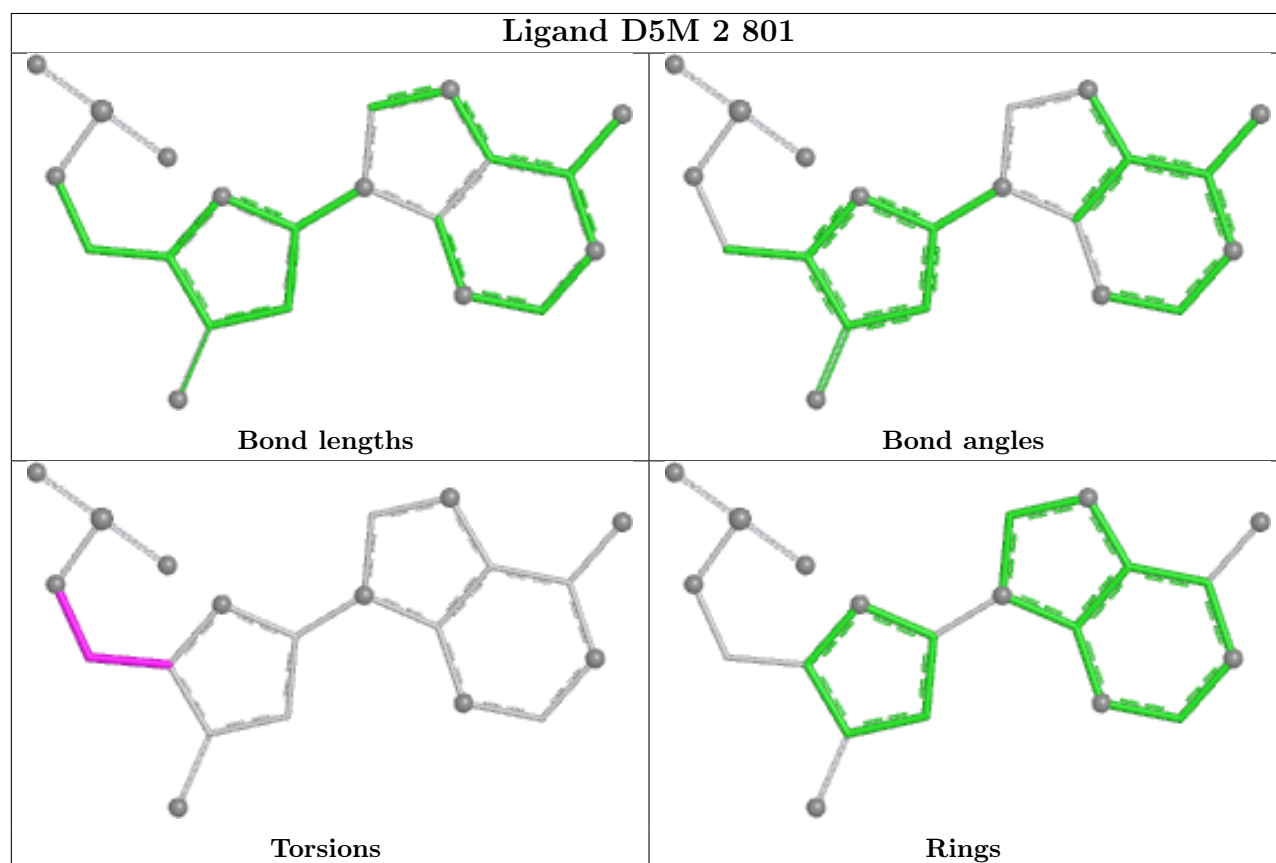
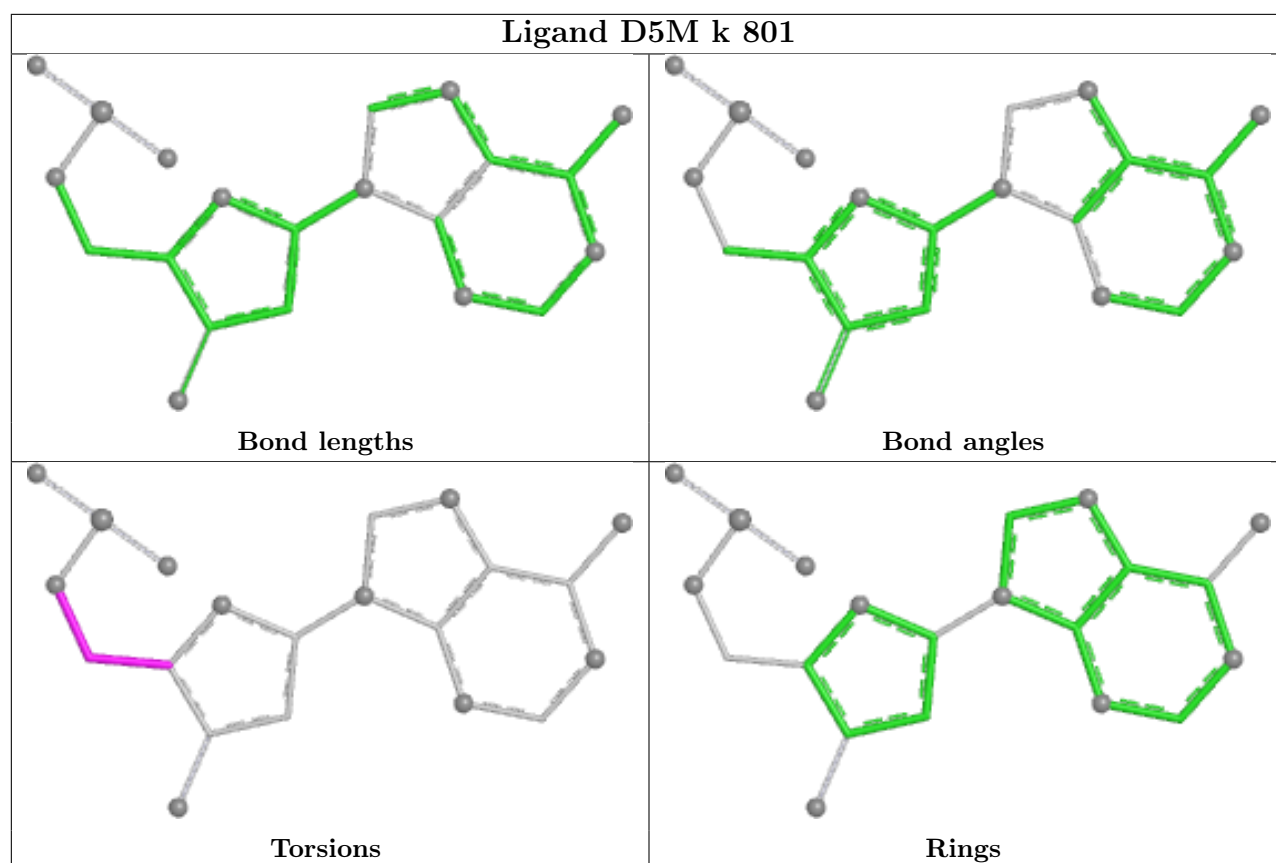


