



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 12:00 PM UTC

PDB ID : 8FYW / pdb_00008fyw
EMDB ID : EMD-29598
Title : Cryo-EM Structure of genome containing AAV2
Authors : Bennett, A.D.; Mckenna, R.
Deposited on : 2023-01-26
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

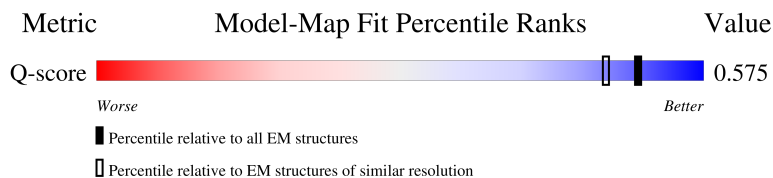
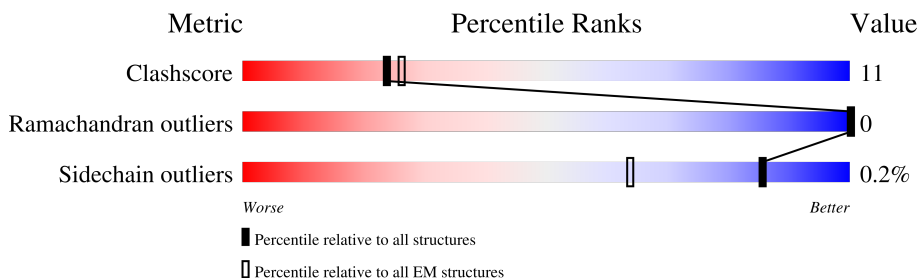
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

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



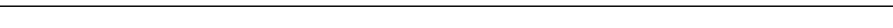
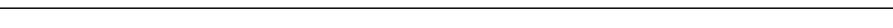
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	735	
1	2	735	
1	3	735	
1	4	735	

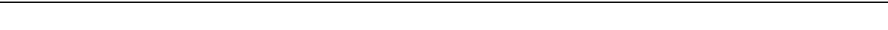
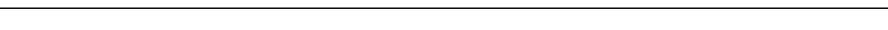
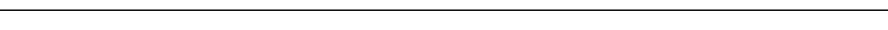
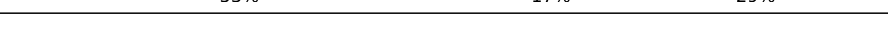
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Mol	Chain	Length	Quality of chain
1	5	735	
1	6	735	
1	7	735	
1	8	735	
1	A	735	
1	B	735	
1	C	735	
1	D	735	
1	E	735	
1	F	735	
1	G	735	
1	H	735	
1	I	735	
1	J	735	
1	K	735	
1	L	735	
1	M	735	
1	N	735	
1	O	735	
1	P	735	
1	Q	735	
1	R	735	
1	S	735	
1	T	735	
1	U	735	

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Mol	Chain	Length	Quality of chain
1	V	735	
1	W	735	
1	X	735	
1	Y	735	
1	Z	735	
1	a	735	
1	b	735	
1	c	735	
1	d	735	
1	e	735	
1	f	735	
1	g	735	
1	h	735	
1	i	735	
1	j	735	
1	k	735	
1	l	735	
1	m	735	
1	n	735	
1	o	735	
1	p	735	
1	q	735	
1	r	735	
1	s	735	
1	t	735	

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Mol	Chain	Length	Quality of chain
1	u	735	 52%18%29%
1	v	735	 53%17%29%
1	w	735	 53%18%29%
1	x	735	 53%17%29%
1	y	735	 53%17%29%
1	z	735	 54%17%29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 251220 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	B	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	C	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	D	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	E	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	F	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	G	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	H	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	I	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	J	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	K	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	L	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	M	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	N	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	O	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	P	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Q	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	S	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	T	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	U	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	V	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	W	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	X	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Y	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	Z	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	a	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	b	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	c	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	d	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	e	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	f	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	g	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	h	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	i	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	j	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	k	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	l	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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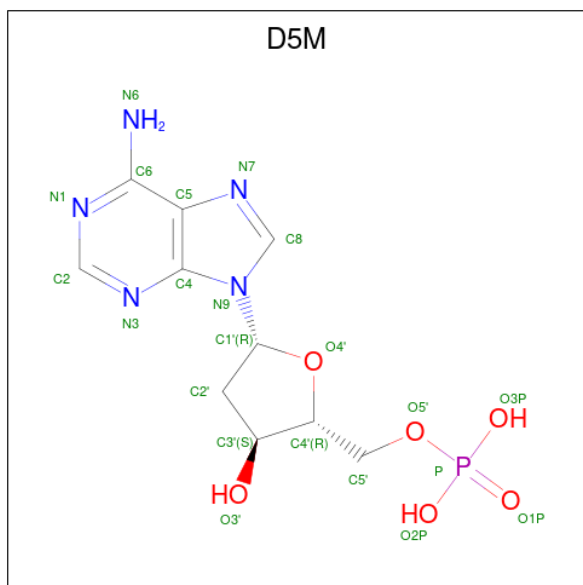
Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	n	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	o	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	p	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	q	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	r	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	s	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	t	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	u	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	v	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	w	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	x	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	y	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	z	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	1	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	2	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	3	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	4	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	5	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	6	519	Total 4166	C 2620	N 731	O 802	S 13	2	0
1	7	519	Total 4166	C 2620	N 731	O 802	S 13	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	519	Total	C	N	O	S	2	0
			4166	2620	731	802	13		

- 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	C	N	O	P	0
			21	10	5	5	1	
2	B	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	C	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	D	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	E	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	F	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	G	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	H	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	I	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	J	1	Total	C	N	O	P	0
			21	10	5	5	1	

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Mol	Chain	Residues	Atoms					AltConf
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
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

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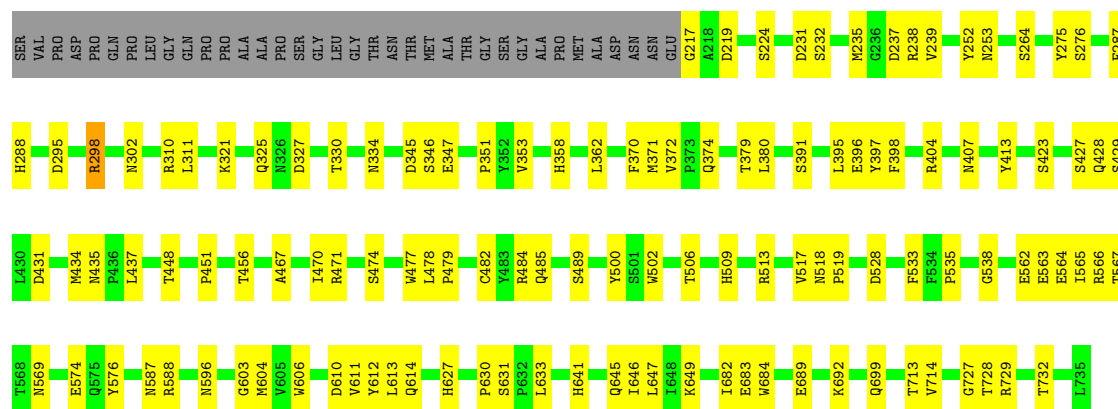
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Mol	Chain	Residues	Atoms					AltConf
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2	g	1	Total 21	C 10	N 5	O 5	P 1	0
2	h	1	Total 21	C 10	N 5	O 5	P 1	0
2	i	1	Total 21	C 10	N 5	O 5	P 1	0
2	j	1	Total 21	C 10	N 5	O 5	P 1	0
2	k	1	Total 21	C 10	N 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
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

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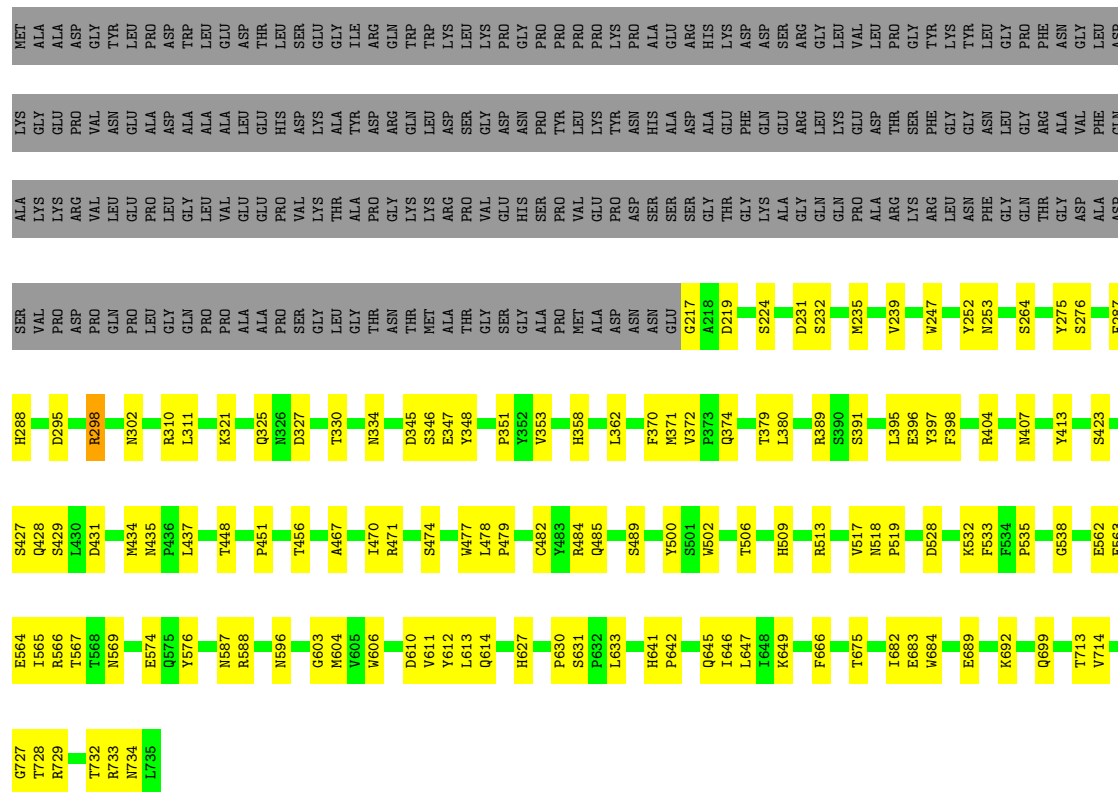
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Mol	Chain	Residues	Atoms					AltConf
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			21	10	5	5	1	
2	2	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	3	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	4	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	5	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	6	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	7	1	Total	C	N	O	P	0
			21	10	5	5	1	
2	8	1	Total	C	N	O	P	0
			21	10	5	5	1	



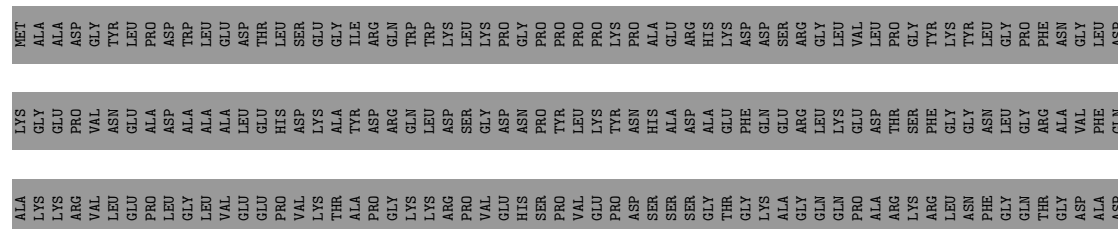
• Molecule 1: Capsid protein VP1

Chain C: 53% 17% 29%

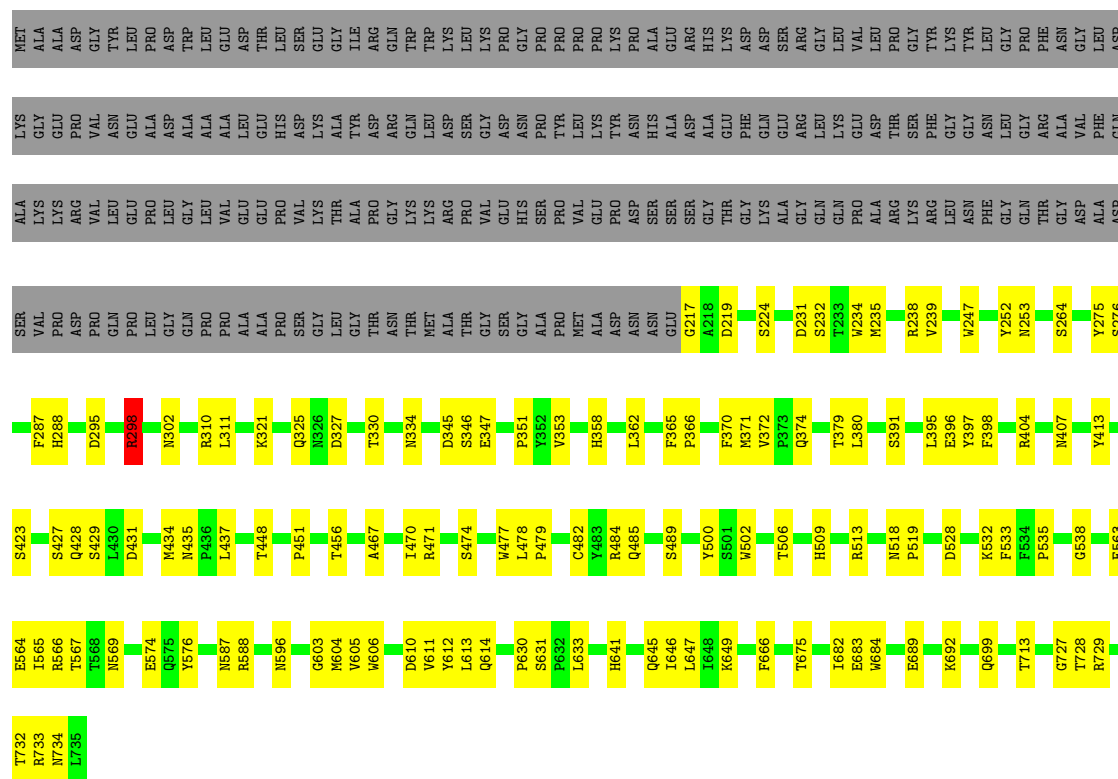


• Molecule 1: Capsid protein VP1

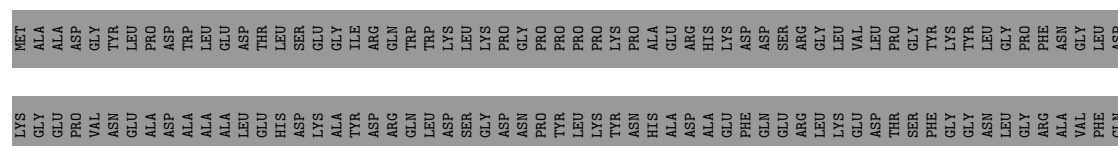
Chain D: 54% 17% 29%

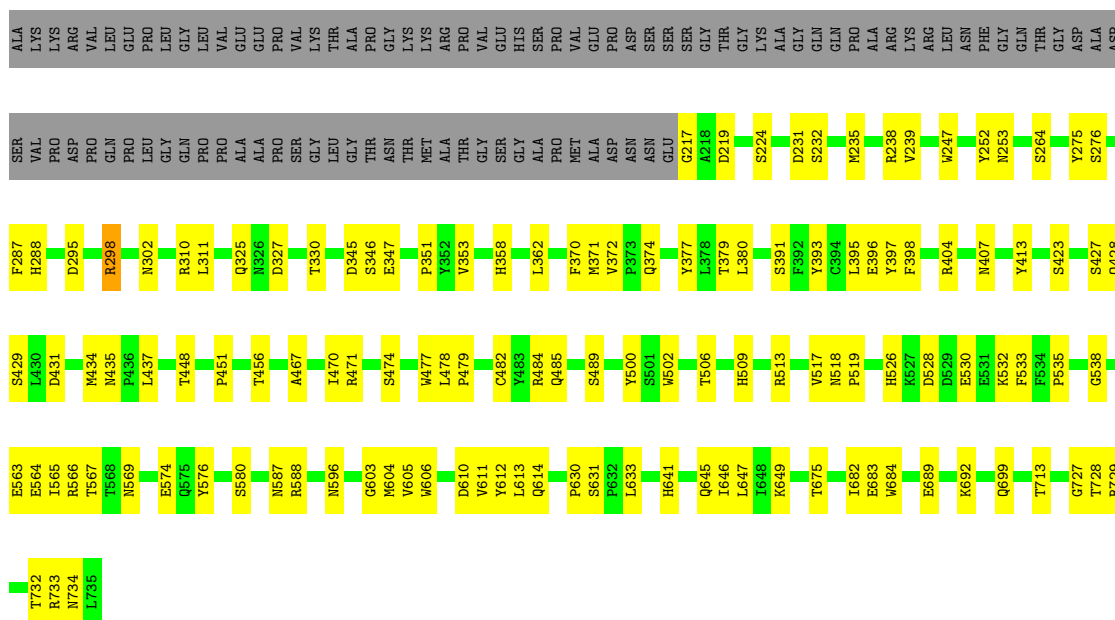


- Molecule 1: Capsid protein VP1

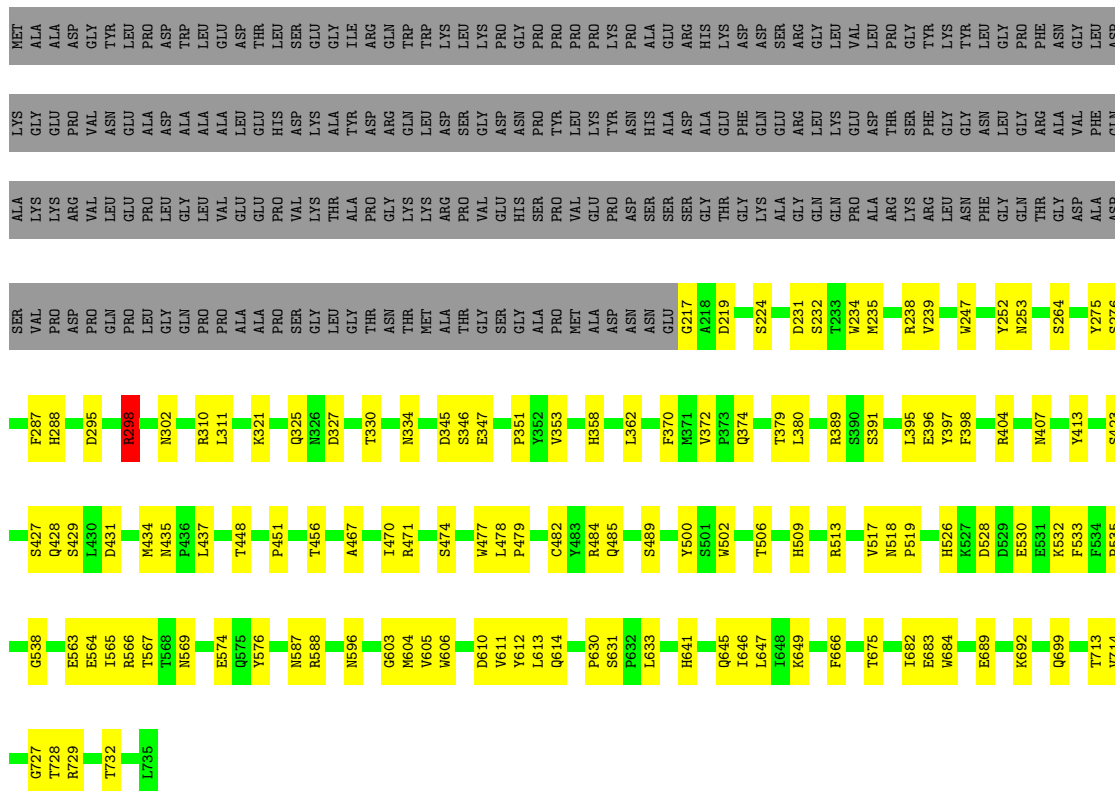


- Molecule 1: Capsid protein VP1





- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



Lysine	G727	M558	S429	R294	SER	ALA	LYS	MET
	T728	E563	L430	D295	VAL	LYS	GLY	
	R729	I565	D431	R298	ASP	ARG	ALA	
	T732	E564	M434	R302	PRO	VAL	ASN	TYR
		R733	I566	P436	R310	GLN	LEU	LEU
		R734	T567	L437	L311	PRO	GLU	GLU
	L735	T568	L438	R310	LEU	PRO	ALA	PRO
		N569	T448	L311	GLN	GLY	ASP	TRP
		E574	P451	K321	PRO	ALA	ALA	LEU
		G575	P451	Q325	PRO	VAL	LEU	GLU
Threonine	T728	Y576	T456	R326	ALA	GLU	THR	ASP
		N587	D327	D327	PRO	GLU	HIS	THR
		R588	A467	T330	SER	VAL	ASP	SER
		N596	L470	T330	GLY	LYS	LYS	GLY
		G603	L471	N334	LEU	THR	ALA	GLY
		M604	R471	T339	THR	ALA	TLE	ARG
		V605	S474	T339	ASN	GLY	ASP	ARG
		V606	L477	D345	MET	LYS	LYS	TRP
			L478	S346	THR	ARG	LEU	TRP
			P479	E347	ALA	ASP	ASP	LYS
Proline					THR	PRO	LEU	LEU
		D610	C482	P351	GLY	VAL	GLY	LYS
		Y612	Y483	R352	SER	GLU	ASP	PRO
		L613	R484	V353	GLY	HIS	ASN	GLY
		Q614	Q485	V353	ALA	SER	PRO	PRO
					PRO	PRO	TYR	PRO
		P630	S489	H358	MET	VAL	LEU	PRO
		S632	Y500	L362	ALA	GLU	LYS	LYS
		L633	S601	F370	ASN	ASP	ASN	PRO
			W502	H371	ASN	SER	HIS	GLU
Alanine		H641	T506	P372	GLU	SER	ALA	GLU
		Q645		Q374	D217	GLY	ALA	ARG
		I646	H509	Q374	D219	THR	ALA	HIS
		L647				GLY	PHE	LYS
		I648		T379	S224	LYS	GLN	ASP
		K649	R513	L380		ALA	GLN	SER
		F666	V517	S391	D231	GLY	ARG	ARG
		T675	N518		S232	GLN	LEU	GLY
		I682	P519	L395	V239	GLN	GLU	VAL
		E683	H526	E396	V239	ALA	ASP	LEU
Tyrosine	T732	I682	K527	Y397	W247	ARG	THR	PRO
	R733	E683	D528	F396	Y253	LYS	SER	GLY
	L735	W684	D529	R404	N252	ARG	PHE	TYR
						LEU	GLY	LYS
						ASN	GLY	TYR
		E689	E530	N407	S264	PHE	ASN	LEU
						GLY		GLY
		K692	F533	Y413	Y275	GLN	PRO	PRO
		T701	P635	S423	S276	THR	GLY	PHE
						GLY	ASN	ALA
Valine					F287	ASP	VAL	GLY
		T713	G538	S427	H288	GLY	VAL	PHE
						ASN	THR	LYS
						ASP	THR	LEU
						ALA	THR	LEU
						ASP	THR	LEU
						ALA	THR	LEU
						ALA	THR	LEU
						ALA	THR	LEU
						ALA	THR	LEU

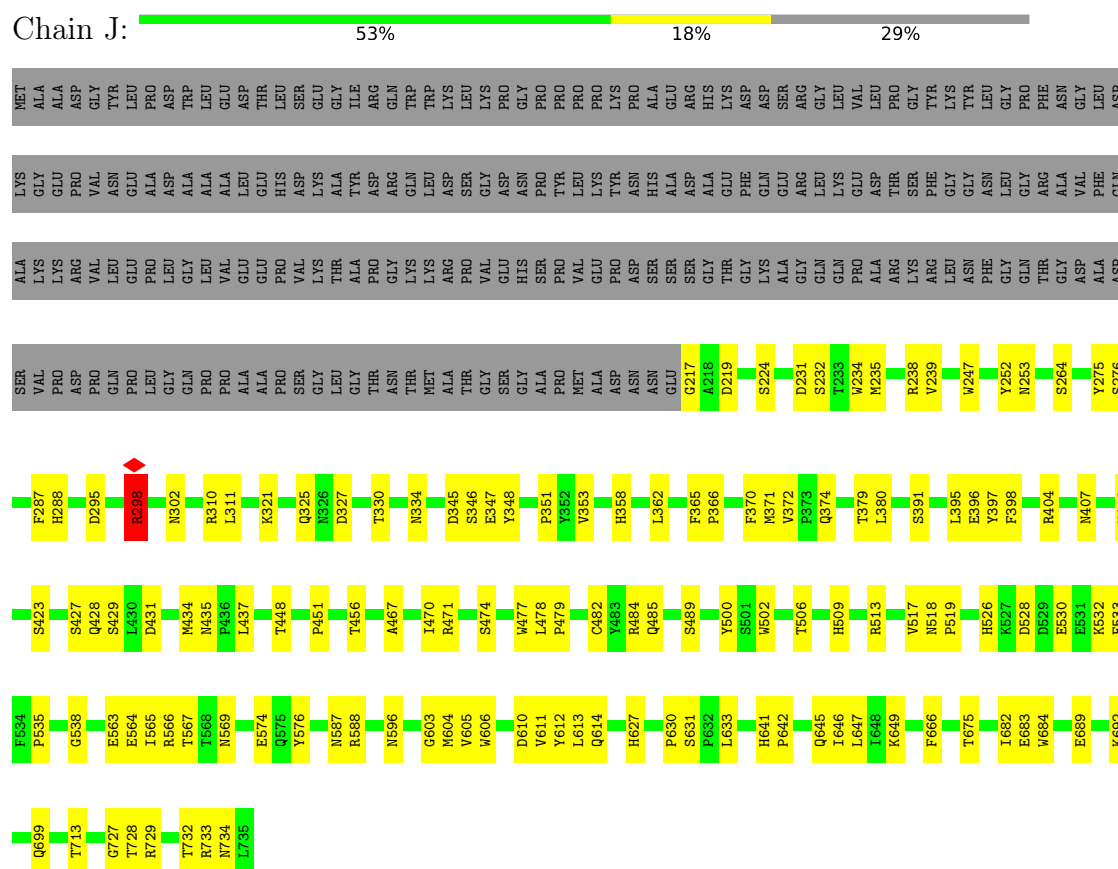
- Molecule 1: Capsid protein VP1

Chain I: 53% 18% 29%

T713	F642	S429	F287	SER	ALA	LYS	MET
V714	M558	L430 D431	H288	VAL	LYS	GLY	ALA
G727				ASP	ARG	PRO	ASP
T728	E562	M434	D295	PRO	VAL	VAL	GLY
R729	E563	N435		GLN	LEU	ASN	TVR
	E564	F436	R298	PRO	GLU	GLU	LEU
T732	R565	L437		LEU	PRO	ALA	PRO
R733	R566	T448		GLY	GLY	ASP	TRP
N734	T567		N302	GLN	ALA	ALA	LEU
L735	T568	P451	R310	PRO	LEU	LEU	GLU
	N569		L311	PRO	VAL	ALA	ASP
				ALA	GLU	LEU	THR
	E574	T456	Q325	ALA	GLU	GLU	LEU
	Q575		N326	PRO	PRO	HIS	LEU
	Y576	A467	D327	SER	VAL	ASP	SER
				GLY	GLY	LYS	GLU
	N587	I470	T330	LEU	THR	ALA	GLY
R588	R471			GLY	ALA	TYR	ILE
			D345	THR	PRO	ASP	ARG
N596		S474	S346	ASN	GLN	GLN	TRP
			E347	THR	LYS	LYS	TRP
G603		W477		MET	LYS	LEU	TRP
M604	L478			ALA	ARG	ASP	LYS
V605	P479		P351	THR	PRO	SER	LEU
W606			Y352	GLY	VAL	GLY	LYS
		C482	V353	SER	GLU	ASP	PRO
D610	Y483			SER	GLU	GLY	PRO
V611	R484		H358	GLY	HIS	ASN	GLY
Y612	Q485			ALA	SER	PRO	PRO
L613			L362	PRO	PRO	TYR	PRO
Q614		S489		MET	VAL	LEU	PRO
			F365	ALA	GLU	LYS	PRO
P630	Y500		P366	ASP	PRO	TYR	LYS
S631	S501			ASN	ASN	ASN	PRO
R632	W502		F370	ASN	SER	HIS	ALA
L633			M371	GLU	SER	ALA	GLU
	T506		W372	G217	SER	ASP	ARG
			P373	G218	GLY	ALA	HIS
H641			Q374	D219	THR	LYS	LYS
					GLY	PHE	ASP
		H509			LYS	GLN	ASP
Q645			T379	S224	LYS	GLN	ASP
I646		R513	L380		ALA	GLU	SER
L647				D231	GLY	ARG	GLY
I648	V517		S391	S232	GLN	LEU	ARG
K649	N518			T233	GLN	LYS	LEU
	P519		L395	W234	PRO	GLU	VAL
			E396	M235	ALA	ASP	LEU
	H526		Y397		ARG	THR	PRO
T675	R527		F398	R238	LYS	SER	GLY
	D528			V239	LYS	SER	TYR
I682	D529				ARG	PHE	TYR
E683	E530		R404		LEU	GLY	TVR
W684	E531		M407	W247	ASN	ASN	LEU
	K532				PHE	GLY	GLY
E689	F533		Y413	Y252	GLY	LEU	TVR
	F534			N253	GLN	ARG	PRO
K692	P535		S423	S264	THR	ARG	ASN
					GLY	ALA	GLY
T701	G538		S427	Y276	ASP	VAL	GLY
				S275	ALA	PHE	LEU
					ASN	TYR	ASP

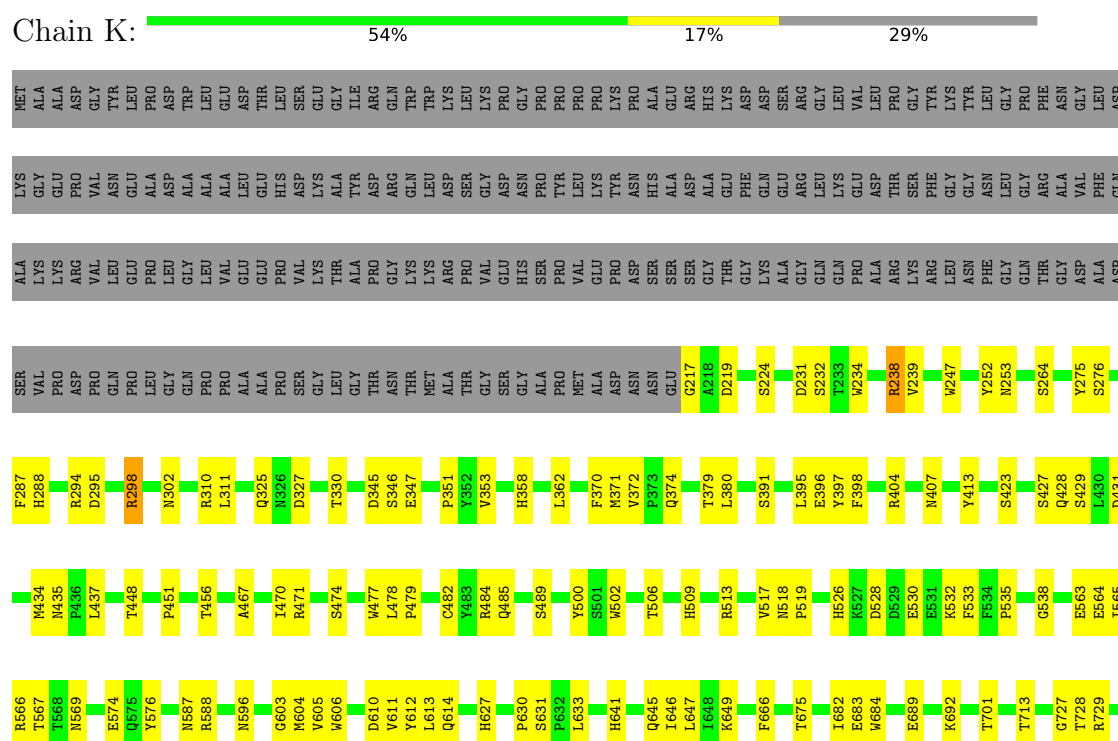
- Molecule 1: Capsid protein VP1

Chain J:



- Molecule 1: Capsid protein VP1

Chain K:





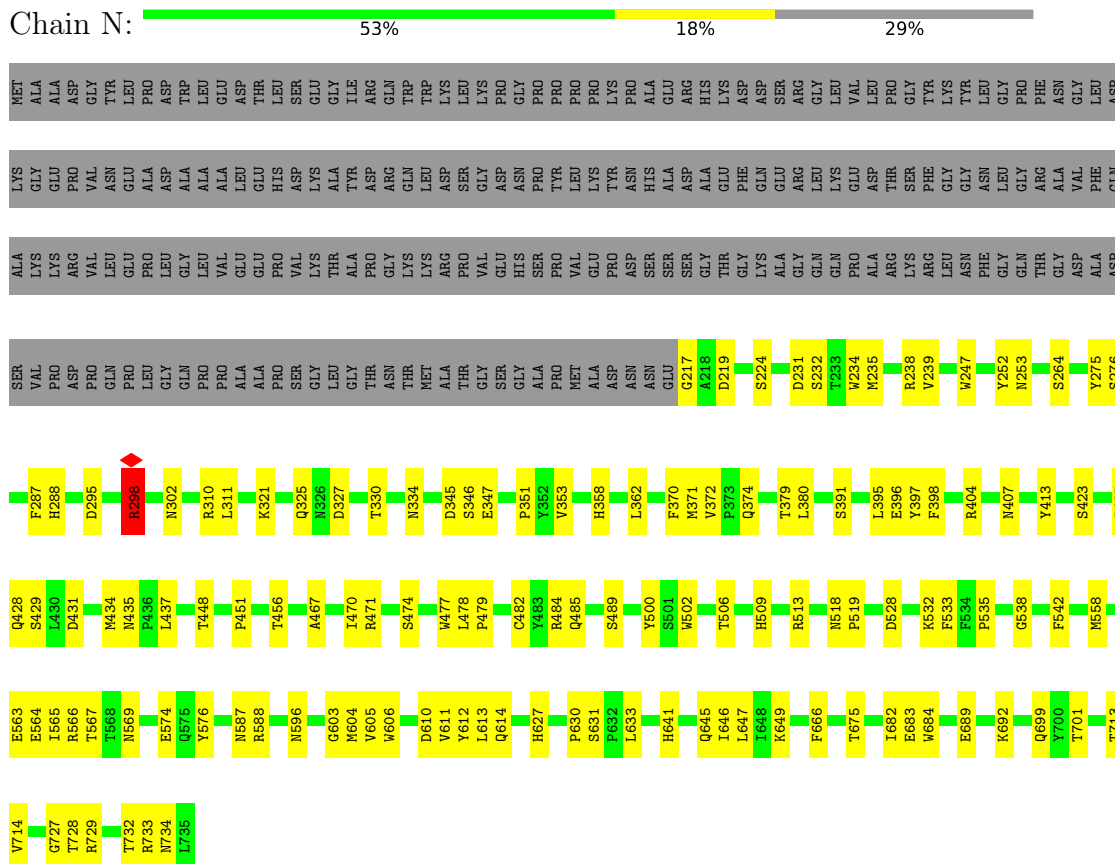
Response	Percentage
Used	53%
Not used	17%
Don't know	29%



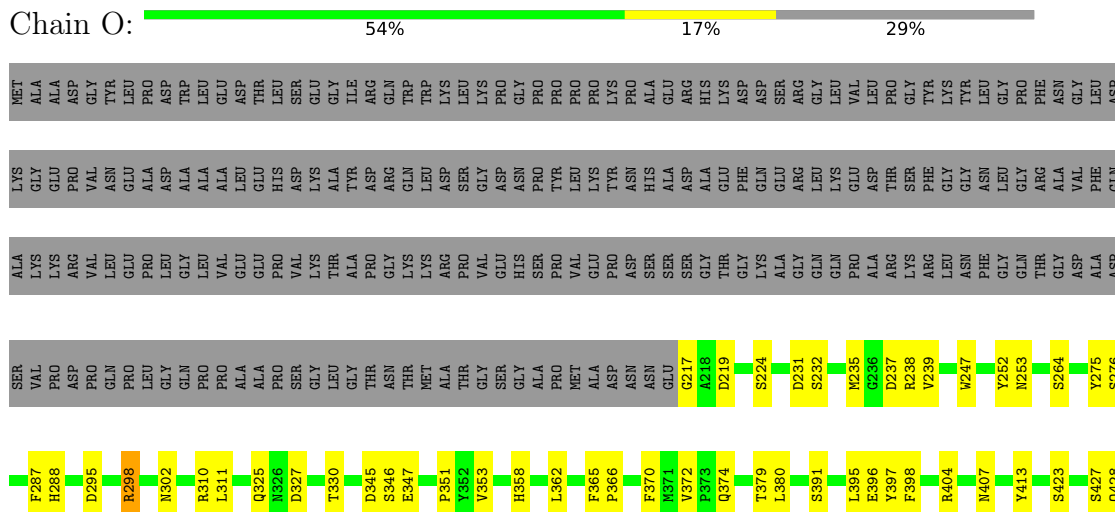
Category	Percentage
Very bad	53%
Bad	17%
Good	29%

