



Full wwPDB EM Validation Report ⓘ

Nov 1, 2023 – 04:53 PM EDT

PDB ID : 8TEY
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 Full wwPDB EM Validation 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



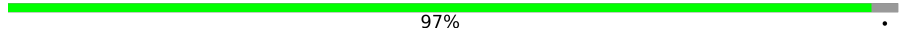
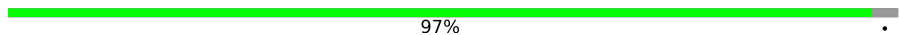
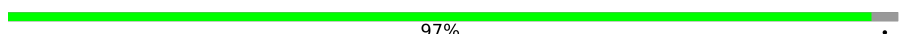
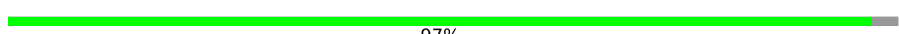


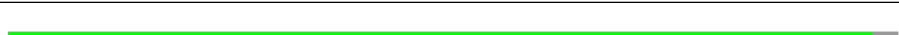
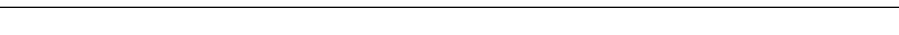
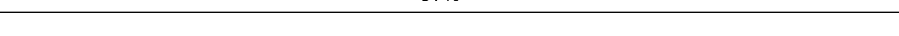
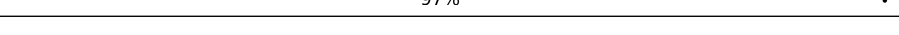
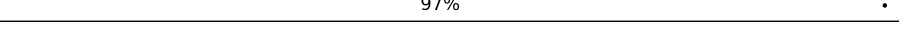
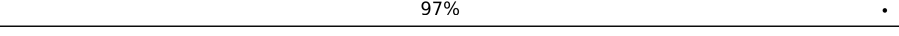
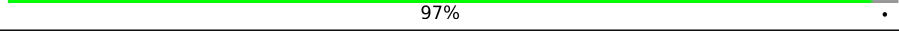
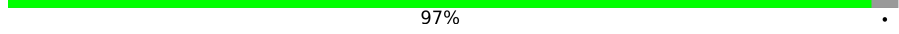
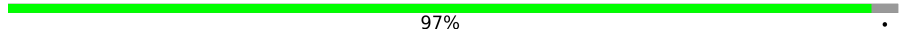
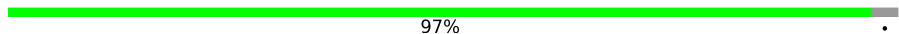
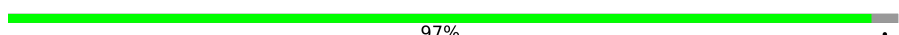
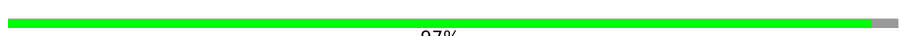





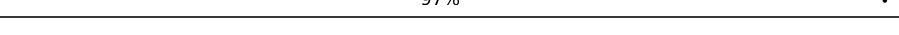
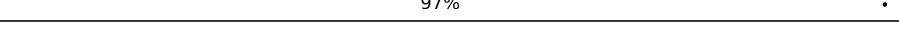
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	97% .
1	2	535	97% .
1	3	535	97% .
1	4	535	97% .
1	5	535	97% .
1	6	535	97% .
1	7	535	97% .
1	8	535	97% .
1	A	535	97% .

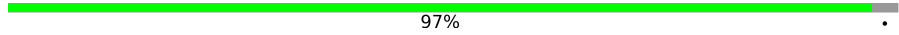
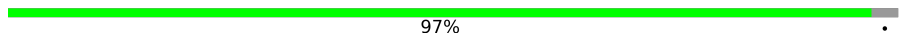
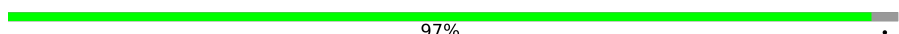
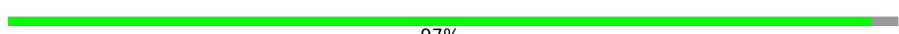


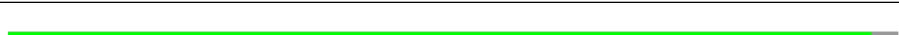
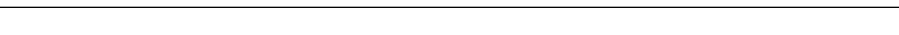
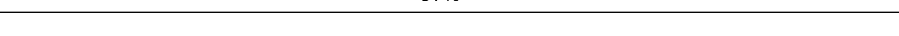
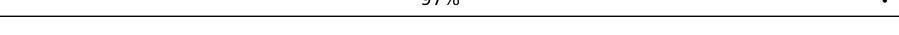
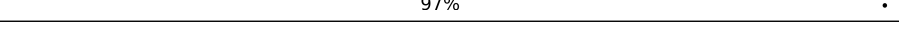
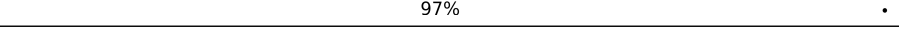

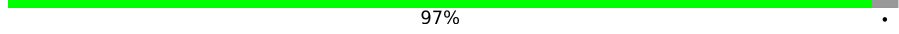
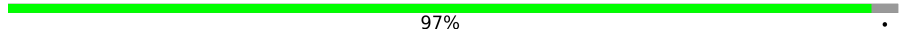
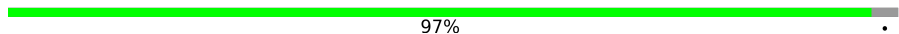
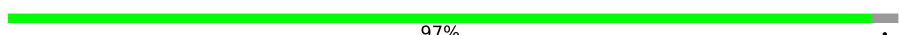
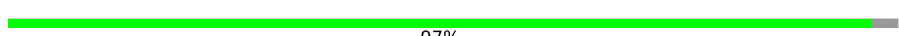





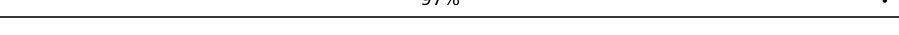
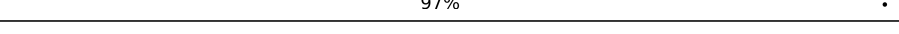
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Mol	Chain	Length	Quality of chain
1	B	535	 97%
1	C	535	 97%
1	D	535	 97%
1	E	535	 97%
1	F	535	 97%
1	G	535	 97%
1	H	535	 97%
1	I	535	 97%
1	J	535	 97%
1	K	535	 97%
1	L	535	 97%
1	M	535	 97%
1	N	535	 97%
1	O	535	 97%
1	P	535	 97%
1	Q	535	 97%
1	R	535	 97%
1	S	535	 97%
1	T	535	 97%
1	U	535	 97%
1	V	535	 97%
1	W	535	 97%
1	X	535	 97%
1	Y	535	 97%
1	Z	535	 97%

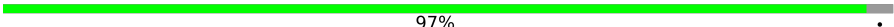
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Mol	Chain	Length	Quality of chain
1	a	535	 97%
1	b	535	 97%
1	c	535	 97%
1	d	535	 97%
1	e	535	 97%
1	f	535	 97%
1	g	535	 97%
1	h	535	 97%
1	i	535	 97%
1	j	535	 97%
1	k	535	 97%
1	l	535	 97%
1	m	535	 97%
1	n	535	 97%
1	o	535	 97%
1	p	535	 97%
1	q	535	 97%
1	r	535	 97%
1	s	535	 97%
1	t	535	 97%
1	u	535	 97%
1	v	535	 97%
1	w	535	 97%
1	x	535	 97%
1	y	535	 97%

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Mol	Chain	Length	Quality of chain
1	z	535	 97%

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
			Total	C	N	O	S		
1	A	519	4167	2642	725	786	14	0	0
1	B	519	4167	2642	725	786	14	0	0
1	C	519	4167	2642	725	786	14	0	0
1	D	519	4167	2642	725	786	14	0	0
1	E	519	4167	2642	725	786	14	0	0
1	F	519	4167	2642	725	786	14	0	0
1	G	519	4167	2642	725	786	14	0	0
1	H	519	4167	2642	725	786	14	0	0
1	I	519	4167	2642	725	786	14	0	0
1	J	519	4167	2642	725	786	14	0	0
1	K	519	4167	2642	725	786	14	0	0
1	L	519	4167	2642	725	786	14	0	0
1	M	519	4167	2642	725	786	14	0	0
1	N	519	4167	2642	725	786	14	0	0
1	O	519	4167	2642	725	786	14	0	0
1	P	519	4167	2642	725	786	14	0	0
1	Q	519	4167	2642	725	786	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	C	N	O	S	0	0
			4167	2642	725	786	14		
1	n	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	o	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	p	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	q	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	r	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	s	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	t	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	u	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	v	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	w	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	x	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	y	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	z	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	1	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	2	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	3	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	4	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	5	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	6	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		
1	7	519	Total	C	N	O	S	0	0
			4167	2642	725	786	14		

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

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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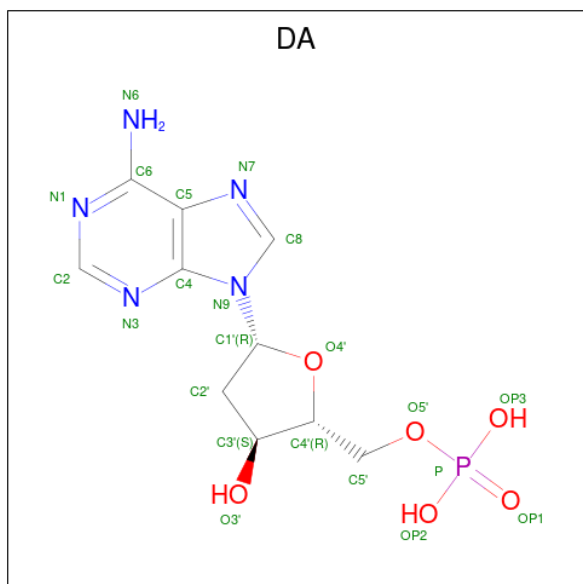
Chain	Residue	Modelled	Actual	Comment	Reference
z	626	TRP	LEU	conflict	UNP Q7TG43
z	644	GLY	ARG	conflict	UNP Q7TG43
1	334	SER	PHE	conflict	UNP Q7TG43
1	339	ALA	GLY	conflict	UNP Q7TG43
1	621	LEU	PRO	conflict	UNP Q7TG43
1	622	GLN	THR	conflict	UNP Q7TG43
1	624	PRO	THR	conflict	UNP Q7TG43
1	625	ILE	HIS	conflict	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 (three-letter code: DA) (formula: C₁₀H₁₄N₅O₆P) (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
			Total	C	N	O	P	
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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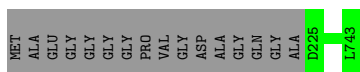
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	r	1	Total 21	C 10	N 5	O 5	P 1	0
2	s	1	Total 21	C 10	N 5	O 5	P 1	0
2	t	1	Total 21	C 10	N 5	O 5	P 1	0
2	u	1	Total 21	C 10	N 5	O 5	P 1	0
2	v	1	Total 21	C 10	N 5	O 5	P 1	0
2	w	1	Total 21	C 10	N 5	O 5	P 1	0
2	x	1	Total 21	C 10	N 5	O 5	P 1	0
2	y	1	Total 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.

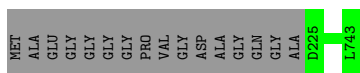
- Molecule 1: Capsid protein

Chain A:  97%



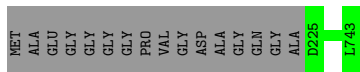
- Molecule 1: Capsid protein

Chain B:  97%



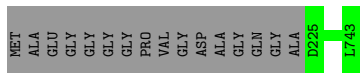
- Molecule 1: Capsid protein

Chain C:  97%



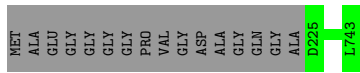
- Molecule 1: Capsid protein

Chain D:  97%



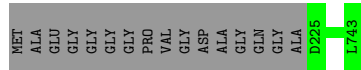
- Molecule 1: Capsid protein

Chain E:  97%



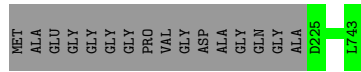
- Molecule 1: Capsid protein

Chain F:  97%



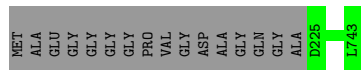
● Molecule 1: Capsid protein

Chain G:  97%



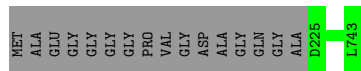
● Molecule 1: Capsid protein

Chain H:  97%



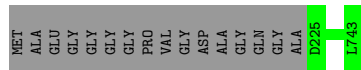
● Molecule 1: Capsid protein

Chain I:  97%



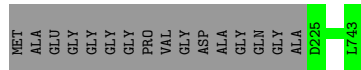
● Molecule 1: Capsid protein

Chain J:  97%



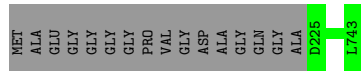
● Molecule 1: Capsid protein

Chain K:  97%



● Molecule 1: Capsid protein

Chain L:  97%



● Molecule 1: Capsid protein

Chain M:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain N:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain O:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain P:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain Q:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain R:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

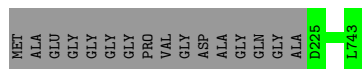
● Molecule 1: Capsid protein

Chain S:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY ALA ALA D225 L743

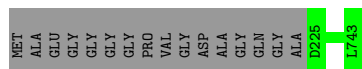
● Molecule 1: Capsid protein

Chain T:  97%



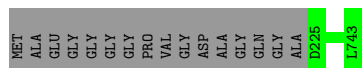
● Molecule 1: Capsid protein

Chain U:  97%



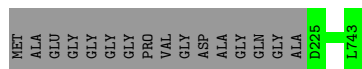
● Molecule 1: Capsid protein

Chain V:  97%



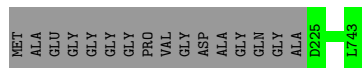
● Molecule 1: Capsid protein

Chain W:  97%



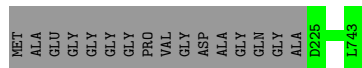
● Molecule 1: Capsid protein

Chain X:  97%



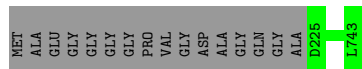
● Molecule 1: Capsid protein

Chain Y:  97%



● Molecule 1: Capsid protein

Chain Z:  97%



● Molecule 1: Capsid protein

Chain a:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain b:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain c:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain d:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain e:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain f:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

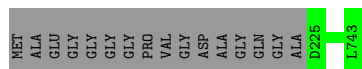
● Molecule 1: Capsid protein

Chain g:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLN GLY GLY ALA ALA D225 L743

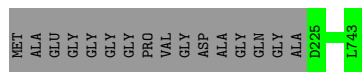
● Molecule 1: Capsid protein

Chain h:  97%



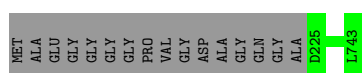
● Molecule 1: Capsid protein

Chain i:  97%



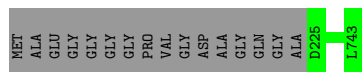
● Molecule 1: Capsid protein

Chain j:  97%



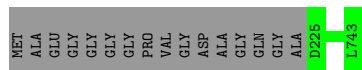
● Molecule 1: Capsid protein

Chain k:  97%



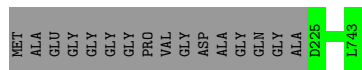
● Molecule 1: Capsid protein

Chain l:  97%



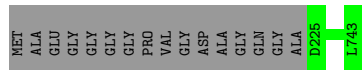
● Molecule 1: Capsid protein

Chain m:  97%



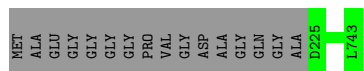
● Molecule 1: Capsid protein

Chain n:  97%



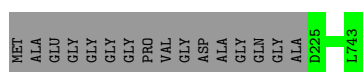
● Molecule 1: Capsid protein

Chain o:  97%



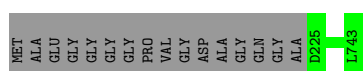
● Molecule 1: Capsid protein

Chain p:  97%



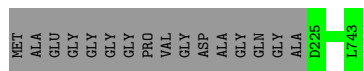
● Molecule 1: Capsid protein

Chain q:  97%



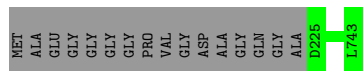
● Molecule 1: Capsid protein

Chain r:  97%



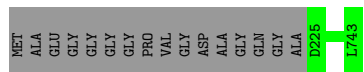
● Molecule 1: Capsid protein

Chain s:  97%



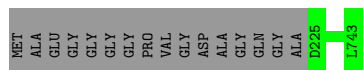
● Molecule 1: Capsid protein

Chain t:  97%



● Molecule 1: Capsid protein

Chain u:  97%



● Molecule 1: Capsid protein

Chain v:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain w:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain x:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain y:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain z:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 1:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 2:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 3:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 4:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 5:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 6:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 7:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

● Molecule 1: Capsid protein

Chain 8:  97%

MET ALA ALA GLU GLY GLY GLY GLY PRO VAL VAL GLY GLY ASP ASP ALA ALA GLY GLN GLY GLY ALA ALA D225 L743

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	2.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/4297	0.53	0/5867
1	2	0.49	0/4297	0.53	0/5867
1	3	0.49	0/4297	0.53	0/5867
1	4	0.49	0/4297	0.53	0/5867
1	5	0.49	0/4297	0.53	0/5867
1	6	0.49	0/4297	0.53	0/5867
1	7	0.49	0/4297	0.53	0/5867
1	8	0.49	0/4297	0.53	0/5867
1	A	0.49	0/4297	0.53	0/5867
1	B	0.49	0/4297	0.53	0/5867
1	C	0.49	0/4297	0.53	0/5867
1	D	0.49	0/4297	0.53	0/5867
1	E	0.49	0/4297	0.53	0/5867
1	F	0.49	0/4297	0.53	0/5867
1	G	0.49	0/4297	0.53	0/5867
1	H	0.49	0/4297	0.53	0/5867
1	I	0.49	0/4297	0.53	0/5867
1	J	0.49	0/4297	0.53	0/5867
1	K	0.49	0/4297	0.53	0/5867
1	L	0.49	0/4297	0.53	0/5867
1	M	0.49	0/4297	0.53	0/5867
1	N	0.49	0/4297	0.53	0/5867
1	O	0.49	0/4297	0.53	0/5867
1	P	0.49	0/4297	0.53	0/5867
1	Q	0.49	0/4297	0.53	0/5867
1	R	0.49	0/4297	0.53	0/5867
1	S	0.49	0/4297	0.53	0/5867
1	T	0.49	0/4297	0.53	0/5867
1	U	0.49	0/4297	0.53	0/5867
1	V	0.49	0/4297	0.53	0/5867
1	W	0.49	0/4297	0.53	0/5867
1	X	0.49	0/4297	0.53	0/5867
1	Y	0.49	0/4297	0.53	0/5867
1	Z	0.49	0/4297	0.53	0/5867

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.49	0/4297	0.53	0/5867
1	b	0.49	0/4297	0.53	0/5867
1	c	0.49	0/4297	0.53	0/5867
1	d	0.49	0/4297	0.53	0/5867
1	e	0.49	0/4297	0.53	0/5867
1	f	0.49	0/4297	0.53	0/5867
1	g	0.49	0/4297	0.53	0/5867
1	h	0.49	0/4297	0.53	0/5867
1	i	0.49	0/4297	0.53	0/5867
1	j	0.49	0/4297	0.53	0/5867
1	k	0.49	0/4297	0.53	0/5867
1	l	0.49	0/4297	0.53	0/5867
1	m	0.49	0/4297	0.53	0/5867
1	n	0.49	0/4297	0.53	0/5867
1	o	0.49	0/4297	0.53	0/5867
1	p	0.49	0/4297	0.53	0/5867
1	q	0.49	0/4297	0.53	0/5867
1	r	0.49	0/4297	0.53	0/5867
1	s	0.49	0/4297	0.53	0/5867
1	t	0.49	0/4297	0.53	0/5867
1	u	0.49	0/4297	0.53	0/5867
1	v	0.49	0/4297	0.53	0/5867
1	w	0.49	0/4297	0.53	0/5867
1	x	0.49	0/4297	0.53	0/5867
1	y	0.49	0/4297	0.53	0/5867
1	z	0.49	0/4297	0.53	0/5867
All	All	0.49	0/257820	0.53	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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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. All (754) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	276	ASN
1	A	307	ASN
1	A	323	ASN
1	A	413	ASN
1	A	433	ASN
1	A	434	GLN
1	A	502	ASN
1	A	521	ASN
1	A	543	GLN
1	A	592	GLN
1	A	615	GLN
1	A	653	GLN
1	B	274	ASN
1	B	276	ASN
1	B	323	ASN
1	B	413	ASN
1	B	433	ASN
1	B	434	GLN

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Mol	Chain	Res	Type
1	B	502	ASN
1	B	521	ASN
1	B	543	GLN
1	B	592	GLN
1	B	615	GLN
1	B	653	GLN
1	C	274	ASN
1	C	276	ASN
1	C	323	ASN
1	C	413	ASN
1	C	427	HIS
1	C	433	ASN
1	C	434	GLN
1	C	502	ASN
1	C	521	ASN
1	C	543	GLN
1	C	592	GLN
1	C	615	GLN
1	C	653	GLN
1	D	274	ASN
1	D	276	ASN
1	D	323	ASN
1	D	413	ASN
1	D	433	ASN
1	D	434	GLN
1	D	502	ASN
1	D	521	ASN
1	D	543	GLN
1	D	592	GLN
1	D	615	GLN
1	D	653	GLN
1	D	707	GLN
1	E	274	ASN
1	E	276	ASN
1	E	323	ASN
1	E	413	ASN
1	E	427	HIS
1	E	433	ASN
1	E	434	GLN
1	E	502	ASN
1	E	521	ASN
1	E	543	GLN

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Mol	Chain	Res	Type
1	E	592	GLN
1	E	615	GLN
1	E	653	GLN
1	F	274	ASN
1	F	276	ASN
1	F	323	ASN
1	F	413	ASN
1	F	433	ASN
1	F	434	GLN
1	F	502	ASN
1	F	521	ASN
1	F	543	GLN
1	F	592	GLN
1	F	615	GLN
1	F	653	GLN
1	F	707	GLN
1	G	274	ASN
1	G	276	ASN
1	G	323	ASN
1	G	413	ASN
1	G	433	ASN
1	G	434	GLN
1	G	502	ASN
1	G	521	ASN
1	G	543	GLN
1	G	592	GLN
1	G	615	GLN
1	G	653	GLN
1	H	274	ASN
1	H	276	ASN
1	H	323	ASN
1	H	413	ASN
1	H	433	ASN
1	H	434	GLN
1	H	502	ASN
1	H	521	ASN
1	H	543	GLN
1	H	592	GLN
1	H	615	GLN
1	H	653	GLN
1	I	274	ASN
1	I	276	ASN

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Mol	Chain	Res	Type
1	I	323	ASN
1	I	413	ASN
1	I	433	ASN
1	I	434	GLN
1	I	502	ASN
1	I	521	ASN
1	I	543	GLN
1	I	592	GLN
1	I	615	GLN
1	I	653	GLN
1	J	274	ASN
1	J	276	ASN
1	J	323	ASN
1	J	413	ASN
1	J	427	HIS
1	J	433	ASN
1	J	434	GLN
1	J	502	ASN
1	J	521	ASN
1	J	543	GLN
1	J	592	GLN
1	J	615	GLN
1	J	653	GLN
1	K	274	ASN
1	K	276	ASN
1	K	323	ASN
1	K	413	ASN
1	K	433	ASN
1	K	434	GLN
1	K	502	ASN
1	K	521	ASN
1	K	543	GLN
1	K	592	GLN
1	K	615	GLN
1	K	653	GLN
1	L	274	ASN
1	L	276	ASN
1	L	323	ASN
1	L	413	ASN
1	L	433	ASN
1	L	434	GLN
1	L	502	ASN

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Mol	Chain	Res	Type
1	L	521	ASN
1	L	543	GLN
1	L	592	GLN
1	L	615	GLN
1	L	653	GLN
1	M	274	ASN
1	M	276	ASN
1	M	307	ASN
1	M	323	ASN
1	M	413	ASN
1	M	427	HIS
1	M	433	ASN
1	M	502	ASN
1	M	521	ASN
1	M	543	GLN
1	M	592	GLN
1	M	615	GLN
1	M	653	GLN
1	N	274	ASN
1	N	276	ASN
1	N	323	ASN
1	N	413	ASN
1	N	433	ASN
1	N	434	GLN
1	N	502	ASN
1	N	521	ASN
1	N	543	GLN
1	N	592	GLN
1	N	615	GLN
1	N	653	GLN
1	O	274	ASN
1	O	276	ASN
1	O	323	ASN
1	O	413	ASN
1	O	427	HIS
1	O	433	ASN
1	O	434	GLN
1	O	502	ASN
1	O	521	ASN
1	O	543	GLN
1	O	592	GLN
1	O	615	GLN

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Mol	Chain	Res	Type
1	O	653	GLN
1	P	274	ASN
1	P	276	ASN
1	P	323	ASN
1	P	413	ASN
1	P	433	ASN
1	P	434	GLN
1	P	502	ASN
1	P	521	ASN
1	P	543	GLN
1	P	592	GLN
1	P	615	GLN
1	P	653	GLN
1	Q	274	ASN
1	Q	276	ASN
1	Q	323	ASN
1	Q	413	ASN
1	Q	427	HIS
1	Q	433	ASN
1	Q	434	GLN
1	Q	502	ASN
1	Q	521	ASN
1	Q	543	GLN
1	Q	592	GLN
1	Q	615	GLN
1	Q	653	GLN
1	R	274	ASN
1	R	276	ASN
1	R	323	ASN
1	R	413	ASN
1	R	433	ASN
1	R	434	GLN
1	R	502	ASN
1	R	521	ASN
1	R	543	GLN
1	R	592	GLN
1	R	615	GLN
1	R	653	GLN
1	S	274	ASN
1	S	276	ASN
1	S	323	ASN
1	S	413	ASN

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Mol	Chain	Res	Type
1	S	427	HIS
1	S	433	ASN
1	S	434	GLN
1	S	502	ASN
1	S	521	ASN
1	S	543	GLN
1	S	592	GLN
1	S	615	GLN
1	S	653	GLN
1	T	274	ASN
1	T	276	ASN
1	T	323	ASN
1	T	413	ASN
1	T	433	ASN
1	T	434	GLN
1	T	502	ASN
1	T	521	ASN
1	T	543	GLN
1	T	592	GLN
1	T	615	GLN
1	T	653	GLN
1	U	274	ASN
1	U	276	ASN
1	U	323	ASN
1	U	413	ASN
1	U	433	ASN
1	U	434	GLN
1	U	502	ASN
1	U	521	ASN
1	U	543	GLN
1	U	592	GLN
1	U	615	GLN
1	U	653	GLN
1	U	707	GLN
1	V	274	ASN
1	V	276	ASN
1	V	307	ASN
1	V	323	ASN
1	V	413	ASN
1	V	433	ASN
1	V	434	GLN
1	V	502	ASN

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Mol	Chain	Res	Type
1	V	521	ASN
1	V	543	GLN
1	V	592	GLN
1	V	615	GLN
1	V	653	GLN
1	W	274	ASN
1	W	276	ASN
1	W	323	ASN
1	W	413	ASN
1	W	433	ASN
1	W	434	GLN
1	W	502	ASN
1	W	521	ASN
1	W	543	GLN
1	W	592	GLN
1	W	615	GLN
1	W	653	GLN
1	X	274	ASN
1	X	276	ASN
1	X	323	ASN
1	X	413	ASN
1	X	433	ASN
1	X	434	GLN
1	X	502	ASN
1	X	521	ASN
1	X	543	GLN
1	X	592	GLN
1	X	615	GLN
1	X	653	GLN
1	Y	274	ASN
1	Y	276	ASN
1	Y	323	ASN
1	Y	413	ASN
1	Y	433	ASN
1	Y	434	GLN
1	Y	502	ASN
1	Y	521	ASN
1	Y	543	GLN
1	Y	592	GLN
1	Y	615	GLN
1	Y	653	GLN
1	Z	274	ASN

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Mol	Chain	Res	Type
1	Z	276	ASN
1	Z	323	ASN
1	Z	413	ASN
1	Z	427	HIS
1	Z	433	ASN
1	Z	434	GLN
1	Z	502	ASN
1	Z	521	ASN
1	Z	543	GLN
1	Z	592	GLN
1	Z	615	GLN
1	Z	653	GLN
1	a	274	ASN
1	a	276	ASN
1	a	307	ASN
1	a	323	ASN
1	a	413	ASN
1	a	433	ASN
1	a	434	GLN
1	a	502	ASN
1	a	521	ASN
1	a	543	GLN
1	a	592	GLN
1	a	615	GLN
1	a	653	GLN
1	b	274	ASN
1	b	276	ASN
1	b	323	ASN
1	b	413	ASN
1	b	427	HIS
1	b	433	ASN
1	b	434	GLN
1	b	502	ASN
1	b	521	ASN
1	b	543	GLN
1	b	592	GLN
1	b	615	GLN
1	b	653	GLN
1	b	707	GLN
1	c	274	ASN
1	c	276	ASN
1	c	307	ASN

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Mol	Chain	Res	Type
1	c	323	ASN
1	c	413	ASN
1	c	433	ASN
1	c	434	GLN
1	c	502	ASN
1	c	521	ASN
1	c	543	GLN
1	c	592	GLN
1	c	615	GLN
1	c	653	GLN
1	d	274	ASN
1	d	276	ASN
1	d	323	ASN
1	d	413	ASN
1	d	433	ASN
1	d	434	GLN
1	d	502	ASN
1	d	521	ASN
1	d	543	GLN
1	d	592	GLN
1	d	615	GLN
1	d	653	GLN
1	e	274	ASN
1	e	276	ASN
1	e	307	ASN
1	e	323	ASN
1	e	413	ASN
1	e	433	ASN
1	e	434	GLN
1	e	502	ASN
1	e	521	ASN
1	e	543	GLN
1	e	592	GLN
1	e	615	GLN
1	e	653	GLN
1	f	274	ASN
1	f	276	ASN
1	f	323	ASN
1	f	413	ASN
1	f	427	HIS
1	f	433	ASN
1	f	434	GLN

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Mol	Chain	Res	Type
1	f	502	ASN
1	f	521	ASN
1	f	543	GLN
1	f	592	GLN
1	f	615	GLN
1	f	653	GLN
1	f	707	GLN
1	g	274	ASN
1	g	276	ASN
1	g	323	ASN
1	g	413	ASN
1	g	427	HIS
1	g	433	ASN
1	g	434	GLN
1	g	502	ASN
1	g	521	ASN
1	g	543	GLN
1	g	592	GLN
1	g	615	GLN
1	g	653	GLN
1	h	274	ASN
1	h	276	ASN
1	h	307	ASN
1	h	323	ASN
1	h	413	ASN
1	h	427	HIS
1	h	433	ASN
1	h	502	ASN
1	h	521	ASN
1	h	543	GLN
1	h	592	GLN
1	h	615	GLN
1	h	653	GLN
1	i	274	ASN
1	i	276	ASN
1	i	323	ASN
1	i	413	ASN
1	i	433	ASN
1	i	434	GLN
1	i	502	ASN
1	i	521	ASN
1	i	543	GLN