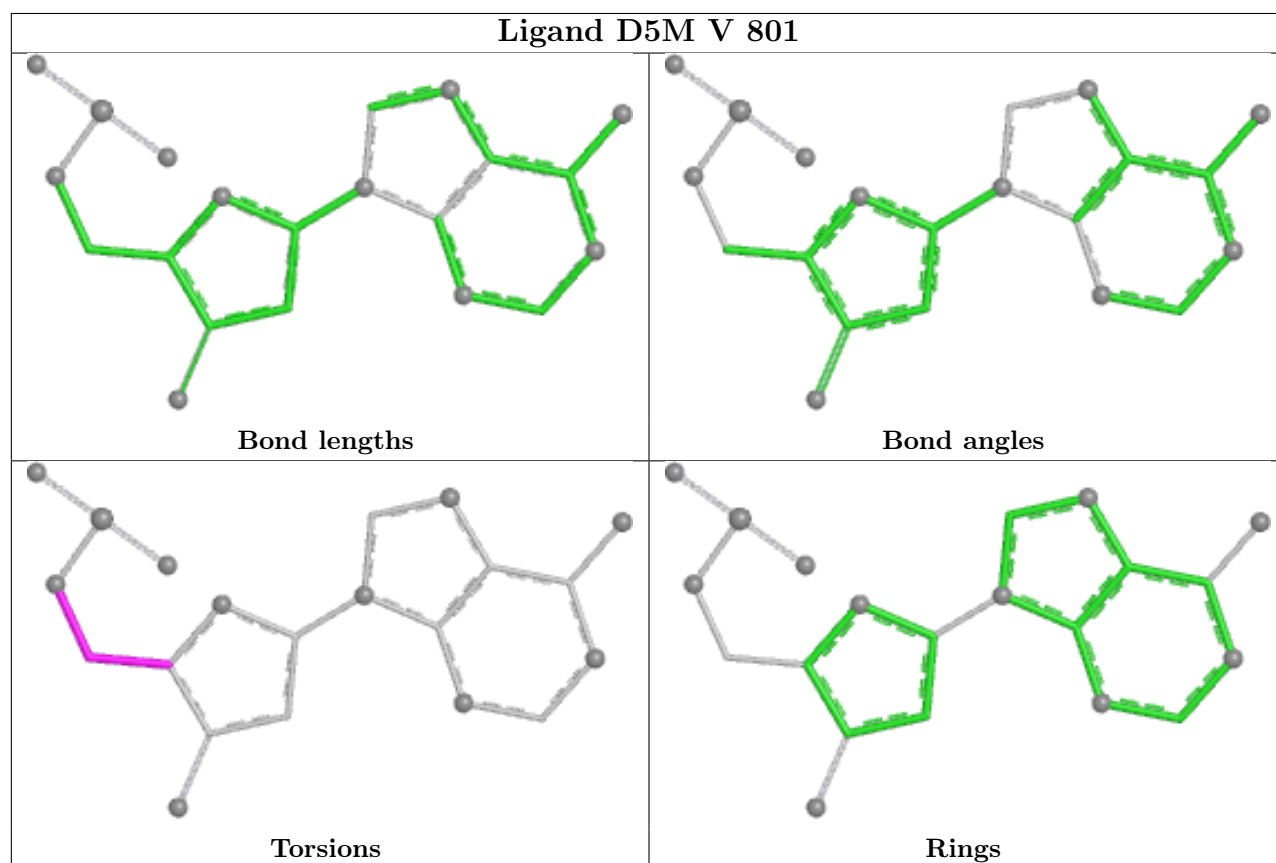
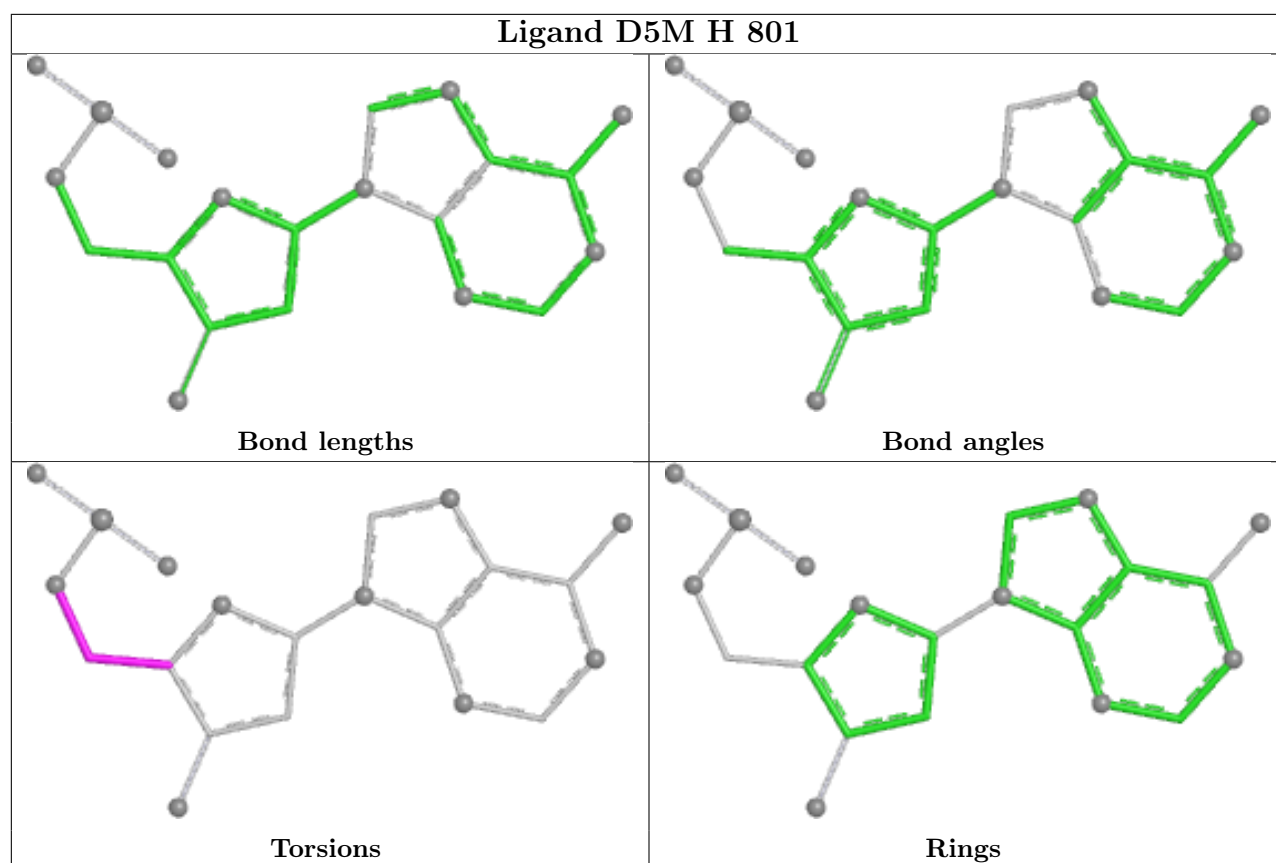


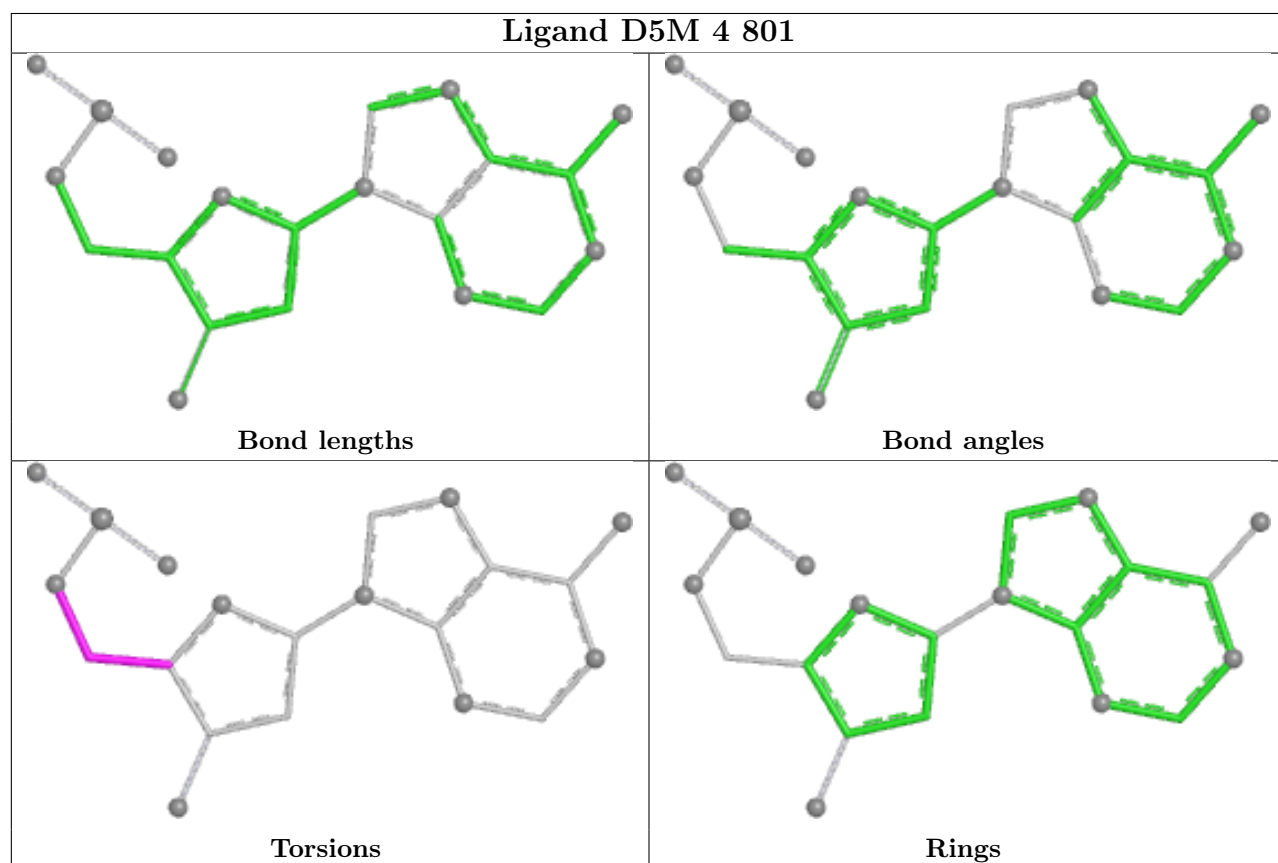
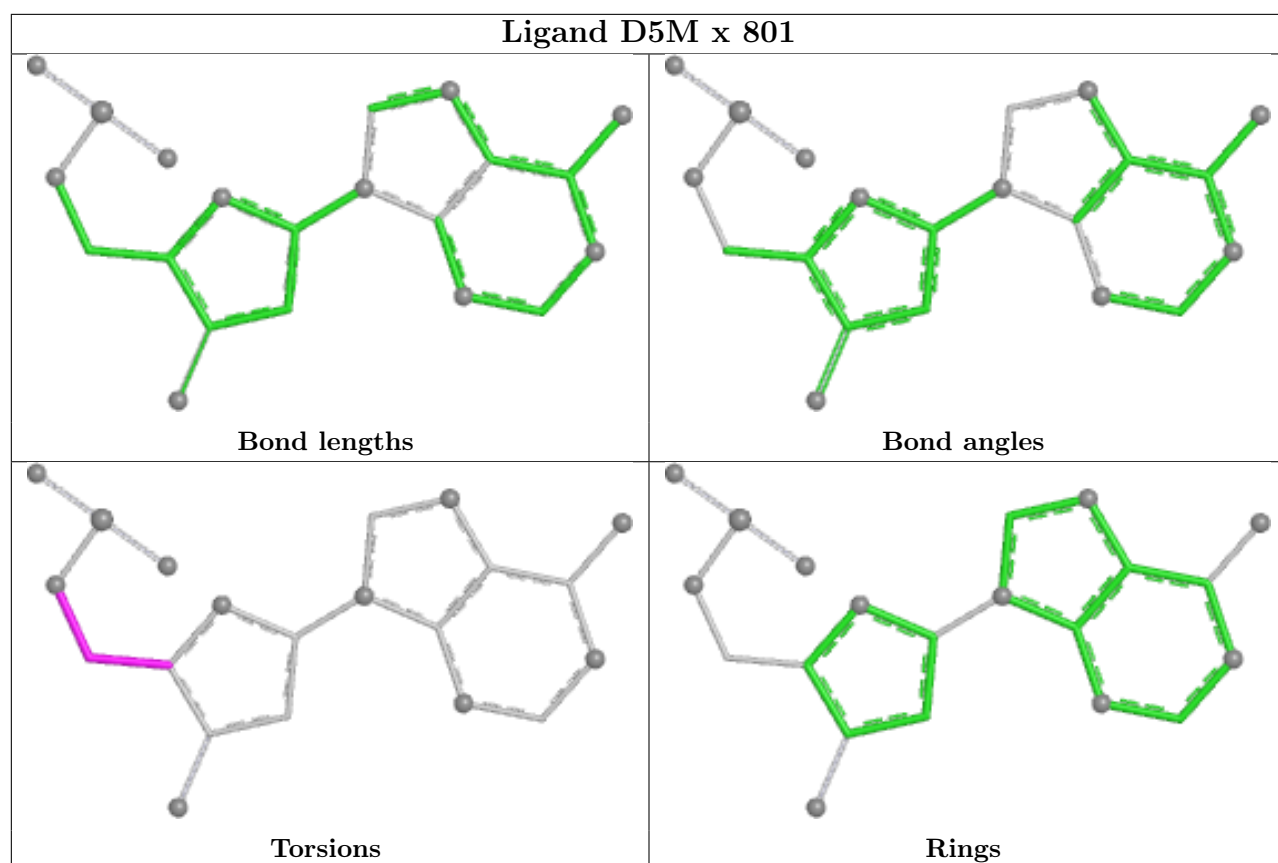


