



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2024 – 12:59 AM EST

PDB ID : 8V82  
EMDB ID : EMD-43015  
Title : Alpha7-nicotinic acetylcholine receptor bound to epibatidine and PNU-120596  
Authors : Burke, S.M.; Noviello, C.M.; Hibbs, R.E.  
Deposited on : 2023-12-04  
Resolution : 2.61 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](mailto: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>.

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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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

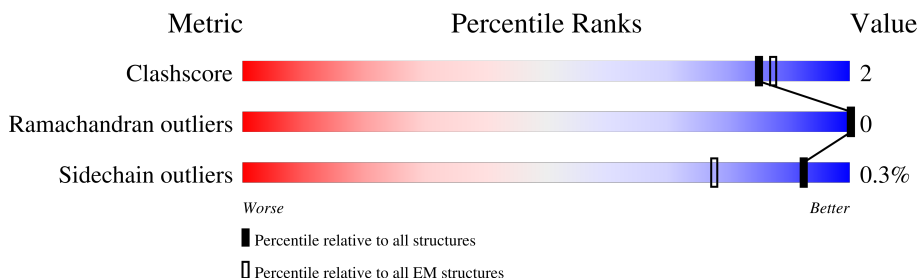
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.61 Å.

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



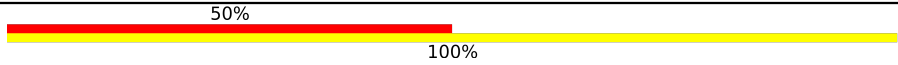
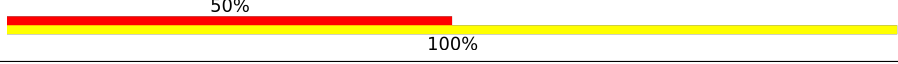


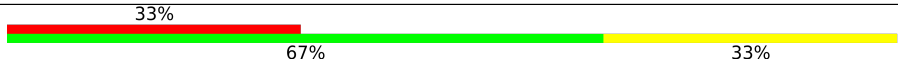


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	599	
1	B	599	
1	C	599	
1	D	599	
1	E	599	
2	F	2	
2	H	2	
2	J	2	

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Mol	Chain	Length	Quality of chain
2	L	2	 50% 100%
2	N	2	 50% 100%
3	G	3	 67% 33%
3	I	3	 67% 33%
3	K	3	 33% 67% 33%
3	M	3	 67% 33%
3	O	3	 67% 33%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 35045 atoms, of which 17605 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 Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	394	6353	2081	3165	516	568	23	1	0
1	B	394	6353	2081	3165	516	568	23	1	0
1	C	394	6353	2081	3165	516	568	23	1	0
1	D	394	6353	2081	3165	516	568	23	1	0
1	E	394	6353	2081	3165	516	568	23	1	0

There are 475 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	?	-	GLU	deletion	UNP P36544
A	?	-	MET	deletion	UNP P36544
A	?	-	SER	deletion	UNP P36544
A	?	-	ALA	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	?	-	ALA	deletion	UNP P36544
A	?	-	PRO	deletion	UNP P36544
A	?	-	PRO	deletion	UNP P36544
A	?	-	PRO	deletion	UNP P36544
A	?	-	ALA	deletion	UNP P36544
A	?	-	SER	deletion	UNP P36544
A	?	-	ASN	deletion	UNP P36544
A	?	-	GLY	deletion	UNP P36544
A	?	-	ASN	deletion	UNP P36544
A	?	-	LEU	deletion	UNP P36544
A	?	-	LEU	deletion	UNP P36544
A	?	-	TYR	deletion	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P36544
A	?	-	GLY	deletion	UNP P36544
A	?	-	PHE	deletion	UNP P36544
A	?	-	ARG	deletion	UNP P36544
A	?	-	GLY	deletion	UNP P36544
A	?	-	LEU	deletion	UNP P36544
A	?	-	ASP	deletion	UNP P36544
A	?	-	GLY	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	?	-	HIS	deletion	UNP P36544
A	?	-	CYS	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	?	-	PRO	deletion	UNP P36544
A	?	-	THR	deletion	UNP P36544
A	?	-	PRO	deletion	UNP P36544
A	?	-	ASP	deletion	UNP P36544
A	?	-	SER	deletion	UNP P36544
A	?	-	GLY	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	?	-	VAL	deletion	UNP P36544
A	324B	ALA	-	linker	UNP P36544
A	324C	GLY	-	linker	UNP P36544
A	324D	ALA	-	linker	UNP P36544
A	324E	MET	-	linker	UNP P36544
A	324L	TRP	MET	conflict	UNP P0ABE7
A	328C	ILE	HIS	conflict	UNP P0ABE7
A	328G	LEU	ARG	conflict	UNP P0ABE7
A	480	TRP	-	expression tag	UNP P36544
A	481	SER	-	expression tag	UNP P36544
A	482	HIS	-	expression tag	UNP P36544
A	483	PRO	-	expression tag	UNP P36544
A	484	GLN	-	expression tag	UNP P36544
A	485	PHE	-	expression tag	UNP P36544
A	486	GLU	-	expression tag	UNP P36544
A	487	LYS	-	expression tag	UNP P36544
A	488	GLY	-	linker	UNP P36544
A	489	GLY	-	linker	UNP P36544
A	490	GLY	-	linker	UNP P36544
A	491	SER	-	linker	UNP P36544
A	492	GLY	-	linker	UNP P36544
A	493	GLY	-	linker	UNP P36544
A	494	GLY	-	linker	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
A	495	SER	-	linker	UNP P36544
A	496	GLY	-	linker	UNP P36544
A	497	GLY	-	linker	UNP P36544
A	498	SER	-	linker	UNP P36544
A	499	SER	-	linker	UNP P36544
A	500	ALA	-	linker	UNP P36544
A	501	TRP	-	expression tag	UNP P36544
A	502	SER	-	expression tag	UNP P36544
A	503	HIS	-	expression tag	UNP P36544
A	504	PRO	-	expression tag	UNP P36544
A	505	GLN	-	expression tag	UNP P36544
A	506	PHE	-	expression tag	UNP P36544
A	507	GLU	-	expression tag	UNP P36544
A	508	LYS	-	expression tag	UNP P36544
A	509	GLY	-	linker	UNP P36544
A	510	SER	-	linker	UNP P36544
A	511	GLY	-	linker	UNP P36544
A	512	GLU	-	linker	UNP P36544
A	513	GLY	-	linker	UNP P36544
A	514	ARG	-	linker	UNP P36544
A	515	GLY	-	linker	UNP P36544
A	516	SER	-	linker	UNP P36544
A	517	LEU	-	linker	UNP P36544
A	518	LEU	-	linker	UNP P36544
A	519	THR	-	linker	UNP P36544
A	520	CYS	-	linker	UNP P36544
A	521	GLY	-	linker	UNP P36544
A	522	ASP	-	linker	UNP P36544
A	523	VAL	-	linker	UNP P36544
A	524	GLU	-	linker	UNP P36544
A	525	GLU	-	linker	UNP P36544
A	526	ASN	-	linker	UNP P36544
A	527	PRO	-	linker	UNP P36544
A	528	GLY	-	linker	UNP P36544
B	?	-	SER	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	?	-	GLU	deletion	UNP P36544
B	?	-	MET	deletion	UNP P36544
B	?	-	SER	deletion	UNP P36544
B	?	-	ALA	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	?	-	ALA	deletion	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P36544
B	?	-	PRO	deletion	UNP P36544
B	?	-	PRO	deletion	UNP P36544
B	?	-	ALA	deletion	UNP P36544
B	?	-	SER	deletion	UNP P36544
B	?	-	ASN	deletion	UNP P36544
B	?	-	GLY	deletion	UNP P36544
B	?	-	ASN	deletion	UNP P36544
B	?	-	LEU	deletion	UNP P36544
B	?	-	LEU	deletion	UNP P36544
B	?	-	TYR	deletion	UNP P36544
B	?	-	ILE	deletion	UNP P36544
B	?	-	GLY	deletion	UNP P36544
B	?	-	PHE	deletion	UNP P36544
B	?	-	ARG	deletion	UNP P36544
B	?	-	GLY	deletion	UNP P36544
B	?	-	LEU	deletion	UNP P36544
B	?	-	ASP	deletion	UNP P36544
B	?	-	GLY	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	?	-	HIS	deletion	UNP P36544
B	?	-	CYS	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	?	-	PRO	deletion	UNP P36544
B	?	-	THR	deletion	UNP P36544
B	?	-	PRO	deletion	UNP P36544
B	?	-	ASP	deletion	UNP P36544
B	?	-	SER	deletion	UNP P36544
B	?	-	GLY	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	?	-	VAL	deletion	UNP P36544
B	324B	ALA	-	linker	UNP P36544
B	324C	GLY	-	linker	UNP P36544
B	324D	ALA	-	linker	UNP P36544
B	324E	MET	-	linker	UNP P36544
B	324L	TRP	MET	conflict	UNP P0ABE7
B	328C	ILE	HIS	conflict	UNP P0ABE7
B	328G	LEU	ARG	conflict	UNP P0ABE7
B	480	TRP	-	expression tag	UNP P36544
B	481	SER	-	expression tag	UNP P36544
B	482	HIS	-	expression tag	UNP P36544
B	483	PRO	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	GLN	-	expression tag	UNP P36544
B	485	PHE	-	expression tag	UNP P36544
B	486	GLU	-	expression tag	UNP P36544
B	487	LYS	-	expression tag	UNP P36544
B	488	GLY	-	linker	UNP P36544
B	489	GLY	-	linker	UNP P36544
B	490	GLY	-	linker	UNP P36544
B	491	SER	-	linker	UNP P36544
B	492	GLY	-	linker	UNP P36544
B	493	GLY	-	linker	UNP P36544
B	494	GLY	-	linker	UNP P36544
B	495	SER	-	linker	UNP P36544
B	496	GLY	-	linker	UNP P36544
B	497	GLY	-	linker	UNP P36544
B	498	SER	-	linker	UNP P36544
B	499	SER	-	linker	UNP P36544
B	500	ALA	-	linker	UNP P36544
B	501	TRP	-	expression tag	UNP P36544
B	502	SER	-	expression tag	UNP P36544
B	503	HIS	-	expression tag	UNP P36544
B	504	PRO	-	expression tag	UNP P36544
B	505	GLN	-	expression tag	UNP P36544
B	506	PHE	-	expression tag	UNP P36544
B	507	GLU	-	expression tag	UNP P36544
B	508	LYS	-	expression tag	UNP P36544
B	509	GLY	-	linker	UNP P36544
B	510	SER	-	linker	UNP P36544
B	511	GLY	-	linker	UNP P36544
B	512	GLU	-	linker	UNP P36544
B	513	GLY	-	linker	UNP P36544
B	514	ARG	-	linker	UNP P36544
B	515	GLY	-	linker	UNP P36544
B	516	SER	-	linker	UNP P36544
B	517	LEU	-	linker	UNP P36544
B	518	LEU	-	linker	UNP P36544
B	519	THR	-	linker	UNP P36544
B	520	CYS	-	linker	UNP P36544
B	521	GLY	-	linker	UNP P36544
B	522	ASP	-	linker	UNP P36544
B	523	VAL	-	linker	UNP P36544
B	524	GLU	-	linker	UNP P36544
B	525	GLU	-	linker	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
B	526	ASN	-	linker	UNP P36544
B	527	PRO	-	linker	UNP P36544
B	528	GLY	-	linker	UNP P36544
C	?	-	SER	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544
C	?	-	GLU	deletion	UNP P36544
C	?	-	MET	deletion	UNP P36544
C	?	-	SER	deletion	UNP P36544
C	?	-	ALA	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544
C	?	-	ALA	deletion	UNP P36544
C	?	-	PRO	deletion	UNP P36544
C	?	-	PRO	deletion	UNP P36544
C	?	-	ALA	deletion	UNP P36544
C	?	-	SER	deletion	UNP P36544
C	?	-	ASN	deletion	UNP P36544
C	?	-	GLY	deletion	UNP P36544
C	?	-	ASN	deletion	UNP P36544
C	?	-	LEU	deletion	UNP P36544
C	?	-	LEU	deletion	UNP P36544
C	?	-	TYR	deletion	UNP P36544
C	?	-	ILE	deletion	UNP P36544
C	?	-	GLY	deletion	UNP P36544
C	?	-	PHE	deletion	UNP P36544
C	?	-	ARG	deletion	UNP P36544
C	?	-	GLY	deletion	UNP P36544
C	?	-	LEU	deletion	UNP P36544
C	?	-	ASP	deletion	UNP P36544
C	?	-	GLY	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544
C	?	-	HIS	deletion	UNP P36544
C	?	-	CYS	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544
C	?	-	PRO	deletion	UNP P36544
C	?	-	THR	deletion	UNP P36544
C	?	-	PRO	deletion	UNP P36544
C	?	-	ASP	deletion	UNP P36544
C	?	-	SER	deletion	UNP P36544
C	?	-	GLY	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544
C	?	-	VAL	deletion	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	324B	ALA	-	linker	UNP P36544
C	324C	GLY	-	linker	UNP P36544
C	324D	ALA	-	linker	UNP P36544
C	324E	MET	-	linker	UNP P36544
C	324L	TRP	MET	conflict	UNP P0ABE7
C	328C	ILE	HIS	conflict	UNP P0ABE7
C	328G	LEU	ARG	conflict	UNP P0ABE7
C	480	TRP	-	expression tag	UNP P36544
C	481	SER	-	expression tag	UNP P36544
C	482	HIS	-	expression tag	UNP P36544
C	483	PRO	-	expression tag	UNP P36544
C	484	GLN	-	expression tag	UNP P36544
C	485	PHE	-	expression tag	UNP P36544
C	486	GLU	-	expression tag	UNP P36544
C	487	LYS	-	expression tag	UNP P36544
C	488	GLY	-	linker	UNP P36544
C	489	GLY	-	linker	UNP P36544
C	490	GLY	-	linker	UNP P36544
C	491	SER	-	linker	UNP P36544
C	492	GLY	-	linker	UNP P36544
C	493	GLY	-	linker	UNP P36544
C	494	GLY	-	linker	UNP P36544
C	495	SER	-	linker	UNP P36544
C	496	GLY	-	linker	UNP P36544
C	497	GLY	-	linker	UNP P36544
C	498	SER	-	linker	UNP P36544
C	499	SER	-	linker	UNP P36544
C	500	ALA	-	linker	UNP P36544
C	501	TRP	-	expression tag	UNP P36544
C	502	SER	-	expression tag	UNP P36544
C	503	HIS	-	expression tag	UNP P36544
C	504	PRO	-	expression tag	UNP P36544
C	505	GLN	-	expression tag	UNP P36544
C	506	PHE	-	expression tag	UNP P36544
C	507	GLU	-	expression tag	UNP P36544
C	508	LYS	-	expression tag	UNP P36544
C	509	GLY	-	linker	UNP P36544
C	510	SER	-	linker	UNP P36544
C	511	GLY	-	linker	UNP P36544
C	512	GLU	-	linker	UNP P36544
C	513	GLY	-	linker	UNP P36544
C	514	ARG	-	linker	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	515	GLY	-	linker	UNP P36544
C	516	SER	-	linker	UNP P36544
C	517	LEU	-	linker	UNP P36544
C	518	LEU	-	linker	UNP P36544
C	519	THR	-	linker	UNP P36544
C	520	CYS	-	linker	UNP P36544
C	521	GLY	-	linker	UNP P36544
C	522	ASP	-	linker	UNP P36544
C	523	VAL	-	linker	UNP P36544
C	524	GLU	-	linker	UNP P36544
C	525	GLU	-	linker	UNP P36544
C	526	ASN	-	linker	UNP P36544
C	527	PRO	-	linker	UNP P36544
C	528	GLY	-	linker	UNP P36544
D	?	-	SER	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544
D	?	-	GLU	deletion	UNP P36544
D	?	-	MET	deletion	UNP P36544
D	?	-	SER	deletion	UNP P36544
D	?	-	ALA	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544
D	?	-	ALA	deletion	UNP P36544
D	?	-	PRO	deletion	UNP P36544
D	?	-	PRO	deletion	UNP P36544
D	?	-	PRO	deletion	UNP P36544
D	?	-	ALA	deletion	UNP P36544
D	?	-	SER	deletion	UNP P36544
D	?	-	ASN	deletion	UNP P36544
D	?	-	GLY	deletion	UNP P36544
D	?	-	ASN	deletion	UNP P36544
D	?	-	LEU	deletion	UNP P36544
D	?	-	LEU	deletion	UNP P36544
D	?	-	TYR	deletion	UNP P36544
D	?	-	ILE	deletion	UNP P36544
D	?	-	GLY	deletion	UNP P36544
D	?	-	PHE	deletion	UNP P36544
D	?	-	ARG	deletion	UNP P36544
D	?	-	GLY	deletion	UNP P36544
D	?	-	LEU	deletion	UNP P36544
D	?	-	ASP	deletion	UNP P36544
D	?	-	GLY	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	HIS	deletion	UNP P36544
D	?	-	CYS	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544
D	?	-	PRO	deletion	UNP P36544
D	?	-	THR	deletion	UNP P36544
D	?	-	PRO	deletion	UNP P36544
D	?	-	ASP	deletion	UNP P36544
D	?	-	SER	deletion	UNP P36544
D	?	-	GLY	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544
D	?	-	VAL	deletion	UNP P36544
D	324B	ALA	-	linker	UNP P36544
D	324C	GLY	-	linker	UNP P36544
D	324D	ALA	-	linker	UNP P36544
D	324E	MET	-	linker	UNP P36544
D	324L	TRP	MET	conflict	UNP P0ABE7
D	328C	ILE	HIS	conflict	UNP P0ABE7
D	328G	LEU	ARG	conflict	UNP P0ABE7
D	480	TRP	-	expression tag	UNP P36544
D	481	SER	-	expression tag	UNP P36544
D	482	HIS	-	expression tag	UNP P36544
D	483	PRO	-	expression tag	UNP P36544
D	484	GLN	-	expression tag	UNP P36544
D	485	PHE	-	expression tag	UNP P36544
D	486	GLU	-	expression tag	UNP P36544
D	487	LYS	-	expression tag	UNP P36544
D	488	GLY	-	linker	UNP P36544
D	489	GLY	-	linker	UNP P36544
D	490	GLY	-	linker	UNP P36544
D	491	SER	-	linker	UNP P36544
D	492	GLY	-	linker	UNP P36544
D	493	GLY	-	linker	UNP P36544
D	494	GLY	-	linker	UNP P36544
D	495	SER	-	linker	UNP P36544
D	496	GLY	-	linker	UNP P36544
D	497	GLY	-	linker	UNP P36544
D	498	SER	-	linker	UNP P36544
D	499	SER	-	linker	UNP P36544
D	500	ALA	-	linker	UNP P36544
D	501	TRP	-	expression tag	UNP P36544
D	502	SER	-	expression tag	UNP P36544
D	503	HIS	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	504	PRO	-	expression tag	UNP P36544
D	505	GLN	-	expression tag	UNP P36544
D	506	PHE	-	expression tag	UNP P36544
D	507	GLU	-	expression tag	UNP P36544
D	508	LYS	-	expression tag	UNP P36544
D	509	GLY	-	linker	UNP P36544
D	510	SER	-	linker	UNP P36544
D	511	GLY	-	linker	UNP P36544
D	512	GLU	-	linker	UNP P36544
D	513	GLY	-	linker	UNP P36544
D	514	ARG	-	linker	UNP P36544
D	515	GLY	-	linker	UNP P36544
D	516	SER	-	linker	UNP P36544
D	517	LEU	-	linker	UNP P36544
D	518	LEU	-	linker	UNP P36544
D	519	THR	-	linker	UNP P36544
D	520	CYS	-	linker	UNP P36544
D	521	GLY	-	linker	UNP P36544
D	522	ASP	-	linker	UNP P36544
D	523	VAL	-	linker	UNP P36544
D	524	GLU	-	linker	UNP P36544
D	525	GLU	-	linker	UNP P36544
D	526	ASN	-	linker	UNP P36544
D	527	PRO	-	linker	UNP P36544
D	528	GLY	-	linker	UNP P36544
E	?	-	SER	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	?	-	GLU	deletion	UNP P36544
E	?	-	MET	deletion	UNP P36544
E	?	-	SER	deletion	UNP P36544
E	?	-	ALA	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	?	-	ALA	deletion	UNP P36544
E	?	-	PRO	deletion	UNP P36544
E	?	-	PRO	deletion	UNP P36544
E	?	-	PRO	deletion	UNP P36544
E	?	-	ALA	deletion	UNP P36544
E	?	-	SER	deletion	UNP P36544
E	?	-	ASN	deletion	UNP P36544
E	?	-	GLY	deletion	UNP P36544
E	?	-	ASN	deletion	UNP P36544
E	?	-	LEU	deletion	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P36544
E	?	-	TYR	deletion	UNP P36544
E	?	-	ILE	deletion	UNP P36544
E	?	-	GLY	deletion	UNP P36544
E	?	-	PHE	deletion	UNP P36544
E	?	-	ARG	deletion	UNP P36544
E	?	-	GLY	deletion	UNP P36544
E	?	-	LEU	deletion	UNP P36544
E	?	-	ASP	deletion	UNP P36544
E	?	-	GLY	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	?	-	HIS	deletion	UNP P36544
E	?	-	CYS	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	?	-	PRO	deletion	UNP P36544
E	?	-	THR	deletion	UNP P36544
E	?	-	PRO	deletion	UNP P36544
E	?	-	ASP	deletion	UNP P36544
E	?	-	SER	deletion	UNP P36544
E	?	-	GLY	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	?	-	VAL	deletion	UNP P36544
E	324B	ALA	-	linker	UNP P36544
E	324C	GLY	-	linker	UNP P36544
E	324D	ALA	-	linker	UNP P36544
E	324E	MET	-	linker	UNP P36544
E	324L	TRP	MET	conflict	UNP P0ABE7
E	328C	ILE	HIS	conflict	UNP P0ABE7
E	328G	LEU	ARG	conflict	UNP P0ABE7
E	480	TRP	-	expression tag	UNP P36544
E	481	SER	-	expression tag	UNP P36544
E	482	HIS	-	expression tag	UNP P36544
E	483	PRO	-	expression tag	UNP P36544
E	484	GLN	-	expression tag	UNP P36544
E	485	PHE	-	expression tag	UNP P36544
E	486	GLU	-	expression tag	UNP P36544
E	487	LYS	-	expression tag	UNP P36544
E	488	GLY	-	linker	UNP P36544
E	489	GLY	-	linker	UNP P36544
E	490	GLY	-	linker	UNP P36544
E	491	SER	-	linker	UNP P36544
E	492	GLY	-	linker	UNP P36544

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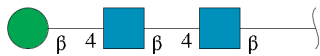
Chain	Residue	Modelled	Actual	Comment	Reference
E	493	GLY	-	linker	UNP P36544
E	494	GLY	-	linker	UNP P36544
E	495	SER	-	linker	UNP P36544
E	496	GLY	-	linker	UNP P36544
E	497	GLY	-	linker	UNP P36544
E	498	SER	-	linker	UNP P36544
E	499	SER	-	linker	UNP P36544
E	500	ALA	-	linker	UNP P36544
E	501	TRP	-	expression tag	UNP P36544
E	502	SER	-	expression tag	UNP P36544
E	503	HIS	-	expression tag	UNP P36544
E	504	PRO	-	expression tag	UNP P36544
E	505	GLN	-	expression tag	UNP P36544
E	506	PHE	-	expression tag	UNP P36544
E	507	GLU	-	expression tag	UNP P36544
E	508	LYS	-	expression tag	UNP P36544
E	509	GLY	-	linker	UNP P36544
E	510	SER	-	linker	UNP P36544
E	511	GLY	-	linker	UNP P36544
E	512	GLU	-	linker	UNP P36544
E	513	GLY	-	linker	UNP P36544
E	514	ARG	-	linker	UNP P36544
E	515	GLY	-	linker	UNP P36544
E	516	SER	-	linker	UNP P36544
E	517	LEU	-	linker	UNP P36544
E	518	LEU	-	linker	UNP P36544
E	519	THR	-	linker	UNP P36544
E	520	CYS	-	linker	UNP P36544
E	521	GLY	-	linker	UNP P36544
E	522	ASP	-	linker	UNP P36544
E	523	VAL	-	linker	UNP P36544
E	524	GLU	-	linker	UNP P36544
E	525	GLU	-	linker	UNP P36544
E	526	ASN	-	linker	UNP P36544
E	527	PRO	-	linker	UNP P36544
E	528	GLY	-	linker	UNP P36544

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	J	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	L	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	N	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
3	I	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
3	K	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
3	M	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
3	O	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	

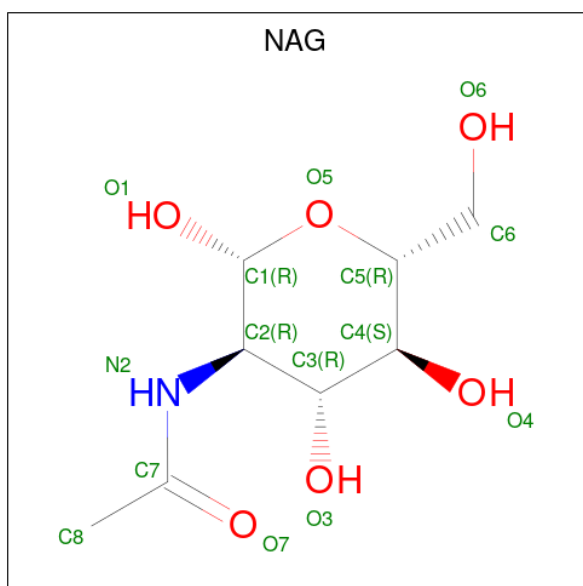
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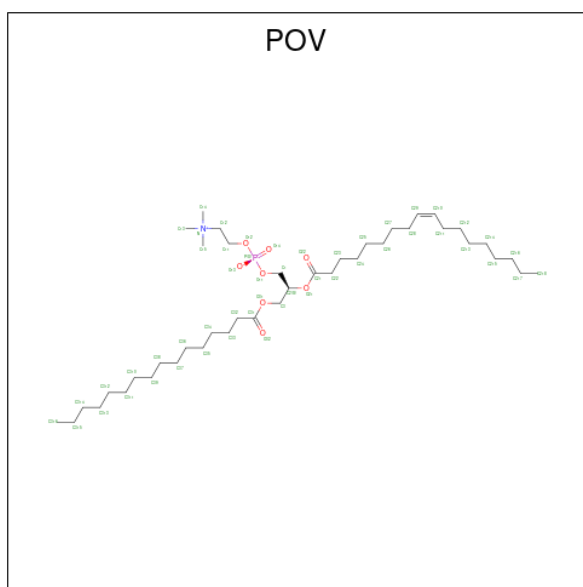
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	D	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	E	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula:  $C_{42}H_{82}NO_8P$ ).