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Mol	Chain	Res	Type
1	i	592	GLN
1	i	615	GLN
1	i	653	GLN
1	j	274	ASN
1	j	276	ASN
1	j	323	ASN
1	j	413	ASN
1	j	433	ASN
1	j	434	GLN
1	j	502	ASN
1	j	521	ASN
1	j	543	GLN
1	j	592	GLN
1	j	615	GLN
1	j	653	GLN
1	k	274	ASN
1	k	276	ASN
1	k	323	ASN
1	k	413	ASN
1	k	433	ASN
1	k	434	GLN
1	k	502	ASN
1	k	521	ASN
1	k	543	GLN
1	k	592	GLN
1	k	615	GLN
1	k	653	GLN
1	k	707	GLN
1	l	274	ASN
1	l	276	ASN
1	l	323	ASN
1	l	413	ASN
1	l	427	HIS
1	l	433	ASN
1	l	434	GLN
1	l	502	ASN
1	l	521	ASN
1	l	543	GLN
1	l	592	GLN
1	l	615	GLN
1	l	653	GLN
1	m	274	ASN

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Mol	Chain	Res	Type
1	m	276	ASN
1	m	323	ASN
1	m	413	ASN
1	m	433	ASN
1	m	434	GLN
1	m	502	ASN
1	m	521	ASN
1	m	543	GLN
1	m	592	GLN
1	m	615	GLN
1	m	653	GLN
1	n	274	ASN
1	n	276	ASN
1	n	323	ASN
1	n	413	ASN
1	n	433	ASN
1	n	434	GLN
1	n	502	ASN
1	n	521	ASN
1	n	543	GLN
1	n	592	GLN
1	n	615	GLN
1	n	653	GLN
1	o	274	ASN
1	o	276	ASN
1	o	323	ASN
1	o	413	ASN
1	o	433	ASN
1	o	434	GLN
1	o	502	ASN
1	o	521	ASN
1	o	543	GLN
1	o	592	GLN
1	o	615	GLN
1	o	653	GLN
1	p	274	ASN
1	p	276	ASN
1	p	307	ASN
1	p	323	ASN
1	p	413	ASN
1	p	433	ASN
1	p	434	GLN

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Mol	Chain	Res	Type
1	p	502	ASN
1	p	521	ASN
1	p	543	GLN
1	p	592	GLN
1	p	615	GLN
1	p	653	GLN
1	q	274	ASN
1	q	276	ASN
1	q	323	ASN
1	q	413	ASN
1	q	433	ASN
1	q	434	GLN
1	q	502	ASN
1	q	521	ASN
1	q	543	GLN
1	q	592	GLN
1	q	615	GLN
1	q	653	GLN
1	r	274	ASN
1	r	276	ASN
1	r	323	ASN
1	r	413	ASN
1	r	427	HIS
1	r	433	ASN
1	r	434	GLN
1	r	502	ASN
1	r	521	ASN
1	r	543	GLN
1	r	592	GLN
1	r	615	GLN
1	r	653	GLN
1	s	274	ASN
1	s	276	ASN
1	s	323	ASN
1	s	413	ASN
1	s	427	HIS
1	s	433	ASN
1	s	434	GLN
1	s	502	ASN
1	s	521	ASN
1	s	543	GLN
1	s	592	GLN

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Mol	Chain	Res	Type
1	s	615	GLN
1	s	653	GLN
1	s	707	GLN
1	t	274	ASN
1	t	276	ASN
1	t	323	ASN
1	t	413	ASN
1	t	433	ASN
1	t	434	GLN
1	t	502	ASN
1	t	521	ASN
1	t	543	GLN
1	t	592	GLN
1	t	615	GLN
1	t	653	GLN
1	u	274	ASN
1	u	276	ASN
1	u	323	ASN
1	u	413	ASN
1	u	433	ASN
1	u	502	ASN
1	u	521	ASN
1	u	543	GLN
1	u	592	GLN
1	u	615	GLN
1	u	653	GLN
1	v	274	ASN
1	v	276	ASN
1	v	307	ASN
1	v	323	ASN
1	v	413	ASN
1	v	433	ASN
1	v	434	GLN
1	v	502	ASN
1	v	521	ASN
1	v	543	GLN
1	v	592	GLN
1	v	615	GLN
1	v	653	GLN
1	w	274	ASN
1	w	276	ASN
1	w	323	ASN

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Mol	Chain	Res	Type
1	w	413	ASN
1	w	427	HIS
1	w	433	ASN
1	w	434	GLN
1	w	502	ASN
1	w	521	ASN
1	w	543	GLN
1	w	592	GLN
1	w	615	GLN
1	w	653	GLN
1	x	274	ASN
1	x	276	ASN
1	x	323	ASN
1	x	413	ASN
1	x	427	HIS
1	x	433	ASN
1	x	434	GLN
1	x	502	ASN
1	x	521	ASN
1	x	543	GLN
1	x	592	GLN
1	x	615	GLN
1	x	653	GLN
1	y	274	ASN
1	y	276	ASN
1	y	323	ASN
1	y	413	ASN
1	y	433	ASN
1	y	434	GLN
1	y	502	ASN
1	y	521	ASN
1	y	543	GLN
1	y	592	GLN
1	y	615	GLN
1	y	653	GLN
1	y	707	GLN
1	z	274	ASN
1	z	276	ASN
1	z	323	ASN
1	z	413	ASN
1	z	433	ASN
1	z	434	GLN

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Mol	Chain	Res	Type
1	z	502	ASN
1	z	521	ASN
1	z	543	GLN
1	z	592	GLN
1	z	615	GLN
1	z	653	GLN
1	1	274	ASN
1	1	276	ASN
1	1	323	ASN
1	1	413	ASN
1	1	433	ASN
1	1	434	GLN
1	1	502	ASN
1	1	521	ASN
1	1	543	GLN
1	1	592	GLN
1	1	615	GLN
1	1	653	GLN
1	2	274	ASN
1	2	276	ASN
1	2	323	ASN
1	2	413	ASN
1	2	433	ASN
1	2	434	GLN
1	2	502	ASN
1	2	521	ASN
1	2	543	GLN
1	2	592	GLN
1	2	615	GLN
1	2	653	GLN
1	2	707	GLN
1	3	274	ASN
1	3	276	ASN
1	3	323	ASN
1	3	413	ASN
1	3	433	ASN
1	3	434	GLN
1	3	502	ASN
1	3	521	ASN
1	3	543	GLN
1	3	592	GLN
1	3	615	GLN

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Mol	Chain	Res	Type
1	3	653	GLN
1	3	707	GLN
1	4	274	ASN
1	4	276	ASN
1	4	307	ASN
1	4	323	ASN
1	4	413	ASN
1	4	433	ASN
1	4	502	ASN
1	4	521	ASN
1	4	543	GLN
1	4	592	GLN
1	4	615	GLN
1	4	653	GLN
1	5	274	ASN
1	5	276	ASN
1	5	323	ASN
1	5	413	ASN
1	5	433	ASN
1	5	434	GLN
1	5	502	ASN
1	5	521	ASN
1	5	543	GLN
1	5	592	GLN
1	5	615	GLN
1	5	653	GLN
1	6	274	ASN
1	6	276	ASN
1	6	323	ASN
1	6	413	ASN
1	6	433	ASN
1	6	434	GLN
1	6	502	ASN
1	6	521	ASN
1	6	543	GLN
1	6	592	GLN
1	6	615	GLN
1	6	653	GLN
1	7	274	ASN
1	7	276	ASN
1	7	323	ASN
1	7	413	ASN

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Mol	Chain	Res	Type
1	7	433	ASN
1	7	434	GLN
1	7	502	ASN
1	7	521	ASN
1	7	543	GLN
1	7	592	GLN
1	7	615	GLN
1	7	653	GLN
1	8	274	ASN
1	8	276	ASN
1	8	323	ASN
1	8	413	ASN
1	8	427	HIS
1	8	433	ASN
1	8	434	GLN
1	8	502	ASN
1	8	521	ASN
1	8	543	GLN
1	8	592	GLN
1	8	615	GLN
1	8	653	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	DA	p	801	-	18,23,24	0.88	0	17,33,36	0.75	0
2	DA	k	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	W	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	i	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	K	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	s	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	d	801	-	18,23,24	0.90	0	17,33,36	0.76	0
2	DA	5	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	h	801	-	18,23,24	0.88	0	17,33,36	0.75	0
2	DA	m	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	3	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	J	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	t	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	V	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	f	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	A	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	D	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	z	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	8	801	-	18,23,24	0.90	0	17,33,36	0.75	0
2	DA	P	801	-	18,23,24	0.90	0	17,33,36	0.74	0
2	DA	e	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	w	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	6	801	-	18,23,24	0.89	0	17,33,36	0.74	0
2	DA	7	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	H	801	-	18,23,24	0.88	0	17,33,36	0.76	0
2	DA	1	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	I	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	M	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	b	801	-	18,23,24	0.88	0	17,33,36	0.74	0
2	DA	a	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	E	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	R	801	-	18,23,24	0.88	0	17,33,36	0.75	0
2	DA	x	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	Y	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	y	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	C	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	j	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	F	801	-	18,23,24	0.88	0	17,33,36	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DA	q	801	-	18,23,24	0.88	0	17,33,36	0.76	0
2	DA	2	801	-	18,23,24	0.89	0	17,33,36	0.76	0
2	DA	4	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	v	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	O	801	-	18,23,24	0.89	0	17,33,36	0.74	0
2	DA	X	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	S	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	G	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	T	801	-	18,23,24	0.90	0	17,33,36	0.76	0
2	DA	r	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	o	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	n	801	-	18,23,24	0.88	0	17,33,36	0.74	0
2	DA	l	801	-	18,23,24	0.88	0	17,33,36	0.75	0
2	DA	Z	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	L	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	N	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	U	801	-	18,23,24	0.89	0	17,33,36	0.74	0
2	DA	c	801	-	18,23,24	0.90	0	17,33,36	0.75	0
2	DA	g	801	-	18,23,24	0.89	0	17,33,36	0.74	0
2	DA	u	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	Q	801	-	18,23,24	0.89	0	17,33,36	0.75	0
2	DA	B	801	-	18,23,24	0.89	0	17,33,36	0.75	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	DA	p	801	-	-	2/3/21/22	0/3/3/3
2	DA	k	801	-	-	2/3/21/22	0/3/3/3
2	DA	W	801	-	-	2/3/21/22	0/3/3/3
2	DA	i	801	-	-	2/3/21/22	0/3/3/3
2	DA	K	801	-	-	2/3/21/22	0/3/3/3
2	DA	s	801	-	-	2/3/21/22	0/3/3/3
2	DA	d	801	-	-	2/3/21/22	0/3/3/3
2	DA	5	801	-	-	2/3/21/22	0/3/3/3
2	DA	h	801	-	-	2/3/21/22	0/3/3/3
2	DA	m	801	-	-	2/3/21/22	0/3/3/3
2	DA	3	801	-	-	2/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DA	J	801	-	-	2/3/21/22	0/3/3/3
2	DA	t	801	-	-	2/3/21/22	0/3/3/3
2	DA	V	801	-	-	2/3/21/22	0/3/3/3
2	DA	f	801	-	-	2/3/21/22	0/3/3/3
2	DA	A	801	-	-	2/3/21/22	0/3/3/3
2	DA	D	801	-	-	2/3/21/22	0/3/3/3
2	DA	z	801	-	-	2/3/21/22	0/3/3/3
2	DA	8	801	-	-	2/3/21/22	0/3/3/3
2	DA	P	801	-	-	2/3/21/22	0/3/3/3
2	DA	e	801	-	-	2/3/21/22	0/3/3/3
2	DA	w	801	-	-	2/3/21/22	0/3/3/3
2	DA	6	801	-	-	2/3/21/22	0/3/3/3
2	DA	7	801	-	-	2/3/21/22	0/3/3/3
2	DA	H	801	-	-	2/3/21/22	0/3/3/3
2	DA	1	801	-	-	2/3/21/22	0/3/3/3
2	DA	I	801	-	-	2/3/21/22	0/3/3/3
2	DA	M	801	-	-	2/3/21/22	0/3/3/3
2	DA	b	801	-	-	2/3/21/22	0/3/3/3
2	DA	a	801	-	-	2/3/21/22	0/3/3/3
2	DA	E	801	-	-	2/3/21/22	0/3/3/3
2	DA	R	801	-	-	2/3/21/22	0/3/3/3
2	DA	x	801	-	-	2/3/21/22	0/3/3/3
2	DA	Y	801	-	-	2/3/21/22	0/3/3/3
2	DA	y	801	-	-	2/3/21/22	0/3/3/3
2	DA	C	801	-	-	2/3/21/22	0/3/3/3
2	DA	j	801	-	-	2/3/21/22	0/3/3/3
2	DA	F	801	-	-	2/3/21/22	0/3/3/3
2	DA	q	801	-	-	2/3/21/22	0/3/3/3
2	DA	2	801	-	-	2/3/21/22	0/3/3/3
2	DA	4	801	-	-	2/3/21/22	0/3/3/3
2	DA	v	801	-	-	2/3/21/22	0/3/3/3
2	DA	O	801	-	-	2/3/21/22	0/3/3/3
2	DA	X	801	-	-	2/3/21/22	0/3/3/3
2	DA	S	801	-	-	2/3/21/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DA	G	801	-	-	2/3/21/22	0/3/3/3
2	DA	T	801	-	-	2/3/21/22	0/3/3/3
2	DA	r	801	-	-	2/3/21/22	0/3/3/3
2	DA	o	801	-	-	2/3/21/22	0/3/3/3
2	DA	n	801	-	-	2/3/21/22	0/3/3/3
2	DA	l	801	-	-	2/3/21/22	0/3/3/3
2	DA	Z	801	-	-	2/3/21/22	0/3/3/3
2	DA	L	801	-	-	2/3/21/22	0/3/3/3
2	DA	N	801	-	-	2/3/21/22	0/3/3/3
2	DA	U	801	-	-	2/3/21/22	0/3/3/3
2	DA	c	801	-	-	2/3/21/22	0/3/3/3
2	DA	g	801	-	-	2/3/21/22	0/3/3/3
2	DA	u	801	-	-	2/3/21/22	0/3/3/3
2	DA	Q	801	-	-	2/3/21/22	0/3/3/3
2	DA	B	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.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	DA	C4'-C5'-O5'-P
2	B	801	DA	C4'-C5'-O5'-P
2	C	801	DA	C4'-C5'-O5'-P
2	D	801	DA	C4'-C5'-O5'-P
2	E	801	DA	C4'-C5'-O5'-P
2	F	801	DA	C4'-C5'-O5'-P
2	G	801	DA	C4'-C5'-O5'-P
2	H	801	DA	C4'-C5'-O5'-P
2	I	801	DA	C4'-C5'-O5'-P
2	J	801	DA	C4'-C5'-O5'-P
2	K	801	DA	C4'-C5'-O5'-P
2	L	801	DA	C4'-C5'-O5'-P
2	M	801	DA	C4'-C5'-O5'-P
2	N	801	DA	C4'-C5'-O5'-P
2	O	801	DA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	P	801	DA	C4'-C5'-O5'-P
2	Q	801	DA	C4'-C5'-O5'-P
2	R	801	DA	C4'-C5'-O5'-P
2	S	801	DA	C4'-C5'-O5'-P
2	T	801	DA	C4'-C5'-O5'-P
2	U	801	DA	C4'-C5'-O5'-P
2	V	801	DA	C4'-C5'-O5'-P
2	W	801	DA	C4'-C5'-O5'-P
2	X	801	DA	C4'-C5'-O5'-P
2	Y	801	DA	C4'-C5'-O5'-P
2	Z	801	DA	C4'-C5'-O5'-P
2	a	801	DA	C4'-C5'-O5'-P
2	b	801	DA	C4'-C5'-O5'-P
2	c	801	DA	C4'-C5'-O5'-P
2	d	801	DA	C4'-C5'-O5'-P
2	e	801	DA	C4'-C5'-O5'-P
2	f	801	DA	C4'-C5'-O5'-P
2	g	801	DA	C4'-C5'-O5'-P
2	h	801	DA	C4'-C5'-O5'-P
2	i	801	DA	C4'-C5'-O5'-P
2	j	801	DA	C4'-C5'-O5'-P
2	k	801	DA	C4'-C5'-O5'-P
2	l	801	DA	C4'-C5'-O5'-P
2	m	801	DA	C4'-C5'-O5'-P
2	n	801	DA	C4'-C5'-O5'-P
2	o	801	DA	C4'-C5'-O5'-P
2	p	801	DA	C4'-C5'-O5'-P
2	q	801	DA	C4'-C5'-O5'-P
2	r	801	DA	C4'-C5'-O5'-P
2	s	801	DA	C4'-C5'-O5'-P
2	t	801	DA	C4'-C5'-O5'-P
2	u	801	DA	C4'-C5'-O5'-P
2	v	801	DA	C4'-C5'-O5'-P
2	w	801	DA	C4'-C5'-O5'-P
2	x	801	DA	C4'-C5'-O5'-P
2	y	801	DA	C4'-C5'-O5'-P
2	z	801	DA	C4'-C5'-O5'-P
2	1	801	DA	C4'-C5'-O5'-P
2	2	801	DA	C4'-C5'-O5'-P
2	3	801	DA	C4'-C5'-O5'-P
2	4	801	DA	C4'-C5'-O5'-P
2	5	801	DA	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	6	801	DA	C4'-C5'-O5'-P
2	7	801	DA	C4'-C5'-O5'-P
2	8	801	DA	C4'-C5'-O5'-P
2	A	801	DA	C3'-C4'-C5'-O5'
2	B	801	DA	C3'-C4'-C5'-O5'
2	C	801	DA	C3'-C4'-C5'-O5'
2	D	801	DA	C3'-C4'-C5'-O5'
2	E	801	DA	C3'-C4'-C5'-O5'
2	F	801	DA	C3'-C4'-C5'-O5'
2	G	801	DA	C3'-C4'-C5'-O5'
2	H	801	DA	C3'-C4'-C5'-O5'
2	I	801	DA	C3'-C4'-C5'-O5'
2	J	801	DA	C3'-C4'-C5'-O5'
2	K	801	DA	C3'-C4'-C5'-O5'
2	L	801	DA	C3'-C4'-C5'-O5'
2	M	801	DA	C3'-C4'-C5'-O5'
2	N	801	DA	C3'-C4'-C5'-O5'
2	O	801	DA	C3'-C4'-C5'-O5'
2	P	801	DA	C3'-C4'-C5'-O5'
2	Q	801	DA	C3'-C4'-C5'-O5'
2	R	801	DA	C3'-C4'-C5'-O5'
2	S	801	DA	C3'-C4'-C5'-O5'
2	T	801	DA	C3'-C4'-C5'-O5'
2	U	801	DA	C3'-C4'-C5'-O5'
2	V	801	DA	C3'-C4'-C5'-O5'
2	W	801	DA	C3'-C4'-C5'-O5'
2	X	801	DA	C3'-C4'-C5'-O5'
2	Y	801	DA	C3'-C4'-C5'-O5'
2	Z	801	DA	C3'-C4'-C5'-O5'
2	a	801	DA	C3'-C4'-C5'-O5'
2	b	801	DA	C3'-C4'-C5'-O5'
2	c	801	DA	C3'-C4'-C5'-O5'
2	d	801	DA	C3'-C4'-C5'-O5'
2	e	801	DA	C3'-C4'-C5'-O5'
2	f	801	DA	C3'-C4'-C5'-O5'
2	g	801	DA	C3'-C4'-C5'-O5'
2	h	801	DA	C3'-C4'-C5'-O5'
2	i	801	DA	C3'-C4'-C5'-O5'
2	j	801	DA	C3'-C4'-C5'-O5'
2	k	801	DA	C3'-C4'-C5'-O5'
2	l	801	DA	C3'-C4'-C5'-O5'
2	m	801	DA	C3'-C4'-C5'-O5'

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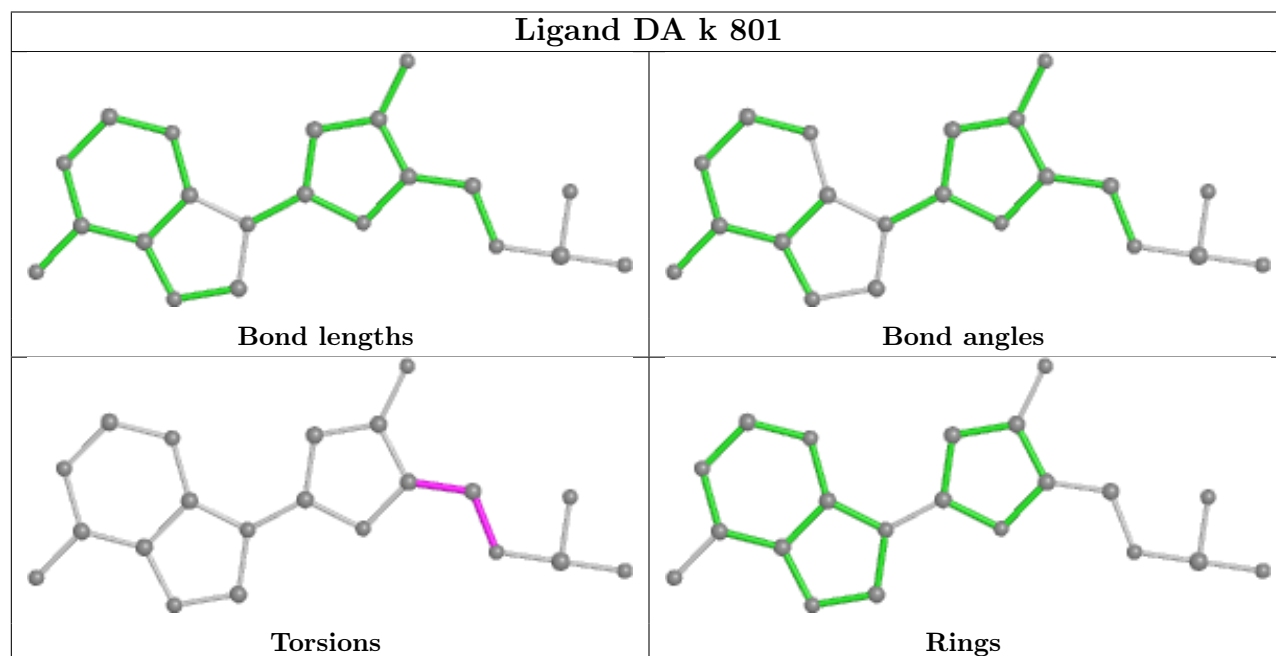
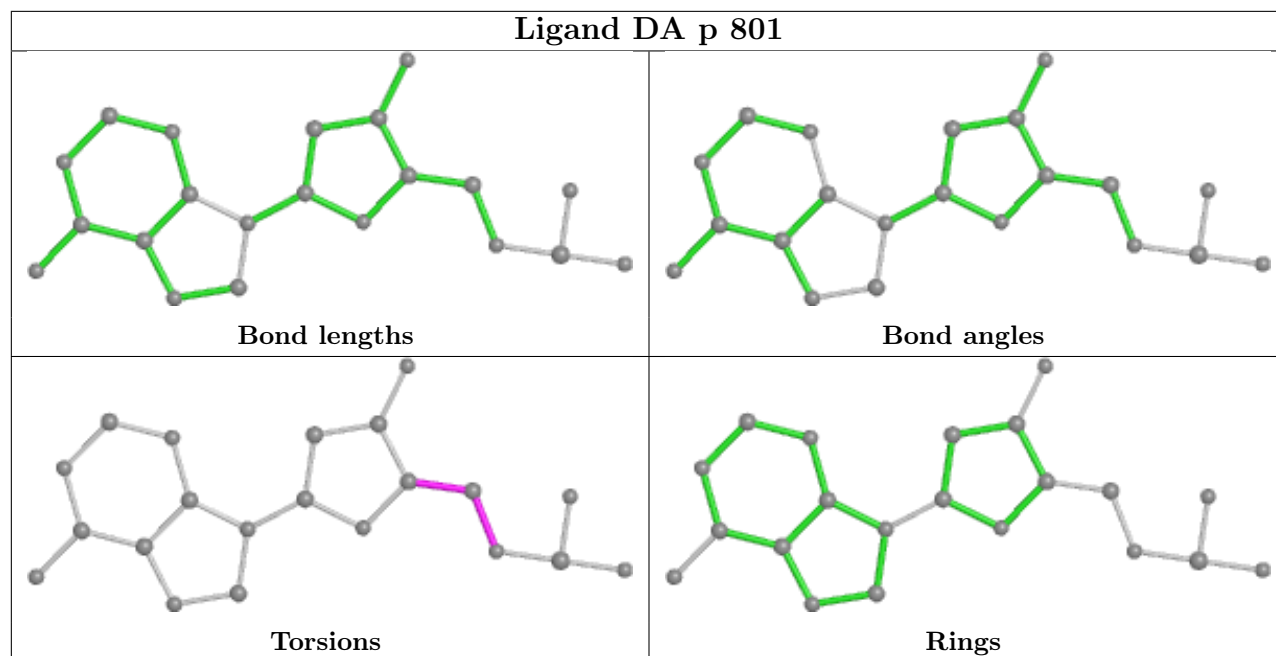
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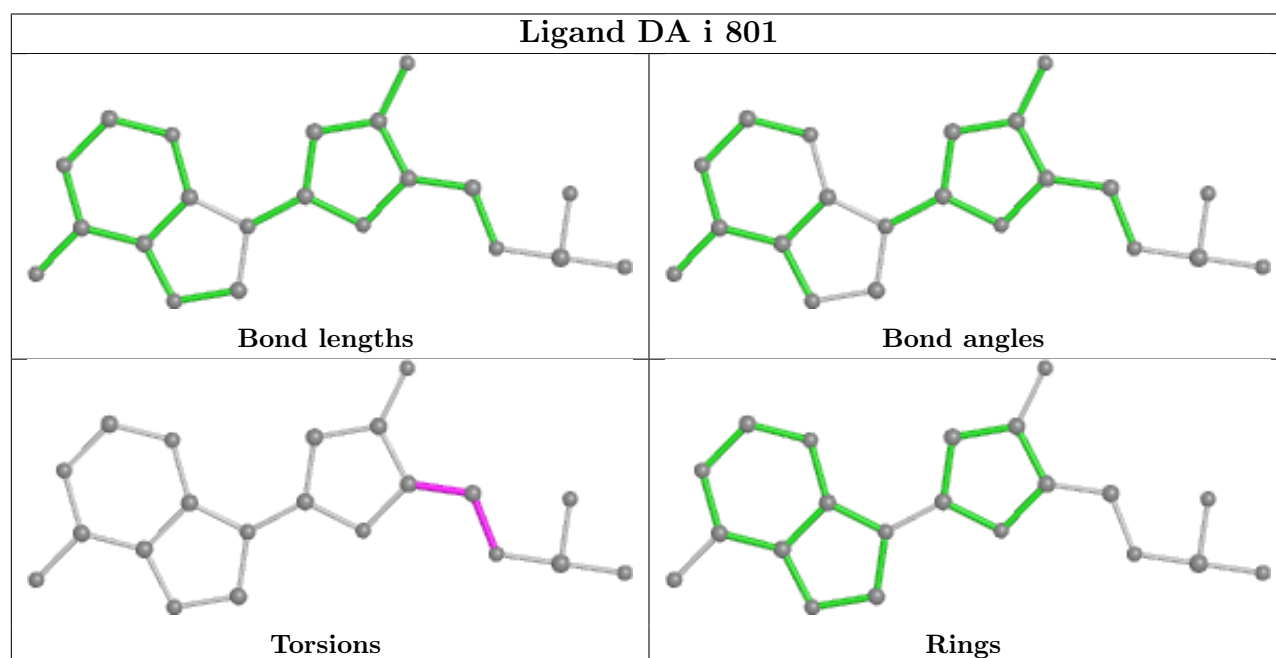
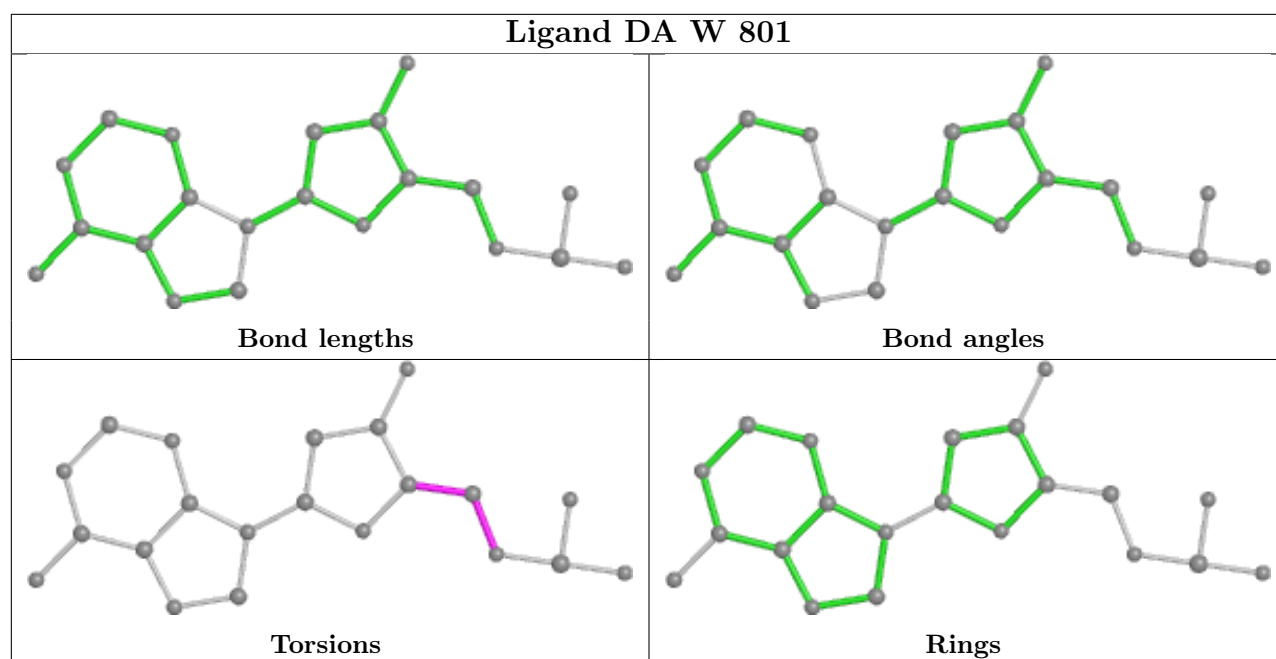
Mol	Chain	Res	Type	Atoms
2	n	801	DA	C3'-C4'-C5'-O5'
2	o	801	DA	C3'-C4'-C5'-O5'
2	p	801	DA	C3'-C4'-C5'-O5'
2	q	801	DA	C3'-C4'-C5'-O5'
2	r	801	DA	C3'-C4'-C5'-O5'
2	s	801	DA	C3'-C4'-C5'-O5'
2	t	801	DA	C3'-C4'-C5'-O5'
2	u	801	DA	C3'-C4'-C5'-O5'
2	v	801	DA	C3'-C4'-C5'-O5'
2	w	801	DA	C3'-C4'-C5'-O5'
2	x	801	DA	C3'-C4'-C5'-O5'
2	y	801	DA	C3'-C4'-C5'-O5'
2	z	801	DA	C3'-C4'-C5'-O5'
2	1	801	DA	C3'-C4'-C5'-O5'
2	2	801	DA	C3'-C4'-C5'-O5'
2	3	801	DA	C3'-C4'-C5'-O5'
2	4	801	DA	C3'-C4'-C5'-O5'
2	5	801	DA	C3'-C4'-C5'-O5'
2	6	801	DA	C3'-C4'-C5'-O5'
2	7	801	DA	C3'-C4'-C5'-O5'
2	8	801	DA	C3'-C4'-C5'-O5'