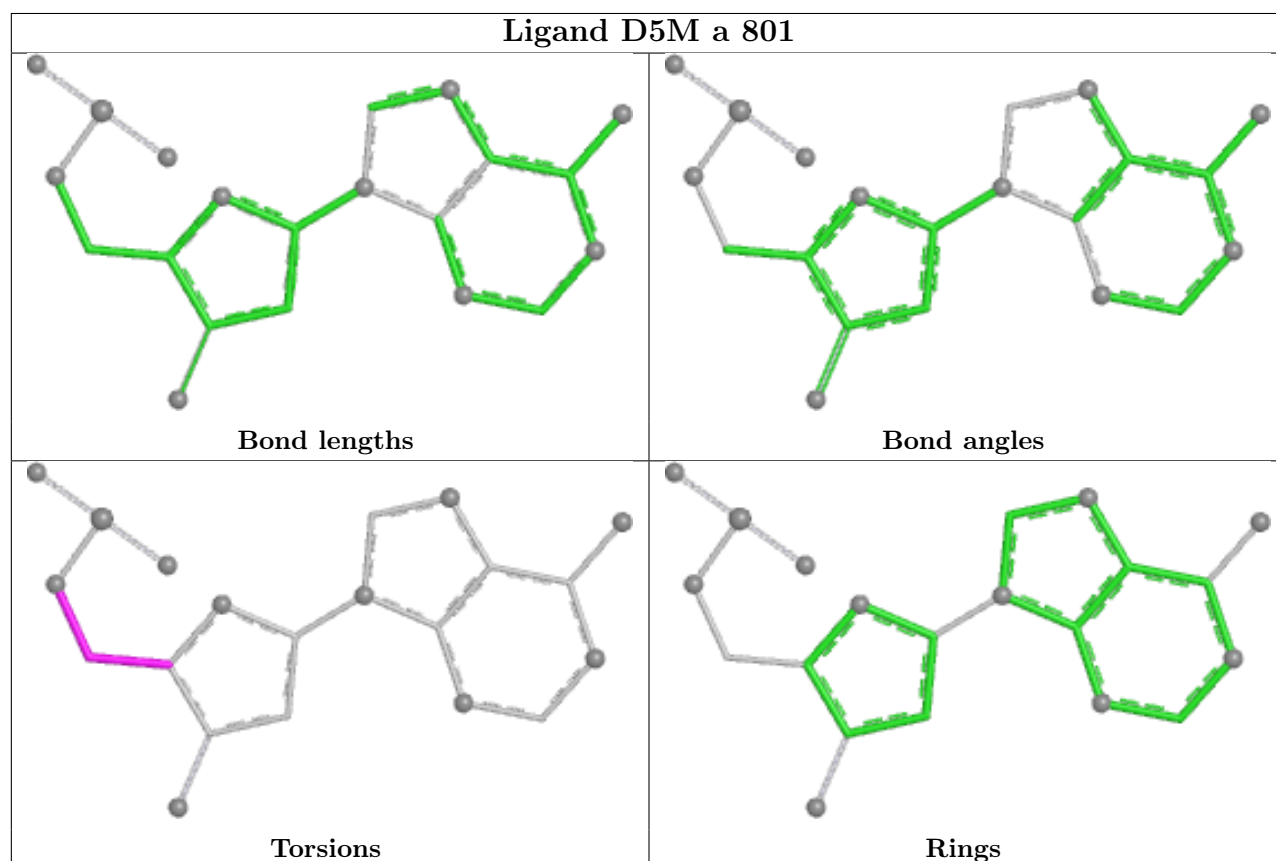
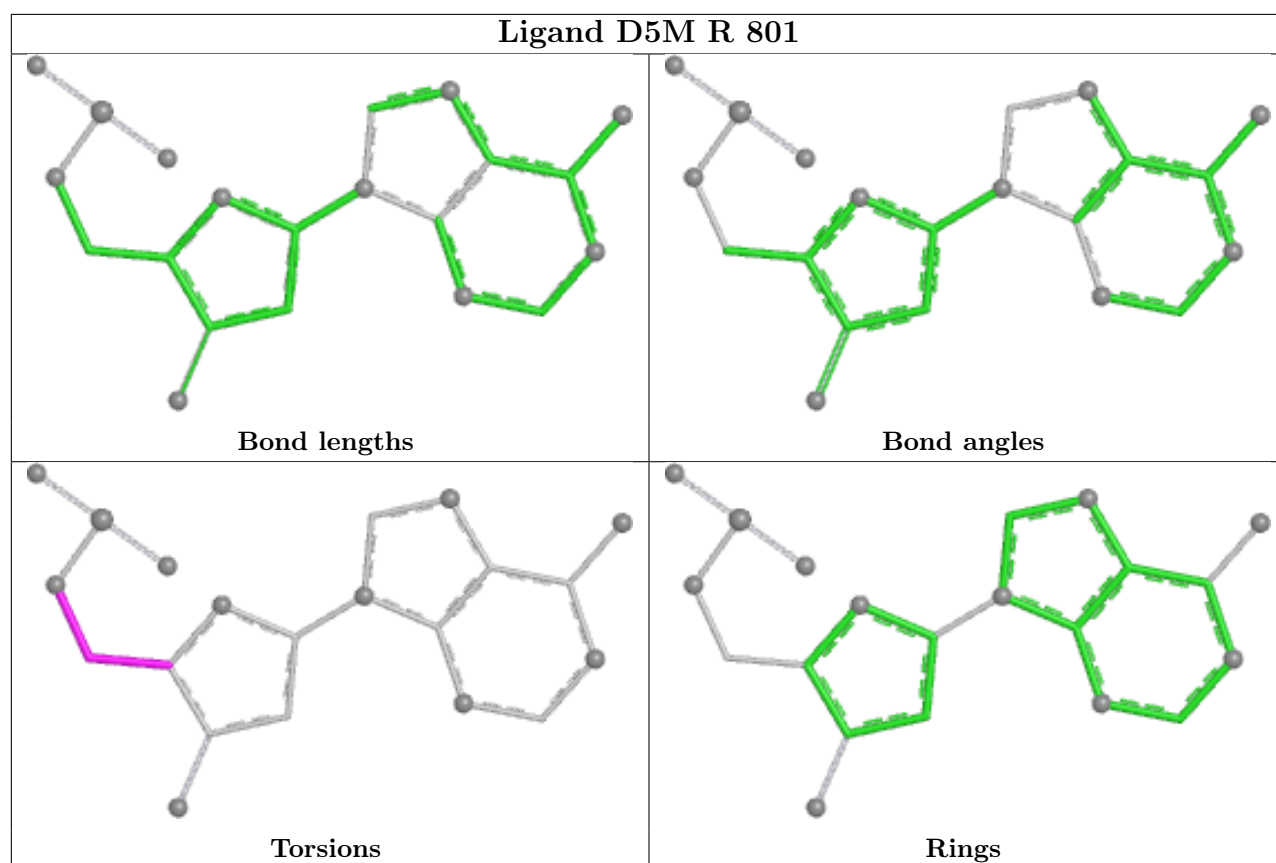