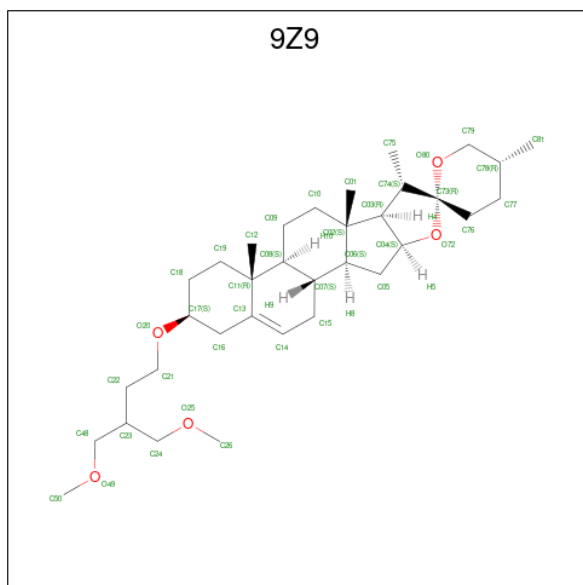
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
6	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
6	A	1	Total 84	C 26	H 48	N 1	O 8	P 1	0
6	A	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
6	A	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
6	B	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
6	B	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
6	B	1	Total 84	C 26	H 48	N 1	O 8	P 1	0
6	C	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
6	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
6	C	1	Total 84	C 26	H 48	N 1	O 8	P 1	0
6	D	1	Total 118	C 37	H 71	N 1	O 8	P 1	0
6	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
6	D	1	Total 84	C 26	H 48	N 1	O 8	P 1	0
6	E	1	Total 118	C 37	H 71	N 1	O 8	P 1	0

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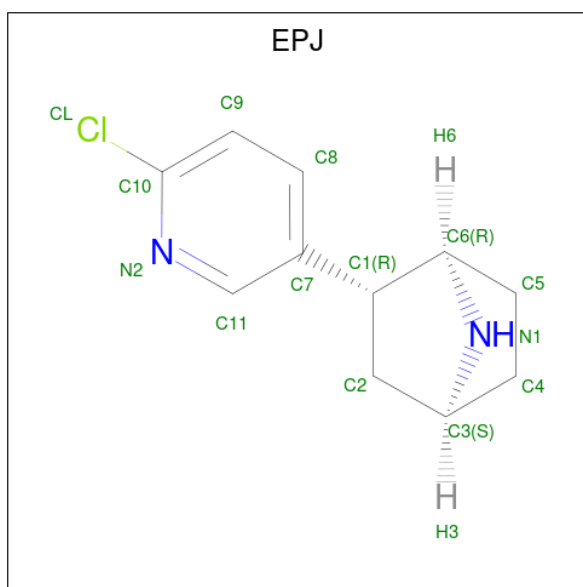
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
6	E	1	84	26	48	1	8	1	0

- Molecule 7 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C<sub>34</sub>H<sub>56</sub>O<sub>5</sub>).



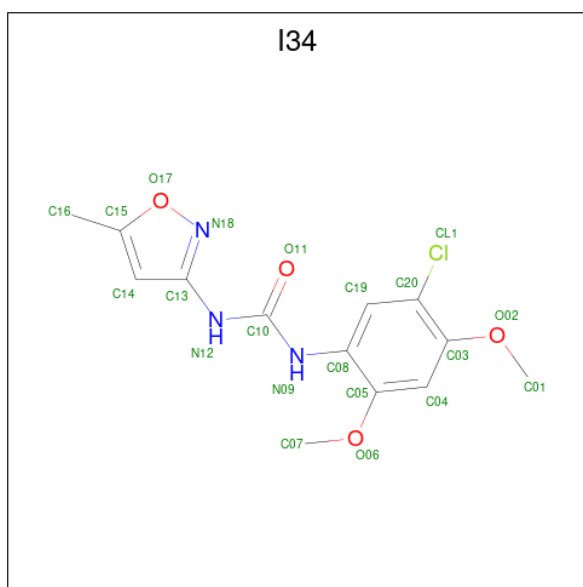
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
7	A	1	95	34	56	5	0
7	B	1	95	34	56	5	0
7	C	1	95	34	56	5	0
7	D	1	95	34	56	5	0
7	E	1	95	34	56	5	0

- Molecule 8 is EPIBATIDINE (three-letter code: EPJ) (formula: C<sub>11</sub>H<sub>13</sub>ClN<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	H		N
8	A	1	27	11	1	13	2	0
8	B	1	27	11	1	13	2	0
8	C	1	27	11	1	13	2	0
8	D	1	27	11	1	13	2	0
8	E	1	27	11	1	13	2	0

- Molecule 9 is N-(5-Chloro-2,4-dimethoxyphenyl)-N'-(5-methyl-3-isoxazolyl)-urea (three-letter code: I34) (formula: C<sub>13</sub>H<sub>14</sub>ClN<sub>3</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	H	N		O
9	A	1	35	13	1	14	3	4	0
9	B	1	35	13	1	14	3	4	0
9	C	1	35	13	1	14	3	4	0
9	D	1	35	13	1	14	3	4	0
9	E	1	35	13	1	14	3	4	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	9	Total	O	0
			9	9	
10	B	9	Total	O	0
			9	9	
10	C	9	Total	O	0
			9	9	
10	D	9	Total	O	0
			9	9	
10	E	9	Total	O	0
			9	9	





GLU  
GLU  
ASN  
PRD  
GLY

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose







- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 67% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 33% 67% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 67% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	151394	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.452	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	276.224, 276.224, 276.224	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, POV, NAG, 9Z9, EPJ, I34, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/3280	0.60	0/4467
1	B	0.36	0/3280	0.60	0/4467
1	C	0.36	0/3280	0.60	0/4467
1	D	0.36	0/3280	0.60	0/4467
1	E	0.36	0/3280	0.60	0/4467
All	All	0.36	0/16400	0.60	0/22335

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3188	3165	3171	12	0
1	B	3188	3165	3171	12	0
1	C	3188	3165	3171	12	0
1	D	3188	3165	3171	12	0
1	E	3188	3165	3171	12	0
2	F	28	25	25	5	0
2	H	28	25	25	5	0
2	J	28	25	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	28	25	25	5	0
2	N	28	25	25	5	0
3	G	39	34	34	1	0
3	I	39	34	34	1	0
3	K	39	34	34	1	0
3	M	39	34	34	1	0
3	O	39	34	34	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	14	13	13	1	0
5	B	14	13	13	1	0
5	C	14	13	13	1	0
5	D	14	13	13	1	0
5	E	14	13	13	1	0
6	A	187	283	277	2	0
6	B	135	201	195	2	0
6	C	135	201	195	1	0
6	D	135	201	195	1	0
6	E	83	119	113	0	0
7	A	39	56	0	0	0
7	B	39	56	0	0	0
7	C	39	56	0	0	0
7	D	39	56	0	0	0
7	E	39	56	0	0	0
8	A	14	13	13	0	0
8	B	14	13	13	0	0
8	C	14	13	13	0	0
8	D	14	13	13	0	0
8	E	14	13	13	0	0
9	A	21	14	0	1	0
9	B	21	14	0	1	0
9	C	21	14	0	1	0
9	D	21	14	0	1	0
9	E	21	14	0	1	0
10	A	9	0	0	0	0
10	B	9	0	0	0	0
10	C	9	0	0	0	0
10	D	9	0	0	0	0
10	E	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17440	17605	17255	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:O	1:C:170:ASN:ND2	2.27	0.67
1:D:39:ILE:O	1:D:170:ASN:ND2	2.27	0.67
1:B:39:ILE:O	1:B:170:ASN:ND2	2.27	0.67
1:E:39:ILE:O	1:E:170:ASN:ND2	2.27	0.67
1:A:39:ILE:O	1:A:170:ASN:ND2	2.27	0.67
1:E:114[A]:HIS:ND1	3:O:1:NAG:H5	2.16	0.61
1:A:114[A]:HIS:ND1	3:G:1:NAG:H5	2.16	0.61
1:C:114[A]:HIS:ND1	3:K:1:NAG:H5	2.16	0.60
1:D:114[A]:HIS:ND1	3:M:1:NAG:H5	2.16	0.59
1:B:114[A]:HIS:ND1	3:I:1:NAG:H5	2.16	0.59
1:D:174:ASP:OD2	1:D:204:ARG:NH2	2.37	0.58
1:A:174:ASP:OD2	1:A:204:ARG:NH2	2.37	0.58
1:B:174:ASP:OD2	1:B:204:ARG:NH2	2.37	0.58
1:E:174:ASP:OD2	1:E:204:ARG:NH2	2.37	0.57
1:C:174:ASP:OD2	1:C:204:ARG:NH2	2.37	0.57
1:D:281:VAL:O	1:D:284:SER:OG	2.20	0.56
1:B:281:VAL:O	1:B:284:SER:OG	2.20	0.56
1:E:281:VAL:O	1:E:284:SER:OG	2.20	0.54
1:A:309:ARG:NH1	1:A:436:GLU:OE2	2.42	0.53
1:D:309:ARG:NH1	1:D:436:GLU:OE2	2.42	0.53
1:E:309:ARG:NH1	1:E:436:GLU:OE2	2.42	0.53
1:B:309:ARG:NH1	1:B:436:GLU:OE2	2.42	0.52
1:C:309:ARG:NH1	1:C:436:GLU:OE2	2.42	0.52
1:A:281:VAL:O	1:A:284:SER:OG	2.20	0.51
6:A:608:POV:H14	1:E:132:ARG:HD3	1.93	0.51
1:B:213:ASN:OD1	9:B:601:I34:N12	2.43	0.51
1:B:132:ARG:HD3	6:B:605:POV:H14	1.93	0.51
1:C:132:ARG:HD3	6:C:605:POV:H14	1.93	0.51
2:H:1:NAG:H61	2:H:2:NAG:C7	2.41	0.51
1:A:213:ASN:OD1	9:A:607:I34:N12	2.44	0.51
1:A:132:ARG:HD3	6:A:603:POV:H14	1.93	0.50
2:N:1:NAG:H61	2:N:2:NAG:C7	2.41	0.50
1:D:132:ARG:HD3	6:D:605:POV:H14	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:NAG:H61	2:J:2:NAG:C7	2.41	0.50
2:L:1:NAG:H61	2:L:2:NAG:C7	2.41	0.50
2:F:1:NAG:H61	2:F:2:NAG:C7	2.41	0.50
1:D:213:ASN:OD1	9:D:601:I34:N12	2.45	0.50
1:C:213:ASN:OD1	9:C:601:I34:N12	2.45	0.49
1:C:281:VAL:O	1:C:284:SER:OG	2.20	0.49
1:E:213:ASN:OD1	9:E:601:I34:N12	2.46	0.49
2:N:1:NAG:H61	2:N:2:NAG:H82	1.94	0.49
2:L:1:NAG:H61	2:L:2:NAG:H82	1.95	0.48
2:H:1:NAG:H61	2:H:2:NAG:H82	1.94	0.48
2:J:1:NAG:H61	2:J:2:NAG:H82	1.95	0.48
2:F:1:NAG:H61	2:F:2:NAG:H82	1.94	0.48
1:C:323:LYS:N	1:C:323:LYS:HD2	2.31	0.46
1:B:323:LYS:HD2	1:B:323:LYS:N	2.31	0.45
1:D:323:LYS:N	1:D:323:LYS:HD2	2.31	0.45
1:A:323:LYS:N	1:A:323:LYS:HD2	2.31	0.45
1:E:323:LYS:HD2	1:E:323:LYS:N	2.31	0.45
2:L:1:NAG:H61	2:L:2:NAG:N2	2.32	0.45
2:J:1:NAG:C6	2:J:2:NAG:H82	2.47	0.45
2:J:1:NAG:H61	2:J:2:NAG:N2	2.32	0.45
2:N:1:NAG:C6	2:N:2:NAG:H82	2.47	0.44
2:F:1:NAG:C6	2:F:2:NAG:H82	2.47	0.44
2:H:1:NAG:C6	2:H:2:NAG:H82	2.47	0.44
1:B:26:GLN:OE1	2:H:1:NAG:H62	2.18	0.44
1:C:67:ASN:HD22	5:C:604:NAG:H83	1.83	0.44
1:D:67:ASN:HD22	5:D:604:NAG:H83	1.83	0.44
2:N:1:NAG:H61	2:N:2:NAG:N2	2.32	0.44
1:D:26:GLN:OE1	2:L:1:NAG:H62	2.18	0.44
1:A:4:ARG:NE	1:E:18:GLU:OE1	2.50	0.44
1:A:67:ASN:HD22	5:A:602:NAG:H83	1.83	0.44
2:L:1:NAG:C6	2:L:2:NAG:H82	2.47	0.44
1:B:67:ASN:HD22	5:B:604:NAG:H83	1.83	0.44
1:C:26:GLN:OE1	2:J:1:NAG:H62	2.18	0.44
1:A:26:GLN:OE1	2:F:1:NAG:H62	2.18	0.43
2:F:1:NAG:H61	2:F:2:NAG:N2	2.32	0.43
2:H:1:NAG:H61	2:H:2:NAG:N2	2.32	0.43
1:B:18:GLU:OE1	1:C:4:ARG:NE	2.52	0.43
1:E:26:GLN:OE1	2:N:1:NAG:H62	2.18	0.43
1:E:67:ASN:HD22	5:E:604:NAG:H83	1.83	0.43
1:A:18:GLU:OE1	1:B:4:ARG:NE	2.49	0.43
1:D:18:GLU:OE1	1:E:4:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:OE1	1:D:4:ARG:NE	2.51	0.41
6:B:606:POV:H13B	6:B:606:POV:H11	1.96	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/599 (65%)	379 (97%)	12 (3%)	0	100	100
1	B	391/599 (65%)	379 (97%)	12 (3%)	0	100	100
1	C	391/599 (65%)	379 (97%)	12 (3%)	0	100	100
1	D	391/599 (65%)	379 (97%)	12 (3%)	0	100	100
1	E	391/599 (65%)	379 (97%)	12 (3%)	0	100	100
All	All	1955/2995 (65%)	1895 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/514 (70%)	356 (100%)	1 (0%)	92	97
1	B	357/514 (70%)	356 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	357/514 (70%)	356 (100%)	1 (0%)	92	97
1	D	357/514 (70%)	356 (100%)	1 (0%)	92	97
1	E	357/514 (70%)	356 (100%)	1 (0%)	92	97
All	All	1785/2570 (70%)	1780 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	B	47	GLN
1	C	47	GLN
1	D	47	GLN
1	E	47	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

25 monosaccharides 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	NAG	F	1	2,1	14,14,15	0.40	0	17,19,21	0.35	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	0.47	0
3	NAG	G	1	3,1	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	G	3	3	11,11,12	0.51	0	15,15,17	0.71	0
2	NAG	H	1	2,1	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	H	2	2	14,14,15	0.42	0	17,19,21	0.46	0
3	NAG	I	1	3,1	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	BMA	I	3	3	11,11,12	0.52	0	15,15,17	0.71	0
2	NAG	J	1	2,1	14,14,15	0.41	0	17,19,21	0.35	0
2	NAG	J	2	2	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	K	1	3,1	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	K	3	3	11,11,12	0.52	0	15,15,17	0.71	0
2	NAG	L	1	2,1	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	L	2	2	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	M	1	3,1	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	M	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	BMA	M	3	3	11,11,12	0.52	0	15,15,17	0.70	0
2	NAG	N	1	2,1	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	N	2	2	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	O	1	3,1	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	BMA	O	3	3	11,11,12	0.51	0	15,15,17	0.71	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	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 30 short contacts:

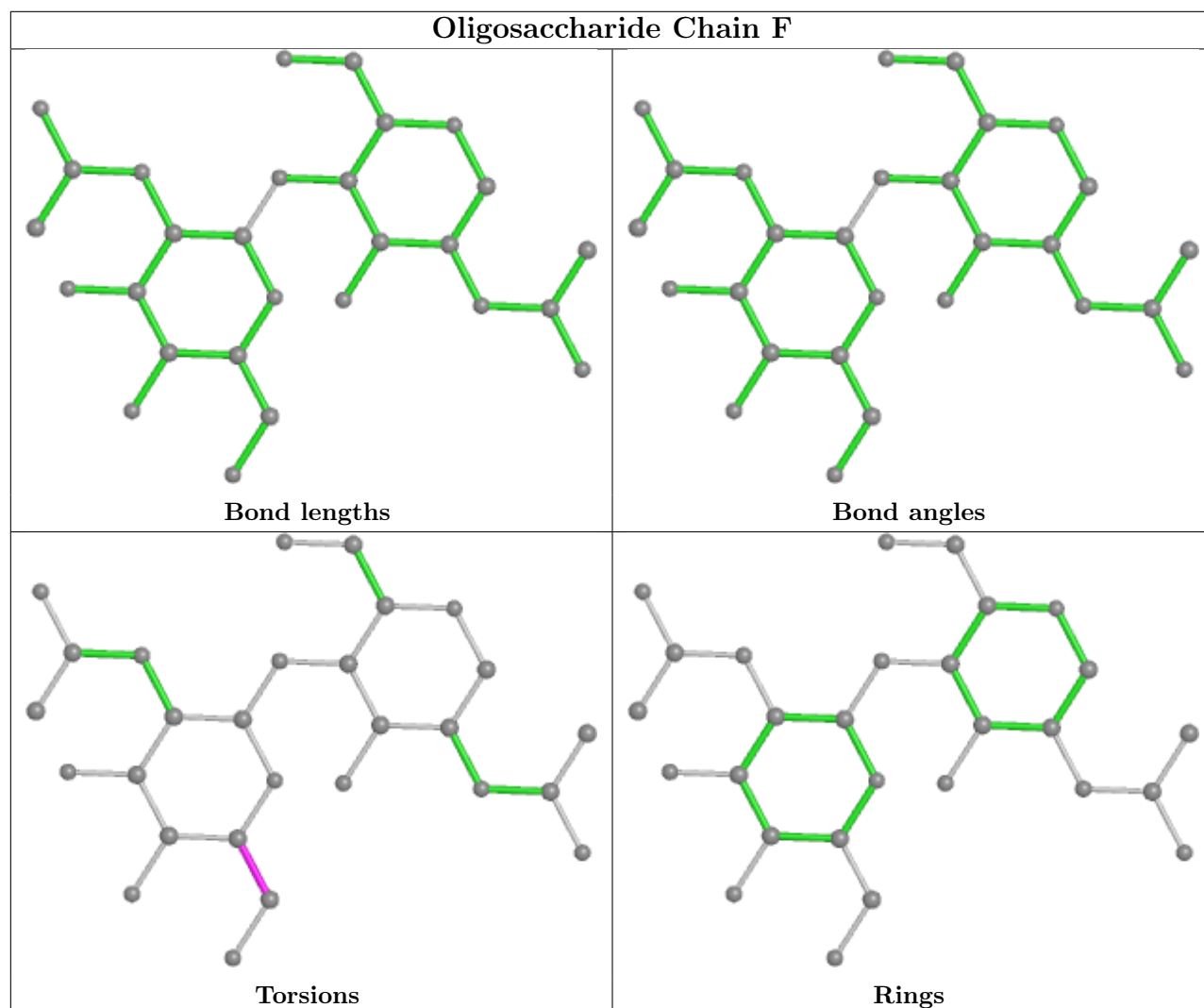
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	5	0
2	H	1	NAG	5	0
3	O	1	NAG	1	0
2	F	1	NAG	5	0

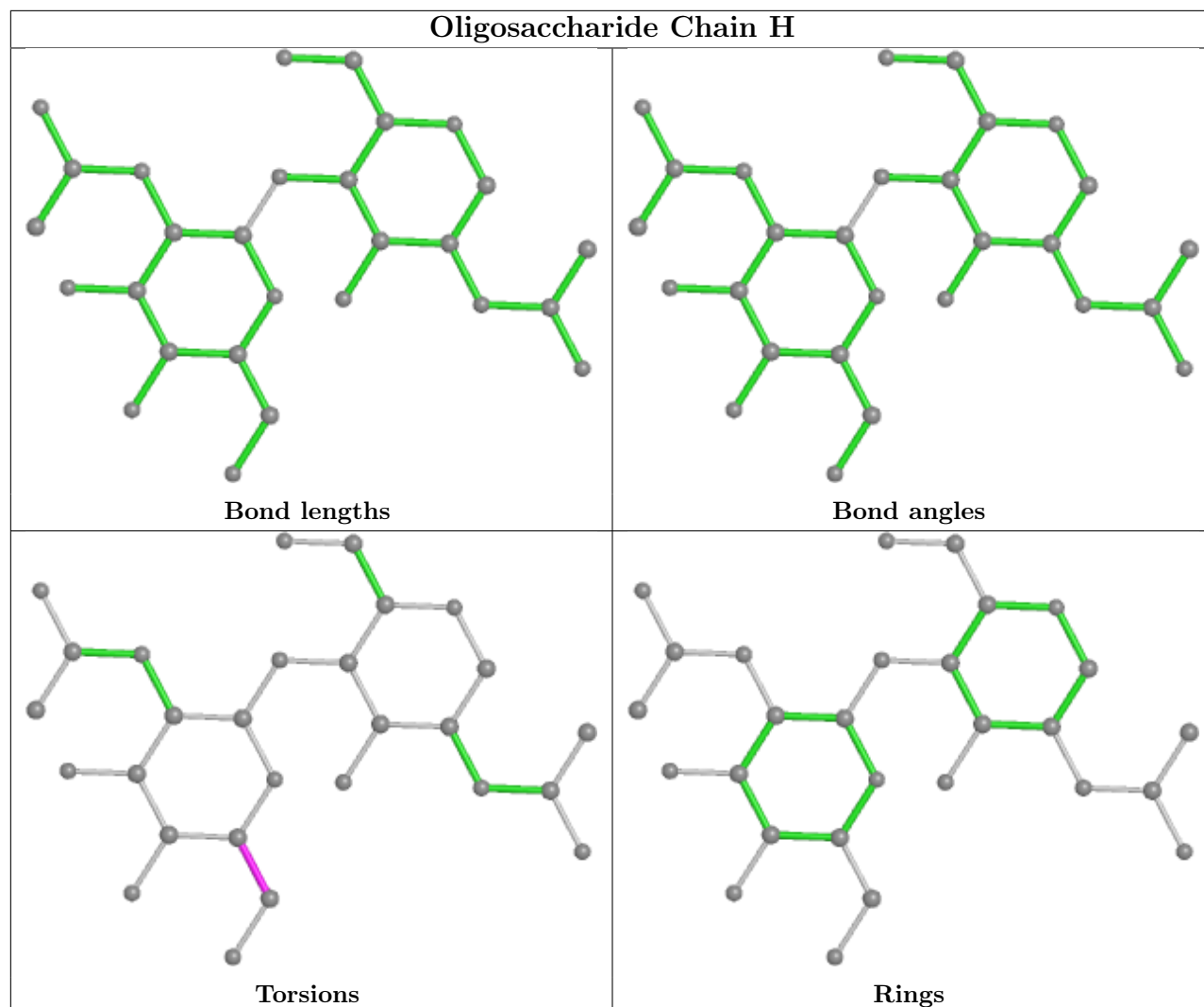
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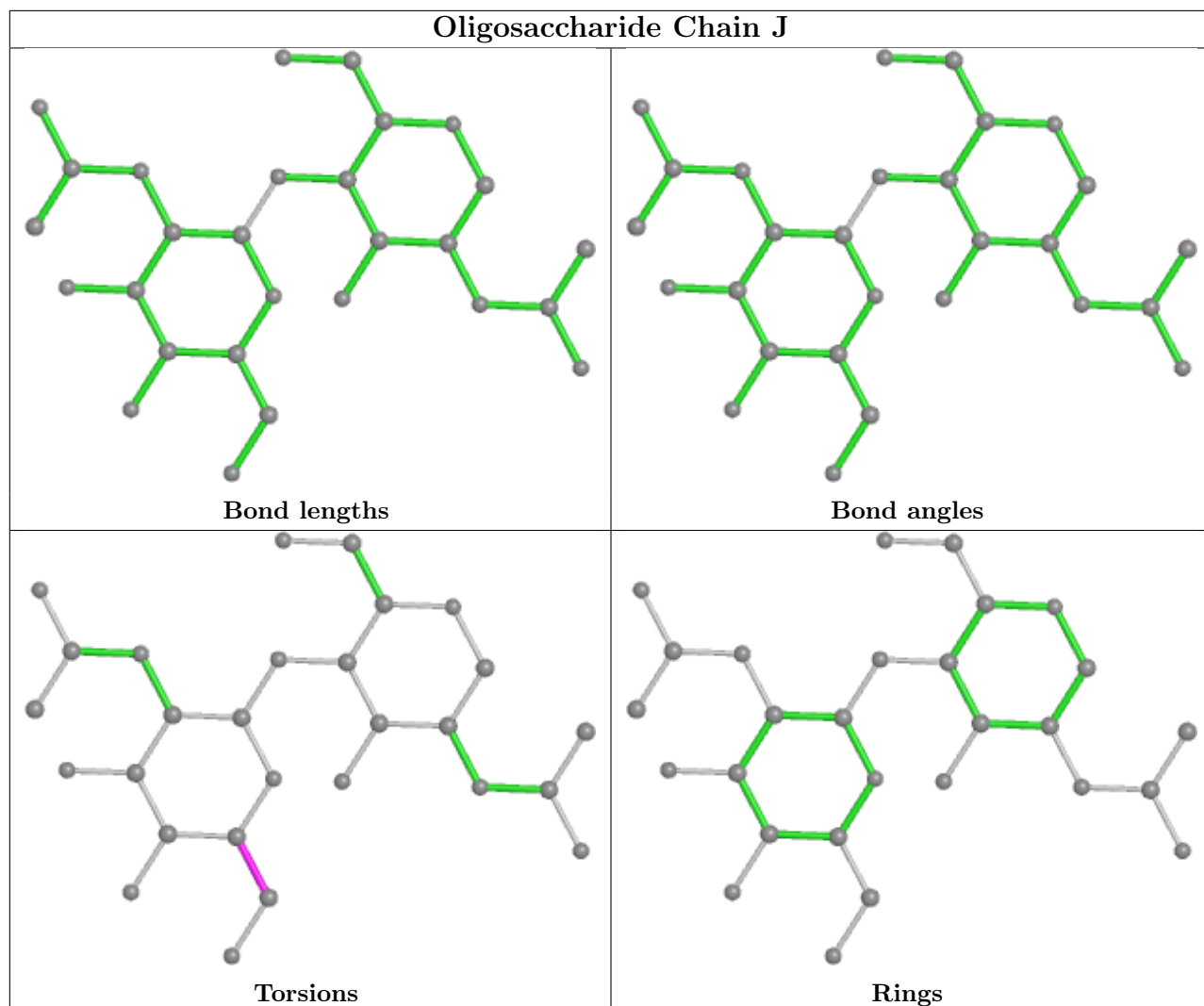
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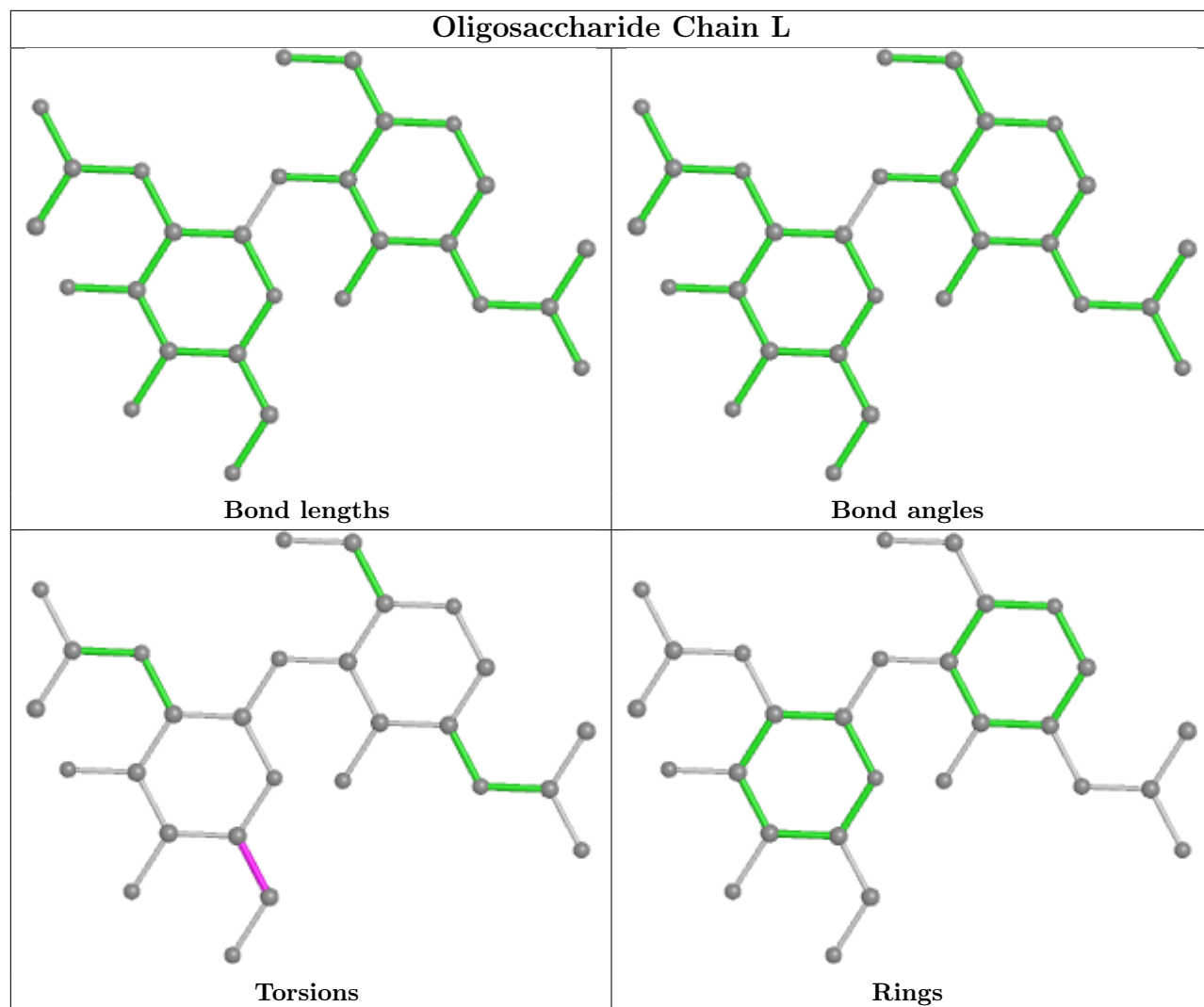
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
2	L	2	NAG	4	0
2	H	2	NAG	4	0
2	J	2	NAG	4	0
3	G	1	NAG	1	0
2	J	1	NAG	5	0
3	I	1	NAG	1	0
3	K	1	NAG	1	0
2	N	1	NAG	5	0
2	F	2	NAG	4	0
2	N	2	NAG	4	0