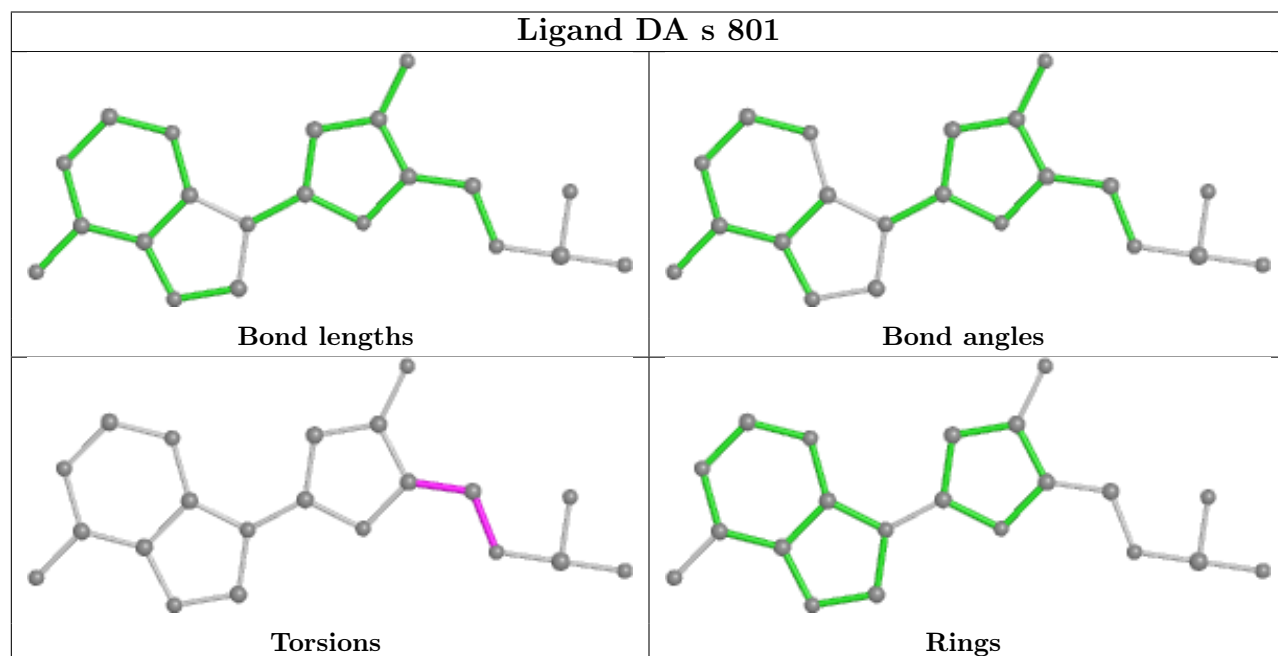
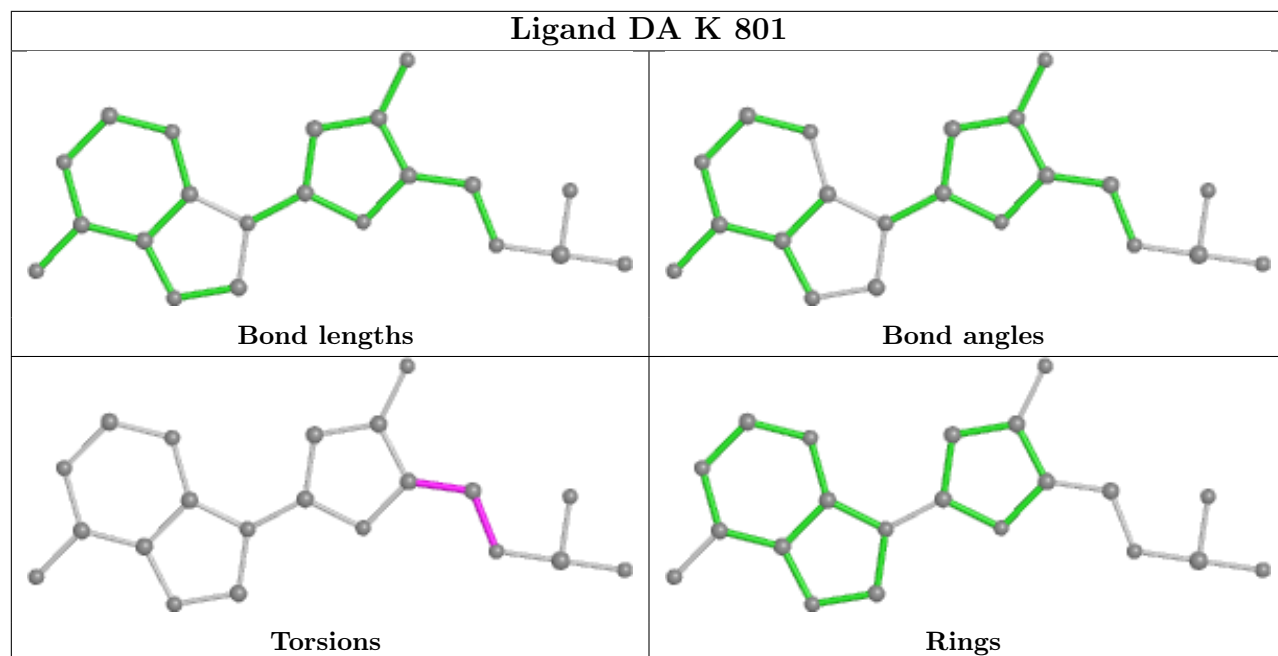
There are no ring outliers.

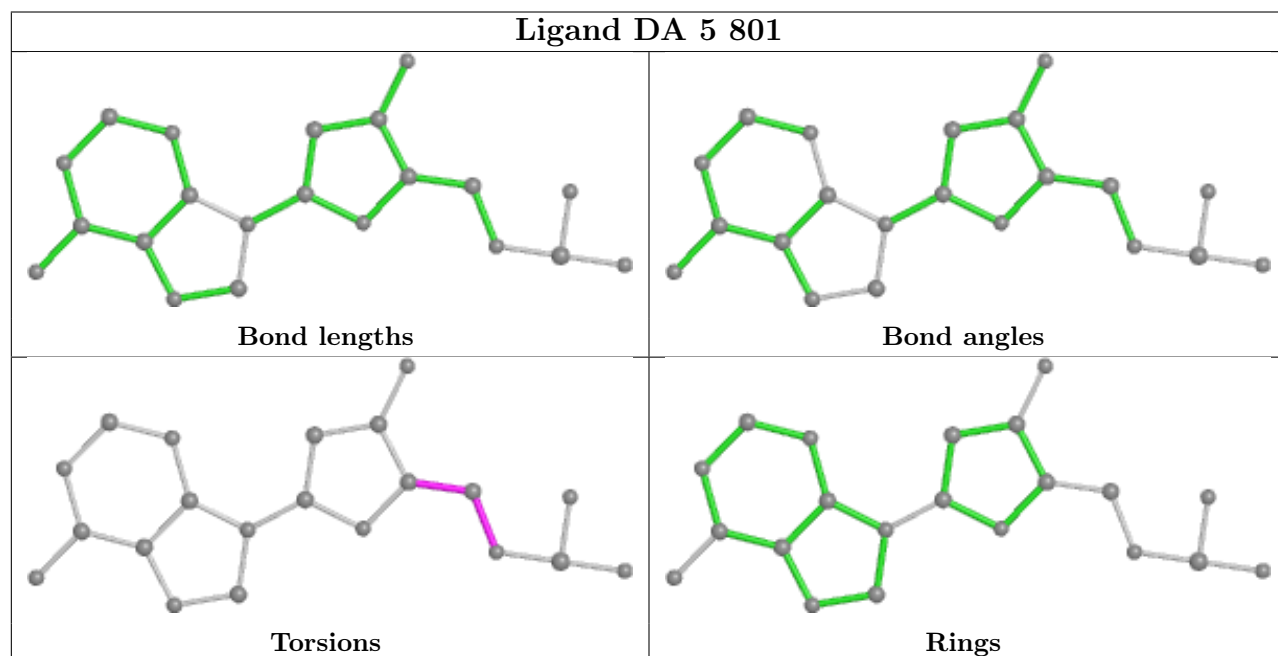
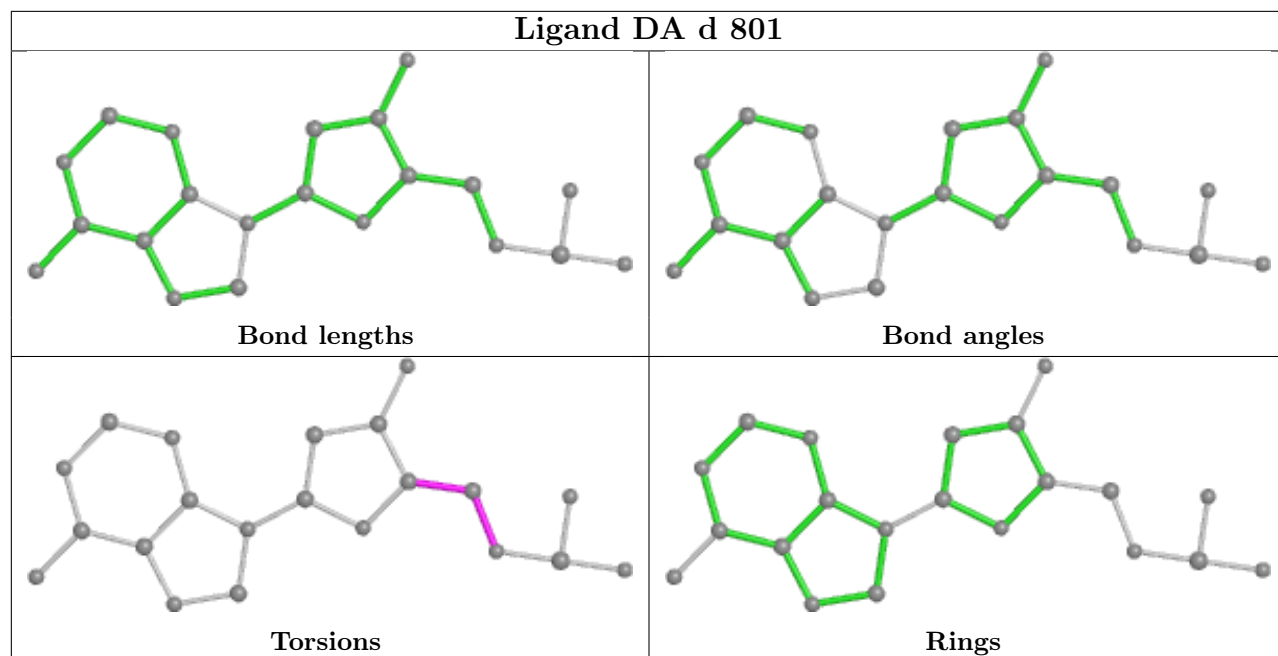
No monomer is involved in short contacts.

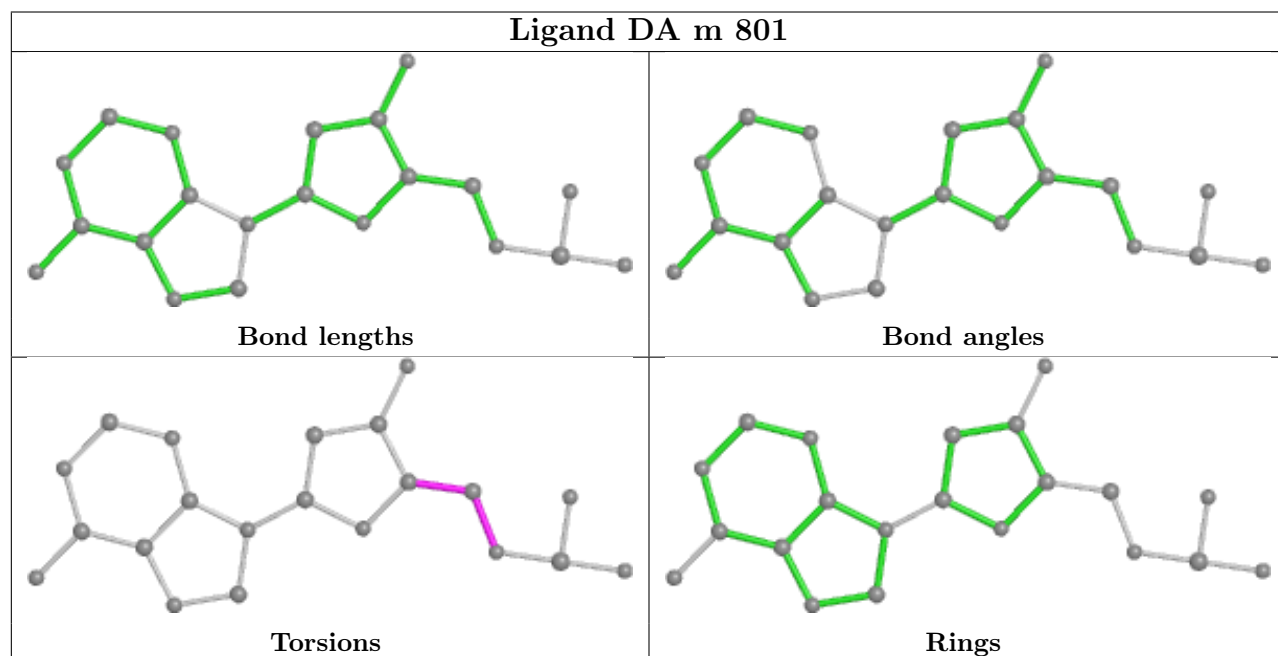
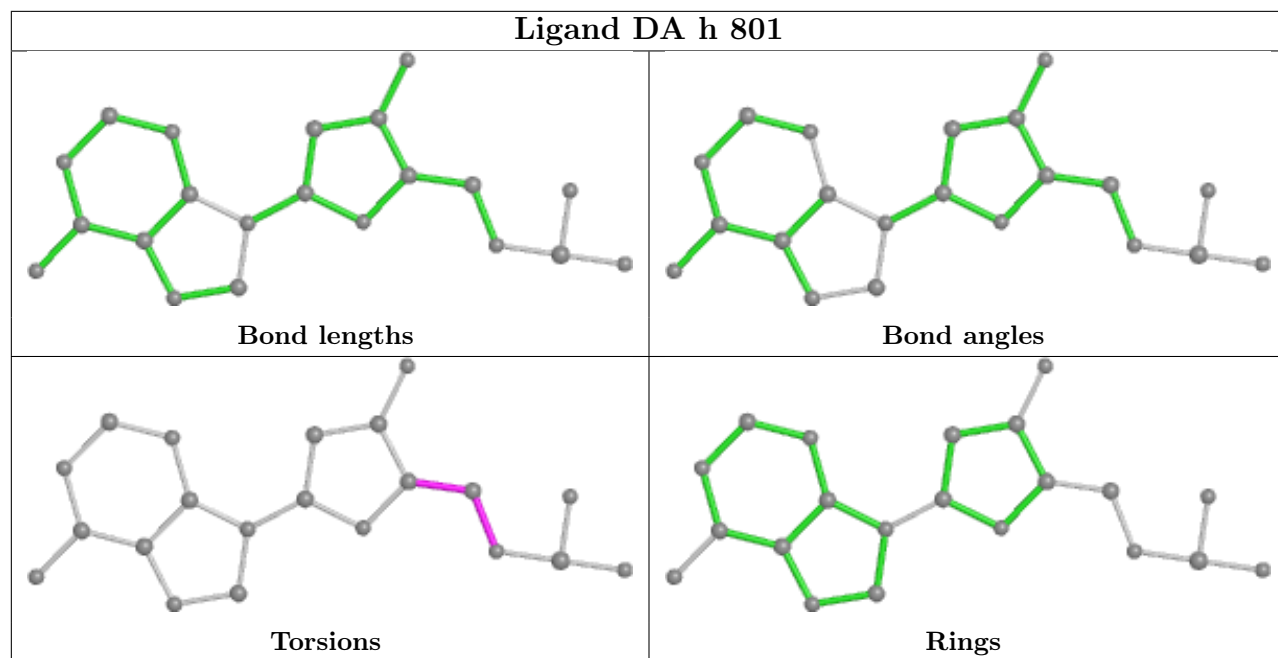
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

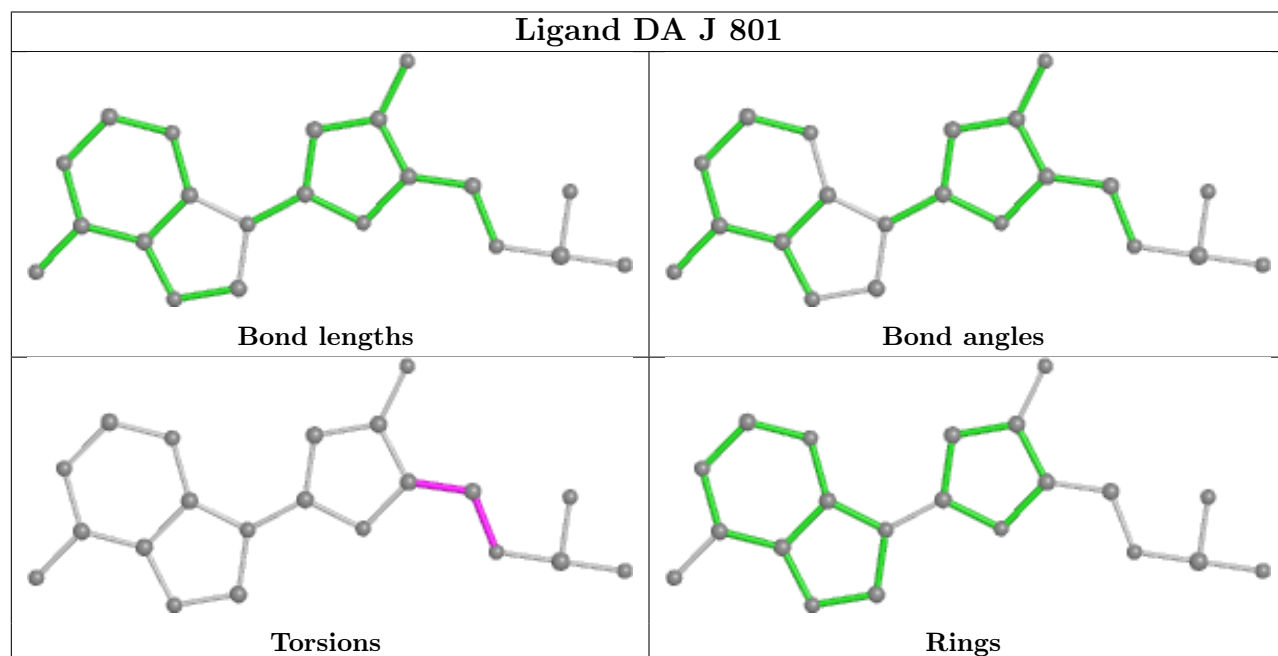
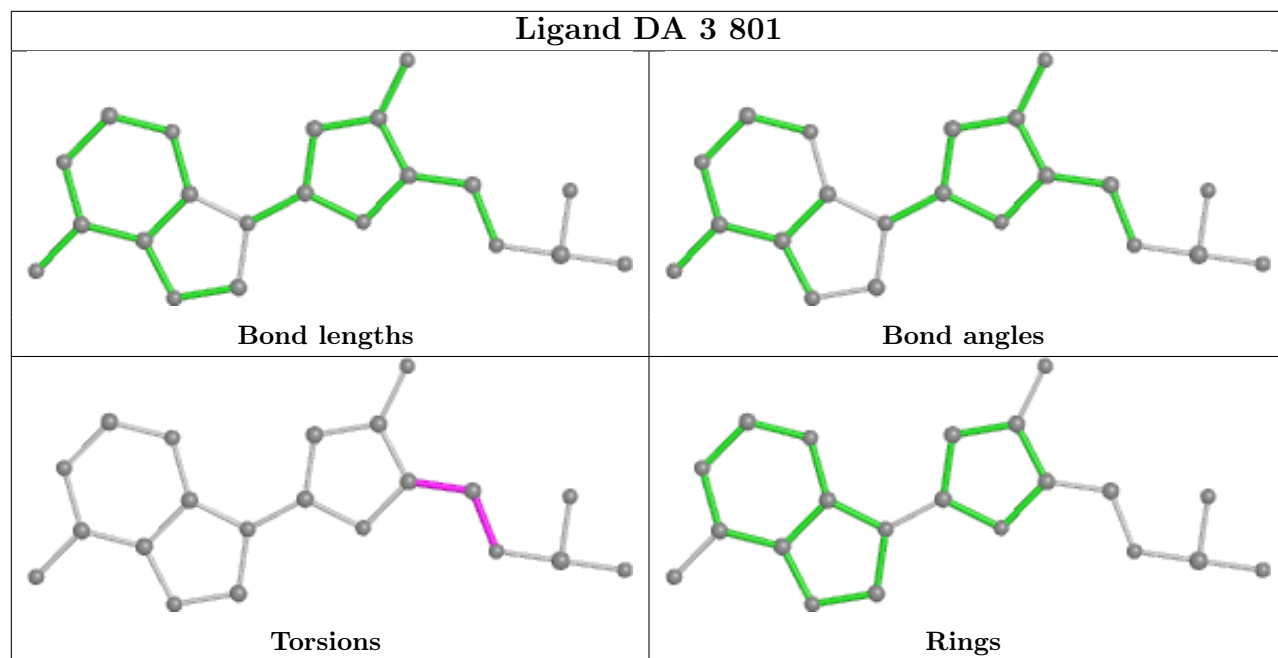


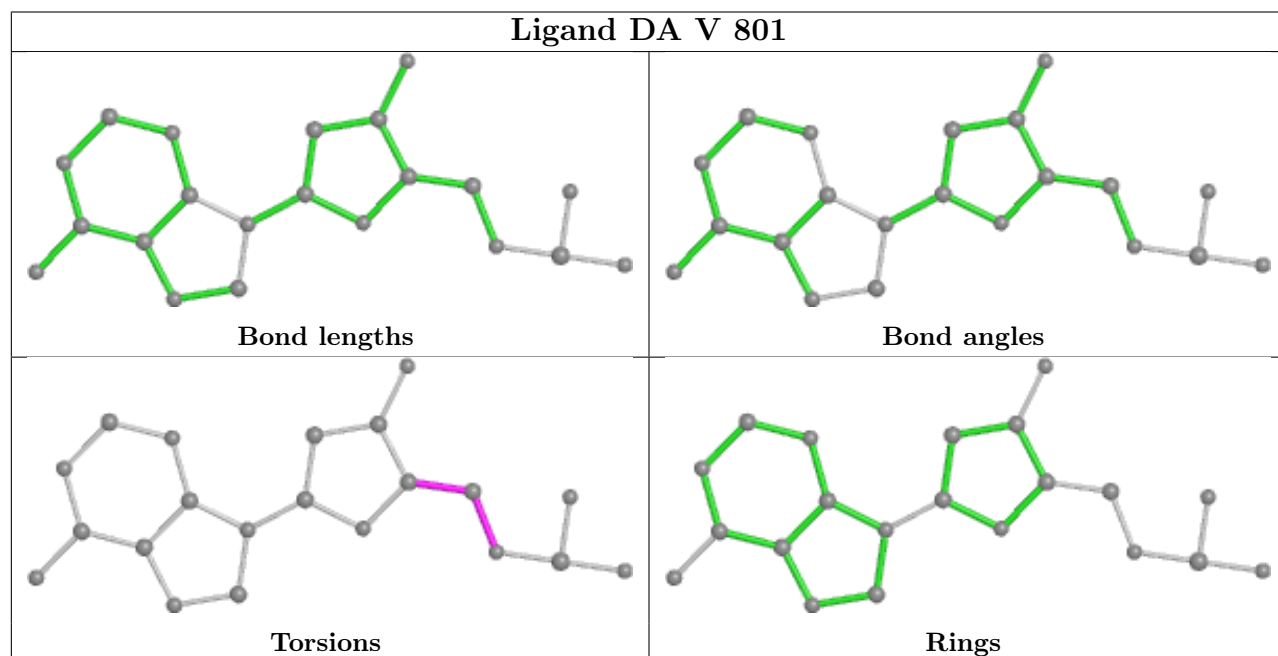
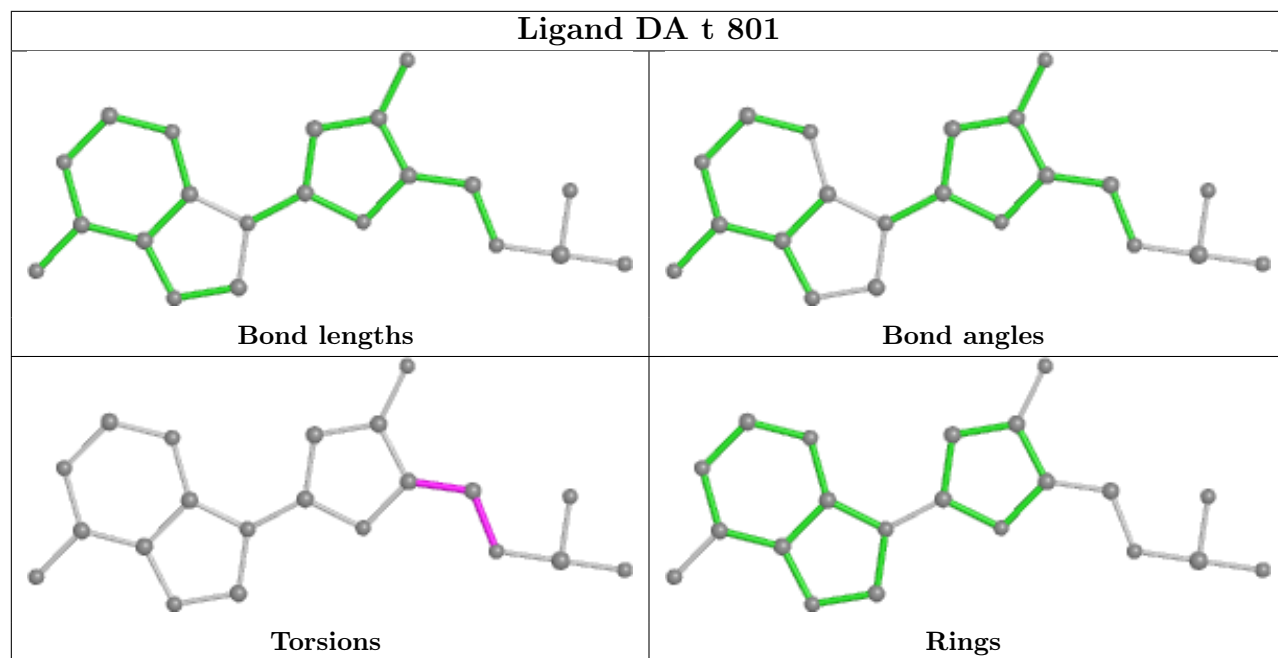


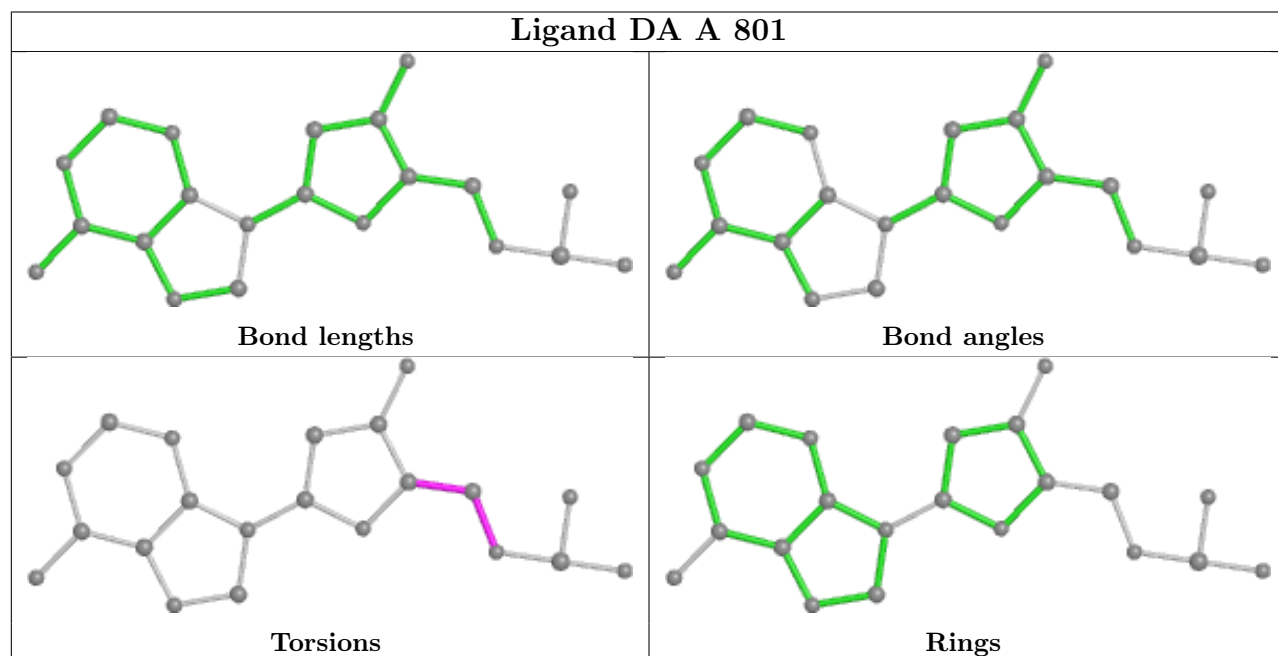
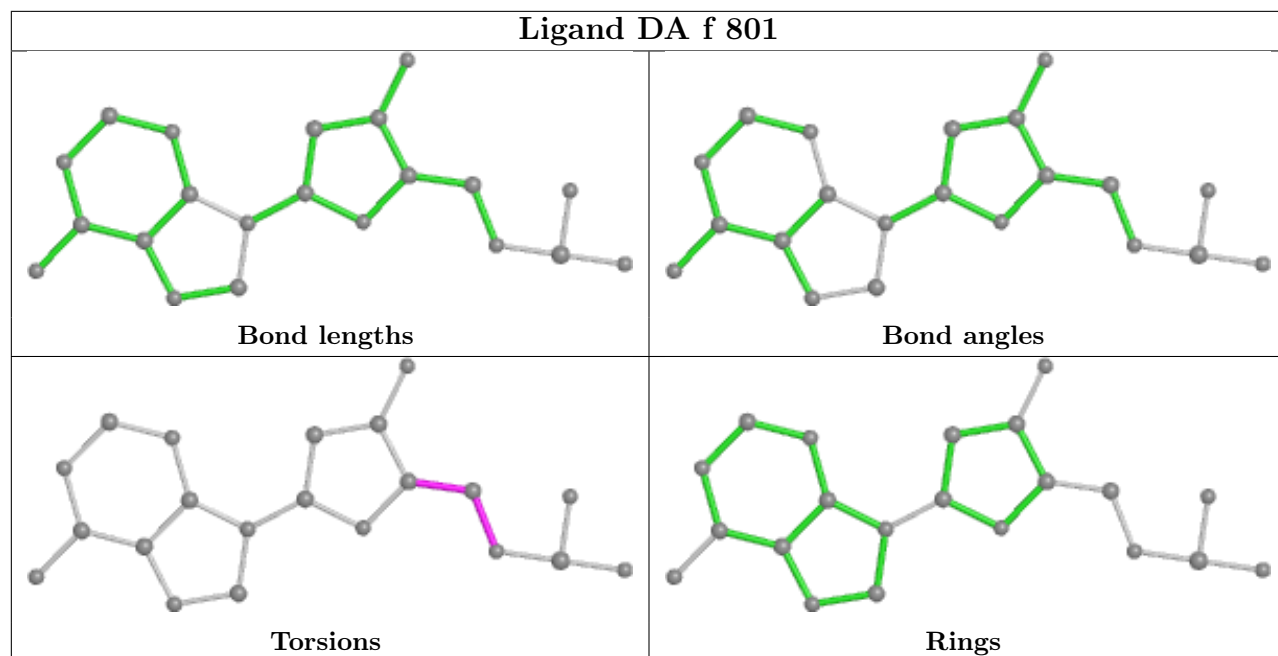