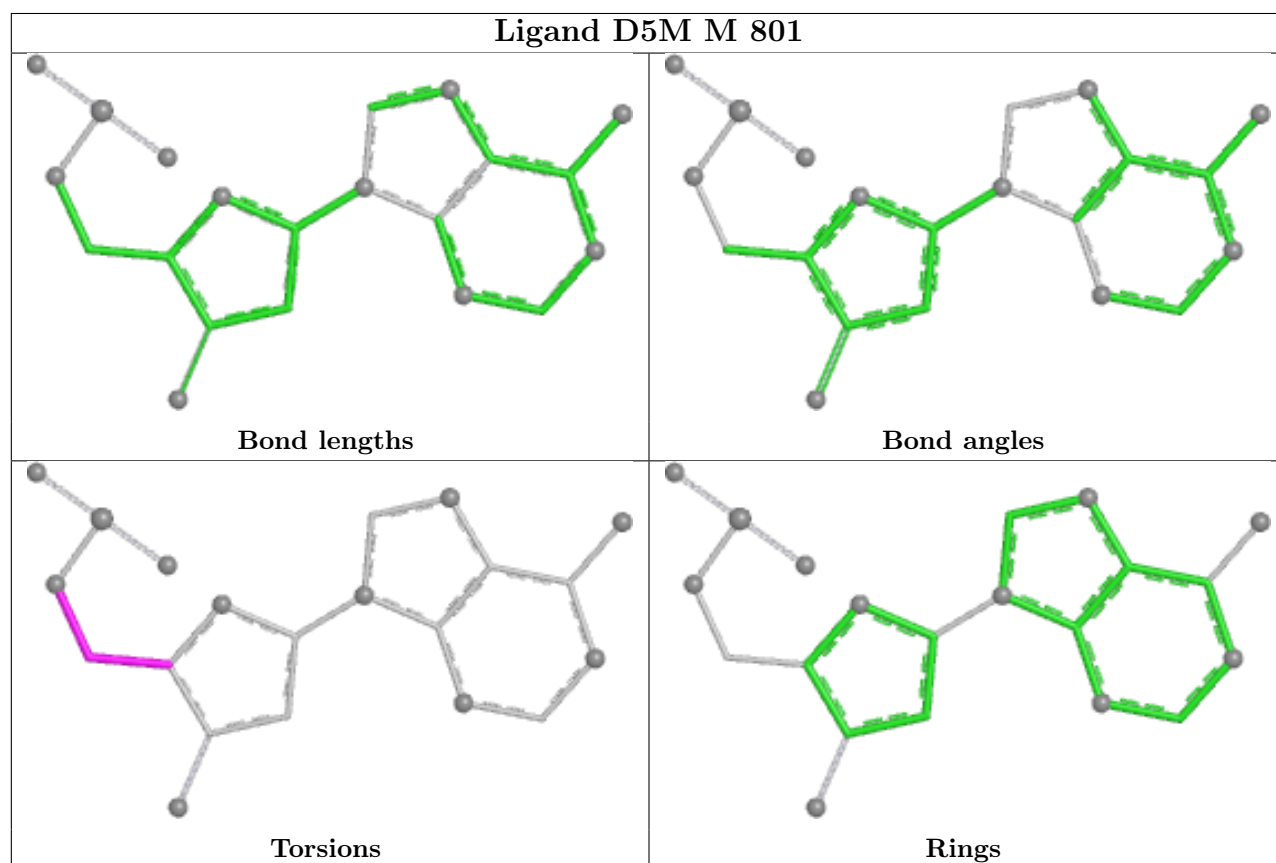
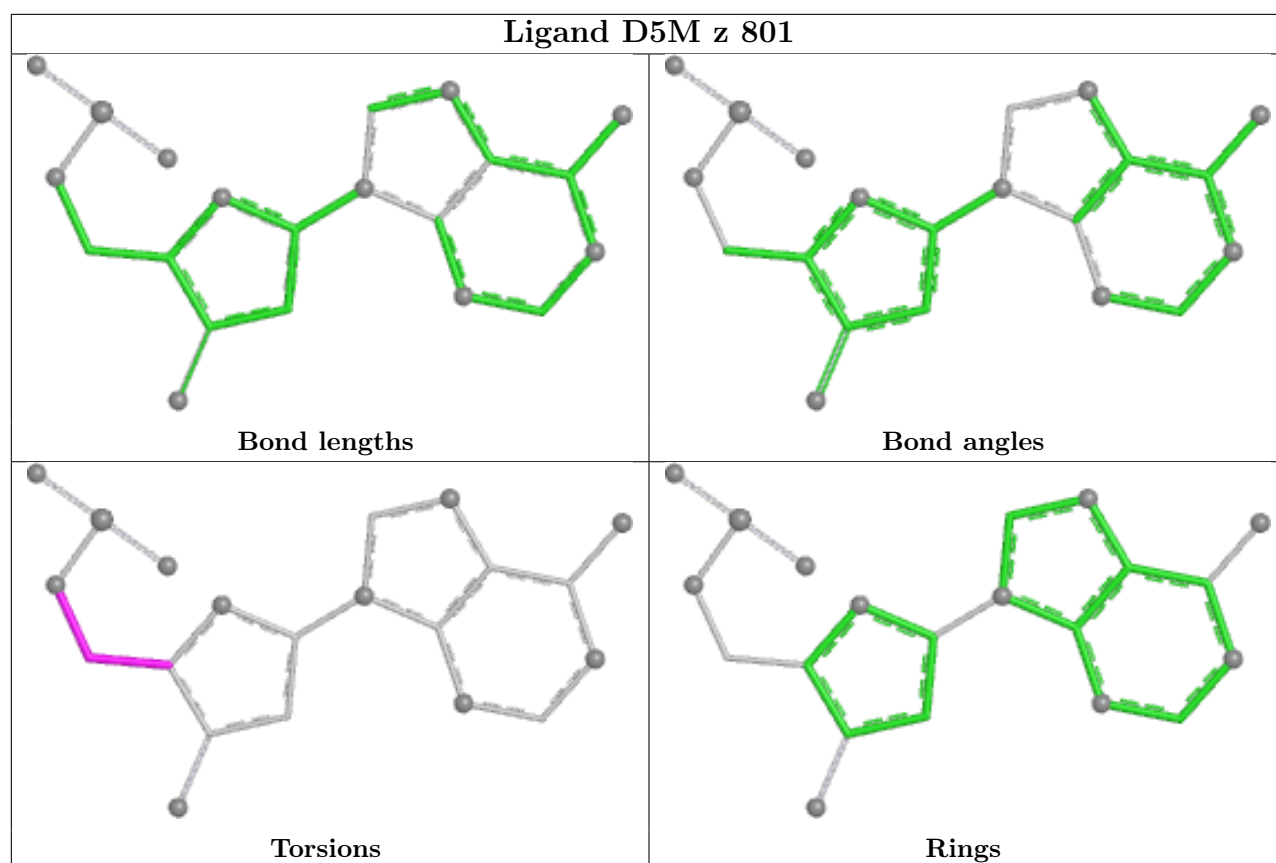












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

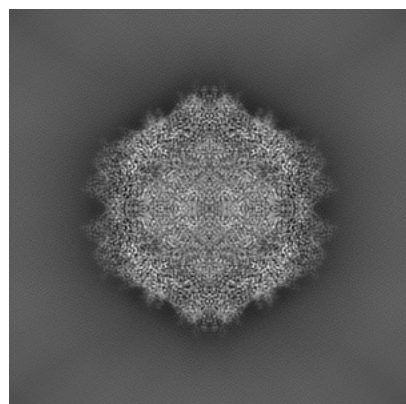
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41209. These allow visual inspection of the internal detail of the map and identification of artifacts.

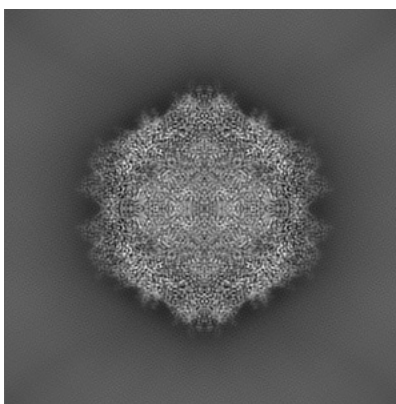
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

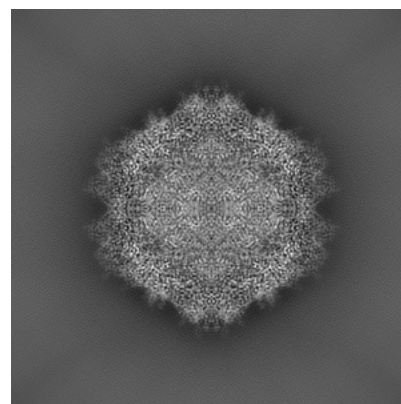
6.1.1 Primary map



X

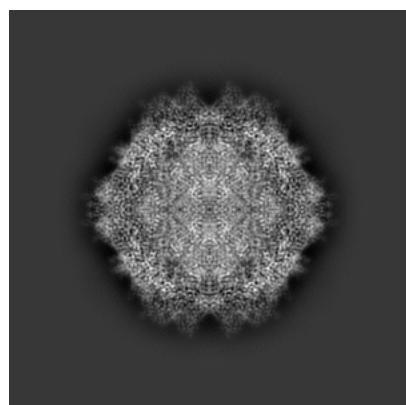


Y

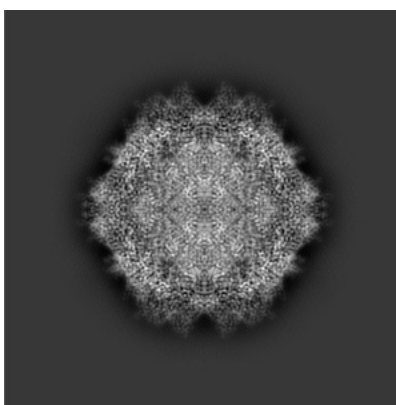


Z

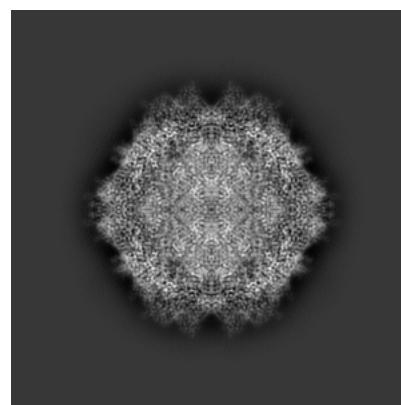
6.1.2 Raw map



X



Y

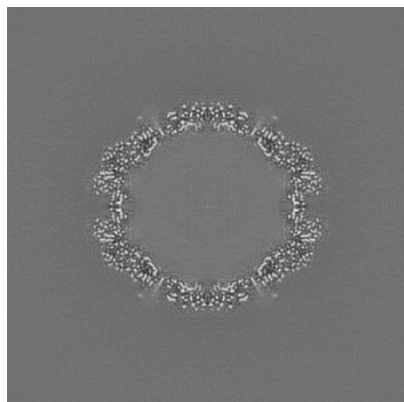


Z

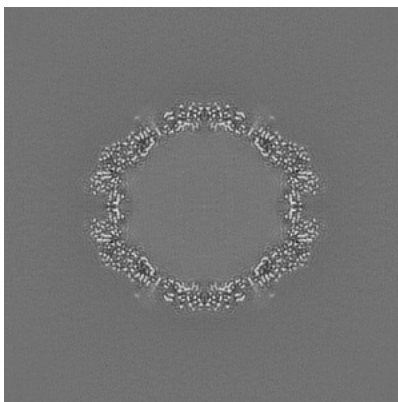
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