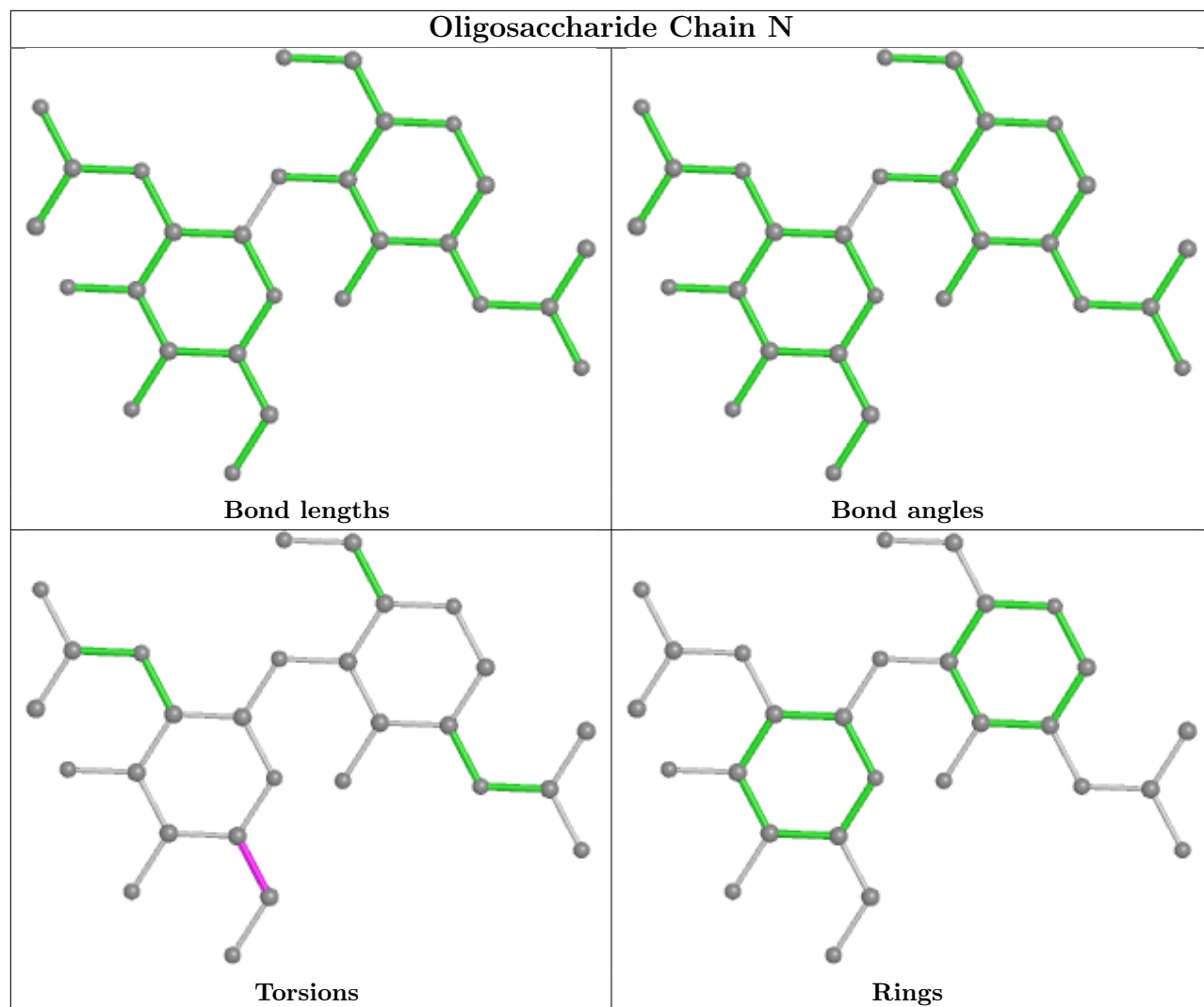
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

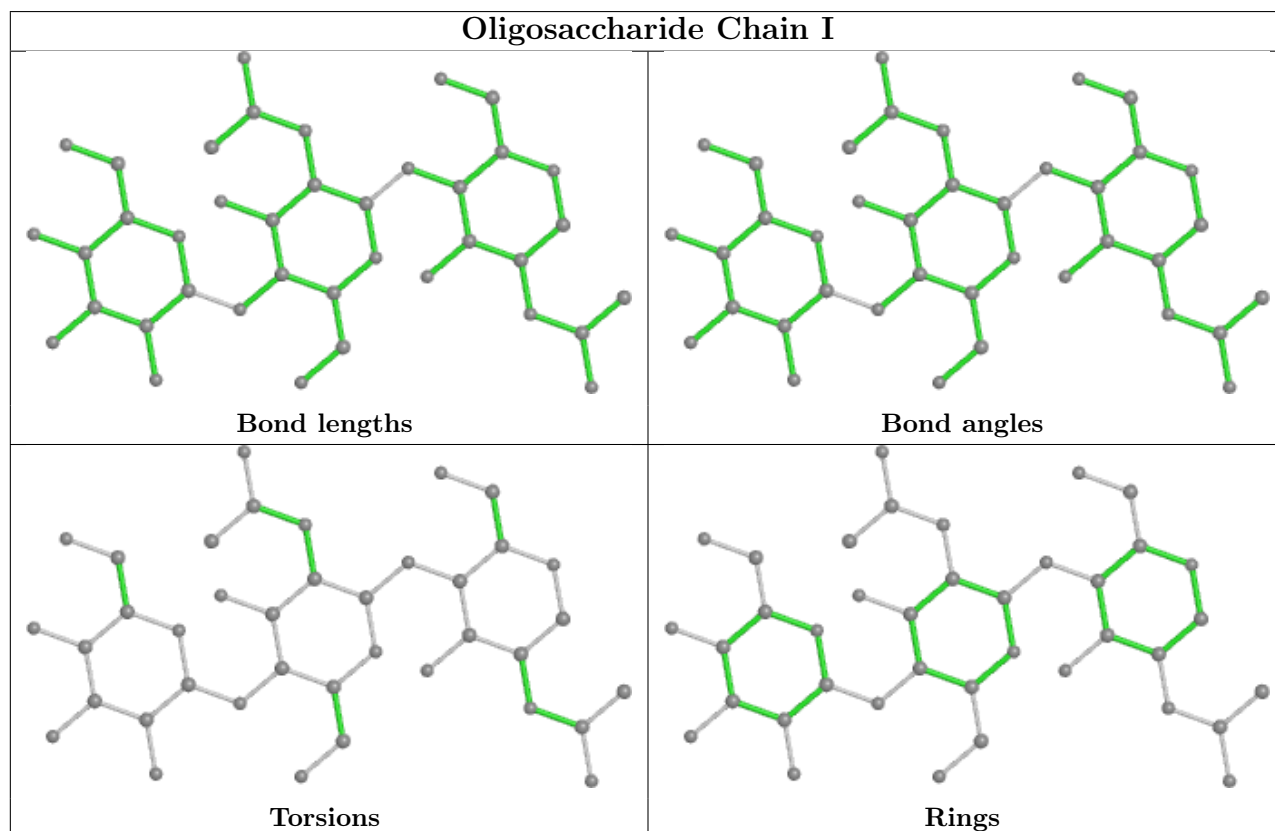
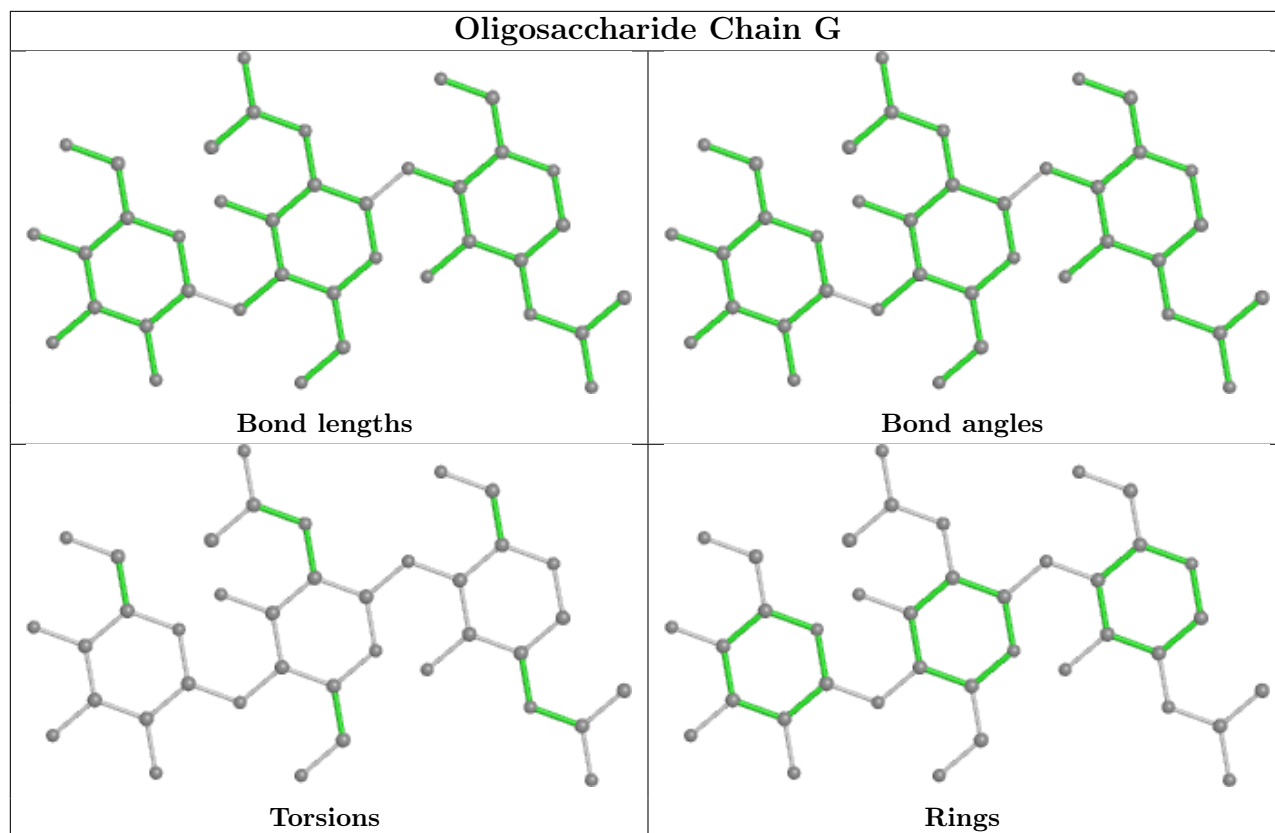




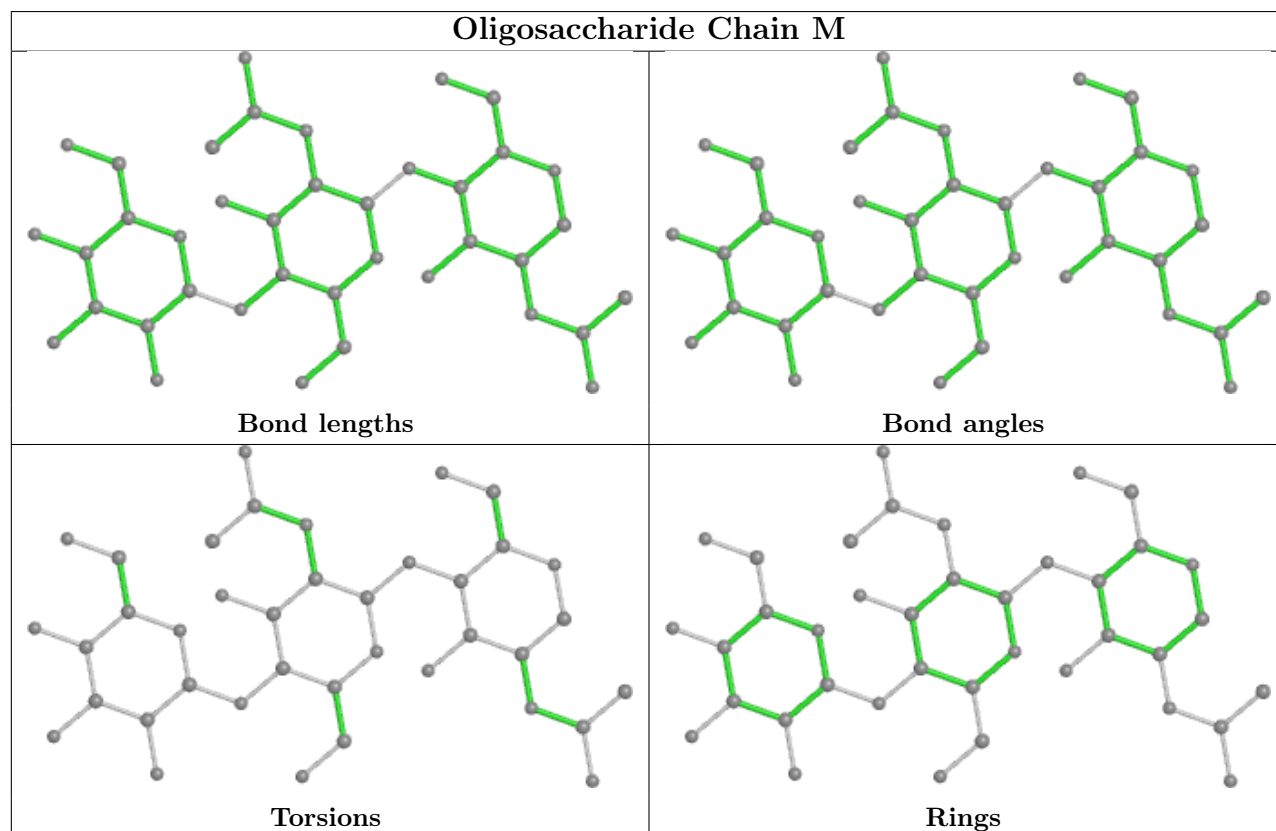
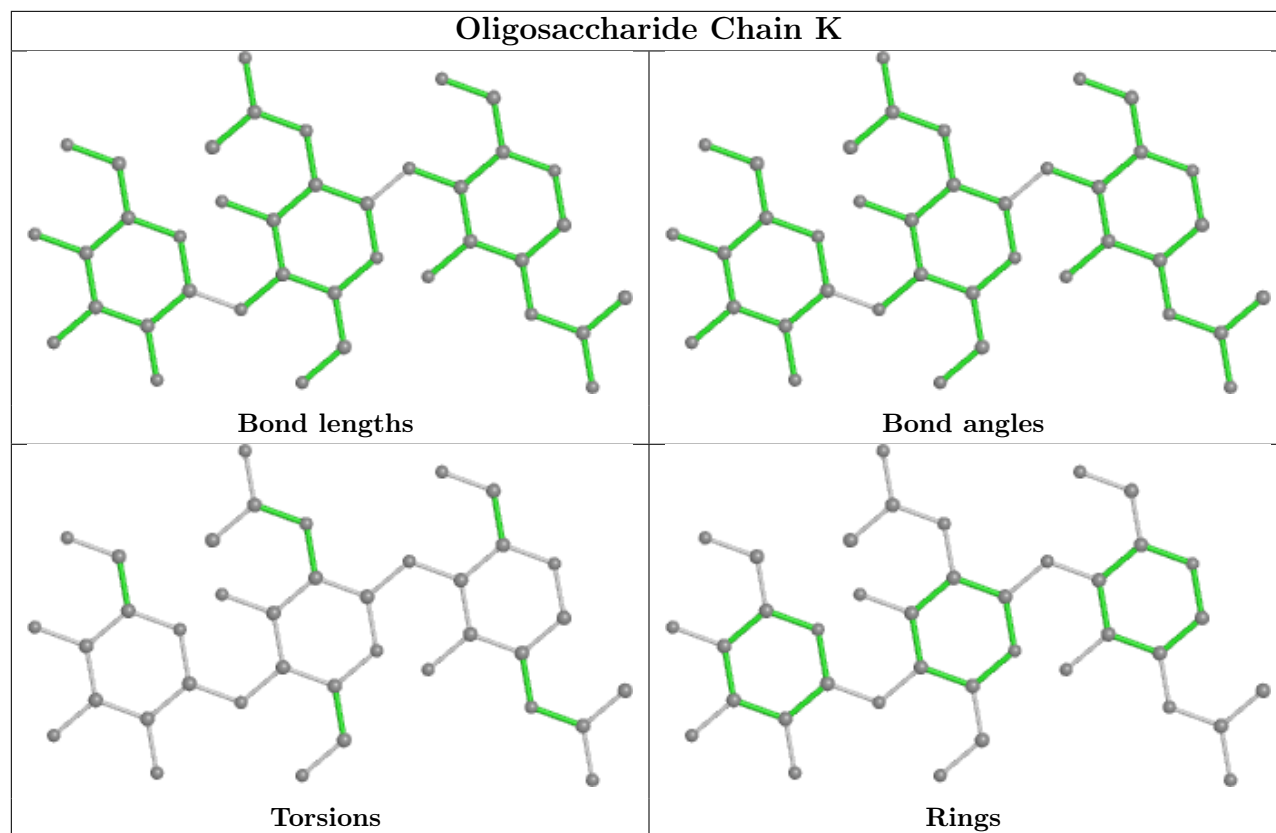


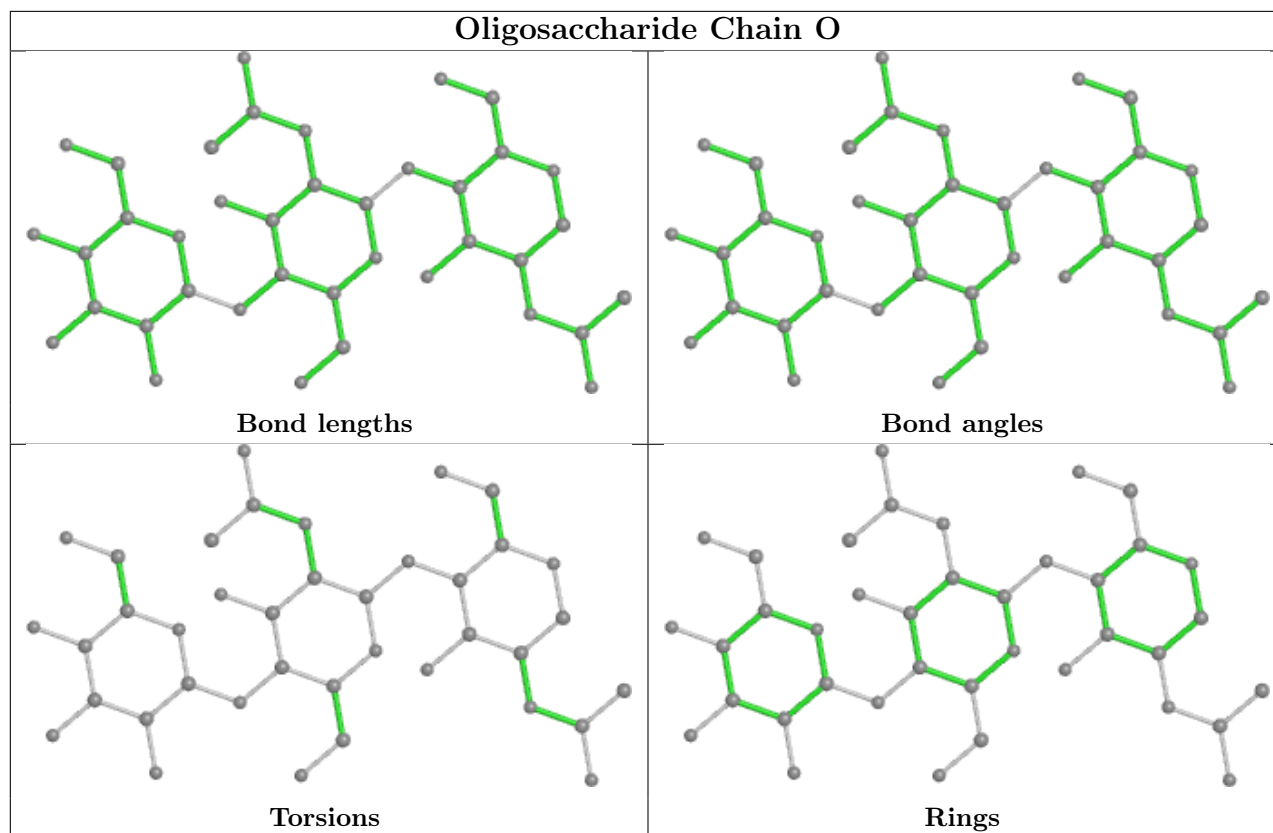












## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 5 are monoatomic - leaving 35 for Mogul analysis.