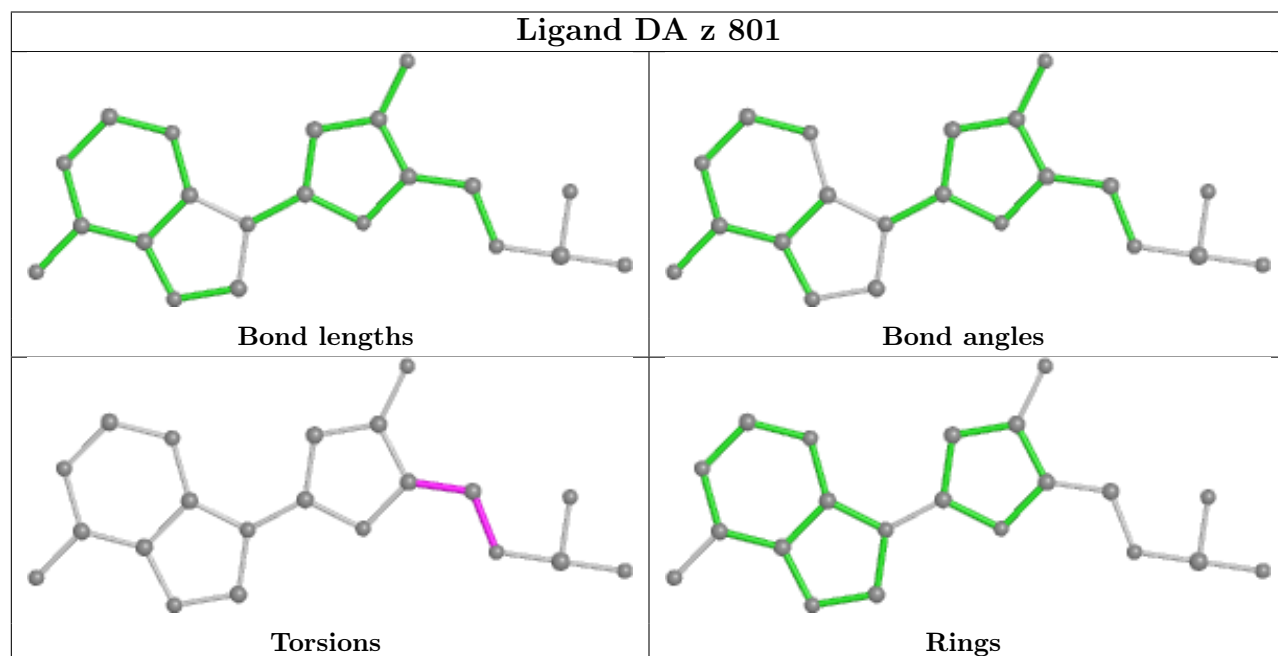
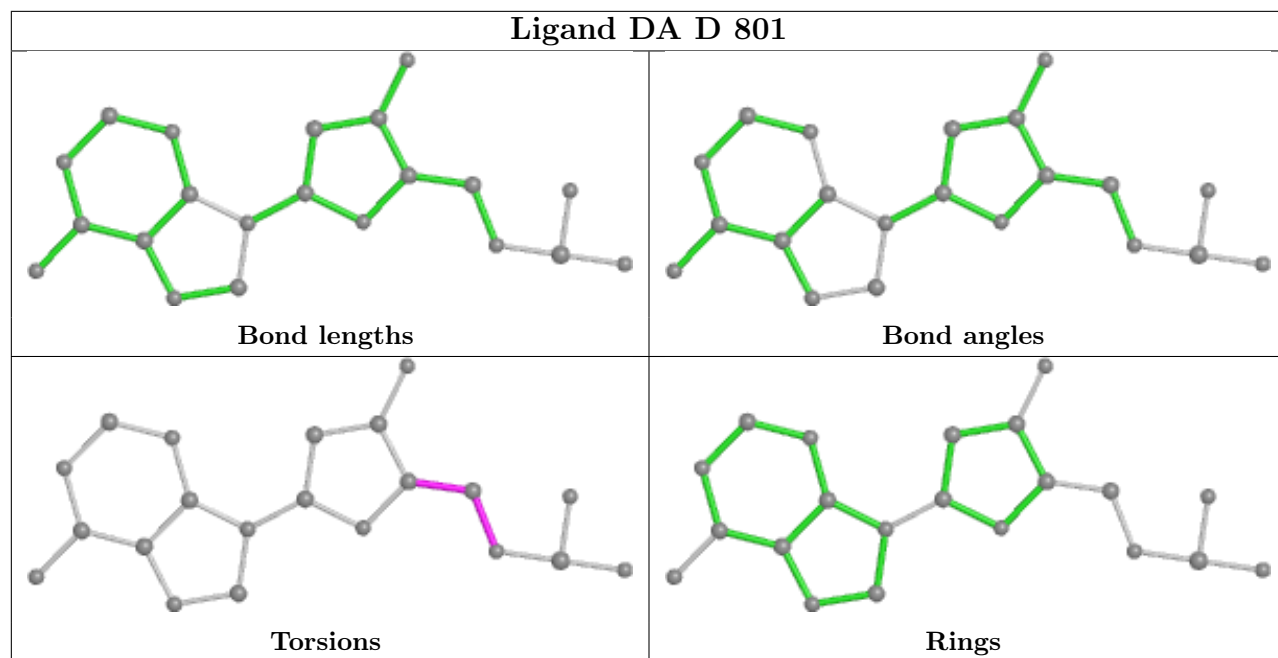


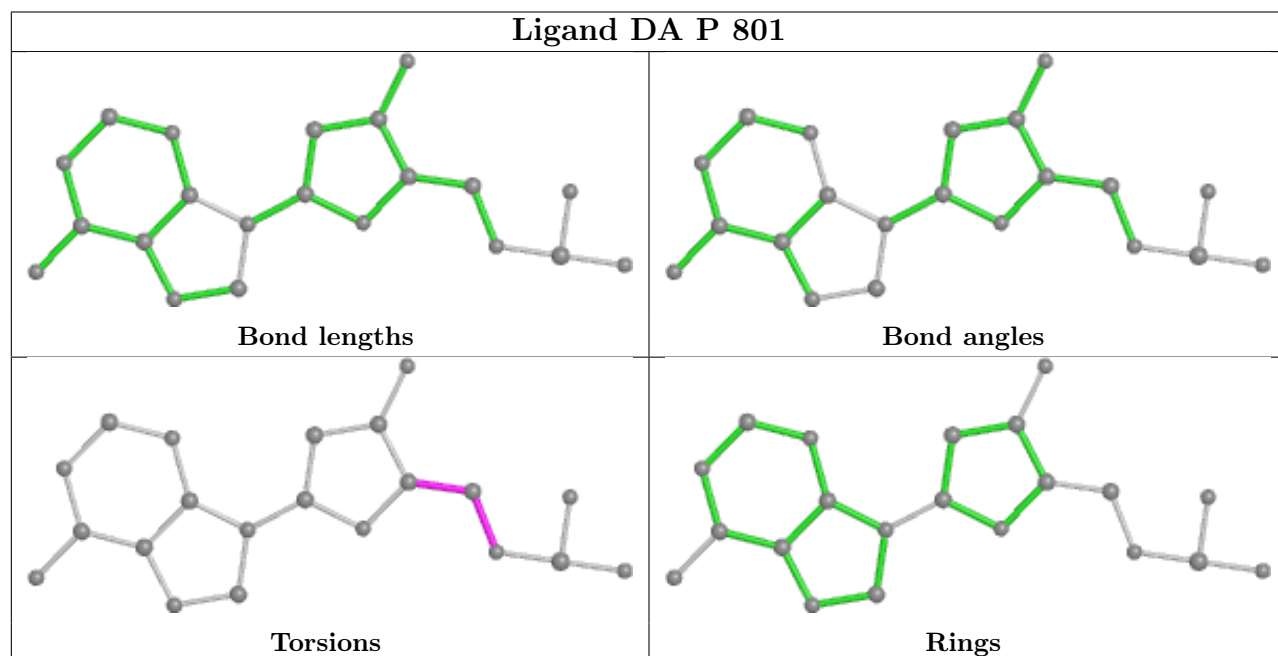
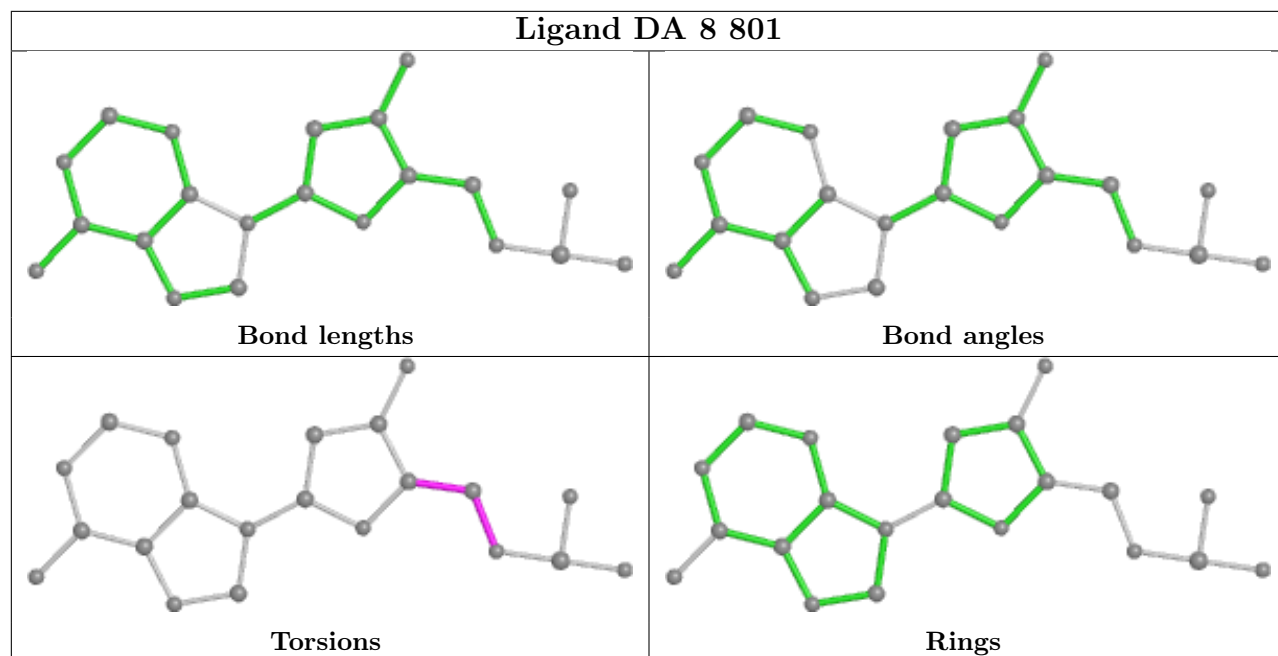


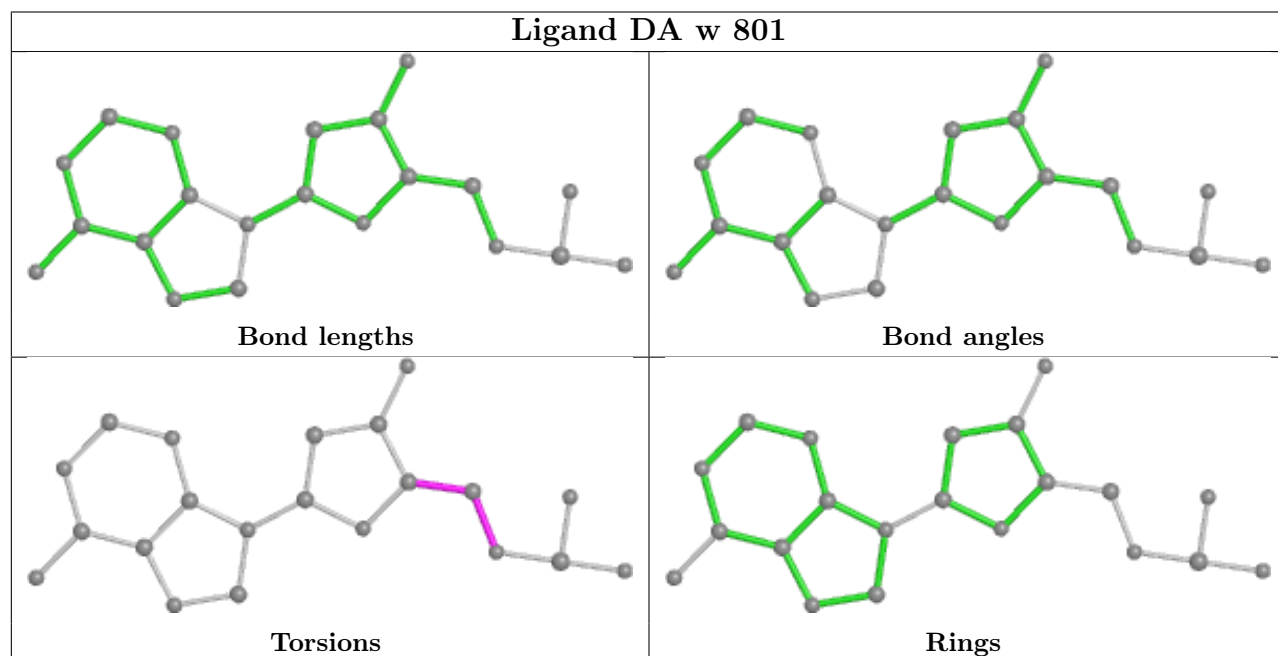
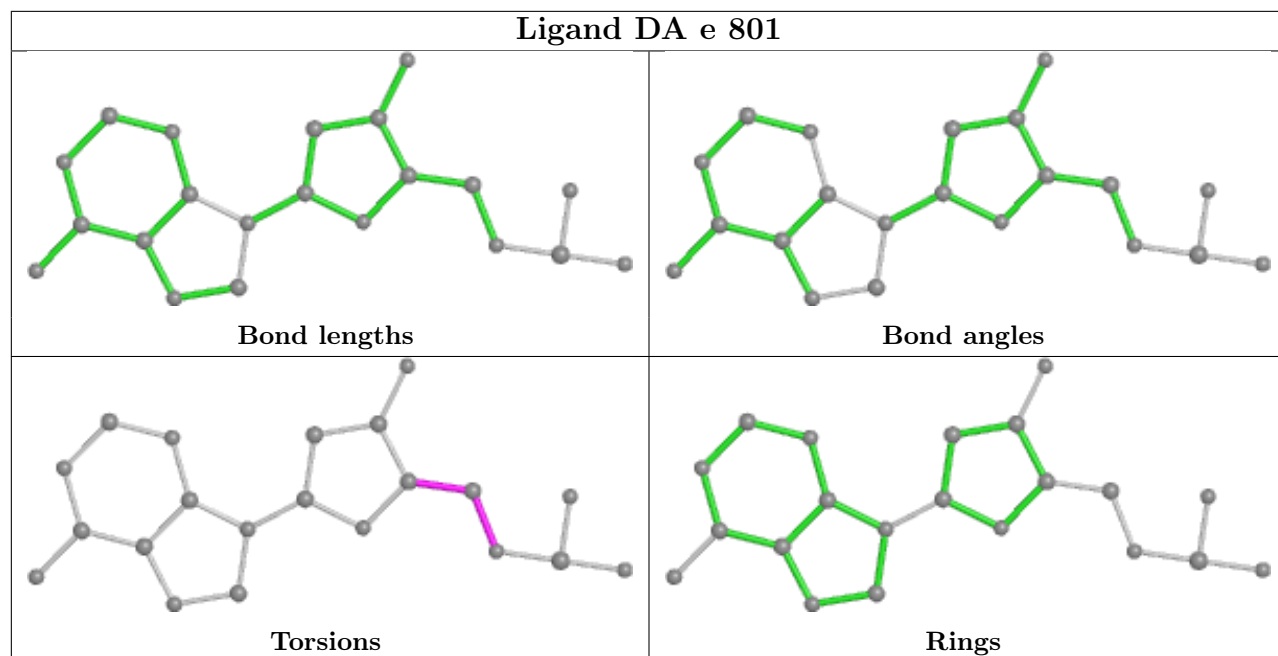


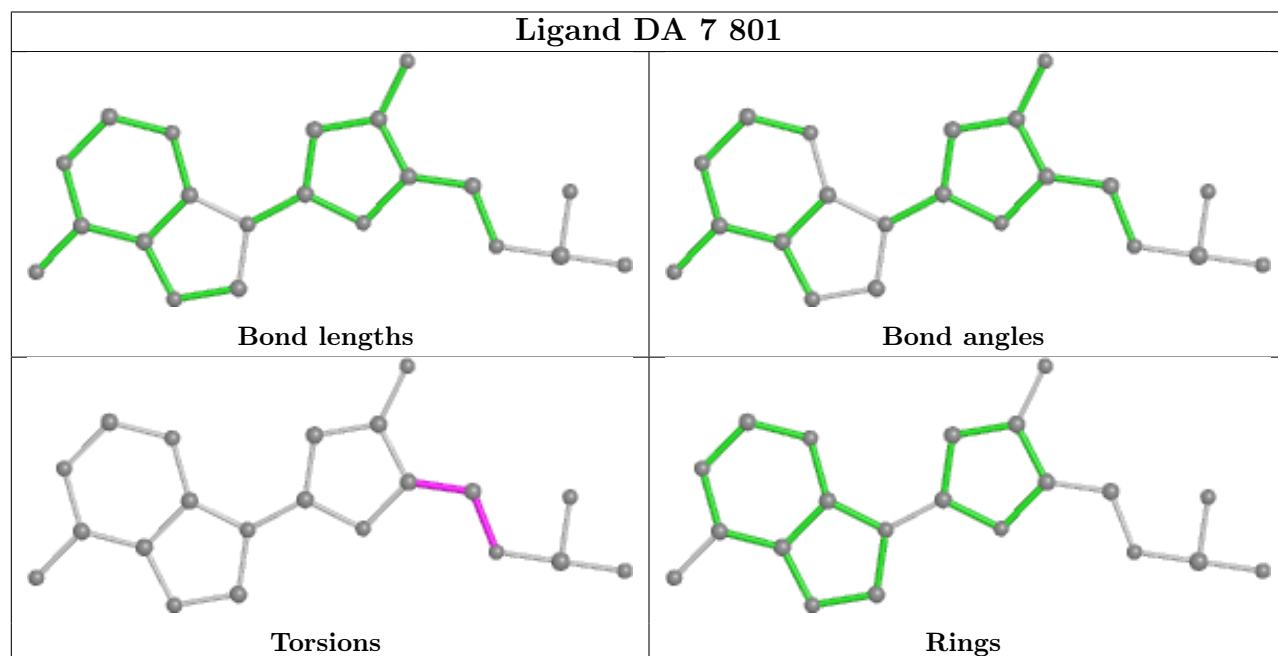
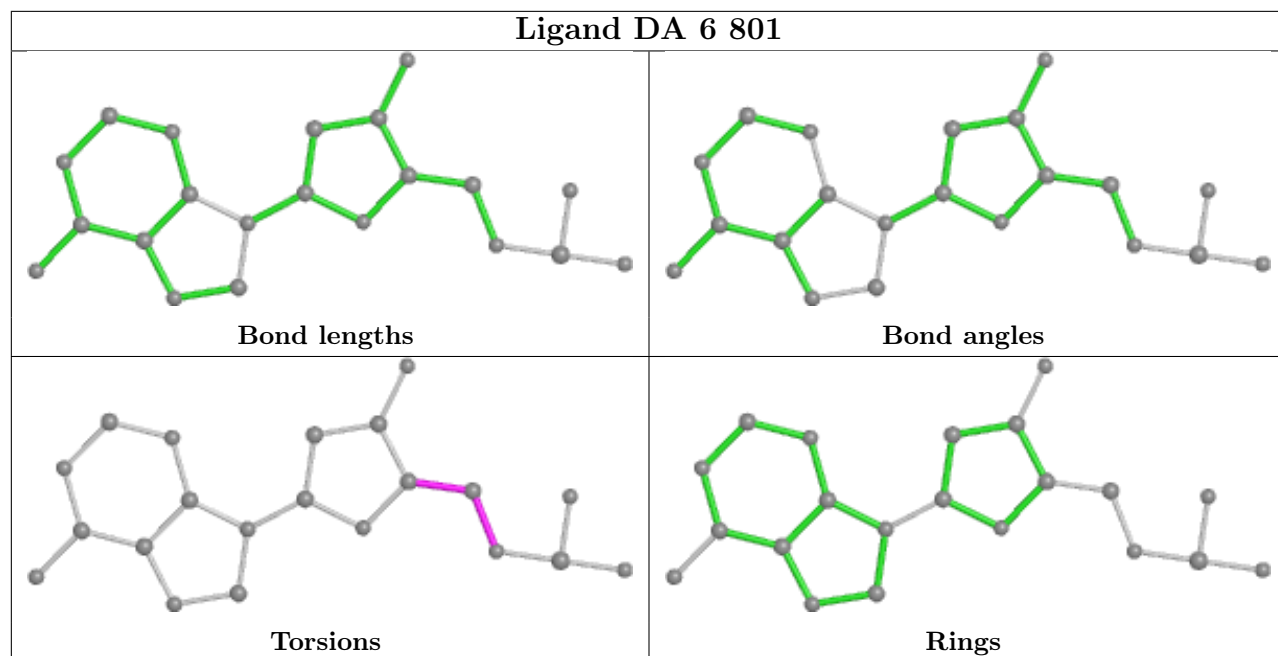


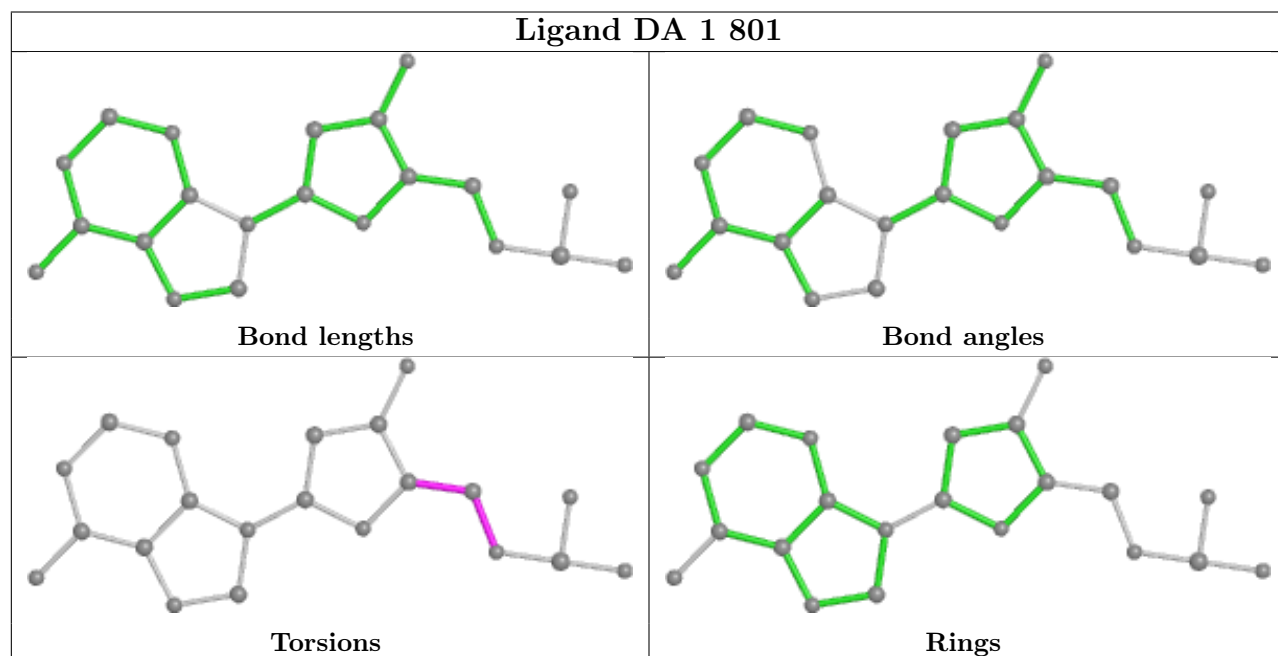
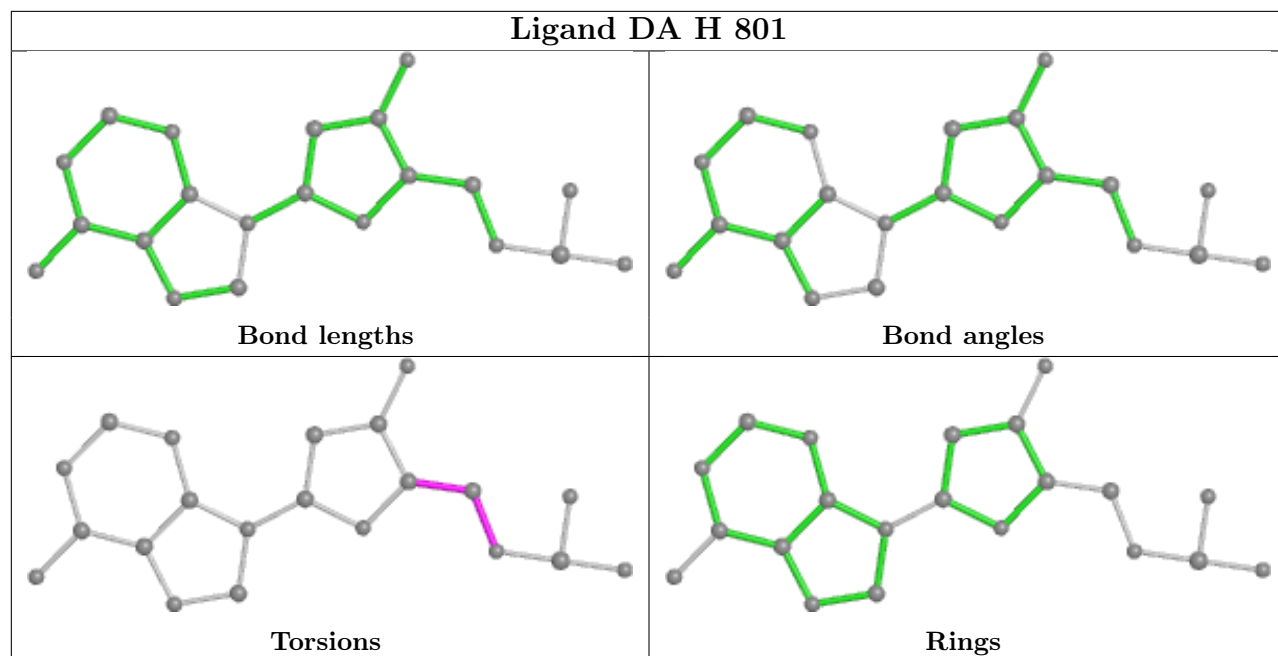


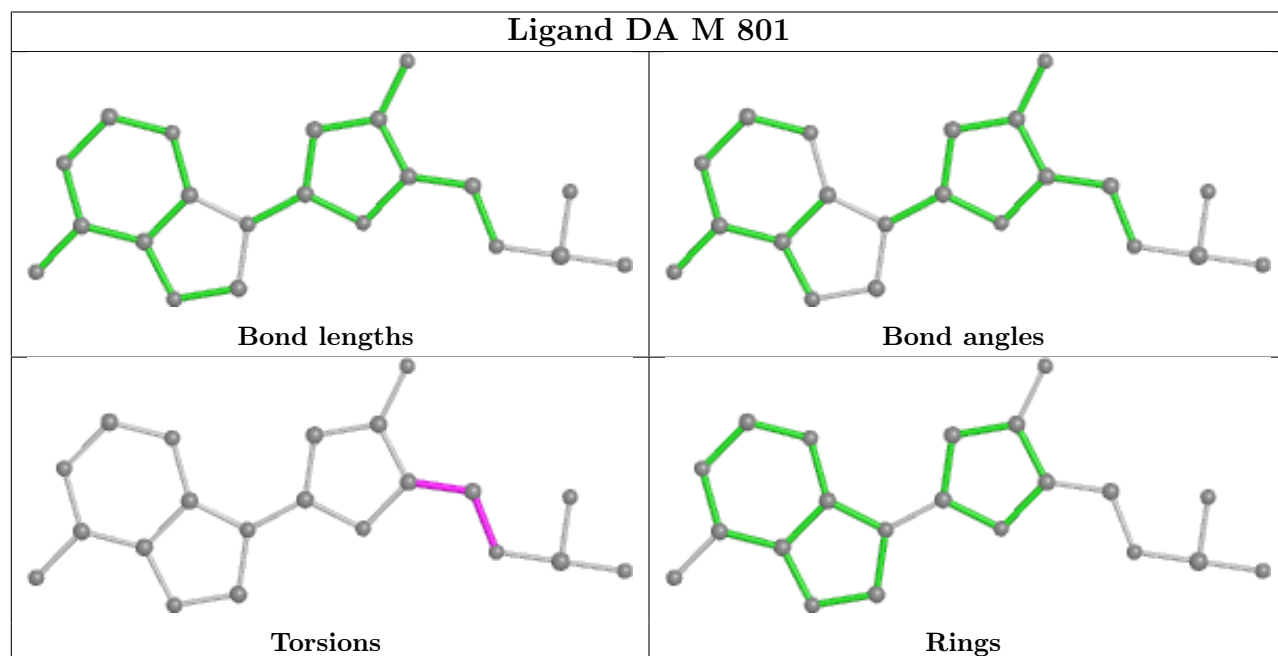
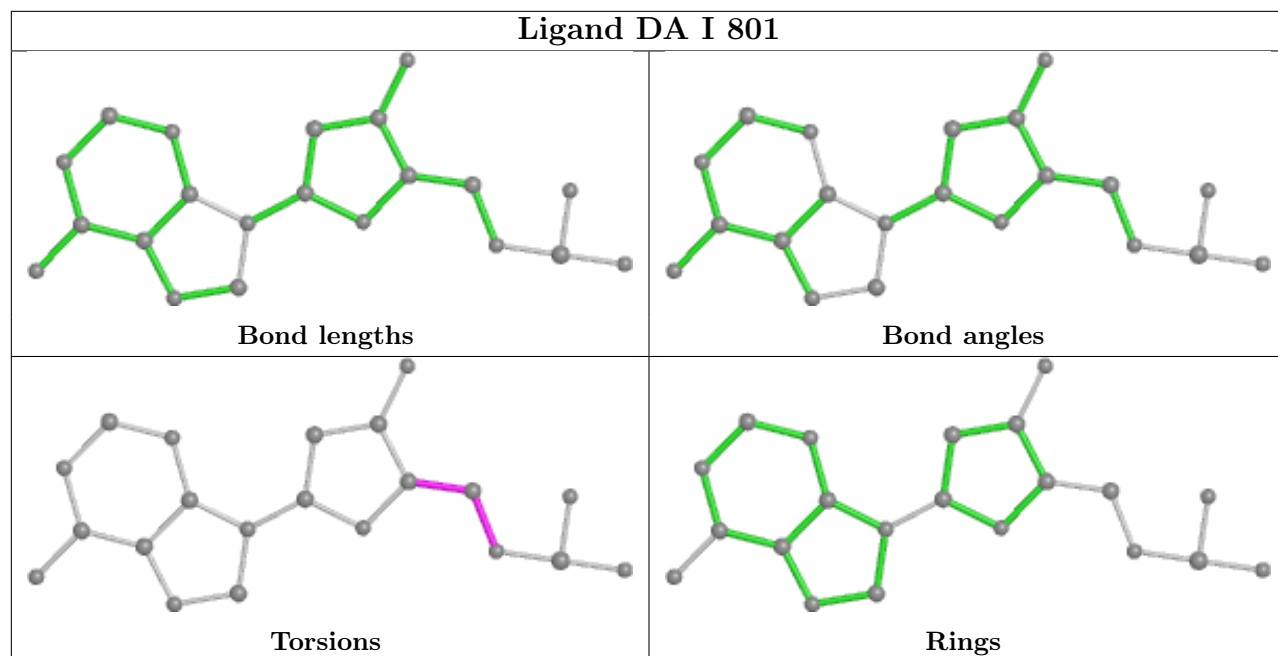