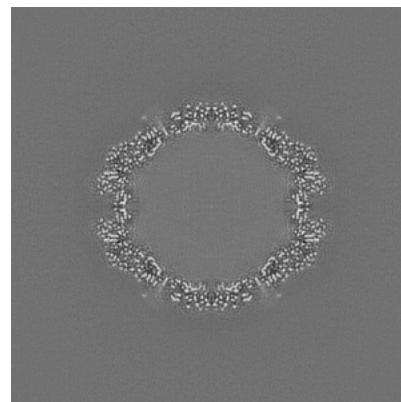
6.2.1 Primary map



X Index: 210

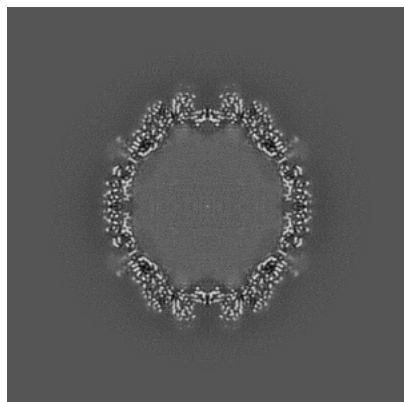


Y Index: 210

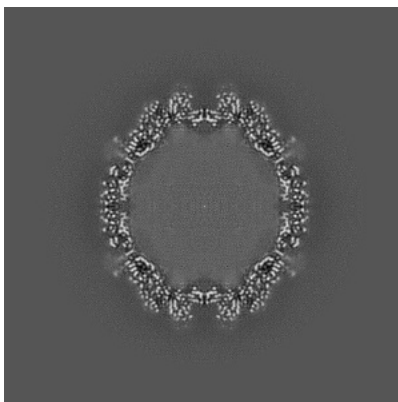


Z Index: 210

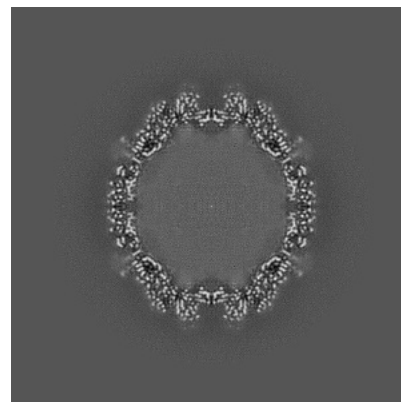
6.2.2 Raw map



X Index: 210



Y Index: 210

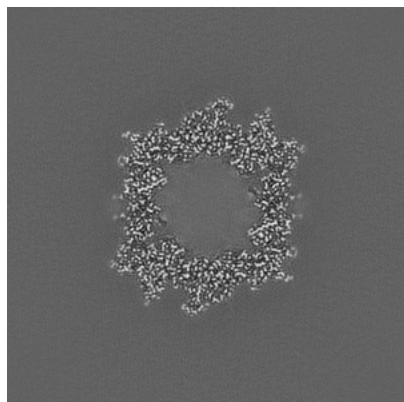


Z Index: 210

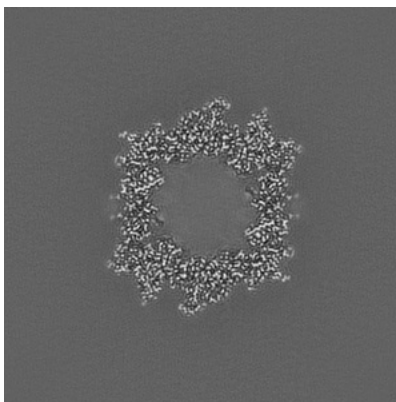
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

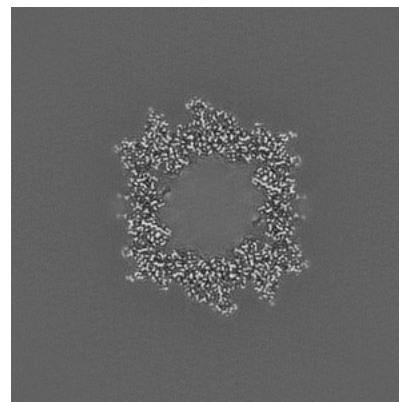
6.3.1 Primary map



X Index: 272

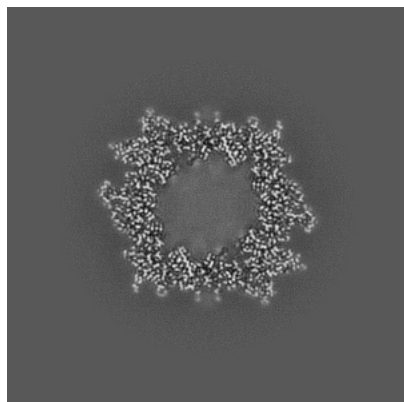


Y Index: 272

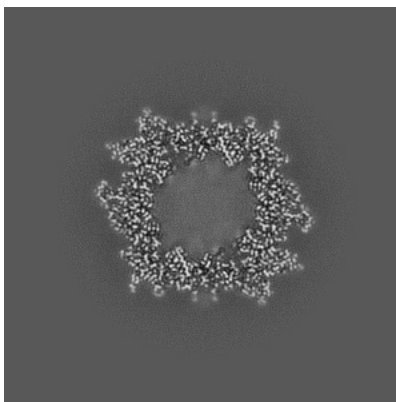


Z Index: 148

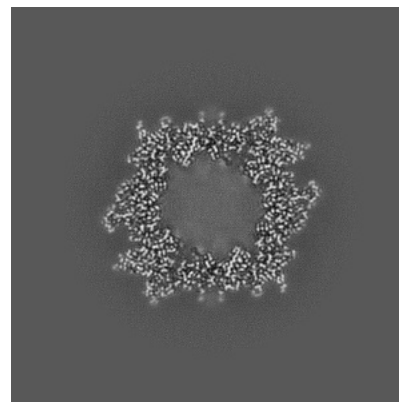
6.3.2 Raw map



X Index: 148



Y Index: 148

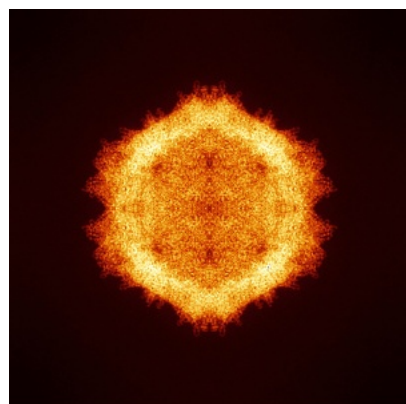


Z Index: 272

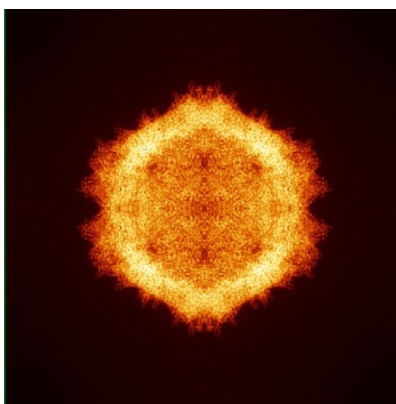
The images above show the largest variance slices of the map in three orthogonal directions.

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

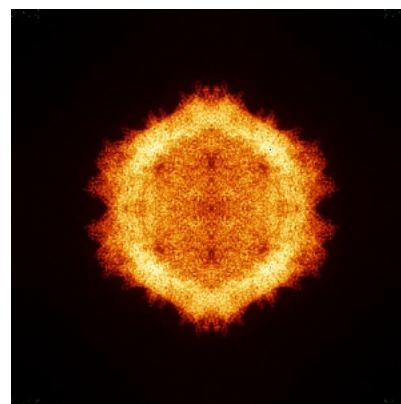
6.4.1 Primary map



X

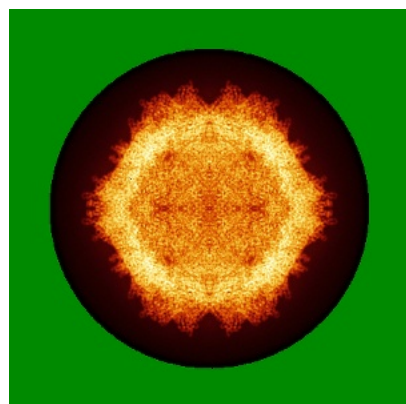


Y

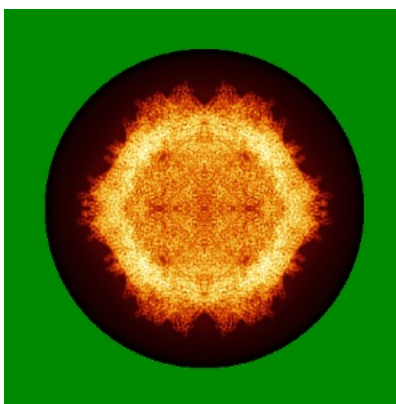


Z

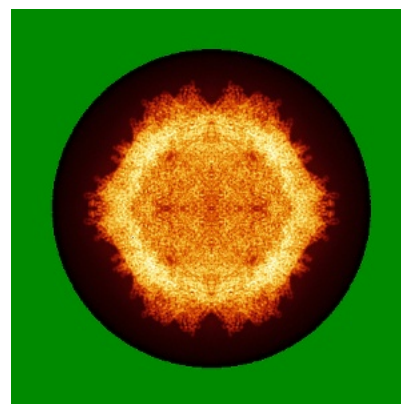
6.4.2 Raw map



X



Y

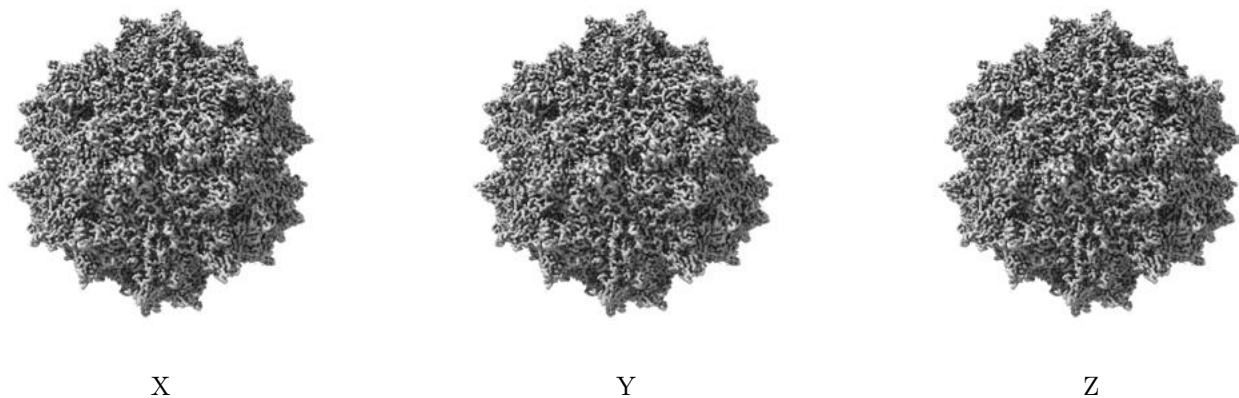


Z

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.