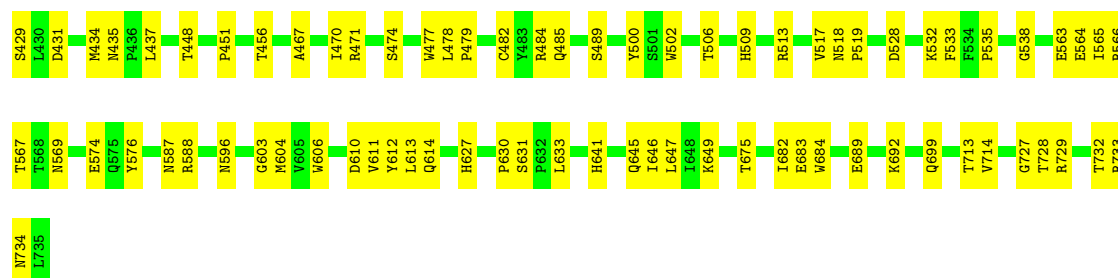


- Molecule 1: Capsid protein VP1

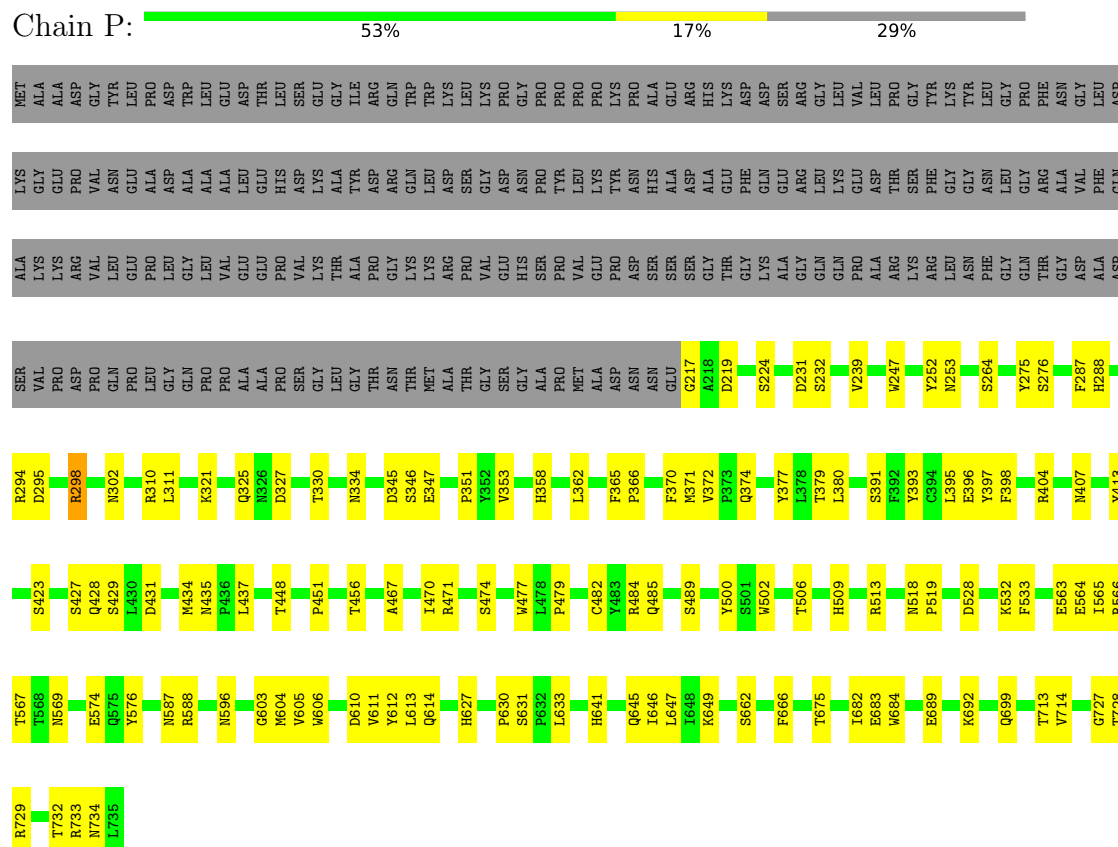


- Molecule 1: Capsid protein VP1

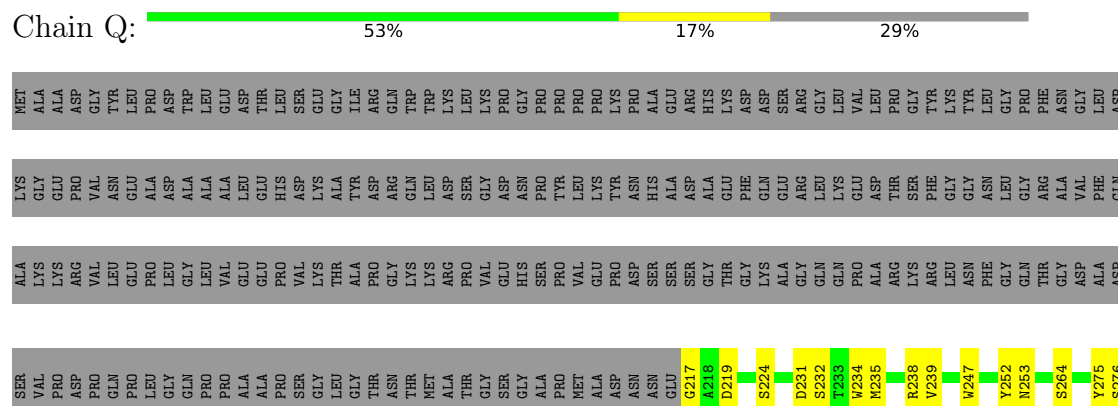


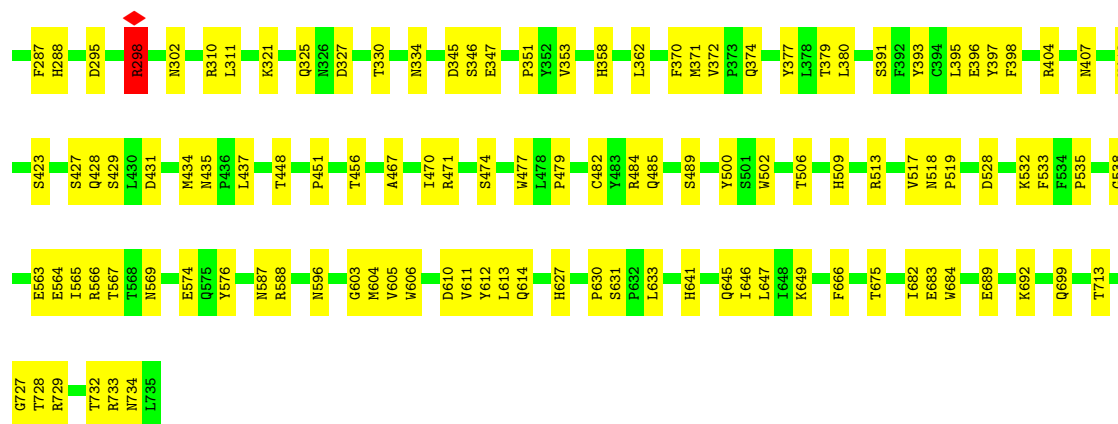


• Molecule 1: Capsid protein VP1



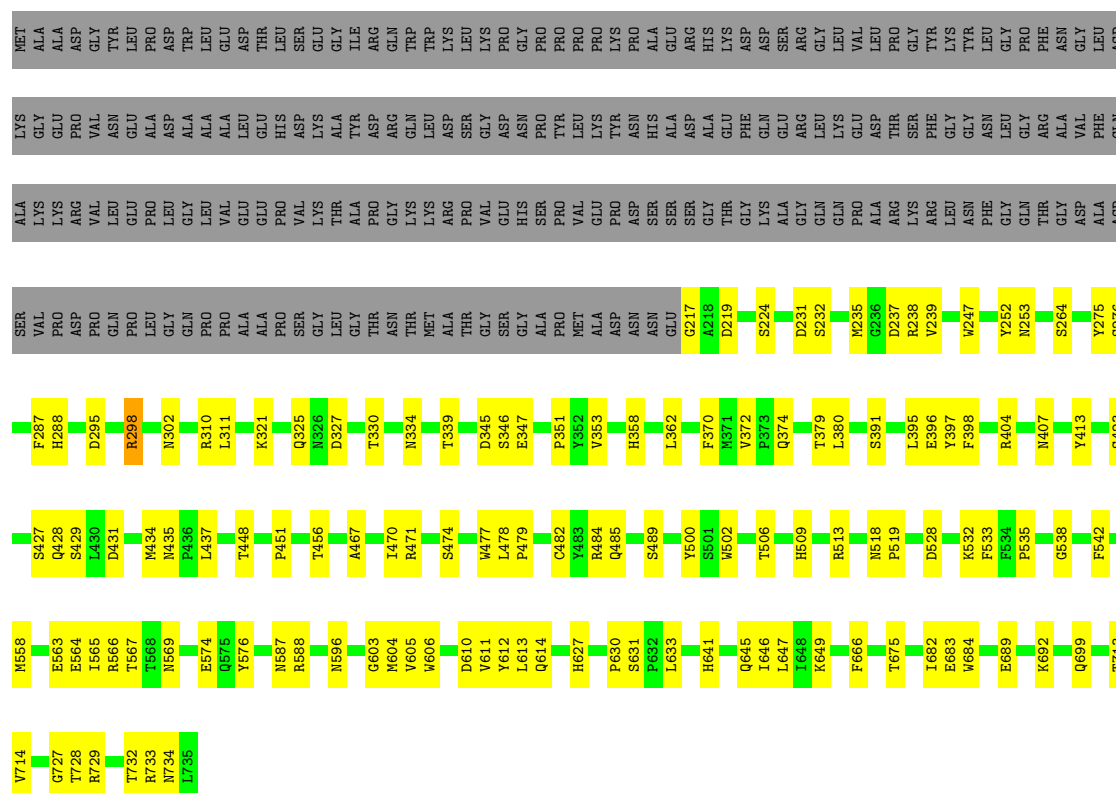
• Molecule 1: Capsid protein VP1





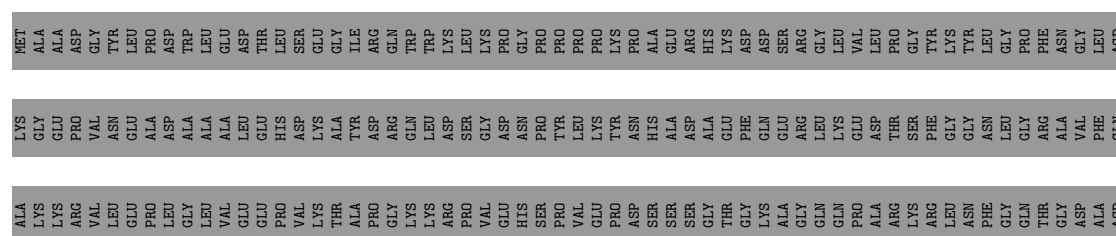
• Molecule 1: Capsid protein VP1

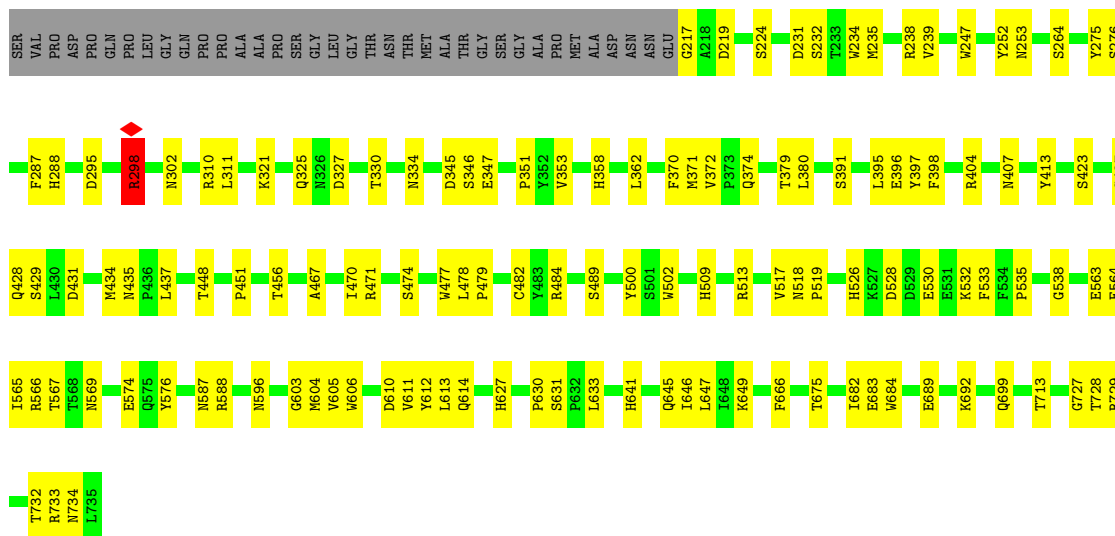
Chain R: 53% 17% 29%



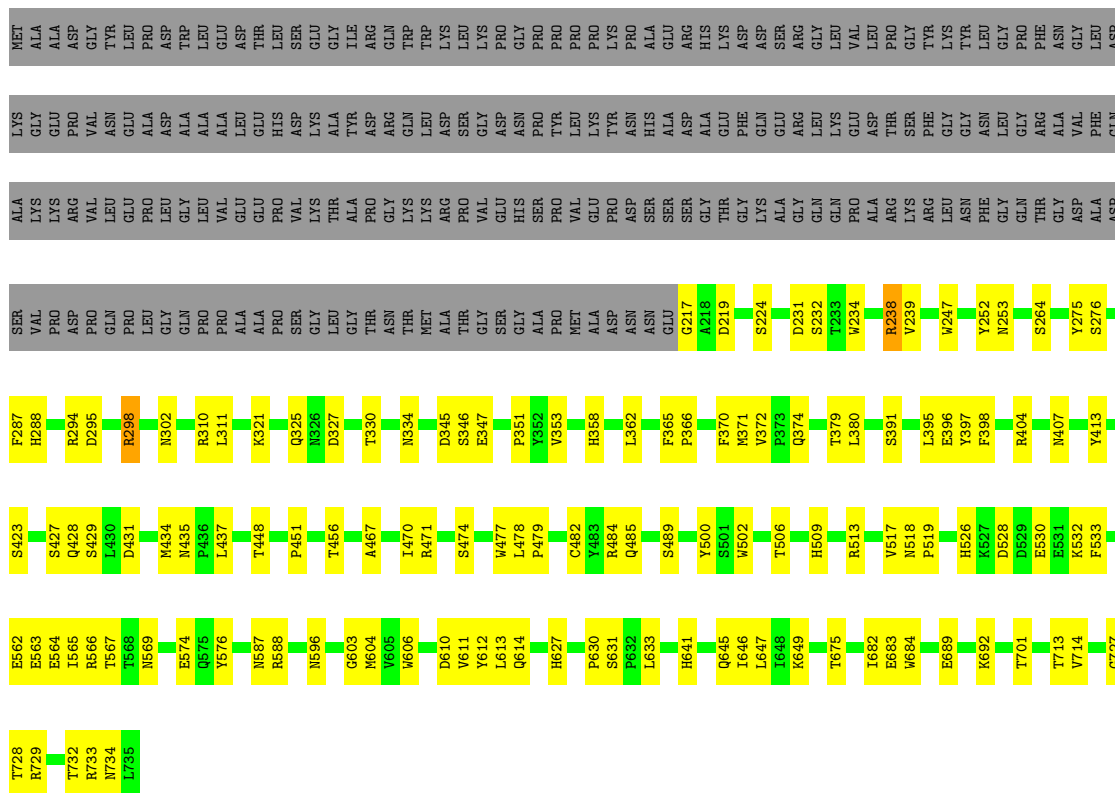
• Molecule 1: Capsid protein VP1

Chain S: 53% 17% 29%

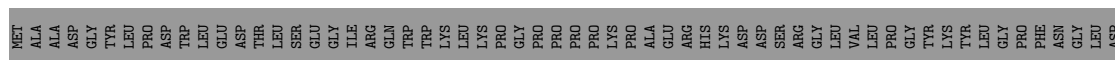




- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

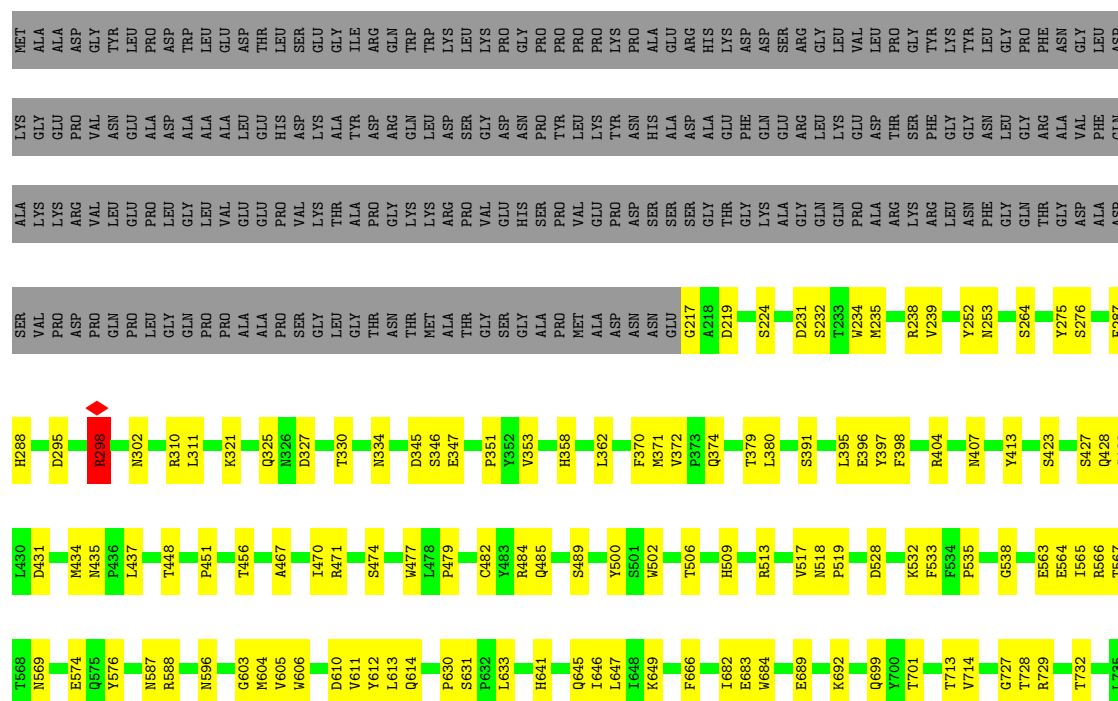


Response	Percentage
Yes	53%
No	17%
Don't know	29%

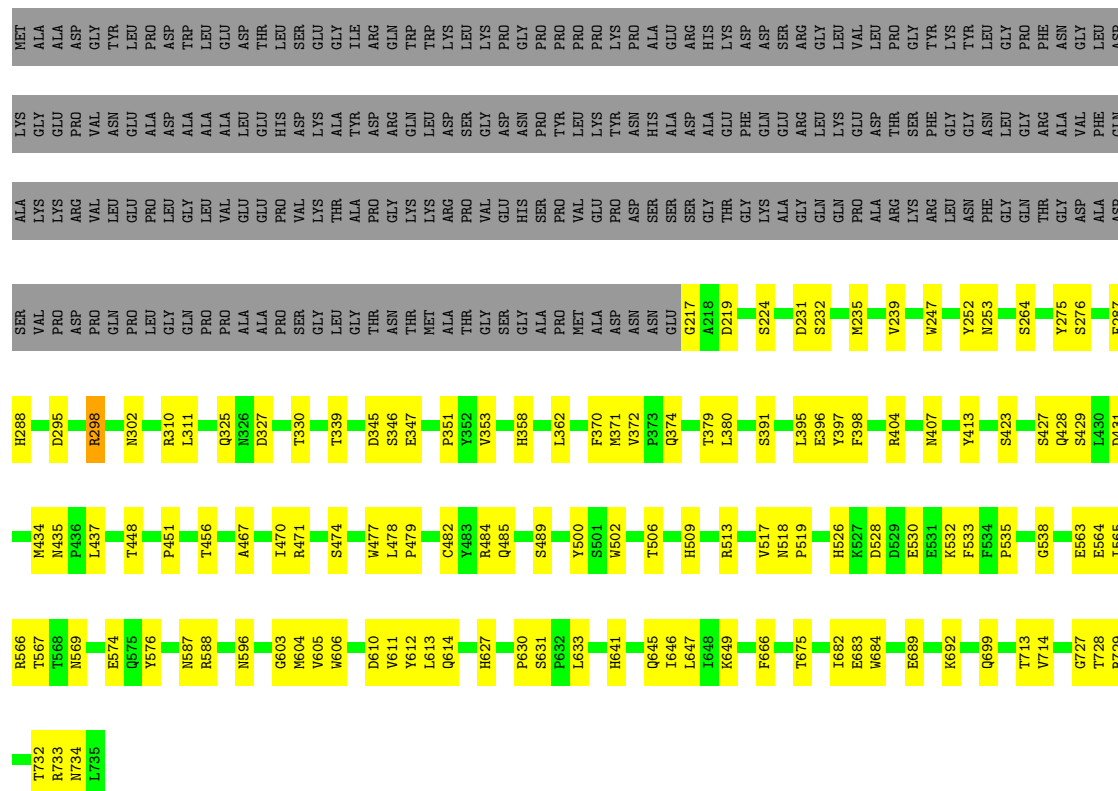


Digital Tool	Percentage
Video conferencing tool	54%
Digital whiteboard	17%
Digital sticky note	29%

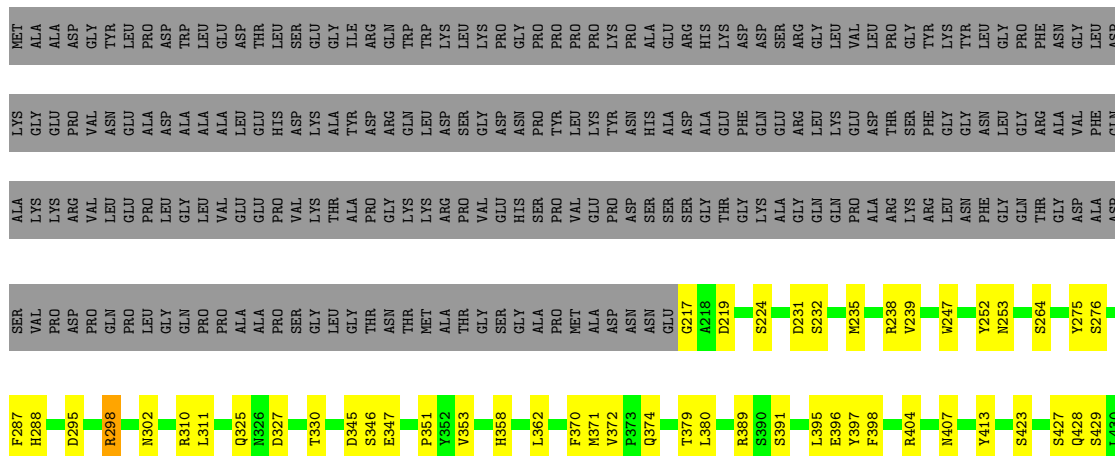


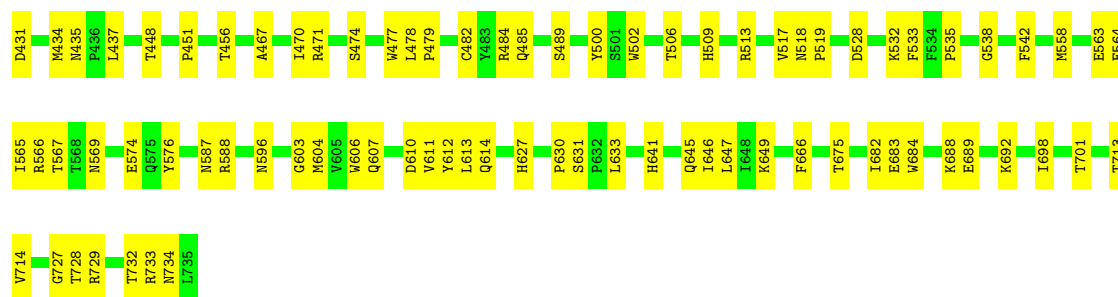


- Molecule 1: Capsid protein VP1



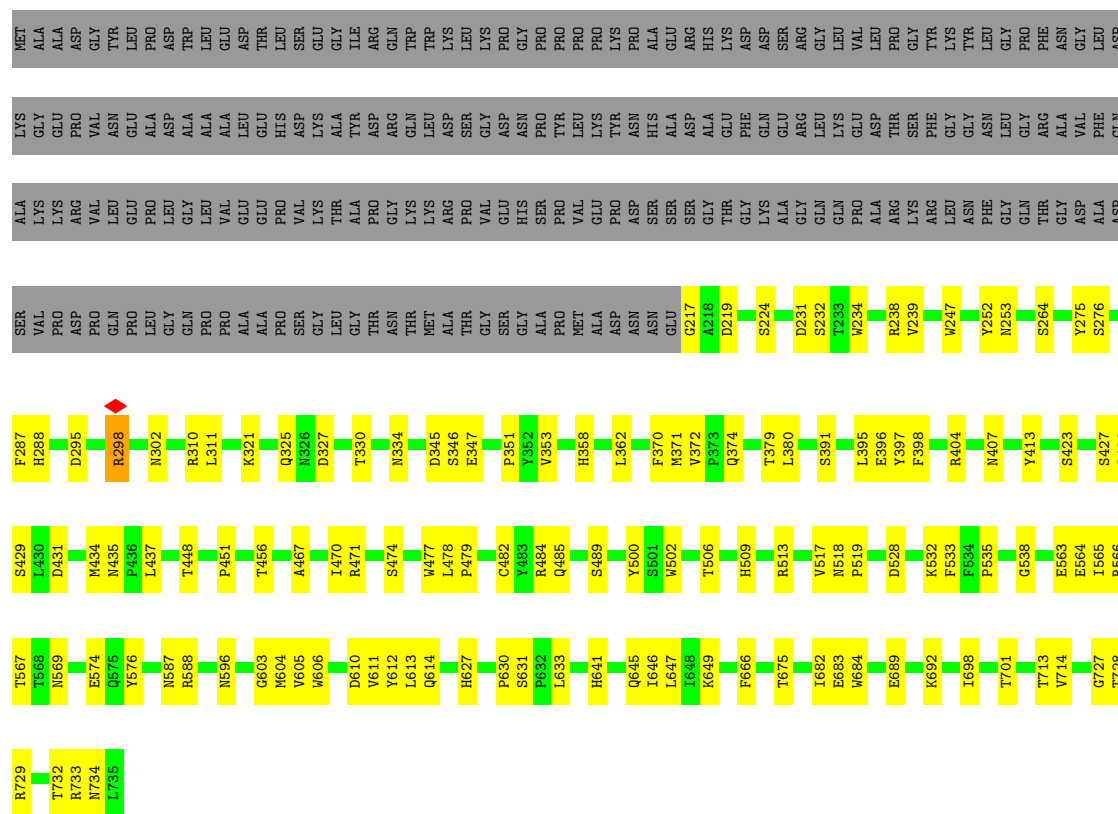
- Molecule 1: Capsid protein VP1





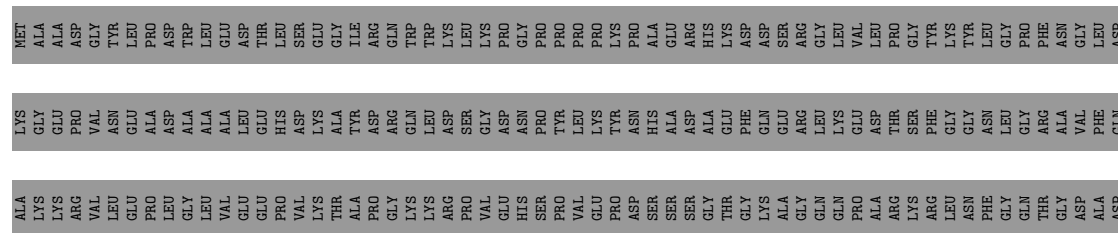
• Molecule 1: Capsid protein VP1

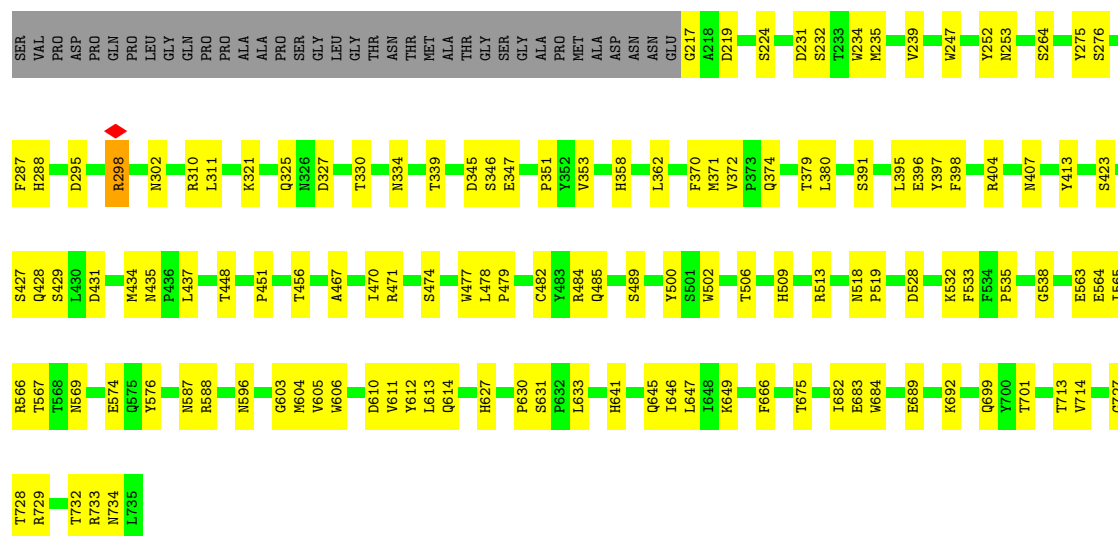
Chain g: 53% 17% 29%



• Molecule 1: Capsid protein VP1

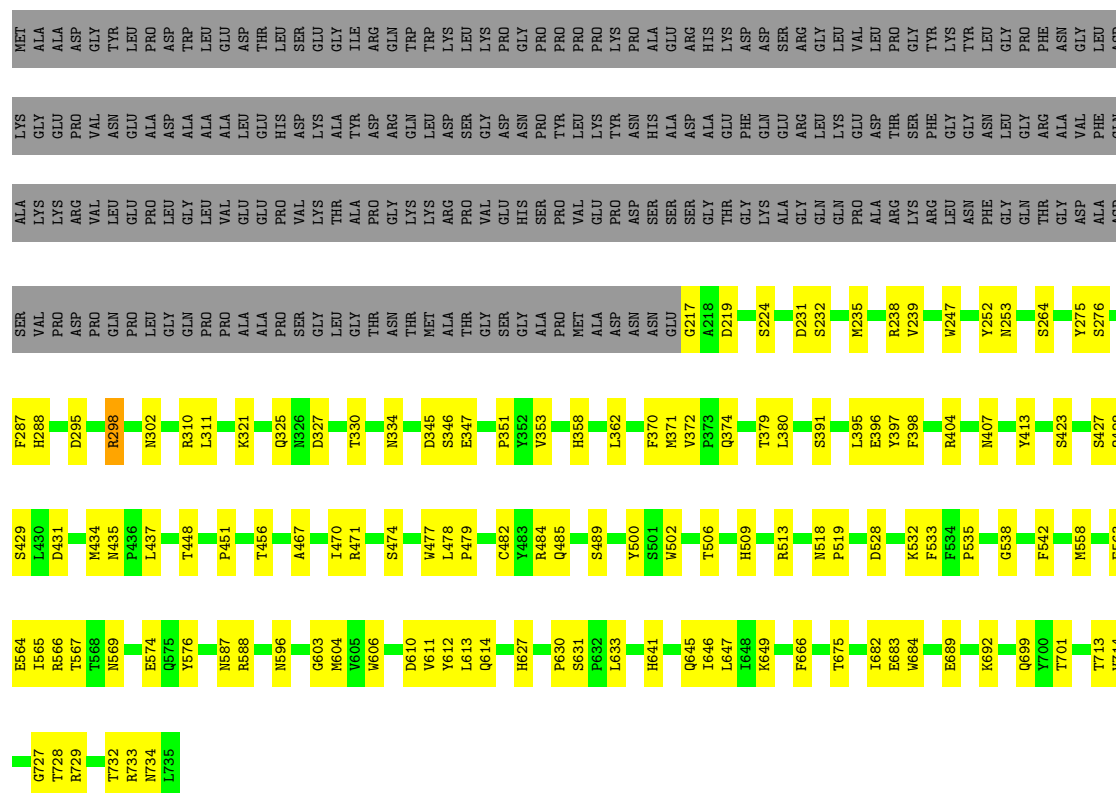
Chain h: 53% 17% 29%





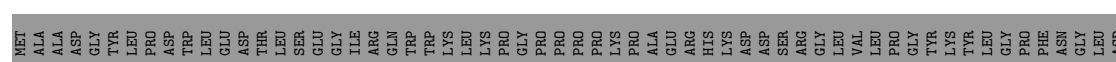
• Molecule 1: Capsid protein VP1

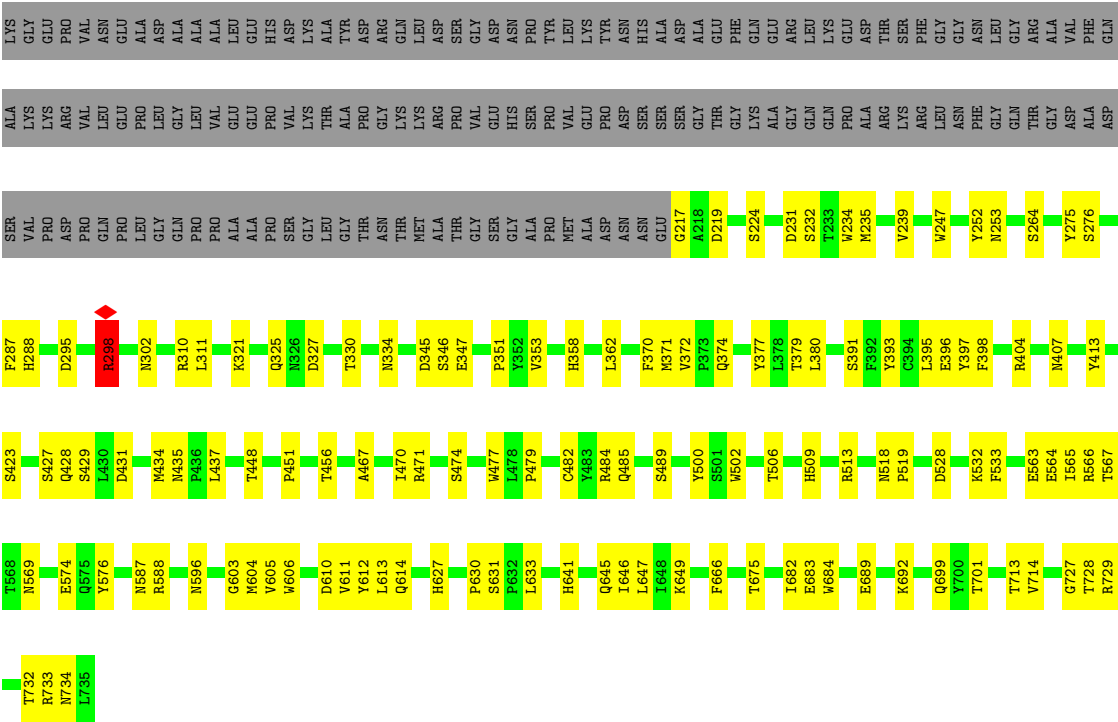
Chain i: 53% 17% 29%



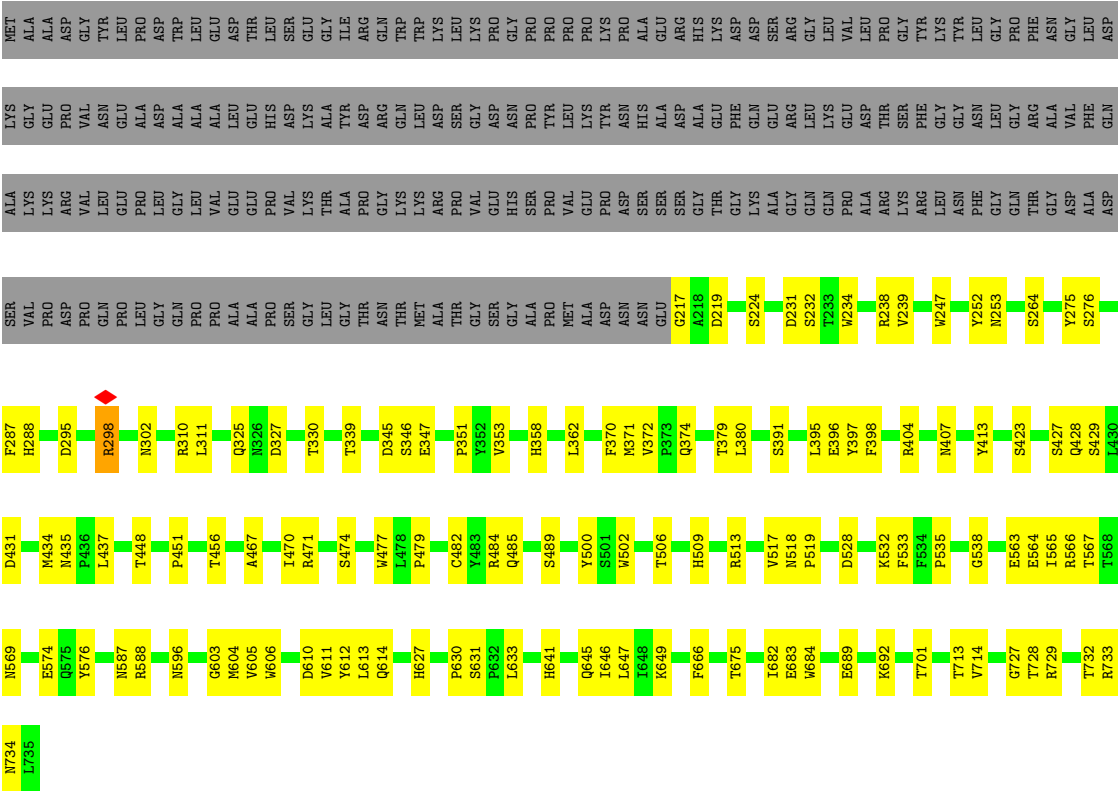
• Molecule 1: Capsid protein VP1

Chain j: 53% 17% 29%



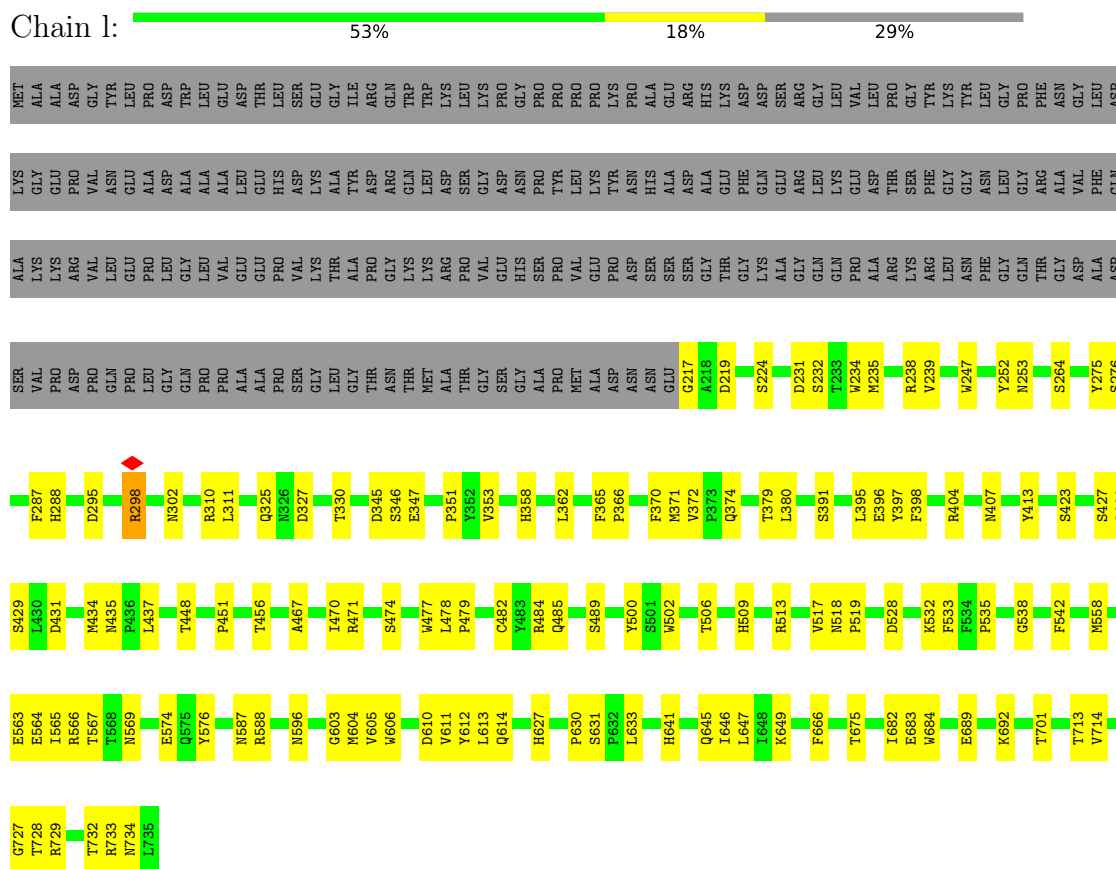


● Molecule 1: Capsid protein VP1



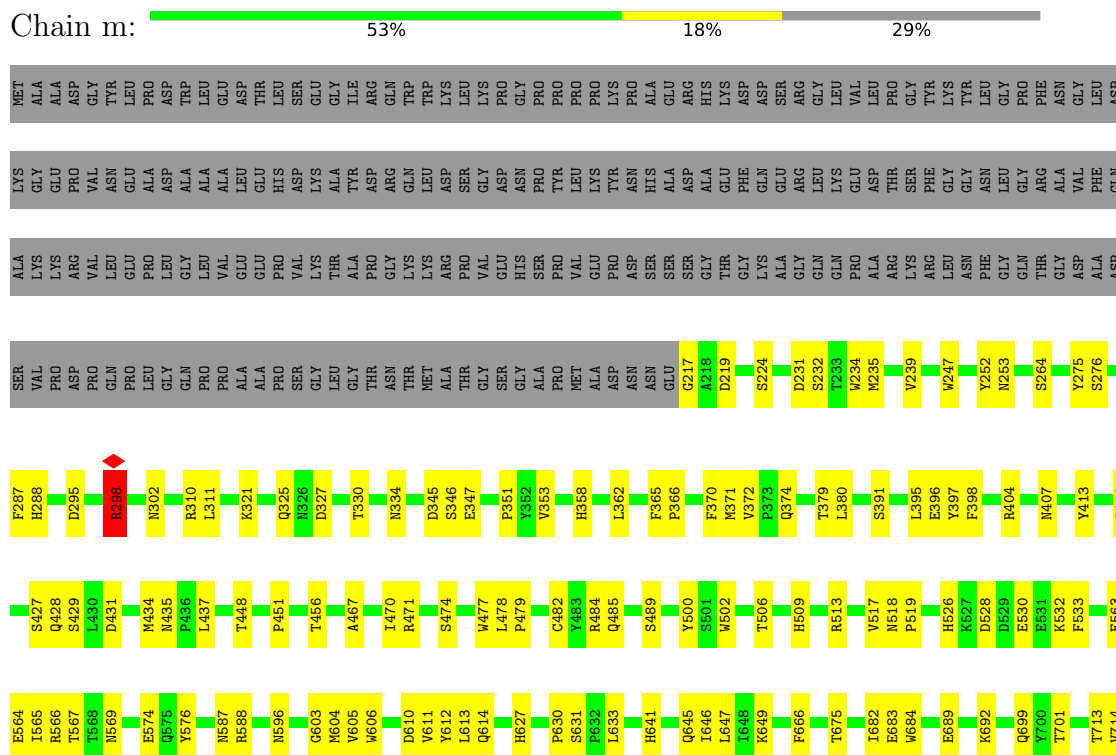
● Molecule 1: Capsid protein VP1

Chain l:



● Molecule 1: Capsid protein VP1

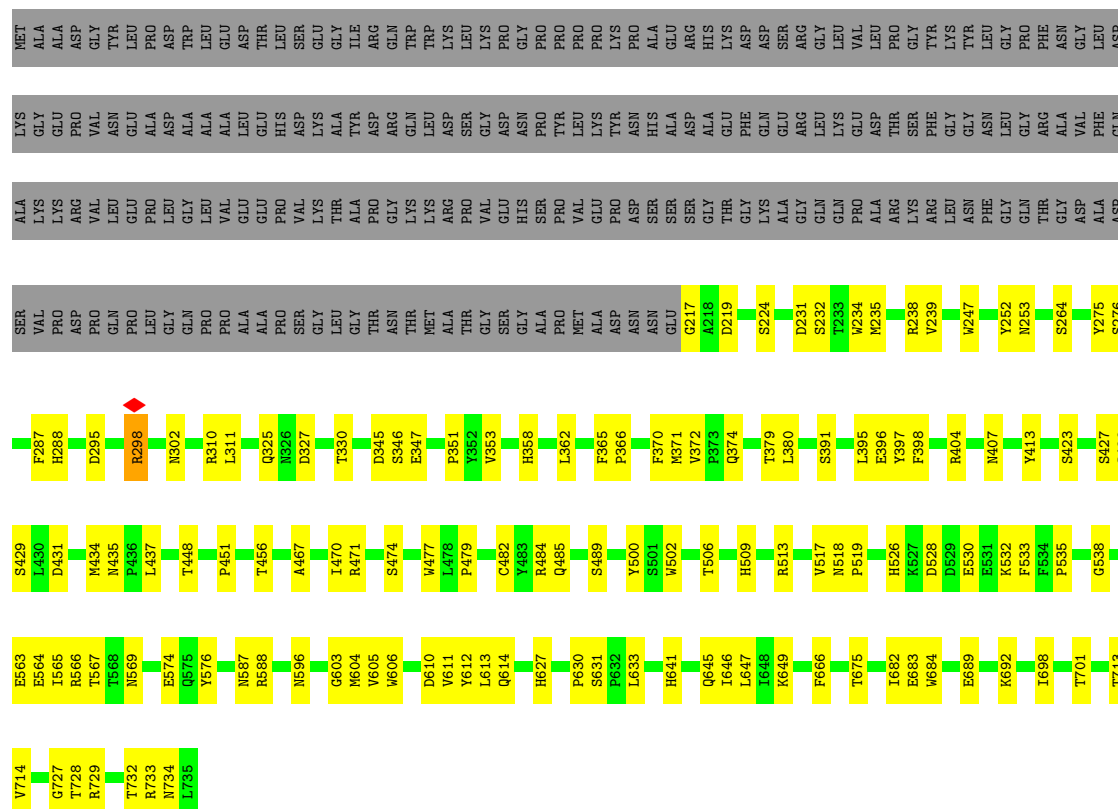
Chain m:





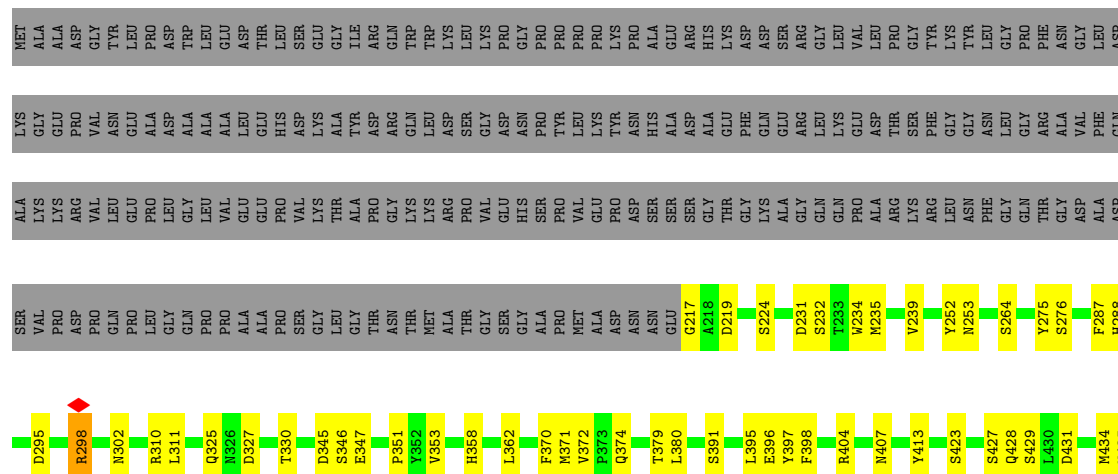
● Molecule 1: Capsid protein VP1

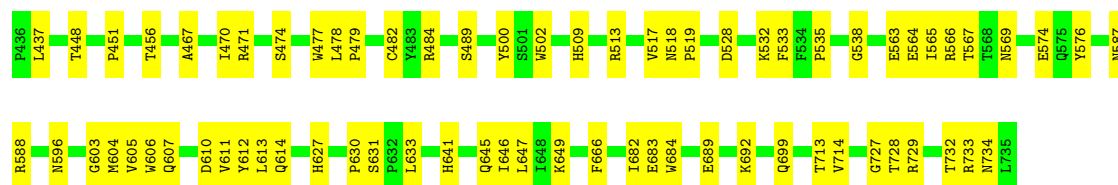
Chain n: 53% 18% 29%



● Molecule 1: Capsid protein VP1

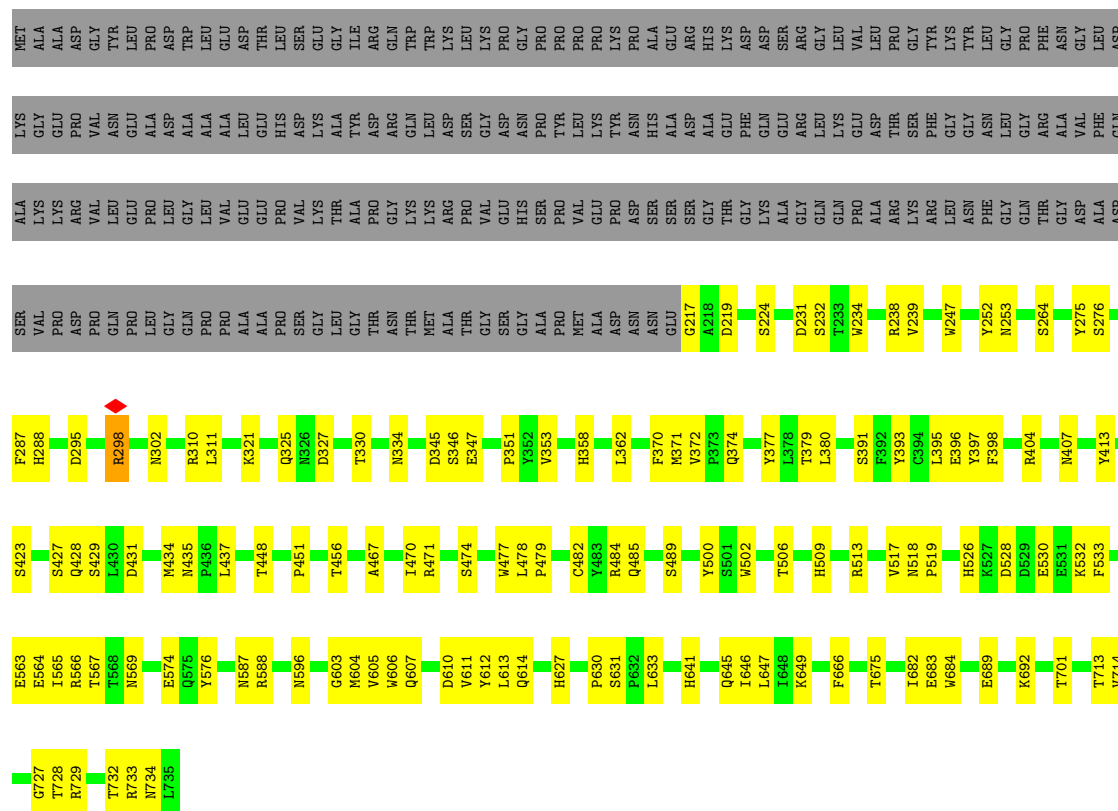
Chain o: 54% 16% 29%





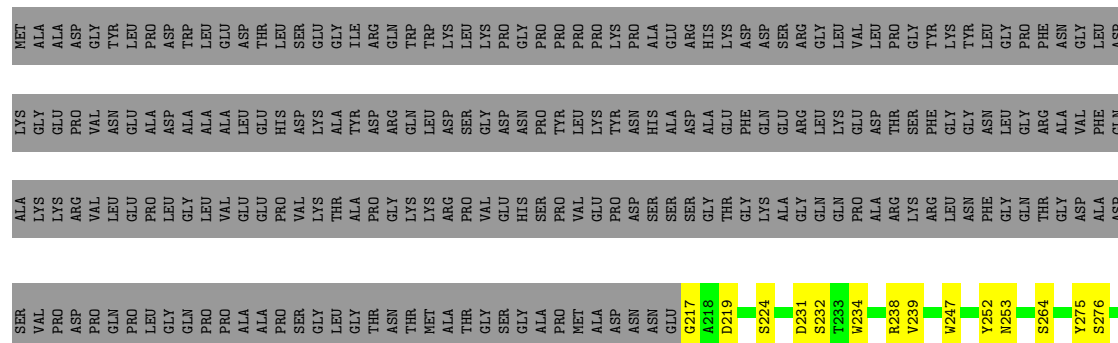
• Molecule 1: Capsid protein VP1

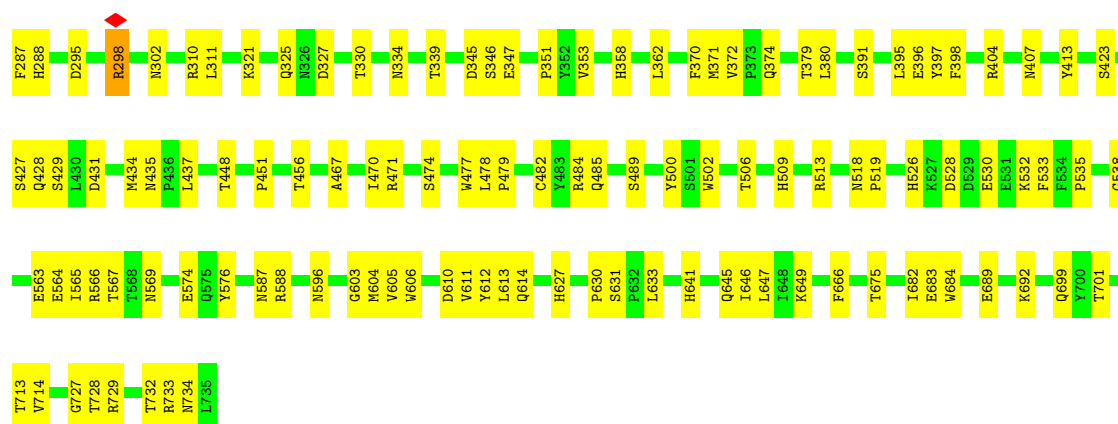
Chain p:  53% 18% 29%



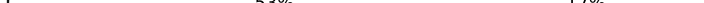
• Molecule 1: Capsid protein VP1

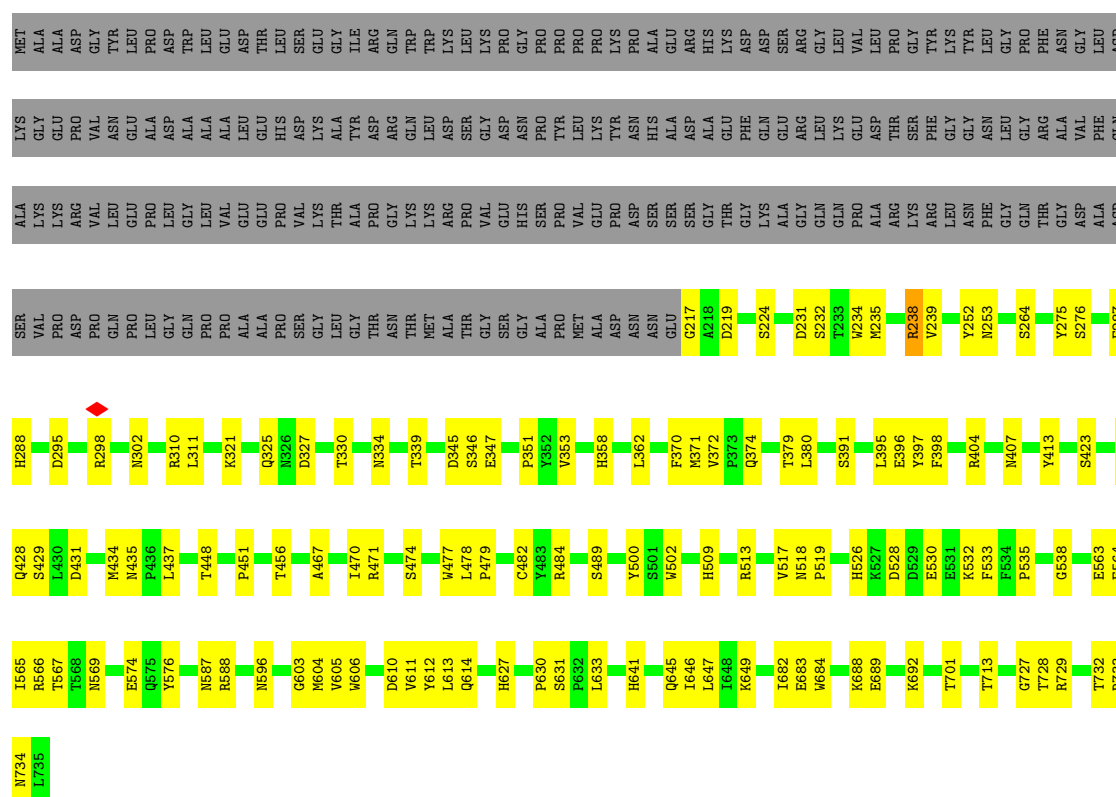
Chain q:  53% 18% 29%





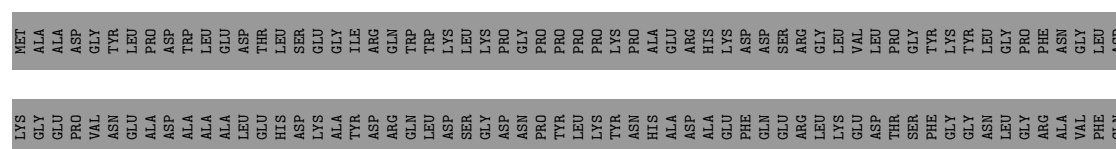
- Molecule 1: Capsid protein VP1

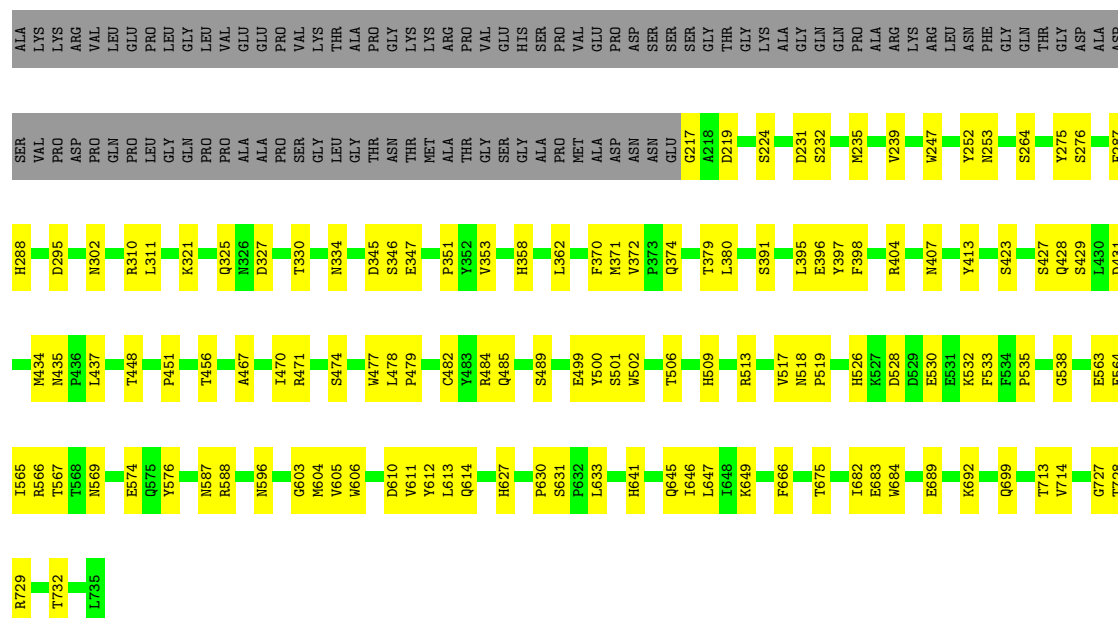
Chain r:  53% 17% 29%



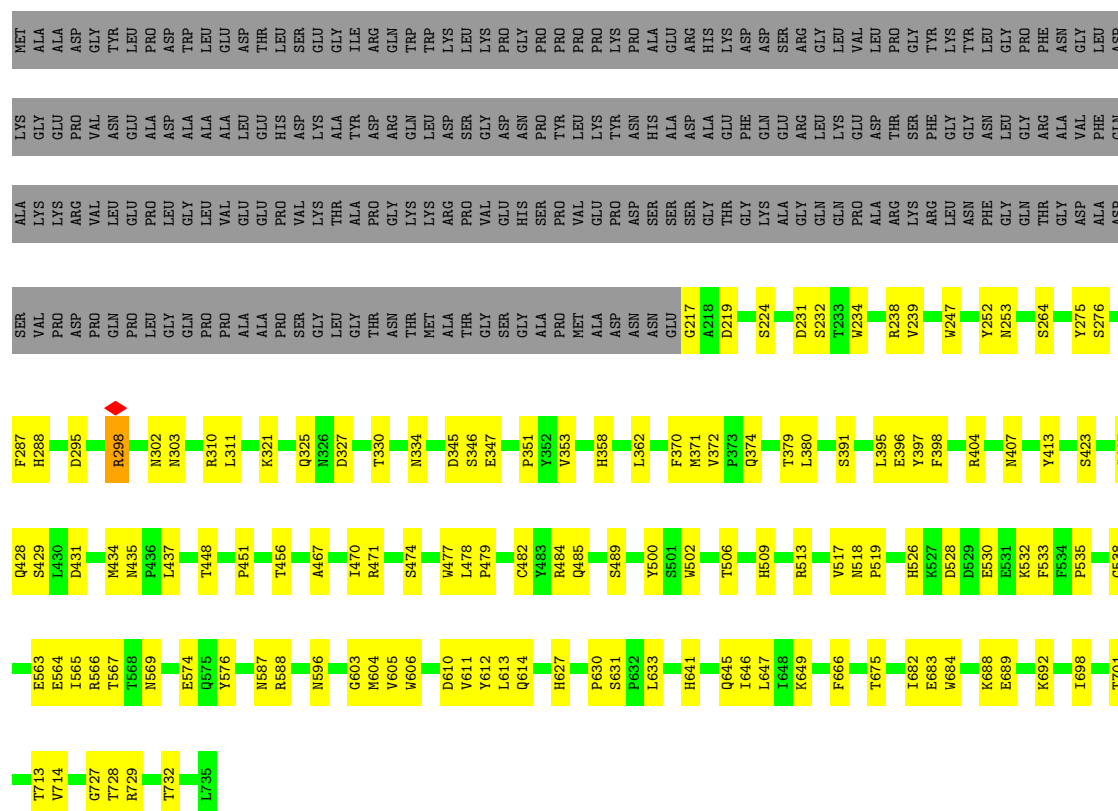
- Molecule 1: Capsid protein VP1

Chain s:



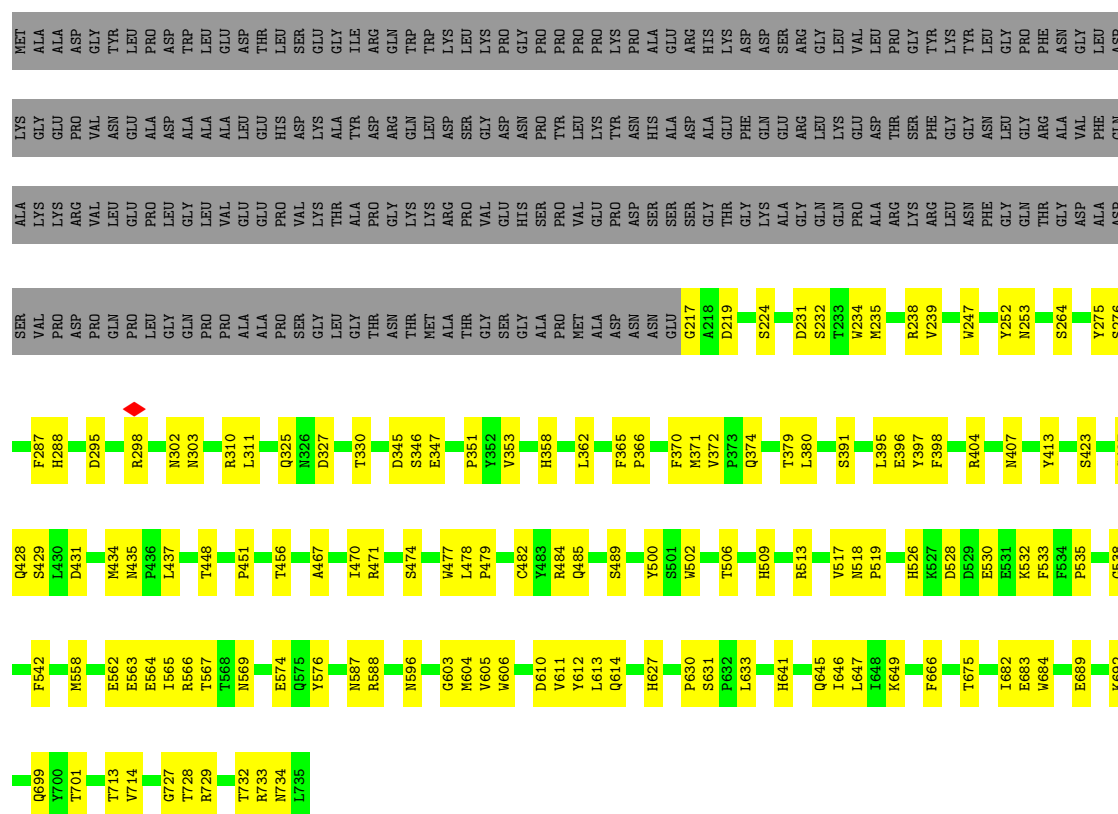


- Molecule 1: Capsid protein VP1

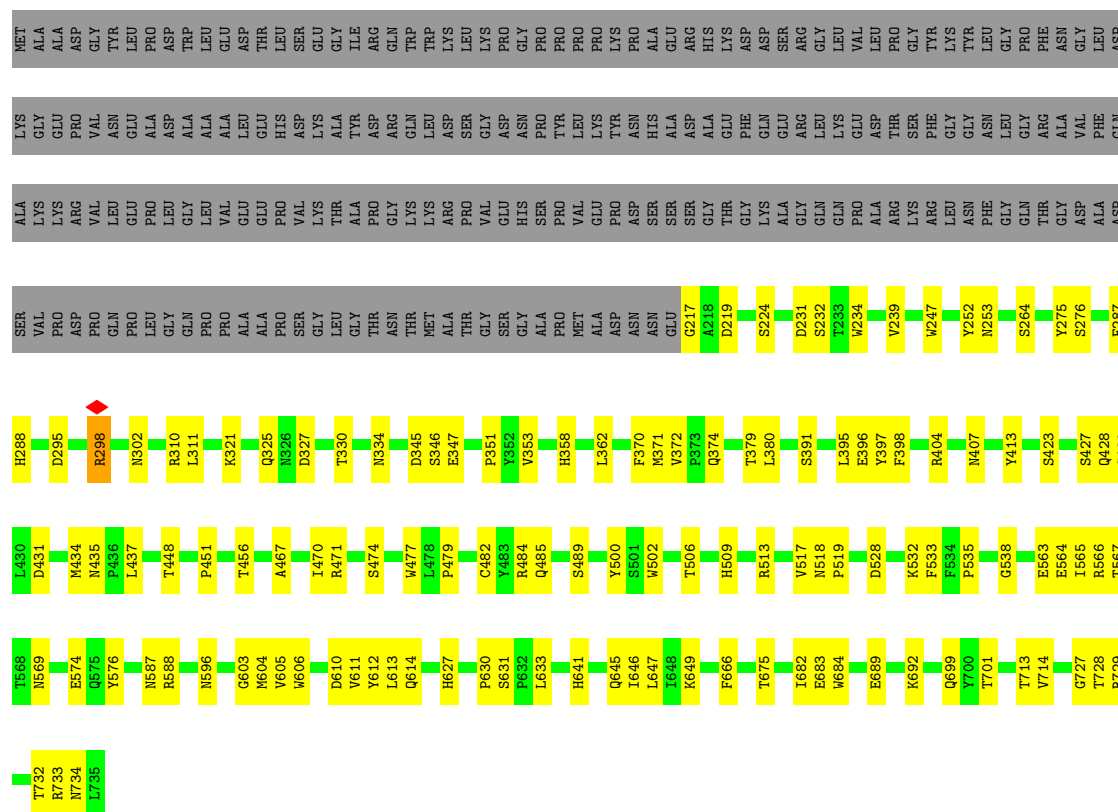


- Molecule 1: Capsid protein VP1

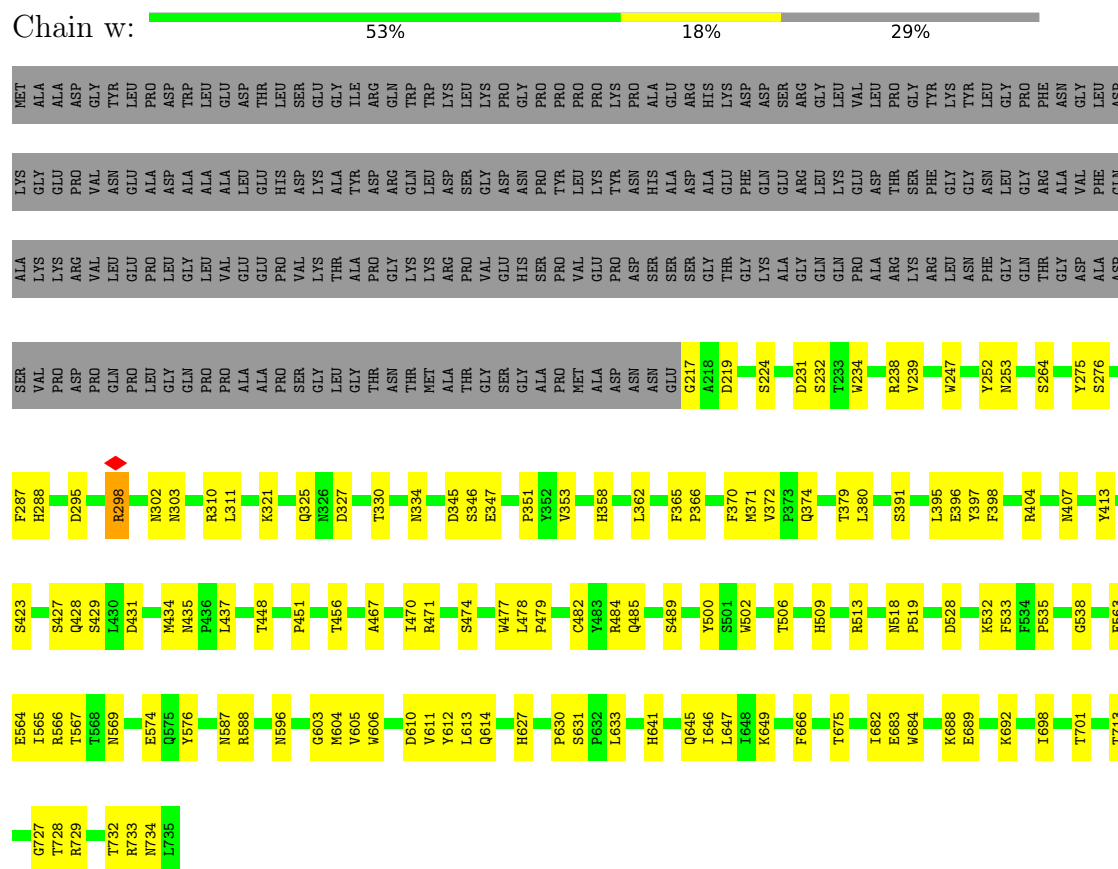




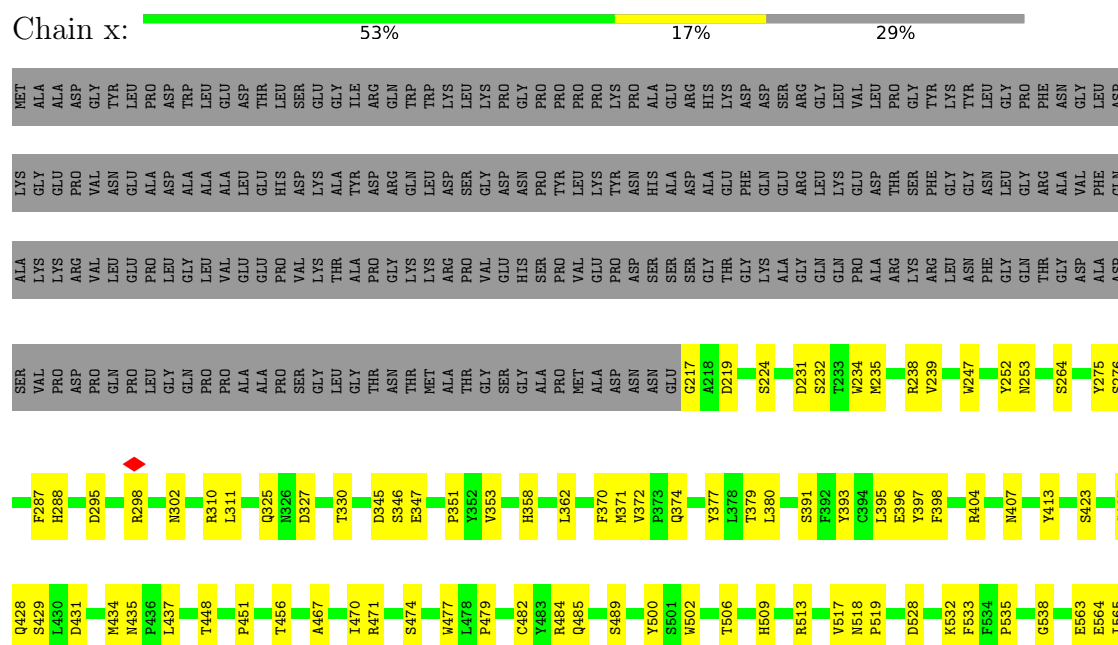
- Molecule 1: Capsid protein VP1

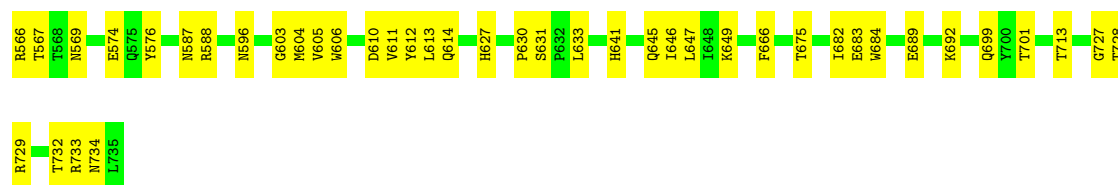


- Molecule 1: Capsid protein VP1



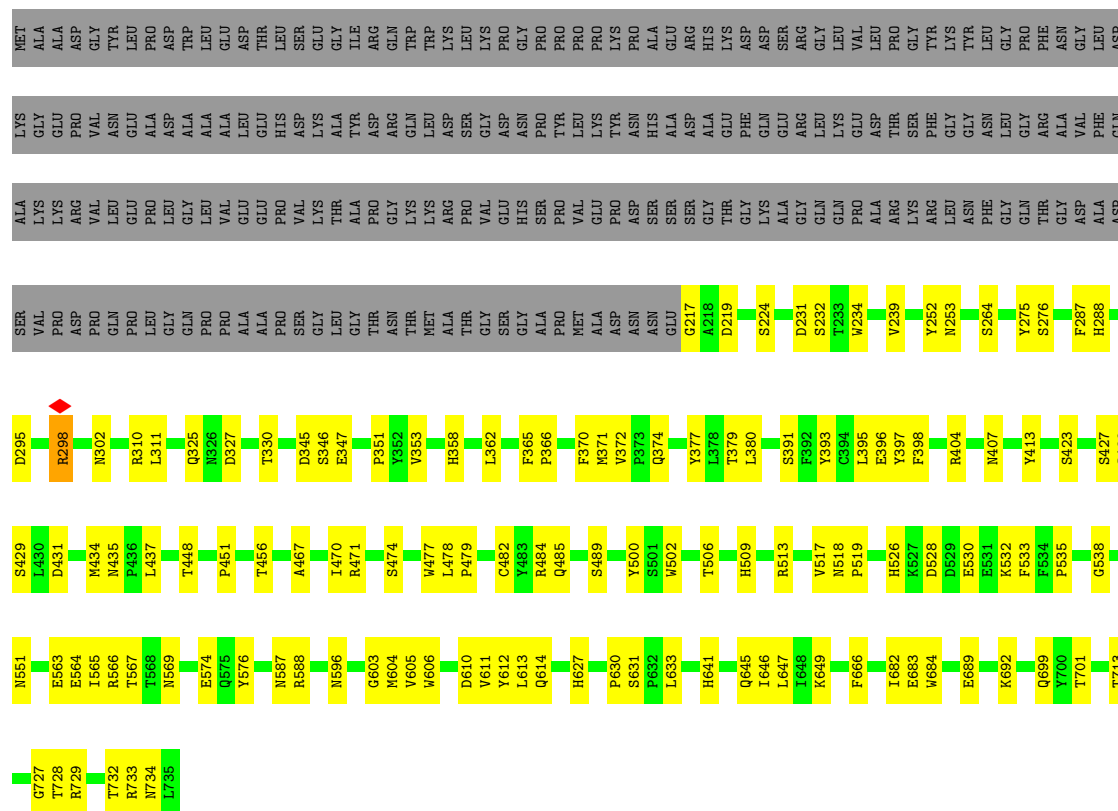
- Molecule 1: Capsid protein VP1





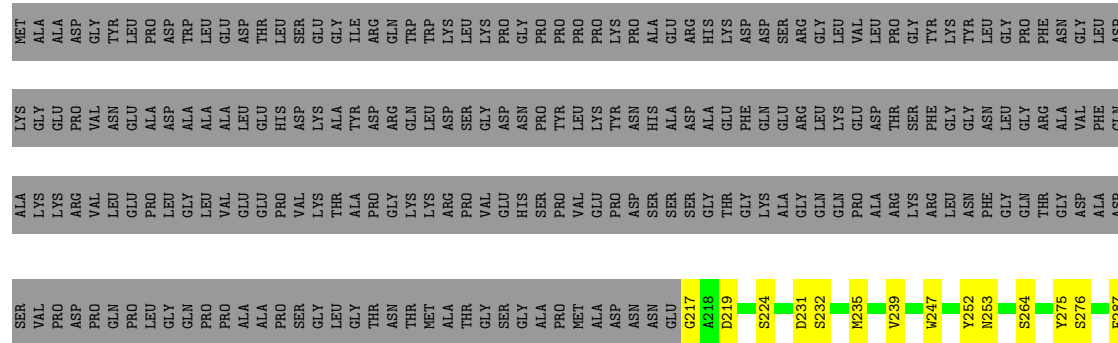
• Molecule 1: Capsid protein VP1

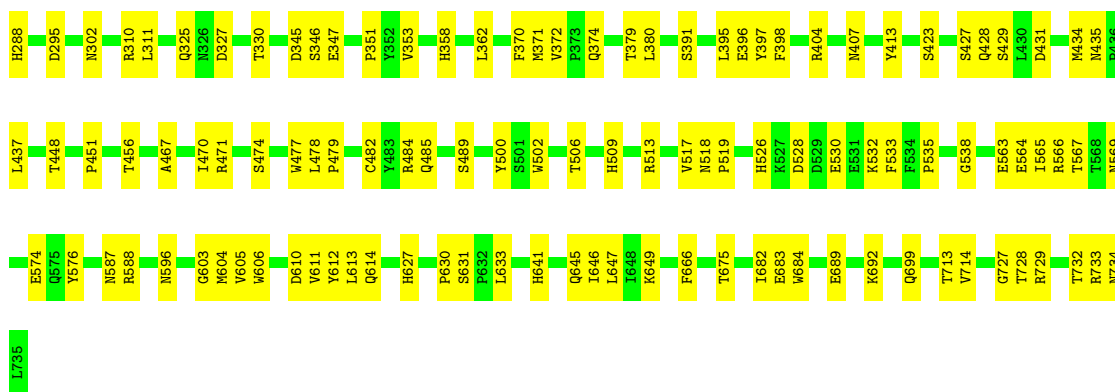
Chain y: 53% 17% 29%



• Molecule 1: Capsid protein VP1

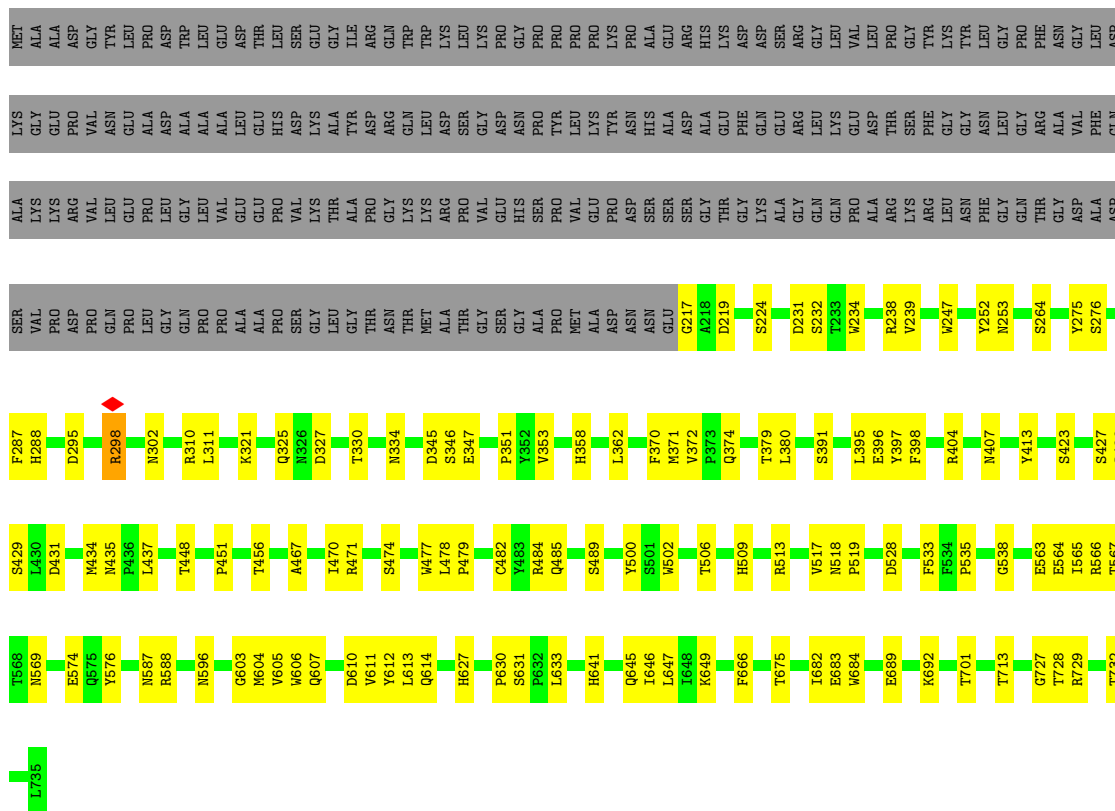
Chain z: 54% 17% 29%





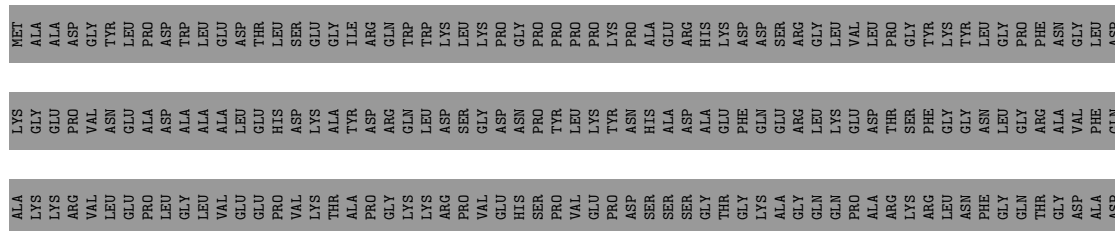
- Molecule 1: Capsid protein VP1

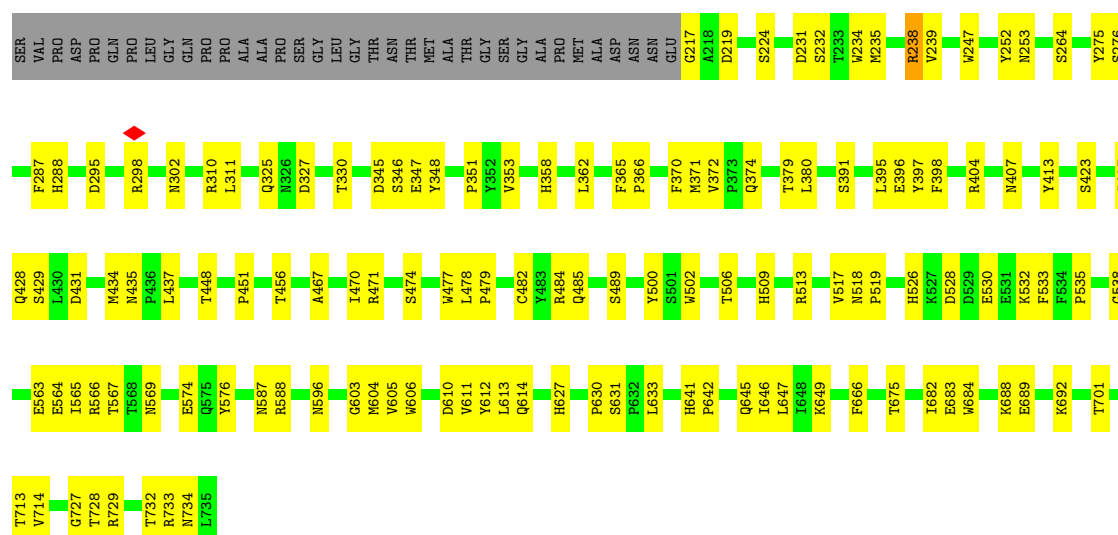
Chain 1: 54% 17% 29%



- Molecule 1: Capsid protein VP1

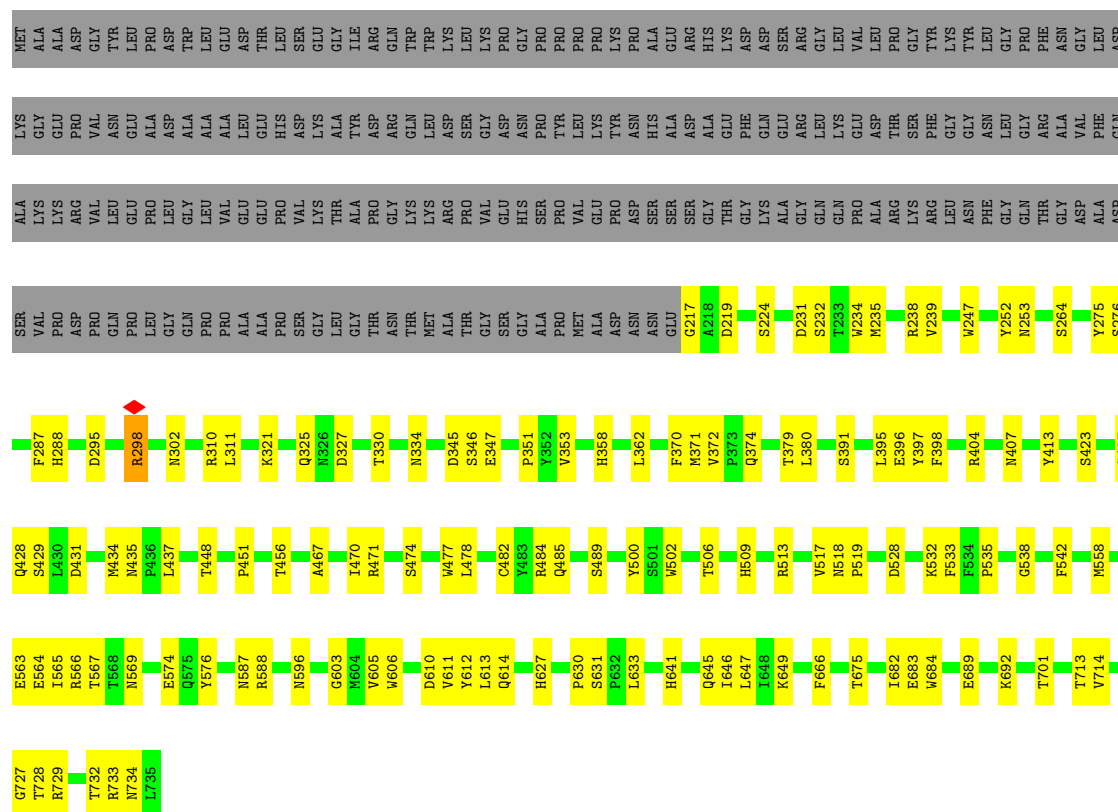
Chain 2: 53% 18% 29%





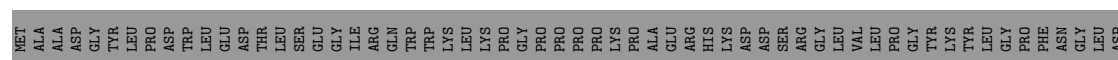
• Molecule 1: Capsid protein VP1

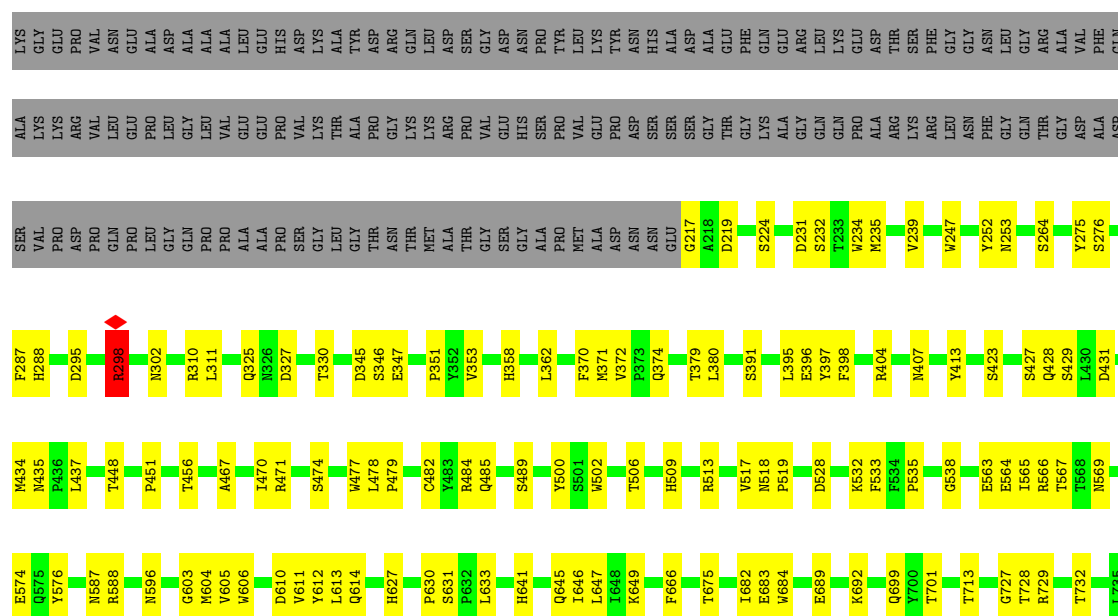
Chain 3: 53% 17% 29%



• Molecule 1: Capsid protein VP1

Chain 4: 54% 17% 29%





• Molecule 1: Capsid protein VP1

Chain 5: 53% 18% 29%



• Molecule 1: Capsid protein VP1

Chain 6: 53% 17% 29%



T732	T567	S429	D296	SER	ALA	LYS	GLY	LYS	GLY	MET
L735	N569	D431	D298	VAL	LYS	LYS	GLY	LYS	ALA	ALA
	E574	M434	N302	ASP	ARG	ARG	VAL	VAL	ASP	ASP
	Q575	M435	N302	PRO	GLN	GLN	LEU	LEU	GLY	TYR
	Y576	P436	R310	PRO	GLU	GLU	PRO	GLU	ALA	PRO
	N587	T448	L311	LEU	LEU	LEU	LEU	LEU	ASP	ASP
	N588			GLN	GLN	GLY	ALA	ALA	TRP	TRP
	N596	P451	K321	PRO	PRO	LEU	LEU	ALA	LEU	LEU
	G603	T456	Q325	ALA	VAL	GLU	VAL	ALA	GLU	ASP
	M604		N326	ALA	GLU	GLU	THR	LEU	LEU	ASP
	V605	A467	D327	PRO	PRO	PRO	HIS	HIS	LEU	LEU
	W606			SER	VAL	ASP	ASP	SER	SER	SER
		I470	T330	GLY	LYS	LYS	LYS	LYS	GLY	GLU
	D610	R471	N334	LEU	THR	THR	ALA	ALA	GLY	GLY
	V611			THR	GLY	GLY	ALA	TYR	ILE	ARG
	Y612	S474	D345	ASN	THR	ASN	PRO	ASP	ARG	ARG
	L613		S346	THR	LYS	GLY	GLN	GLN	GLN	TRP
	Q614	W477	E347	MET	LYS	LYS	LEU	LEU	LEU	TRP
		L478		ALA	ARG	ASP	ASP	ASP	LYS	LYS
	H627	P479	P351	THR	ALA	PRO	SER	SER	LEU	LEU
			Y352	GLY	VAL	GLY	VAL	GLY	GLY	LYS
	P630	C482	V353	SER	GLU	GLU	ASP	ASP	PRO	PRO
	S631	Y483	H358	GLY	HIS	HIS	ASN	GLY	GLY	GLY
	P432	R484		ALA	SER	PRO	PRO	PRO	PRO	PRO
	L633	Q485	L362	PRO	PRO	PRO	TYR	TYR	TYR	PRO
	H641	S489		MET	VAL	LEU	LEU	LEU	LEU	PRO
	Q645	Y500	F370	ALA	ALA	GLU	GLU	LYS	LYS	PRO
	I646	S501	N371	ASP	ASP	PRO	PRO	TYR	TYR	LYS
	L647	W502	V372	ASN	ASN	ASN	ASN	ASN	ASN	PRO
	I648		P373	GLU	SER	SER	ALA	HIS	ALA	GLU
	K649	T506	Q374		SER	GLY	ALA	HIS	ARG	ARG
			T379	D217	GLY	THR	LYS	LYS	HIS	LYS
	F666	H509	L390	D219	GLY	PHE	GLY	PHE	ASP	ASP
	I682	R513	R389	S224	LYS	GLN	GLN	GLN	ASP	SER
	E683		S390		ALA	ALA	GLU	ARG	SER	ARG
	W684	V517	S391	D231	GLY	GLY	ARG	ARG	ARG	ARG
		N518		S232	GLN	GLN	LEU	LEU	LEU	LEU
	E689	P519	L395	M235	PRO	PRO	VAL	VAL	LEU	LEU
			E396		ALA	ALA	ASP	ASP	LEU	LEU
	K692	D528	Y397	R238	ARG	ARG	THR	THR	PRO	PRO
	I698	K532	F398	V239	LYS	LYS	SER	SER	GLY	GLY
	Q699	F533	R404	Y252	ARG	ARG	PHE	PHE	TYR	TYR
	T700	F534		N253	ASN	ASN	GLY	GLY	LYS	LYS
	T701	P535	N407		PHE	PHE	ASN	ASN	TYR	TYR
				S264	GLY	GLY	LEU	LEU	LEU	GLY
	T713	G539	Y413		GLN	GLN	GLY	GLY	PRO	PRO
	T714			Y275	THR	THR	ARG	ARG	PHE	PHE
	G727	E563	S423	S276	GLY	GLY	ALA	ALA	ASN	ASN
	T728	E564			ASP	VAL	VAL	VAL	GLY	GLY
	T729	P565	S427	F287	ALA	PHE	PHE	PHE	LEU	LEU
			O458	P288	ASP	THR	THR	THR	ASP	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3838	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	13.476	Depositor
Minimum map value	-8.449	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	373.66, 373.66, 373.66	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.099, 1.099, 1.099	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	0.60	3/5855 (0.1%)
1	2	0.38	0/4297	0.60	3/5855 (0.1%)
1	3	0.37	0/4297	0.59	3/5855 (0.1%)
1	4	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	5	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	6	0.38	0/4297	0.60	3/5855 (0.1%)
1	7	0.38	0/4297	0.59	3/5855 (0.1%)
1	8	0.40	0/4297	0.60	3/5855 (0.1%)
1	A	0.38	0/4297	0.59	3/5855 (0.1%)
1	B	0.38	0/4297	0.60	3/5855 (0.1%)
1	C	0.38	0/4297	0.59	3/5855 (0.1%)
1	D	0.40	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	E	0.39	0/4297	0.60	7/5855 (0.1%)
1	F	0.38	0/4297	0.59	3/5855 (0.1%)
1	G	0.39	0/4297	0.60	7/5855 (0.1%)
1	H	0.38	0/4297	0.60	3/5855 (0.1%)
1	I	0.37	0/4297	0.60	7/5855 (0.1%)
1	J	0.42	2/4297 (0.0%)	0.61	3/5855 (0.1%)
1	K	0.38	0/4297	0.60	3/5855 (0.1%)
1	L	0.36	0/4297	0.59	3/5855 (0.1%)
1	M	0.37	0/4297	0.59	3/5855 (0.1%)
1	N	0.38	0/4297	0.59	7/5855 (0.1%)
1	O	0.37	0/4297	0.59	3/5855 (0.1%)
1	P	0.38	0/4297	0.60	3/5855 (0.1%)
1	Q	0.37	0/4297	0.60	7/5855 (0.1%)
1	R	0.38	0/4297	0.59	3/5855 (0.1%)
1	S	0.42	2/4297 (0.0%)	0.61	3/5855 (0.1%)
1	T	0.38	0/4297	0.60	3/5855 (0.1%)
1	U	0.36	0/4297	0.60	3/5855 (0.1%)
1	V	0.37	0/4297	0.59	3/5855 (0.1%)
1	W	0.40	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	X	0.37	0/4297	0.59	3/5855 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.37	0/4297	0.59	7/5855 (0.1%)
1	Z	0.37	0/4297	0.59	3/5855 (0.1%)
1	a	0.39	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	b	0.41	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	c	0.38	0/4297	0.59	3/5855 (0.1%)
1	d	0.39	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	e	0.41	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	f	0.38	0/4297	0.60	3/5855 (0.1%)
1	g	0.38	0/4297	0.59	3/5855 (0.1%)
1	h	0.42	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	i	0.38	0/4297	0.59	3/5855 (0.1%)
1	j	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	k	0.38	0/4297	0.60	3/5855 (0.1%)
1	l	0.40	0/4297	0.60	3/5855 (0.1%)
1	m	0.43	2/4297 (0.0%)	0.60	3/5855 (0.1%)
1	n	0.37	0/4297	0.58	3/5855 (0.1%)
1	o	0.42	2/4297 (0.0%)	0.59	3/5855 (0.1%)
1	p	0.38	0/4297	0.59	3/5855 (0.1%)
1	q	0.42	0/4297	0.60	3/5855 (0.1%)
1	r	0.38	0/4297	0.60	3/5855 (0.1%)
1	s	0.39	0/4297	0.59	3/5855 (0.1%)
1	t	0.40	0/4297	0.60	3/5855 (0.1%)
1	u	0.40	0/4297	0.59	3/5855 (0.1%)
1	v	0.42	0/4297	0.60	3/5855 (0.1%)
1	w	0.40	0/4297	0.60	3/5855 (0.1%)
1	x	0.40	0/4297	0.60	3/5855 (0.1%)
1	y	0.42	0/4297	0.60	3/5855 (0.1%)
1	z	0.39	0/4297	0.59	3/5855 (0.1%)
All	All	0.39	28/257820 (0.0%)	0.60	204/351300 (0.1%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	298[A]	ARG	CA-CB	6.99	1.65	1.53
1	m	298[B]	ARG	CA-CB	6.99	1.65	1.53
1	4	298[A]	ARG	CA-CB	6.99	1.65	1.53
1	4	298[B]	ARG	CA-CB	6.99	1.65	1.53
1	S	298[A]	ARG	CA-CB	6.28	1.64	1.53

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	264	SER	CB-CA-C	-6.12	109.50	116.54
1	1	264	SER	CB-CA-C	-6.12	109.51	116.54
1	j	264	SER	CB-CA-C	-6.11	109.52	116.54
1	5	264	SER	CB-CA-C	-6.11	109.52	116.54
1	c	264	SER	CB-CA-C	-6.10	109.52	116.54

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	4166	0	3926	109	0
1	2	4166	0	3926	116	0
1	3	4166	0	3926	108	0
1	4	4166	0	3926	108	0
1	5	4166	0	3926	115	0
1	6	4166	0	3926	111	0
1	7	4166	0	3926	106	0
1	8	4166	0	3926	118	0
1	A	4166	0	3926	108	0
1	B	4166	0	3926	104	0
1	C	4166	0	3926	112	0
1	D	4166	0	3926	105	0
1	E	4166	0	3926	110	0
1	F	4166	0	3926	108	0
1	G	4166	0	3926	108	0
1	H	4166	0	3926	108	0
1	I	4166	0	3926	115	0
1	J	4166	0	3926	112	0
1	K	4166	0	3926	107	0
1	L	4166	0	3926	118	0
1	M	4166	0	3926	110	0
1	N	4166	0	3926	115	0
1	O	4166	0	3926	106	0
1	P	4166	0	3926	104	0
1	Q	4166	0	3926	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4166	0	3926	107	0
1	S	4166	0	3926	108	0
1	T	4166	0	3926	111	0
1	U	4166	0	3926	115	0
1	V	4166	0	3926	107	0
1	W	4166	0	3926	108	0
1	X	4166	0	3926	107	0
1	Y	4166	0	3926	112	0
1	Z	4166	0	3926	108	0
1	a	4166	0	3926	105	0
1	b	4166	0	3926	116	0
1	c	4166	0	3926	103	0
1	d	4166	0	3926	104	0
1	e	4166	0	3926	114	0
1	f	4166	0	3926	111	0
1	g	4166	0	3926	113	0
1	h	4166	0	3926	108	0
1	i	4166	0	3926	108	0
1	j	4166	0	3926	108	0
1	k	4166	0	3926	107	0
1	l	4166	0	3926	118	0
1	m	4166	0	3926	115	0
1	n	4166	0	3926	112	0
1	o	4166	0	3926	104	0
1	p	4166	0	3926	111	0
1	q	4166	0	3926	114	0
1	r	4166	0	3926	111	0
1	s	4166	0	3926	105	0
1	t	4166	0	3926	118	0
1	u	4166	0	3926	114	0
1	v	4166	0	3926	109	0
1	w	4166	0	3926	115	0
1	x	4166	0	3926	108	0
1	y	4166	0	3926	112	0
1	z	4166	0	3926	106	0
2	1	21	0	12	1	0
2	2	21	0	12	1	0
2	3	21	0	12	1	0
2	4	21	0	12	1	0
2	5	21	0	12	1	0
2	6	21	0	12	1	0
2	7	21	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8	21	0	12	1	0
2	A	21	0	12	1	0
2	B	21	0	12	1	0
2	C	21	0	12	1	0
2	D	21	0	12	1	0
2	E	21	0	12	1	0
2	F	21	0	12	1	0
2	G	21	0	12	1	0
2	H	21	0	12	1	0
2	I	21	0	12	1	0
2	J	21	0	12	1	0
2	K	21	0	12	1	0
2	L	21	0	12	1	0
2	M	21	0	12	1	0
2	N	21	0	12	1	0
2	O	21	0	12	1	0
2	P	21	0	12	1	0
2	Q	21	0	12	1	0
2	R	21	0	12	1	0
2	S	21	0	12	1	0
2	T	21	0	12	1	0
2	U	21	0	12	1	0
2	V	21	0	12	1	0
2	W	21	0	12	1	0
2	X	21	0	12	1	0
2	Y	21	0	12	1	0
2	Z	21	0	12	1	0
2	a	21	0	12	1	0
2	b	21	0	12	1	0
2	c	21	0	12	1	0
2	d	21	0	12	1	0
2	e	21	0	12	1	0
2	f	21	0	12	1	0
2	g	21	0	12	1	0
2	h	21	0	12	1	0
2	i	21	0	12	1	0
2	j	21	0	12	1	0
2	k	21	0	12	1	0
2	l	21	0	12	1	0
2	m	21	0	12	1	0
2	n	21	0	12	1	0
2	o	21	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	p	21	0	12	1	0
2	q	21	0	12	1	0
2	r	21	0	12	1	0
2	s	21	0	12	1	0
2	t	21	0	12	1	0
2	u	21	0	12	1	0
2	v	21	0	12	1	0
2	w	21	0	12	1	0
2	x	21	0	12	1	0
2	y	21	0	12	1	0
2	z	21	0	12	1	0
All	All	251220	0	236280	5297	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 11.

The worst 5 of 5297 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:298[A]:ARG:HH21	1:U:298[A]:ARG:HG2	1.31	0.94
1:L:298[A]:ARG:HG2	1:L:298[A]:ARG:HH21	1.31	0.93
1:3:298[A]:ARG:HG2	1:3:298[A]:ARG:HH21	1.38	0.87
1:n:298[A]:ARG:HG2	1:n:298[A]:ARG:HH21	1.38	0.87
1:C:431:ASP:OD2	1:Y:513:ARG:NH1	2.14	0.81

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	519/735 (71%)	499 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	3	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	4	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	5	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	6	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	7	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	8	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	A	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	B	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	C	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	D	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	E	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	F	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	G	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	H	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	I	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	J	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	K	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	L	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	M	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	N	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	O	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	P	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	Q	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	R	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	S	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	T	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	U	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	V	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	W	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	X	519/735 (71%)	499 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	Z	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	a	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	b	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	c	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	d	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	e	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	f	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	g	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	h	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	i	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	j	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	k	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	l	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	m	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	n	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	o	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	p	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	q	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	r	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	s	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
1	t	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	u	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	v	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	w	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	x	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	y	519/735 (71%)	499 (96%)	20 (4%)	0	100	100
1	z	519/735 (71%)	500 (96%)	19 (4%)	0	100	100
All	All	31140/44100 (71%)	29964 (96%)	1176 (4%)	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	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	2	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	3	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	4	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	5	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	6	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	7	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	8	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	A	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	B	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	C	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	D	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	E	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	F	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	G	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	H	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	I	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	J	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	K	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	L	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	M	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	N	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	O	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	P	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Q	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	R	461/630 (73%)	459 (100%)	2 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	T	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	U	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	V	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	W	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	X	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Y	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	Z	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	a	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	b	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	c	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	d	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	e	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	f	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	g	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	h	461/630 (73%)	461 (100%)	0	100	100
1	i	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	j	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	k	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	l	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	m	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	n	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	o	461/630 (73%)	461 (100%)	0	100	100
1	p	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	q	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	r	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	s	461/630 (73%)	461 (100%)	0	100	100
1	t	461/630 (73%)	457 (99%)	4 (1%)	70	84
1	u	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	v	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	w	461/630 (73%)	457 (99%)	4 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	y	461/630 (73%)	459 (100%)	2 (0%)	84	92
1	z	461/630 (73%)	461 (100%)	0	100	100
All	All	27660/37800 (73%)	27532 (100%)	128 (0%)	85	90

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	298[B]	ARG
1	5	298[B]	ARG
1	W	298[A]	ARG
1	V	298[B]	ARG
1	6	298[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 861 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	229	HIS
1	n	518	ASN
1	4	584	GLN
1	g	645	GLN
1	f	717	ASN

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	e	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	2	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	x	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	W	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	P	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	K	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	L	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	q	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	z	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	M	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	v	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	F	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	4	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	D	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	J	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	p	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	f	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	H	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	m	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	Z	901	-	20,23,24	0.38	0	28,33,36	0.28	0
2	D5M	7	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	a	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	l	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	X	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	i	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	E	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	k	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	t	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	u	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	3	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	T	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	S	901	-	20,23,24	0.38	0	28,33,36	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D5M	A	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	R	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	I	901	-	20,23,24	0.38	0	28,33,36	0.28	0
2	D5M	O	901	-	20,23,24	0.37	0	28,33,36	0.28	0
2	D5M	V	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	b	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	G	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	Y	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	B	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	C	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	N	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	y	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	c	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	5	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	l	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	j	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	g	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	Q	901	-	20,23,24	0.37	0	28,33,36	0.28	0
2	D5M	d	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	6	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	h	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	U	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	s	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	r	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	n	901	-	20,23,24	0.38	0	28,33,36	0.27	0
2	D5M	8	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	o	901	-	20,23,24	0.37	0	28,33,36	0.27	0
2	D5M	w	901	-	20,23,24	0.37	0	28,33,36	0.27	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	e	901	-	-	5/7/21/22	0/3/3/3
2	D5M	2	901	-	-	5/7/21/22	0/3/3/3
2	D5M	x	901	-	-	5/7/21/22	0/3/3/3
2	D5M	W	901	-	-	5/7/21/22	0/3/3/3
2	D5M	P	901	-	-	5/7/21/22	0/3/3/3
2	D5M	K	901	-	-	5/7/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	L	901	-	-	5/7/21/22	0/3/3/3
2	D5M	q	901	-	-	5/7/21/22	0/3/3/3
2	D5M	z	901	-	-	5/7/21/22	0/3/3/3
2	D5M	M	901	-	-	5/7/21/22	0/3/3/3
2	D5M	v	901	-	-	5/7/21/22	0/3/3/3
2	D5M	F	901	-	-	5/7/21/22	0/3/3/3
2	D5M	4	901	-	-	5/7/21/22	0/3/3/3
2	D5M	D	901	-	-	5/7/21/22	0/3/3/3
2	D5M	J	901	-	-	5/7/21/22	0/3/3/3
2	D5M	p	901	-	-	5/7/21/22	0/3/3/3
2	D5M	f	901	-	-	5/7/21/22	0/3/3/3
2	D5M	H	901	-	-	5/7/21/22	0/3/3/3
2	D5M	m	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Z	901	-	-	5/7/21/22	0/3/3/3
2	D5M	7	901	-	-	5/7/21/22	0/3/3/3
2	D5M	a	901	-	-	5/7/21/22	0/3/3/3
2	D5M	1	901	-	-	5/7/21/22	0/3/3/3
2	D5M	X	901	-	-	5/7/21/22	0/3/3/3
2	D5M	i	901	-	-	5/7/21/22	0/3/3/3
2	D5M	E	901	-	-	5/7/21/22	0/3/3/3
2	D5M	k	901	-	-	5/7/21/22	0/3/3/3
2	D5M	t	901	-	-	5/7/21/22	0/3/3/3
2	D5M	u	901	-	-	5/7/21/22	0/3/3/3
2	D5M	3	901	-	-	5/7/21/22	0/3/3/3
2	D5M	T	901	-	-	5/7/21/22	0/3/3/3
2	D5M	S	901	-	-	5/7/21/22	0/3/3/3
2	D5M	A	901	-	-	5/7/21/22	0/3/3/3
2	D5M	R	901	-	-	5/7/21/22	0/3/3/3
2	D5M	I	901	-	-	5/7/21/22	0/3/3/3
2	D5M	O	901	-	-	5/7/21/22	0/3/3/3
2	D5M	V	901	-	-	5/7/21/22	0/3/3/3
2	D5M	b	901	-	-	5/7/21/22	0/3/3/3
2	D5M	G	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Y	901	-	-	5/7/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	B	901	-	-	5/7/21/22	0/3/3/3
2	D5M	C	901	-	-	5/7/21/22	0/3/3/3
2	D5M	N	901	-	-	5/7/21/22	0/3/3/3
2	D5M	y	901	-	-	5/7/21/22	0/3/3/3
2	D5M	c	901	-	-	5/7/21/22	0/3/3/3
2	D5M	5	901	-	-	5/7/21/22	0/3/3/3
2	D5M	l	901	-	-	5/7/21/22	0/3/3/3
2	D5M	j	901	-	-	5/7/21/22	0/3/3/3
2	D5M	g	901	-	-	5/7/21/22	0/3/3/3
2	D5M	Q	901	-	-	5/7/21/22	0/3/3/3
2	D5M	d	901	-	-	5/7/21/22	0/3/3/3
2	D5M	6	901	-	-	5/7/21/22	0/3/3/3
2	D5M	h	901	-	-	5/7/21/22	0/3/3/3
2	D5M	U	901	-	-	5/7/21/22	0/3/3/3
2	D5M	s	901	-	-	5/7/21/22	0/3/3/3
2	D5M	r	901	-	-	5/7/21/22	0/3/3/3
2	D5M	n	901	-	-	5/7/21/22	0/3/3/3
2	D5M	8	901	-	-	5/7/21/22	0/3/3/3
2	D5M	o	901	-	-	5/7/21/22	0/3/3/3
2	D5M	w	901	-	-	5/7/21/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 300 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	D5M	O4'-C1'-N9-C4
2	B	901	D5M	O4'-C1'-N9-C4
2	C	901	D5M	O4'-C1'-N9-C4
2	D	901	D5M	O4'-C1'-N9-C4
2	E	901	D5M	O4'-C1'-N9-C4

There are no ring outliers.