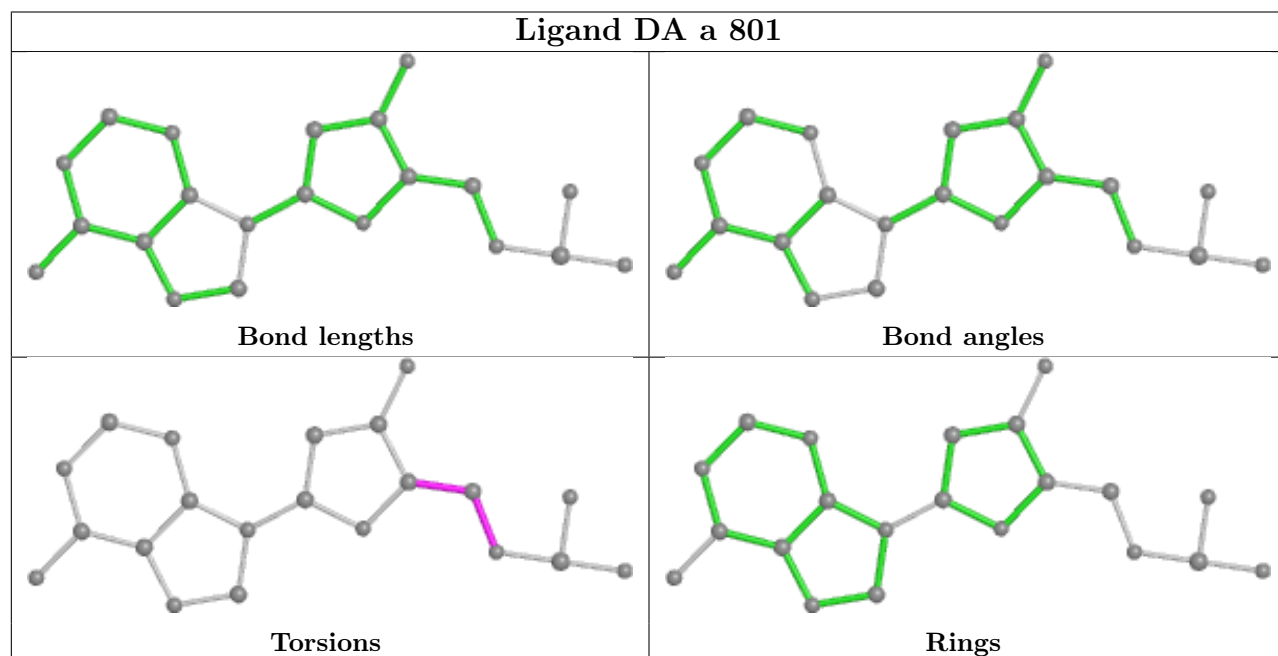
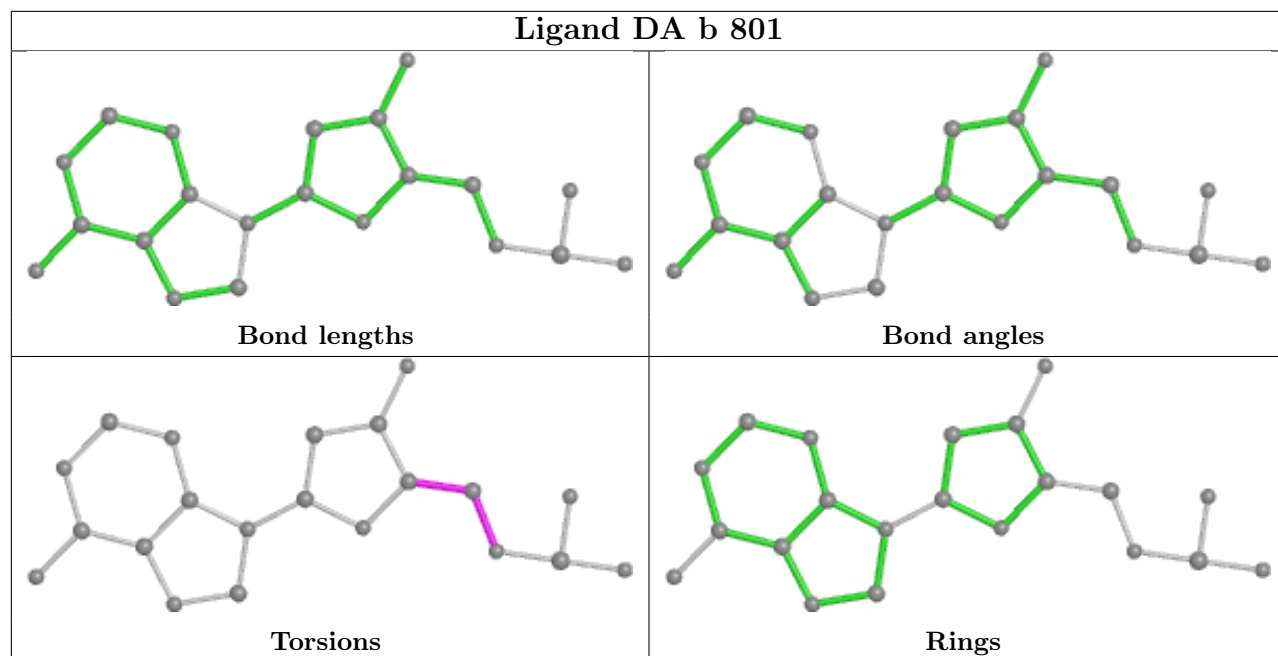


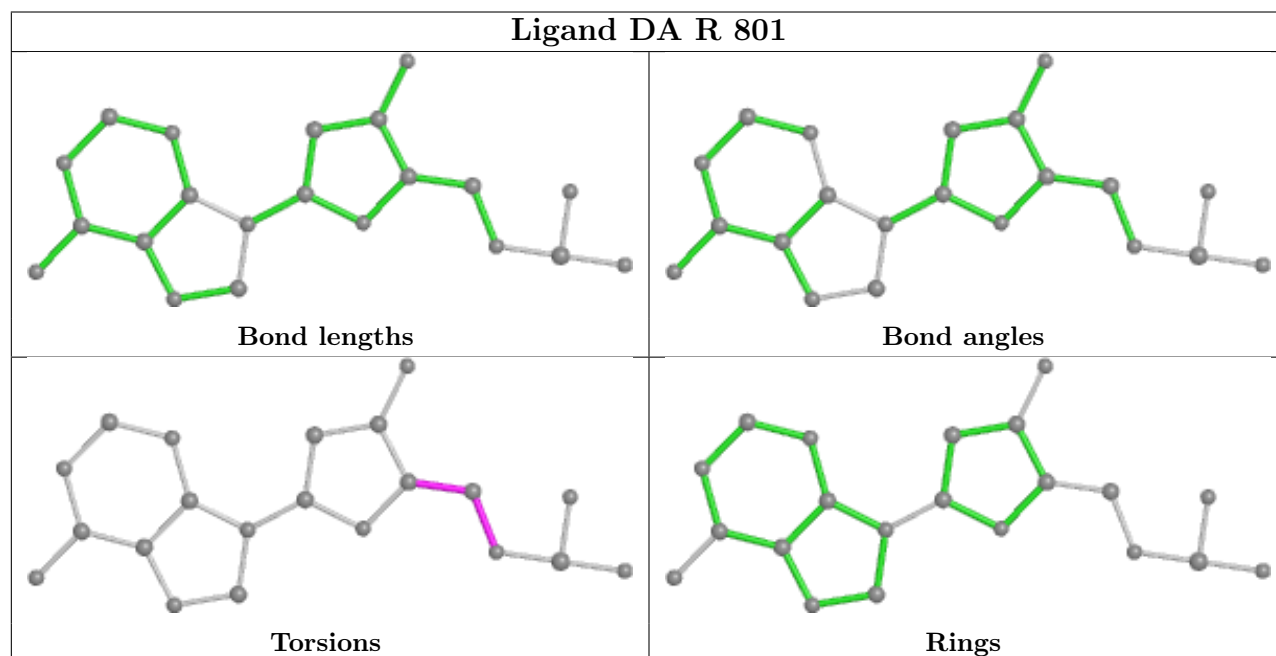
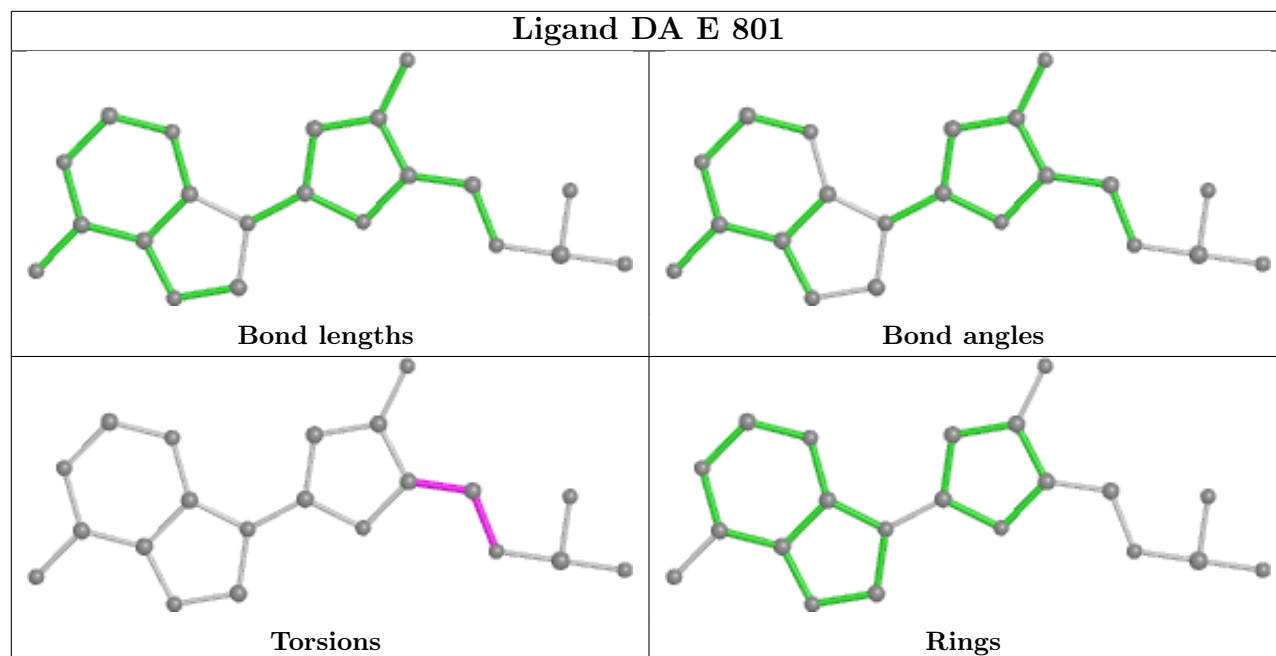


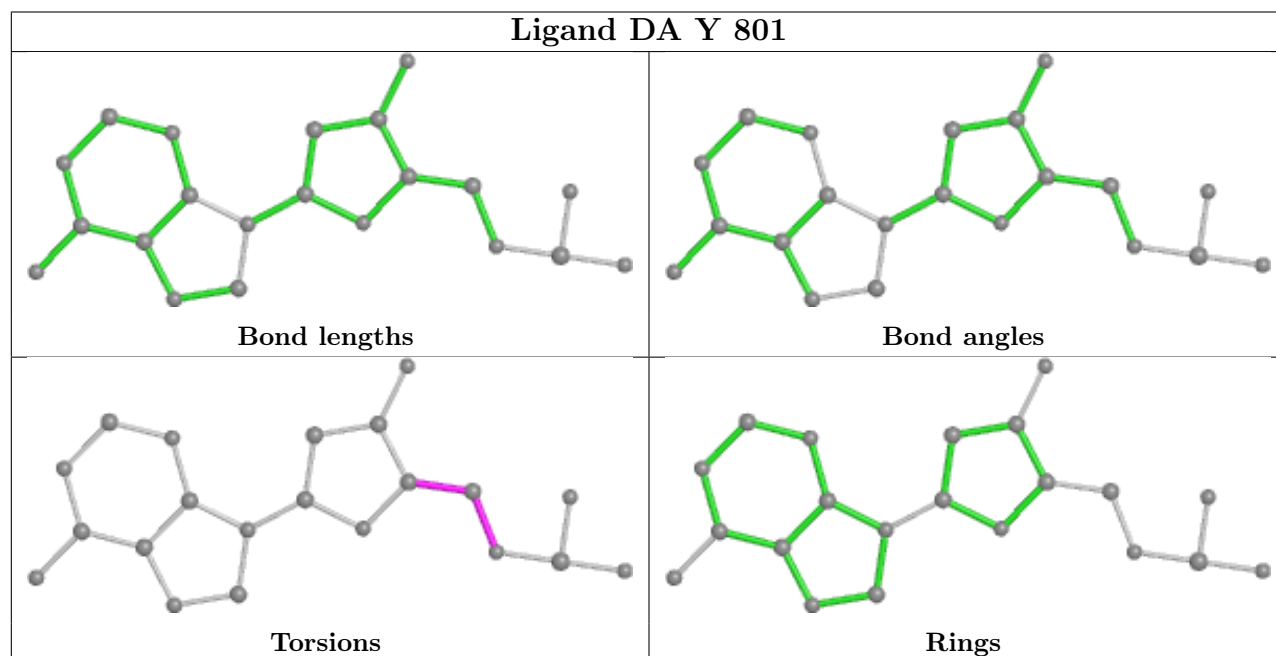
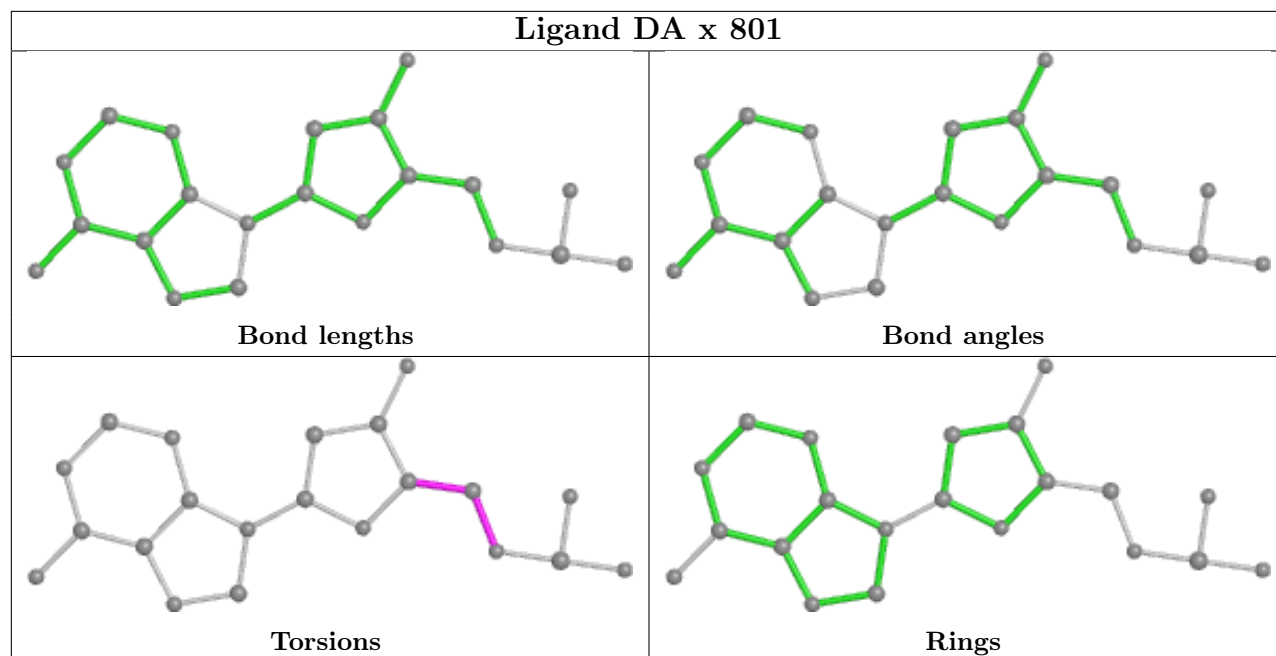


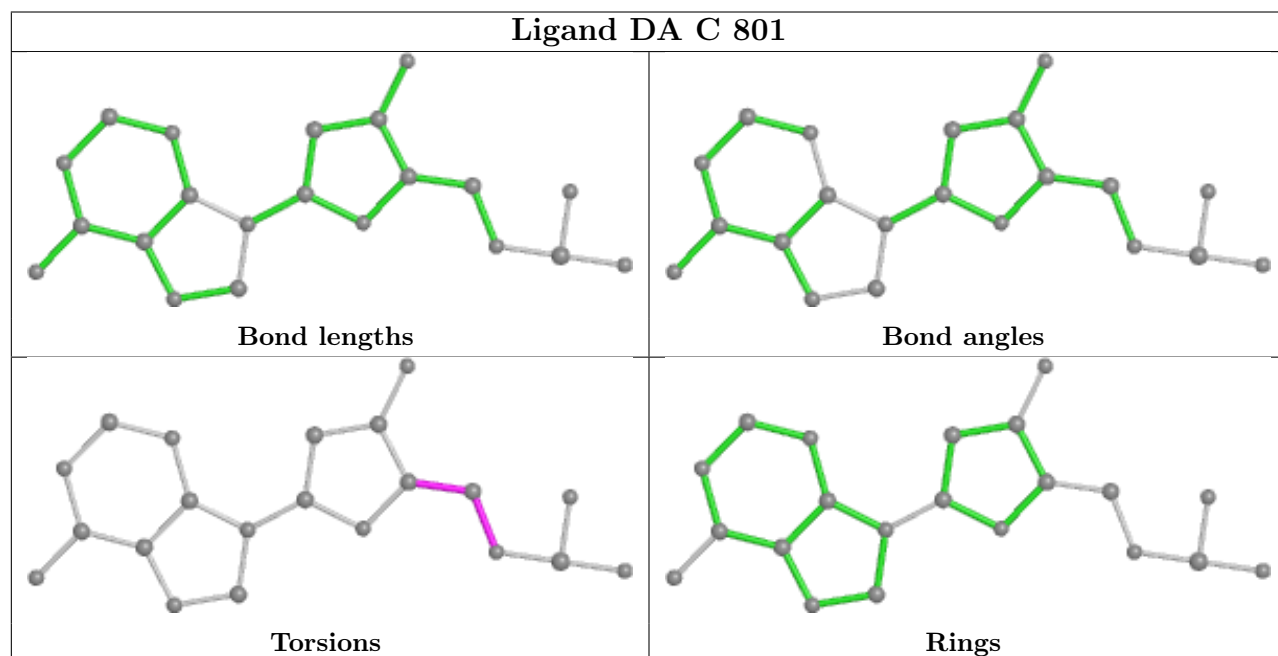
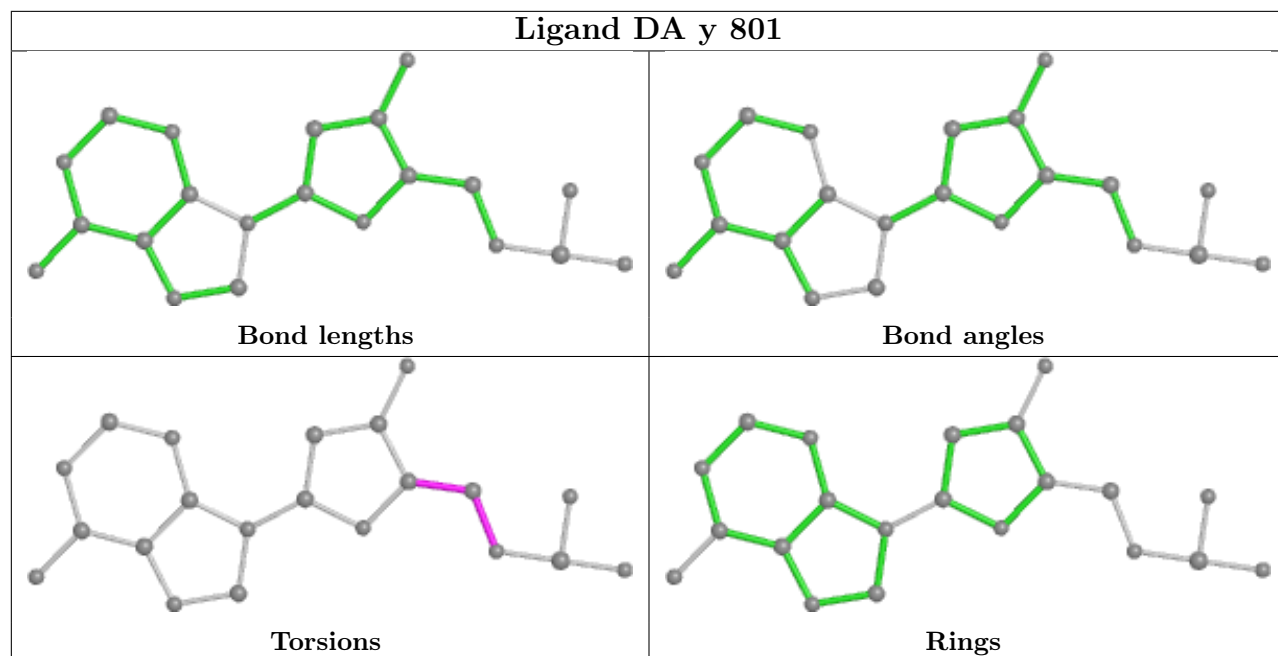


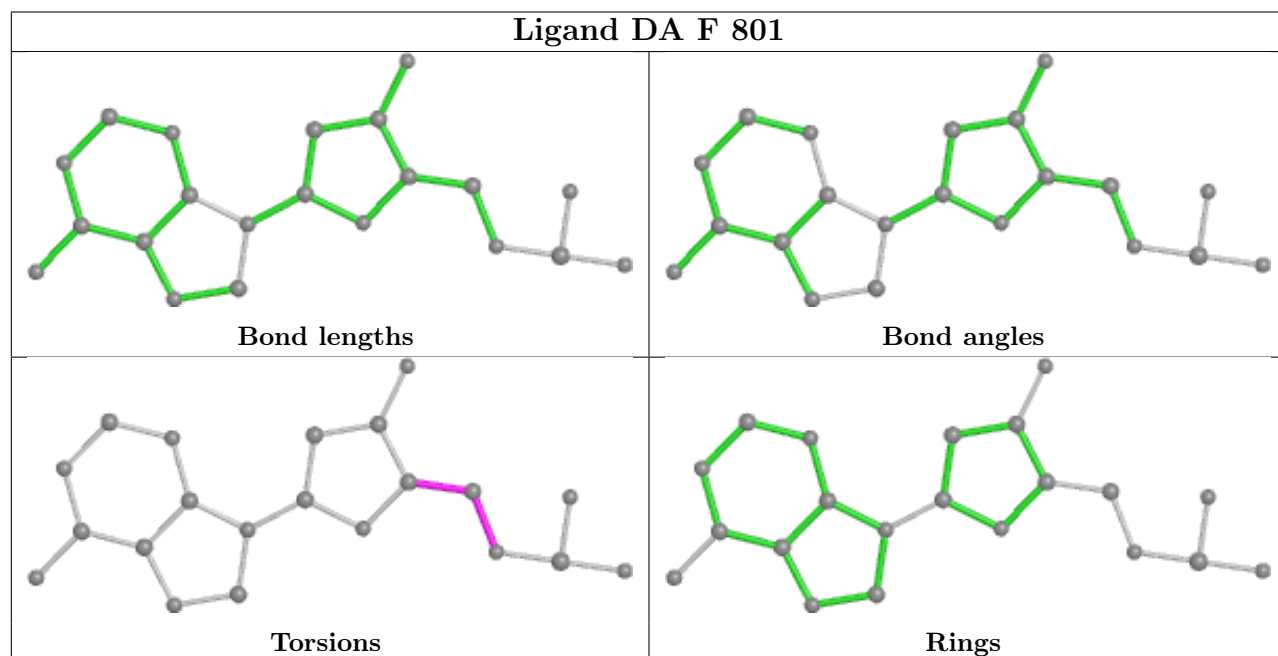
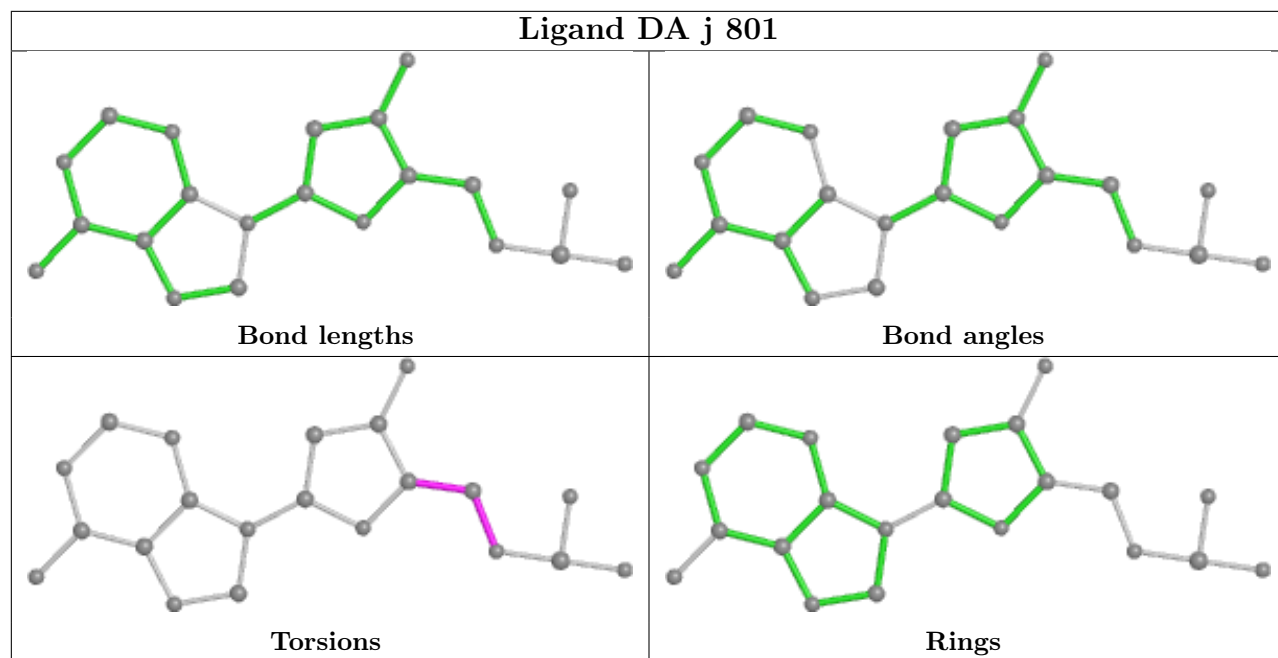


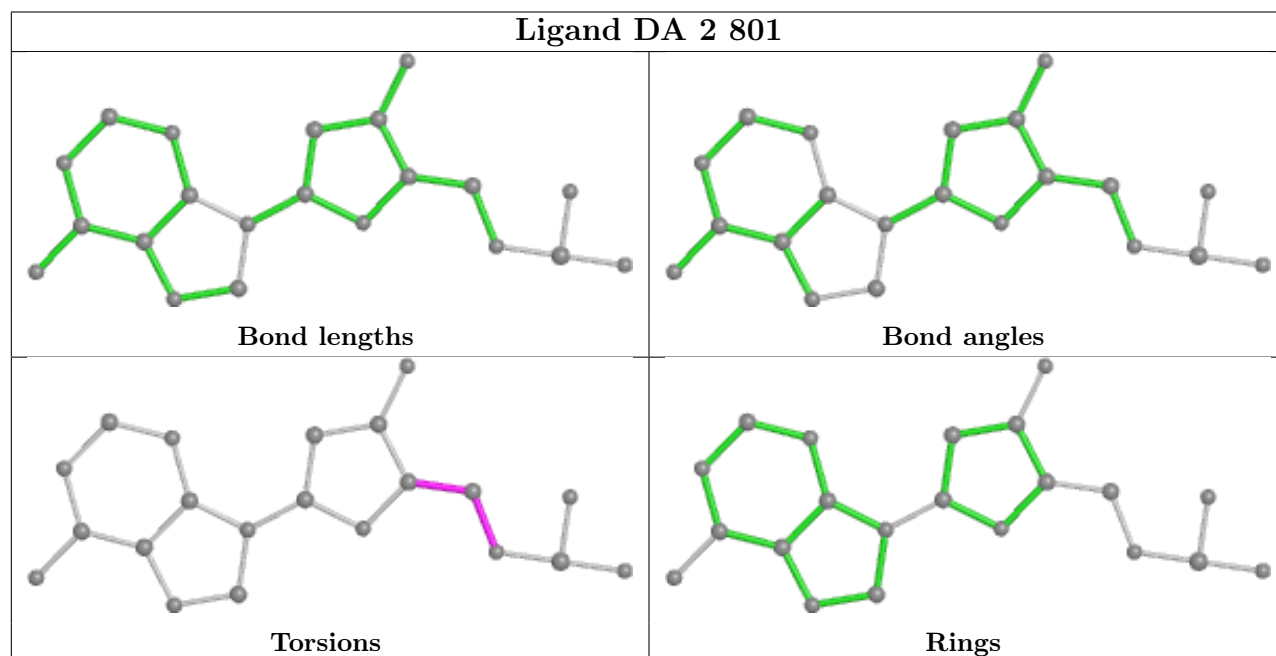
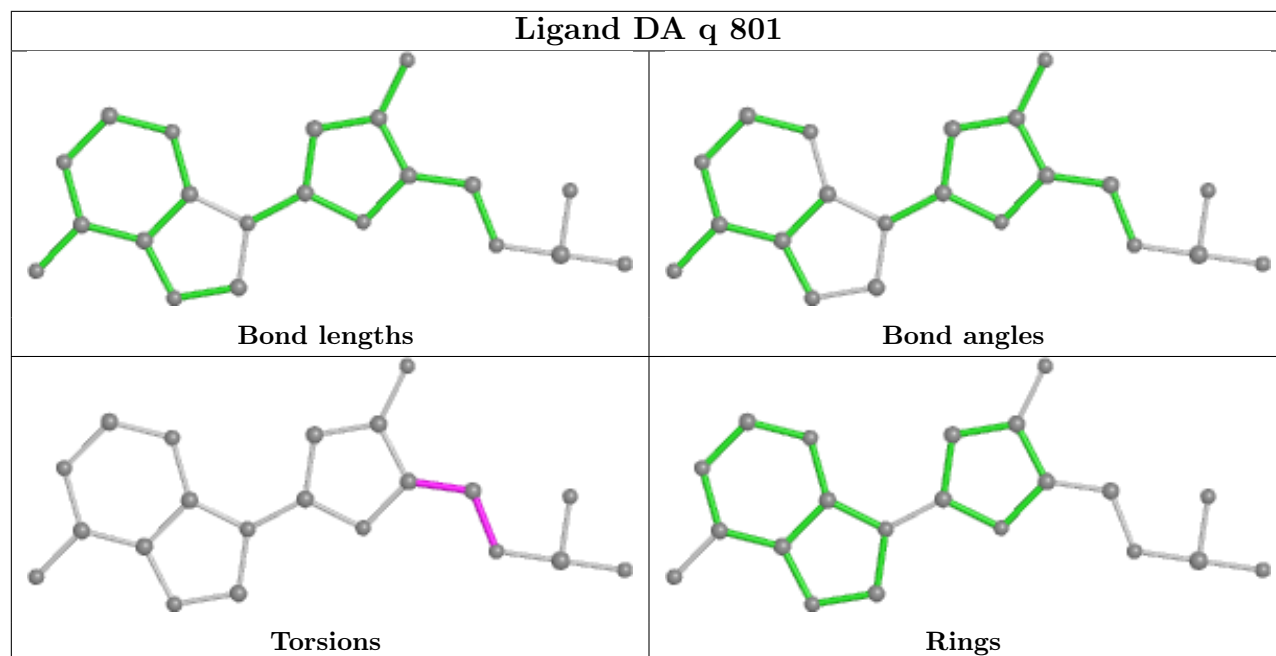