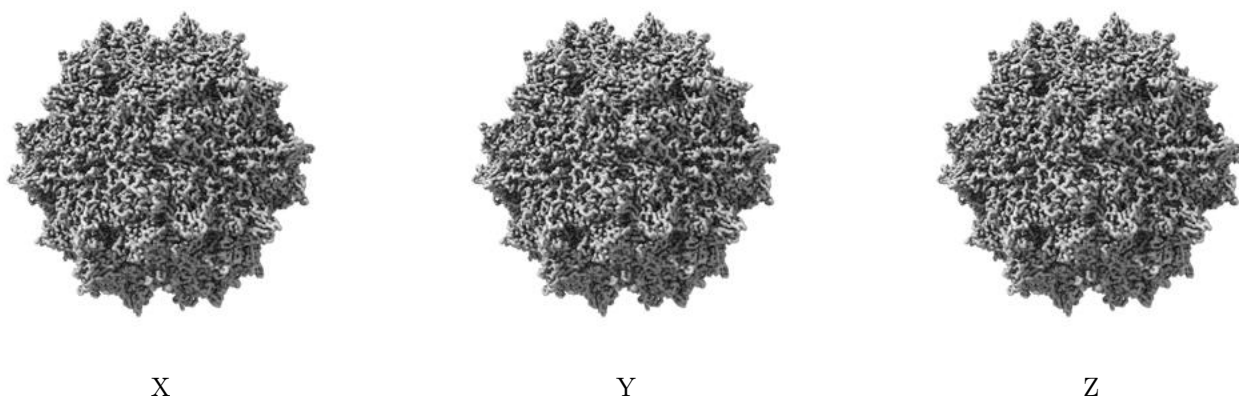
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. 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



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.

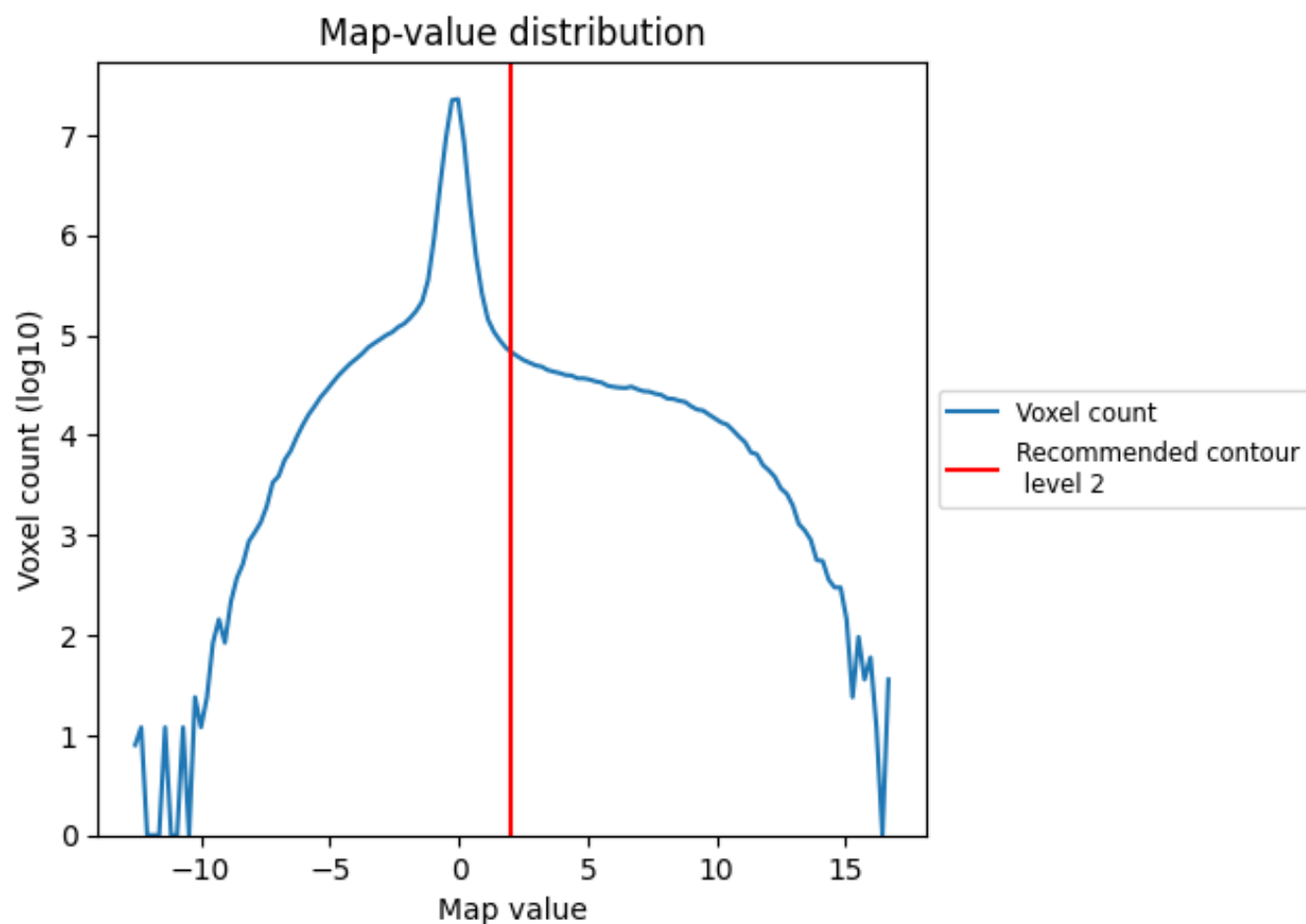
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

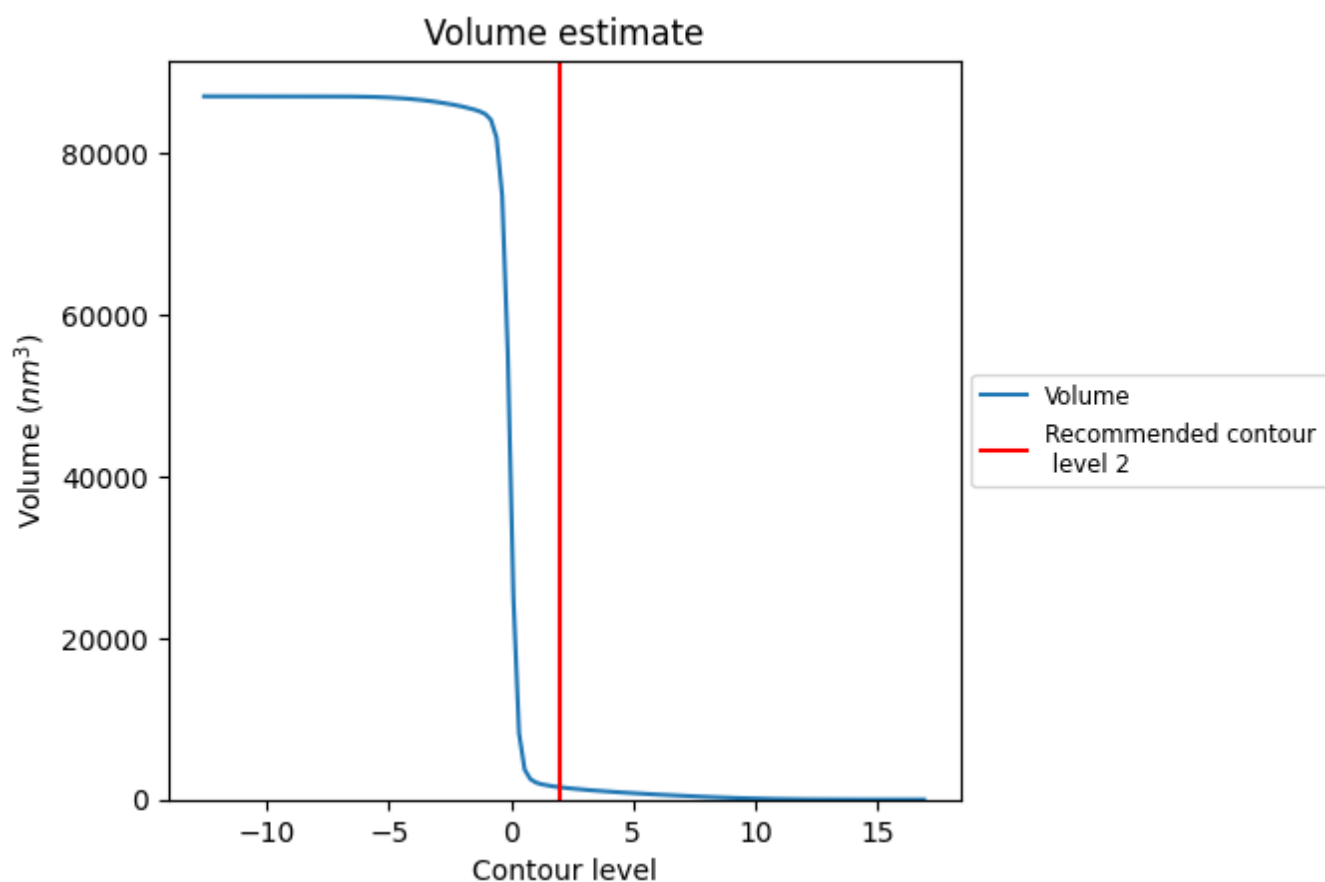
This section contains the results of statistical analysis of the map.