60 monomers are involved in 60 short contacts:

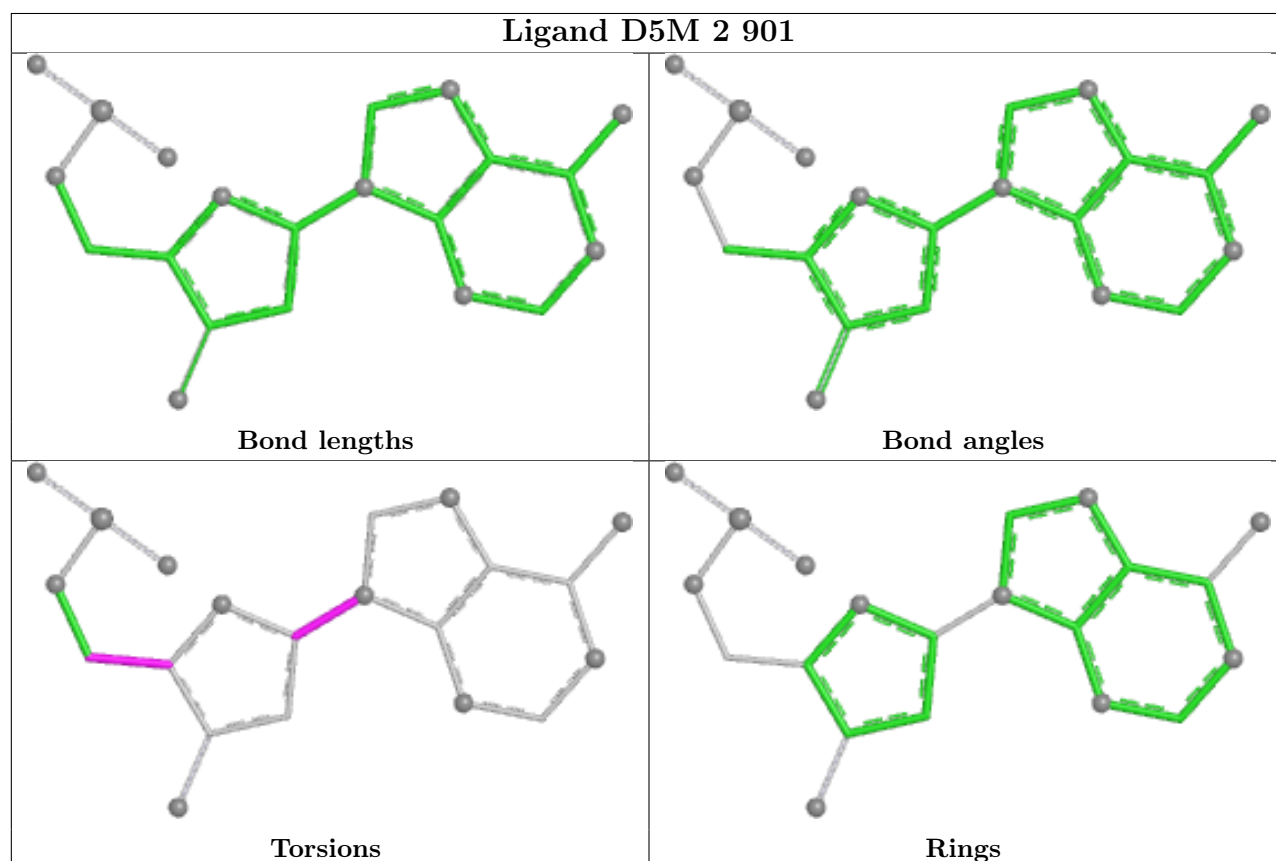
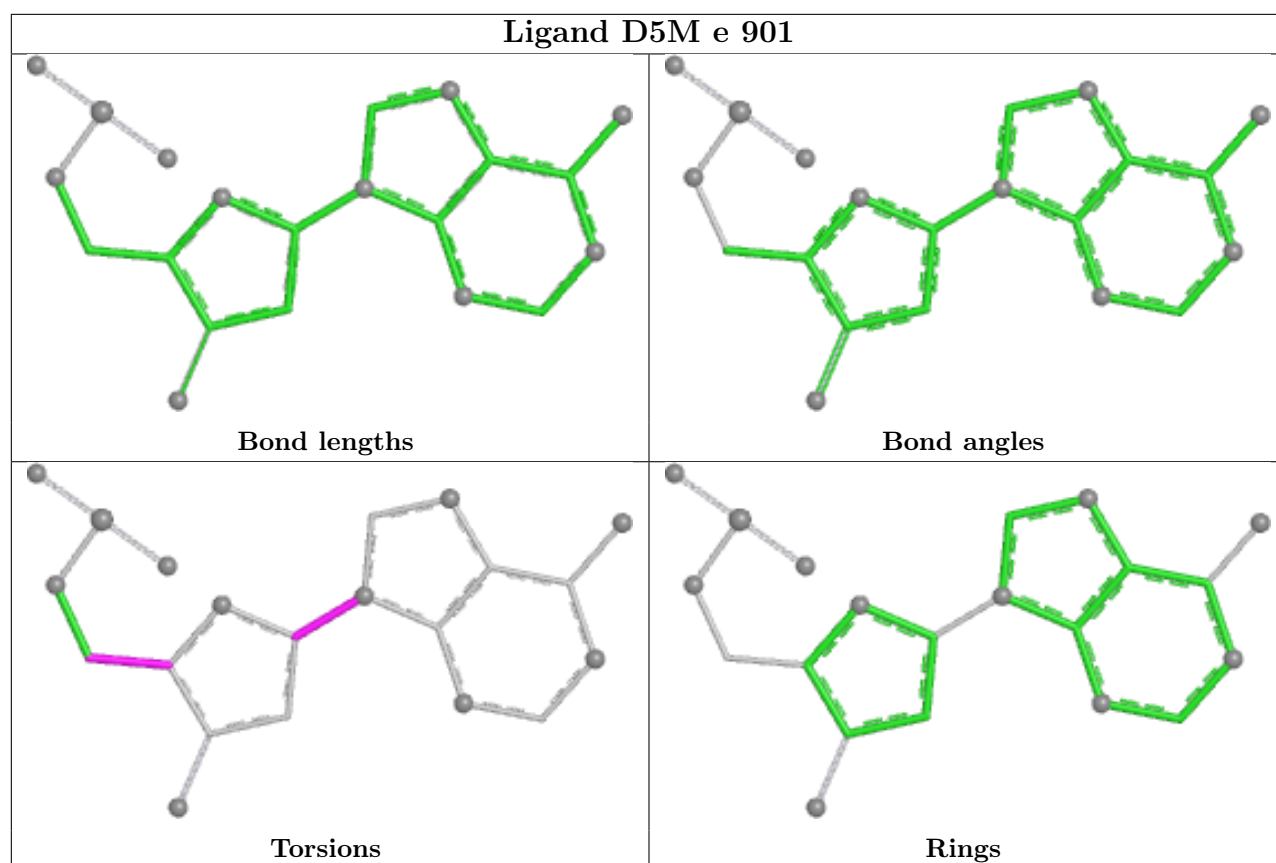
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	901	D5M	1	0
2	2	901	D5M	1	0
2	x	901	D5M	1	0
2	W	901	D5M	1	0
2	P	901	D5M	1	0
2	K	901	D5M	1	0
2	L	901	D5M	1	0
2	q	901	D5M	1	0
2	z	901	D5M	1	0
2	M	901	D5M	1	0
2	v	901	D5M	1	0
2	F	901	D5M	1	0
2	4	901	D5M	1	0
2	D	901	D5M	1	0
2	J	901	D5M	1	0
2	p	901	D5M	1	0
2	f	901	D5M	1	0
2	H	901	D5M	1	0
2	m	901	D5M	1	0
2	Z	901	D5M	1	0
2	7	901	D5M	1	0
2	a	901	D5M	1	0
2	1	901	D5M	1	0
2	X	901	D5M	1	0
2	i	901	D5M	1	0
2	E	901	D5M	1	0
2	k	901	D5M	1	0
2	t	901	D5M	1	0
2	u	901	D5M	1	0
2	3	901	D5M	1	0
2	T	901	D5M	1	0
2	S	901	D5M	1	0
2	A	901	D5M	1	0
2	R	901	D5M	1	0
2	I	901	D5M	1	0
2	O	901	D5M	1	0
2	V	901	D5M	1	0
2	b	901	D5M	1	0
2	G	901	D5M	1	0
2	Y	901	D5M	1	0
2	B	901	D5M	1	0
2	C	901	D5M	1	0
2	N	901	D5M	1	0

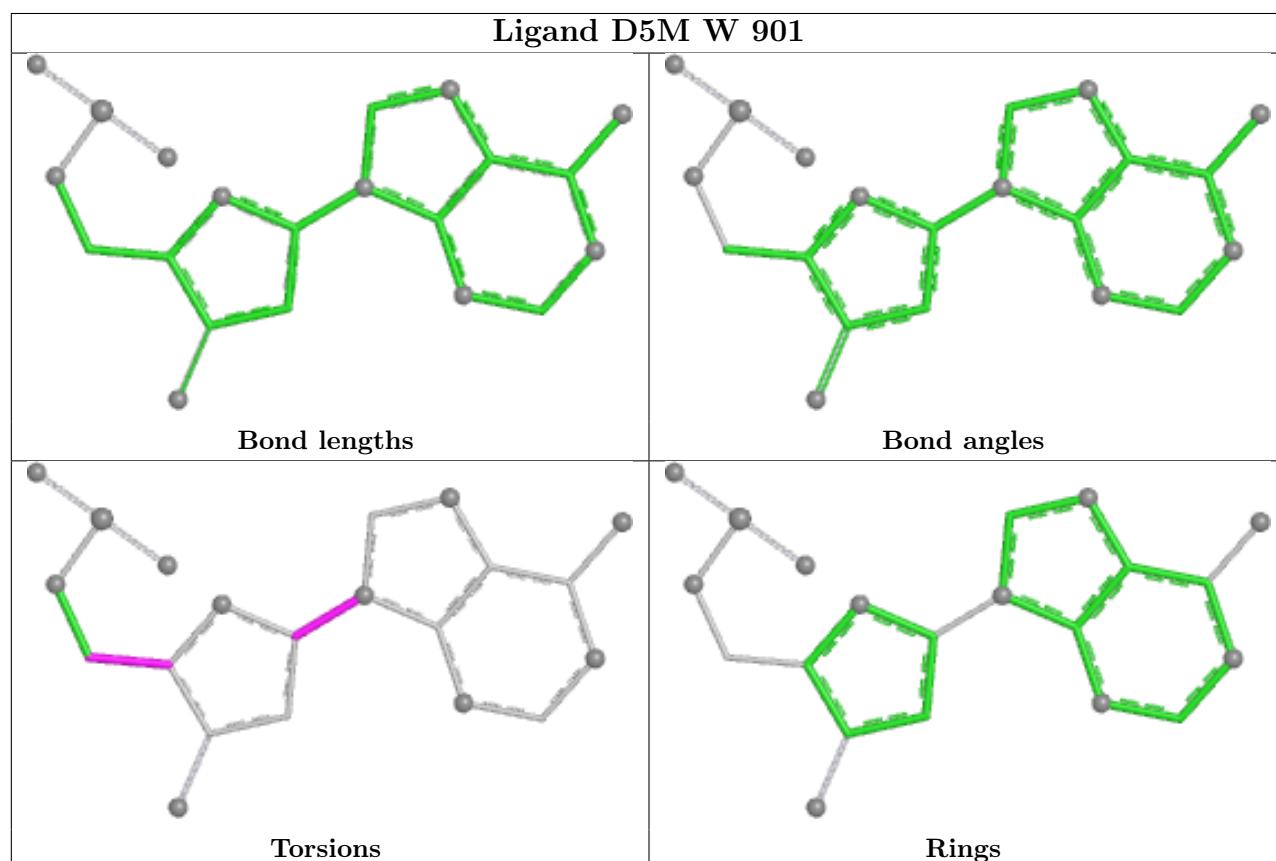
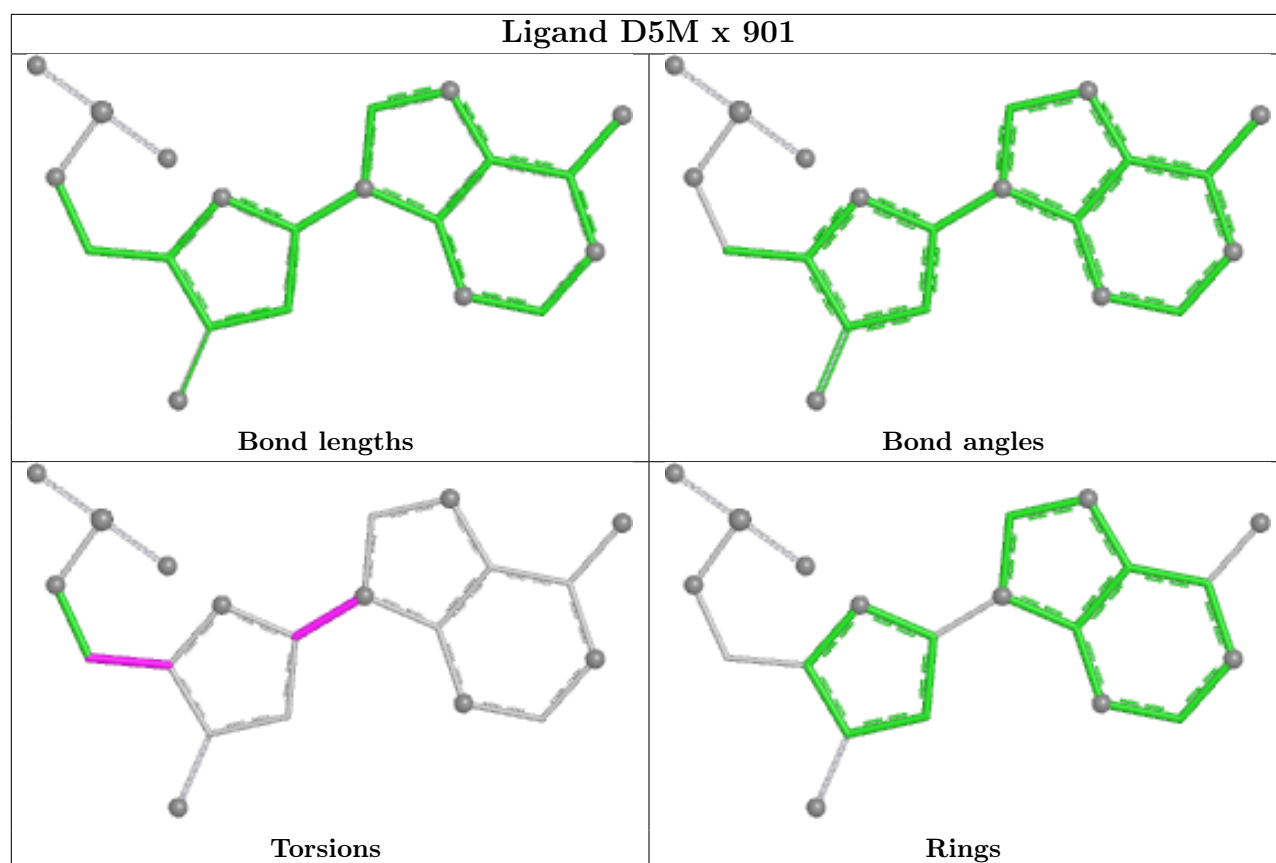
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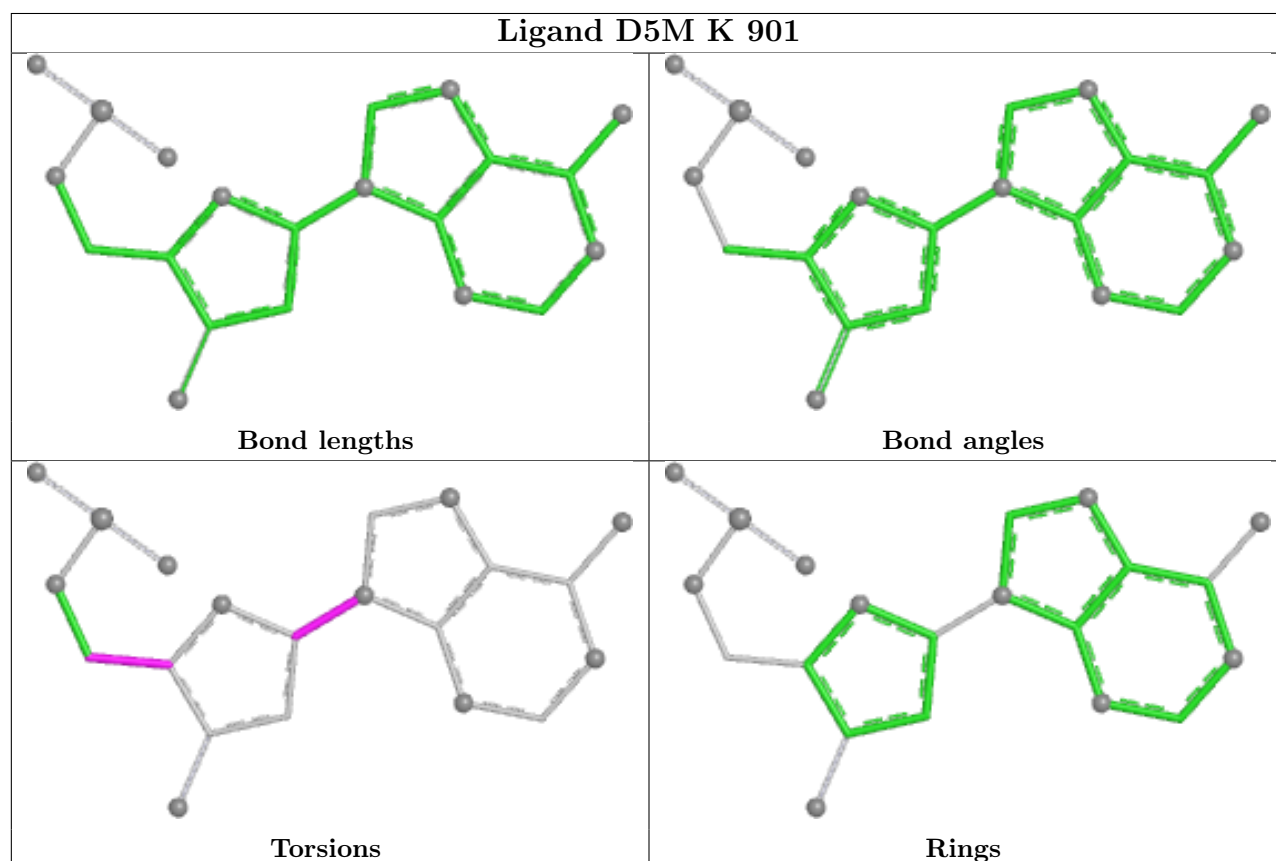
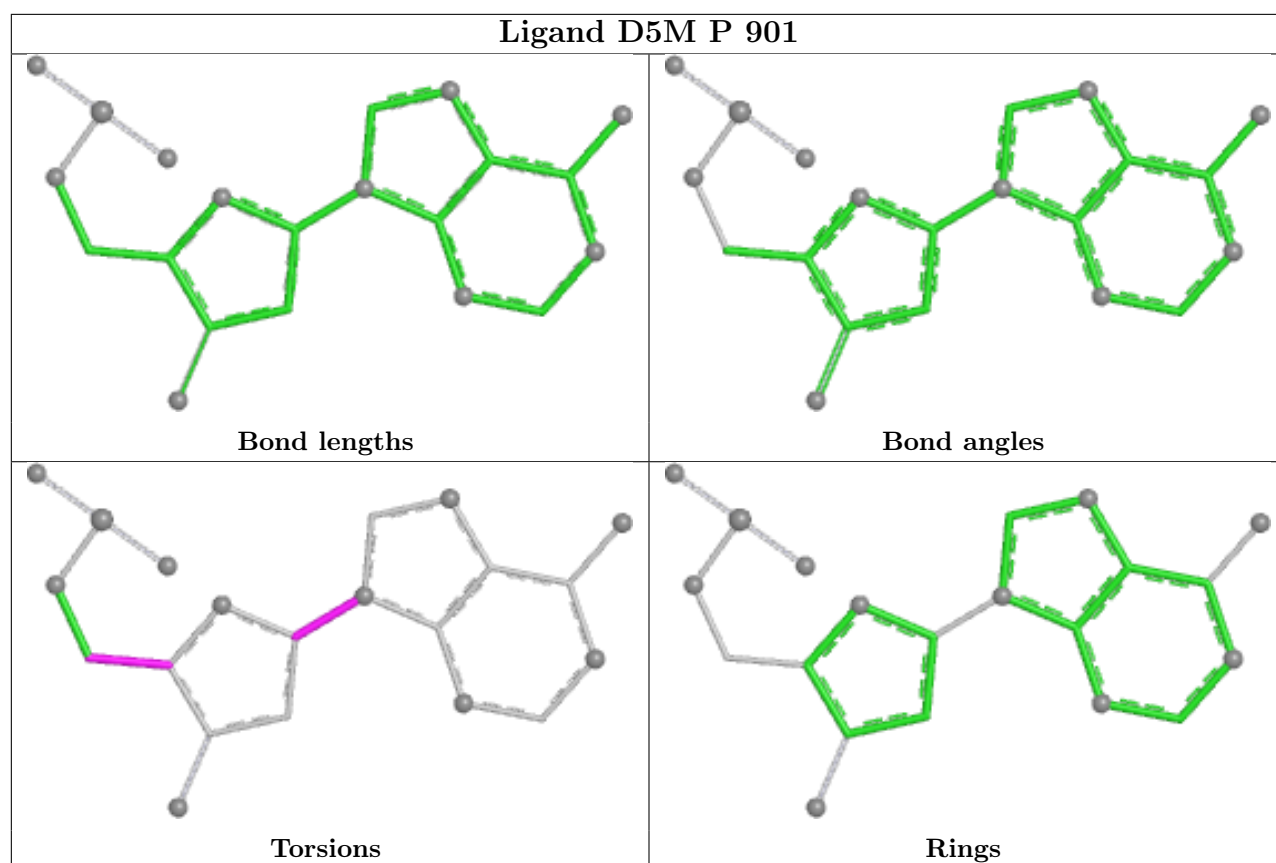
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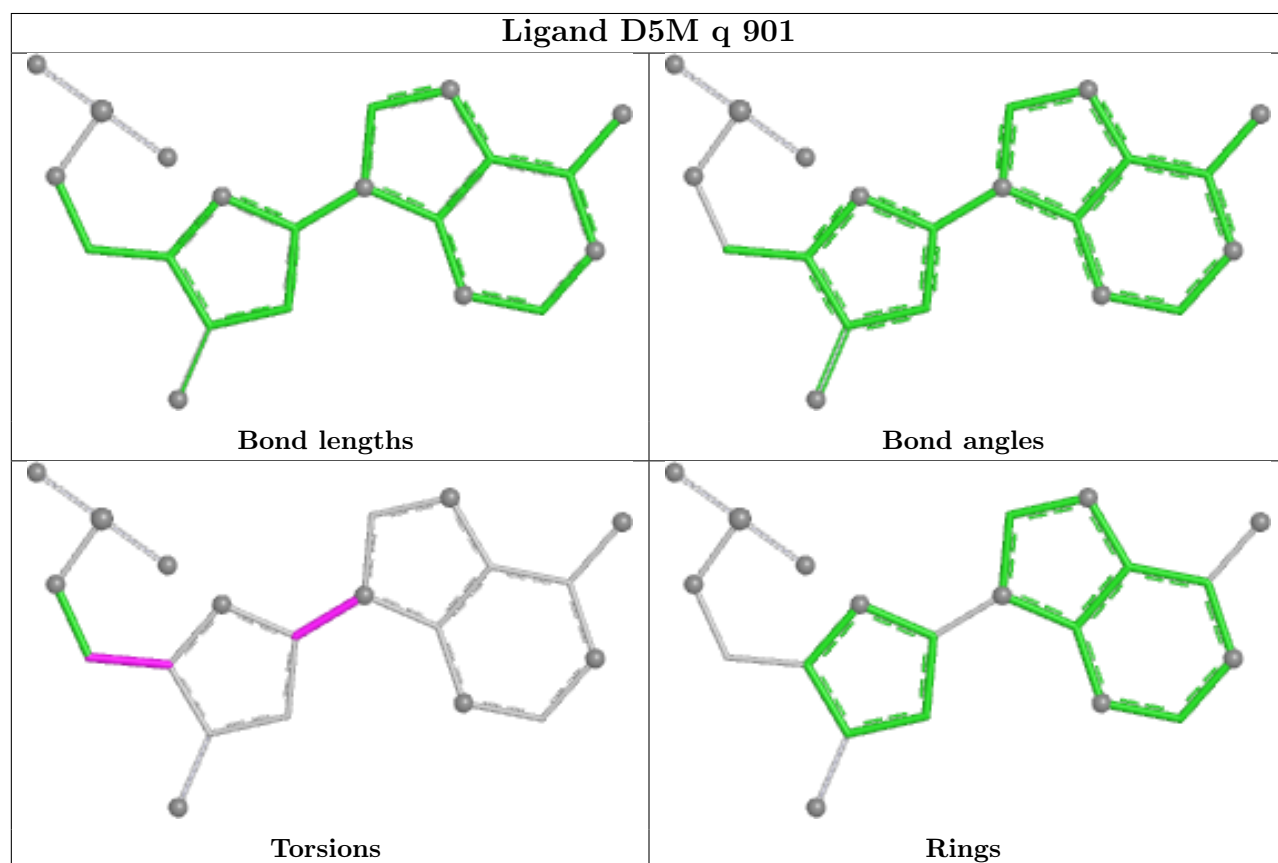
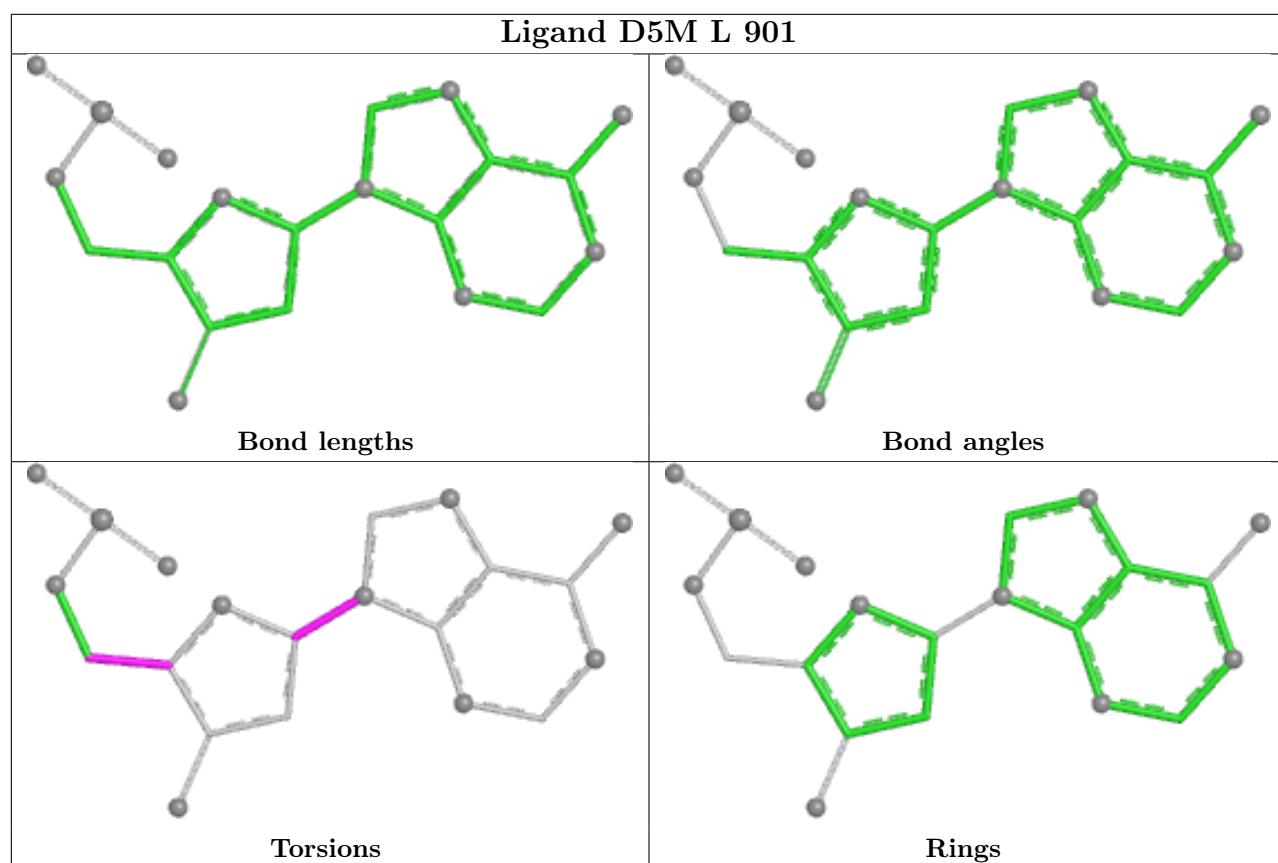
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	y	901	D5M	1	0
2	c	901	D5M	1	0
2	5	901	D5M	1	0
2	l	901	D5M	1	0
2	j	901	D5M	1	0
2	g	901	D5M	1	0
2	Q	901	D5M	1	0
2	d	901	D5M	1	0
2	6	901	D5M	1	0
2	h	901	D5M	1	0
2	U	901	D5M	1	0
2	s	901	D5M	1	0
2	r	901	D5M	1	0
2	n	901	D5M	1	0
2	8	901	D5M	1	0
2	o	901	D5M	1	0
2	w	901	D5M	1	0

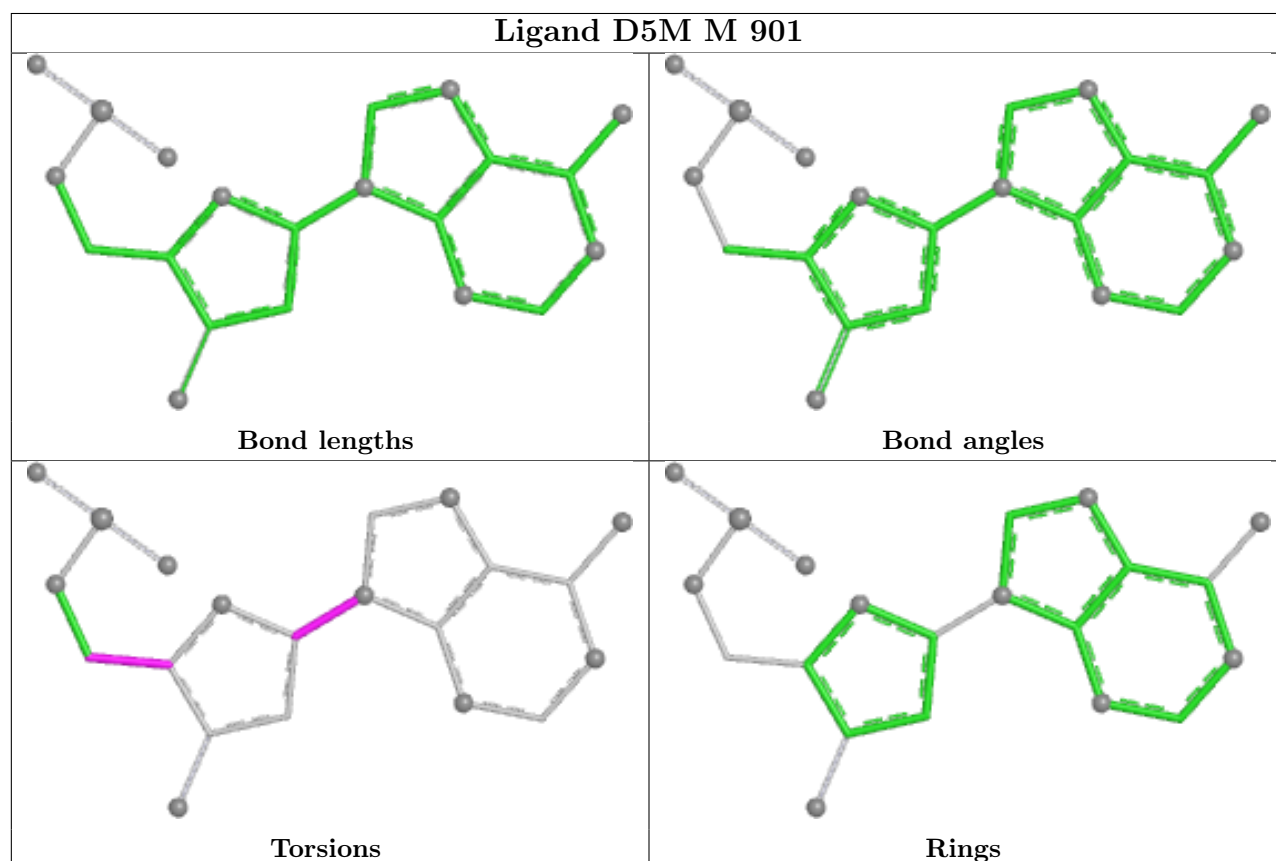
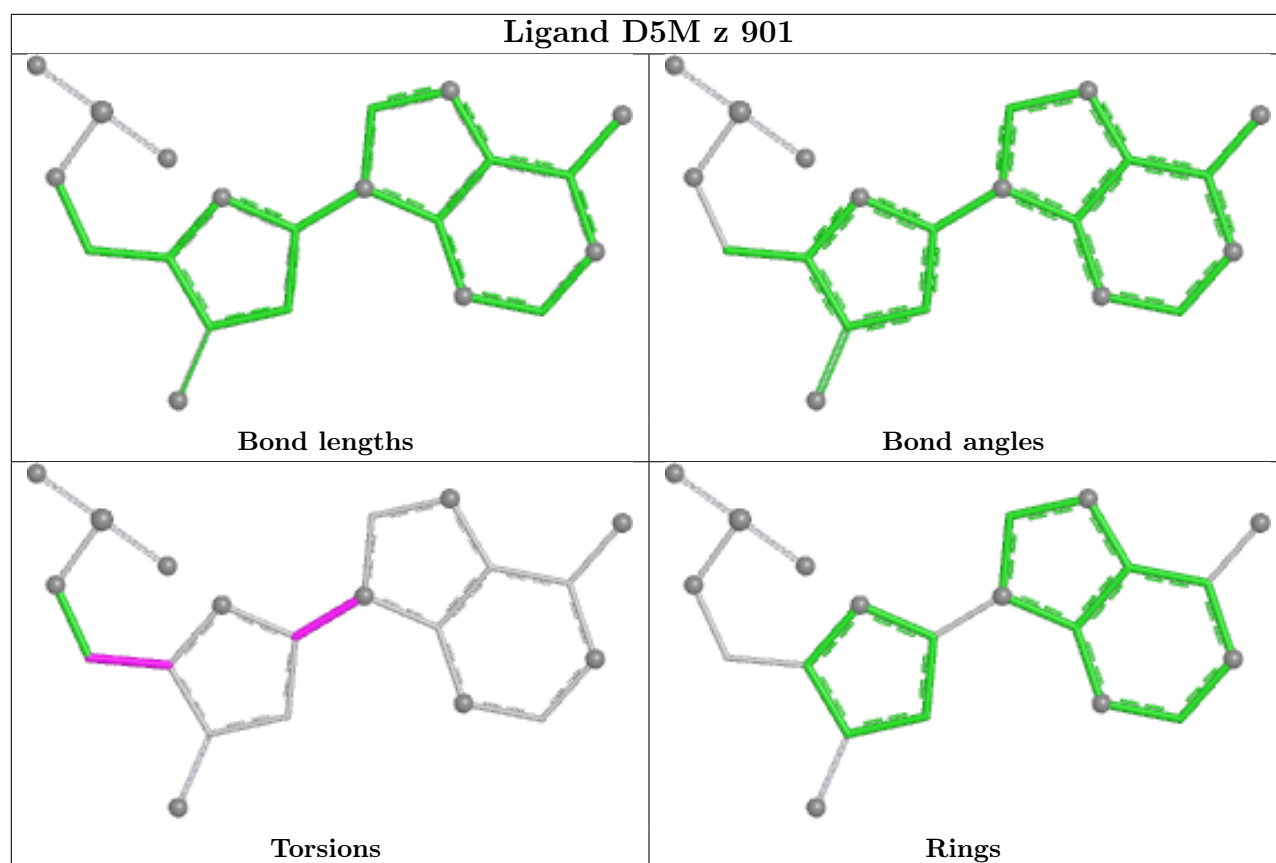
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

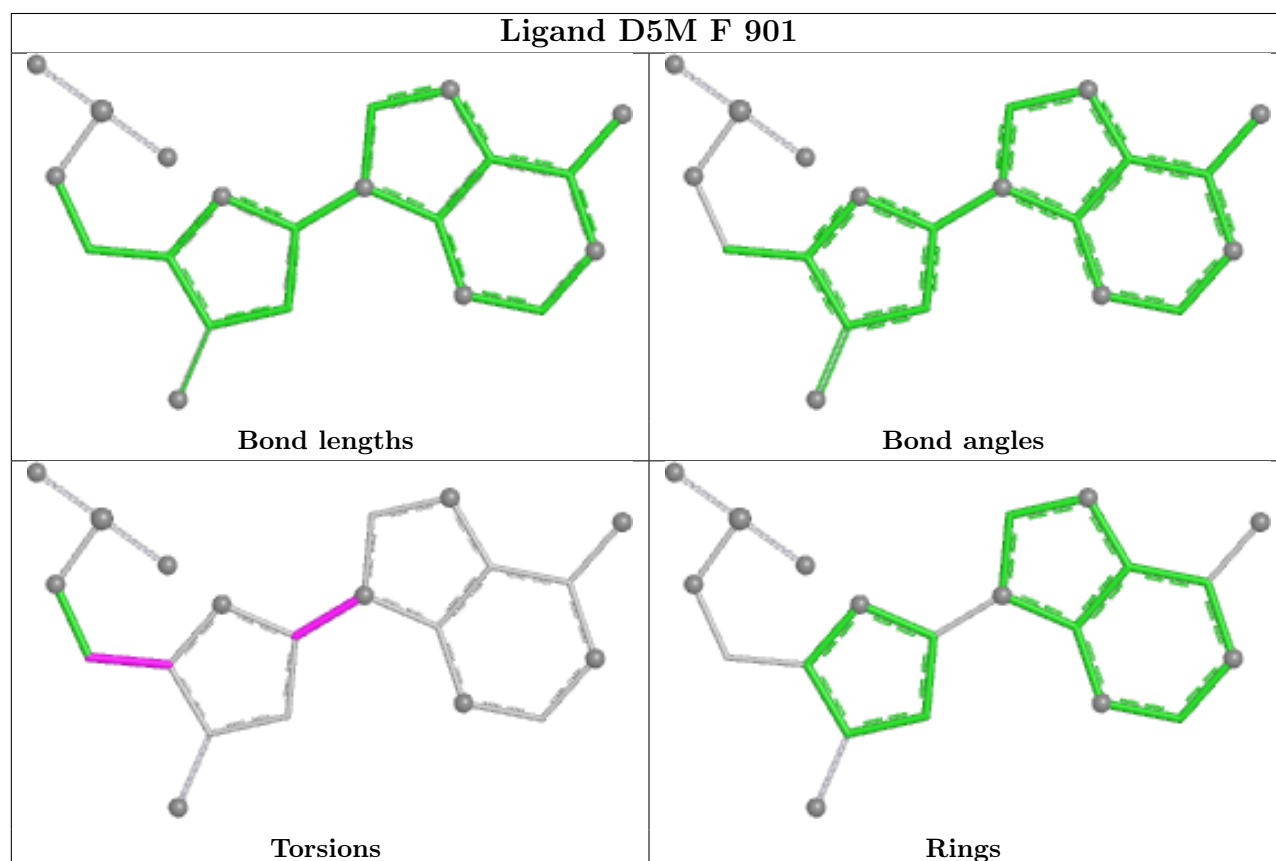
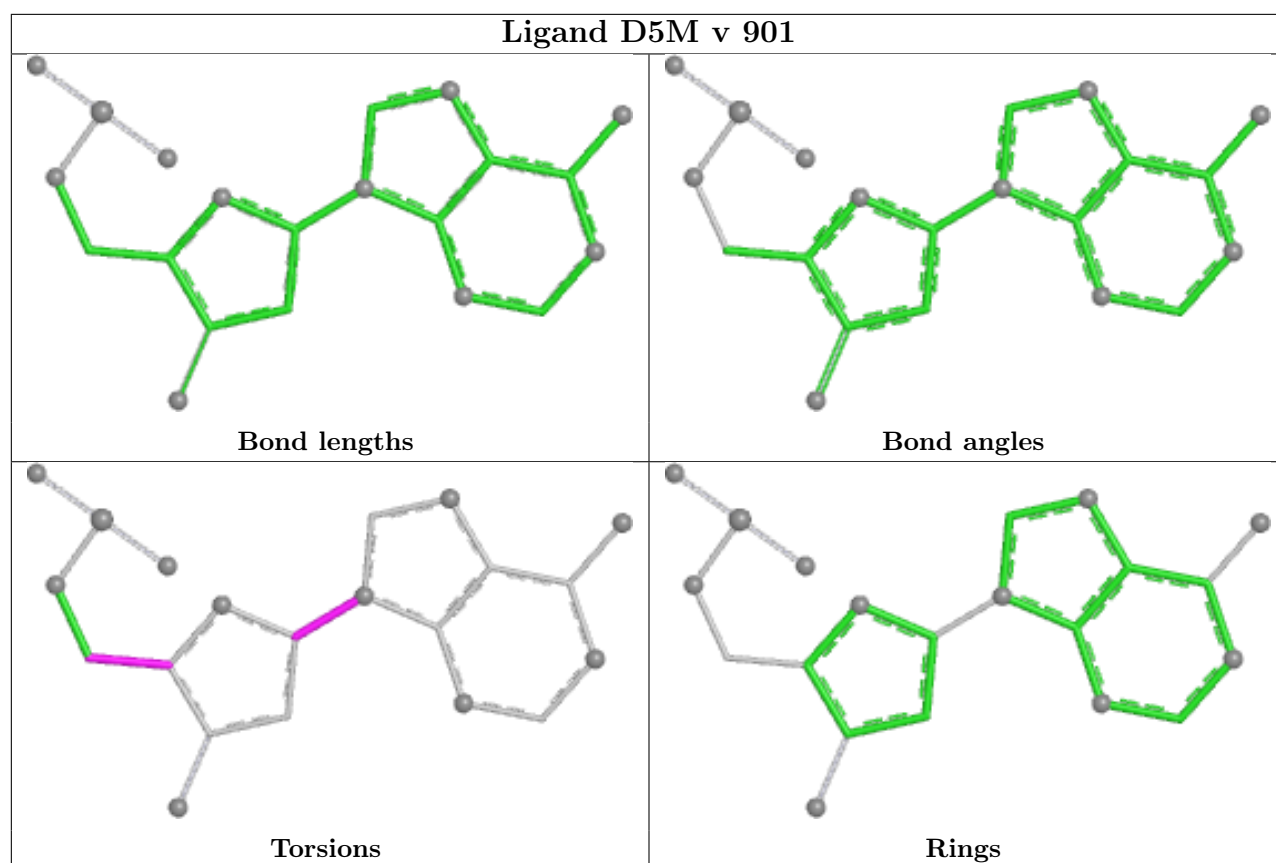


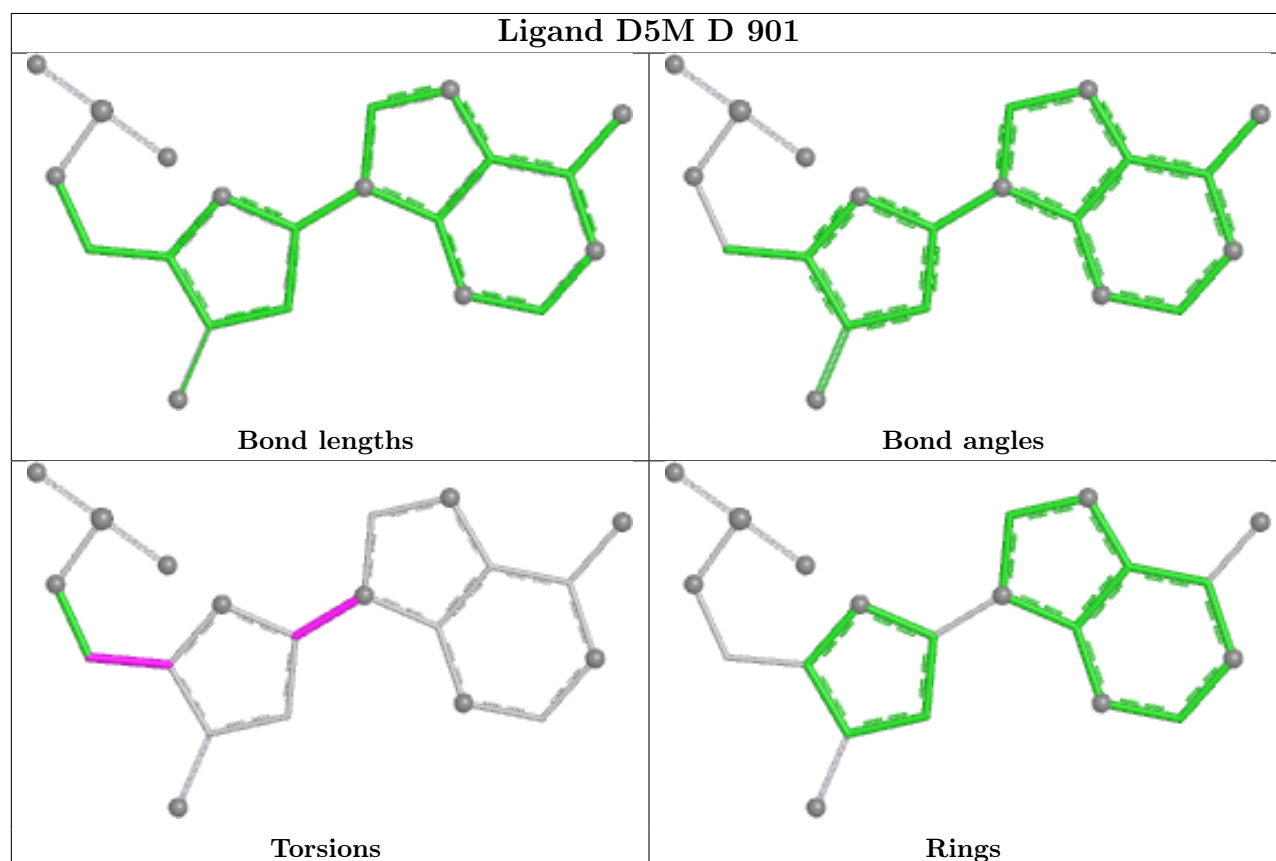
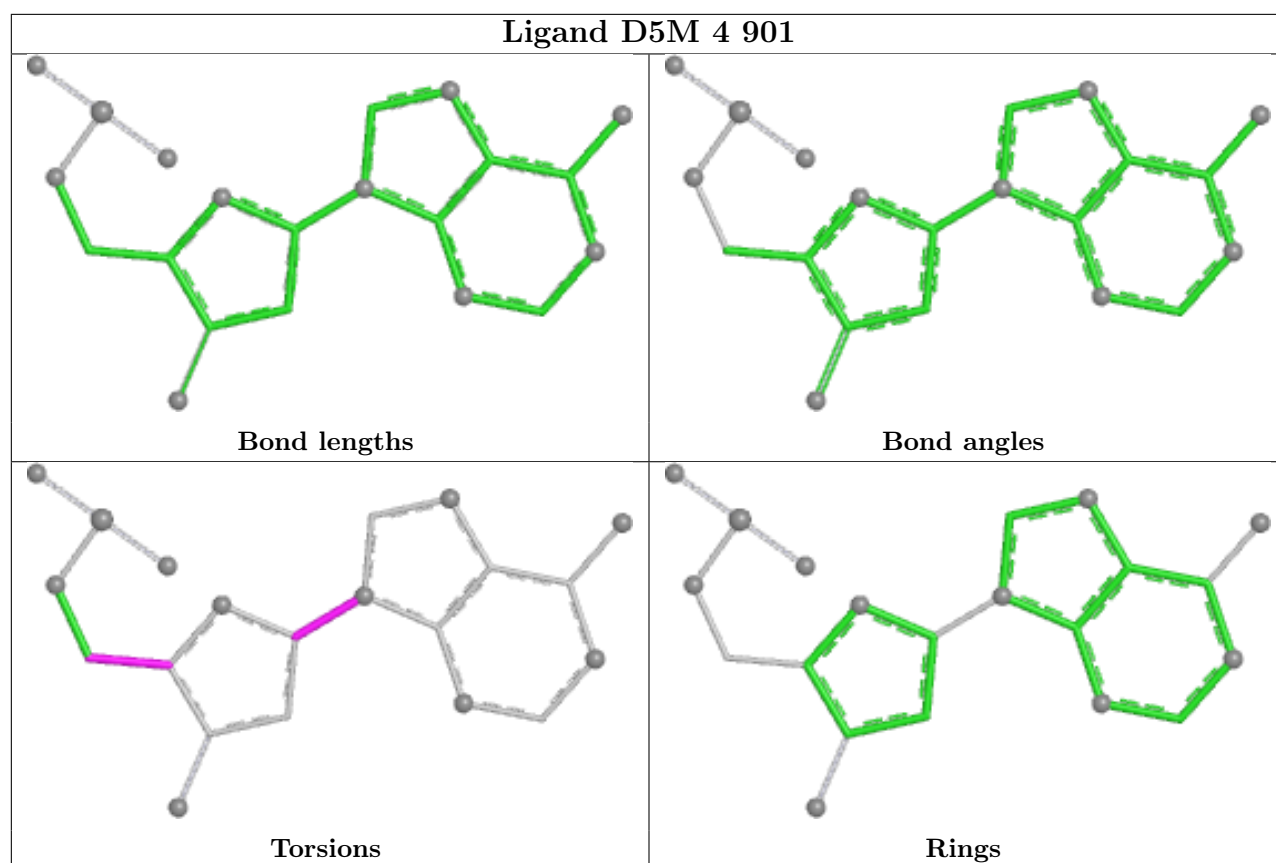