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	$\# Z  > 2$
8	EPJ	D	608	-	16,16,16	0.20	0	20,23,23	0.54	0
5	NAG	C	604	1	14,14,15	0.38	0	17,19,21	0.61	0
5	NAG	D	604	1	14,14,15	0.38	0	17,19,21	0.61	0
6	POV	C	606	-	35,35,51	0.41	0	41,43,59	0.46	0
6	POV	A	604	-	35,35,51	0.41	0	41,43,59	0.46	0
6	POV	D	602	-	46,46,51	0.32	0	52,54,59	0.28	0
6	POV	B	606	-	35,35,51	0.42	0	41,43,59	0.46	0
6	POV	B	602	-	46,46,51	0.32	0	52,54,59	0.28	0
9	I34	B	601	-	19,22,22	0.94	1 (5%)	23,30,30	0.82	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	POV	E	605	-	35,35,51	0.41	0	41,43,59	0.46	0
9	I34	E	601	-	19,22,22	0.94	1 (5%)	23,30,30	0.82	1 (4%)
9	I34	D	601	-	19,22,22	0.95	1 (5%)	23,30,30	0.82	1 (4%)
7	9Z9	A	605	-	44,44,44	0.17	0	66,68,68	0.35	0
8	EPJ	A	606	-	16,16,16	0.19	0	20,23,23	0.54	0
7	9Z9	C	607	-	44,44,44	0.17	0	66,68,68	0.35	0
5	NAG	B	604	1	14,14,15	0.37	0	17,19,21	0.61	0
6	POV	D	606	-	35,35,51	0.42	0	41,43,59	0.46	0
8	EPJ	E	607	-	16,16,16	0.19	0	20,23,23	0.54	0
9	I34	C	601	-	19,22,22	0.95	1 (5%)	23,30,30	0.82	1 (4%)
7	9Z9	E	606	-	44,44,44	0.18	0	66,68,68	0.35	0
5	NAG	A	602	1	14,14,15	0.38	0	17,19,21	0.61	0
6	POV	C	605	-	51,51,51	0.37	0	57,59,59	0.52	1 (1%)
8	EPJ	C	608	-	16,16,16	0.19	0	20,23,23	0.54	0
7	9Z9	D	607	-	44,44,44	0.17	0	66,68,68	0.35	0
9	I34	A	607	-	19,22,22	0.94	1 (5%)	23,30,30	0.82	1 (4%)
6	POV	A	608	-	51,51,51	0.37	0	57,59,59	0.52	1 (1%)
5	NAG	E	604	1	14,14,15	0.37	0	17,19,21	0.61	0
7	9Z9	B	607	-	44,44,44	0.17	0	66,68,68	0.35	0
6	POV	E	602	-	46,46,51	0.32	0	52,54,59	0.28	0
6	POV	C	602	-	46,46,51	0.32	0	52,54,59	0.28	0
6	POV	A	603	-	51,51,51	0.37	0	57,59,59	0.52	1 (1%)
6	POV	D	605	-	51,51,51	0.37	0	57,59,59	0.52	1 (1%)
6	POV	A	609	-	46,46,51	0.32	0	52,54,59	0.28	0
6	POV	B	605	-	51,51,51	0.37	0	57,59,59	0.52	1 (1%)
8	EPJ	B	608	-	16,16,16	0.19	0	20,23,23	0.54	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
8	EPJ	D	608	-	-	2/4/21/21	0/4/3/3
5	NAG	C	604	1	-	4/6/23/26	0/1/1/1
5	NAG	D	604	1	-	4/6/23/26	0/1/1/1
6	POV	C	606	-	-	21/39/39/55	-
6	POV	A	604	-	-	21/39/39/55	-
6	POV	D	602	-	-	22/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	B	606	-	-	21/39/39/55	-
6	POV	B	602	-	-	22/50/50/55	-
9	I34	B	601	-	-	0/10/12/12	0/2/2/2
6	POV	E	605	-	-	21/39/39/55	-
9	I34	E	601	-	-	0/10/12/12	0/2/2/2
9	I34	D	601	-	-	0/10/12/12	0/2/2/2
7	9Z9	A	605	-	-	3/12/100/100	0/6/6/6
8	EPJ	A	606	-	-	2/4/21/21	0/4/3/3
7	9Z9	C	607	-	-	3/12/100/100	0/6/6/6
5	NAG	B	604	1	-	4/6/23/26	0/1/1/1
6	POV	D	606	-	-	21/39/39/55	-
8	EPJ	E	607	-	-	2/4/21/21	0/4/3/3
9	I34	C	601	-	-	0/10/12/12	0/2/2/2
7	9Z9	E	606	-	-	3/12/100/100	0/6/6/6
5	NAG	A	602	1	-	4/6/23/26	0/1/1/1
6	POV	C	605	-	-	21/55/55/55	-
8	EPJ	C	608	-	-	2/4/21/21	0/4/3/3
7	9Z9	D	607	-	-	3/12/100/100	0/6/6/6
9	I34	A	607	-	-	0/10/12/12	0/2/2/2
6	POV	A	608	-	-	21/55/55/55	-
5	NAG	E	604	1	-	4/6/23/26	0/1/1/1
7	9Z9	B	607	-	-	3/12/100/100	0/6/6/6
6	POV	E	602	-	-	23/50/50/55	-
6	POV	C	602	-	-	21/50/50/55	-
6	POV	A	603	-	-	21/55/55/55	-
6	POV	D	605	-	-	21/55/55/55	-
6	POV	A	609	-	-	22/50/50/55	-
6	POV	B	605	-	-	21/55/55/55	-
8	EPJ	B	608	-	-	2/4/21/21	0/4/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	601	I34	C14-C15	-3.96	1.34	1.39
9	D	601	I34	C14-C15	-3.94	1.34	1.39
9	B	601	I34	C14-C15	-3.93	1.34	1.39
9	E	601	I34	C14-C15	-3.92	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	607	I34	C14-C15	-3.90	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	605	POV	C2-O21-C21	2.40	123.70	117.79
6	A	603	POV	C2-O21-C21	2.38	123.65	117.79
6	B	605	POV	C2-O21-C21	2.38	123.65	117.79
6	C	605	POV	C2-O21-C21	2.36	123.61	117.79
6	A	608	POV	C2-O21-C21	2.36	123.60	117.79
9	A	607	I34	C15-C14-C13	-2.30	104.86	107.23
9	D	601	I34	C15-C14-C13	-2.29	104.87	107.23
9	B	601	I34	C15-C14-C13	-2.29	104.87	107.23
9	C	601	I34	C15-C14-C13	-2.28	104.88	107.23
9	E	601	I34	C15-C14-C13	-2.25	104.90	107.23

There are no chirality outliers.

All (365) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C3-C2-N2-C7
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
5	B	604	NAG	C3-C2-N2-C7
5	B	604	NAG	C8-C7-N2-C2
5	B	604	NAG	O7-C7-N2-C2
5	C	604	NAG	C3-C2-N2-C7
5	C	604	NAG	C8-C7-N2-C2
5	C	604	NAG	O7-C7-N2-C2
5	D	604	NAG	C3-C2-N2-C7
5	D	604	NAG	C8-C7-N2-C2
5	D	604	NAG	O7-C7-N2-C2
5	E	604	NAG	C3-C2-N2-C7
5	E	604	NAG	C8-C7-N2-C2
5	E	604	NAG	O7-C7-N2-C2
6	A	603	POV	C11-O12-P-O14
6	A	603	POV	O12-C11-C12-N
6	A	603	POV	C22-C21-O21-C2
6	A	603	POV	O22-C21-O21-C2
6	A	604	POV	C1-O11-P-O13
6	A	604	POV	C11-O12-P-O13
6	A	604	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
6	A	608	POV	C11-O12-P-O14
6	A	608	POV	O12-C11-C12-N
6	A	608	POV	C22-C21-O21-C2
6	A	608	POV	O22-C21-O21-C2
6	A	609	POV	C1-O11-P-O14
6	A	609	POV	C11-O12-P-O14
6	A	609	POV	O12-C11-C12-N
6	B	602	POV	C1-O11-P-O14
6	B	602	POV	C11-O12-P-O14
6	B	602	POV	O12-C11-C12-N
6	B	605	POV	C11-O12-P-O14
6	B	605	POV	O12-C11-C12-N
6	B	605	POV	C22-C21-O21-C2
6	B	605	POV	O22-C21-O21-C2
6	B	606	POV	C1-O11-P-O13
6	B	606	POV	C11-O12-P-O13
6	B	606	POV	C11-O12-P-O14
6	C	602	POV	C1-O11-P-O14
6	C	602	POV	C11-O12-P-O14
6	C	602	POV	O12-C11-C12-N
6	C	605	POV	C11-O12-P-O14
6	C	605	POV	O12-C11-C12-N
6	C	605	POV	C22-C21-O21-C2
6	C	605	POV	O22-C21-O21-C2
6	C	606	POV	C1-O11-P-O13
6	C	606	POV	C11-O12-P-O13
6	C	606	POV	C11-O12-P-O14
6	D	602	POV	C1-O11-P-O14
6	D	602	POV	C11-O12-P-O14
6	D	602	POV	O12-C11-C12-N
6	D	605	POV	C11-O12-P-O14
6	D	605	POV	O12-C11-C12-N
6	D	605	POV	C22-C21-O21-C2
6	D	605	POV	O22-C21-O21-C2
6	D	606	POV	C1-O11-P-O13
6	D	606	POV	C11-O12-P-O13
6	D	606	POV	C11-O12-P-O14
6	E	602	POV	C1-O11-P-O14
6	E	602	POV	C11-O12-P-O14
6	E	602	POV	O12-C11-C12-N
6	E	605	POV	C1-O11-P-O13
6	E	605	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
6	E	605	POV	C11-O12-P-O14
7	A	605	9Z9	C18-C17-O20-C21
7	B	607	9Z9	C18-C17-O20-C21
7	C	607	9Z9	C18-C17-O20-C21
7	D	607	9Z9	C18-C17-O20-C21
7	E	606	9Z9	C18-C17-O20-C21
6	A	604	POV	C1-O11-P-O12
6	A	604	POV	C11-O12-P-O11
6	B	606	POV	C1-O11-P-O12
6	B	606	POV	C11-O12-P-O11
6	C	606	POV	C1-O11-P-O12
6	C	606	POV	C11-O12-P-O11
6	D	606	POV	C1-O11-P-O12
6	D	606	POV	C11-O12-P-O11
6	E	605	POV	C1-O11-P-O12
6	E	605	POV	C11-O12-P-O11
6	A	609	POV	C32-C31-O31-C3
6	B	602	POV	C32-C31-O31-C3
6	C	602	POV	C32-C31-O31-C3
6	D	602	POV	C32-C31-O31-C3
6	E	602	POV	C32-C31-O31-C3
6	B	606	POV	C22-C23-C24-C25
6	E	605	POV	C22-C23-C24-C25
6	E	605	POV	C33-C34-C35-C36
6	A	604	POV	C22-C23-C24-C25
6	A	604	POV	C33-C34-C35-C36
6	B	606	POV	C33-C34-C35-C36
6	C	606	POV	C22-C23-C24-C25
6	C	606	POV	C33-C34-C35-C36
6	D	606	POV	C22-C23-C24-C25
6	D	606	POV	C33-C34-C35-C36
6	A	609	POV	O32-C31-O31-C3
6	B	602	POV	O32-C31-O31-C3
6	C	602	POV	O32-C31-O31-C3
6	D	602	POV	O32-C31-O31-C3
6	E	602	POV	O32-C31-O31-C3
6	A	609	POV	C37-C38-C39-C310
6	B	602	POV	C37-C38-C39-C310
6	D	602	POV	C37-C38-C39-C310
6	E	602	POV	C37-C38-C39-C310
6	C	602	POV	C37-C38-C39-C310
6	A	604	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	B	606	POV	C23-C24-C25-C26
6	C	606	POV	C23-C24-C25-C26
6	D	606	POV	C23-C24-C25-C26
6	E	605	POV	C23-C24-C25-C26
6	A	603	POV	C39-C310-C311-C312
6	A	608	POV	C39-C310-C311-C312
6	B	605	POV	C39-C310-C311-C312
6	C	605	POV	C39-C310-C311-C312
6	D	605	POV	C39-C310-C311-C312
8	A	606	EPJ	C6-C1-C7-C8
8	B	608	EPJ	C6-C1-C7-C8
8	C	608	EPJ	C6-C1-C7-C8
8	D	608	EPJ	C6-C1-C7-C8
8	E	607	EPJ	C6-C1-C7-C8
6	A	603	POV	C32-C31-O31-C3
6	A	608	POV	C32-C31-O31-C3
6	B	605	POV	C32-C31-O31-C3
6	C	605	POV	C32-C31-O31-C3
6	D	605	POV	C32-C31-O31-C3
6	A	604	POV	C2-C3-O31-C31
6	B	606	POV	C2-C3-O31-C31
6	C	606	POV	C2-C3-O31-C31
6	E	605	POV	C2-C3-O31-C31
6	D	606	POV	C2-C3-O31-C31
6	A	603	POV	O32-C31-O31-C3
6	A	608	POV	O32-C31-O31-C3
6	B	605	POV	O32-C31-O31-C3
6	C	605	POV	O32-C31-O31-C3
6	D	605	POV	O32-C31-O31-C3
6	A	603	POV	C25-C26-C27-C28
6	A	608	POV	C25-C26-C27-C28
6	C	605	POV	C25-C26-C27-C28
6	D	605	POV	C25-C26-C27-C28
6	B	605	POV	C25-C26-C27-C28
6	A	603	POV	O11-C1-C2-O21
6	A	608	POV	O11-C1-C2-O21
6	B	605	POV	O11-C1-C2-O21
6	C	605	POV	O11-C1-C2-O21
6	D	605	POV	O11-C1-C2-O21
6	A	604	POV	C26-C27-C28-C29
6	B	606	POV	C26-C27-C28-C29
6	C	606	POV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	D	606	POV	C26-C27-C28-C29
6	E	605	POV	C26-C27-C28-C29
6	A	603	POV	O11-C1-C2-C3
6	A	608	POV	O11-C1-C2-C3
6	A	609	POV	O11-C1-C2-C3
6	B	602	POV	O11-C1-C2-C3
6	B	605	POV	O11-C1-C2-C3
6	C	602	POV	O11-C1-C2-C3
6	C	605	POV	O11-C1-C2-C3
6	D	602	POV	O11-C1-C2-C3
6	D	605	POV	O11-C1-C2-C3
6	E	602	POV	O11-C1-C2-C3
6	A	603	POV	C210-C211-C212-C213
6	A	608	POV	C210-C211-C212-C213
6	B	605	POV	C210-C211-C212-C213
6	C	605	POV	C210-C211-C212-C213
6	D	605	POV	C210-C211-C212-C213
8	A	606	EPJ	C6-C1-C7-C11
8	B	608	EPJ	C6-C1-C7-C11
8	C	608	EPJ	C6-C1-C7-C11
8	D	608	EPJ	C6-C1-C7-C11
8	E	607	EPJ	C6-C1-C7-C11
6	A	609	POV	C311-C312-C313-C314
6	B	602	POV	C311-C312-C313-C314
6	C	602	POV	C311-C312-C313-C314
6	D	602	POV	C311-C312-C313-C314
6	E	602	POV	C311-C312-C313-C314
6	A	603	POV	O31-C31-C32-C33
6	A	608	POV	O31-C31-C32-C33
6	B	605	POV	O31-C31-C32-C33
6	C	605	POV	O31-C31-C32-C33
6	D	605	POV	O31-C31-C32-C33
6	A	603	POV	C313-C314-C315-C316
6	A	608	POV	C313-C314-C315-C316
6	B	605	POV	C313-C314-C315-C316
6	C	605	POV	C313-C314-C315-C316
6	D	605	POV	C313-C314-C315-C316
6	A	609	POV	C26-C27-C28-C29
6	B	602	POV	C26-C27-C28-C29
6	C	602	POV	C26-C27-C28-C29
6	D	602	POV	C26-C27-C28-C29
6	E	602	POV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	A	604	POV	C32-C31-O31-C3
6	B	606	POV	C32-C31-O31-C3
6	C	606	POV	C32-C31-O31-C3
6	D	606	POV	C32-C31-O31-C3
6	E	605	POV	C32-C31-O31-C3
6	A	603	POV	C311-C312-C313-C314
6	A	608	POV	C311-C312-C313-C314
6	B	605	POV	C311-C312-C313-C314
6	C	605	POV	C311-C312-C313-C314
6	D	605	POV	C311-C312-C313-C314
6	A	609	POV	C21-C22-C23-C24
6	B	602	POV	C21-C22-C23-C24
6	C	602	POV	C21-C22-C23-C24
6	D	602	POV	C21-C22-C23-C24
6	E	602	POV	C21-C22-C23-C24
6	A	604	POV	C2-C1-O11-P
6	B	606	POV	C2-C1-O11-P
6	C	606	POV	C2-C1-O11-P
6	D	606	POV	C2-C1-O11-P
6	E	605	POV	C2-C1-O11-P
6	A	603	POV	C34-C35-C36-C37
6	B	605	POV	C34-C35-C36-C37
6	A	604	POV	O11-C1-C2-O21
6	B	606	POV	O11-C1-C2-O21
6	C	606	POV	O11-C1-C2-O21
6	D	606	POV	O11-C1-C2-O21
6	E	605	POV	O11-C1-C2-O21
6	A	608	POV	C34-C35-C36-C37
6	C	605	POV	C34-C35-C36-C37
6	D	605	POV	C34-C35-C36-C37
6	A	603	POV	O21-C2-C3-O31
6	A	608	POV	O21-C2-C3-O31
6	B	605	POV	O21-C2-C3-O31
6	C	605	POV	O21-C2-C3-O31
6	D	605	POV	O21-C2-C3-O31
6	A	609	POV	C2-C1-O11-P
6	B	602	POV	C2-C1-O11-P
6	C	602	POV	C2-C1-O11-P
6	D	602	POV	C2-C1-O11-P
6	E	602	POV	C2-C1-O11-P
6	A	604	POV	O32-C31-O31-C3
6	B	606	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	D	606	POV	O32-C31-O31-C3
6	C	606	POV	O32-C31-O31-C3
6	E	605	POV	O32-C31-O31-C3
6	A	603	POV	C1-C2-C3-O31
6	A	608	POV	C1-C2-C3-O31
6	B	605	POV	C1-C2-C3-O31
6	C	605	POV	C1-C2-C3-O31
6	D	605	POV	C1-C2-C3-O31
6	A	609	POV	O11-C1-C2-O21
6	B	602	POV	O11-C1-C2-O21
6	C	602	POV	O11-C1-C2-O21
6	D	602	POV	O11-C1-C2-O21
6	E	602	POV	O11-C1-C2-O21
6	A	604	POV	O11-C1-C2-C3
6	B	606	POV	O11-C1-C2-C3
6	C	606	POV	O11-C1-C2-C3
6	D	606	POV	O11-C1-C2-C3
6	E	605	POV	O11-C1-C2-C3
6	A	604	POV	O12-C11-C12-N
6	B	606	POV	O12-C11-C12-N
6	C	606	POV	O12-C11-C12-N
6	D	606	POV	O12-C11-C12-N
6	E	605	POV	O12-C11-C12-N
6	E	602	POV	C313-C314-C315-C316
6	A	609	POV	C313-C314-C315-C316
6	B	602	POV	C313-C314-C315-C316
6	C	602	POV	C313-C314-C315-C316
6	D	602	POV	C313-C314-C315-C316
6	C	602	POV	C310-C311-C312-C313
6	A	609	POV	C310-C311-C312-C313
6	B	602	POV	C310-C311-C312-C313
6	D	602	POV	C310-C311-C312-C313
6	E	602	POV	C310-C311-C312-C313
6	A	603	POV	C1-O11-P-O12
6	A	603	POV	C11-O12-P-O11
6	A	608	POV	C1-O11-P-O12
6	A	608	POV	C11-O12-P-O11
6	A	609	POV	C1-O11-P-O12
6	A	609	POV	C11-O12-P-O11
6	B	602	POV	C1-O11-P-O12
6	B	602	POV	C11-O12-P-O11
6	B	605	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
6	B	605	POV	C11-O12-P-O11
6	C	602	POV	C1-O11-P-O12
6	C	602	POV	C11-O12-P-O11
6	C	605	POV	C1-O11-P-O12
6	C	605	POV	C11-O12-P-O11
6	D	602	POV	C1-O11-P-O12
6	D	602	POV	C11-O12-P-O11
6	D	605	POV	C1-O11-P-O12
6	D	605	POV	C11-O12-P-O11
6	E	602	POV	C1-O11-P-O12
6	E	602	POV	C11-O12-P-O11
6	A	608	POV	O32-C31-C32-C33
6	A	603	POV	O32-C31-C32-C33
6	B	605	POV	O32-C31-C32-C33
6	C	605	POV	O32-C31-C32-C33
6	D	605	POV	O32-C31-C32-C33
6	C	602	POV	C312-C313-C314-C315
6	D	602	POV	C312-C313-C314-C315
6	A	609	POV	C312-C313-C314-C315
6	B	602	POV	C312-C313-C314-C315
6	E	602	POV	C312-C313-C314-C315
6	A	609	POV	C210-C211-C212-C213
6	B	602	POV	C210-C211-C212-C213
6	C	602	POV	C210-C211-C212-C213
6	D	602	POV	C210-C211-C212-C213
6	E	602	POV	C210-C211-C212-C213
7	A	605	9Z9	C23-C48-O49-C50
7	B	607	9Z9	C23-C48-O49-C50
7	C	607	9Z9	C23-C48-O49-C50
7	D	607	9Z9	C23-C48-O49-C50
7	E	606	9Z9	C23-C48-O49-C50
5	A	602	NAG	C1-C2-N2-C7
5	B	604	NAG	C1-C2-N2-C7
5	C	604	NAG	C1-C2-N2-C7
5	D	604	NAG	C1-C2-N2-C7
5	E	604	NAG	C1-C2-N2-C7
6	B	602	POV	C24-C25-C26-C27
6	D	602	POV	C24-C25-C26-C27
6	E	602	POV	C24-C25-C26-C27
6	C	602	POV	C24-C25-C26-C27
6	A	609	POV	C24-C25-C26-C27
6	A	609	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
6	C	602	POV	C29-C210-C211-C212
6	D	602	POV	C29-C210-C211-C212
6	B	602	POV	C29-C210-C211-C212
6	E	602	POV	C29-C210-C211-C212
6	A	603	POV	C26-C27-C28-C29
6	A	608	POV	C26-C27-C28-C29
6	B	605	POV	C26-C27-C28-C29
6	C	605	POV	C26-C27-C28-C29
6	D	605	POV	C26-C27-C28-C29
7	A	605	9Z9	O20-C21-C22-C23
7	B	607	9Z9	O20-C21-C22-C23
7	C	607	9Z9	O20-C21-C22-C23
7	D	607	9Z9	O20-C21-C22-C23
7	E	606	9Z9	O20-C21-C22-C23
6	A	604	POV	O31-C31-C32-C33
6	B	606	POV	O31-C31-C32-C33
6	C	606	POV	O31-C31-C32-C33
6	D	606	POV	O31-C31-C32-C33
6	E	605	POV	O31-C31-C32-C33
6	C	606	POV	O32-C31-C32-C33
6	D	606	POV	O32-C31-C32-C33
6	E	605	POV	O32-C31-C32-C33
6	A	604	POV	O32-C31-C32-C33
6	B	606	POV	O32-C31-C32-C33
6	B	606	POV	C25-C26-C27-C28
6	D	606	POV	C25-C26-C27-C28
6	A	604	POV	C11-C12-N-C13
6	B	606	POV	C11-C12-N-C13
6	C	606	POV	C11-C12-N-C13
6	D	606	POV	C11-C12-N-C13
6	E	605	POV	C11-C12-N-C13
6	A	604	POV	C25-C26-C27-C28
6	C	606	POV	C25-C26-C27-C28
6	E	605	POV	C25-C26-C27-C28
6	C	602	POV	O21-C21-C22-C23
6	A	604	POV	C11-C12-N-C15
6	B	606	POV	C11-C12-N-C15
6	C	606	POV	C11-C12-N-C15
6	D	606	POV	C11-C12-N-C15
6	E	605	POV	C11-C12-N-C15
6	A	609	POV	O21-C21-C22-C23
6	B	602	POV	O21-C21-C22-C23