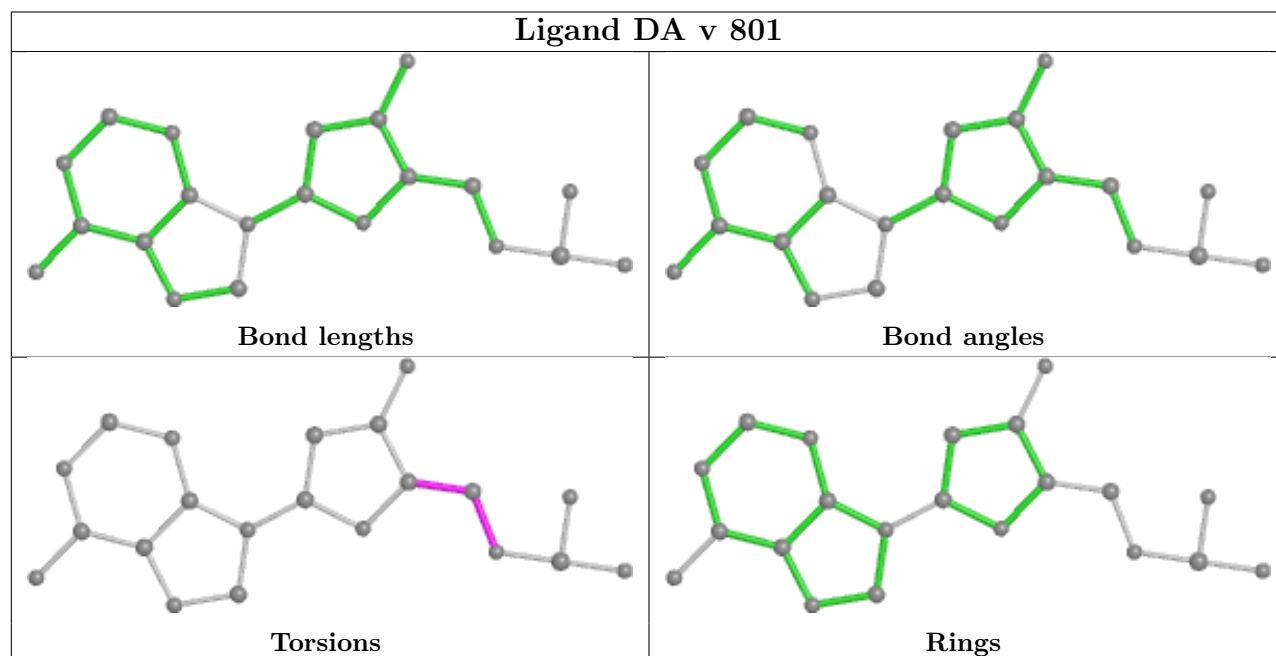
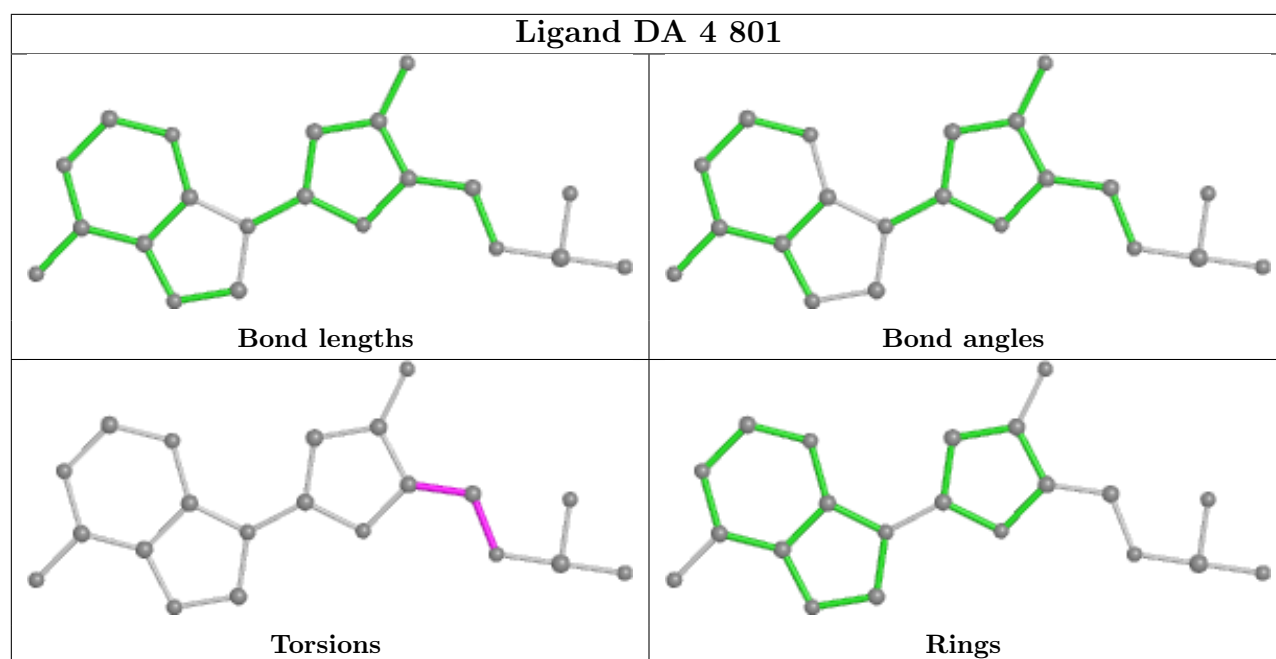


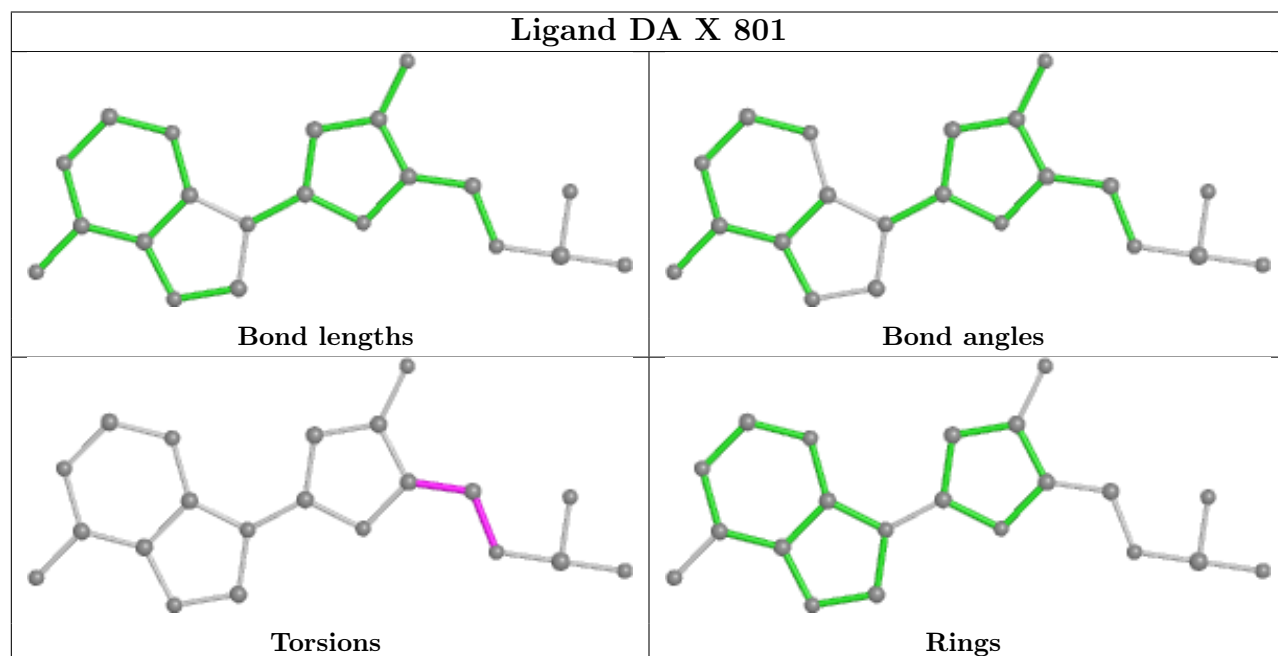
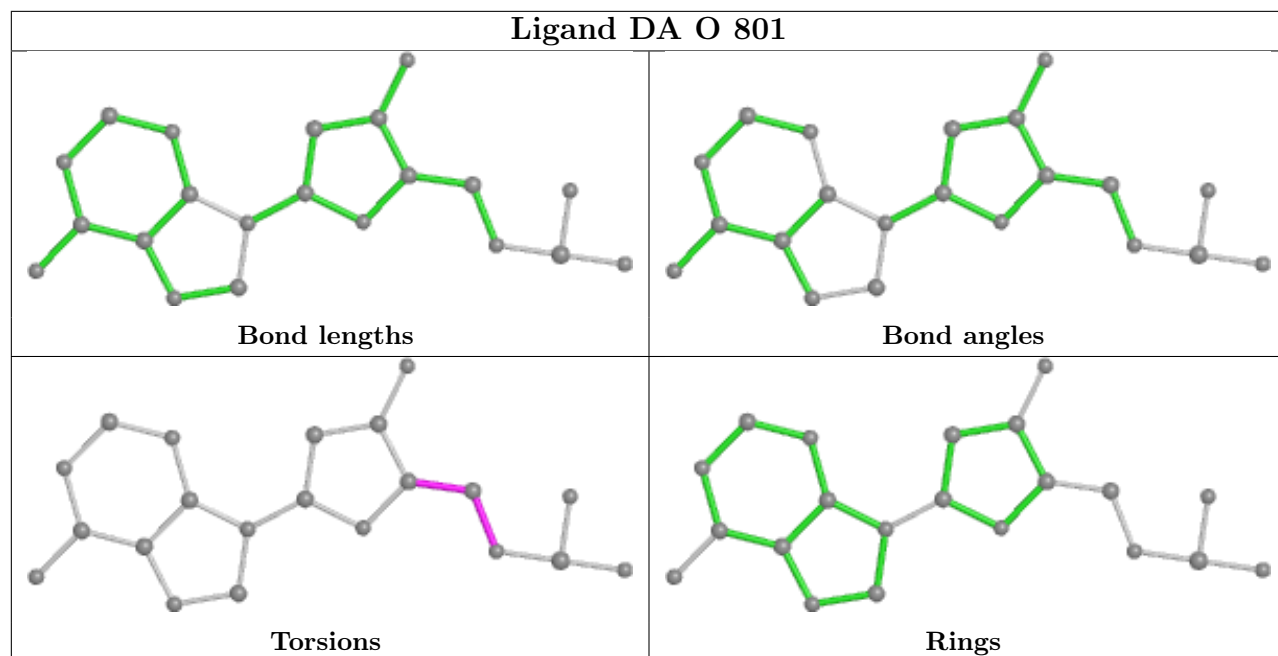


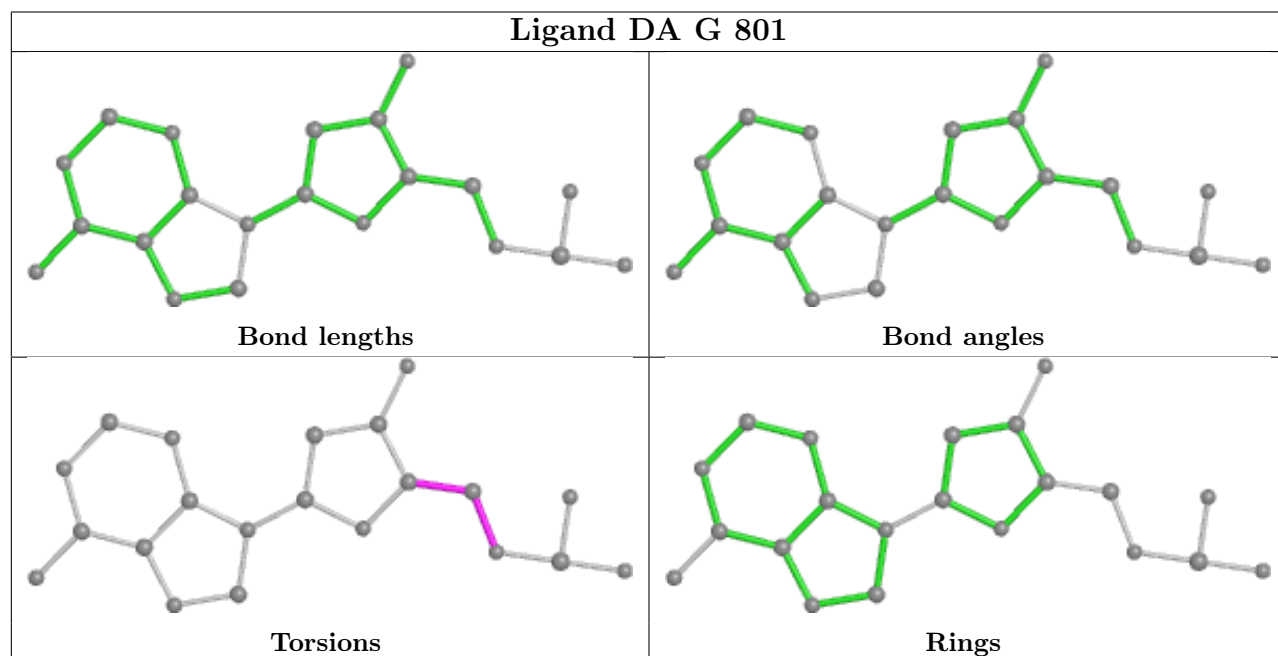
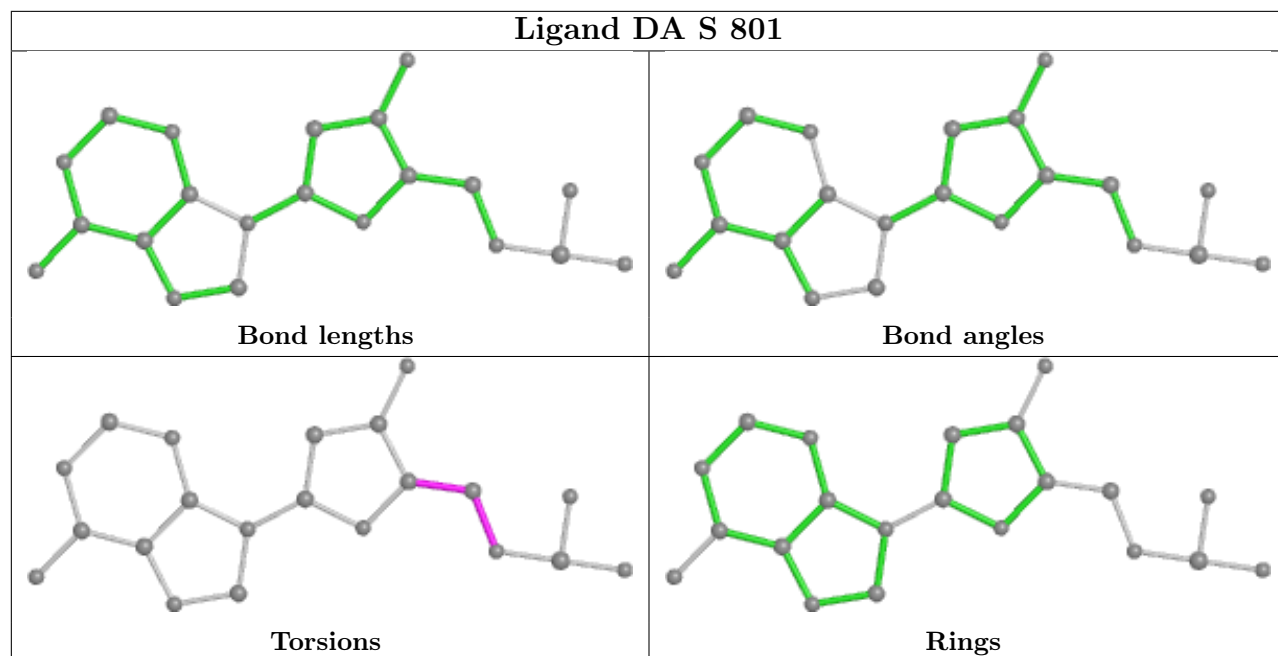


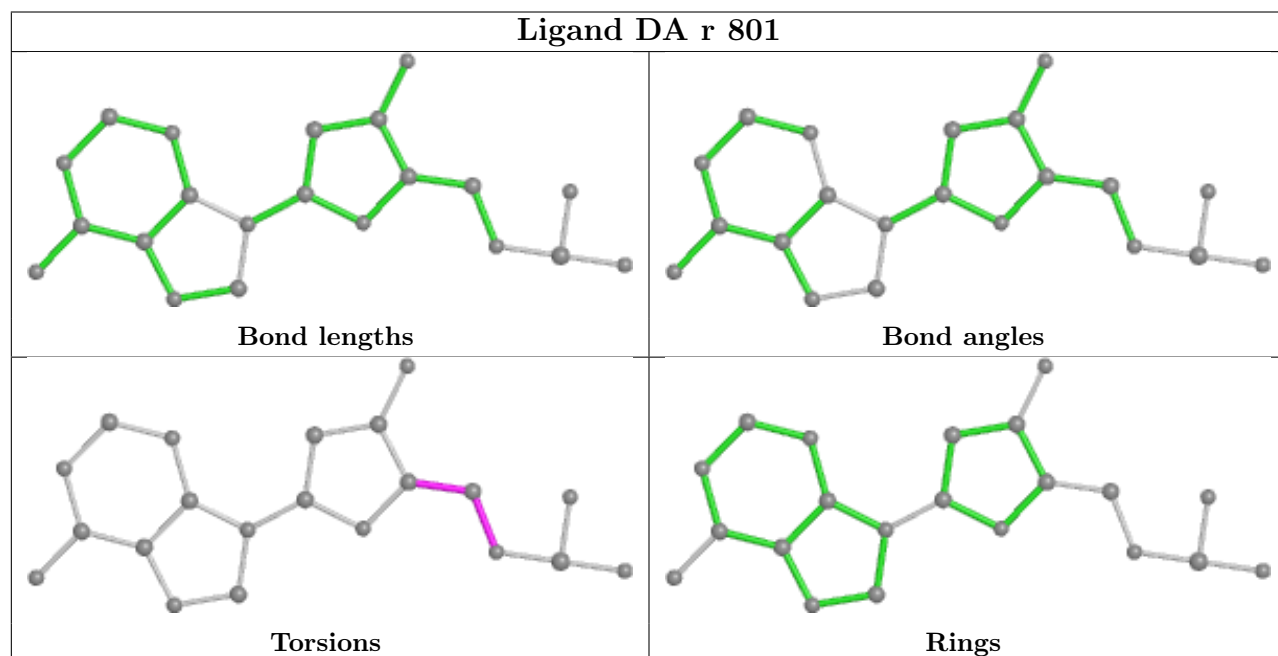
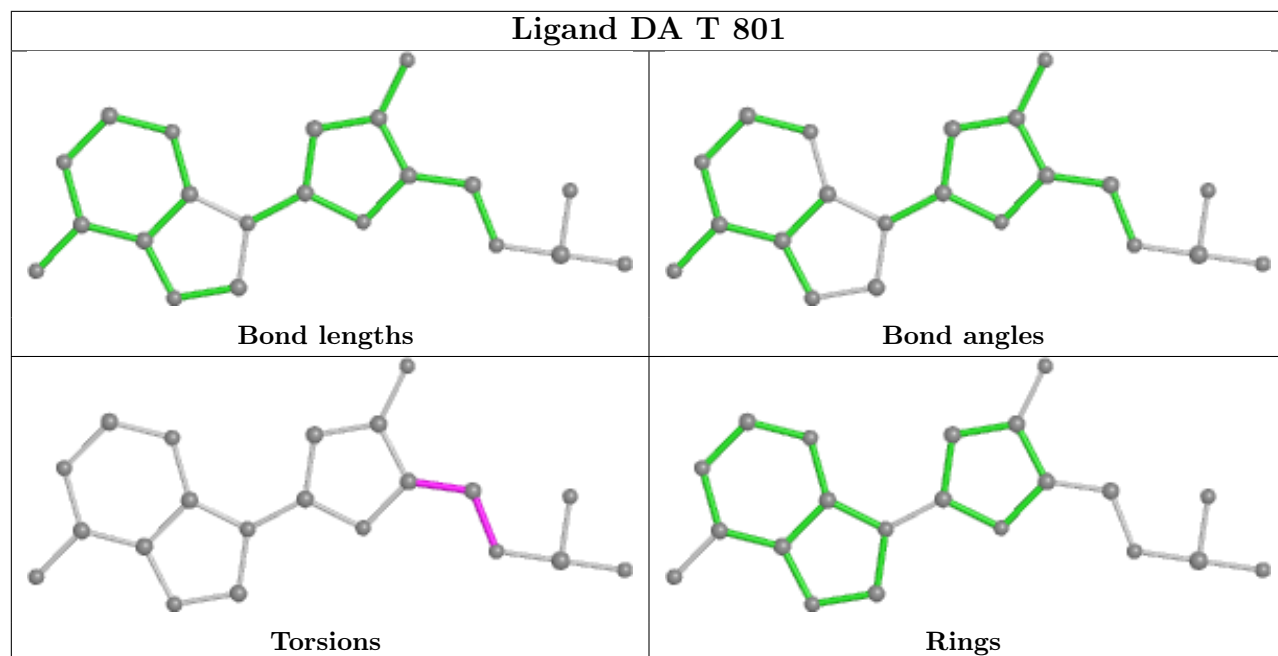


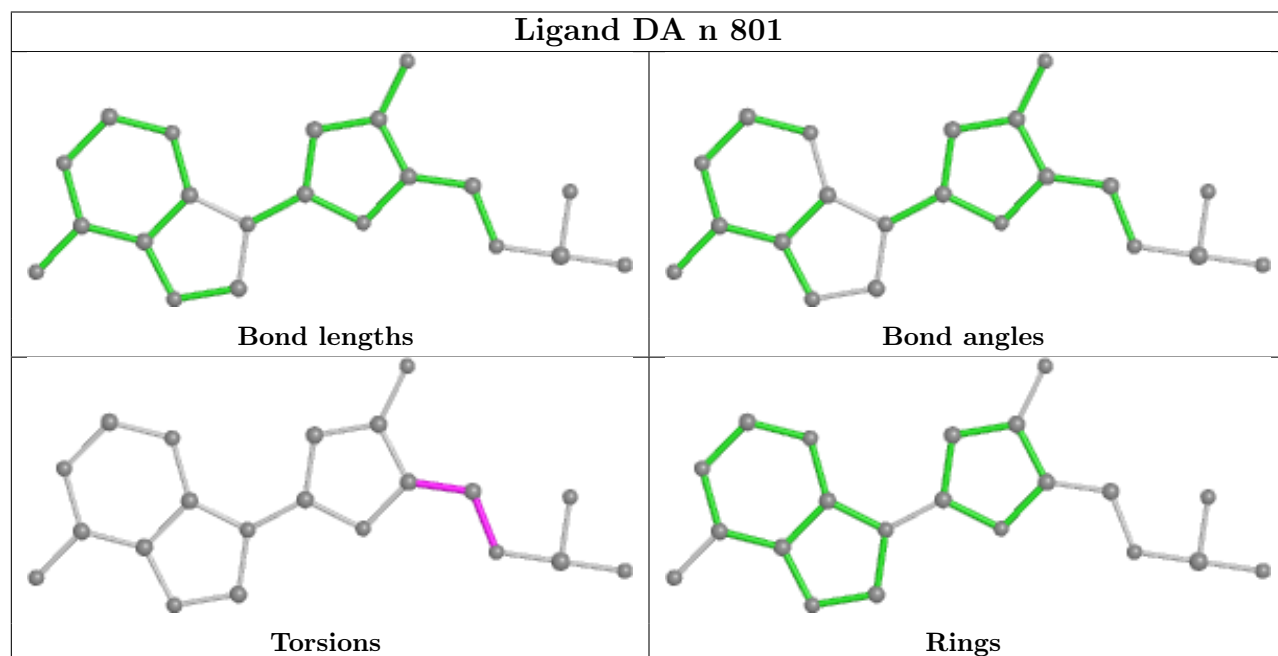
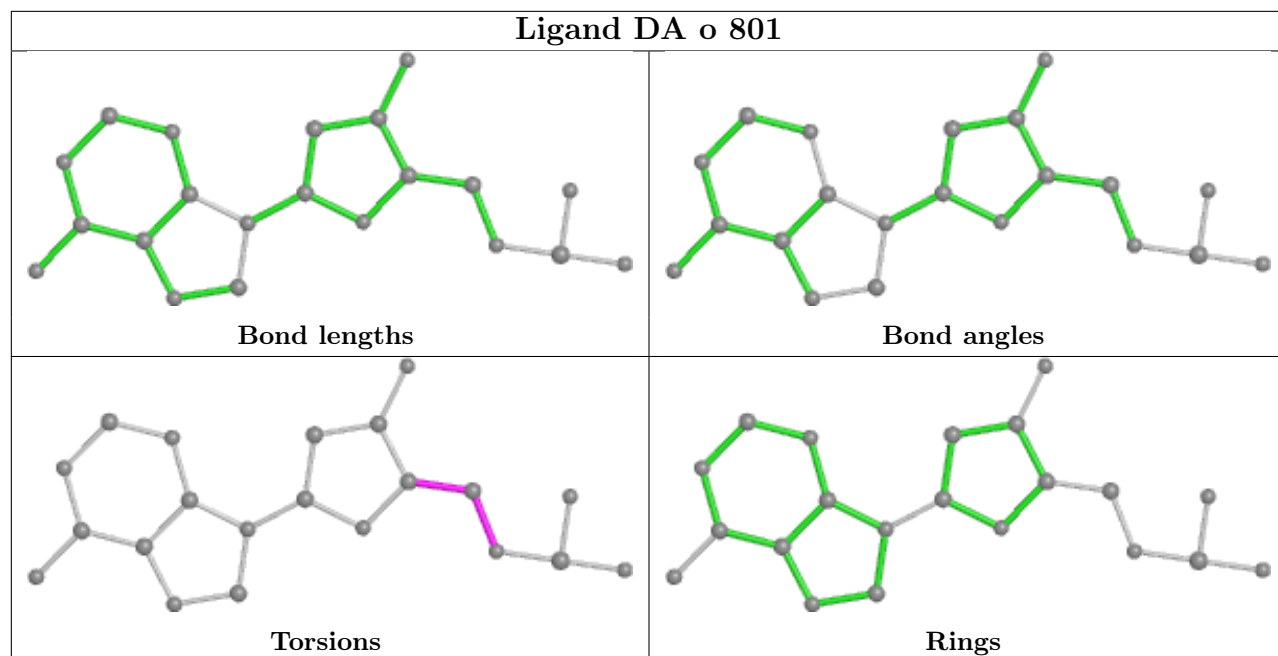


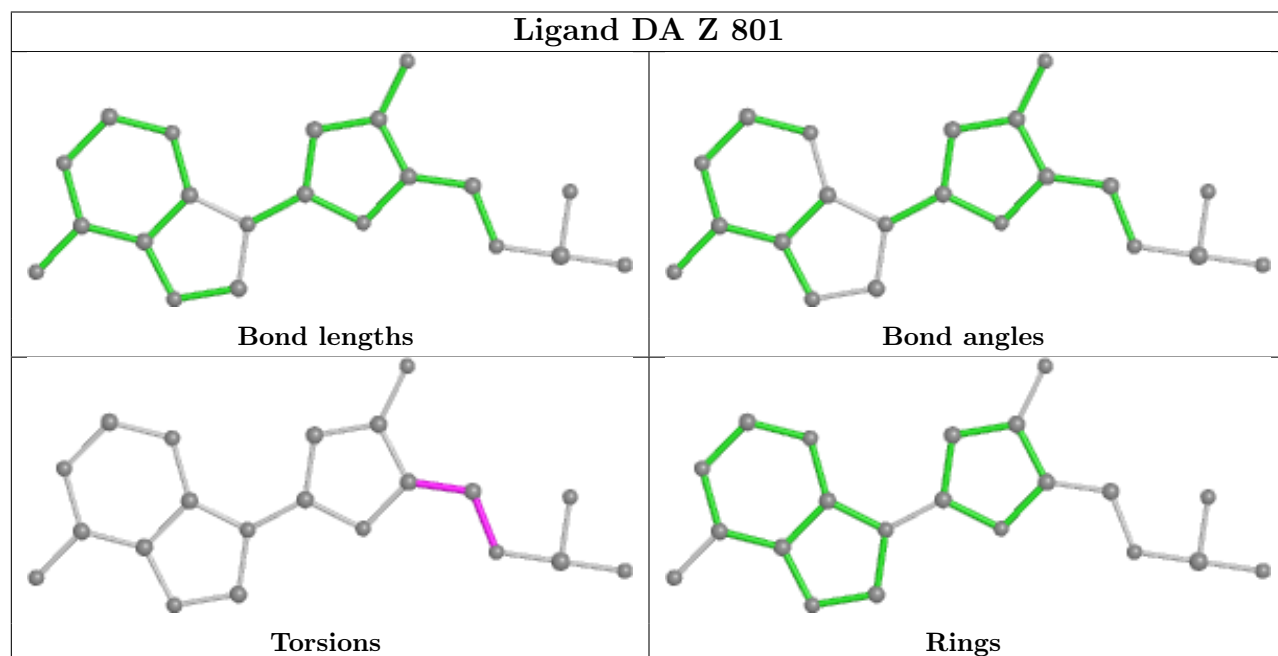
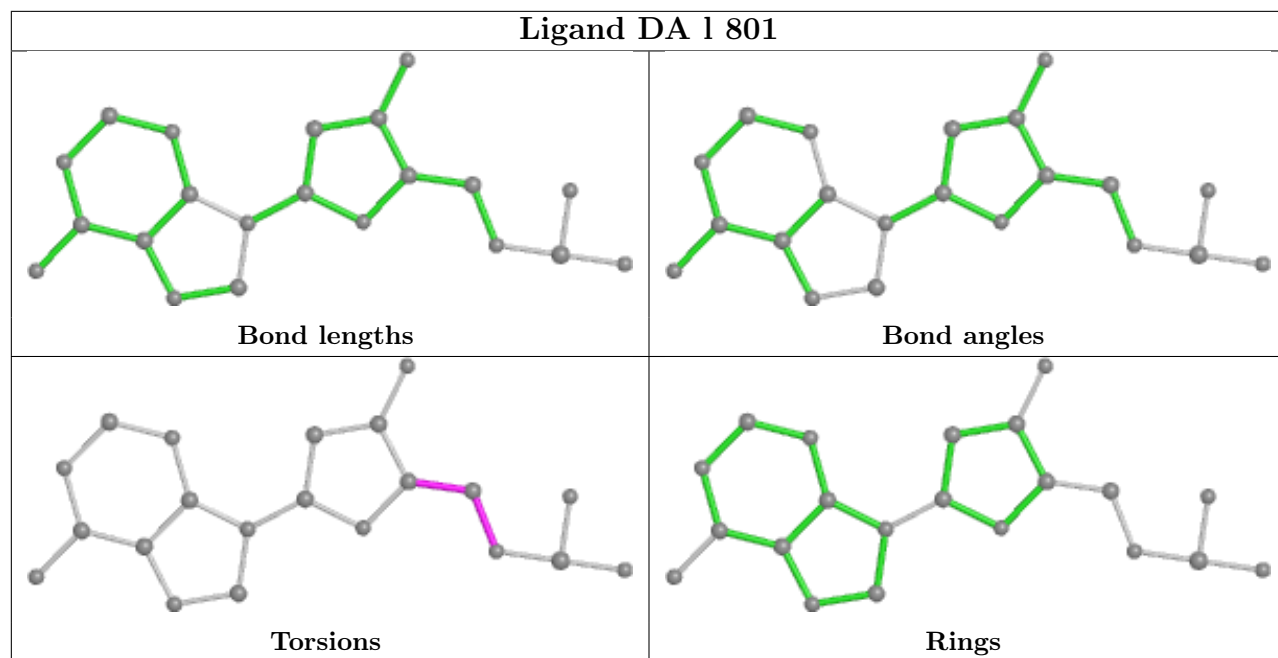