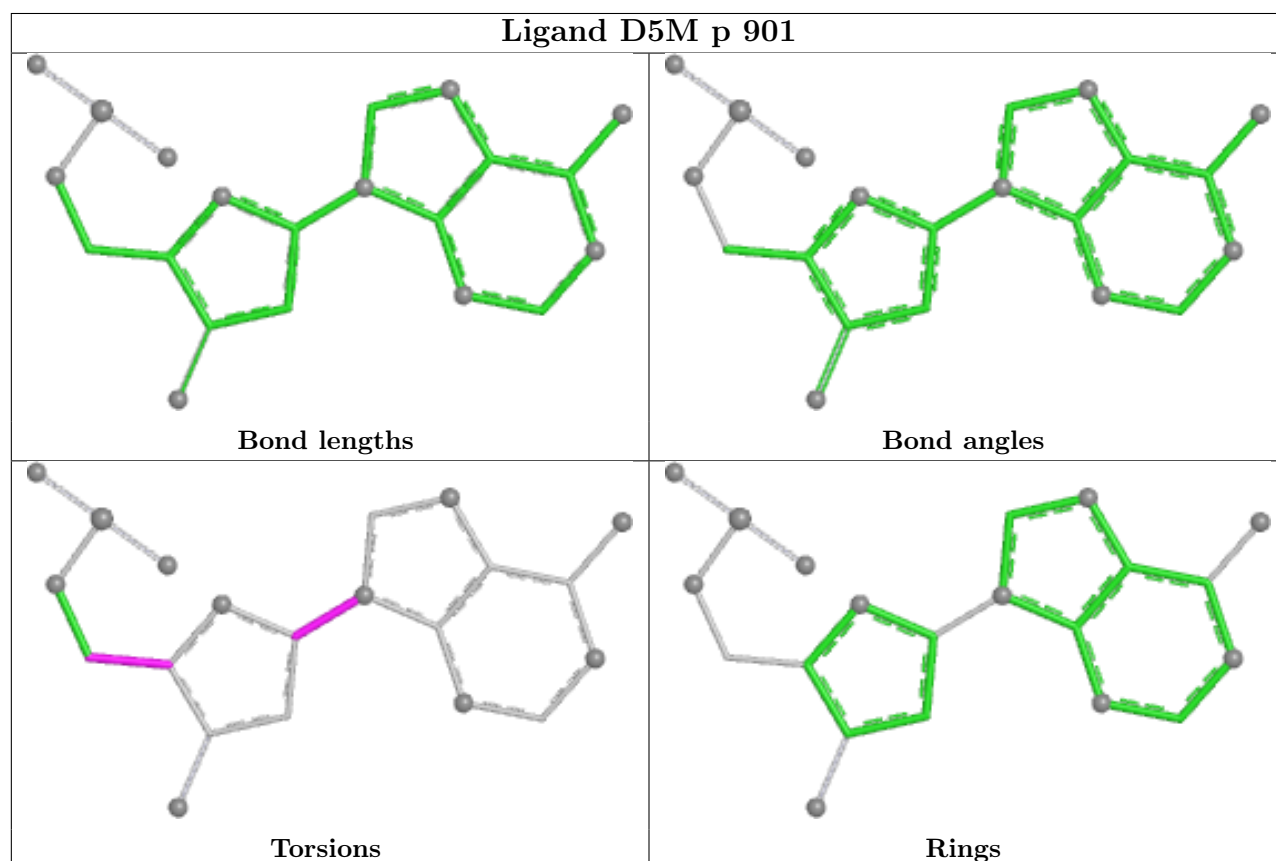
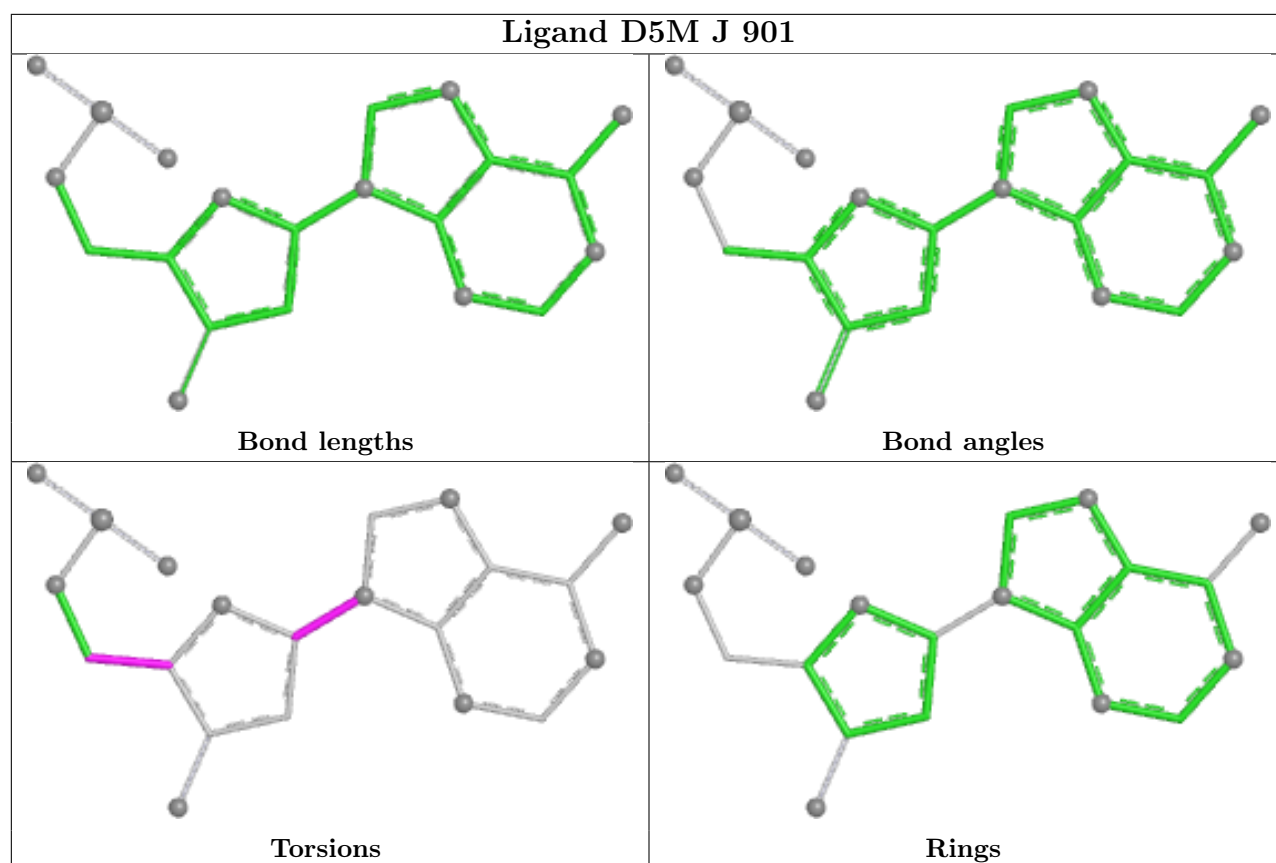


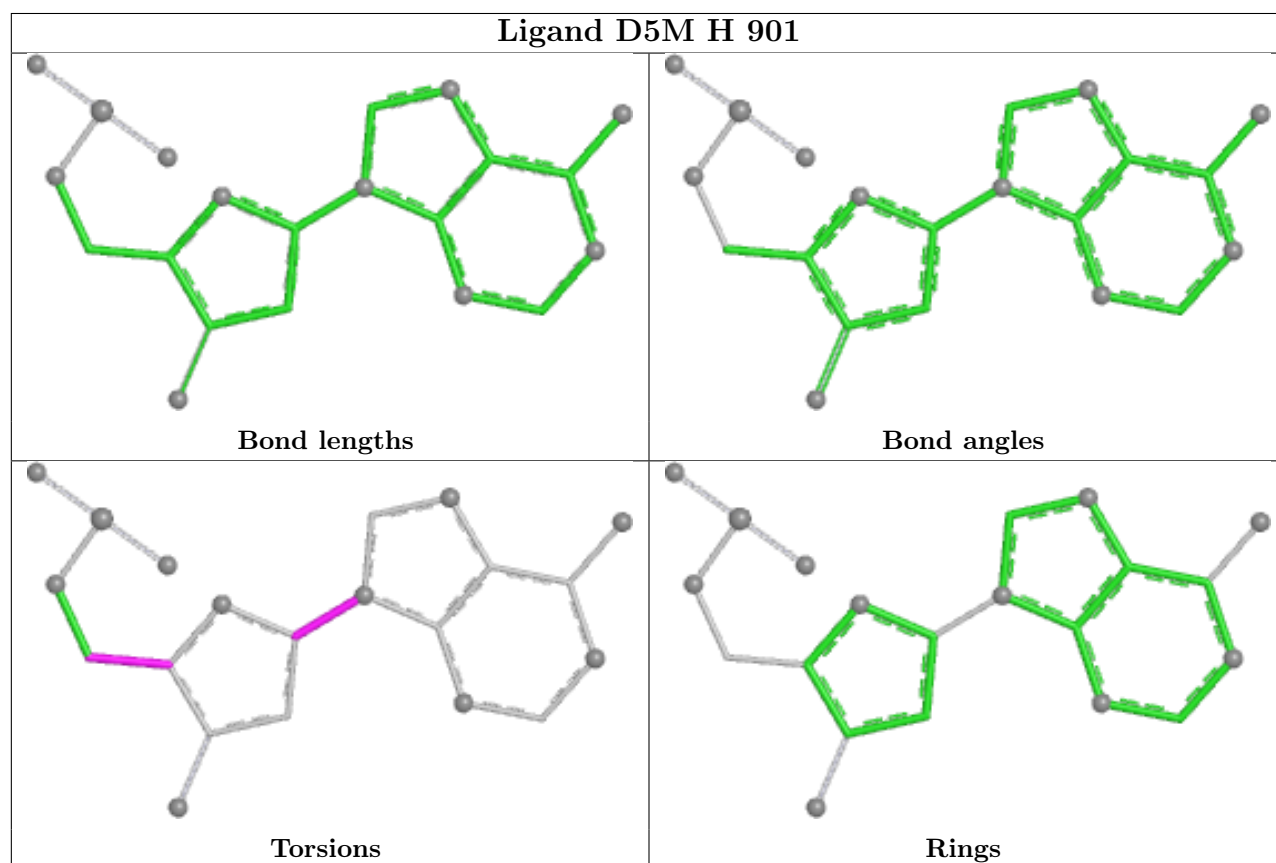
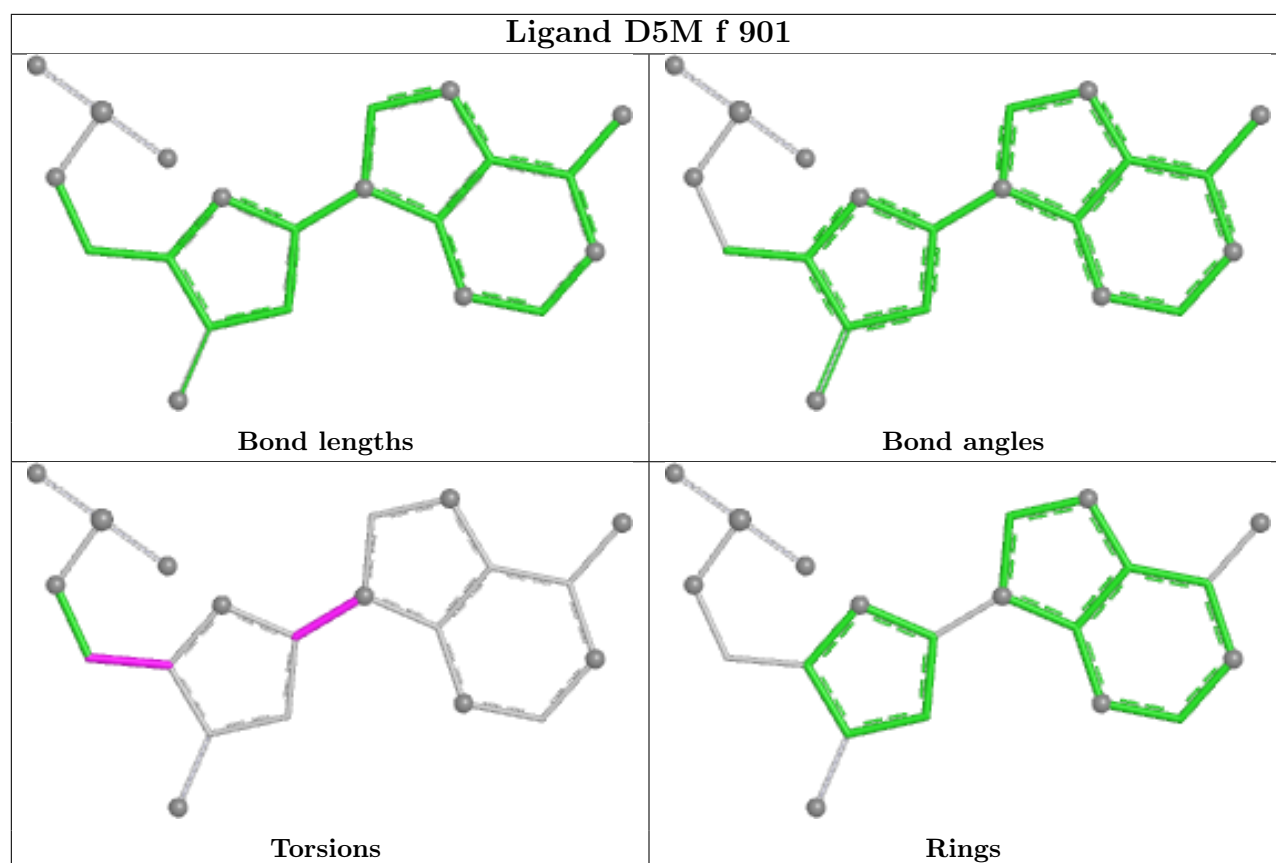


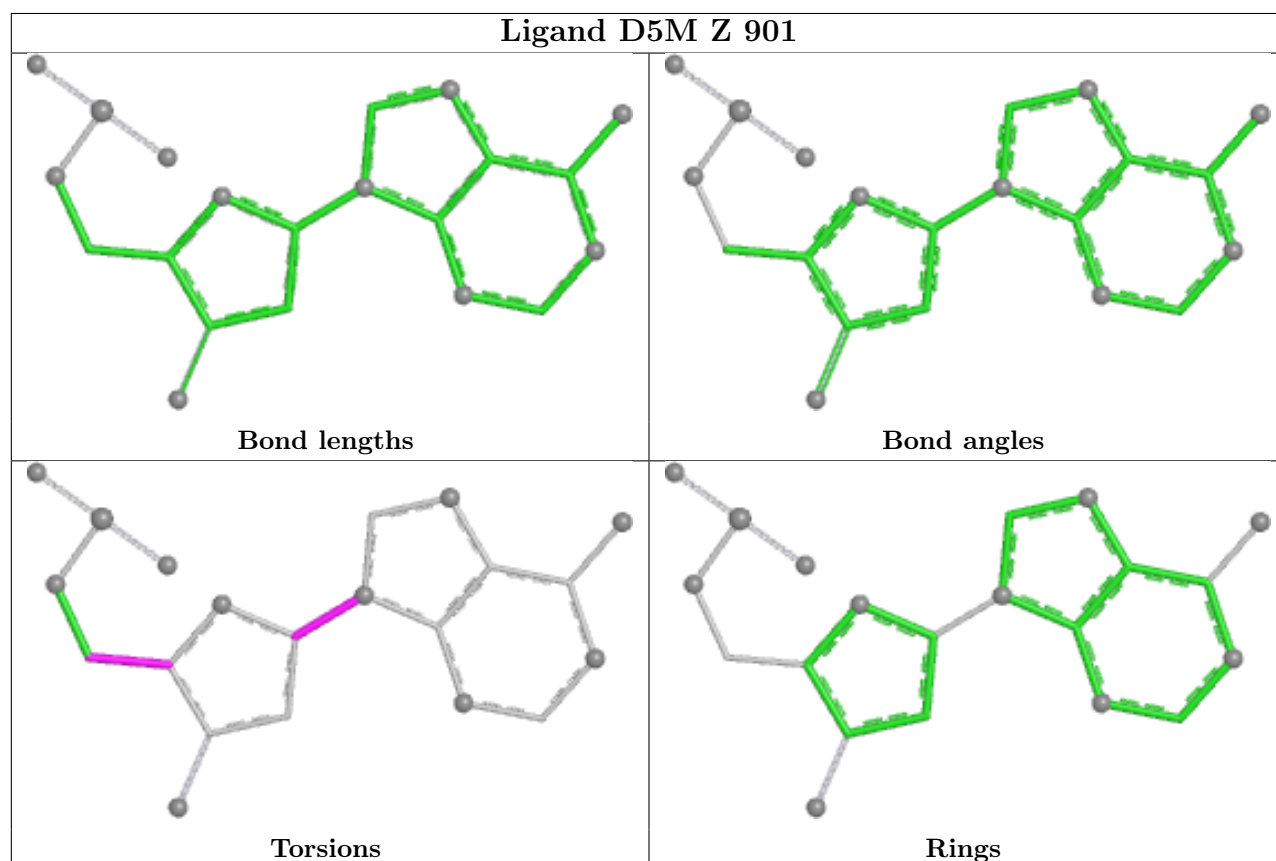
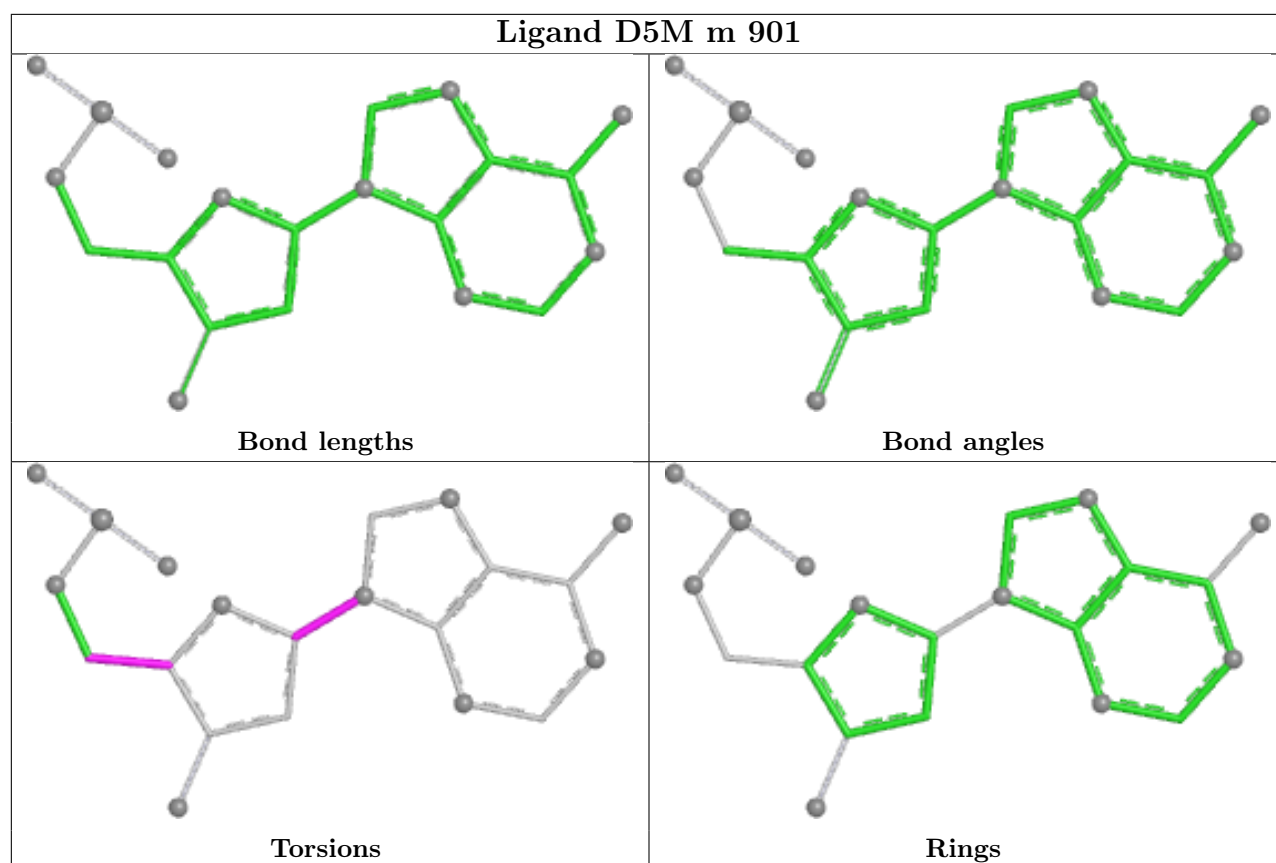




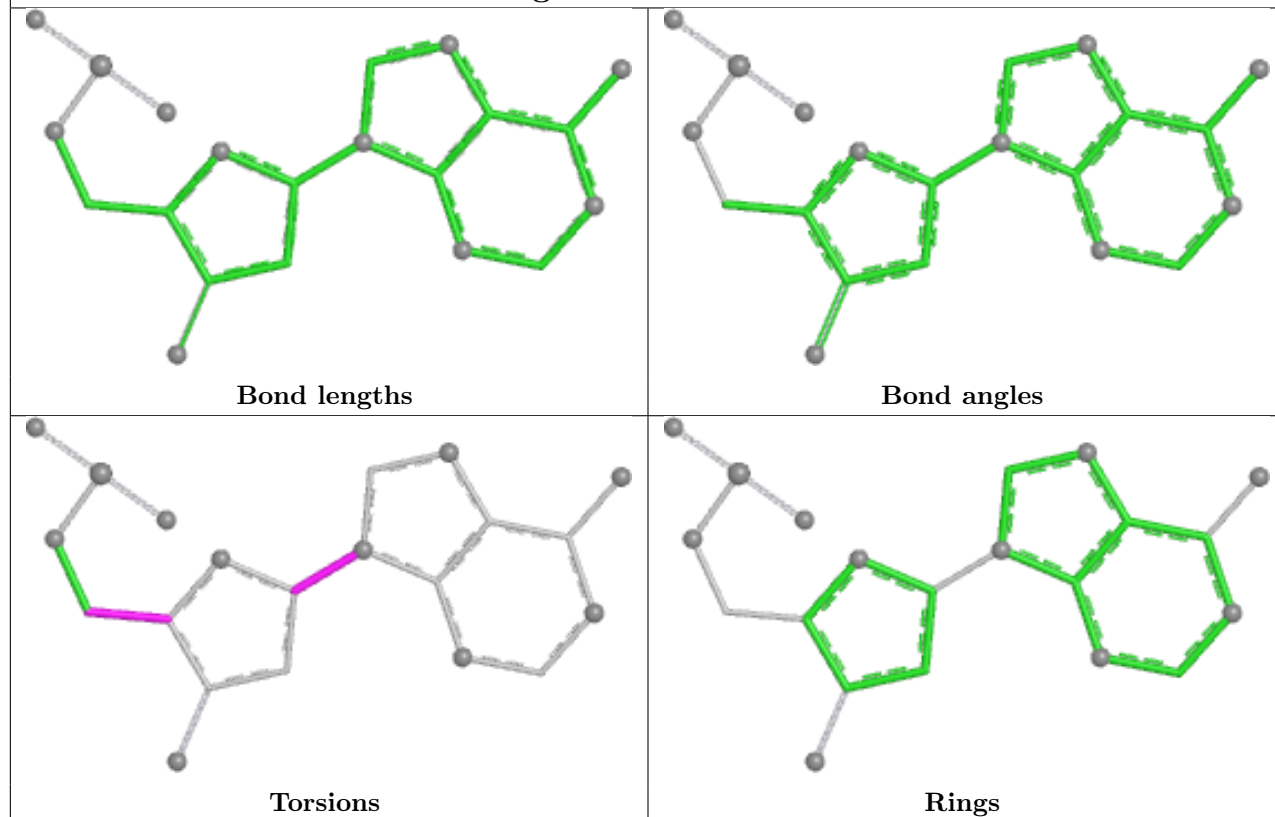




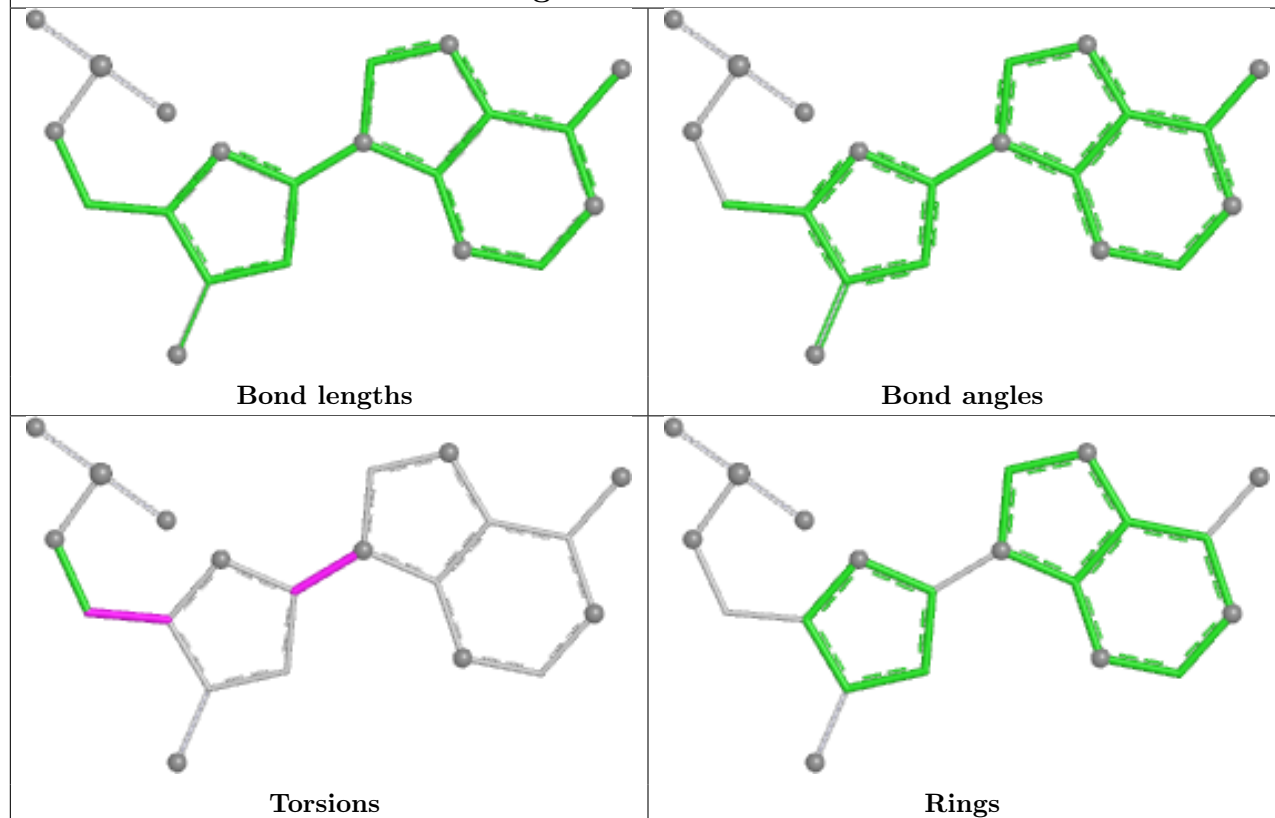




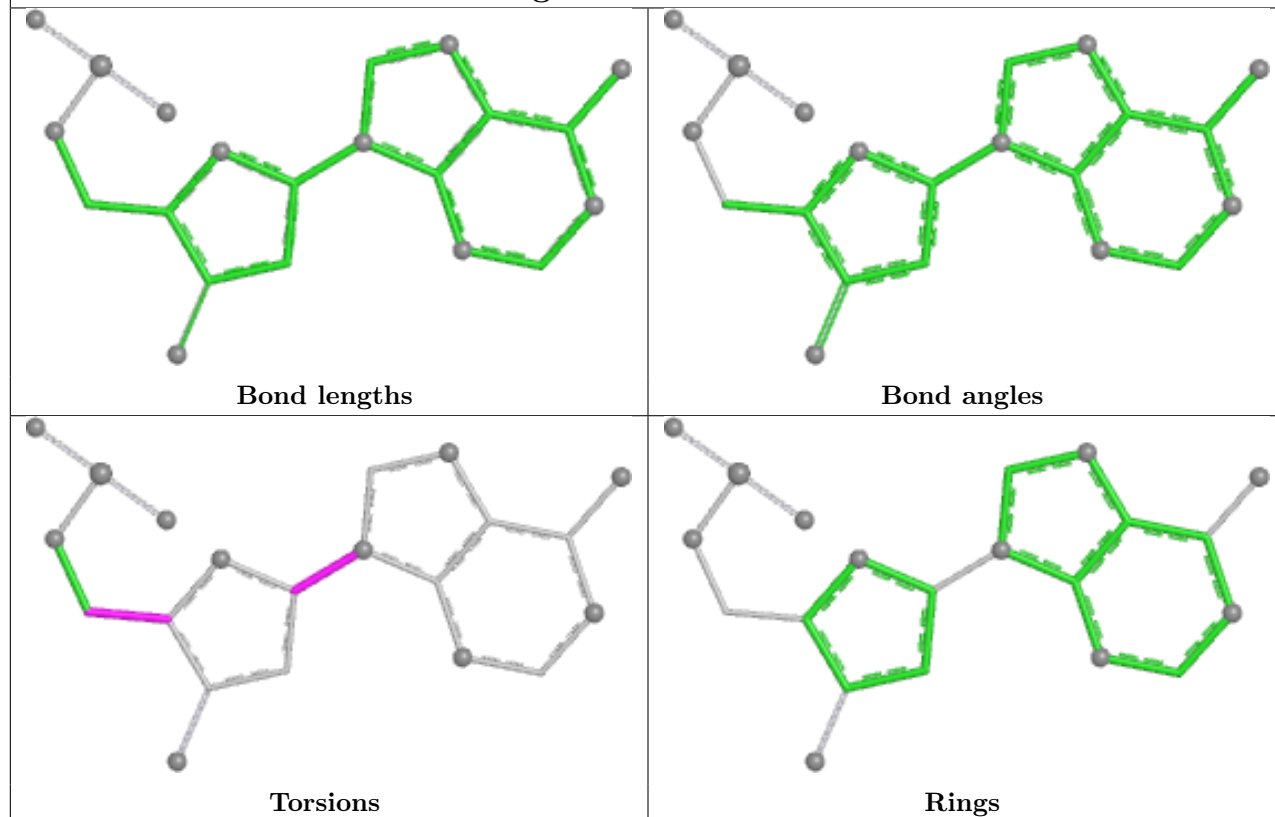
Ligand D5M 7 901



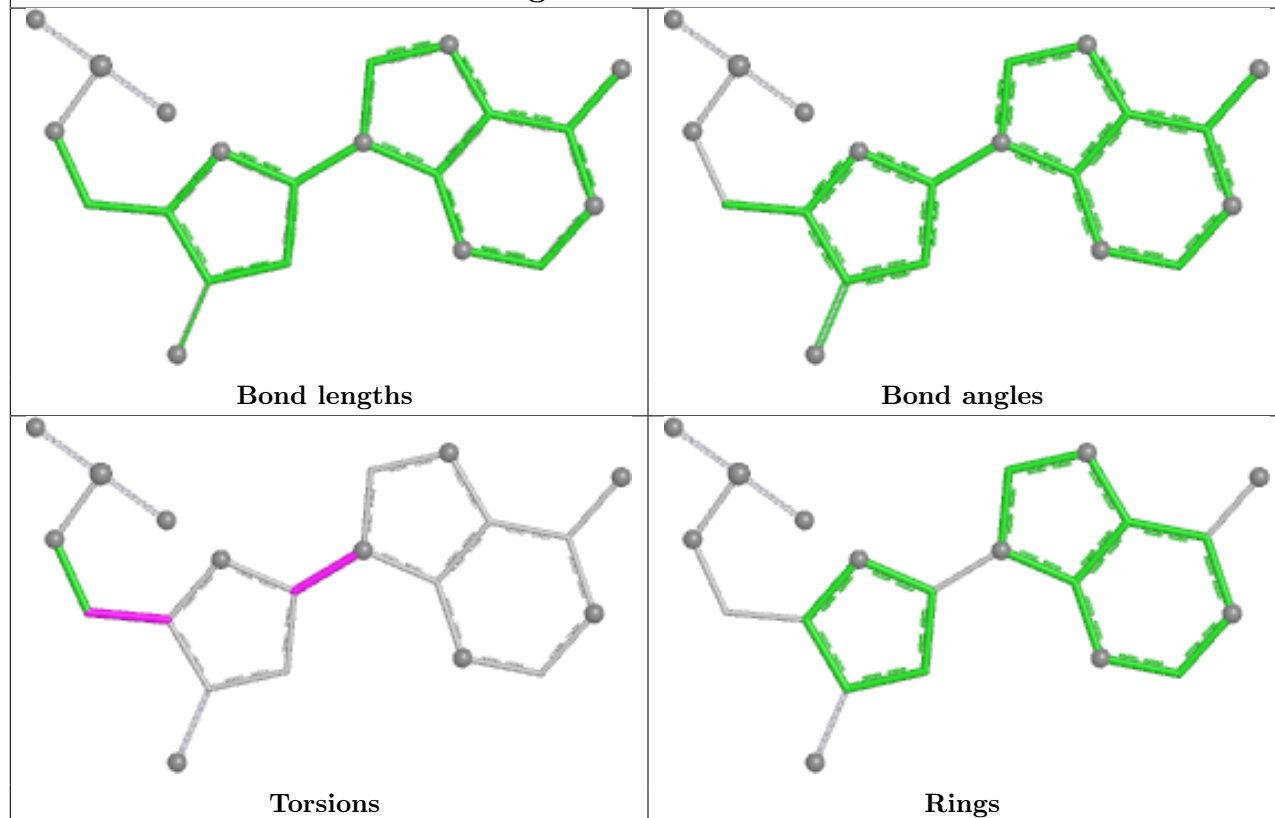
Ligand D5M a 901

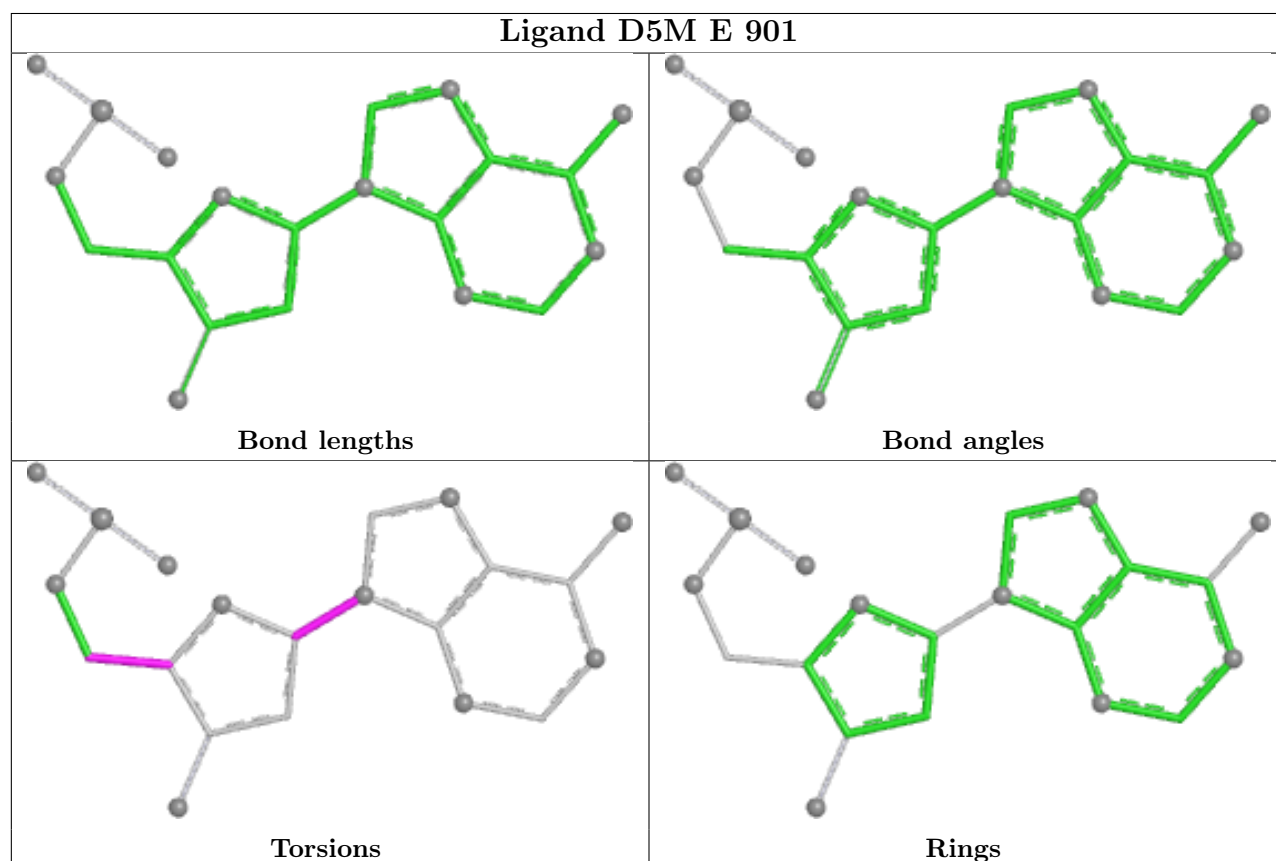
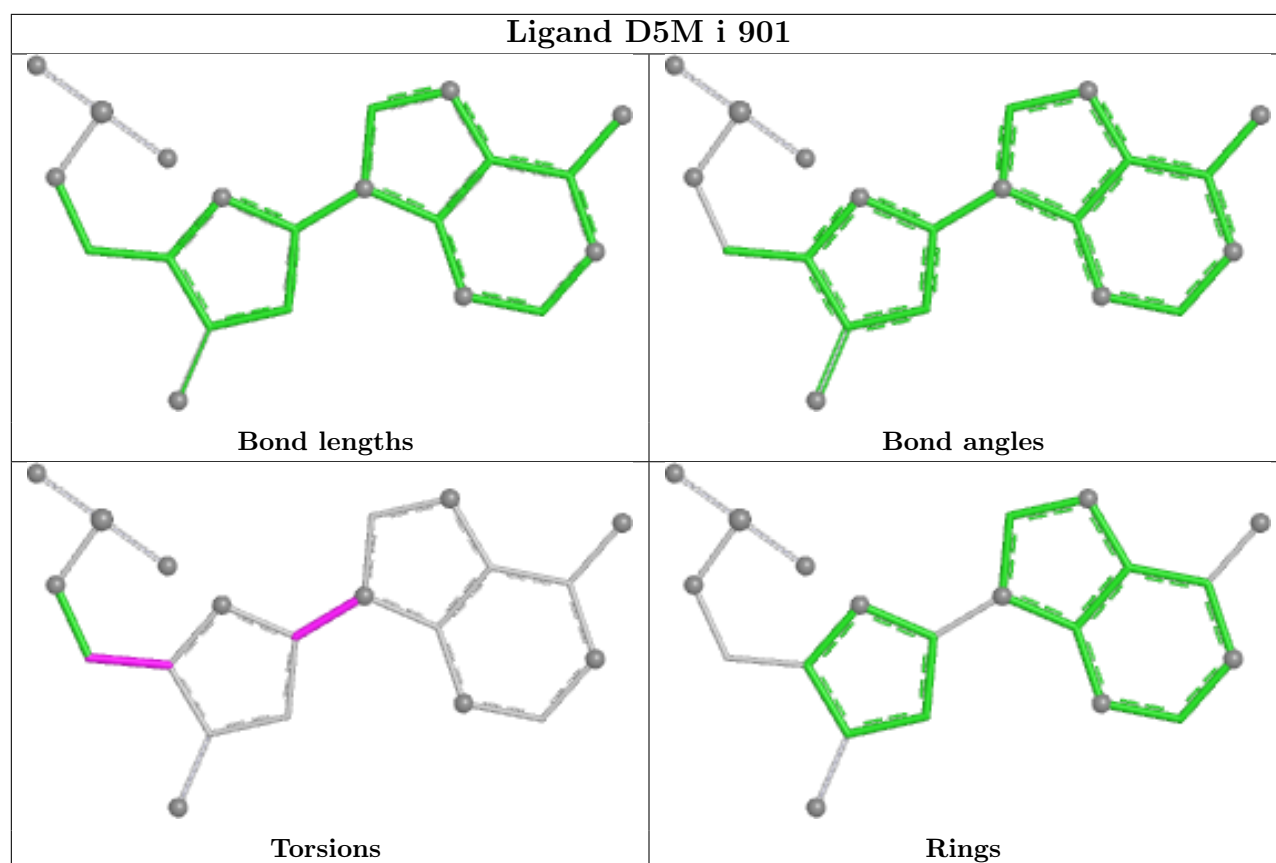


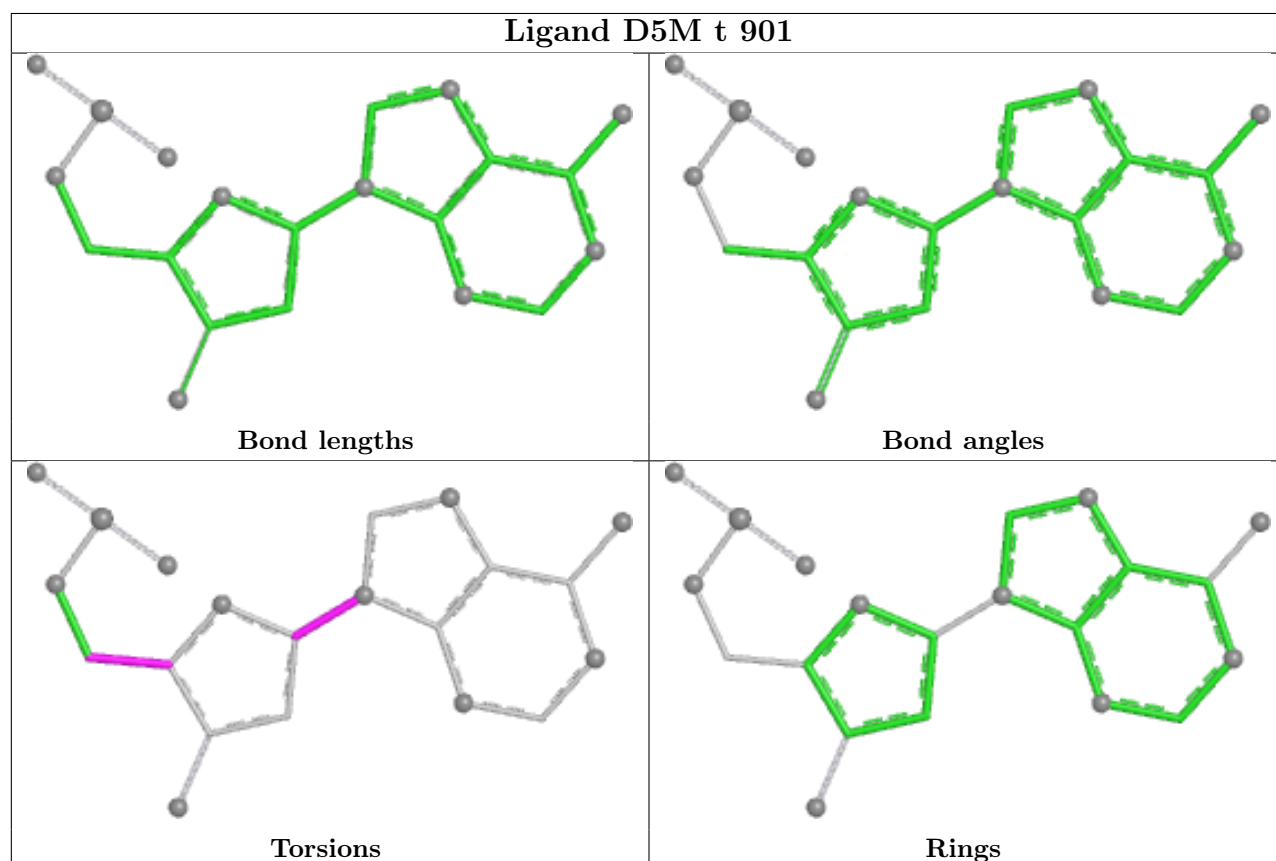
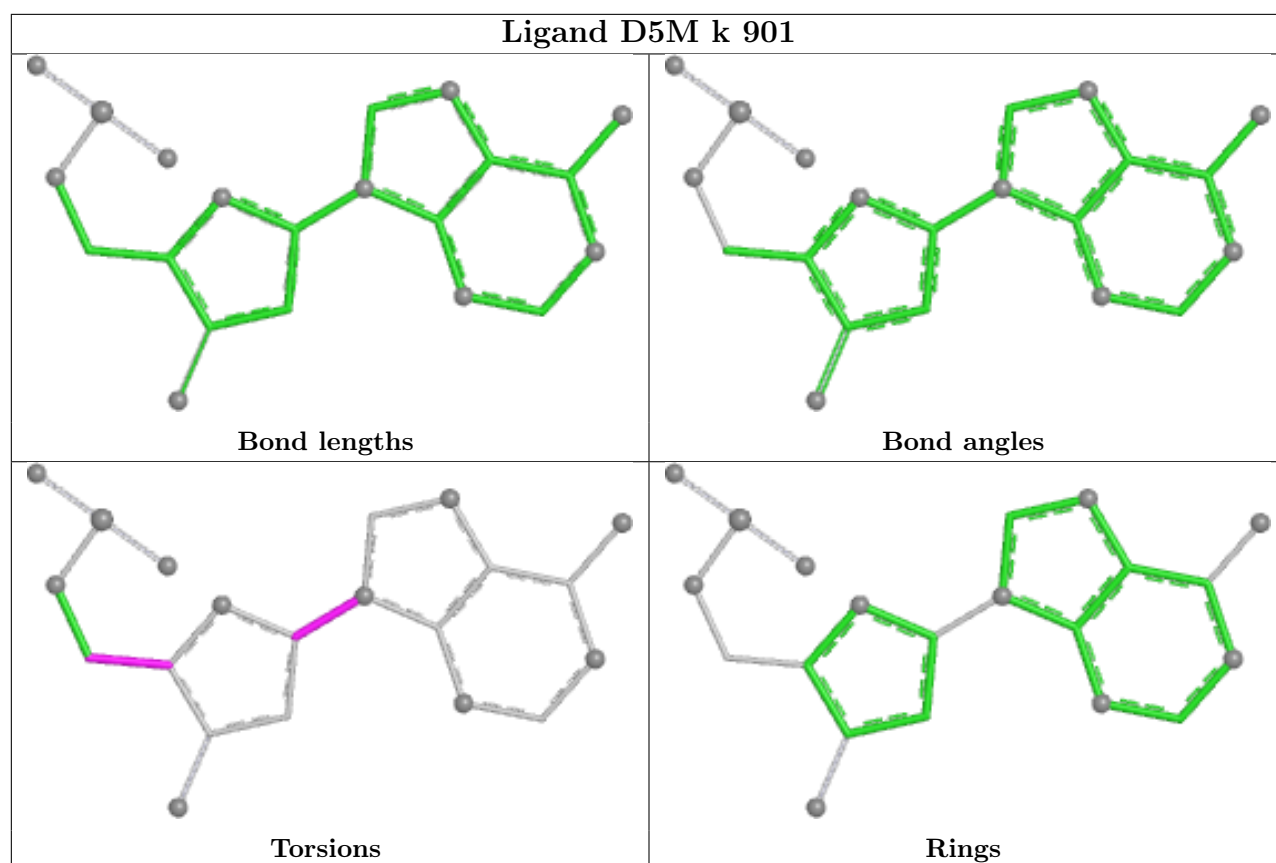
Ligand D5M 1 901