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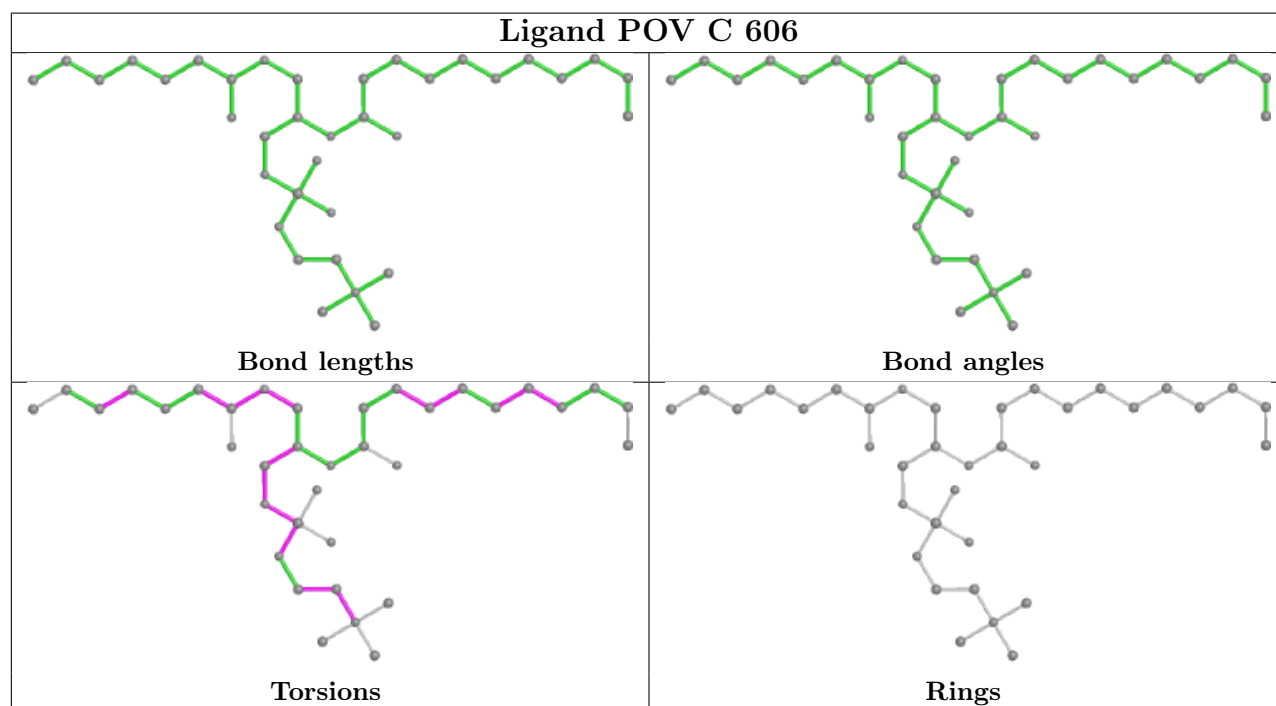
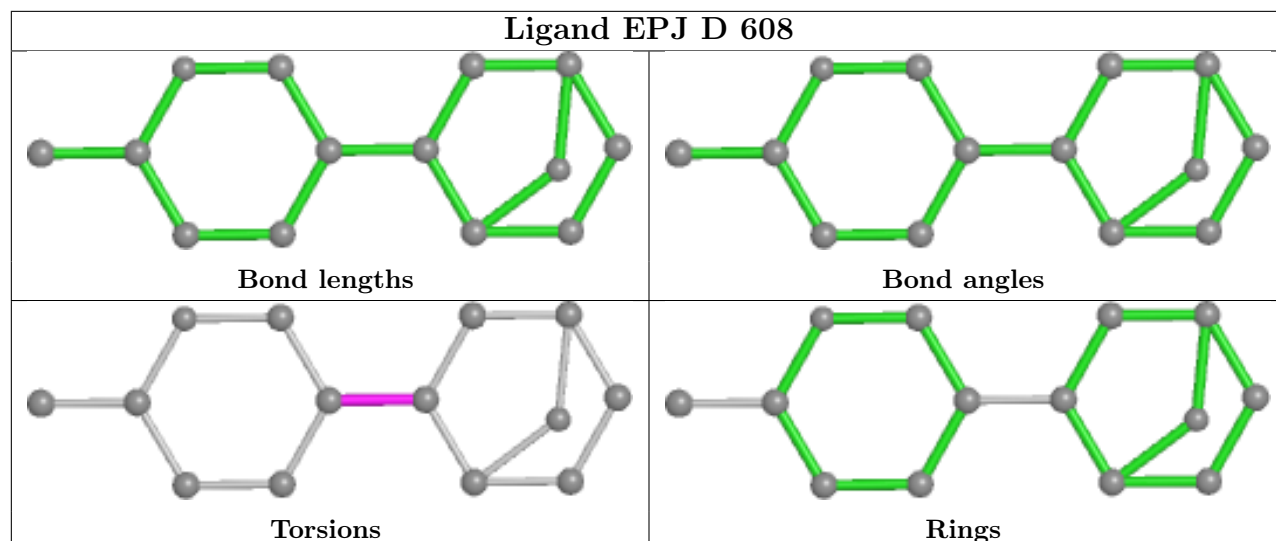
Mol	Chain	Res	Type	Atoms
6	D	602	POV	O21-C21-C22-C23
6	E	602	POV	O21-C21-C22-C23
6	E	602	POV	C311-C310-C39-C38
6	B	602	POV	C311-C310-C39-C38
6	D	602	POV	C311-C310-C39-C38
6	A	609	POV	C311-C310-C39-C38
6	E	602	POV	C32-C33-C34-C35

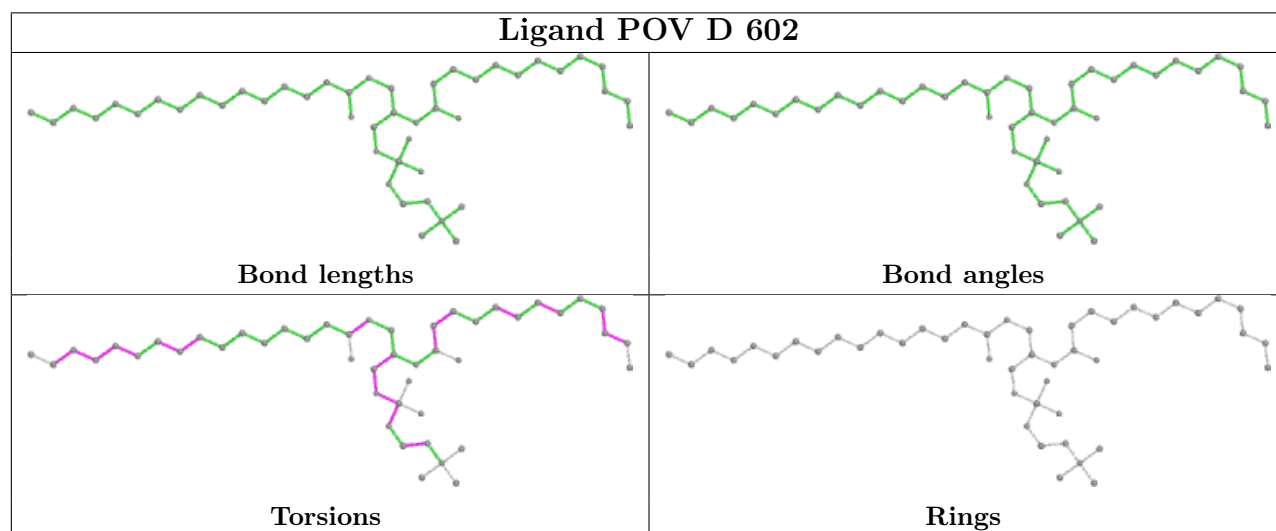
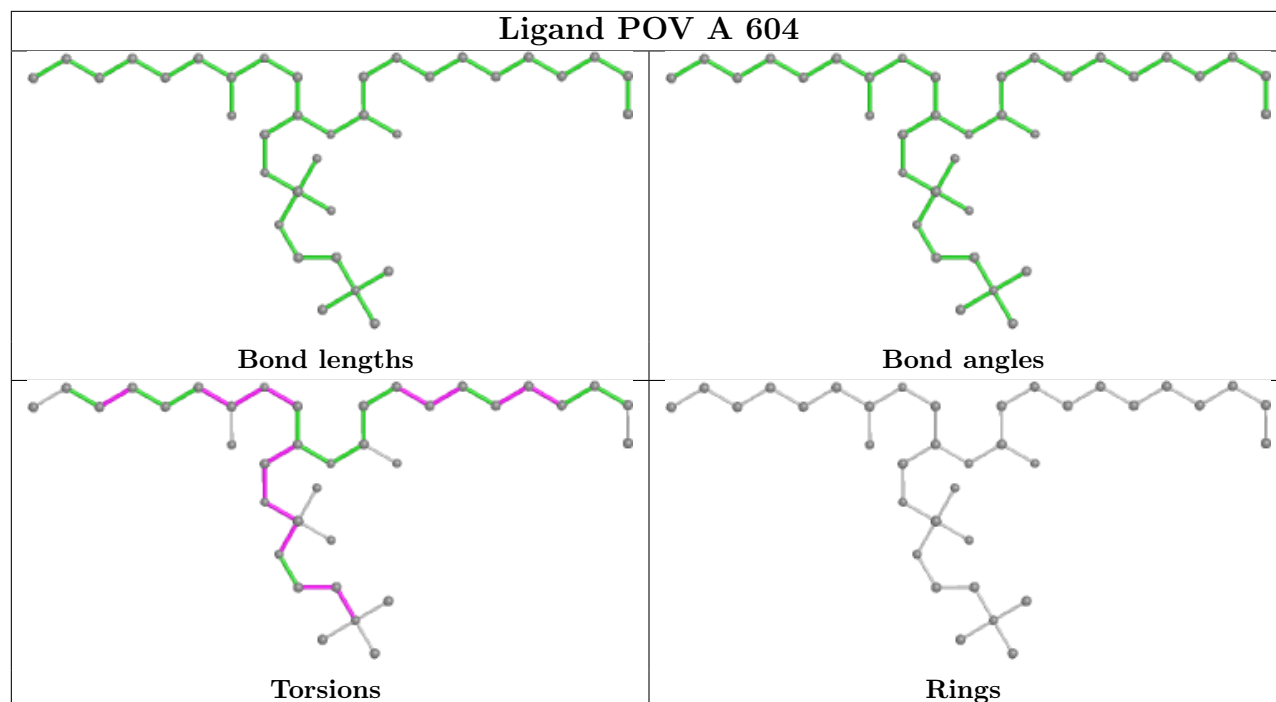
There are no ring outliers.

16 monomers are involved in 16 short contacts:

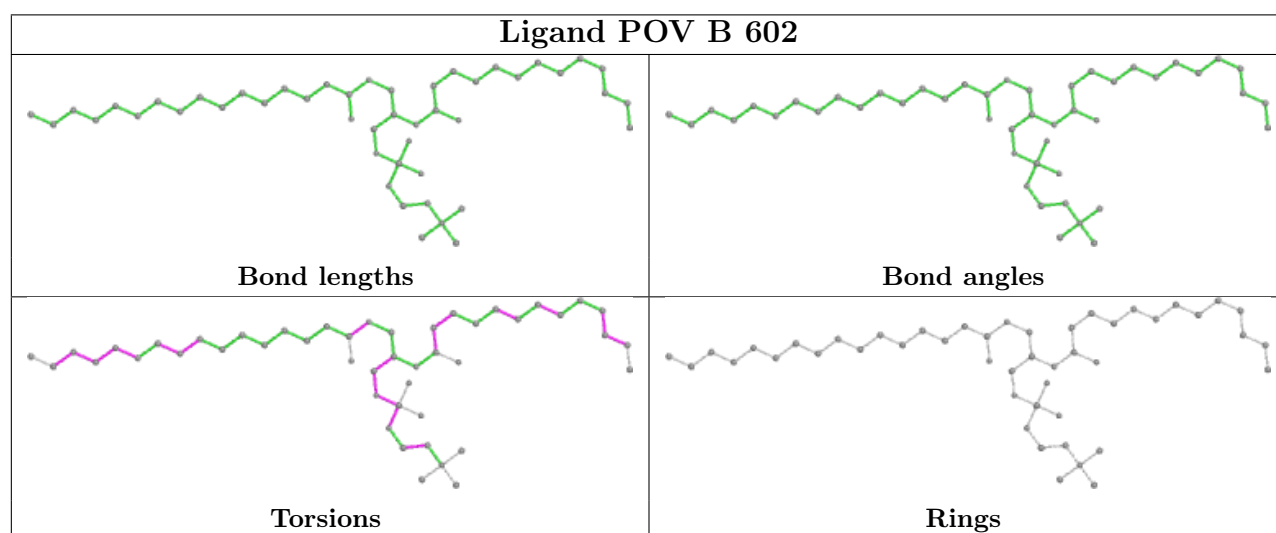
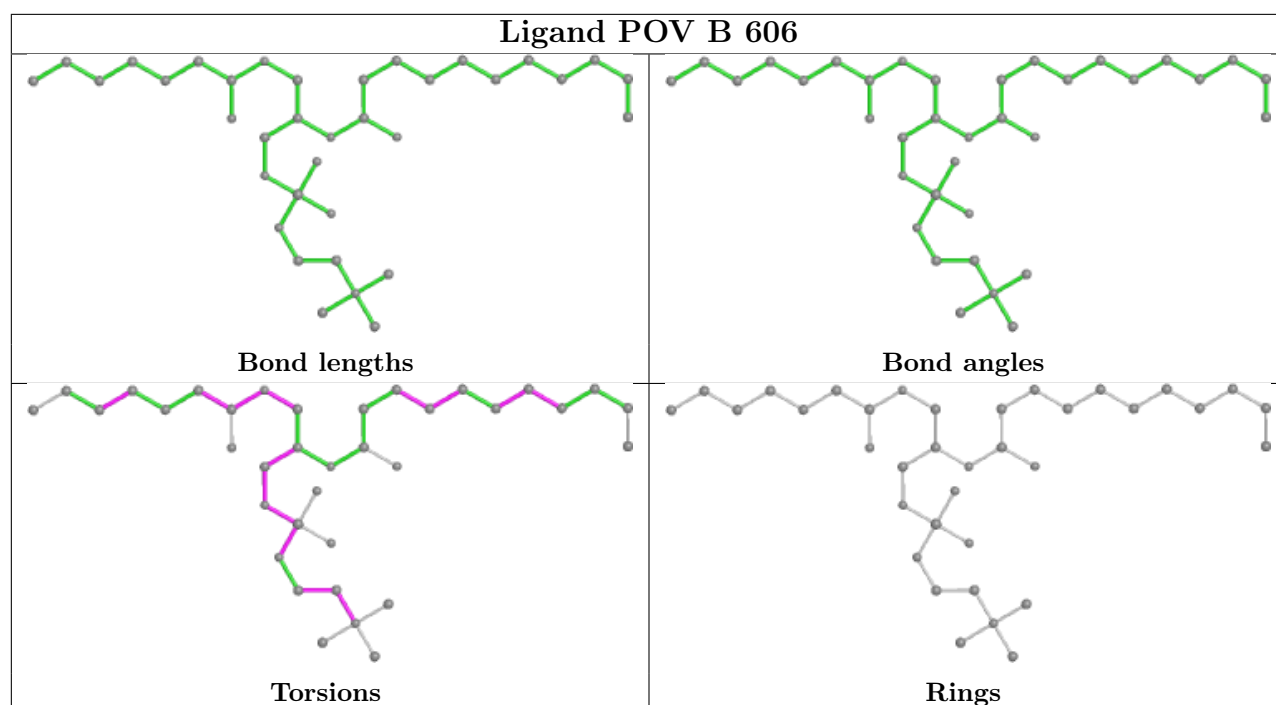
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	604	NAG	1	0
5	D	604	NAG	1	0
6	B	606	POV	1	0
9	B	601	I34	1	0
9	E	601	I34	1	0
9	D	601	I34	1	0
5	B	604	NAG	1	0
9	C	601	I34	1	0
5	A	602	NAG	1	0
6	C	605	POV	1	0
9	A	607	I34	1	0
6	A	608	POV	1	0
5	E	604	NAG	1	0
6	A	603	POV	1	0
6	D	605	POV	1	0
6	B	605	POV	1	0

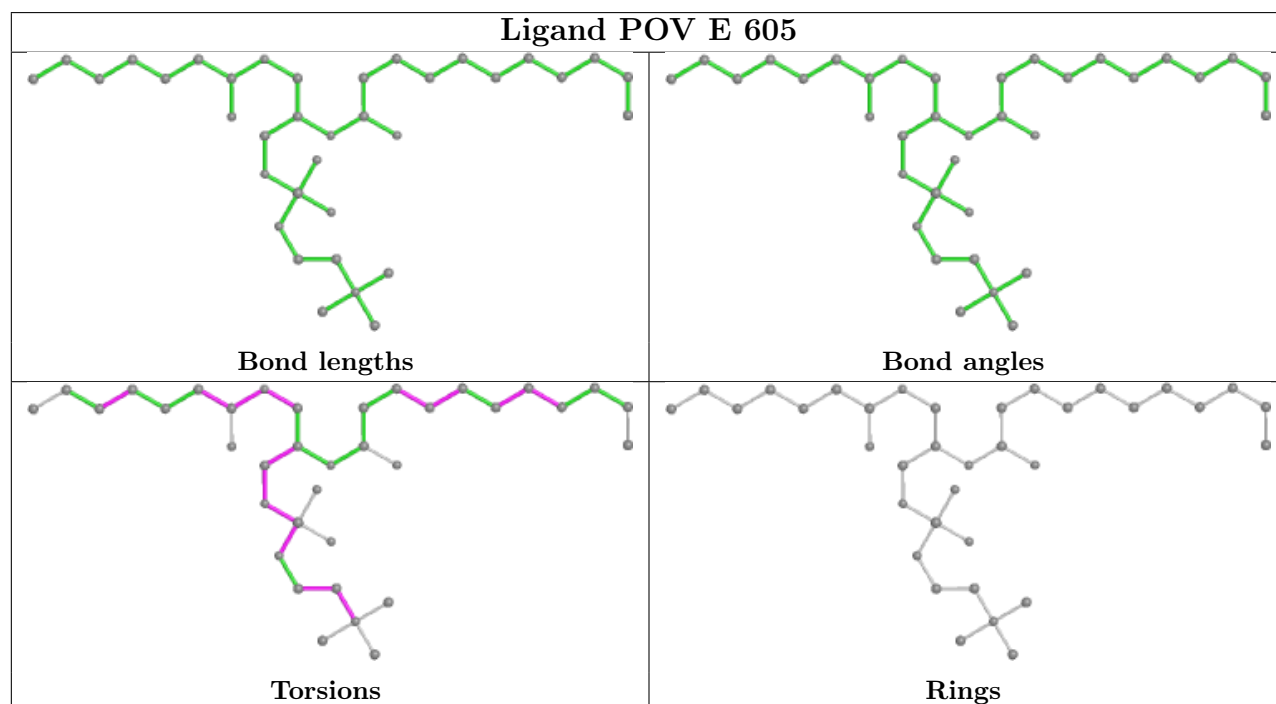
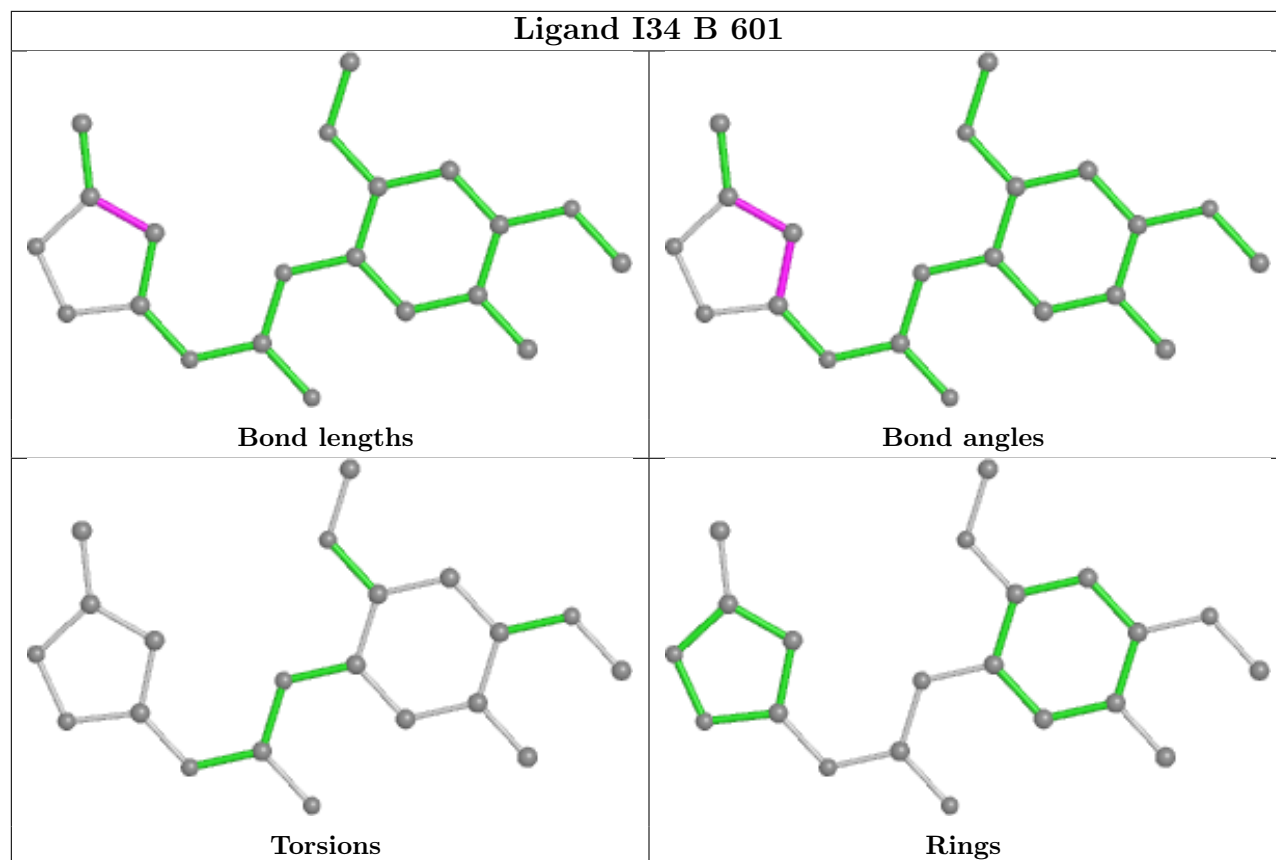
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

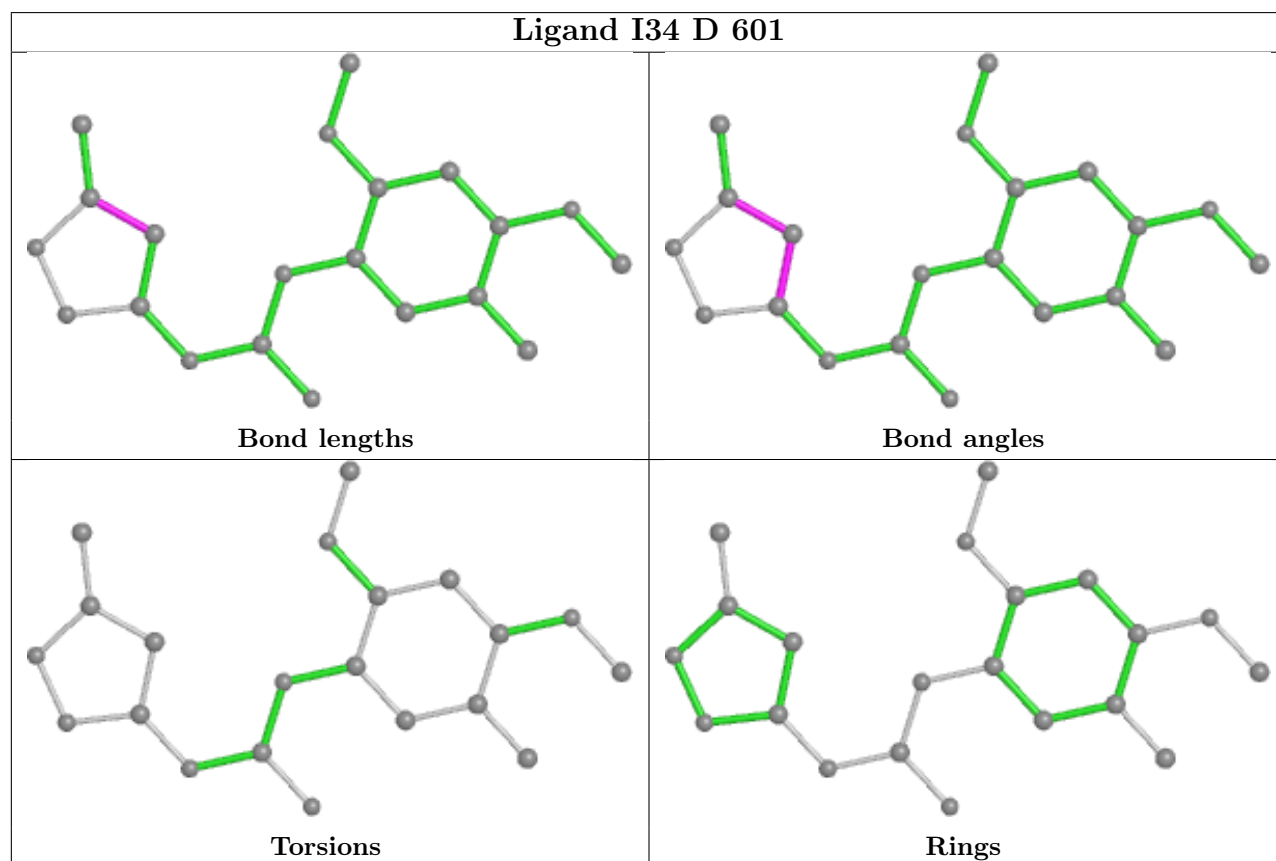
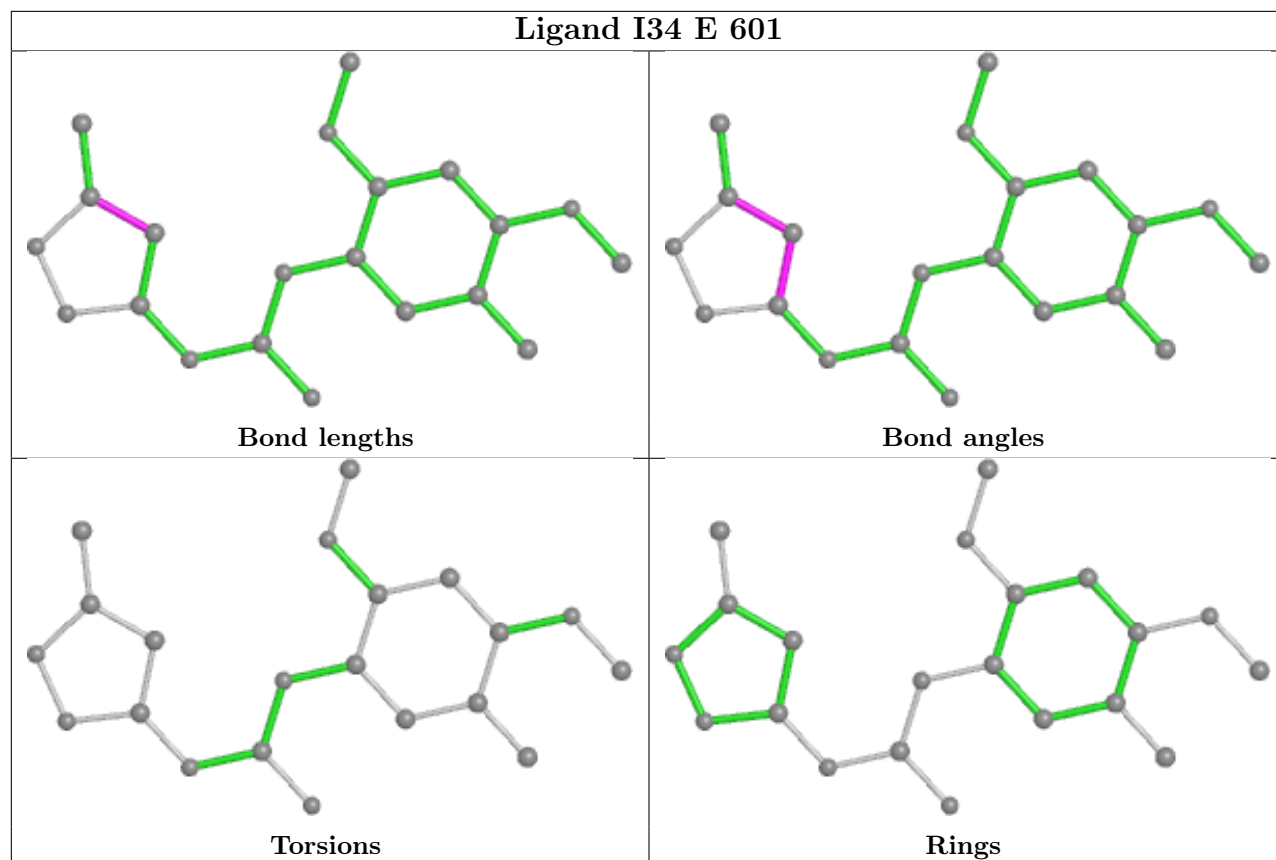