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.

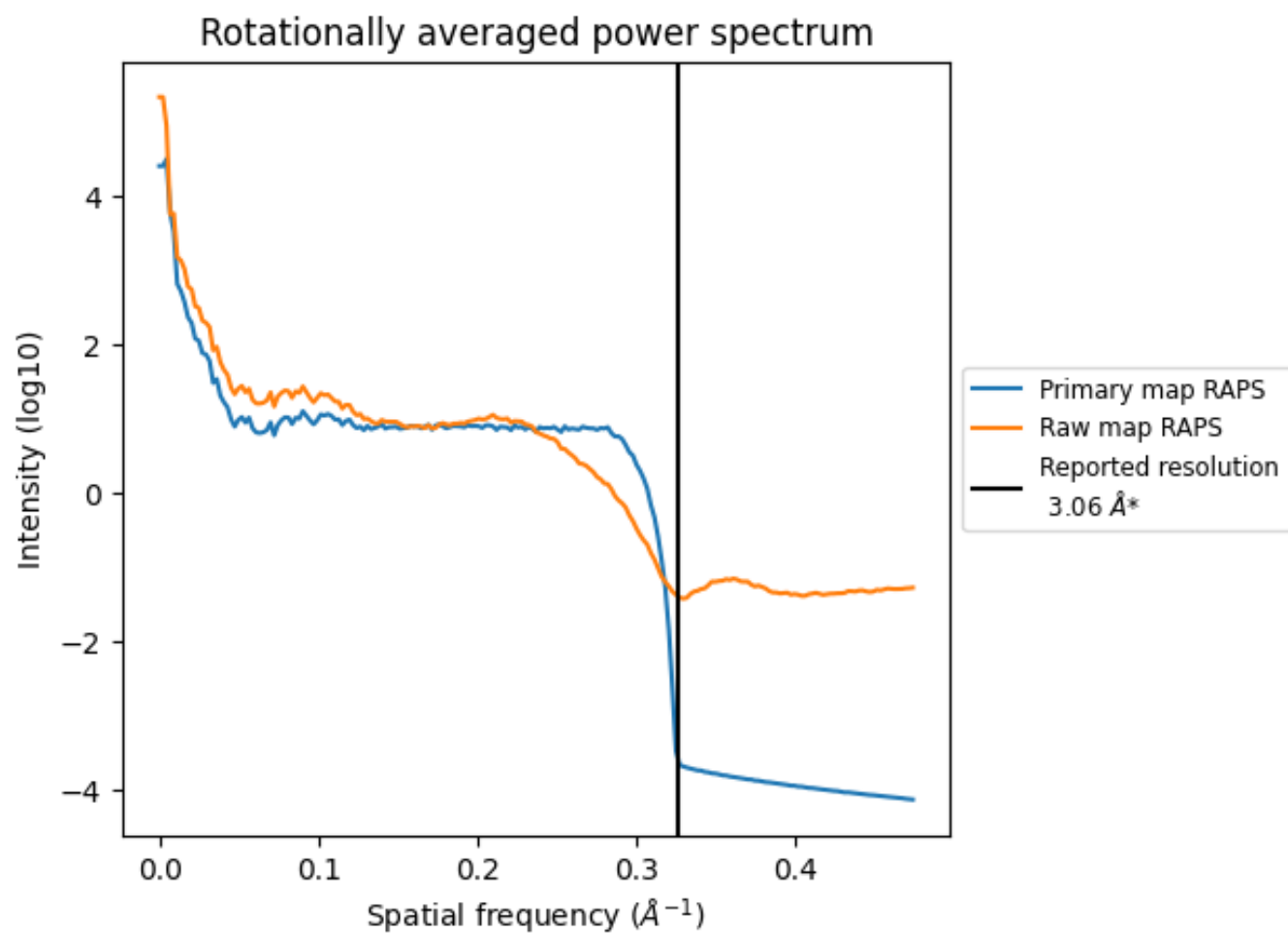
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1526 nm^3 ; this corresponds to an approximate mass of 1378 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

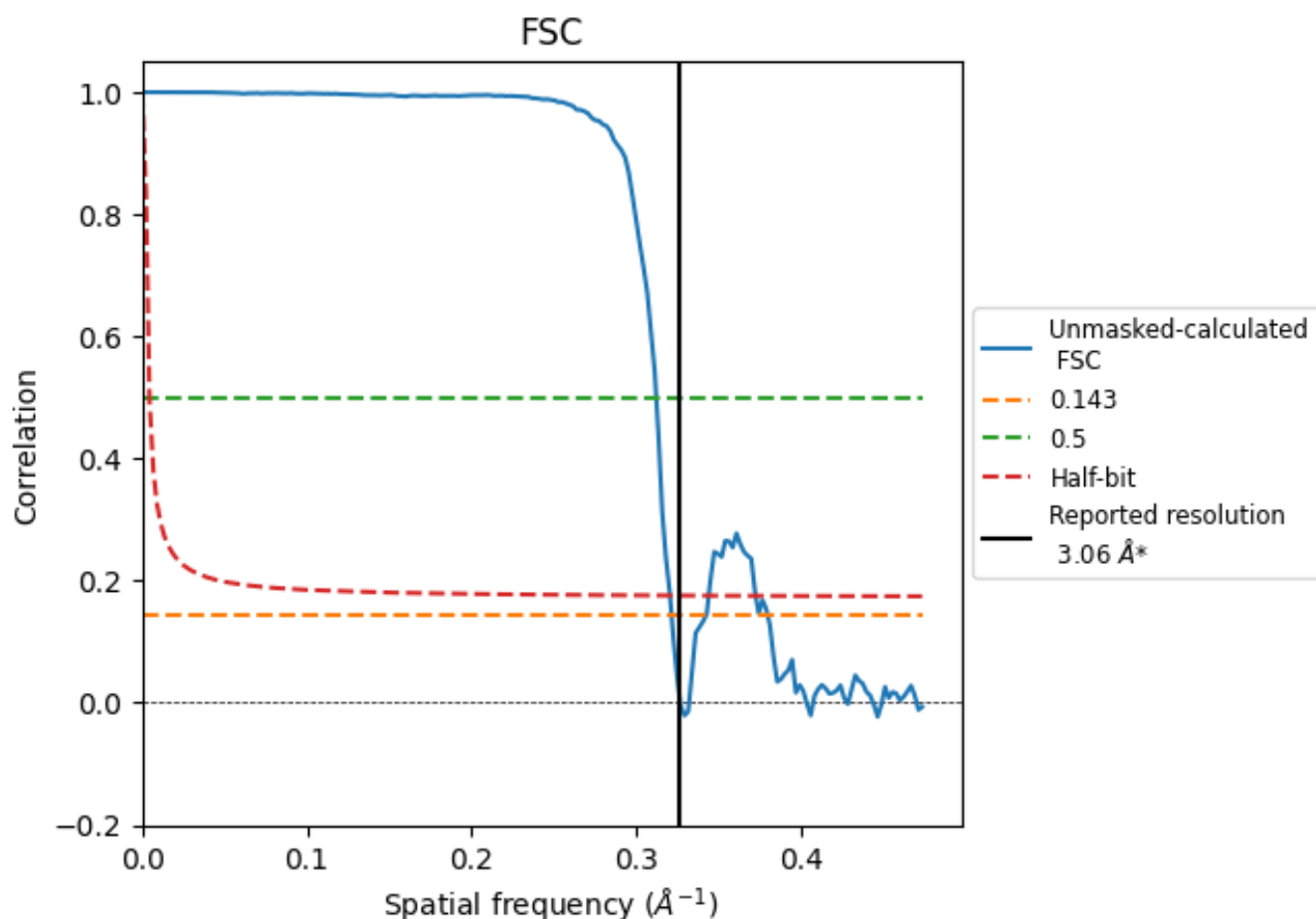


*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

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 0.327\AA^{-1}

8.2 Resolution estimates [i](#)

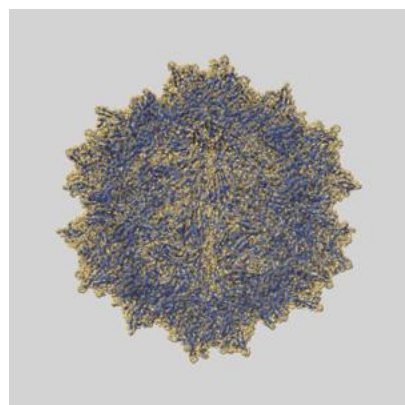
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.20	3.12

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

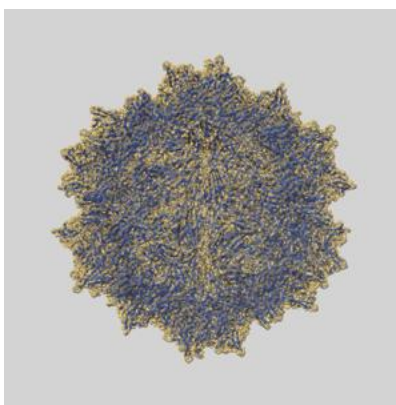
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41209 and PDB model 8TEY. Per-residue inclusion information can be found in section [3](#) on page [24](#).