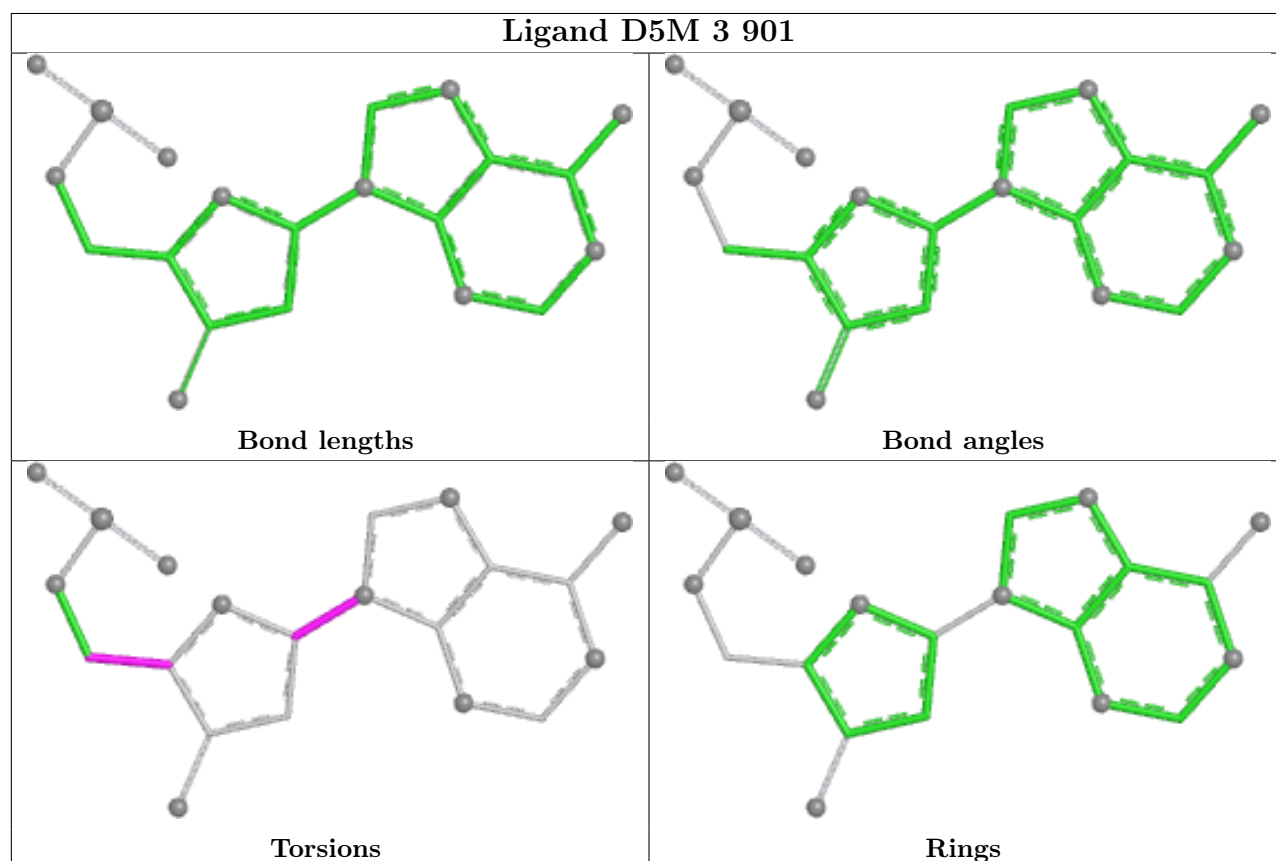
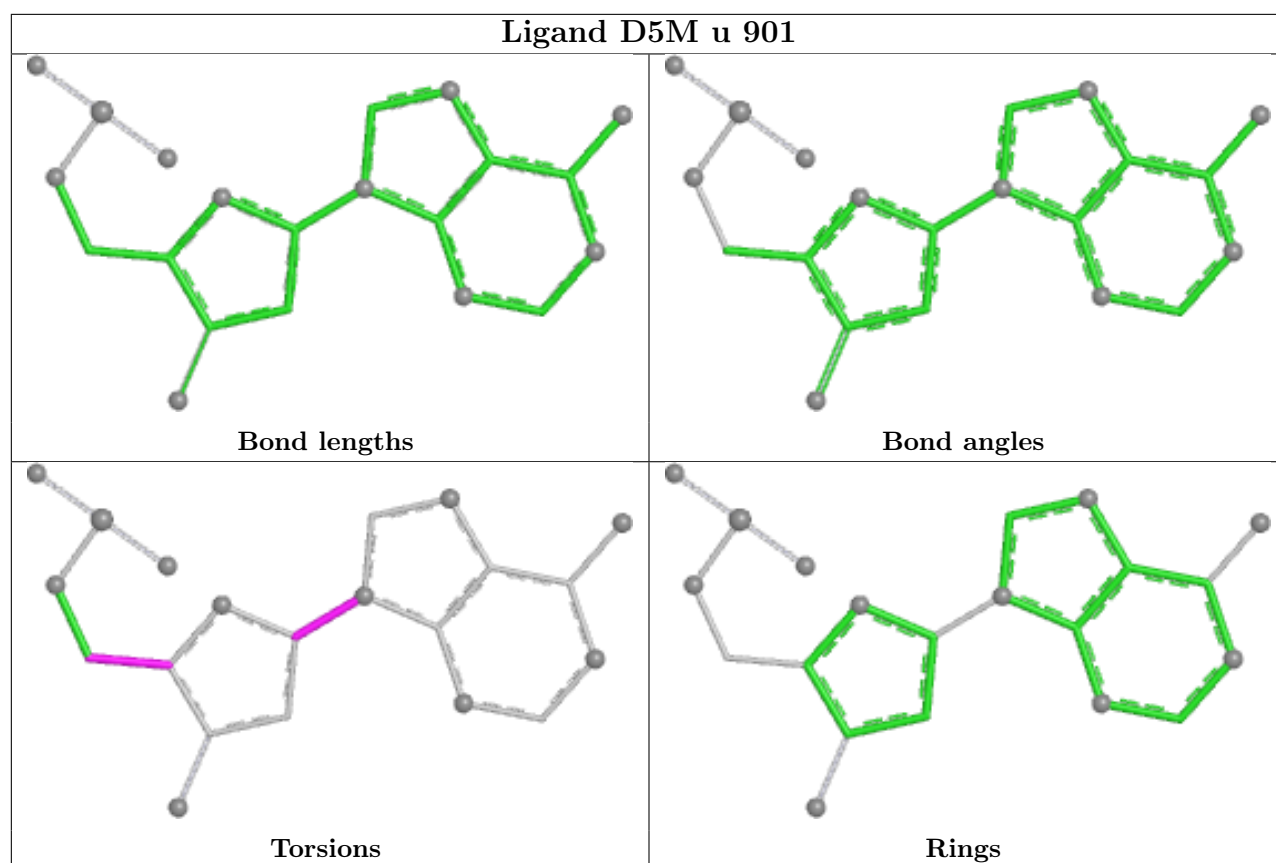


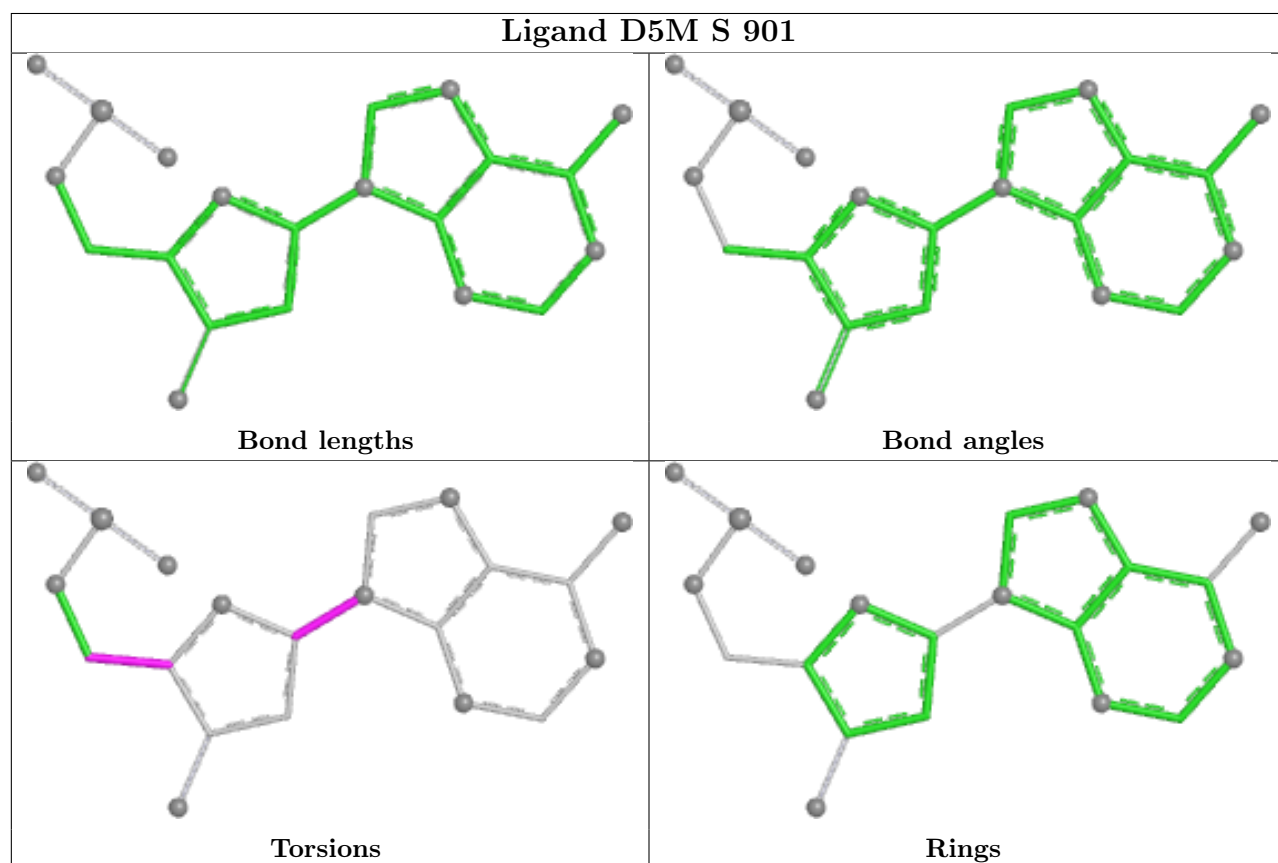
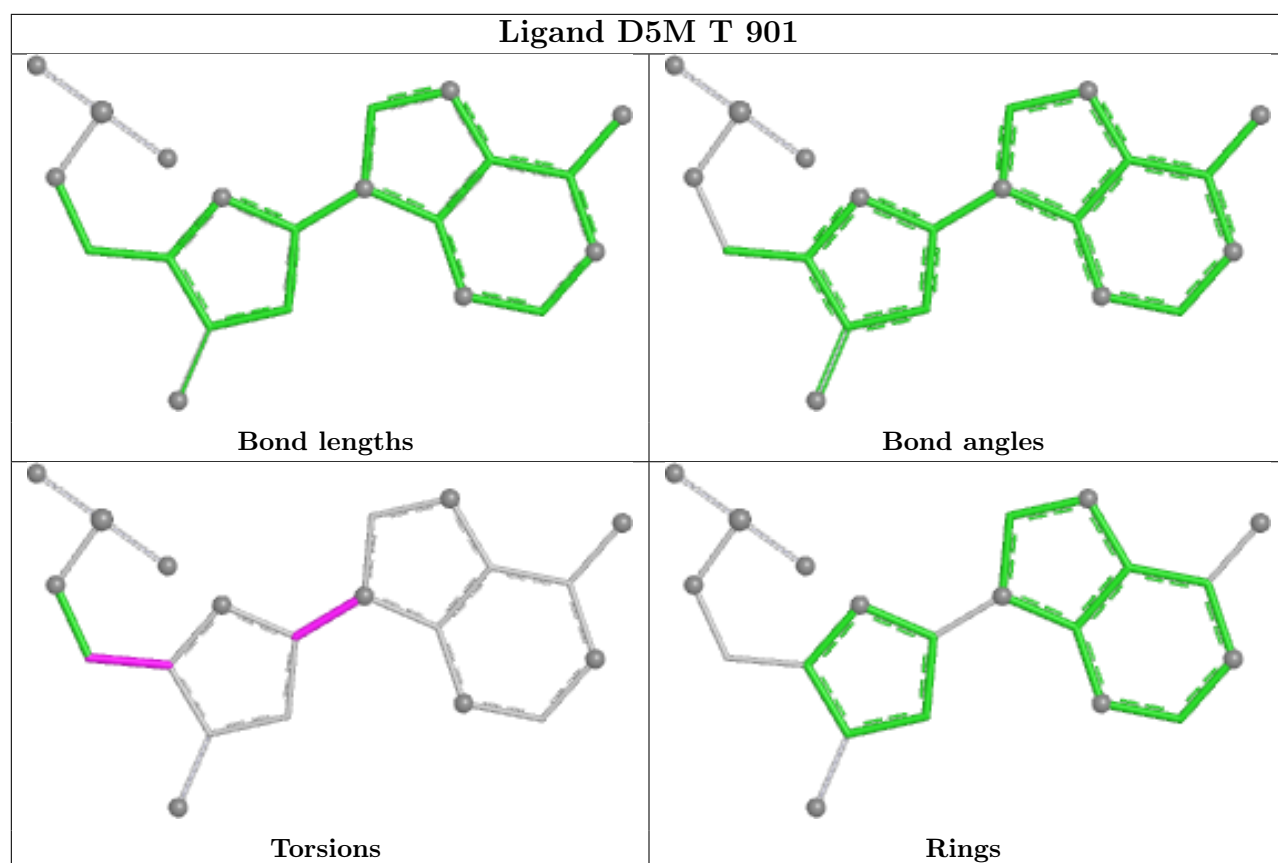
Ligand D5M X 901

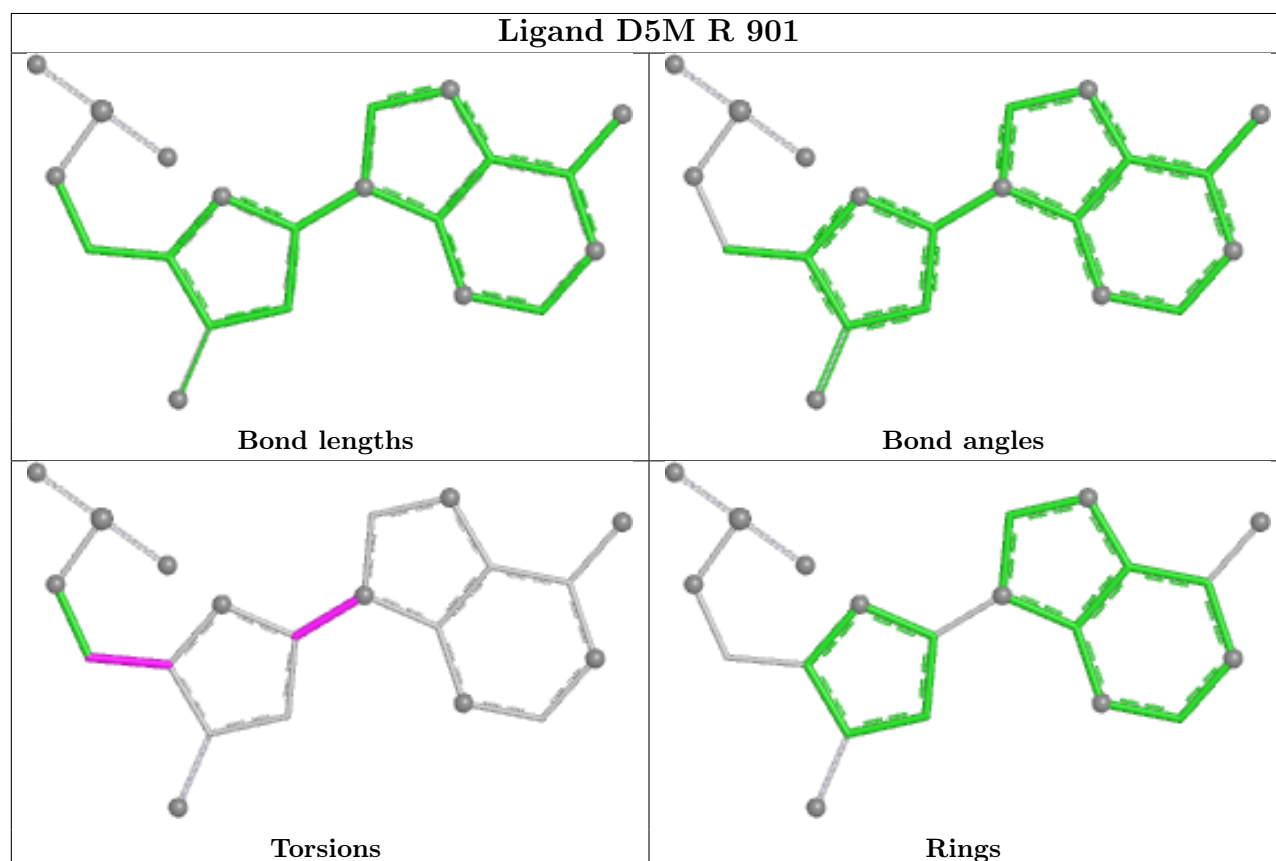
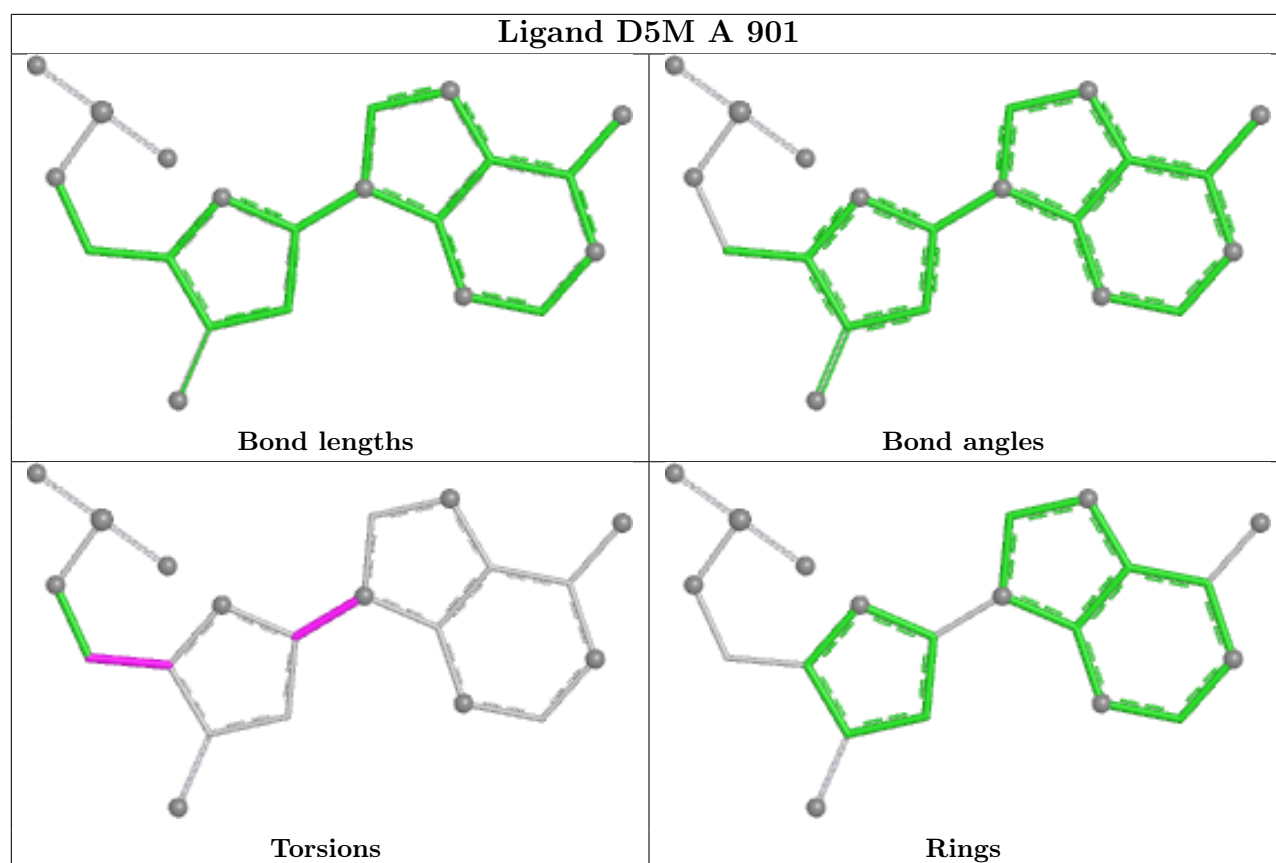




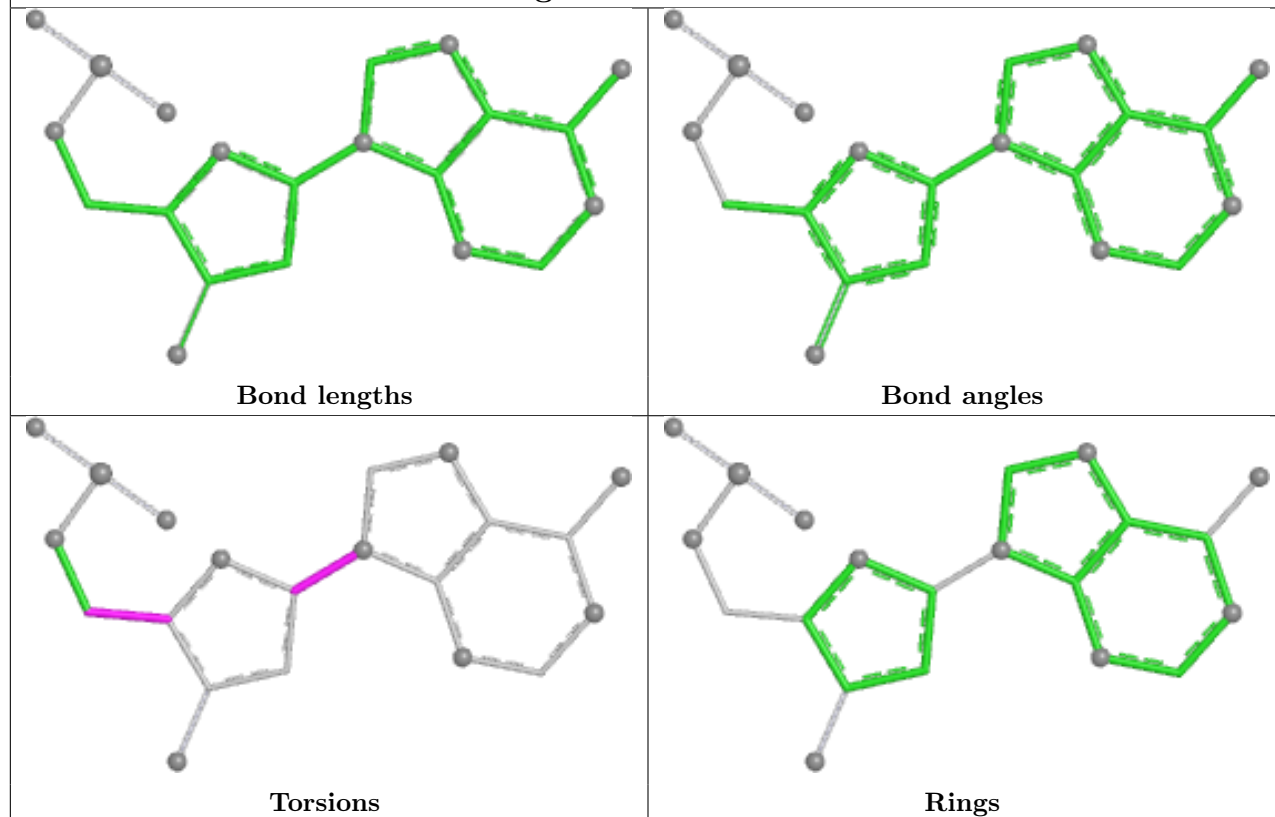




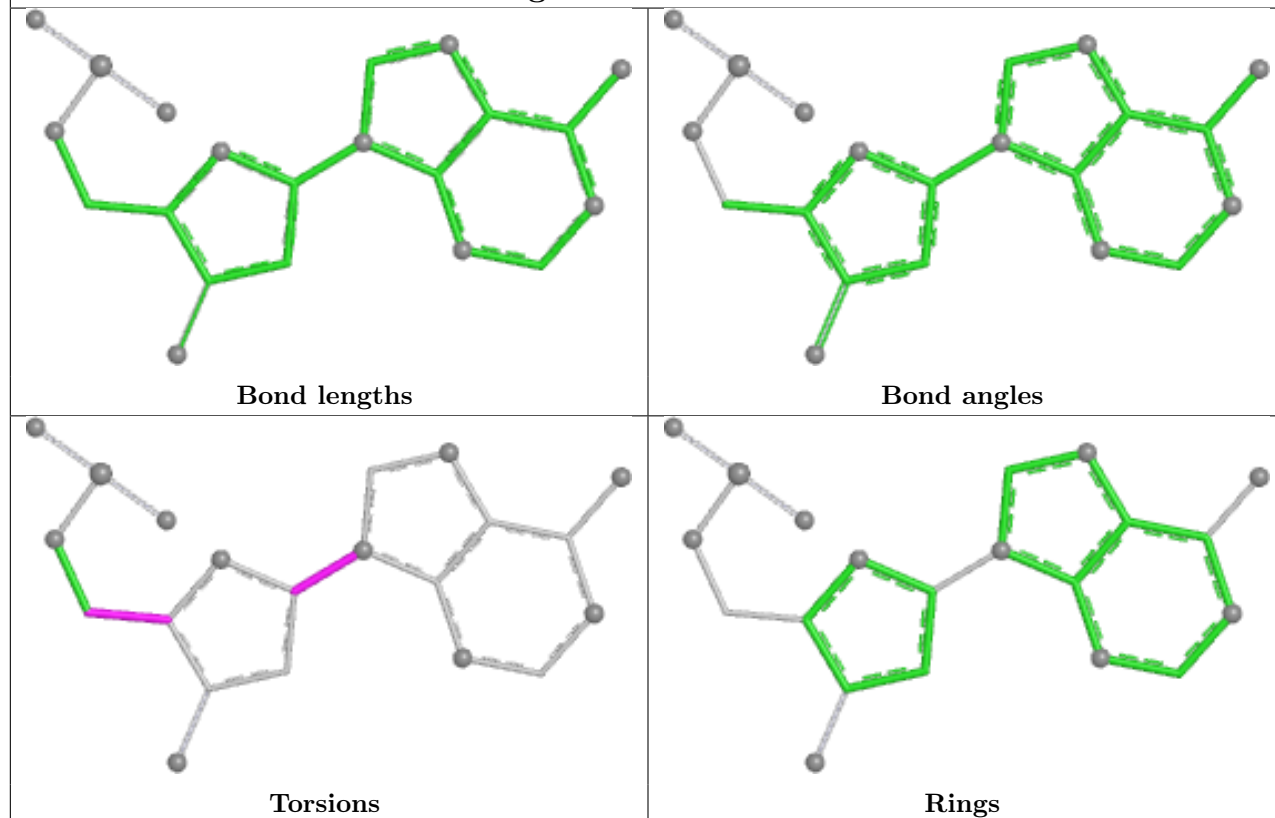


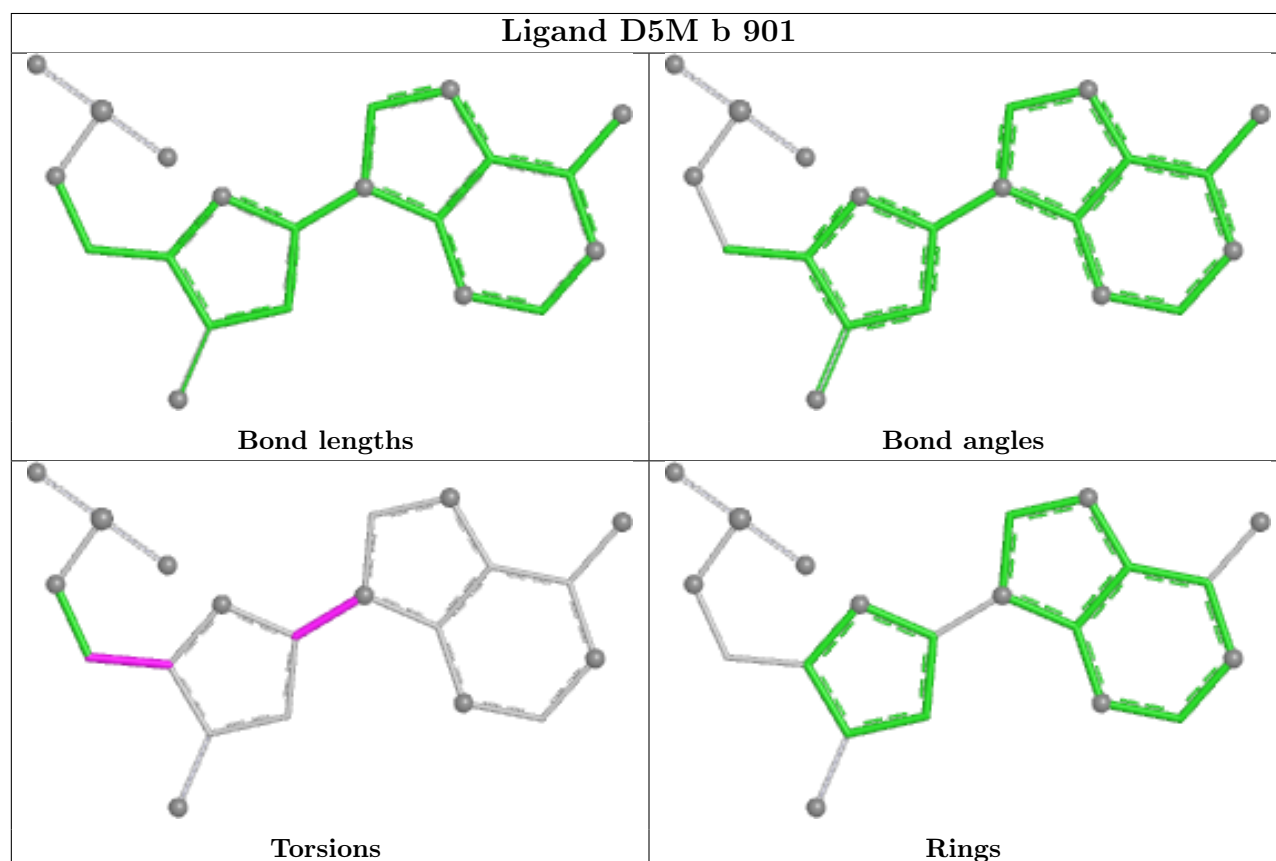
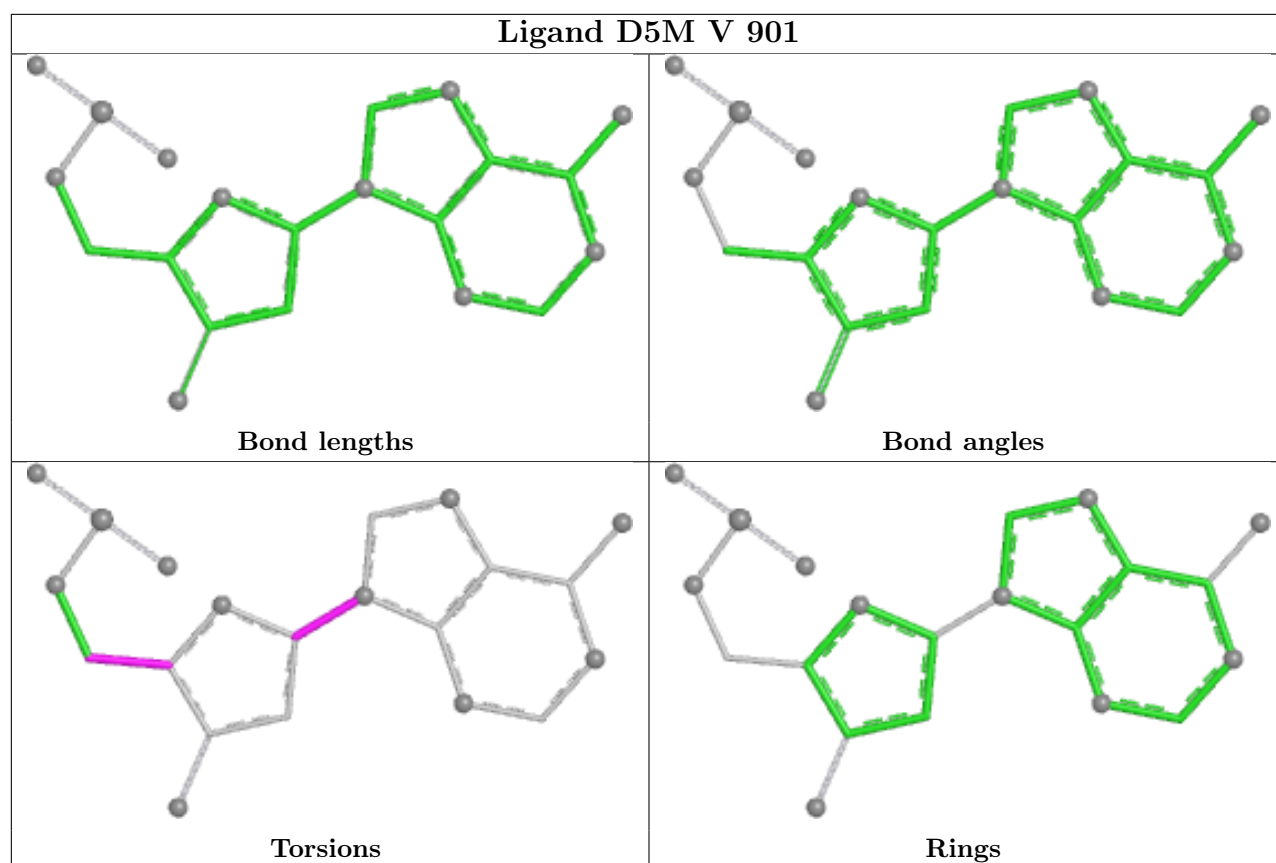


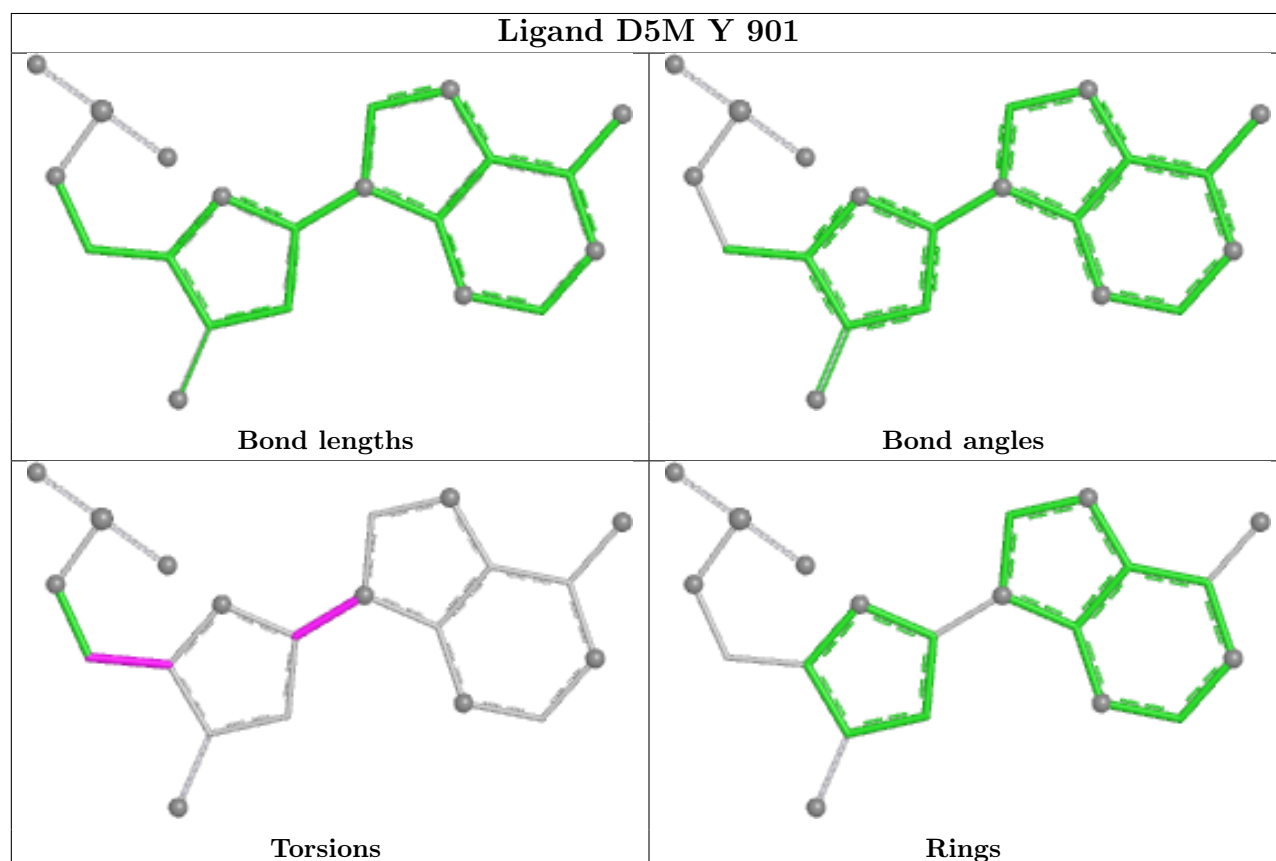
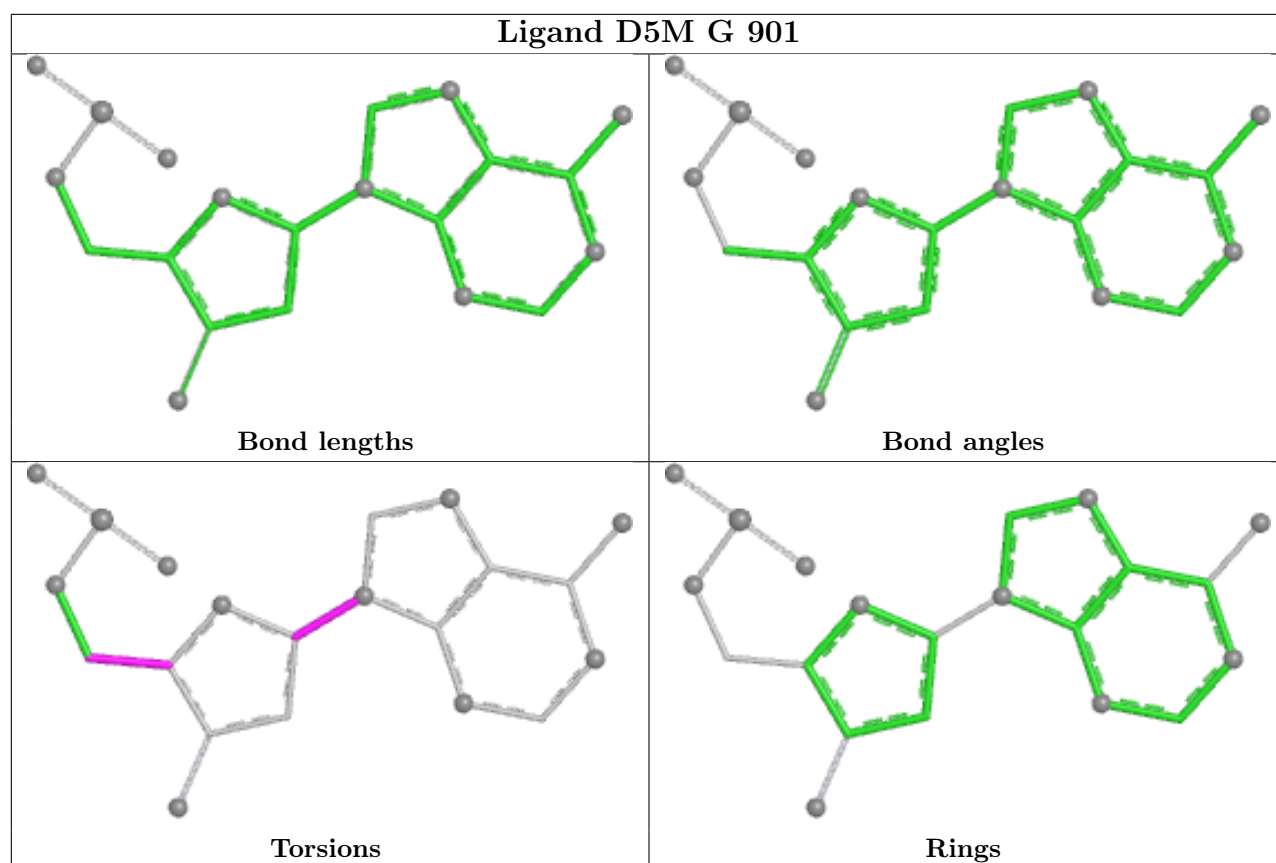
Ligand D5M I 901

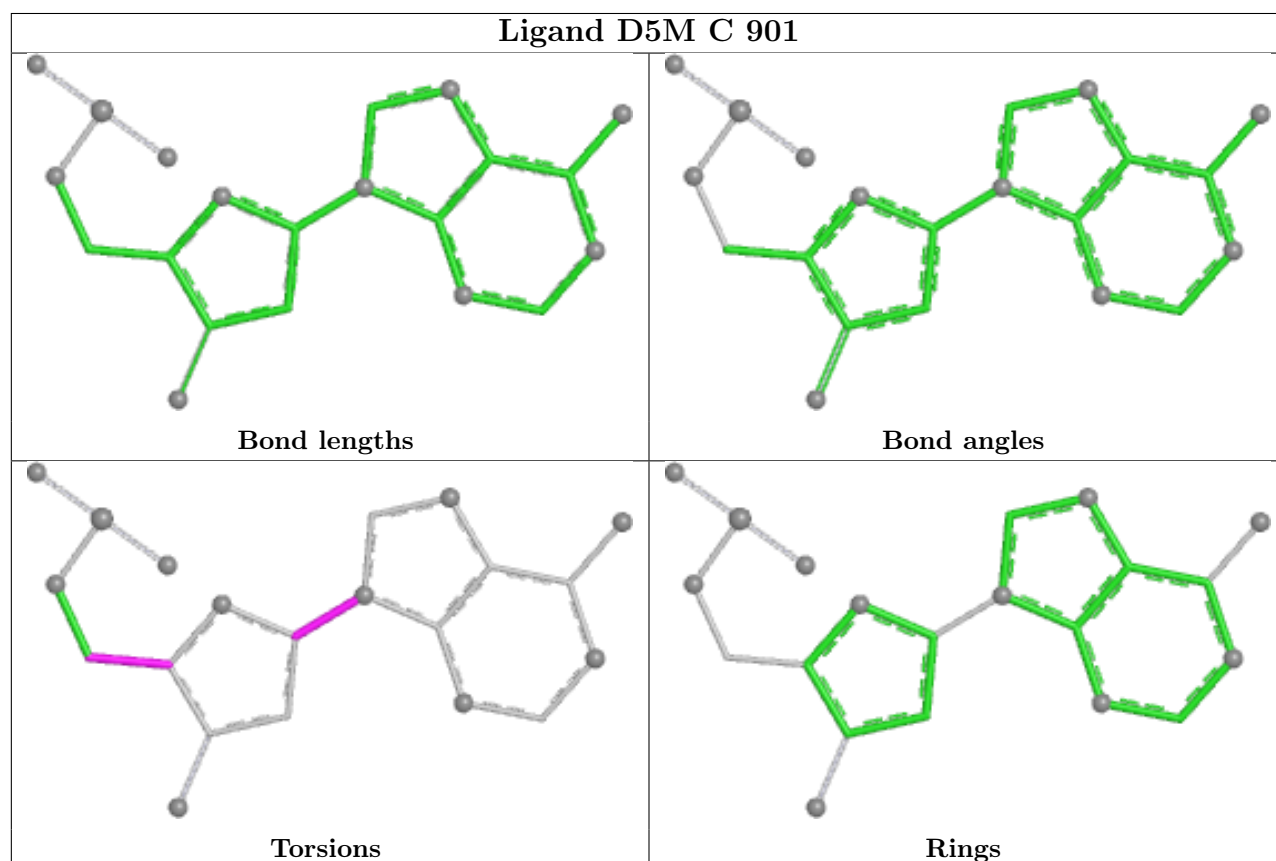
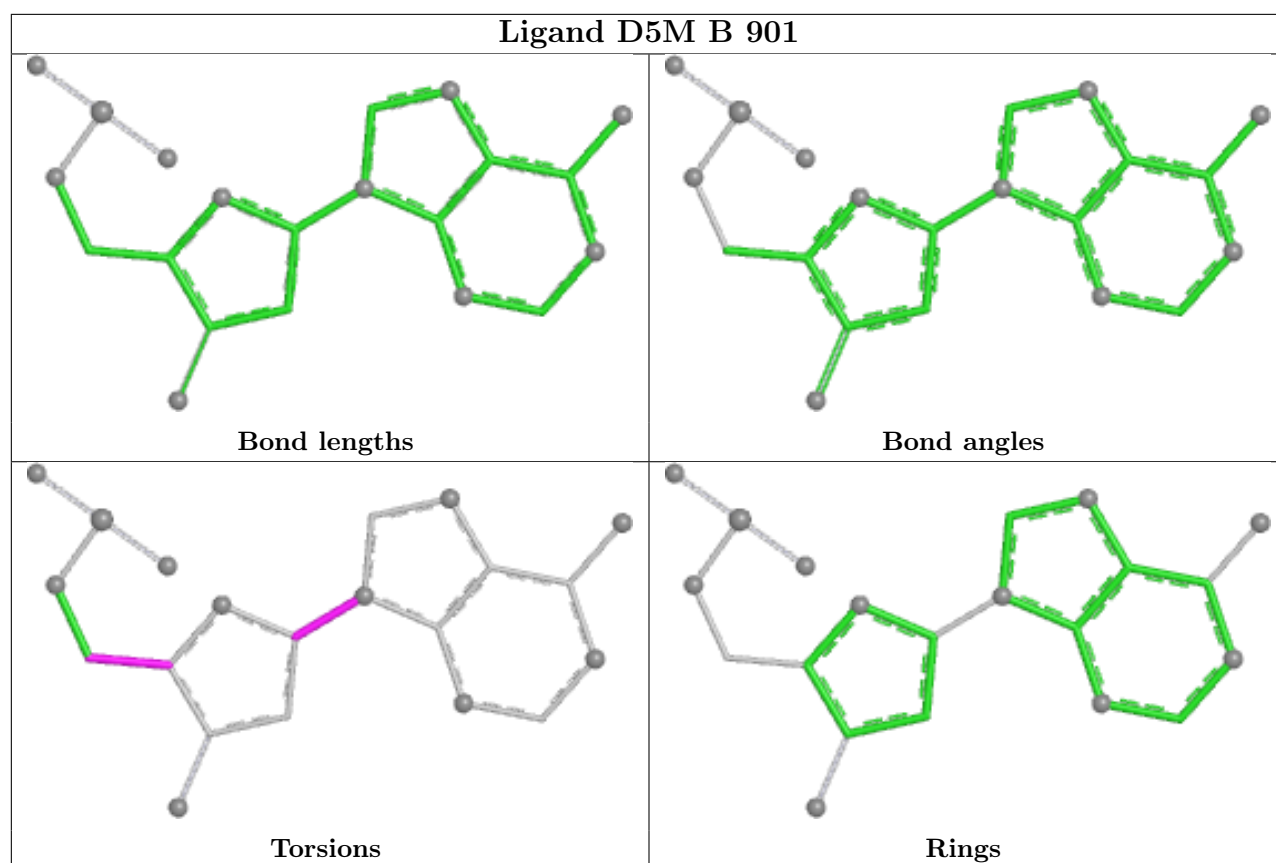


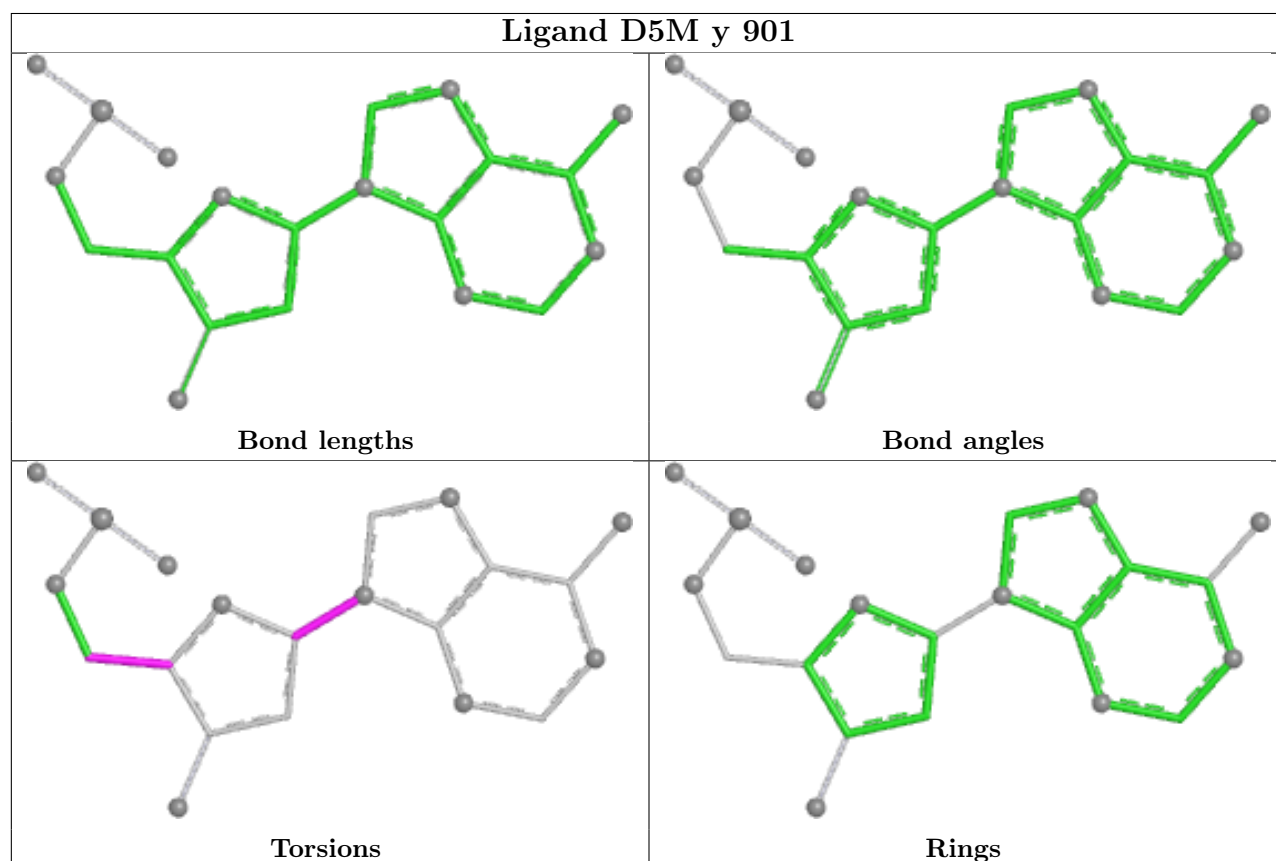
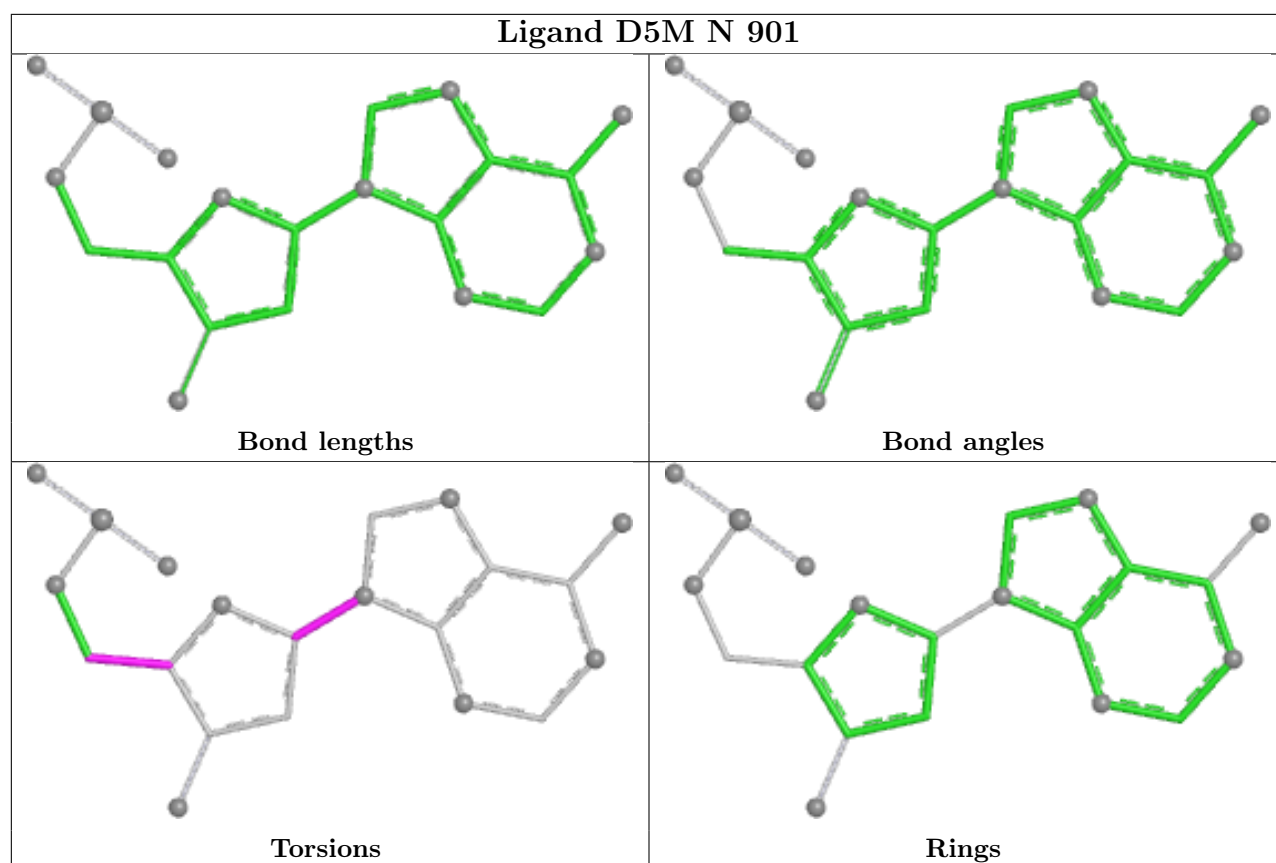
Ligand D5M O 901