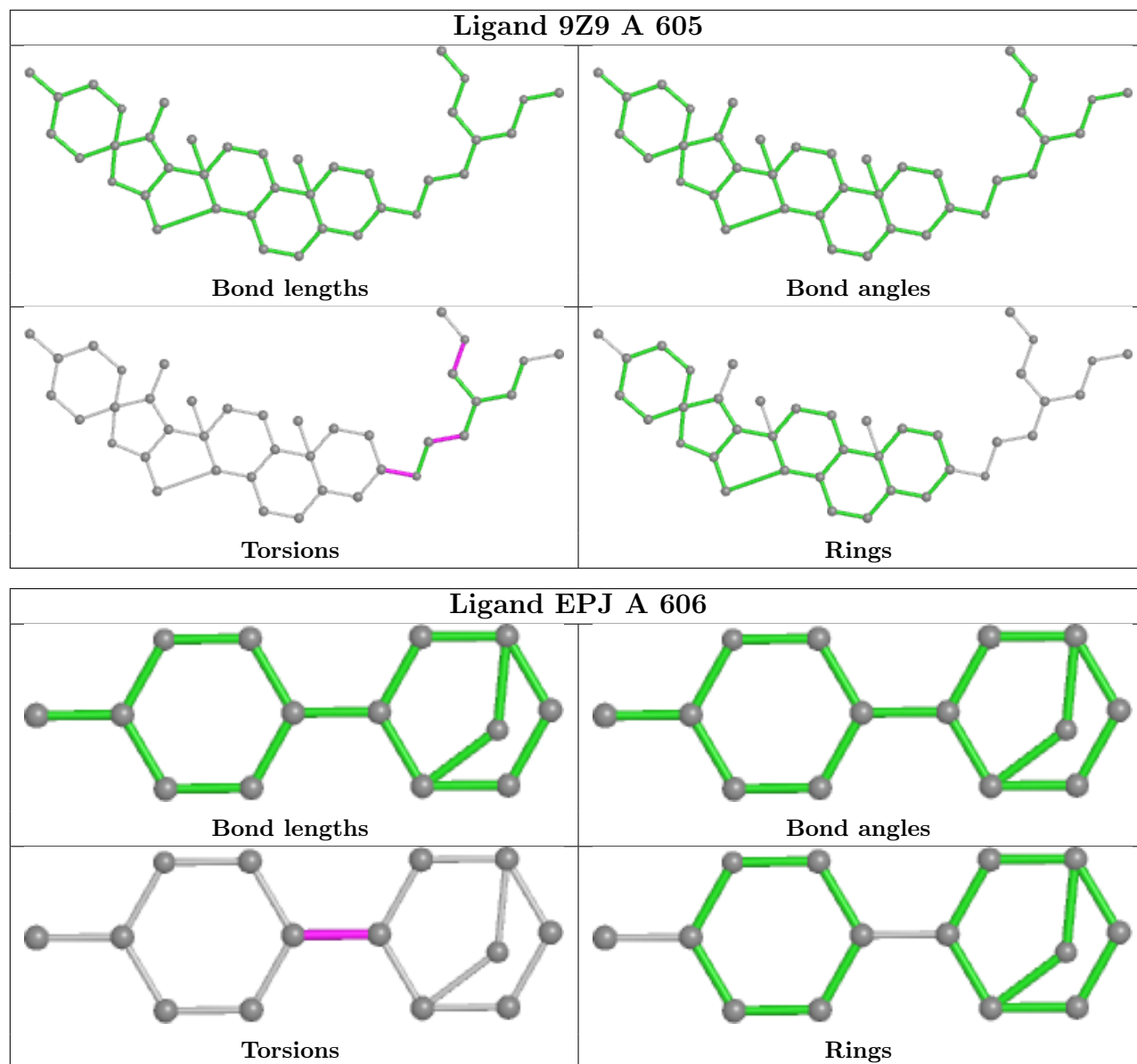


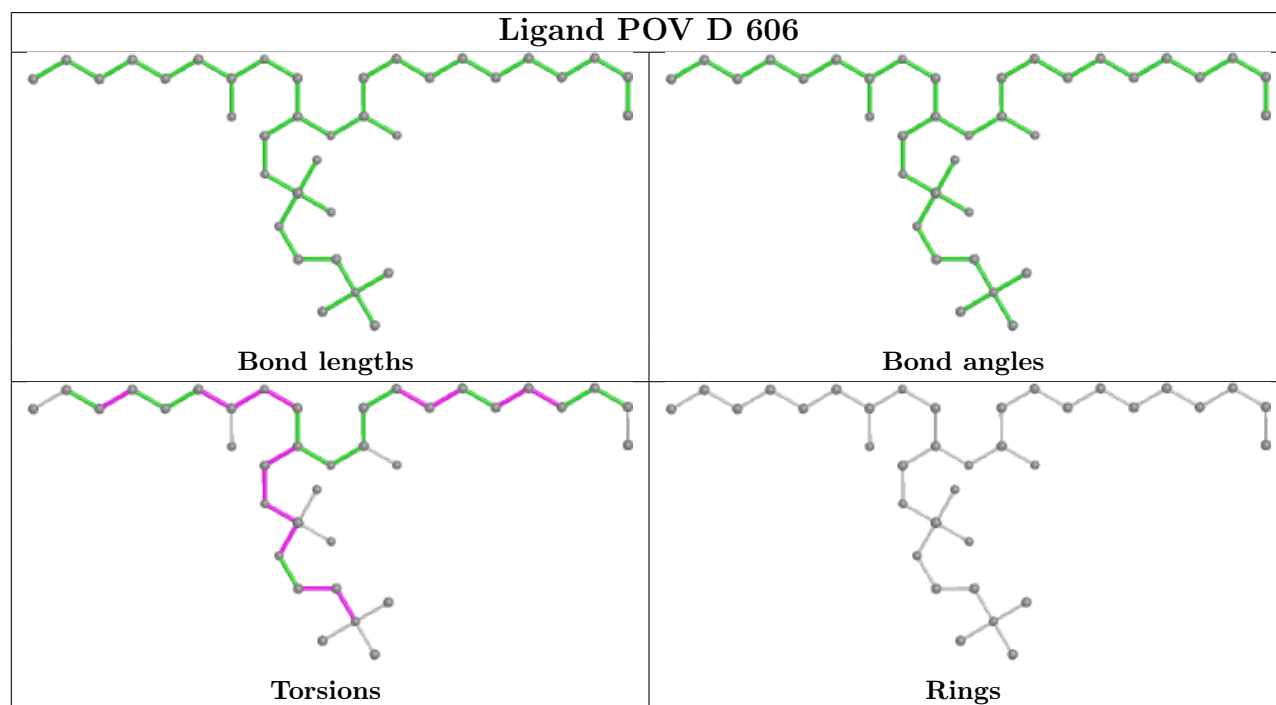
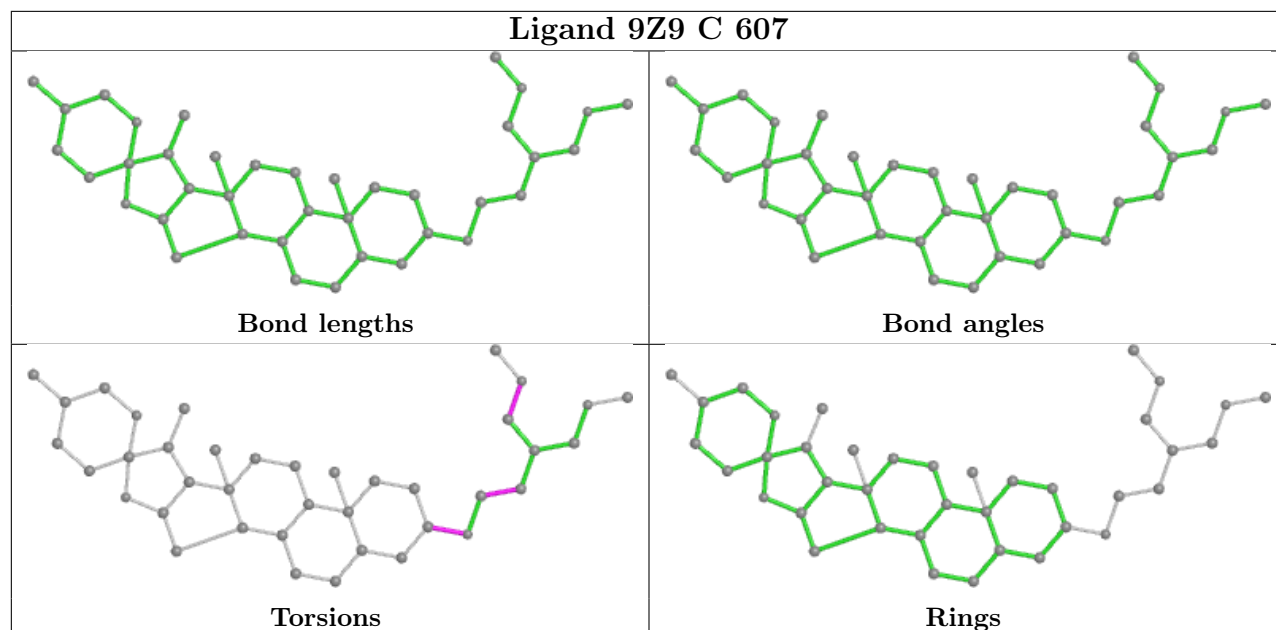


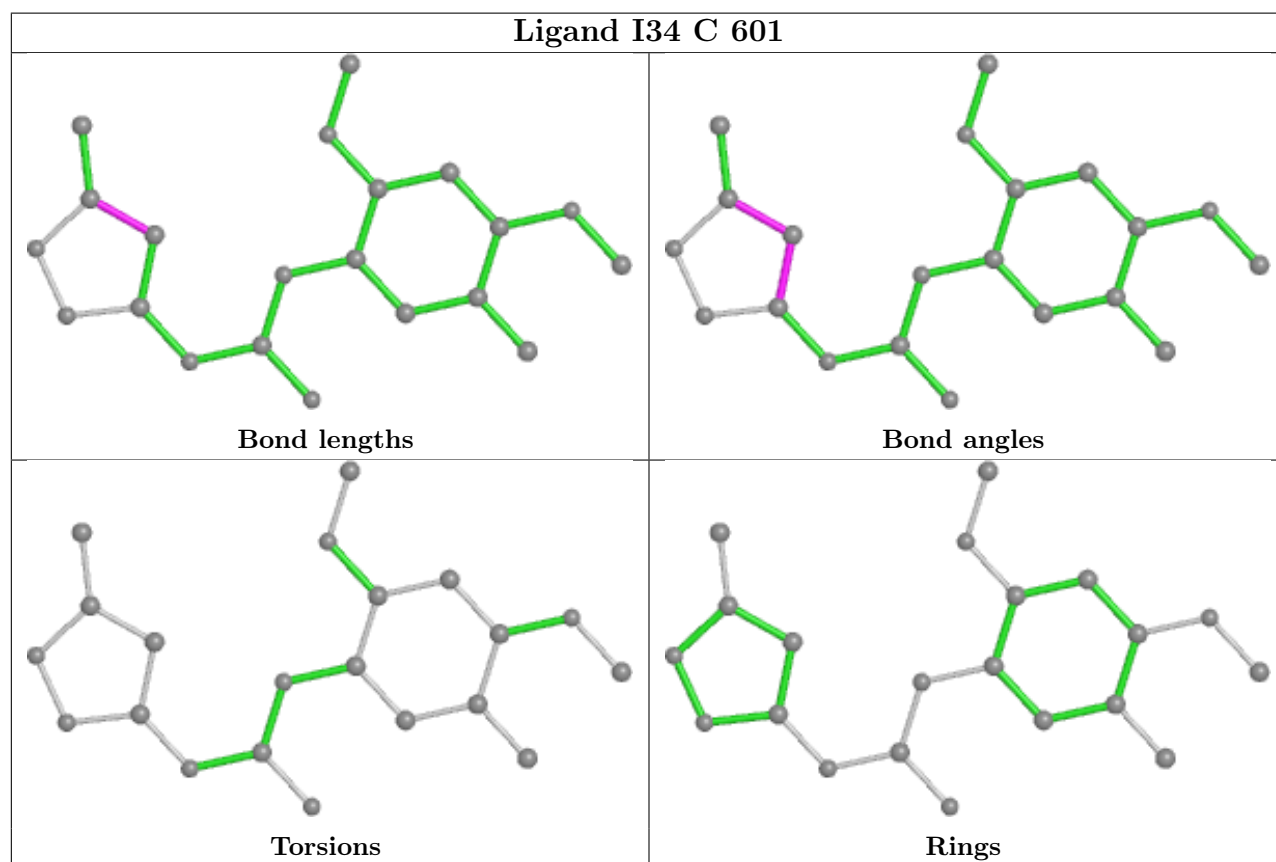
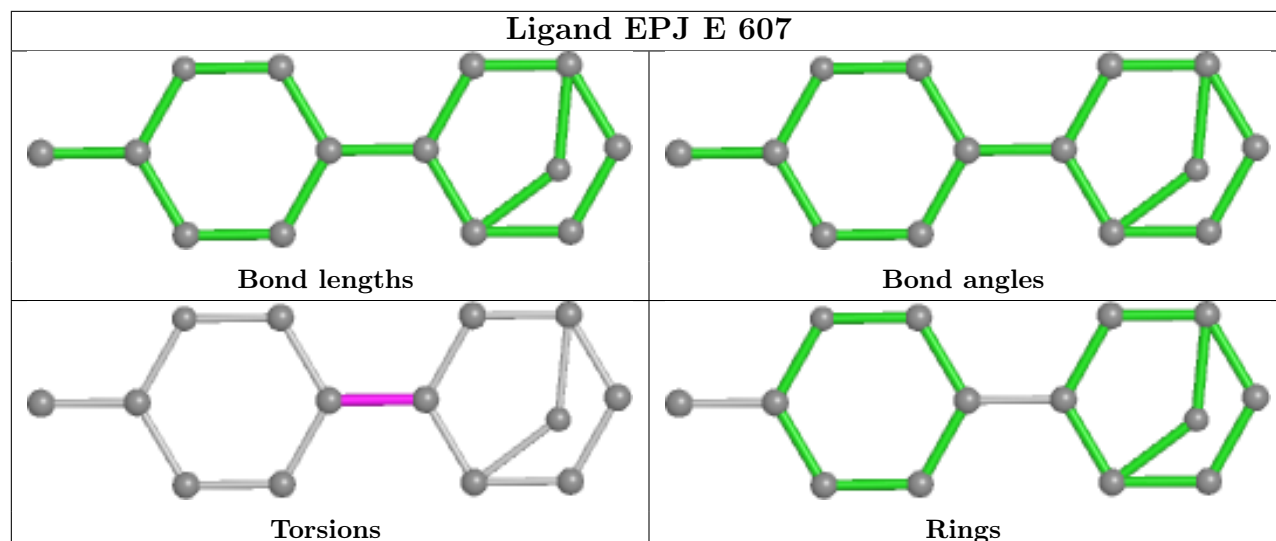


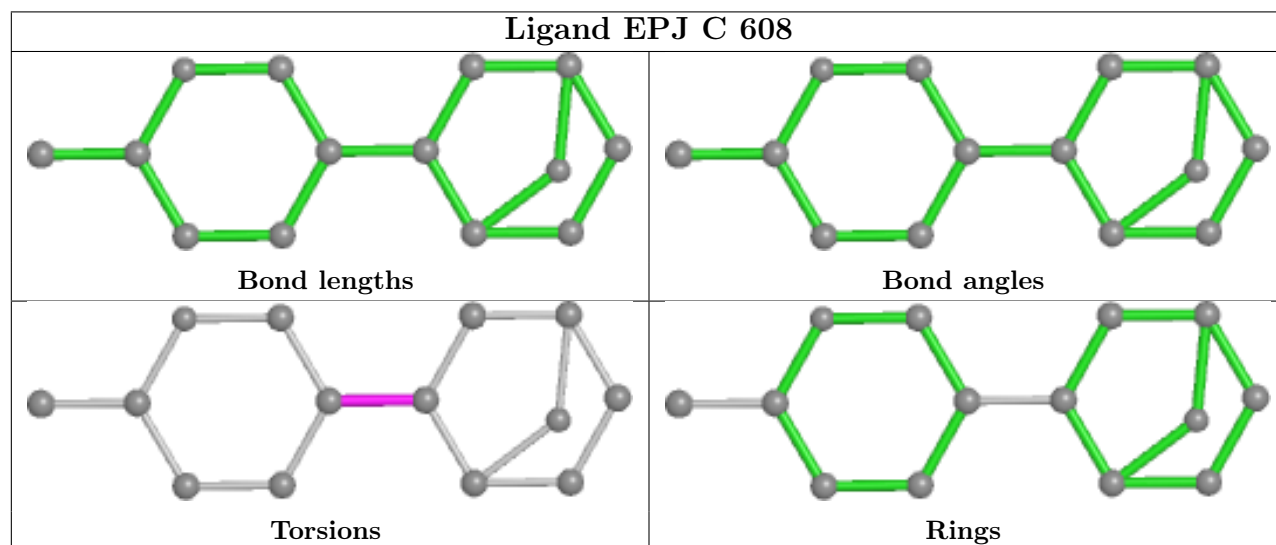
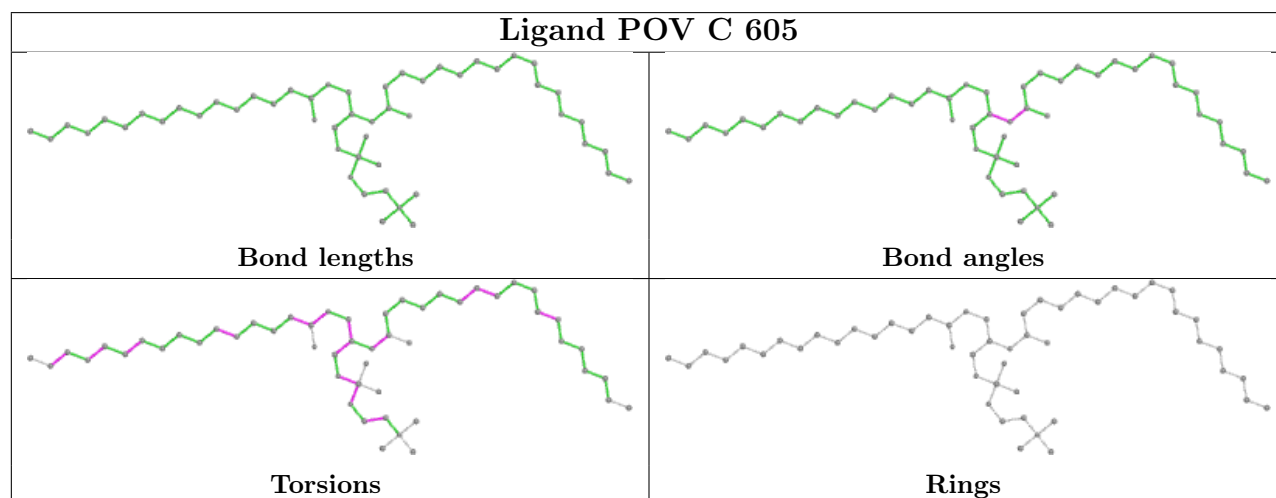
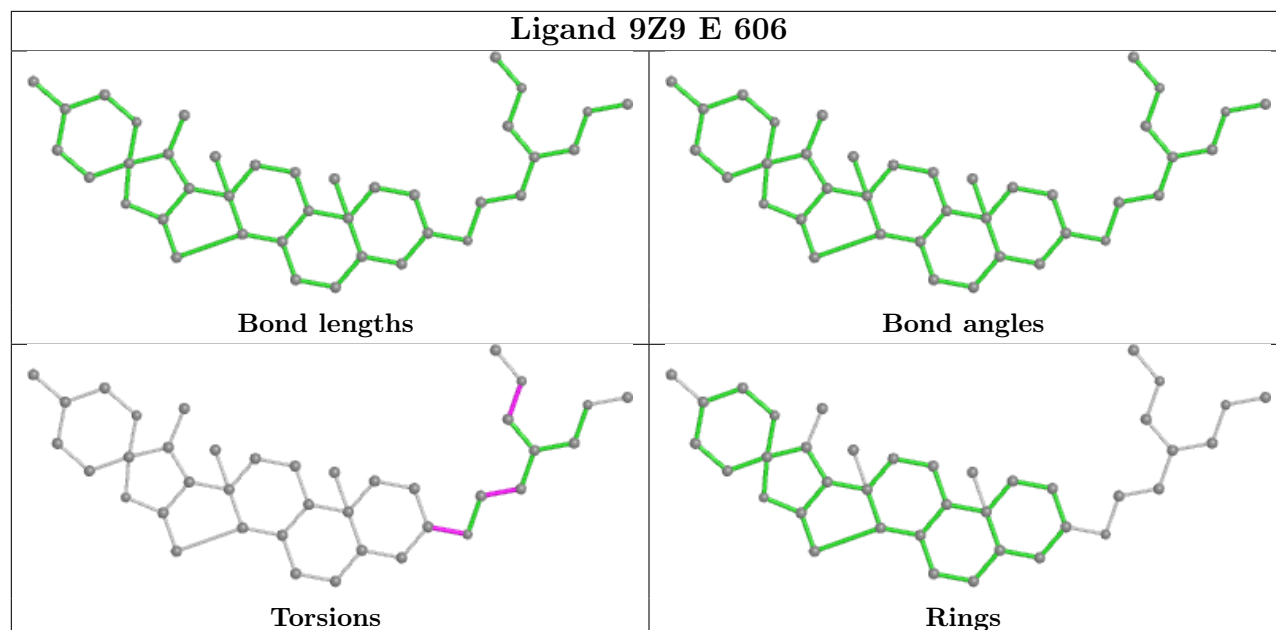