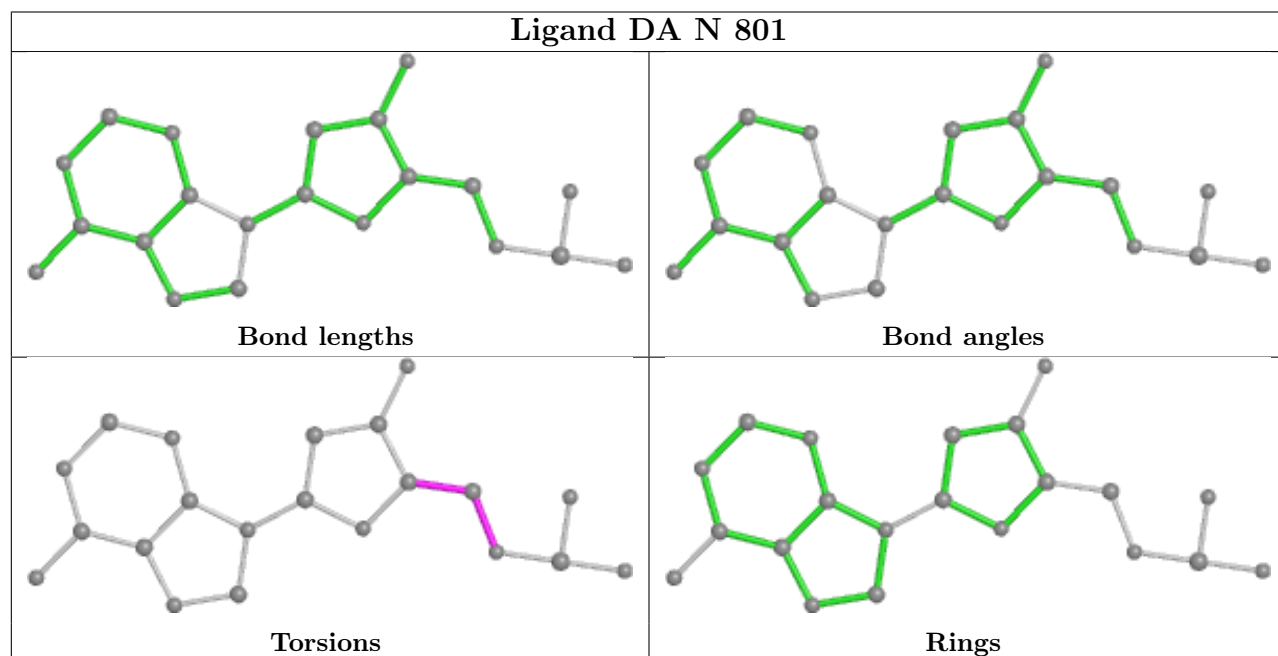
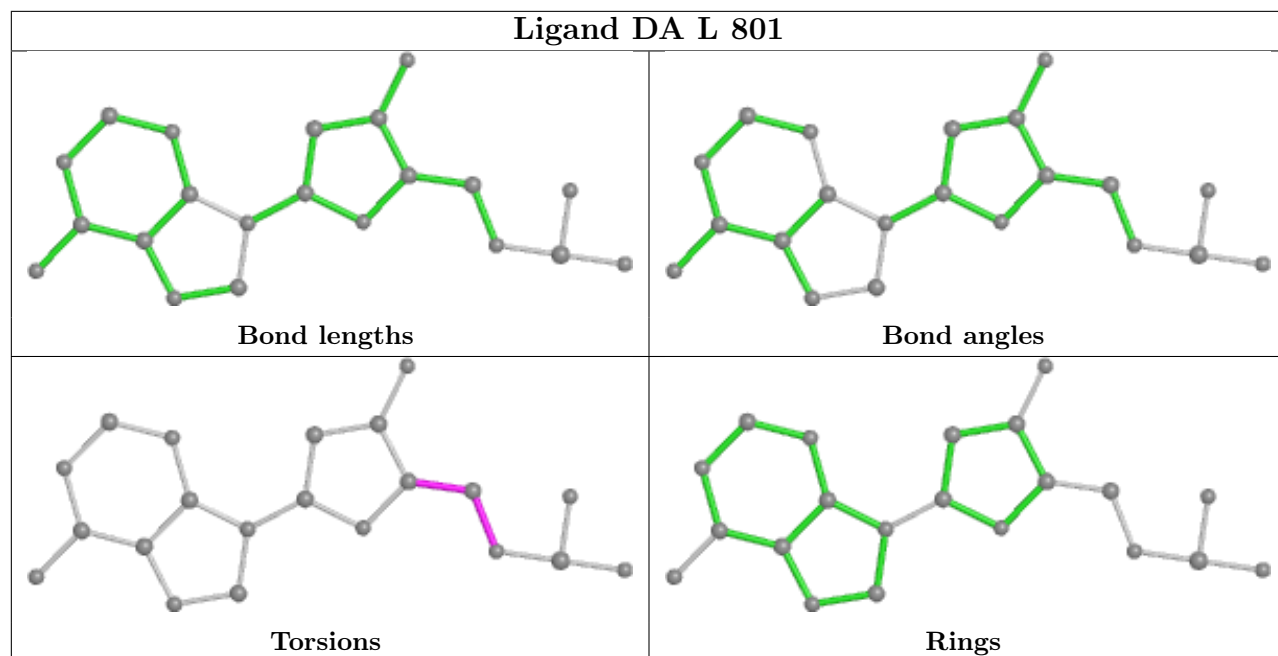


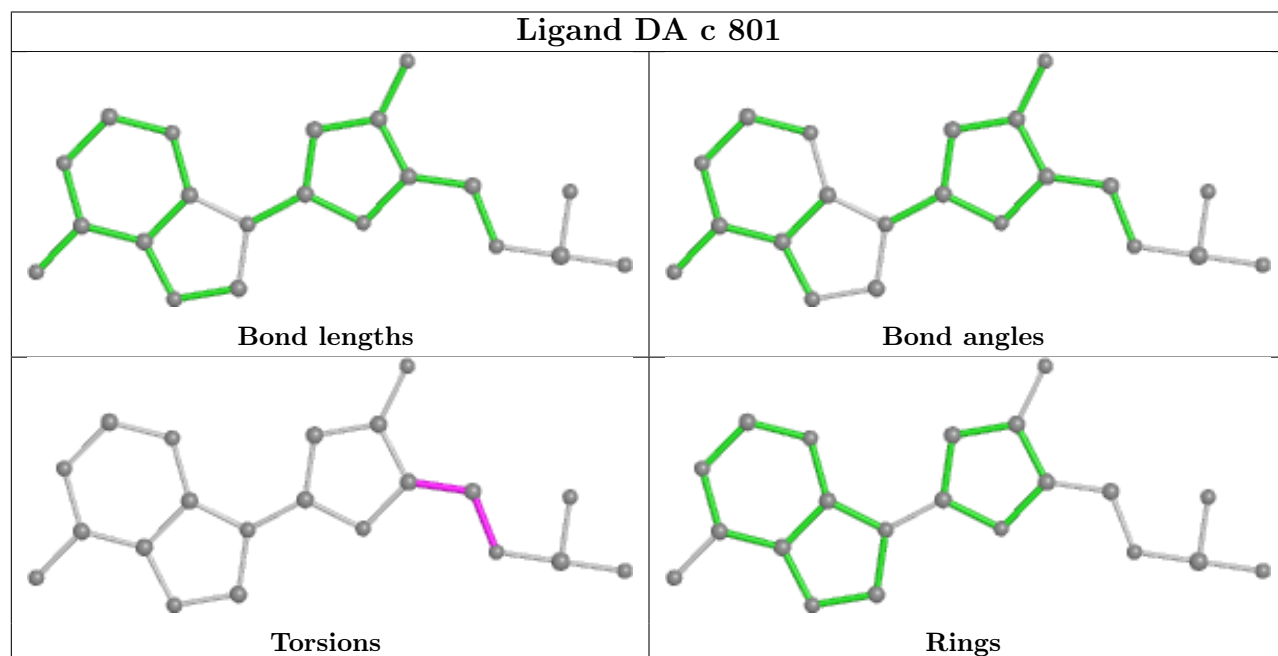
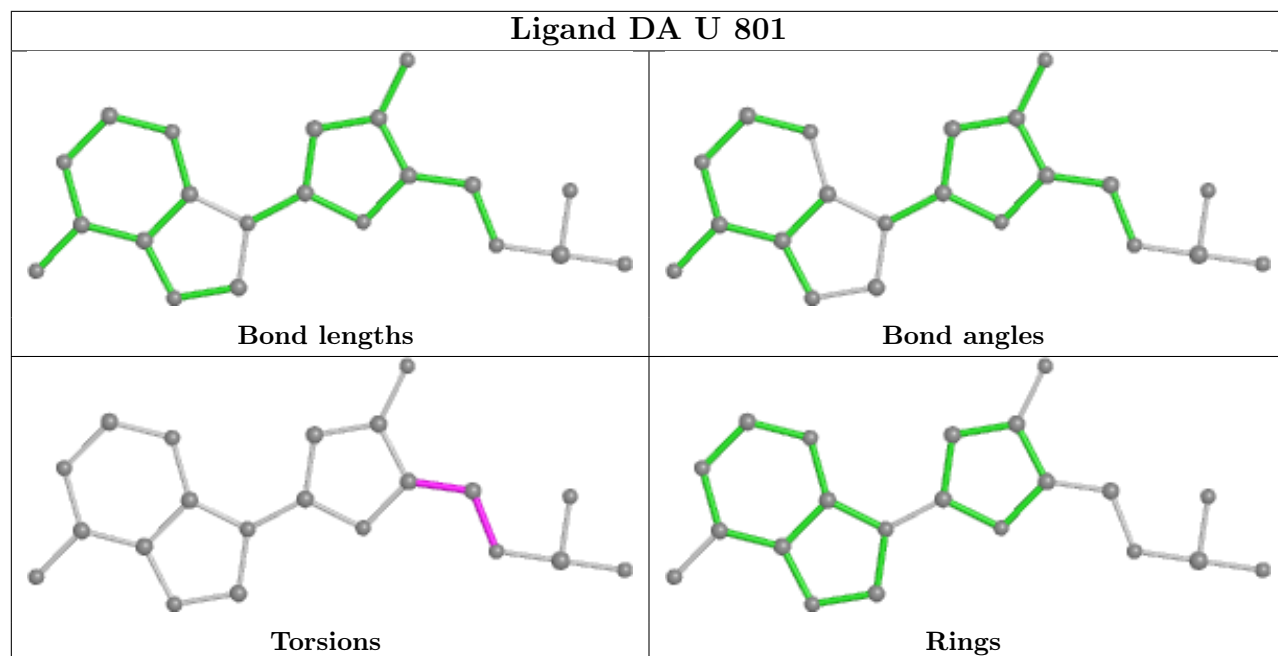


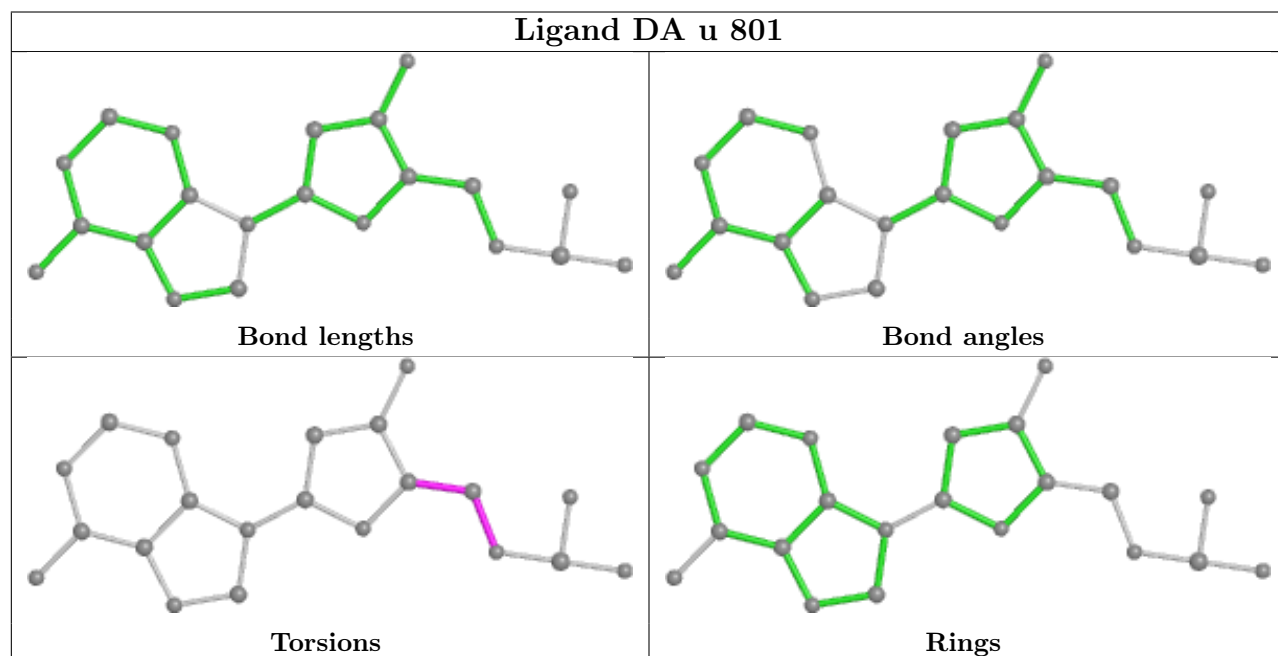
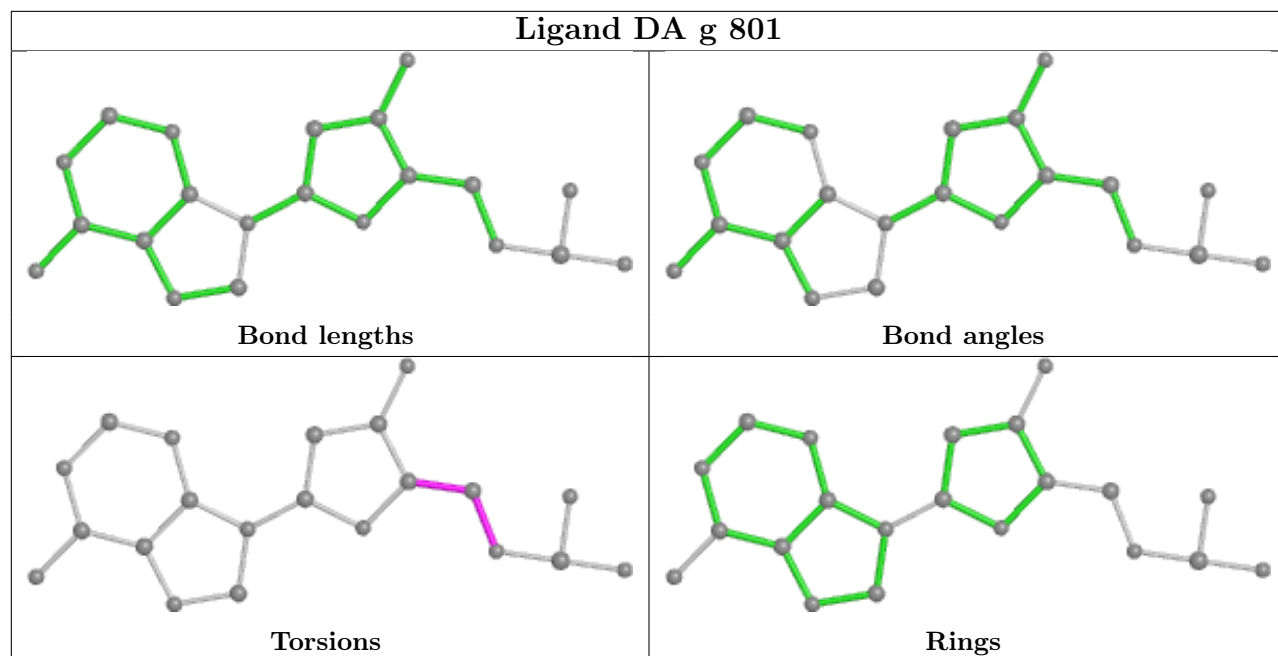


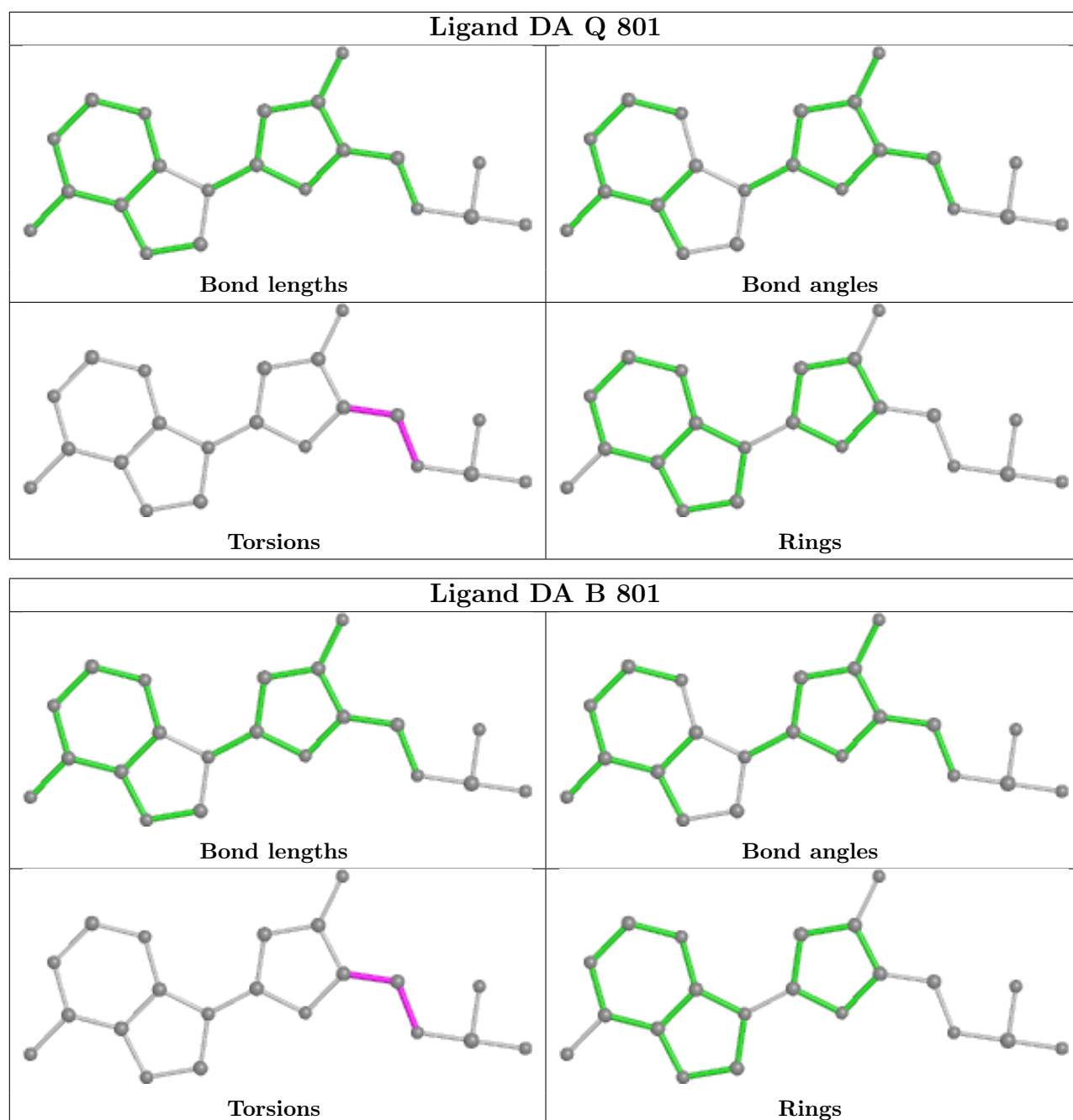












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

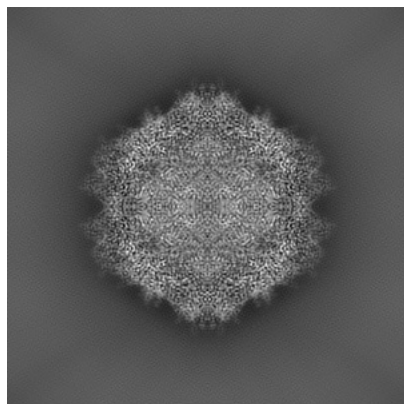
6 Map visualisation [i](#)

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.

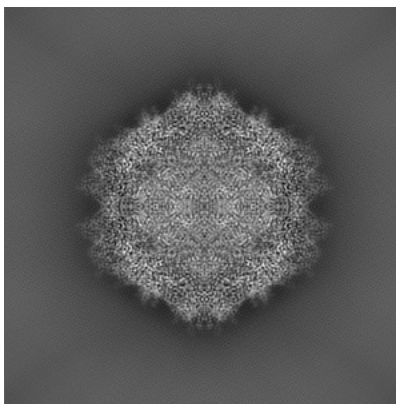
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

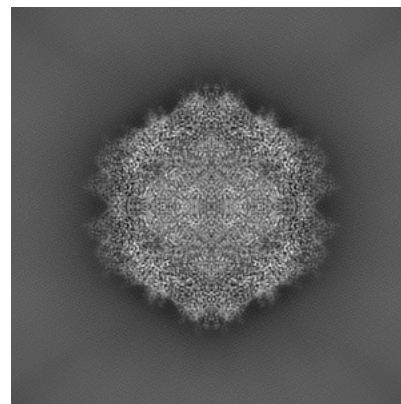
6.1.1 Primary map



X

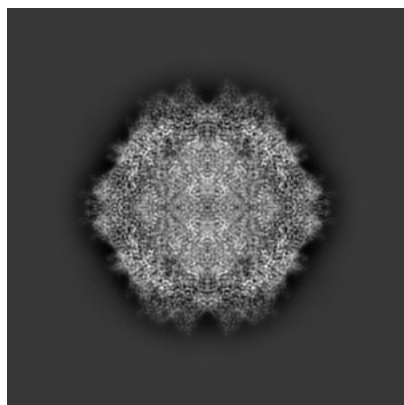


Y

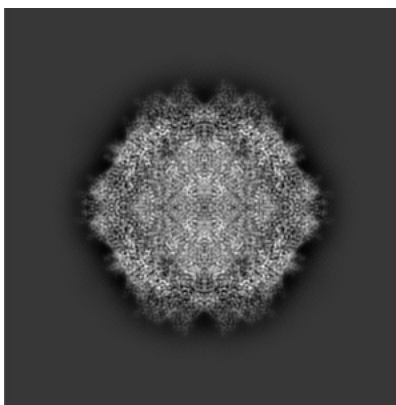


Z

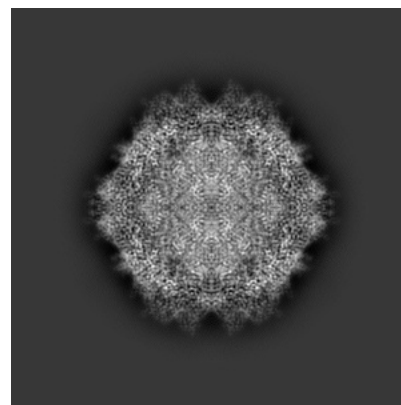
6.1.2 Raw map



X



Y

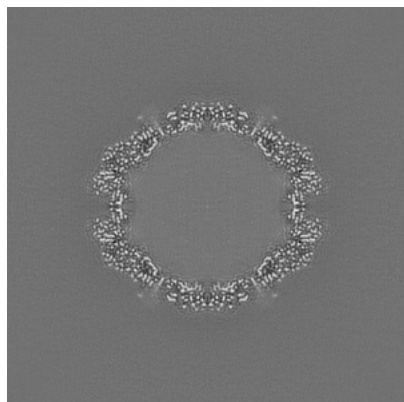


Z

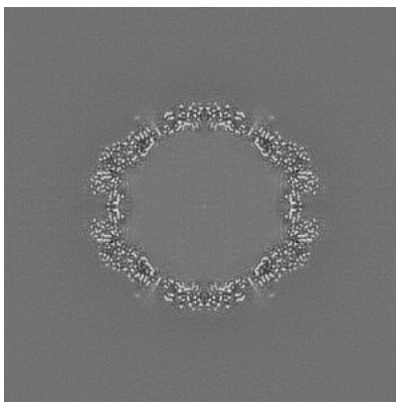
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

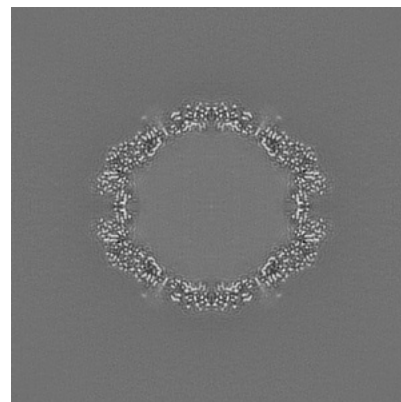
6.2.1 Primary map



X Index: 210

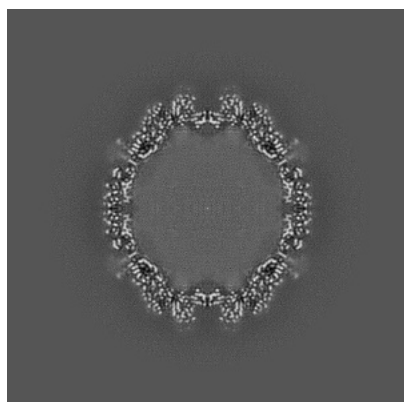


Y Index: 210

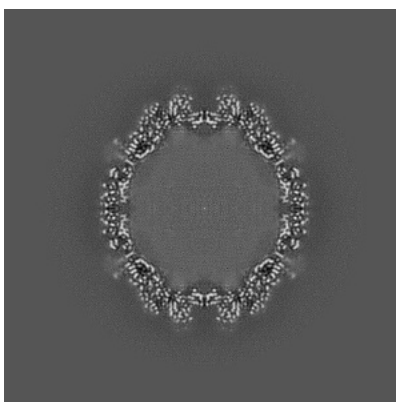


Z Index: 210

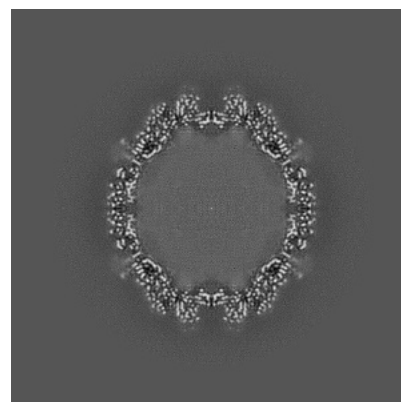
6.2.2 Raw map



X Index: 210



Y Index: 210

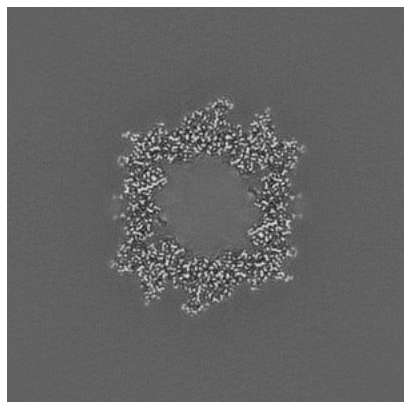


Z Index: 210

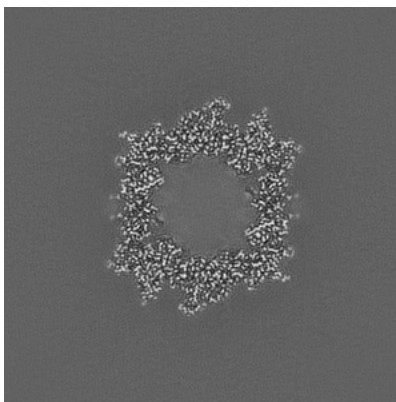
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

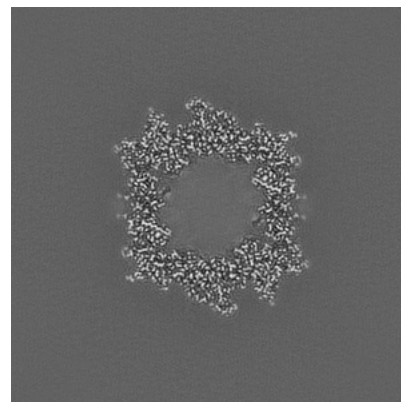
6.3.1 Primary map



X Index: 272

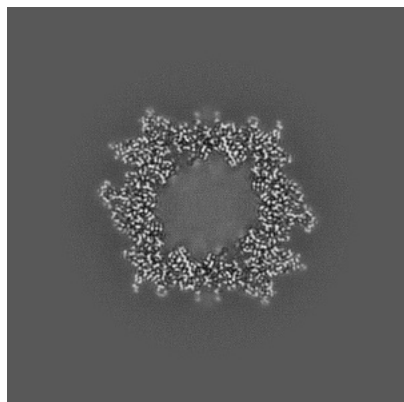


Y Index: 272

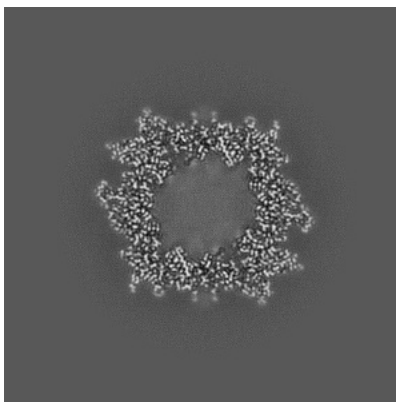


Z Index: 148

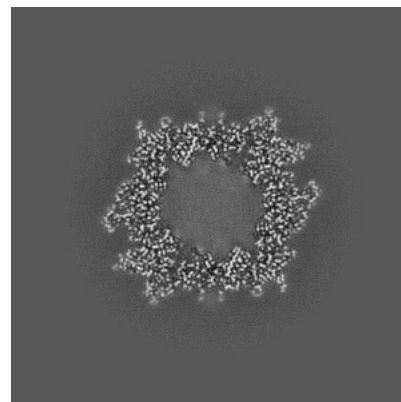
6.3.2 Raw map



X Index: 148



Y Index: 148

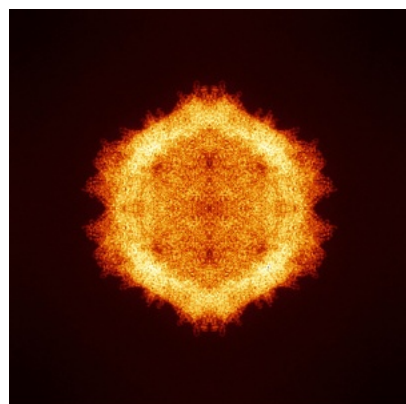


Z Index: 272

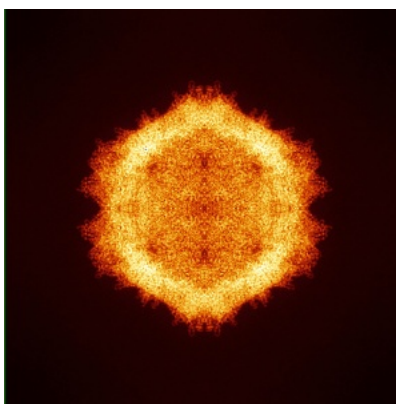
The images above show the largest variance slices of the map in three orthogonal directions.