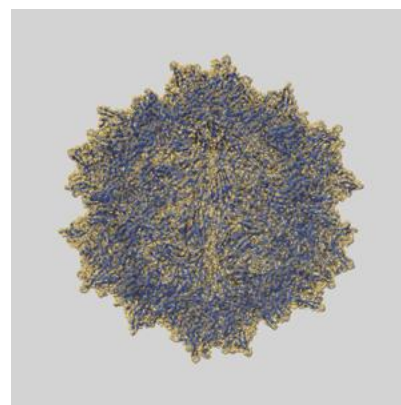
9.1 Map-model overlay [i](#)



X



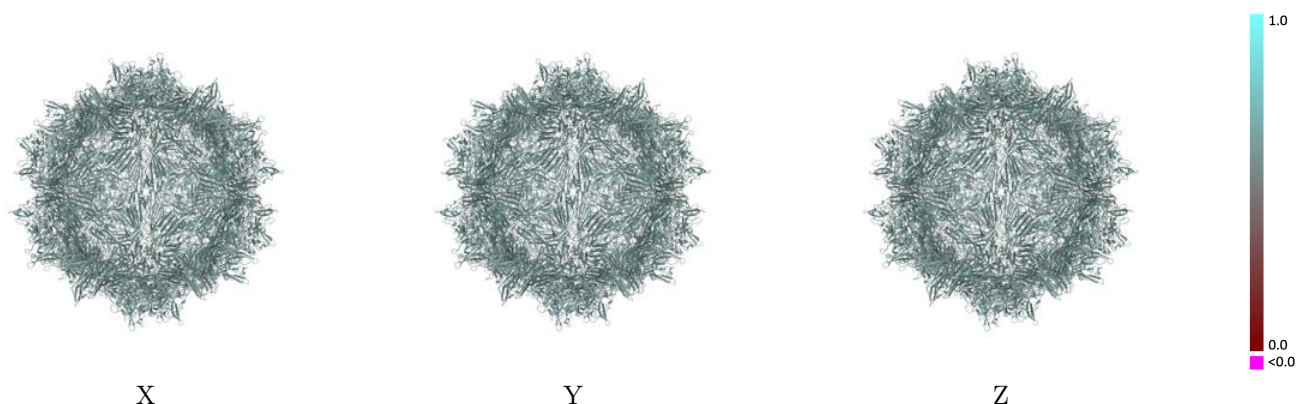
Y



Z

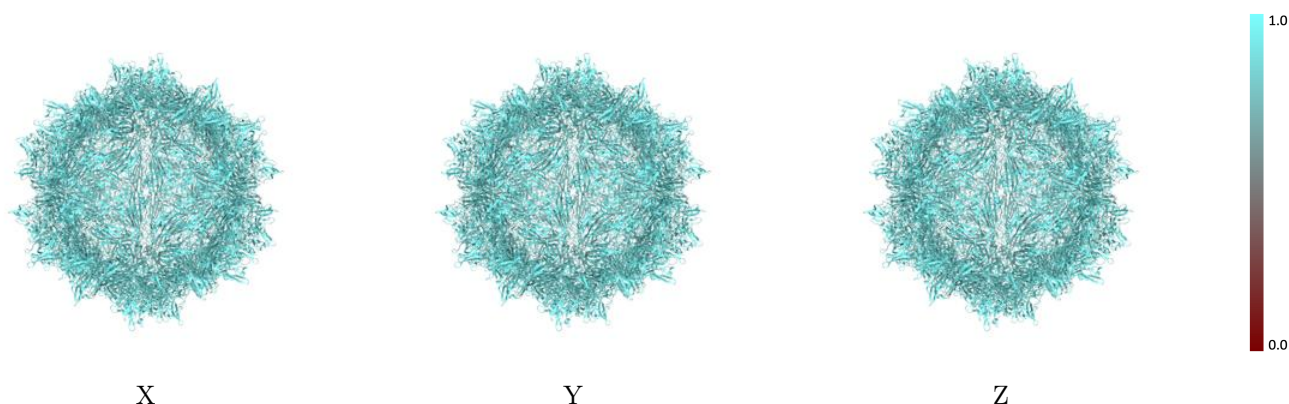
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



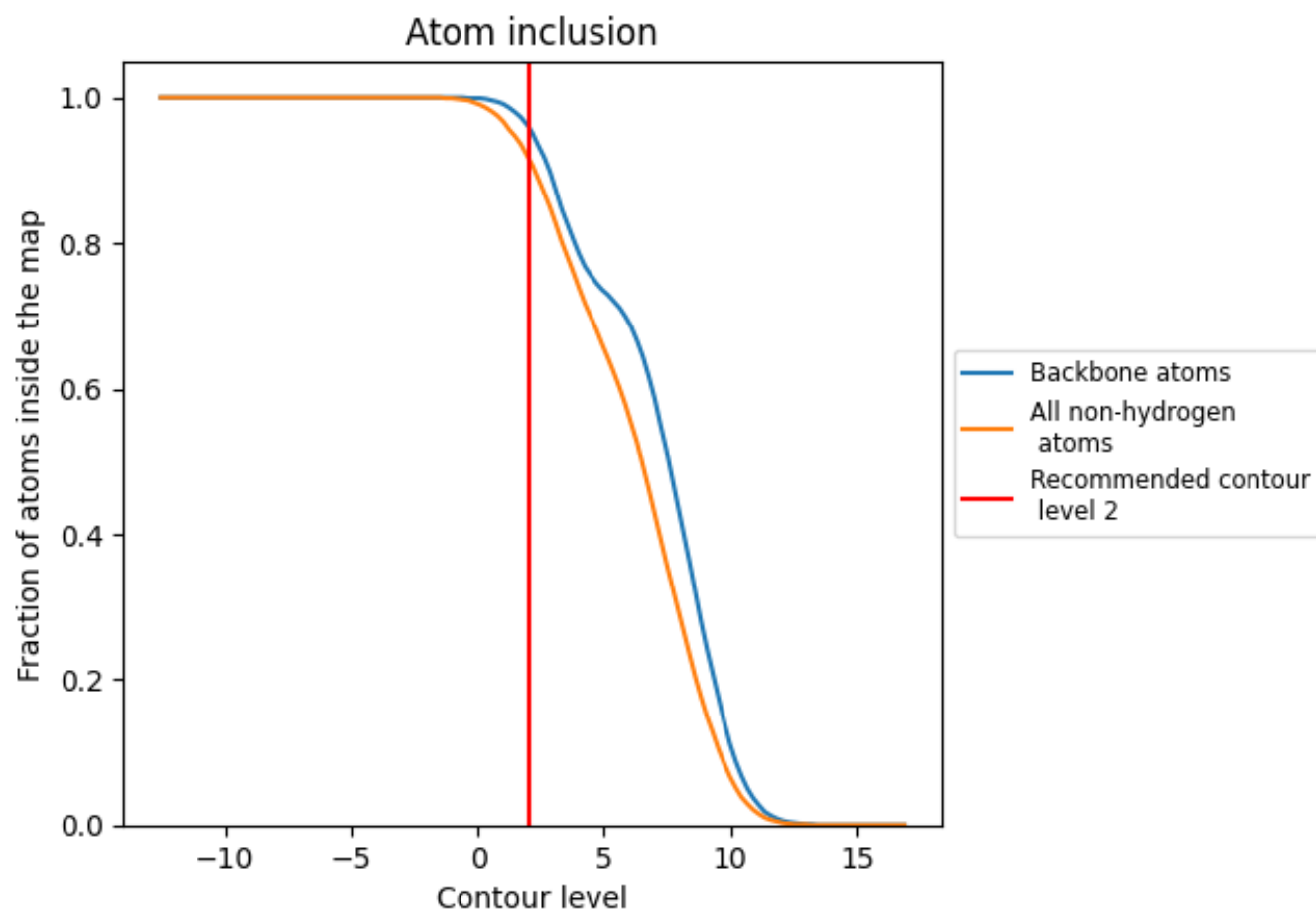
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5910
1	 0.9200	 0.5910
2	 0.9210	 0.5910
3	 0.9170	 0.5910
4	 0.9200	 0.5920
5	 0.9180	 0.5920
6	 0.9180	 0.5910
7	 0.9180	 0.5910
8	 0.9170	 0.5910
A	 0.9180	 0.5910
B	 0.9210	 0.5910
C	 0.9190	 0.5920
D	 0.9180	 0.5920
E	 0.9160	 0.5910
F	 0.9170	 0.5910
G	 0.9170	 0.5910
H	 0.9180	 0.5910
I	 0.9190	 0.5920
J	 0.9210	 0.5910
K	 0.9200	 0.5920
L	 0.9210	 0.5910
M	 0.9170	 0.5910
N	 0.9180	 0.5910
O	 0.9170	 0.5910
P	 0.9180	 0.5920
Q	 0.9190	 0.5920
R	 0.9200	 0.5910
S	 0.9210	 0.5910
T	 0.9190	 0.5920
U	 0.9210	 0.5920
V	 0.9200	 0.5920
W	 0.9180	 0.5920
X	 0.9170	 0.5910
Y	 0.9180	 0.5910
Z	 0.9170	 0.5920



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Chain	Atom inclusion	Q-score
a	 0.9180	 0.5910
b	 0.9180	 0.5920
c	 0.9170	 0.5920
d	 0.9170	 0.5920
e	 0.9180	 0.5910
f	 0.9180	 0.5910
g	 0.9190	 0.5920
h	 0.9170	 0.5910
i	 0.9180	 0.5910
j	 0.9180	 0.5920
k	 0.9180	 0.5910
l	 0.9170	 0.5910
m	 0.9190	 0.5920
n	 0.9170	 0.5930
o	 0.9170	 0.5910
p	 0.9200	 0.5920
q	 0.9210	 0.5910
r	 0.9210	 0.5910
s	 0.9210	 0.5910
t	 0.9160	 0.5910
u	 0.9190	 0.5910
v	 0.9180	 0.5920
w	 0.9170	 0.5900
x	 0.9190	 0.5920
y	 0.9170	 0.5910
z	 0.9210	 0.5910