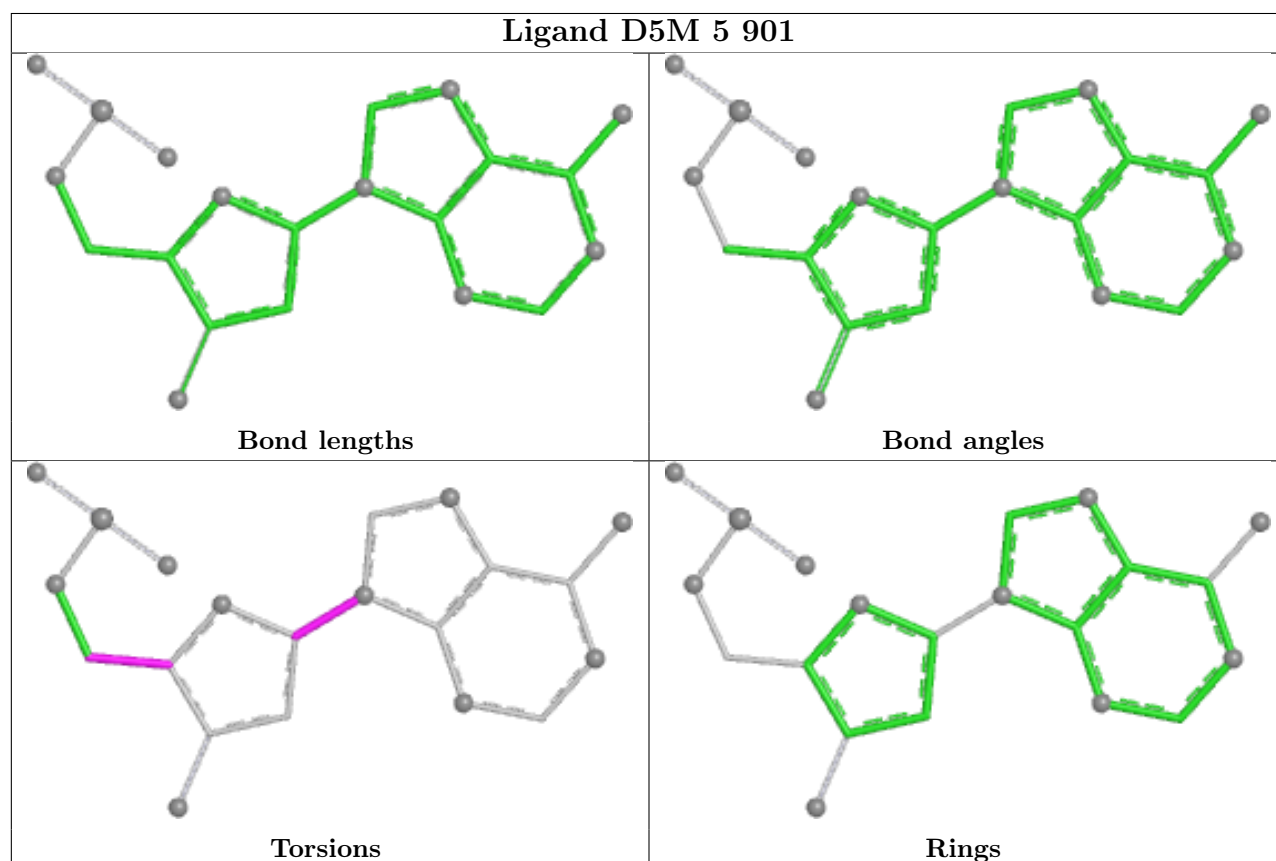
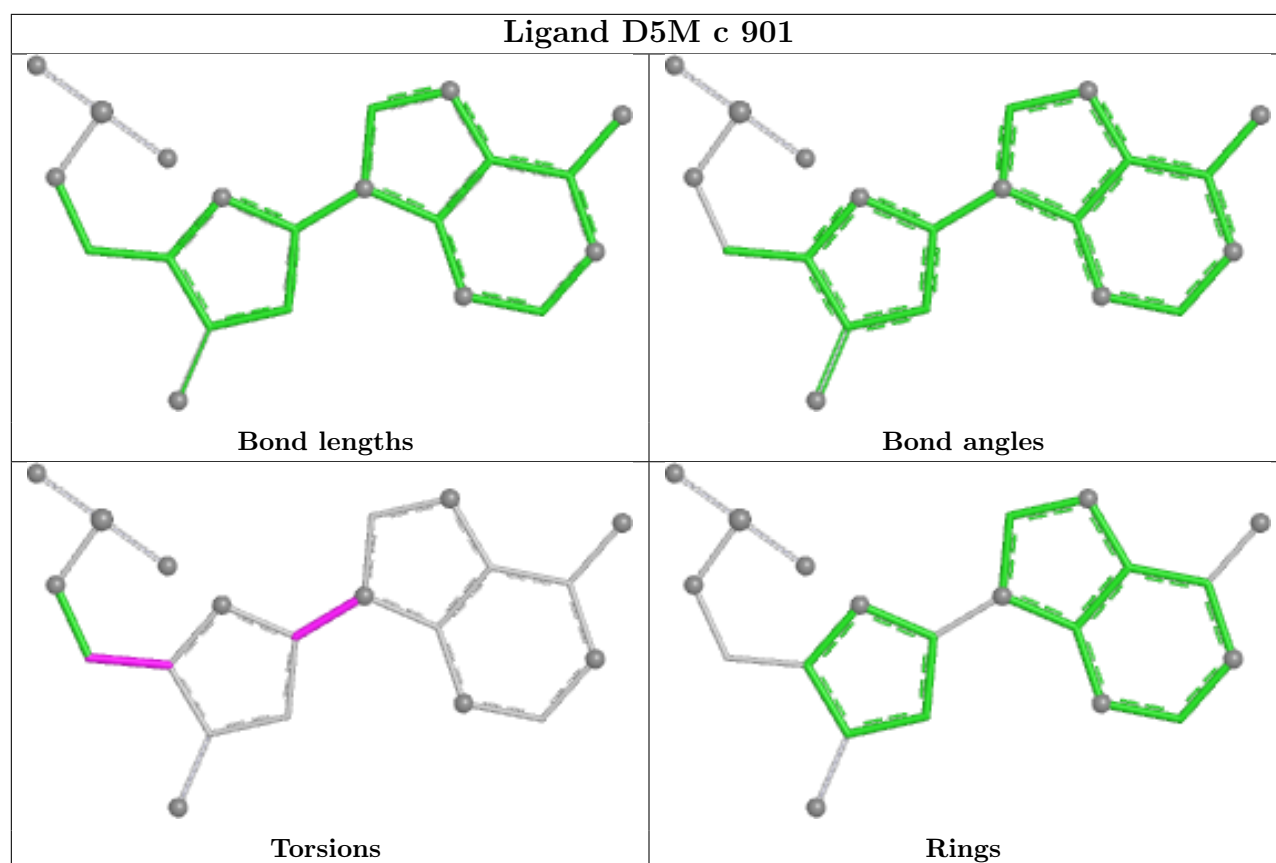




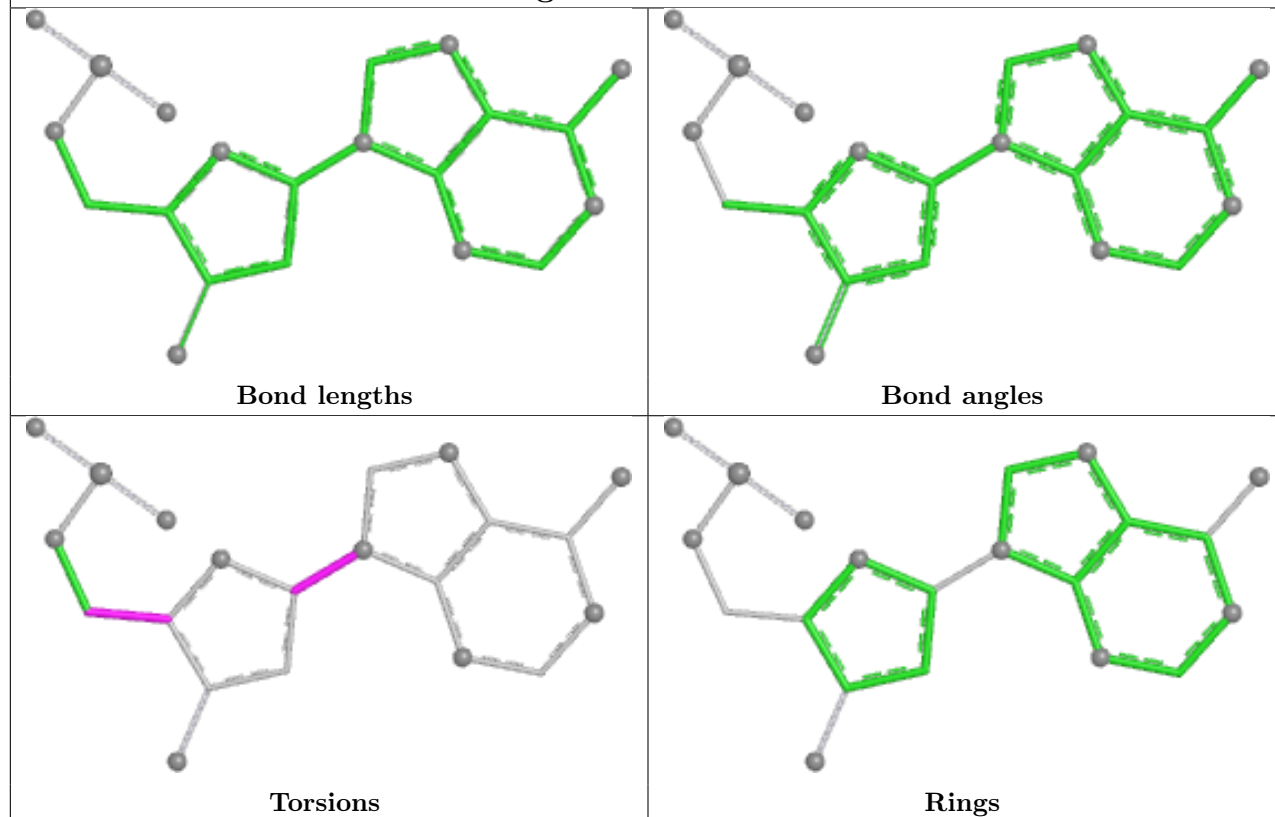




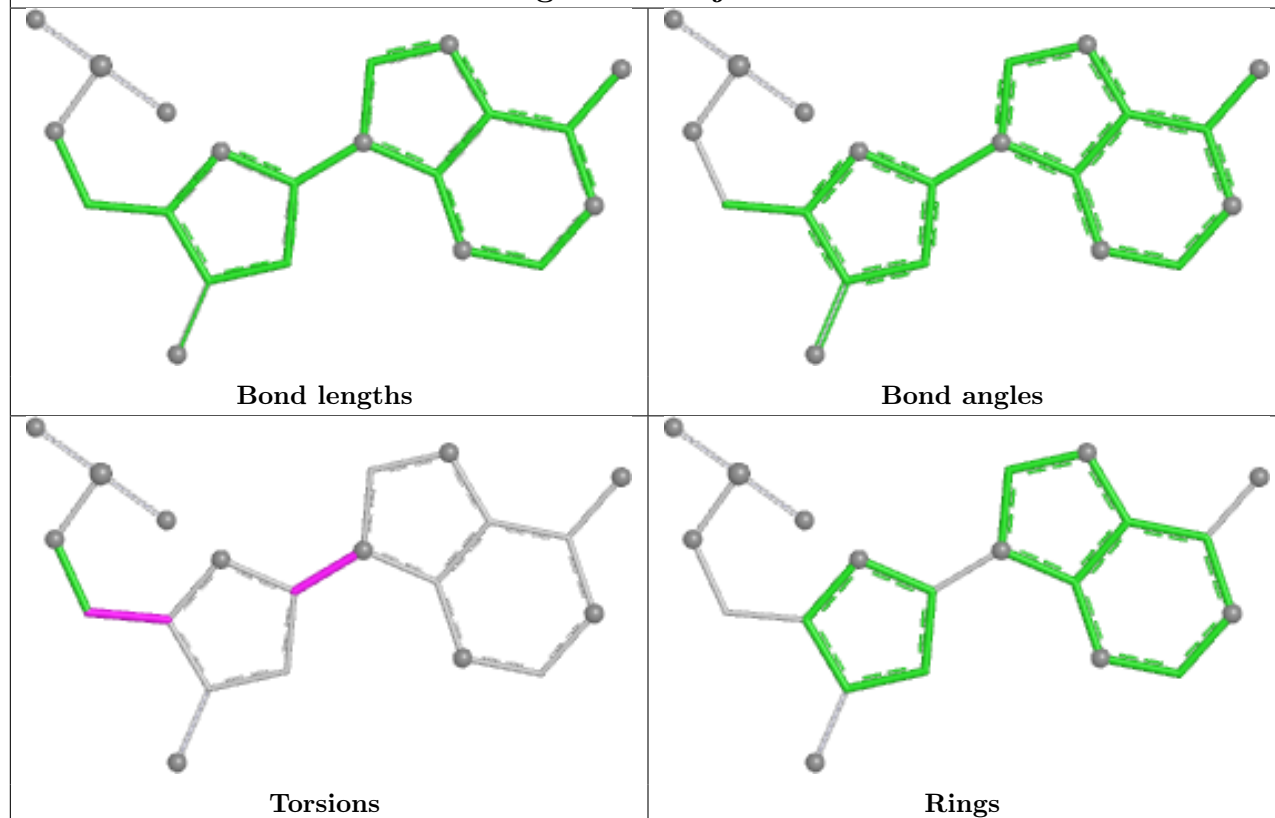


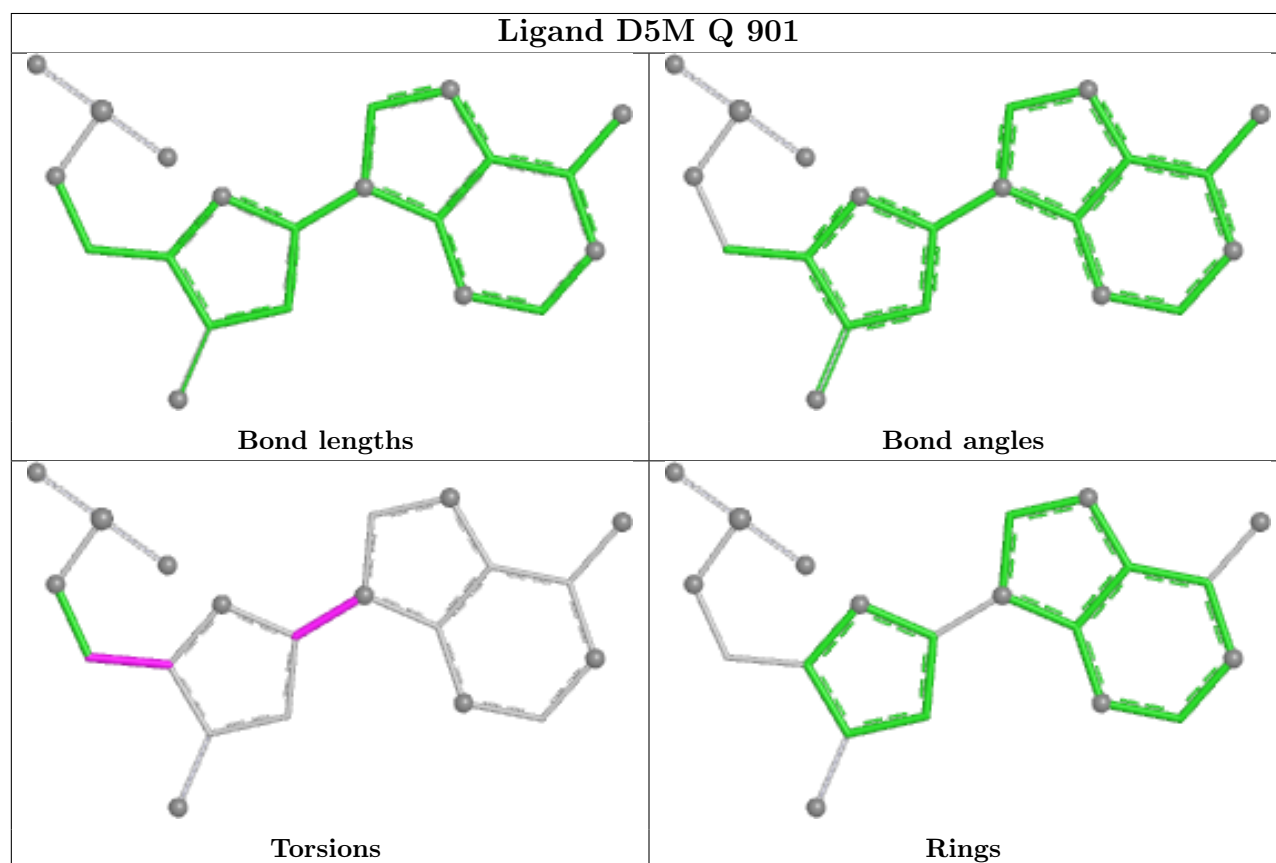
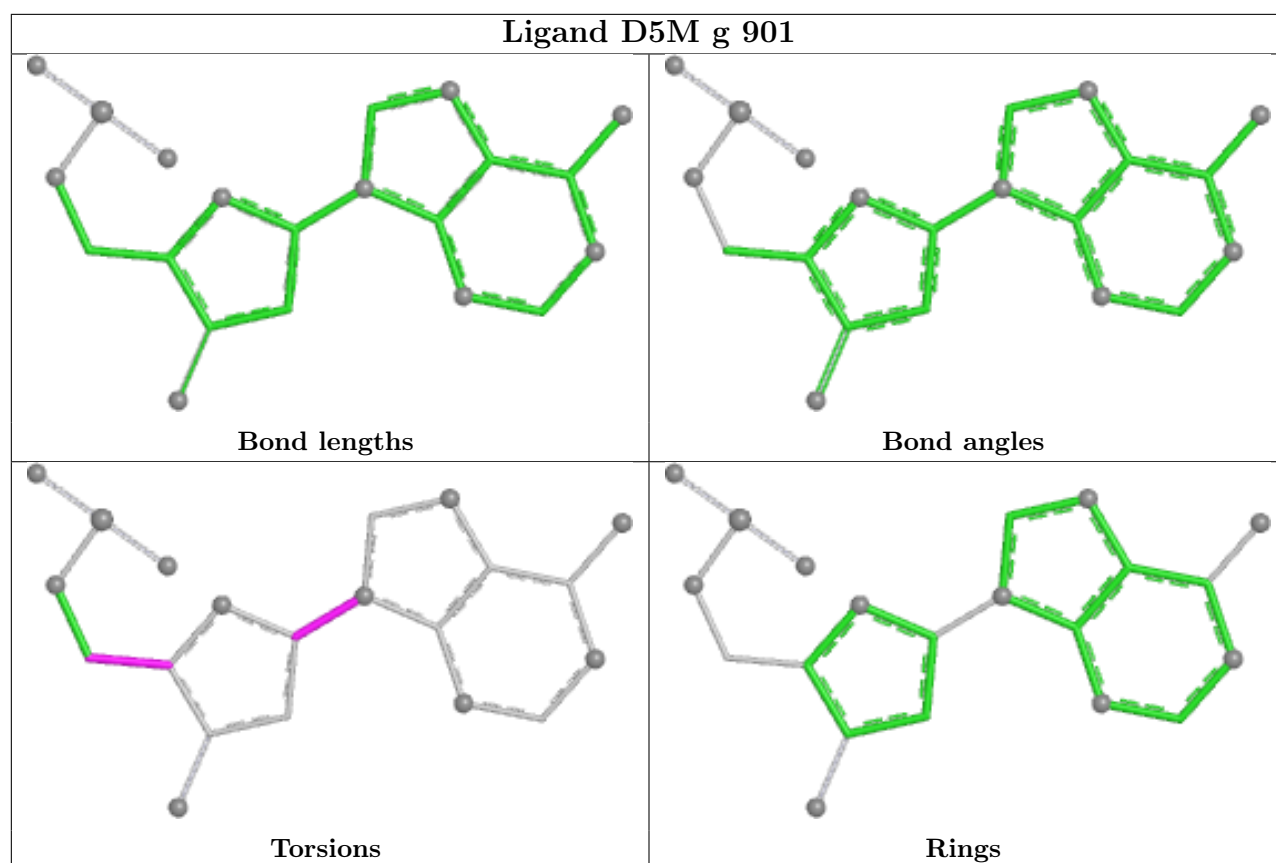


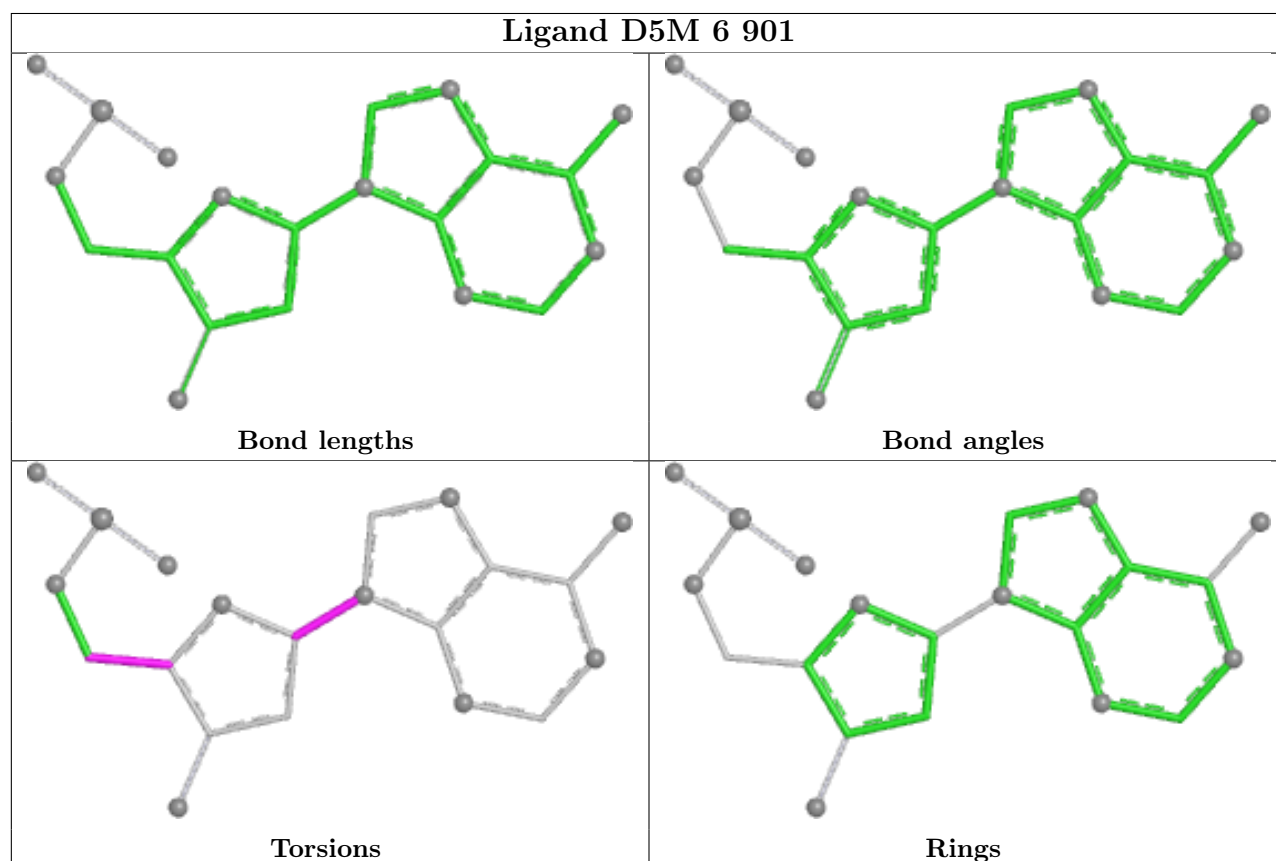
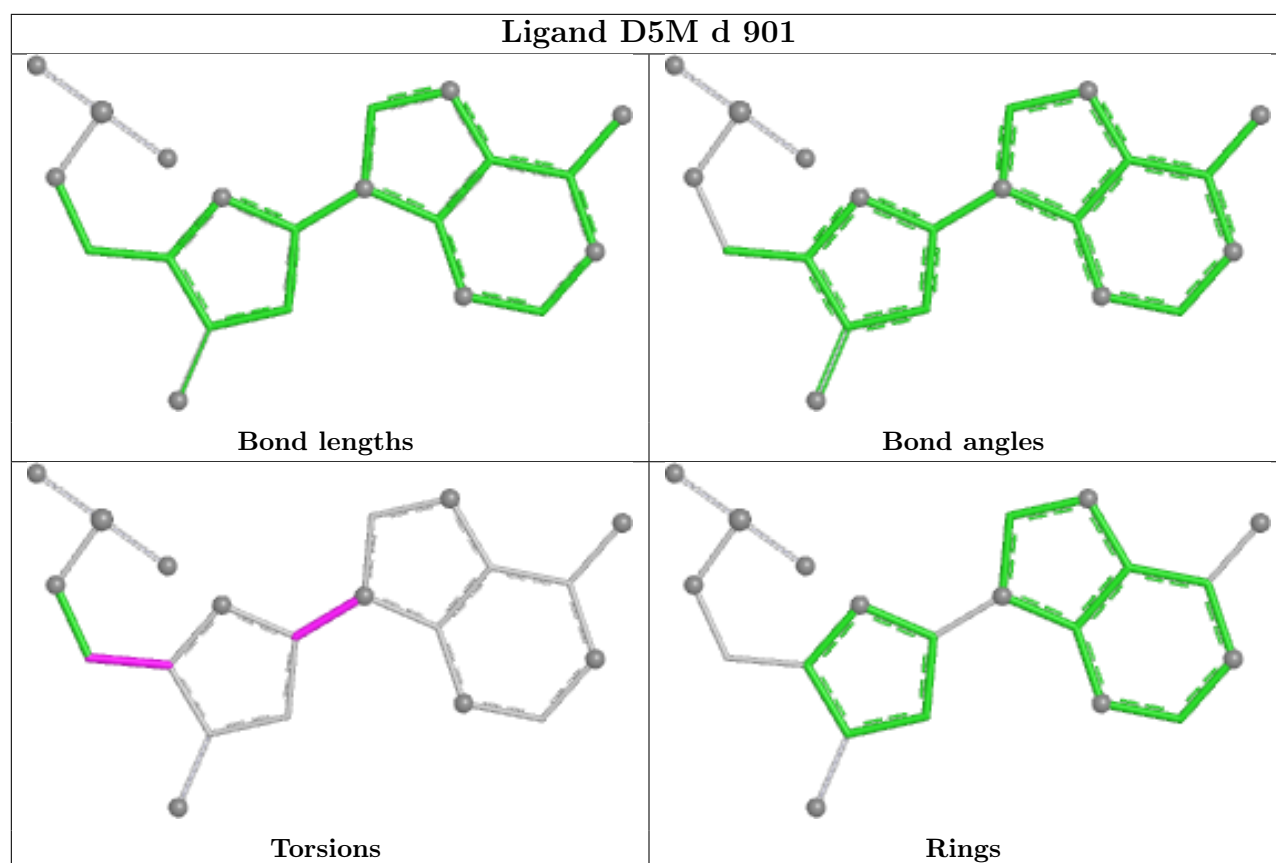
Ligand D5M 1 901

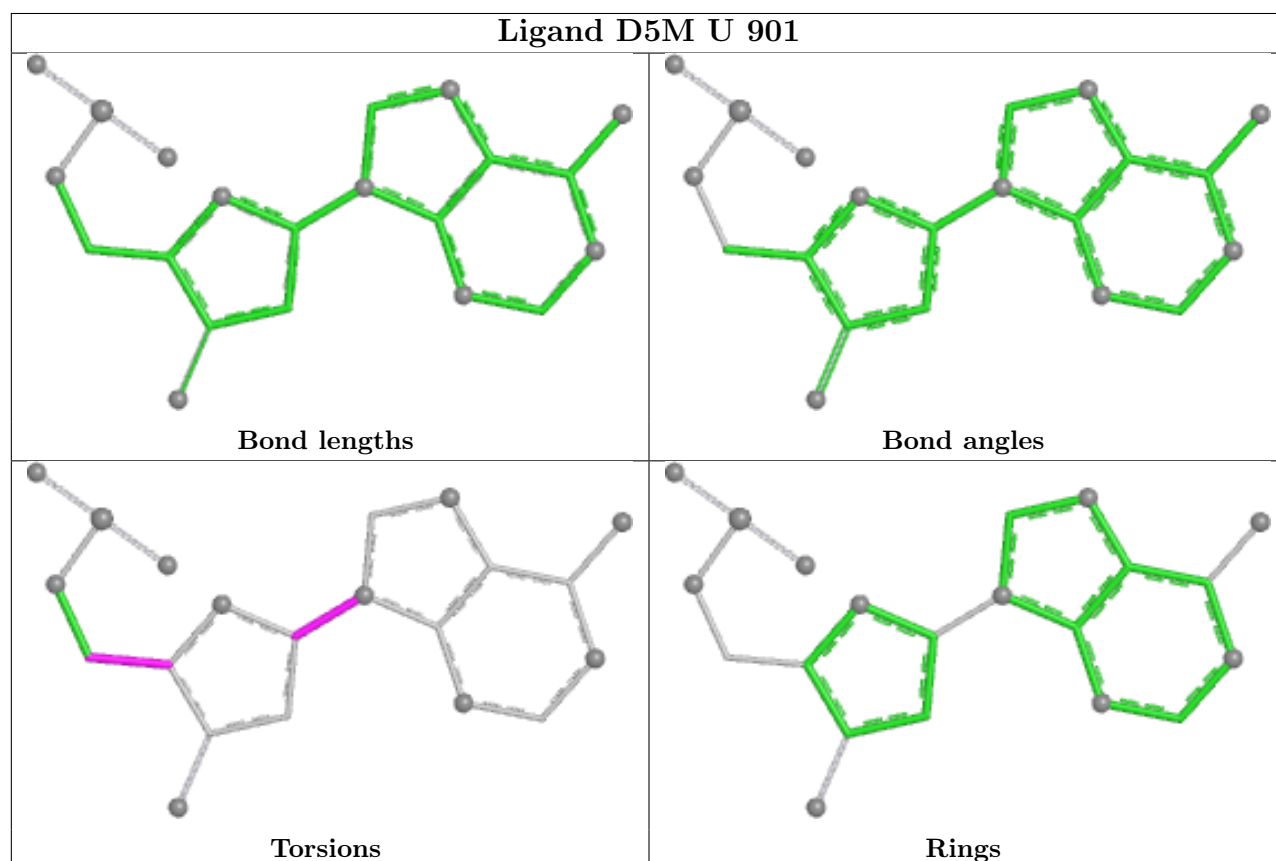
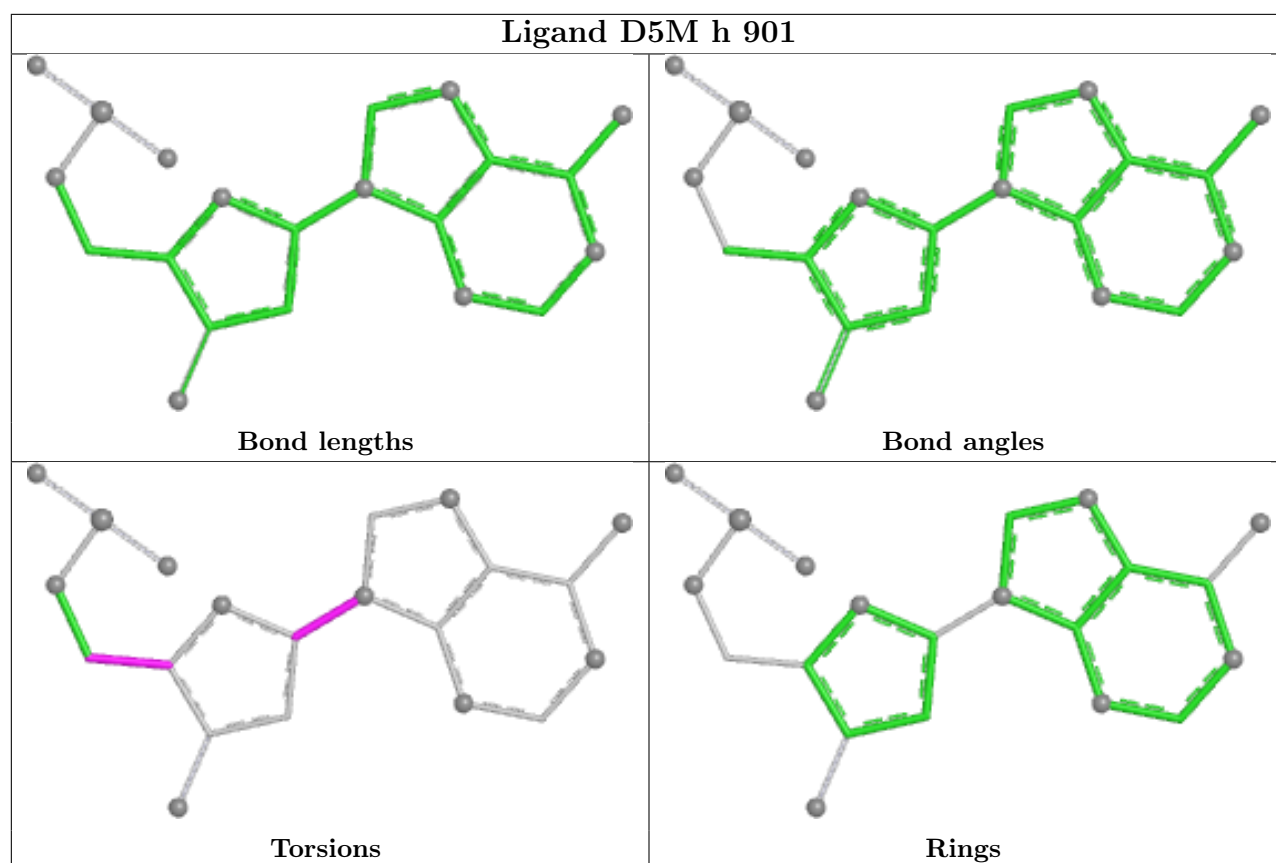


Ligand D5M j 901

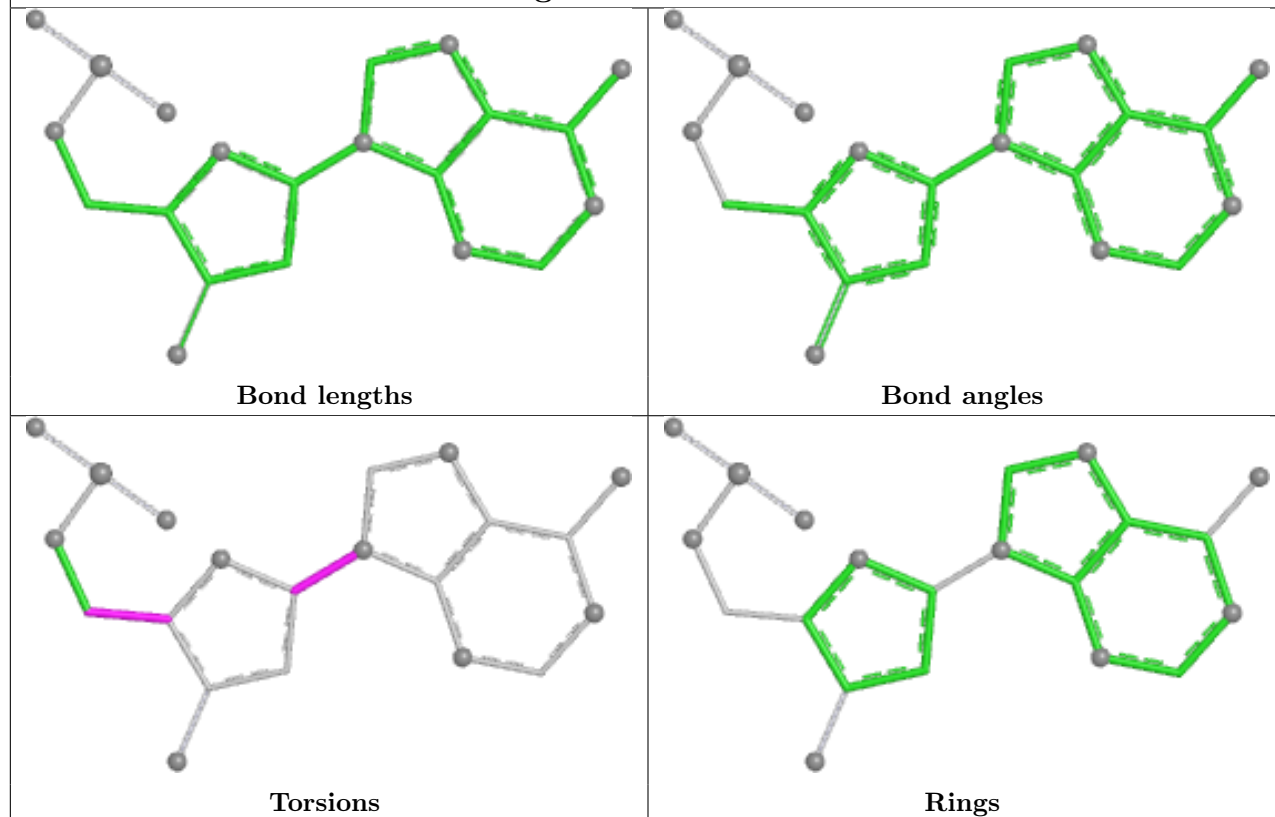




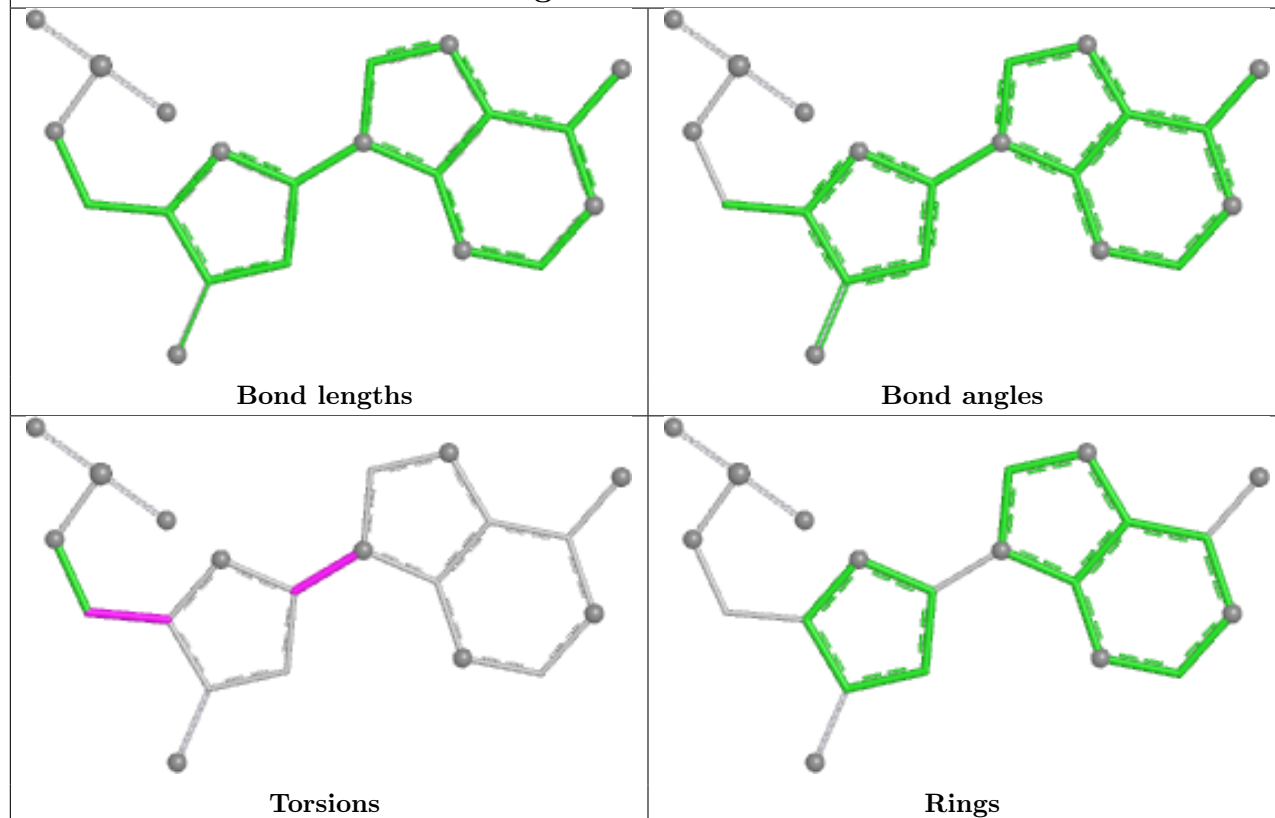


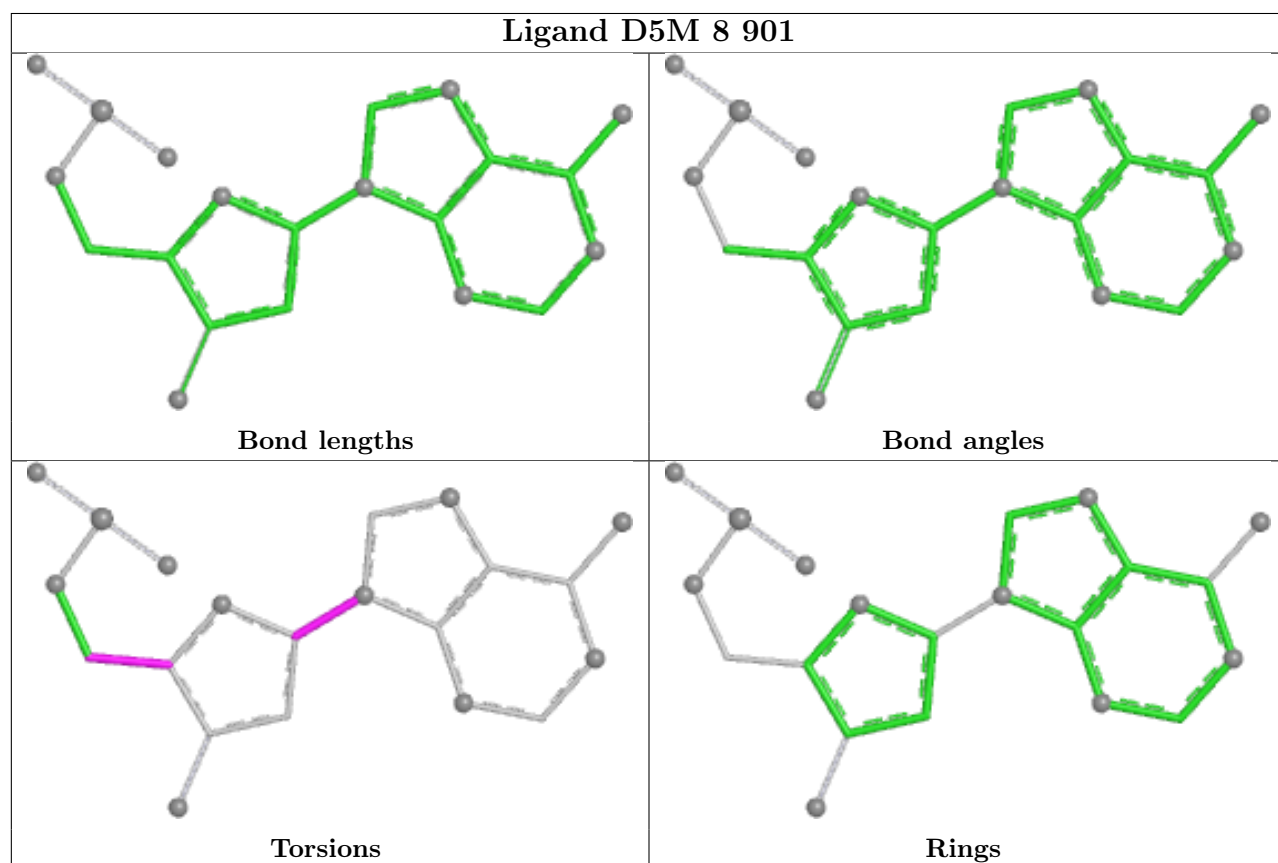
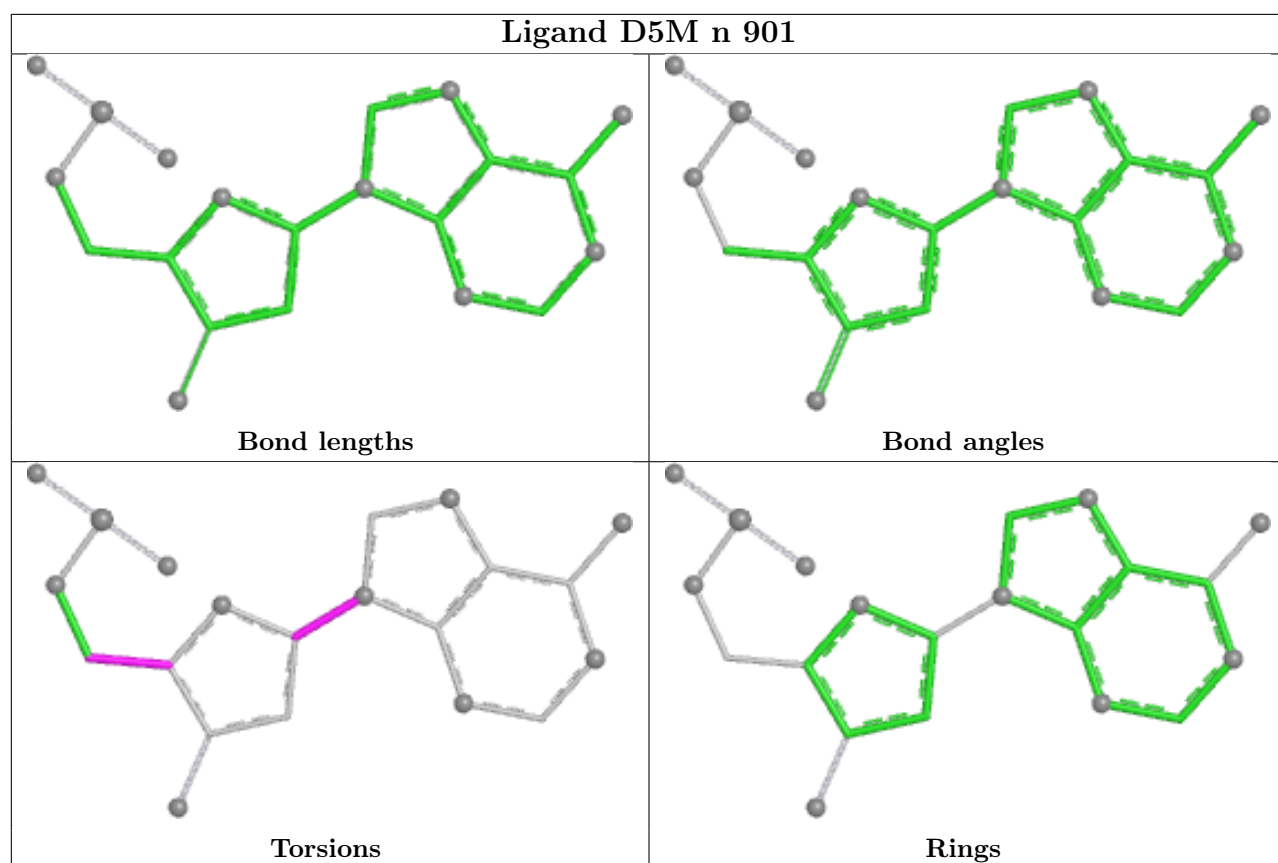


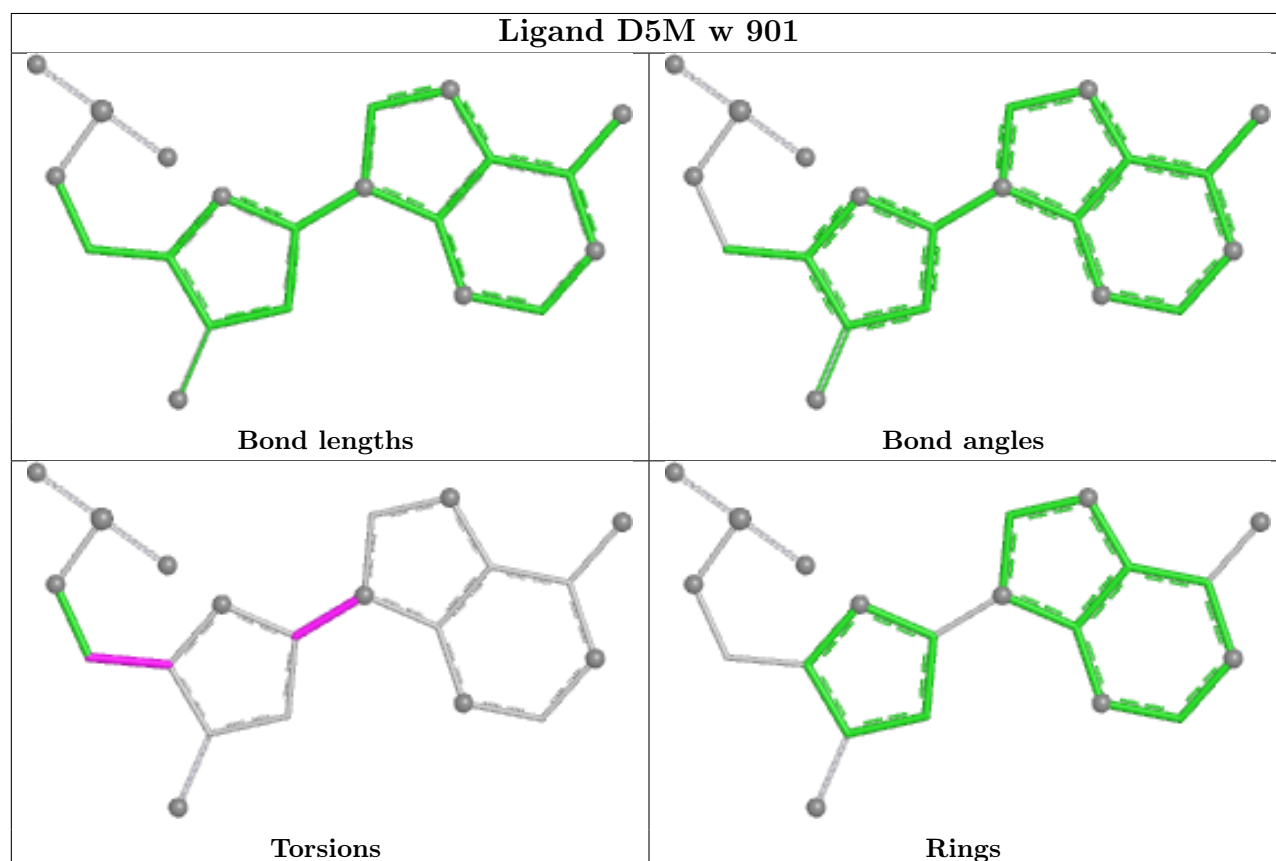
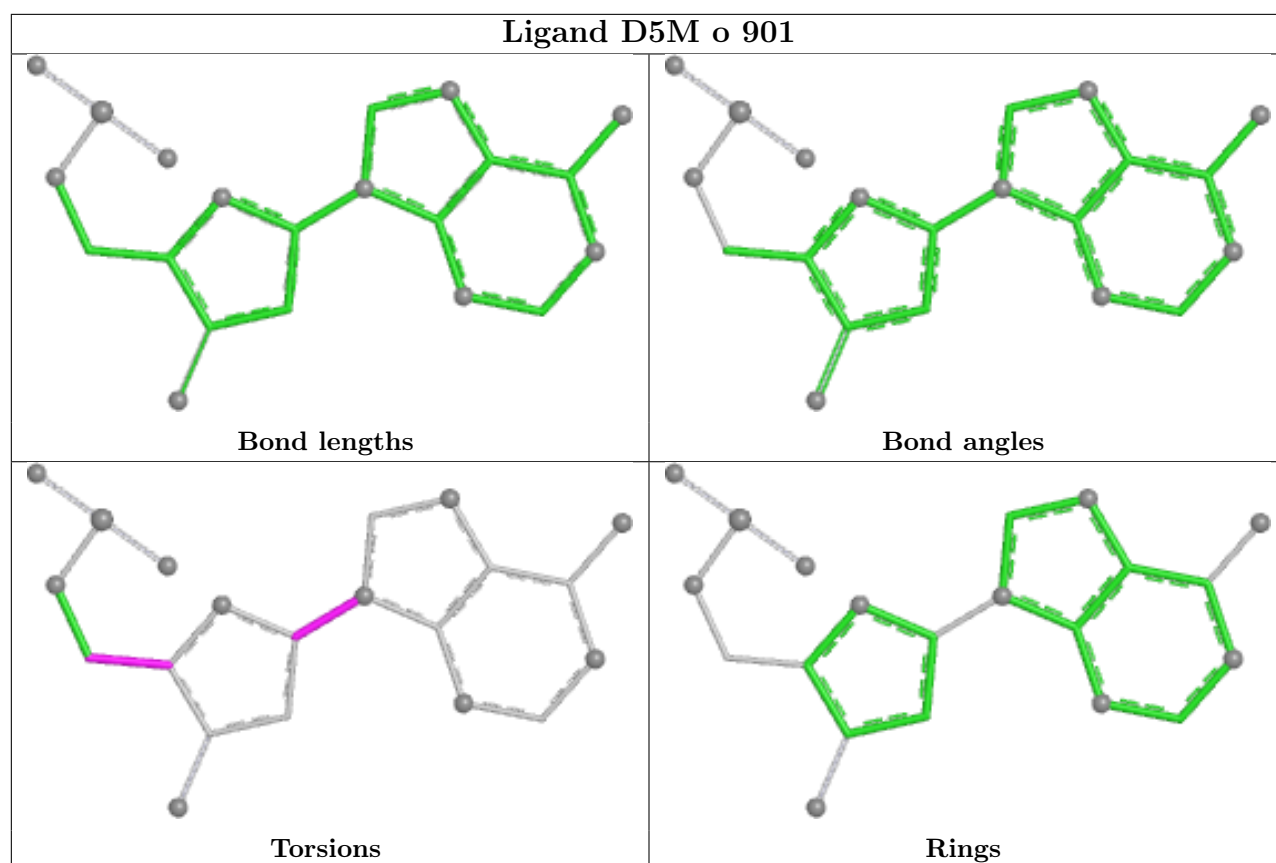
Ligand D5M s 901



Ligand D5M r 901







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.