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

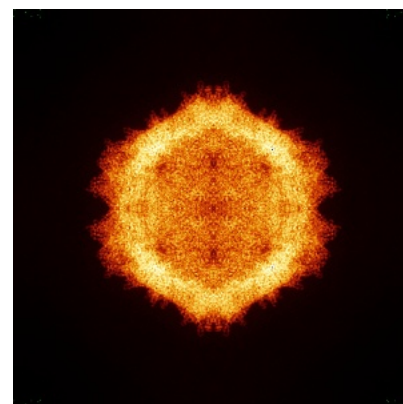
6.4.1 Primary map



X

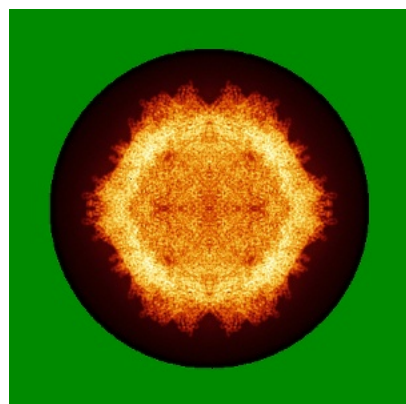


Y

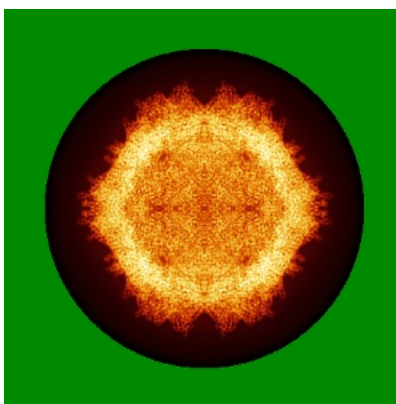


Z

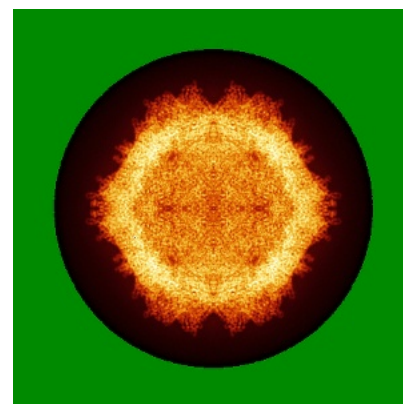
6.4.2 Raw map



X



Y

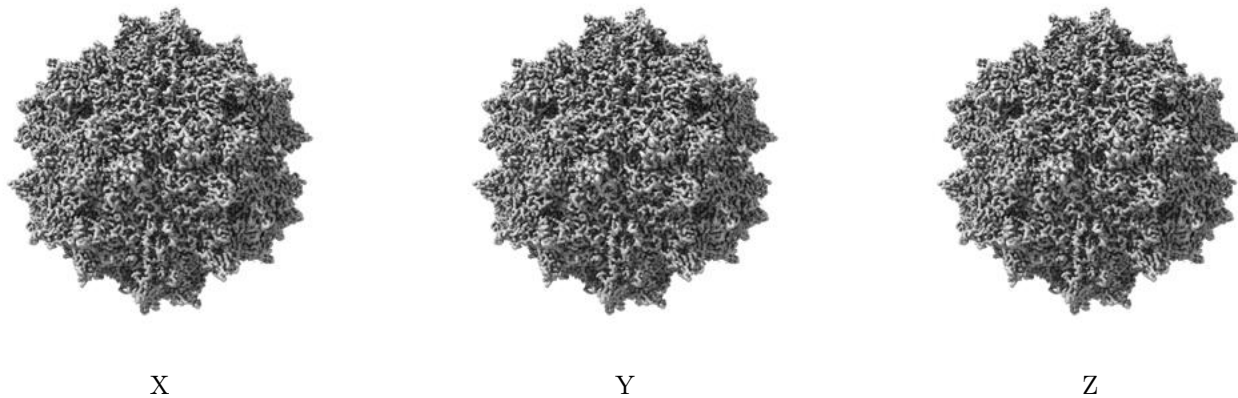


Z

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.

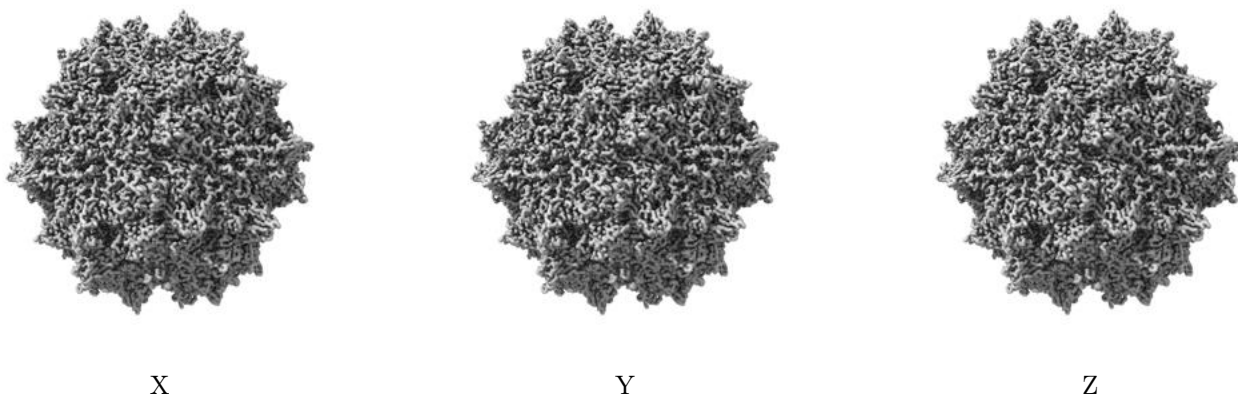
6.5 Orthogonal surface views [i](#)

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.

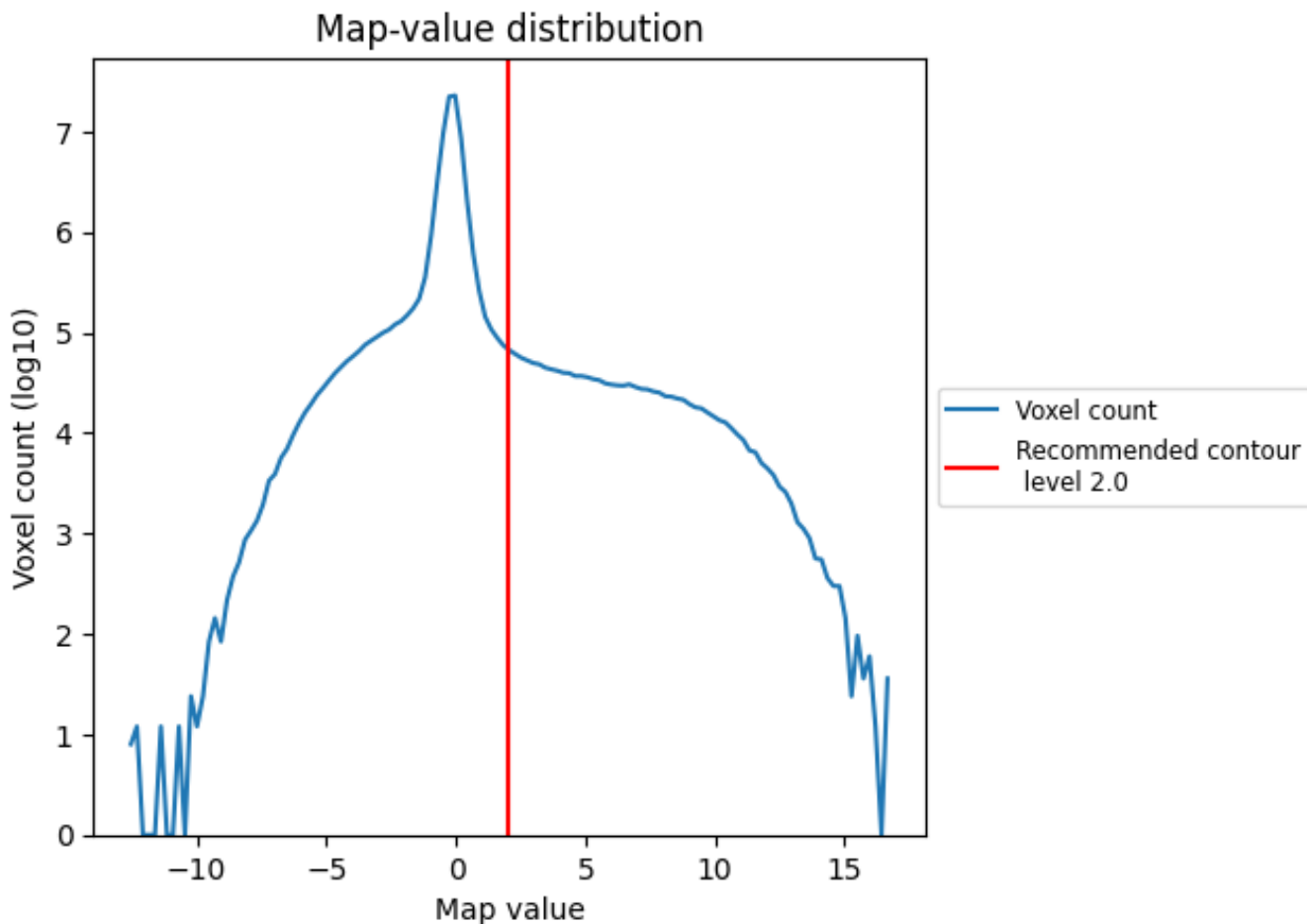
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

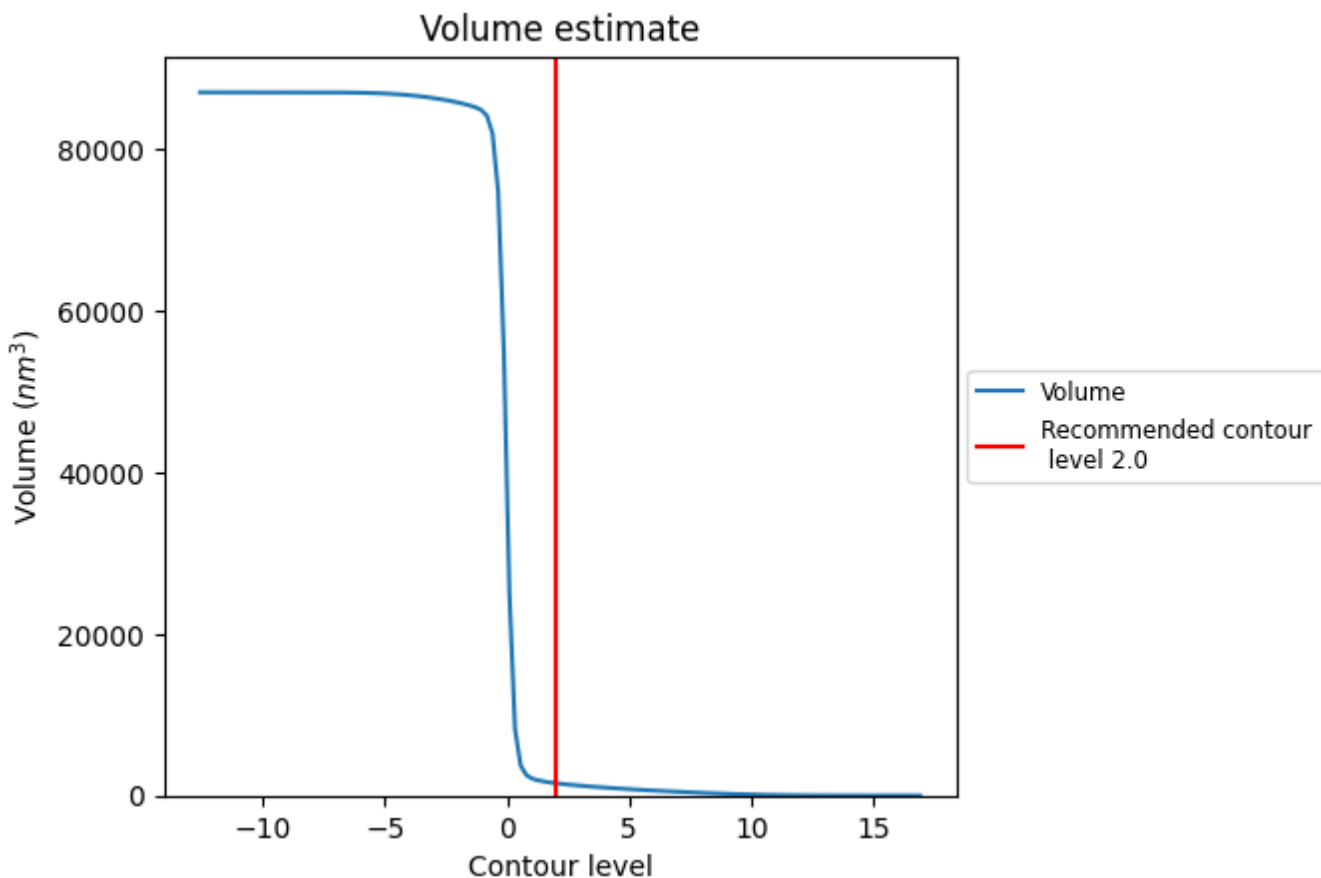
This section contains the results of statistical analysis of the map.

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.

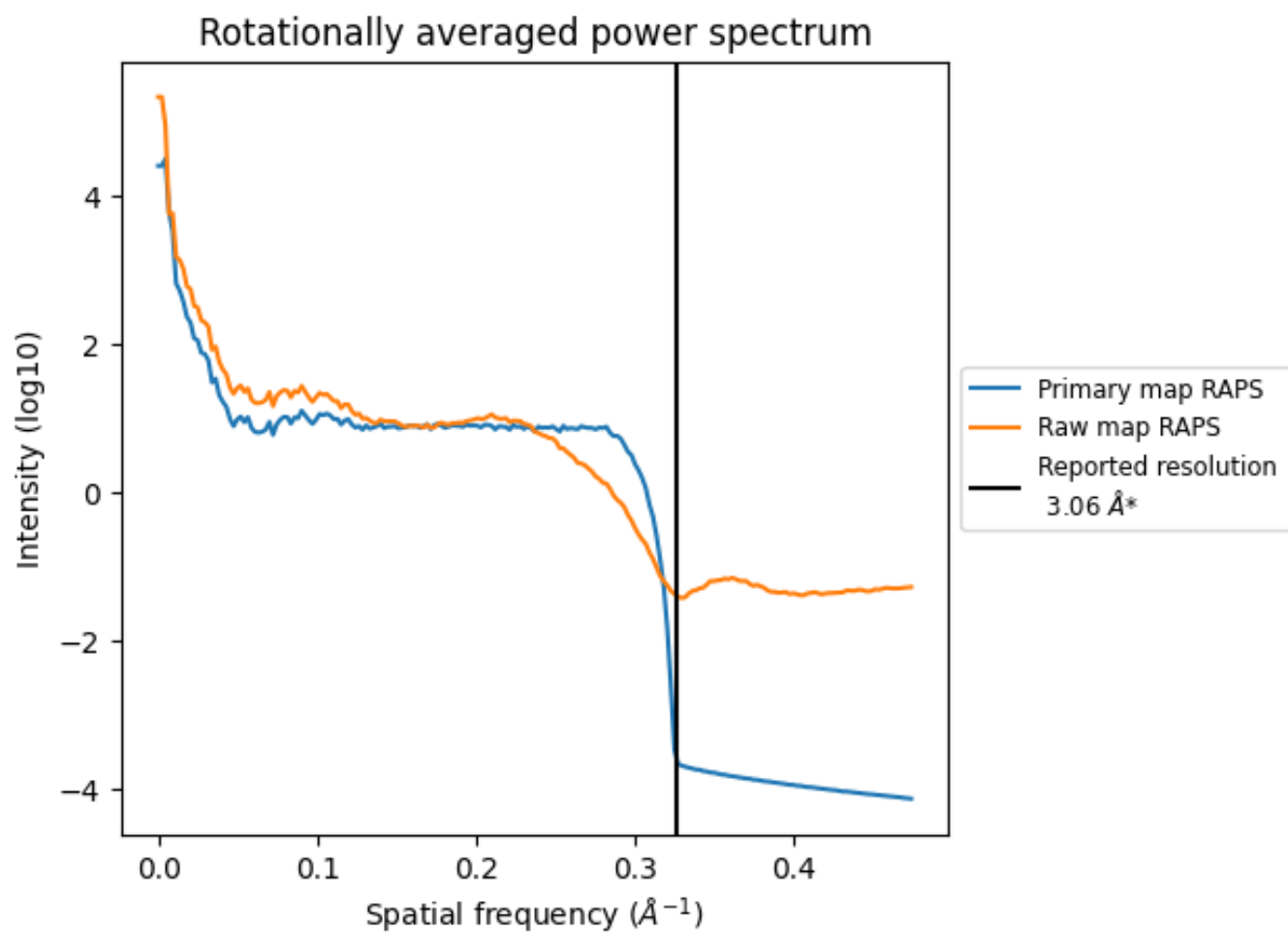
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1526 nm³; 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 [i](#)

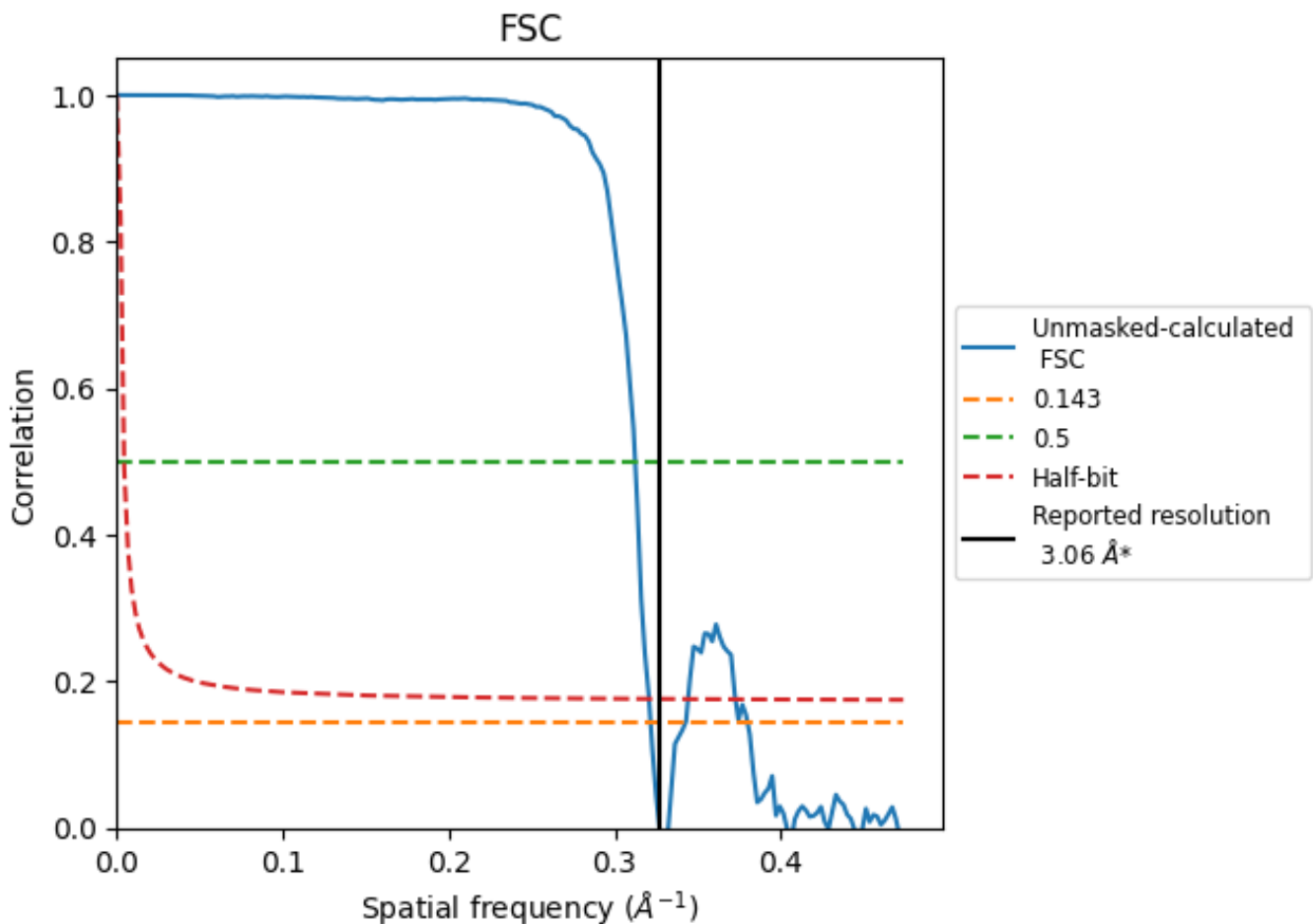


*Reported resolution corresponds to spatial frequency of 0.327 \AA^{-1}

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](#)

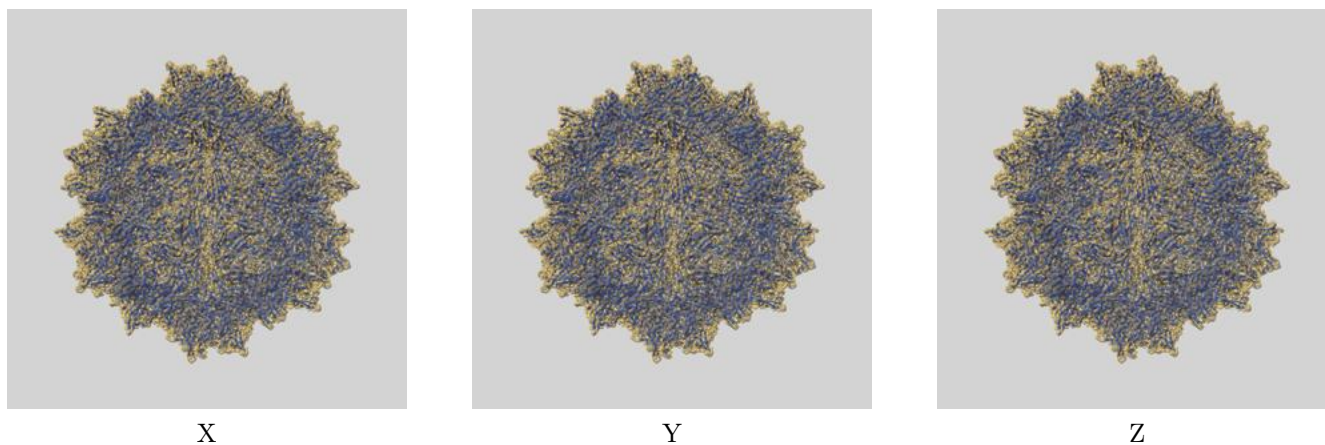
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.20	3.12

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

9 Map-model fit [i](#)

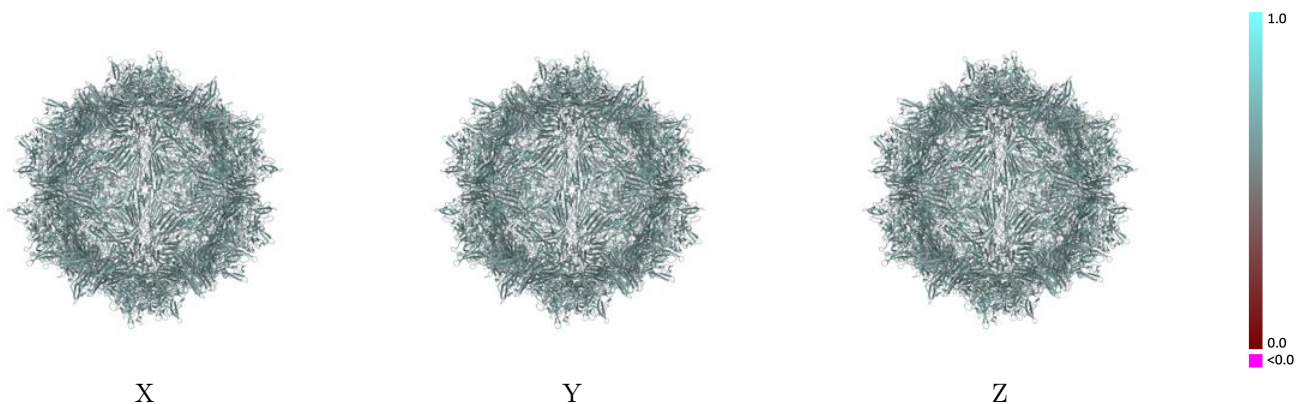
This section contains information regarding the fit between EMDB map EMD-41209 and PDB model 8TEY. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



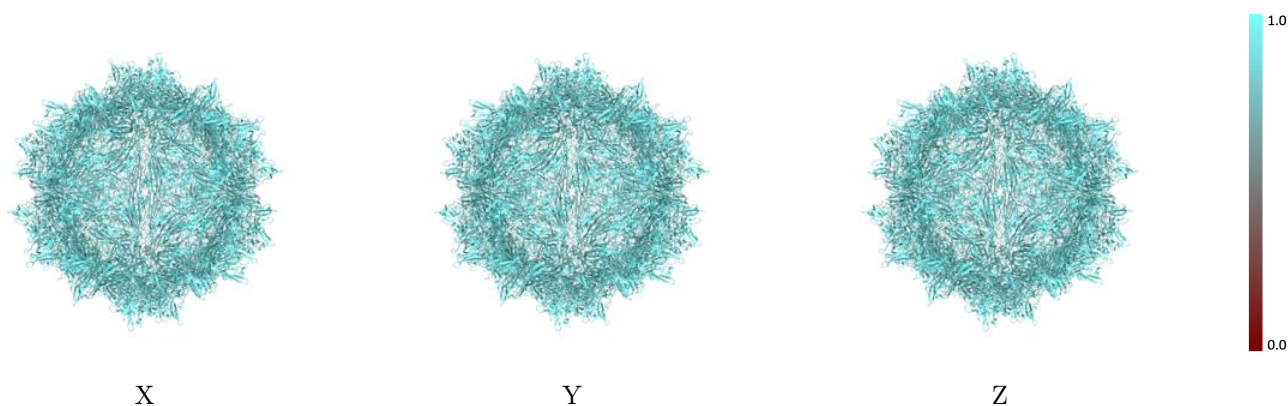
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



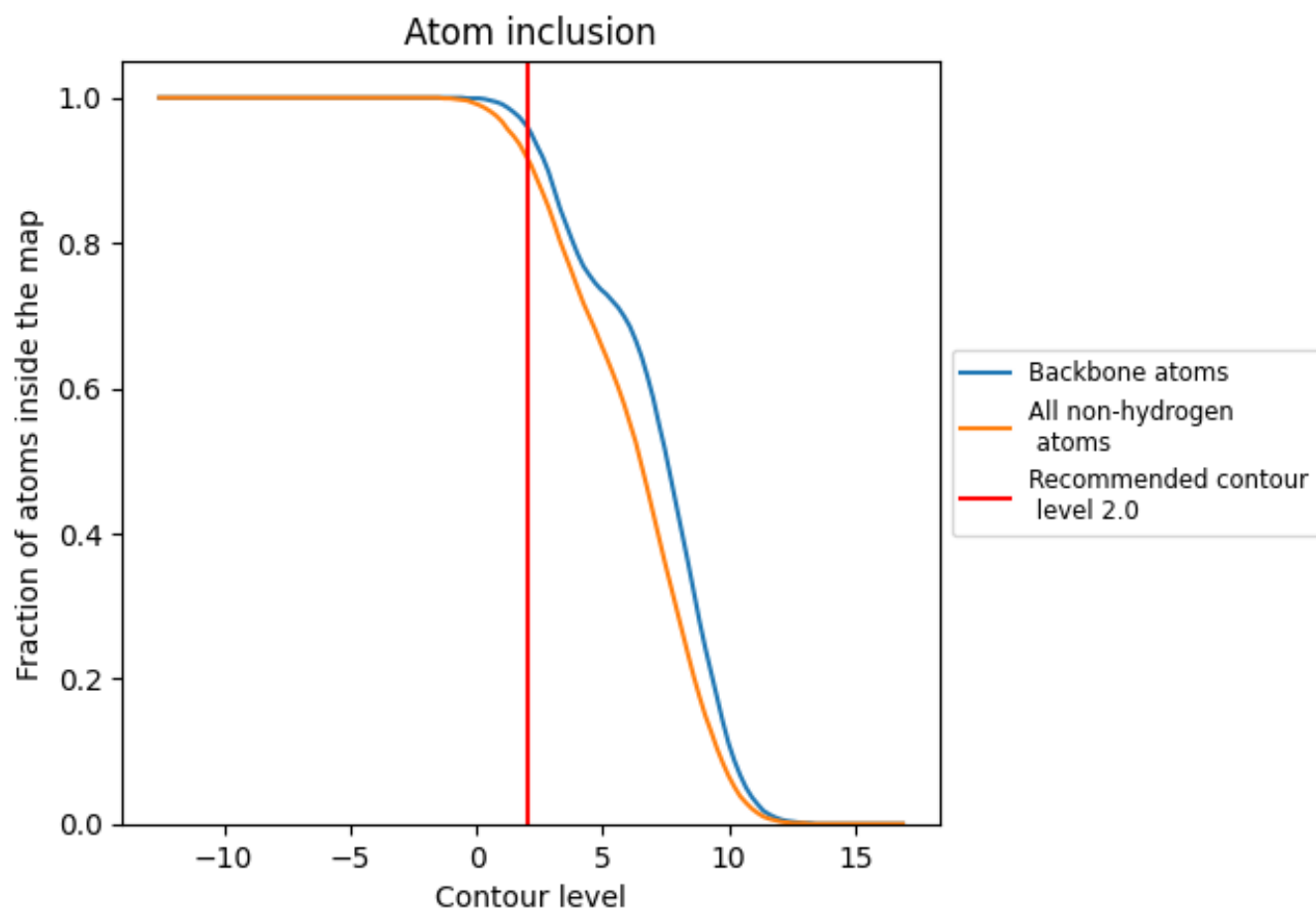
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.0).







































































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 (2.0) 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	 0.5910
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