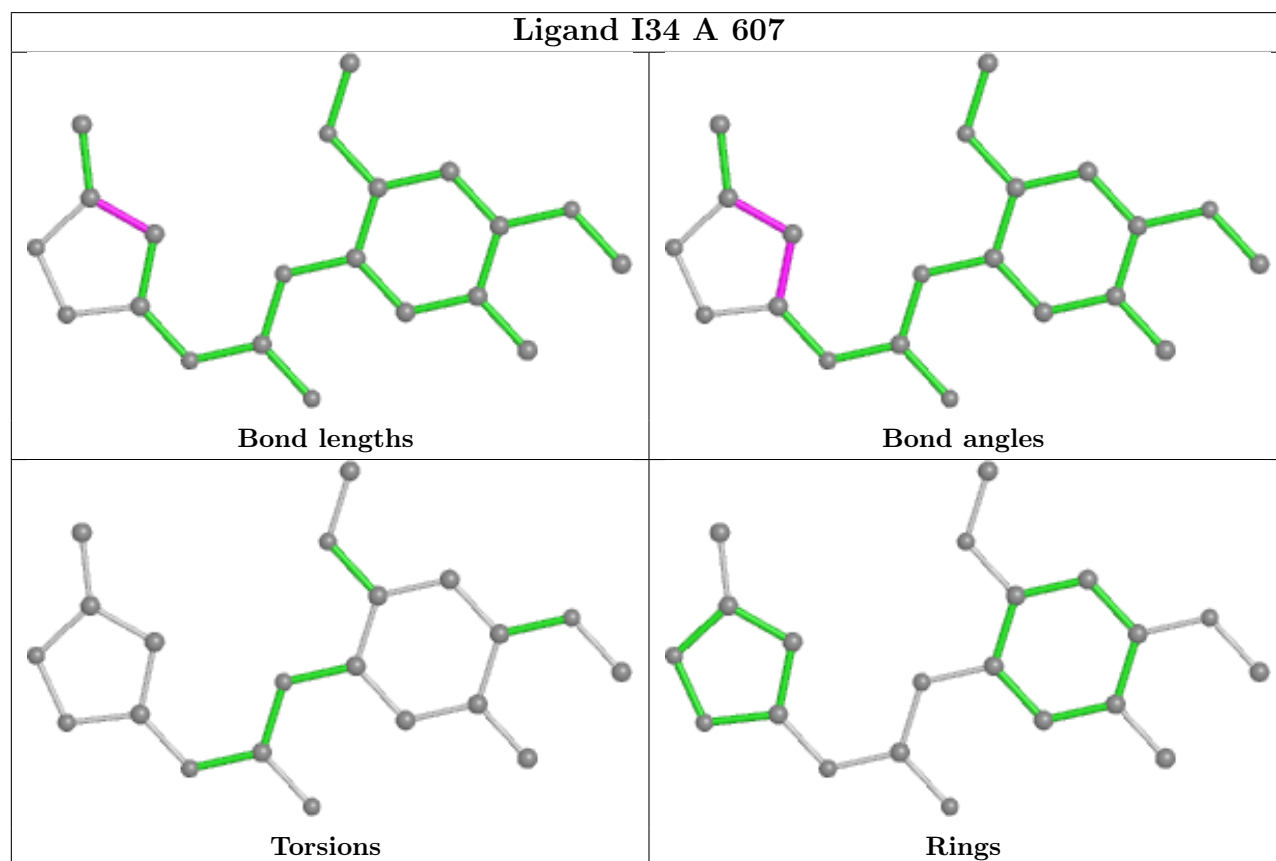
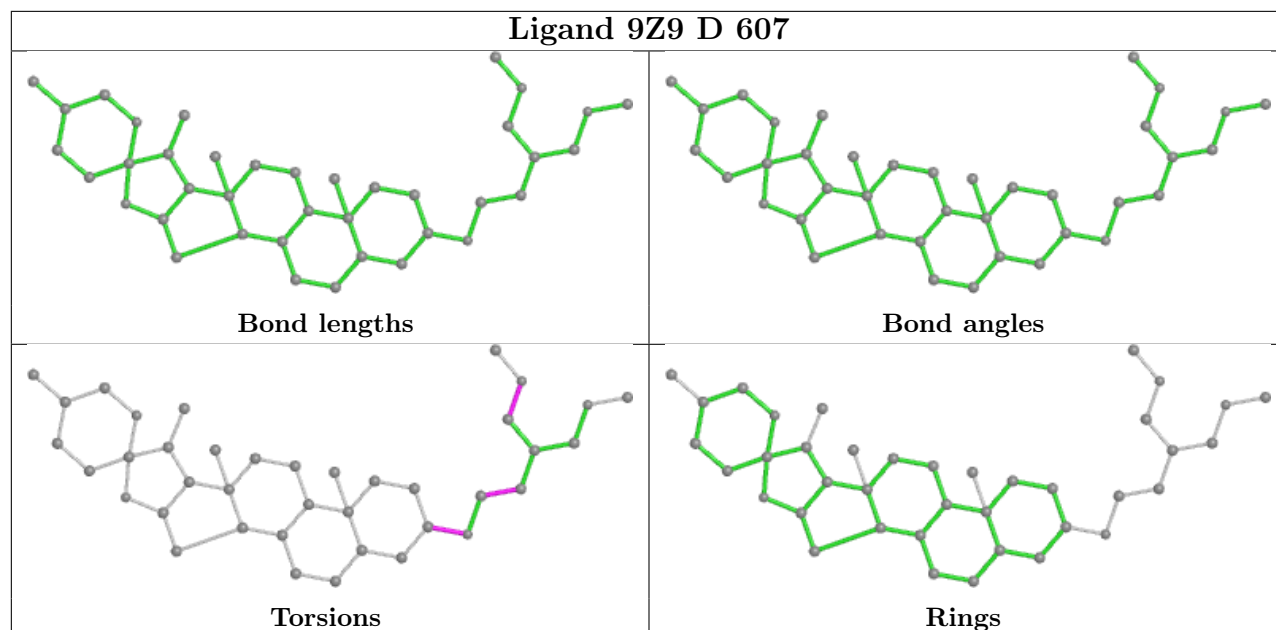




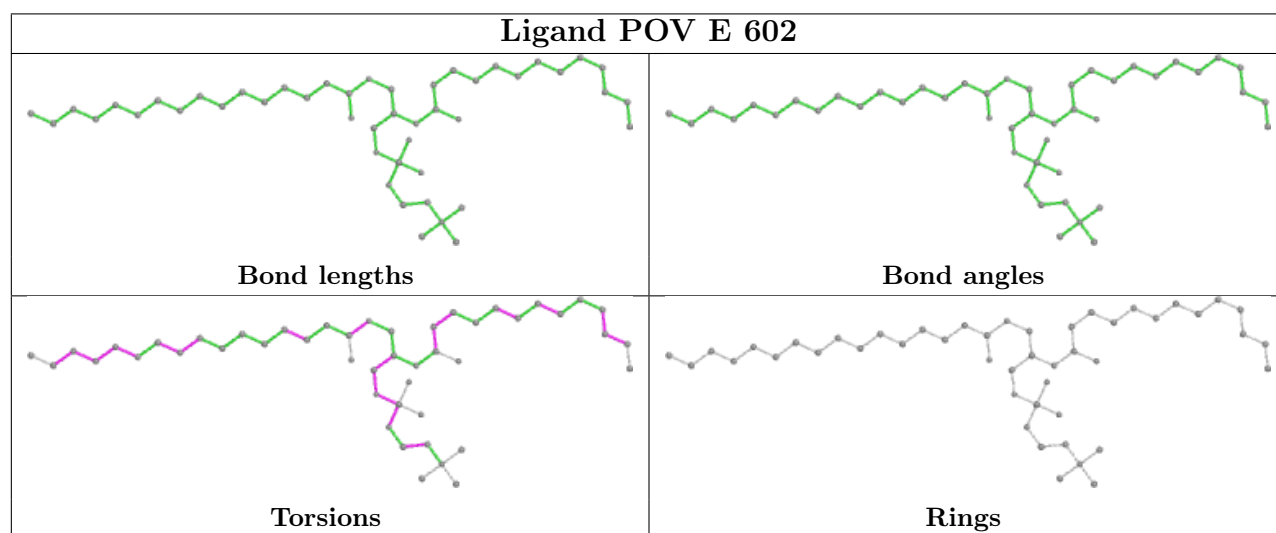
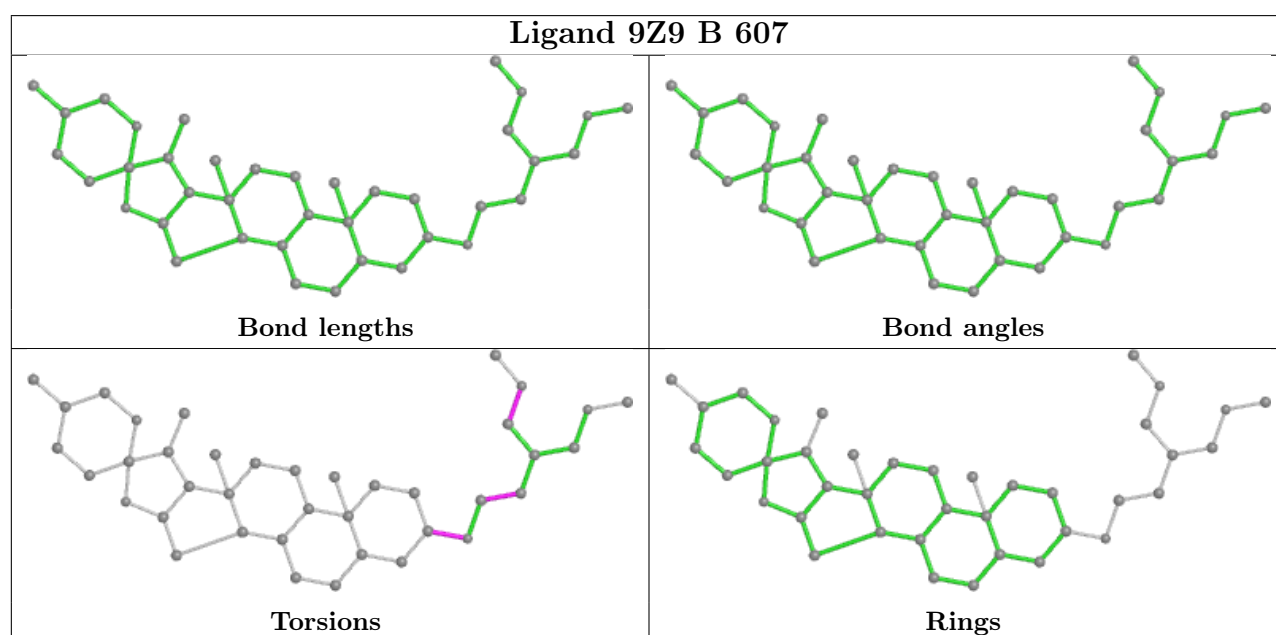
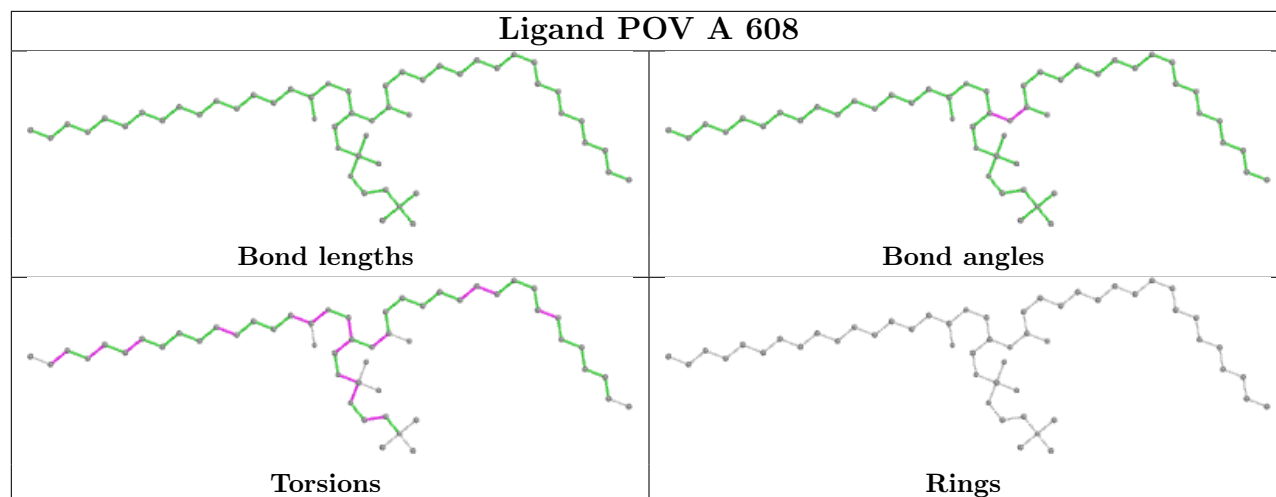


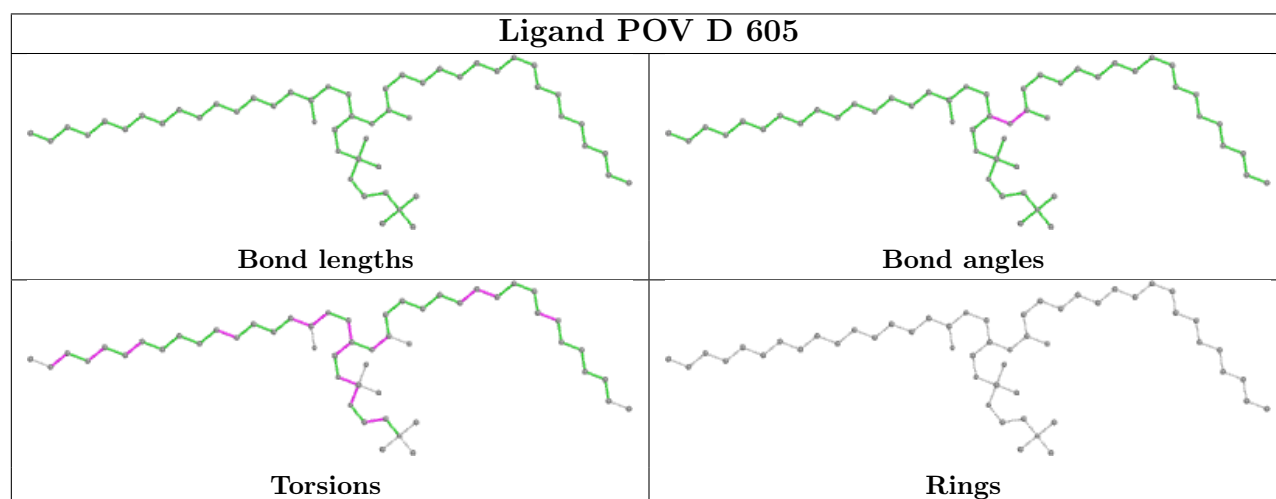
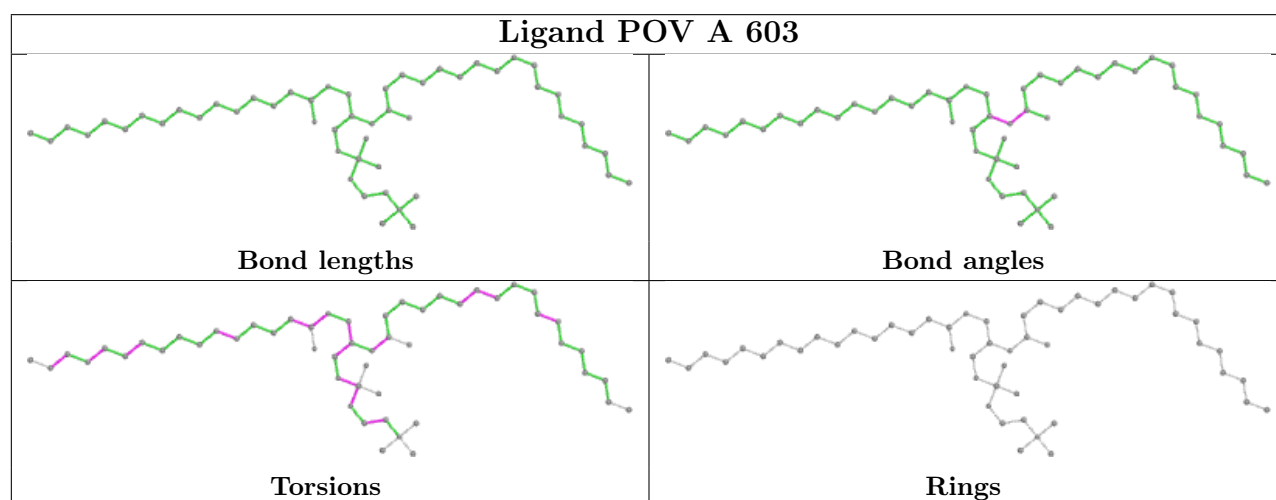
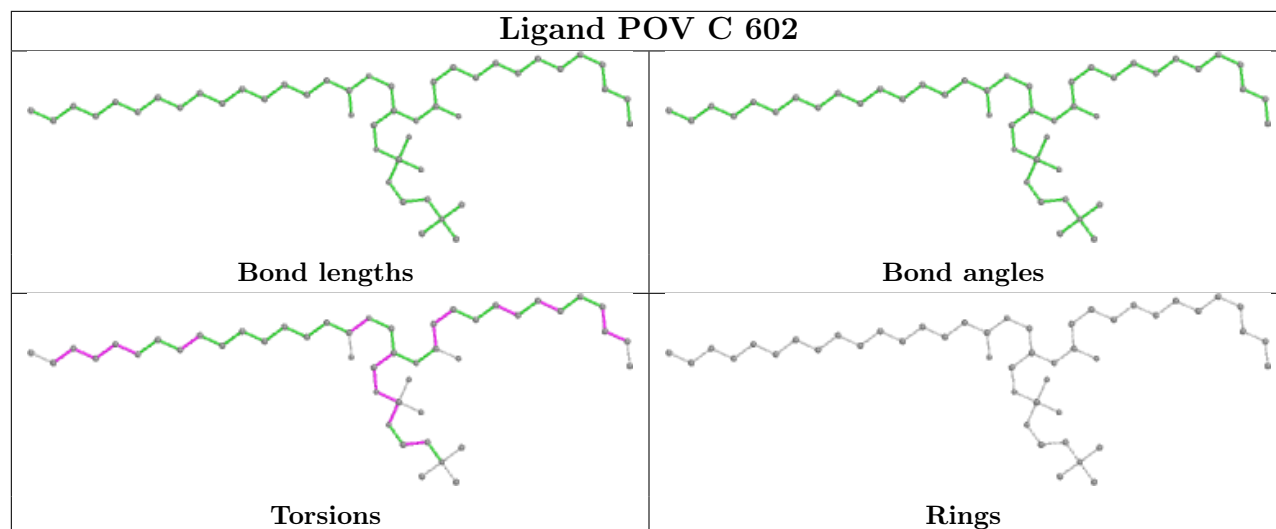


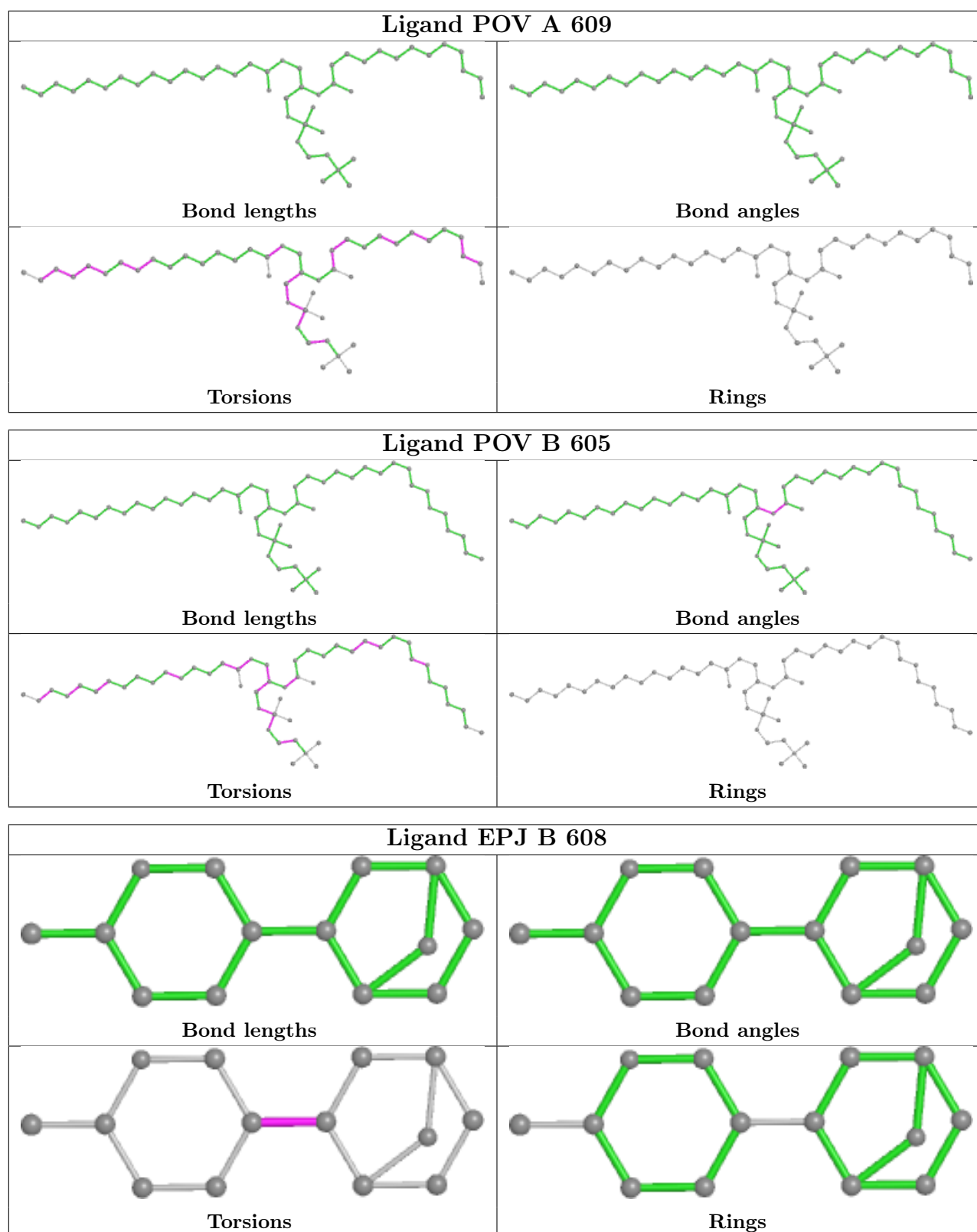












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

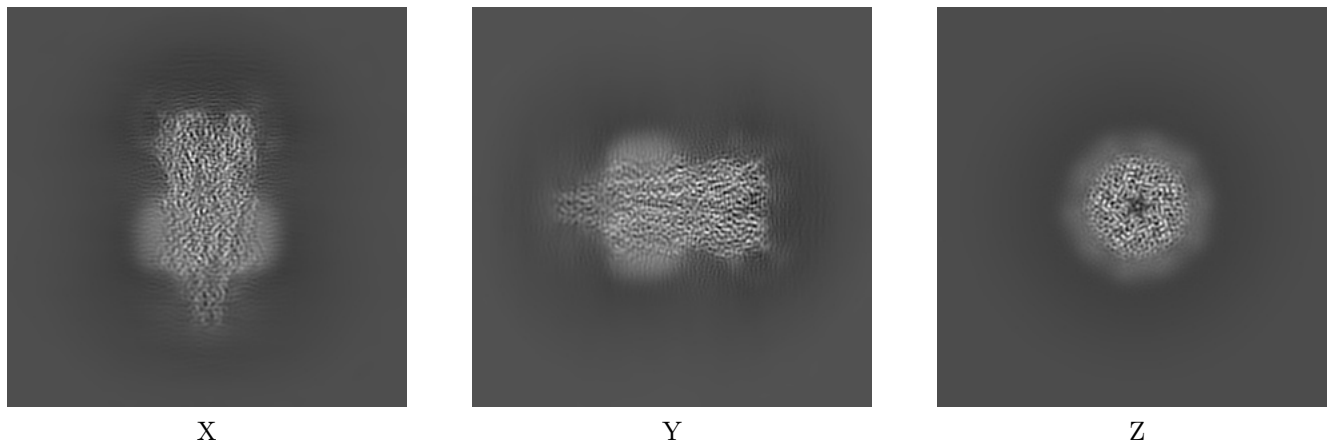
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43015. These allow visual inspection of the internal detail of the map and identification of artifacts.

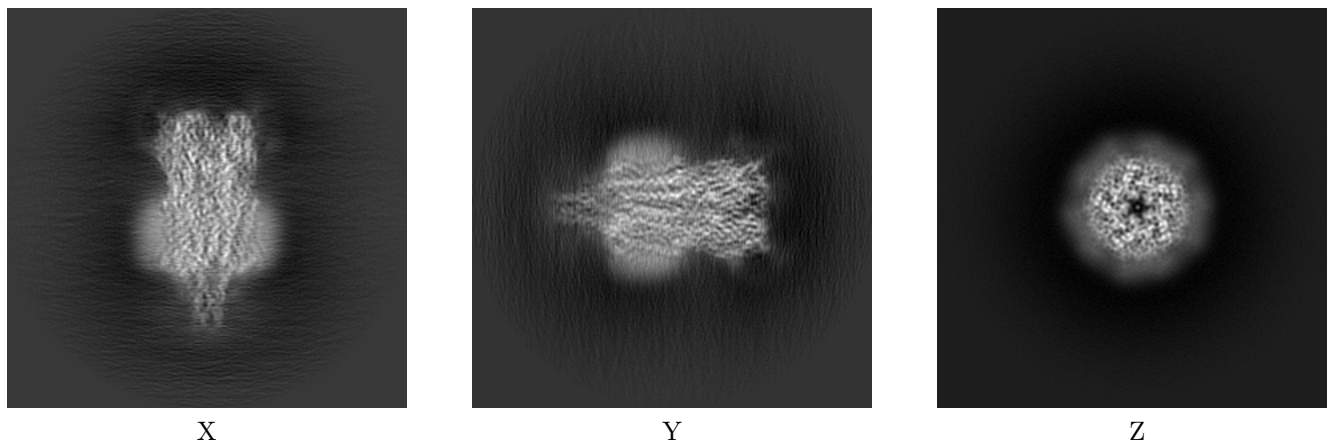
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



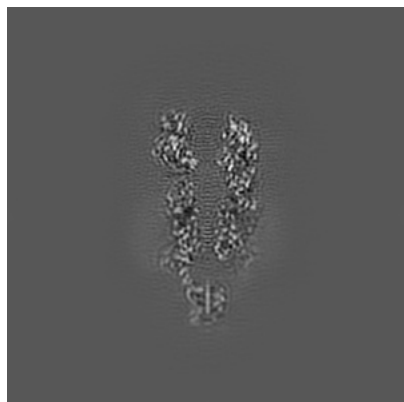
#### 6.1.2 Raw map



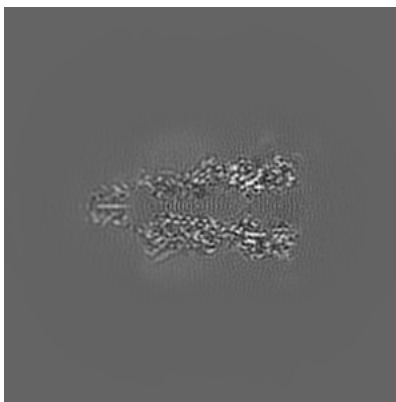
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