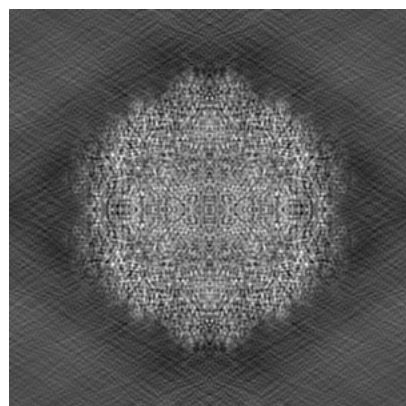
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29598. These allow visual inspection of the internal detail of the map and identification of artifacts.

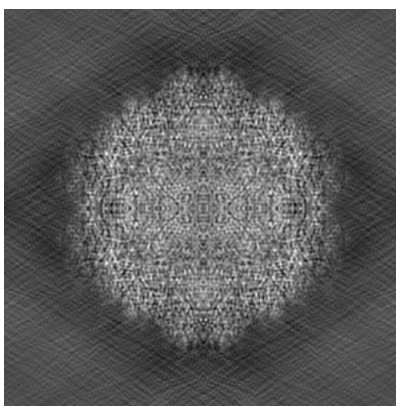
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

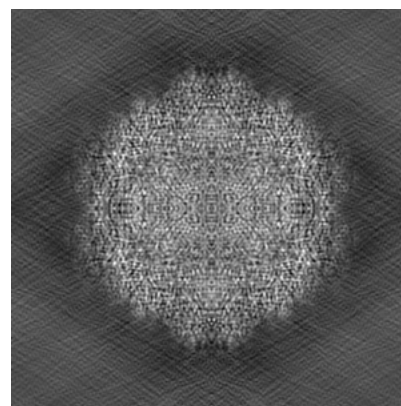
6.1.1 Primary map



X

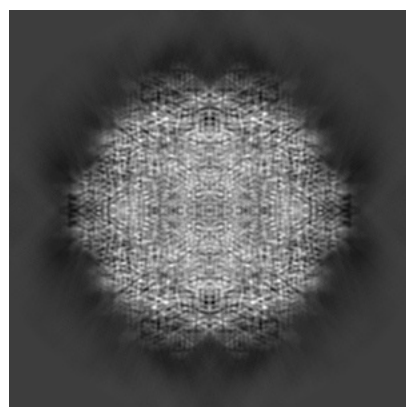


Y

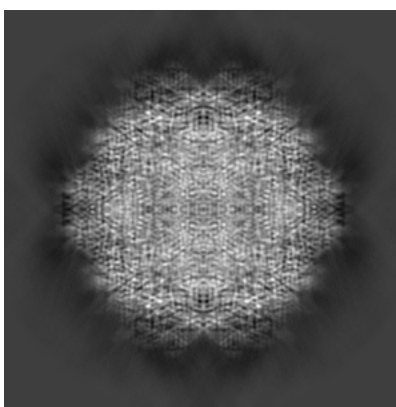


Z

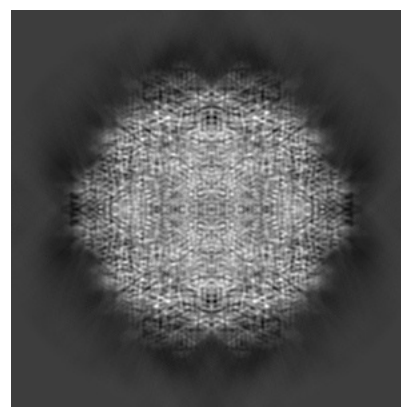
6.1.2 Raw map



X



Y

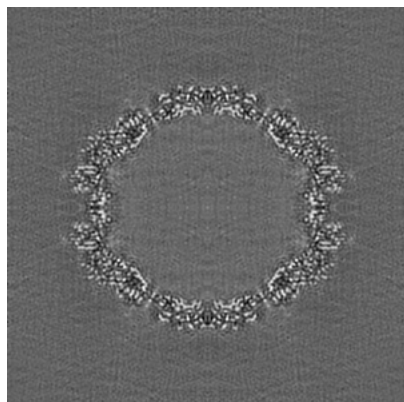


Z

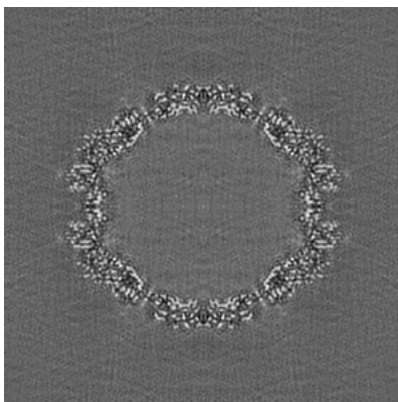
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

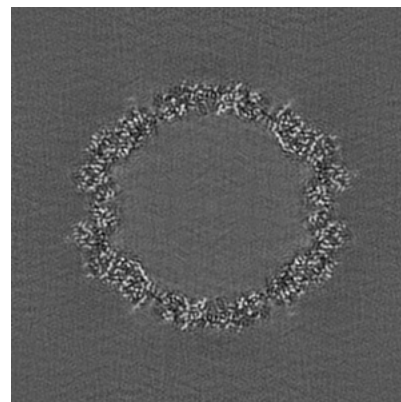
6.2.1 Primary map



X Index: 170

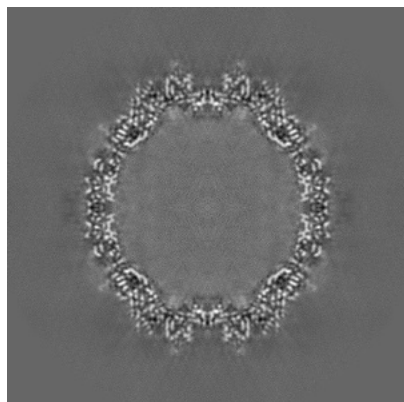


Y Index: 170

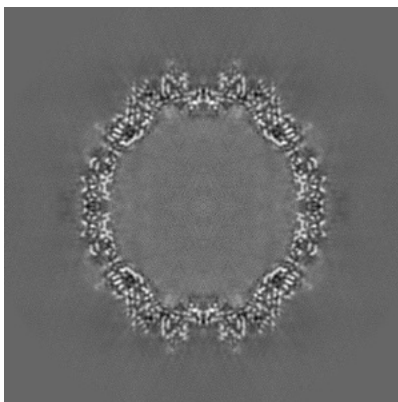


Z Index: 170

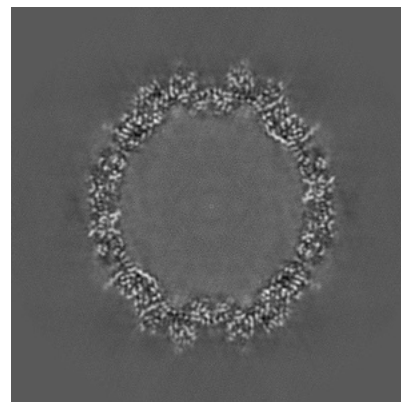
6.2.2 Raw map



X Index: 170



Y Index: 170

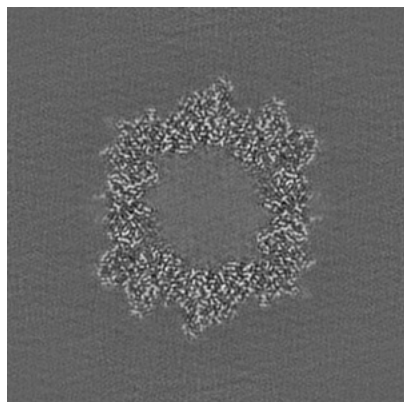


Z Index: 170

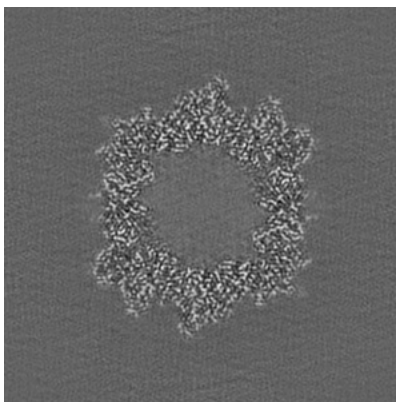
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

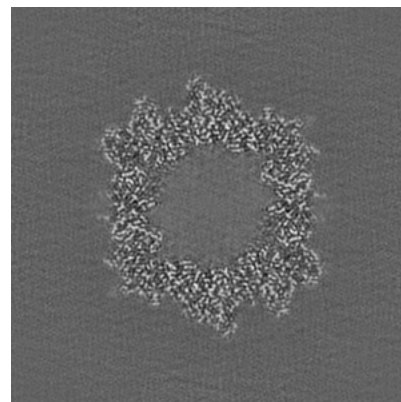
6.3.1 Primary map



X Index: 231

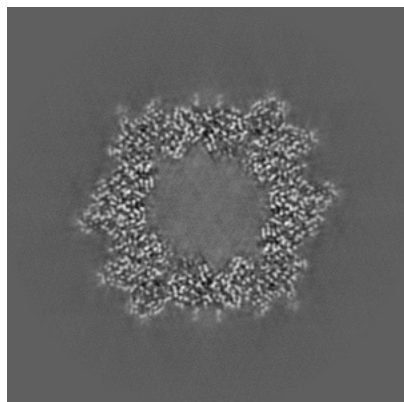


Y Index: 231

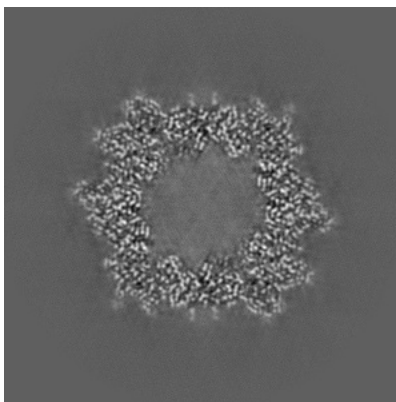


Z Index: 108

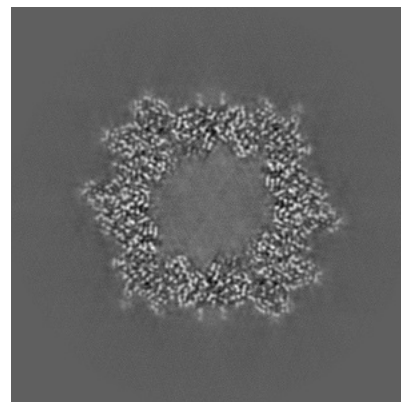
6.3.2 Raw map



X Index: 231



Y Index: 109

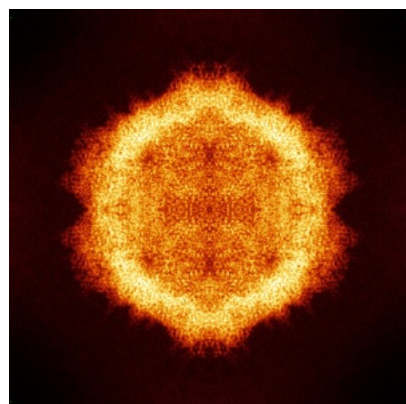


Z Index: 108

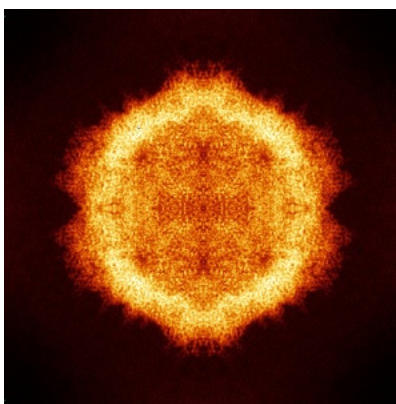
The images above show the largest variance slices of the map in three orthogonal directions.

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

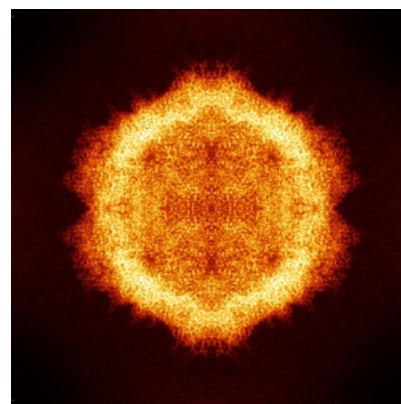
6.4.1 Primary map



X

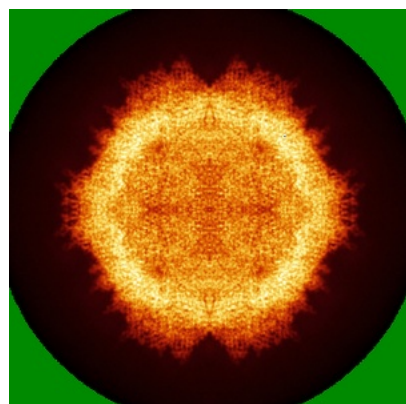


Y

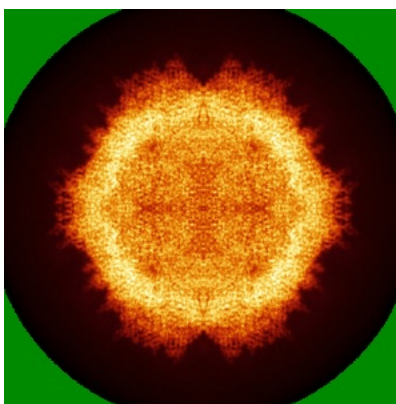


Z

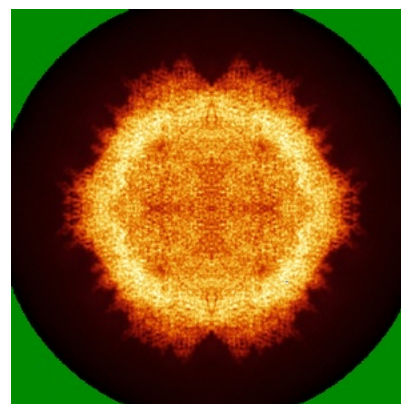
6.4.2 Raw map



X



Y

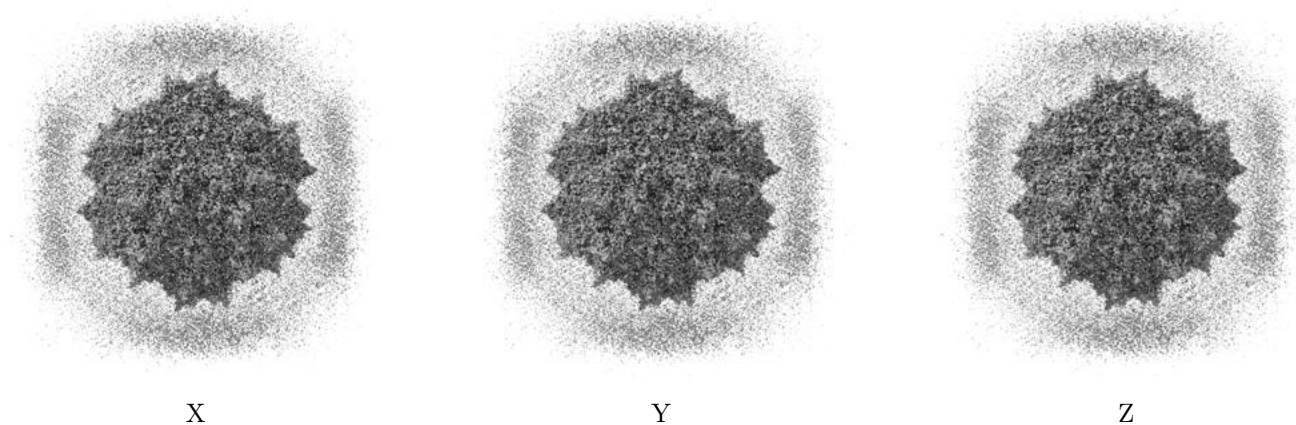


Z

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.

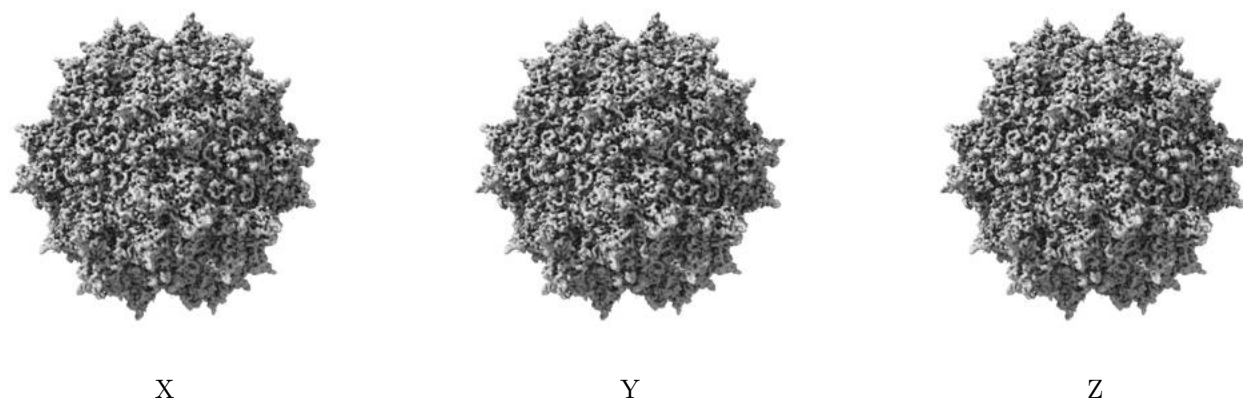
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

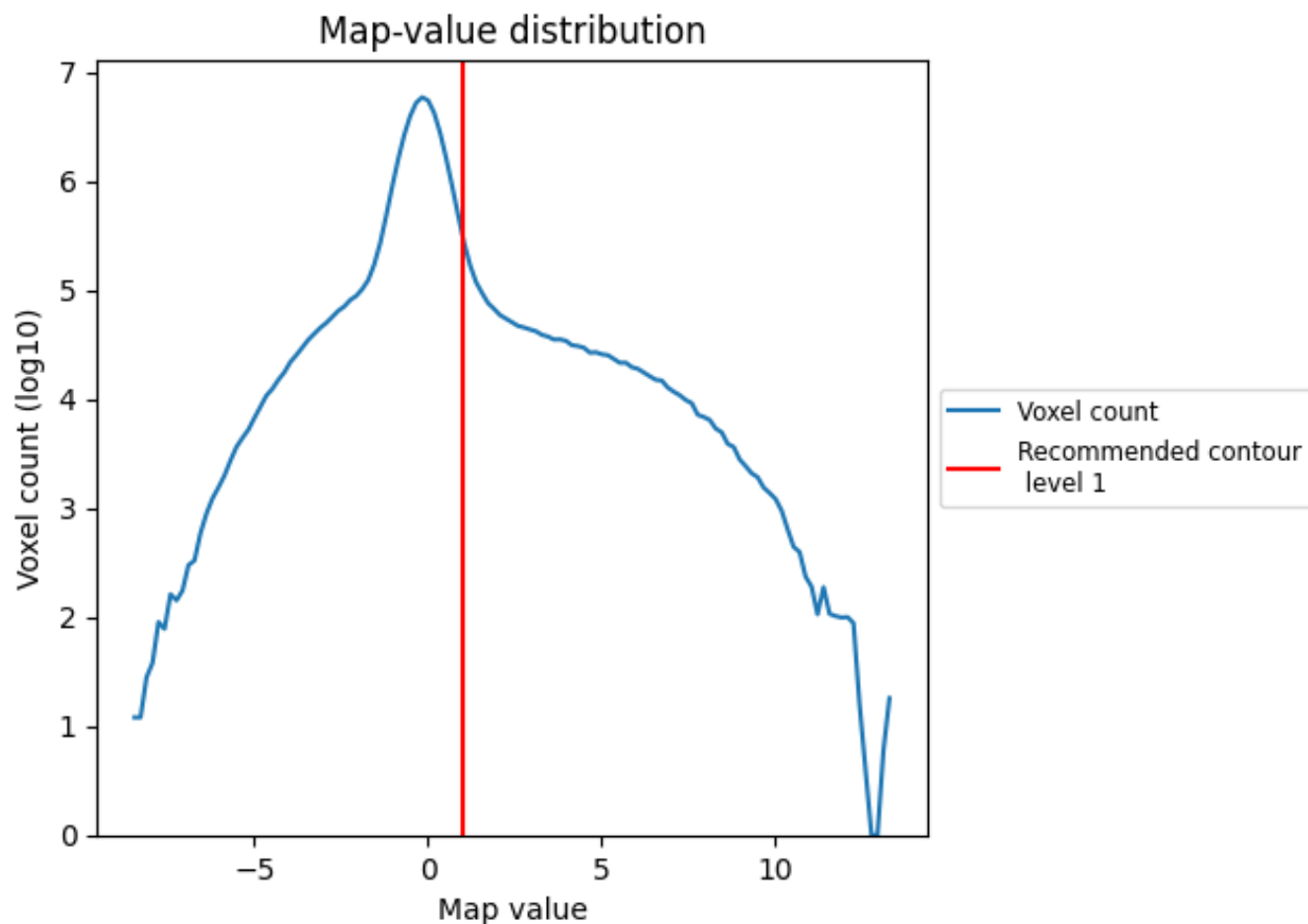
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

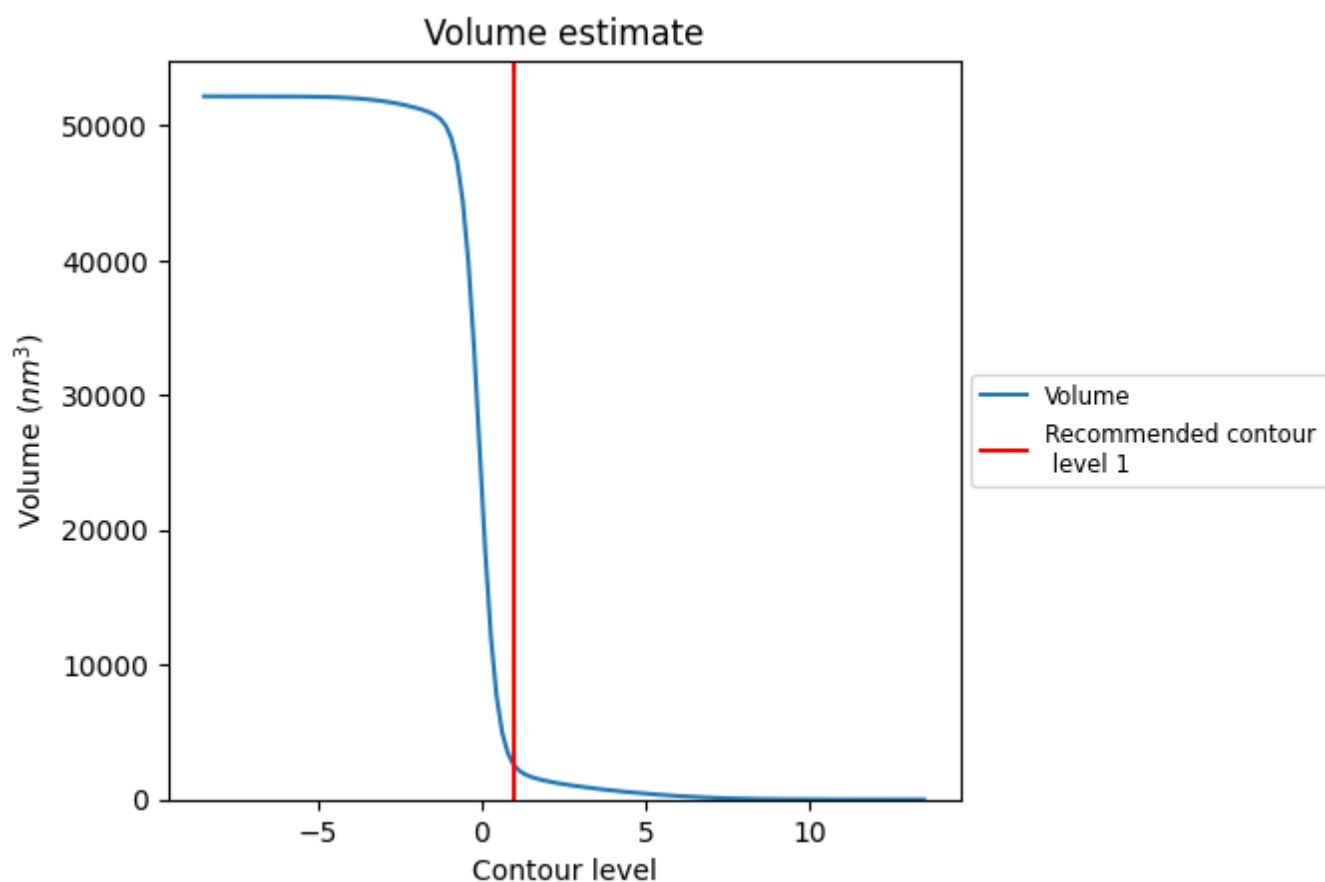
This section contains the results of statistical analysis of the map.

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.

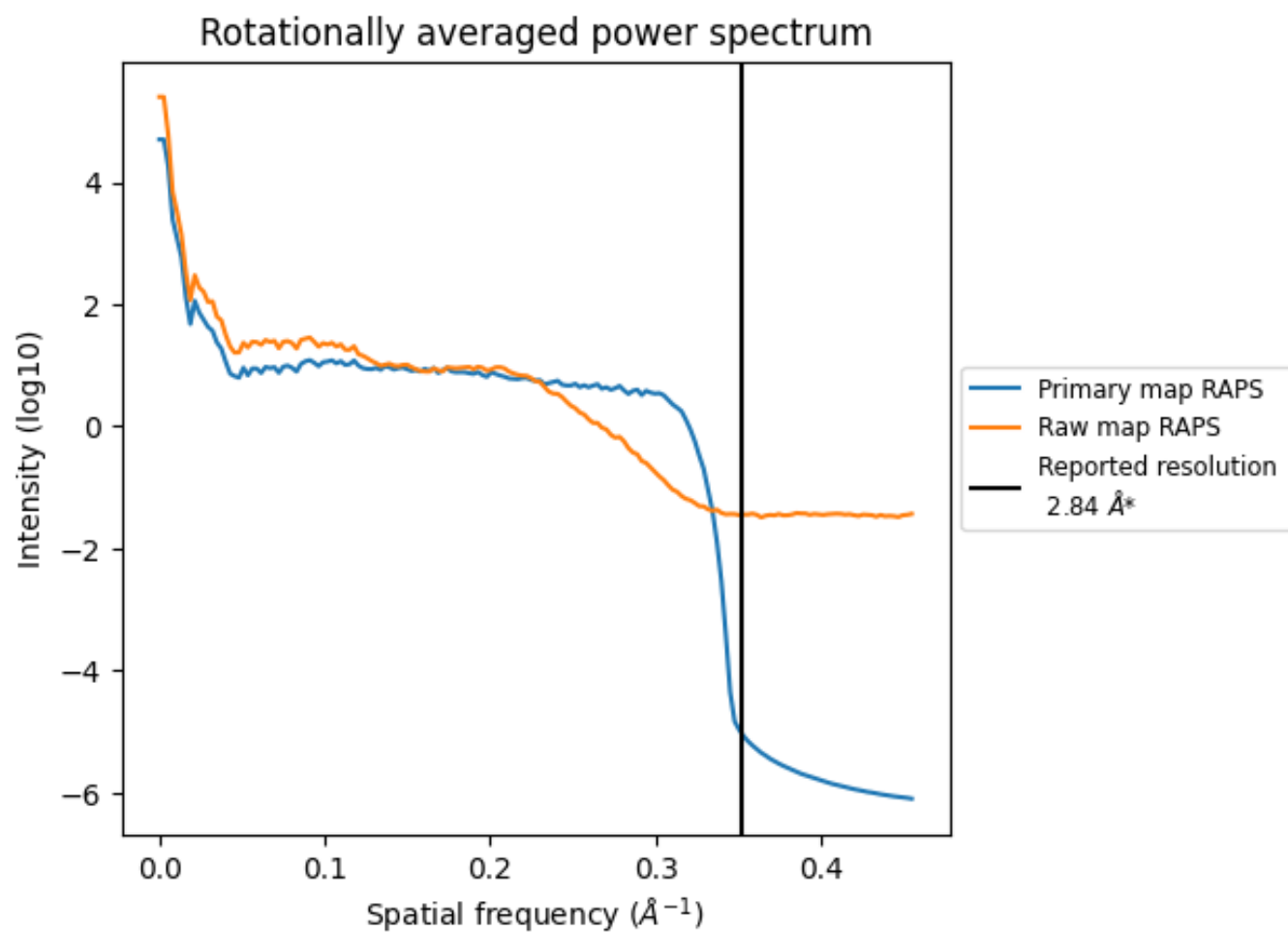
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2536 nm³; this corresponds to an approximate mass of 2291 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 ⓘ

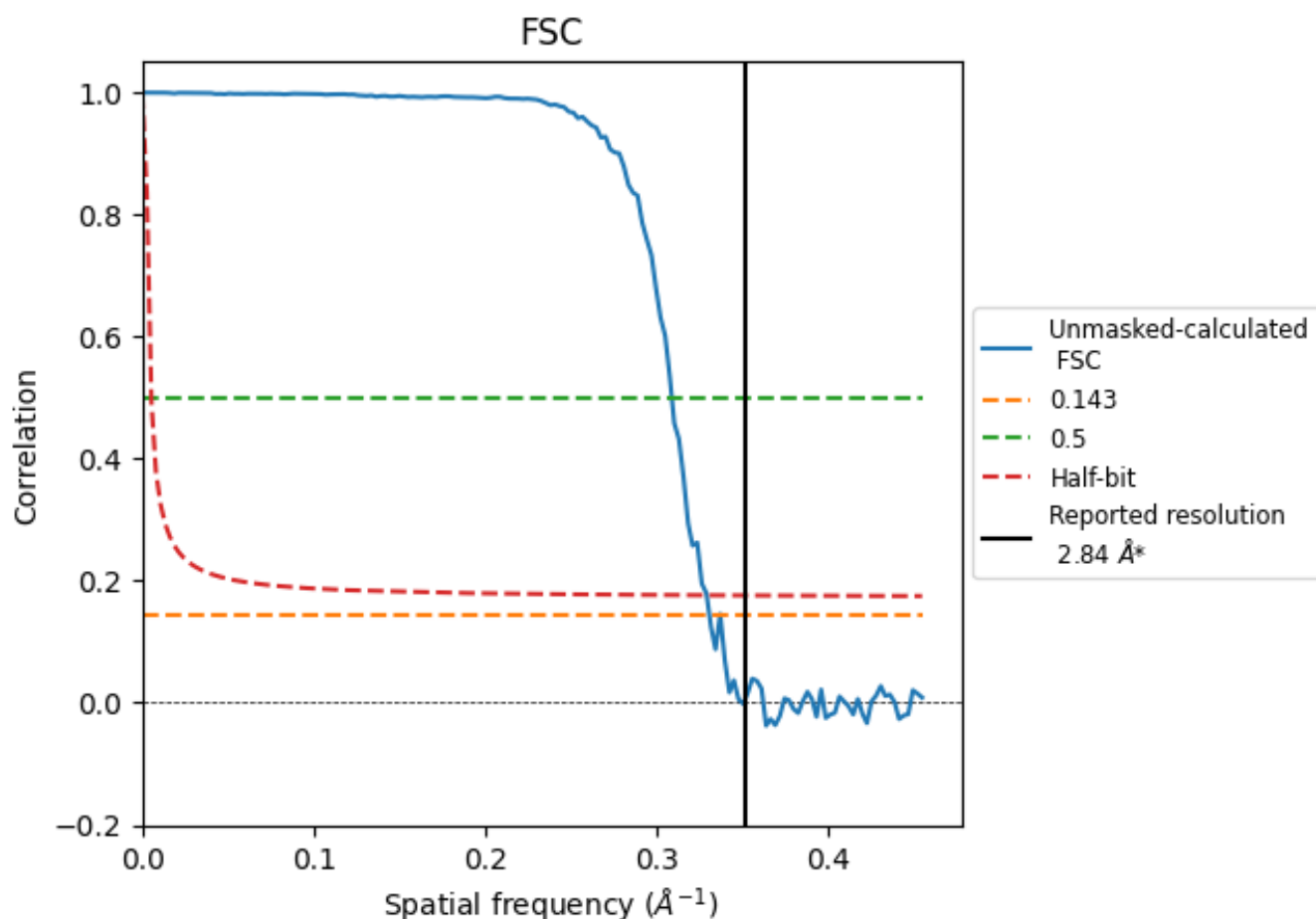


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

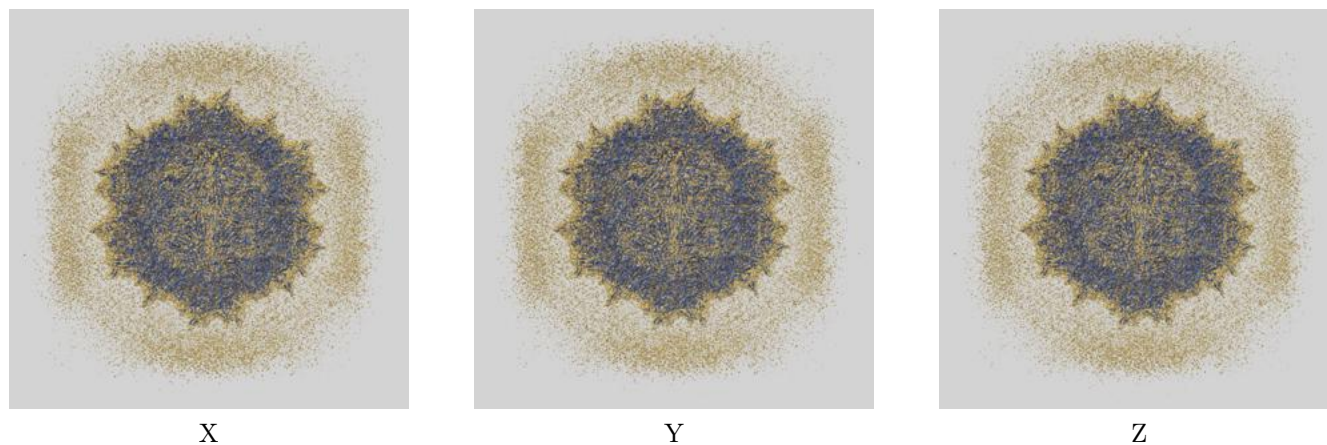
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.24	3.04

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

9 Map-model fit [i](#)

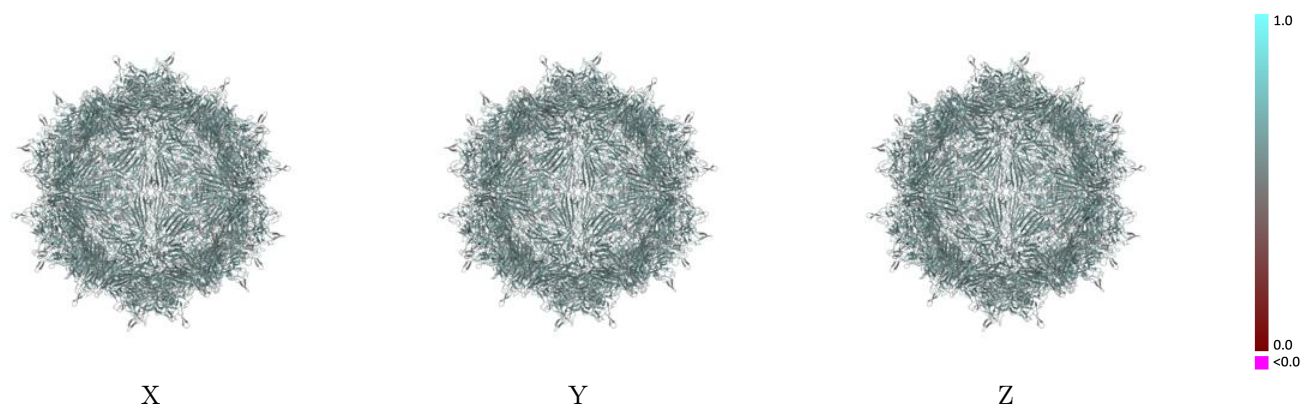
This section contains information regarding the fit between EMDB map EMD-29598 and PDB model 8FYW. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



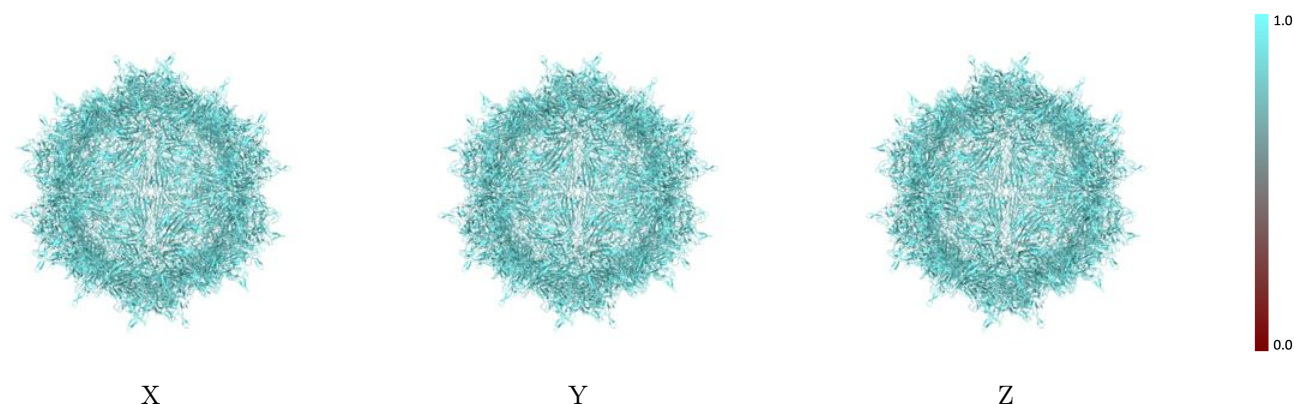
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



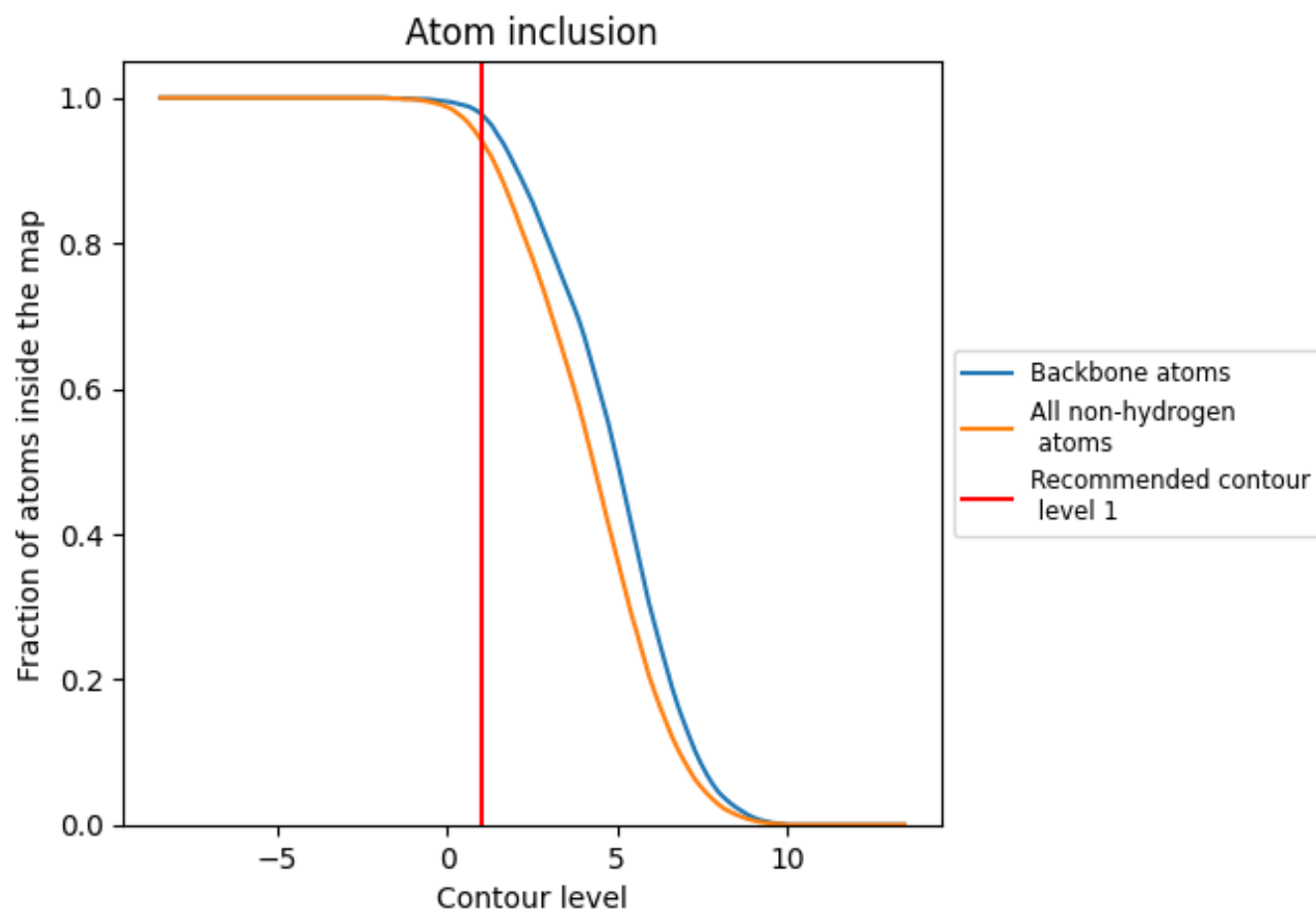
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.5750
1	0.9420	0.5730
2	0.9430	0.5750
3	0.9430	0.5760
4	0.9410	0.5740
5	0.9420	0.5750
6	0.9420	0.5760
7	0.9420	0.5750
8	0.9410	0.5730
A	0.9430	0.5760
B	0.9430	0.5750
C	0.9410	0.5760
D	0.9420	0.5760
E	0.9420	0.5750
F	0.9430	0.5760
G	0.9420	0.5750
H	0.9420	0.5760
I	0.9400	0.5750
J	0.9430	0.5740
K	0.9400	0.5750
L	0.9420	0.5740
M	0.9410	0.5750
N	0.9410	0.5760
O	0.9410	0.5750
P	0.9420	0.5760
Q	0.9400	0.5750
R	0.9430	0.5740
S	0.9430	0.5740
T	0.9400	0.5750
U	0.9420	0.5740
V	0.9410	0.5760
W	0.9420	0.5760
X	0.9410	0.5740
Y	0.9410	0.5750
Z	0.9410	0.5750

1.0

0.0

<0.0

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9440	 0.5760
b	 0.9430	 0.5750
c	 0.9430	 0.5770
d	 0.9440	 0.5760
e	 0.9430	 0.5750
f	 0.9420	 0.5770
g	 0.9400	 0.5750
h	 0.9410	 0.5740
i	 0.9420	 0.5770
j	 0.9420	 0.5740
k	 0.9420	 0.5750
l	 0.9410	 0.5740
m	 0.9410	 0.5740
n	 0.9430	 0.5750
o	 0.9410	 0.5750
p	 0.9400	 0.5740
q	 0.9420	 0.5740
r	 0.9430	 0.5740
s	 0.9430	 0.5750
t	 0.9410	 0.5750
u	 0.9410	 0.5750
v	 0.9440	 0.5740
w	 0.9410	 0.5740
x	 0.9410	 0.5750
y	 0.9440	 0.5760
z	 0.9420	 0.5740