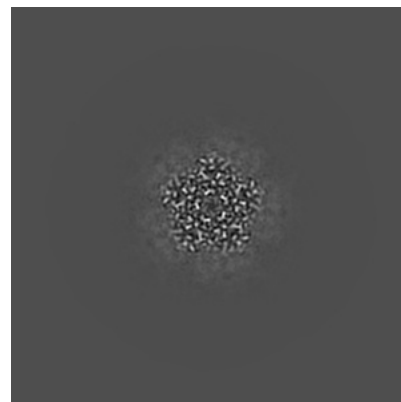
### 6.2.1 Primary map



X Index: 128

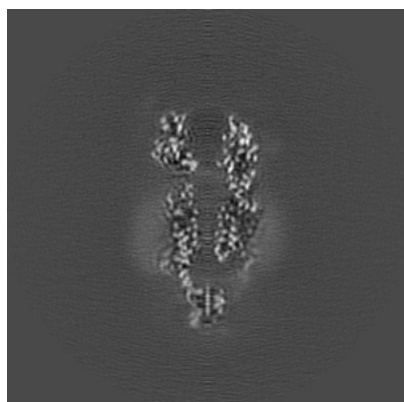


Y Index: 128

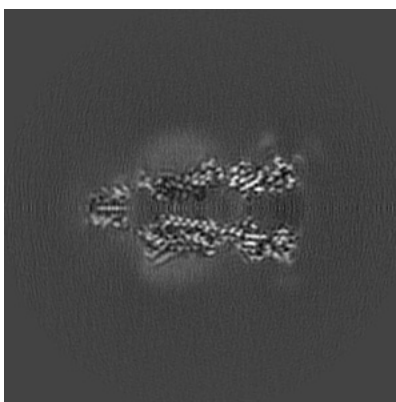


Z Index: 128

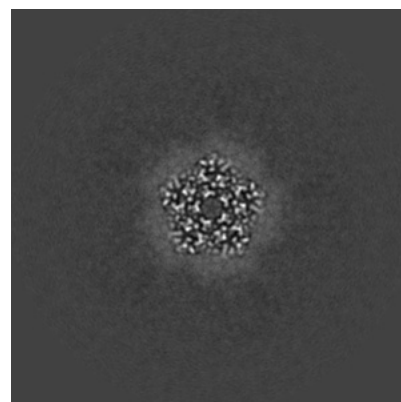
### 6.2.2 Raw map



X Index: 128



Y Index: 128

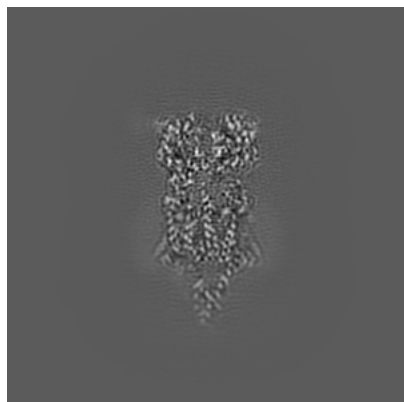


Z Index: 128

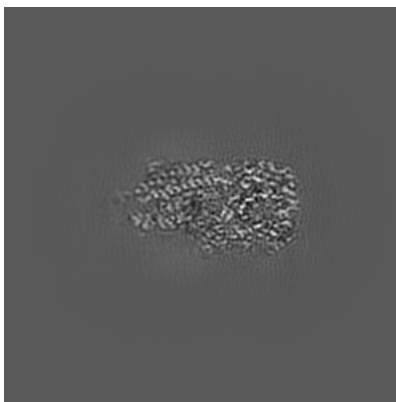
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

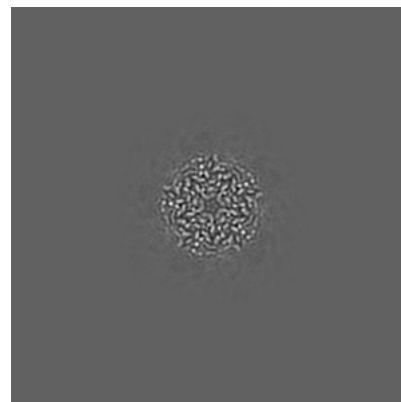
### 6.3.1 Primary map



X Index: 118

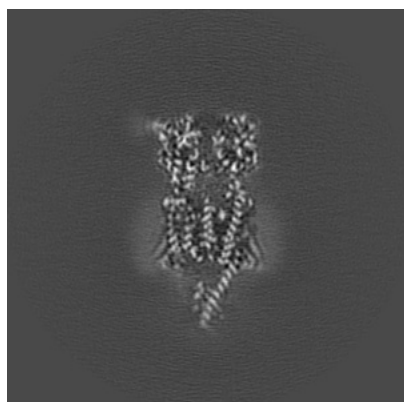


Y Index: 142

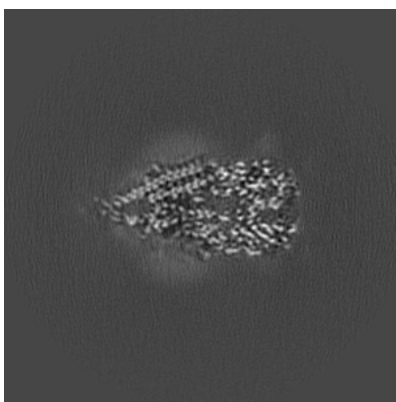


Z Index: 157

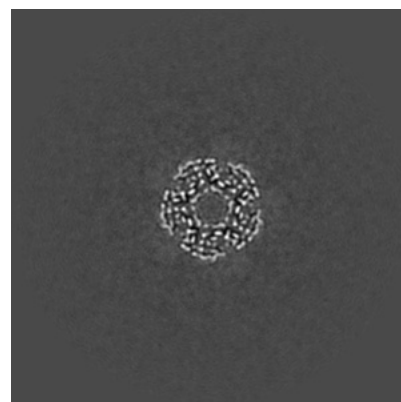
### 6.3.2 Raw map



X Index: 119



Y Index: 139

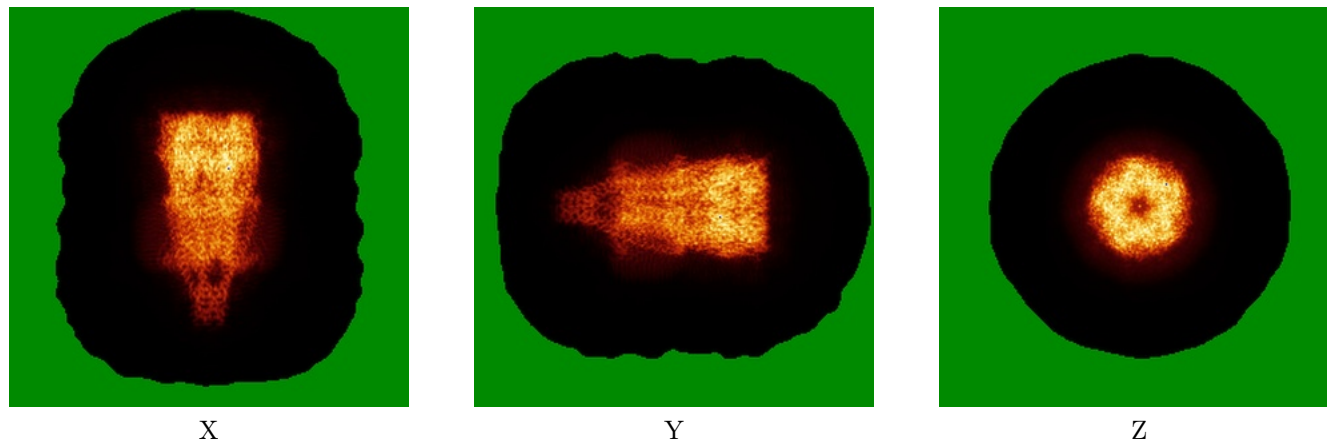


Z Index: 160

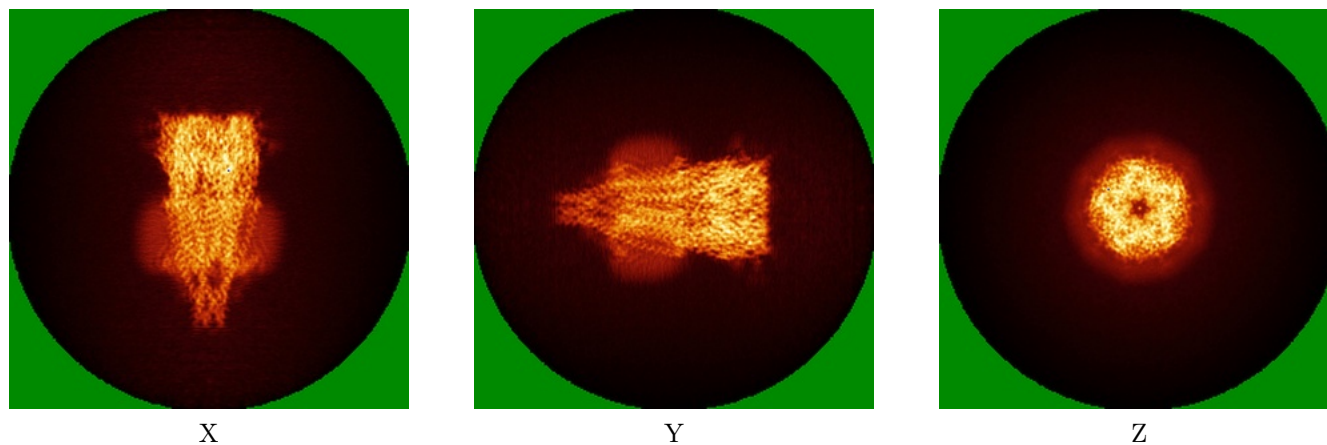
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



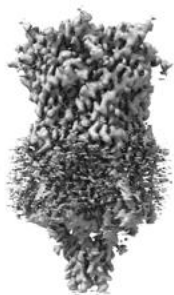
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

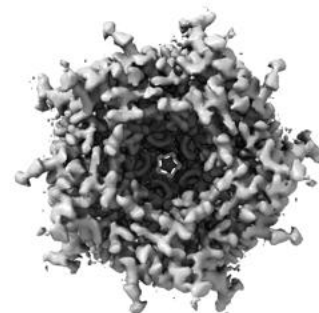
### 6.5.2 Raw map



X



Y



Z

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

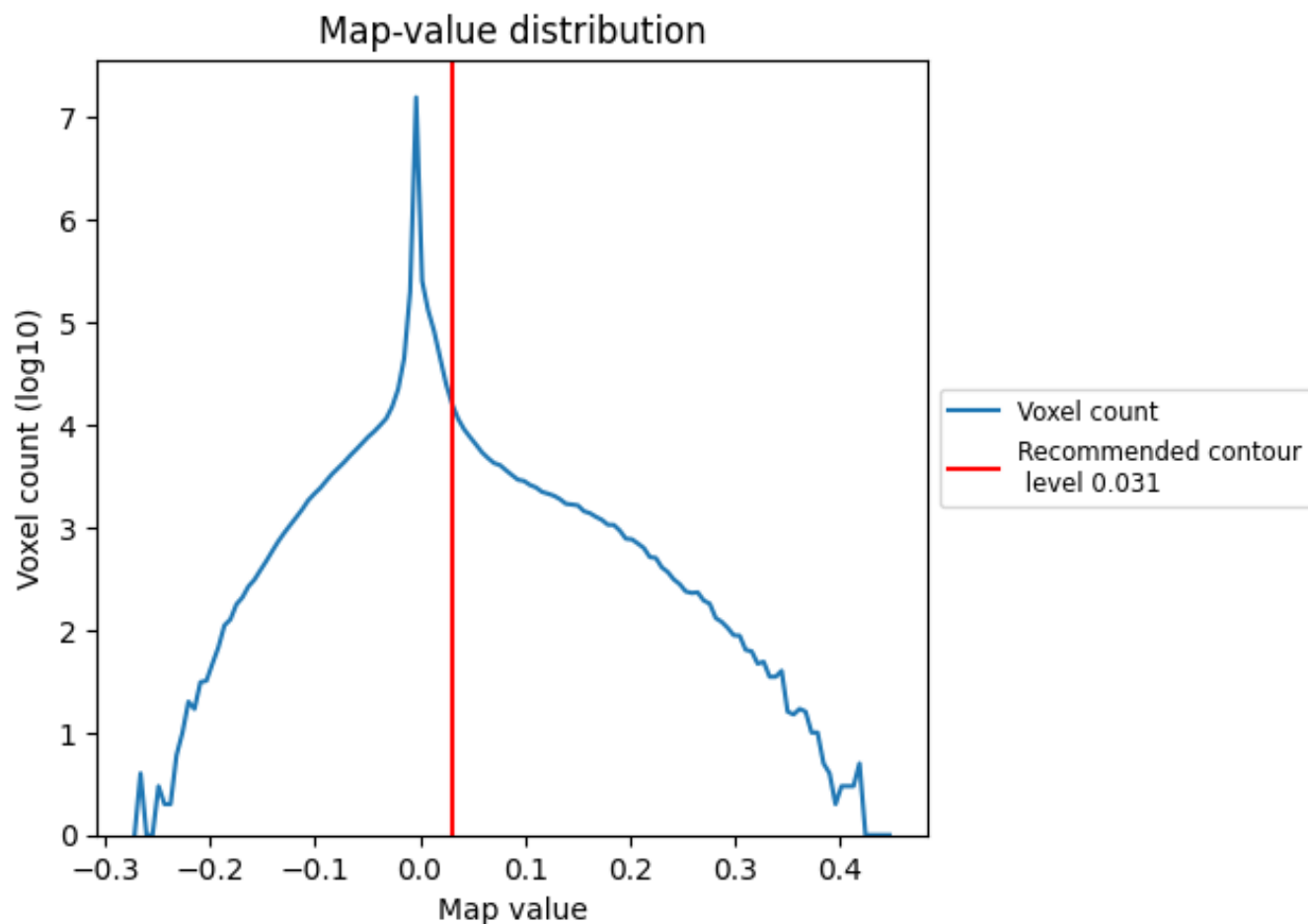
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

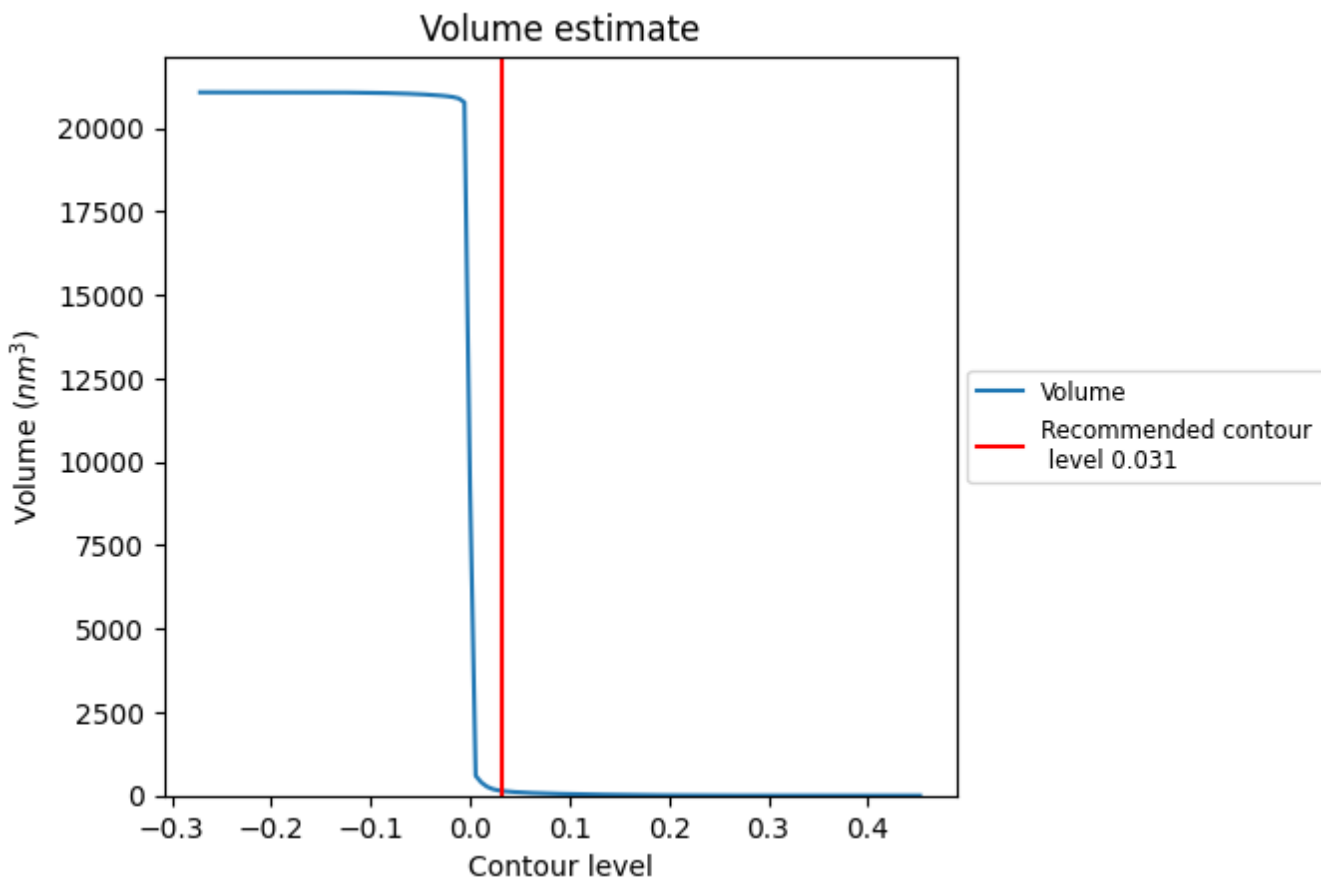
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

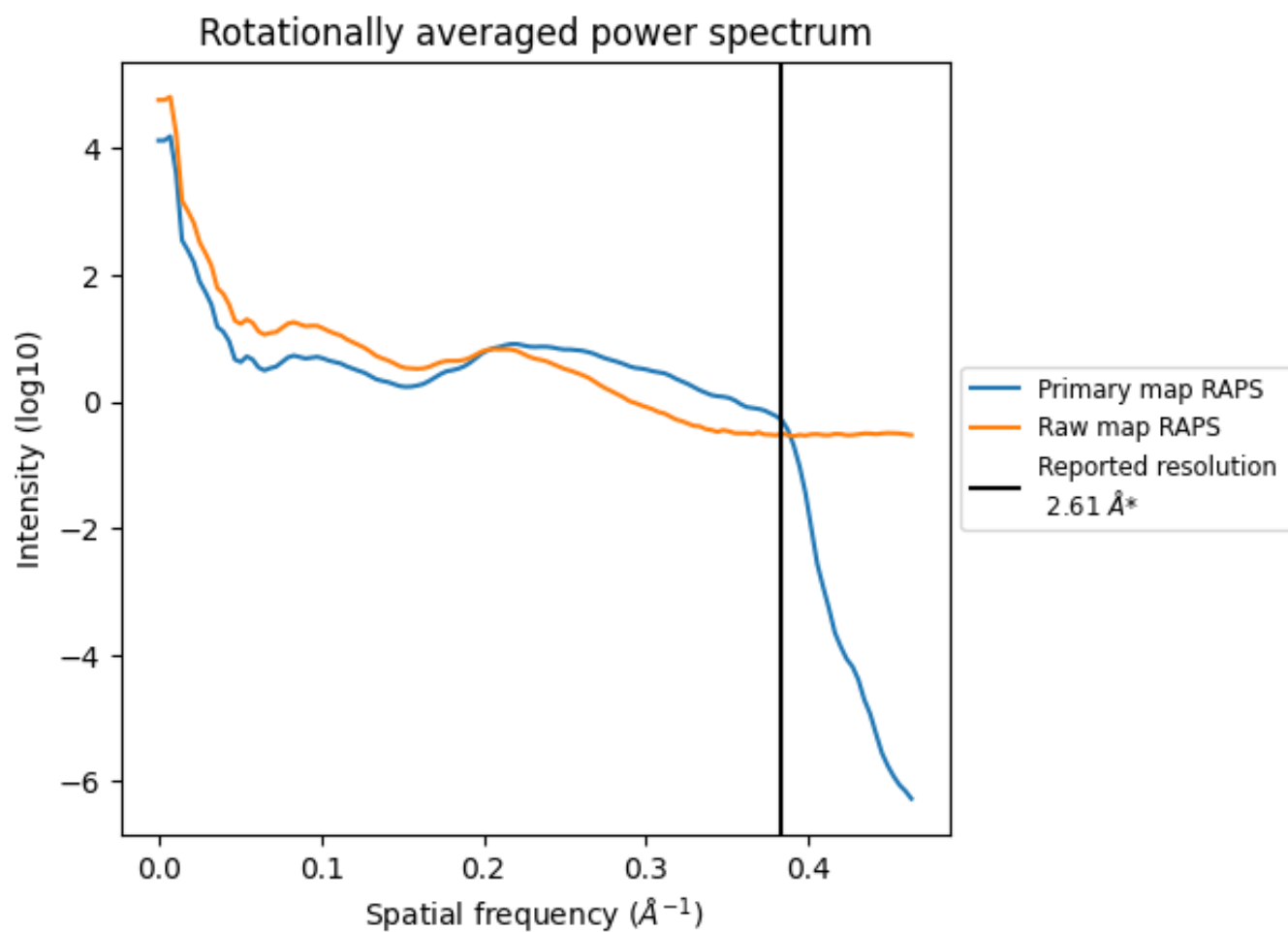
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm<sup>3</sup>; this corresponds to an approximate mass of 131 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

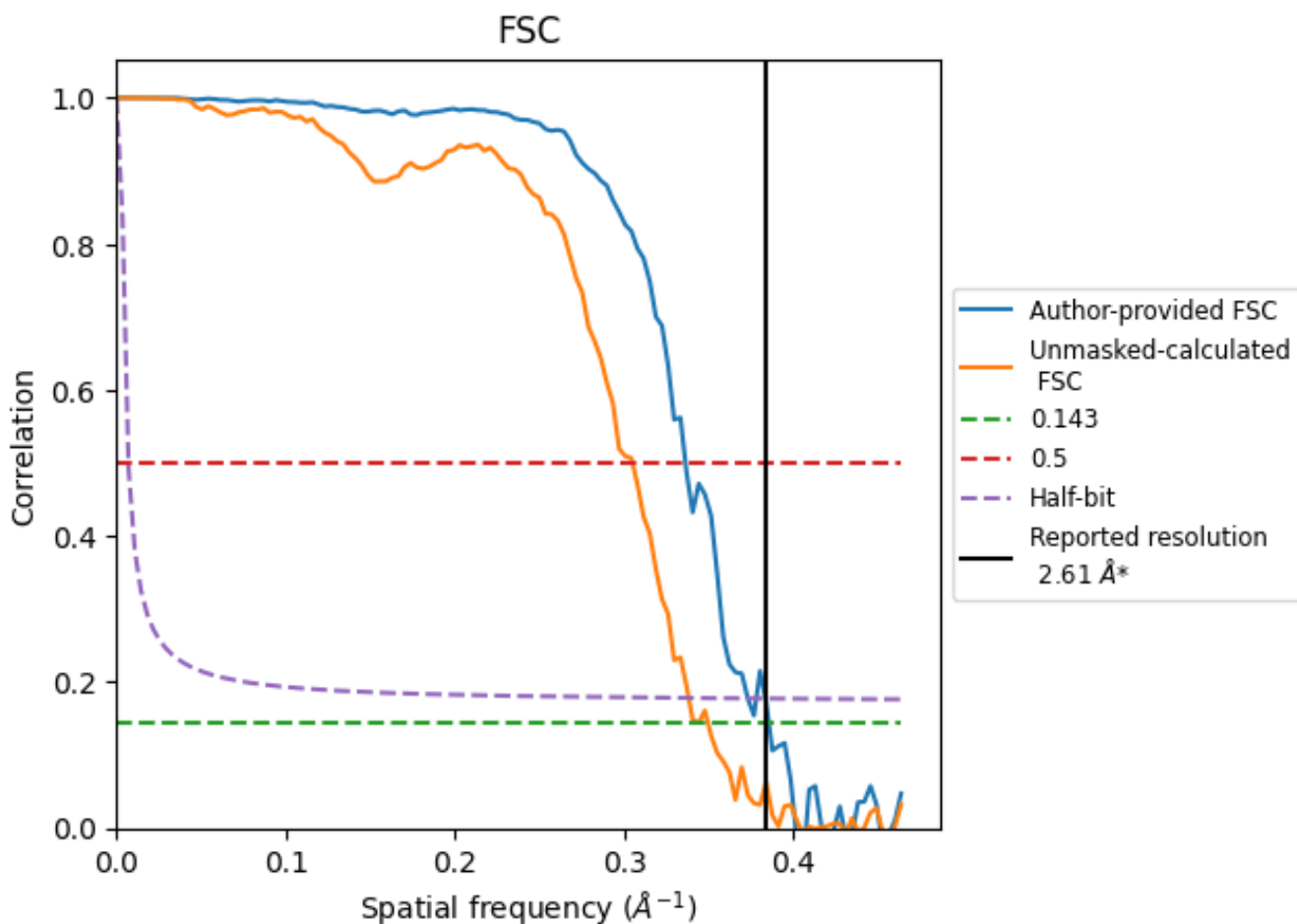


\*Reported resolution corresponds to spatial frequency of  $0.383 \text{ \AA}^{-1}$

## 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 0.383 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

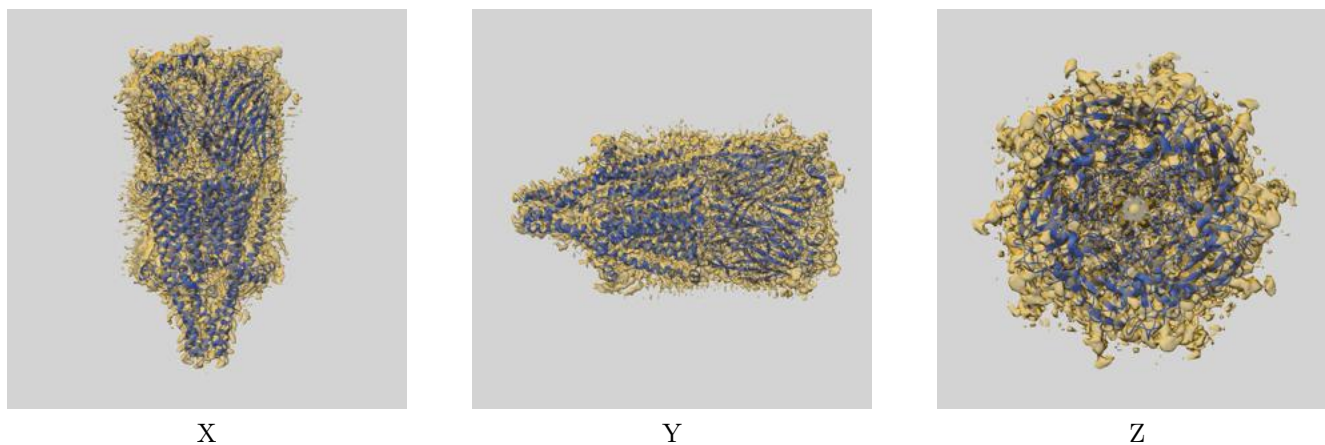
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.60	2.98	2.68
Unmasked-calculated*	2.86	3.28	2.96

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

## 9 Map-model fit [i](#)

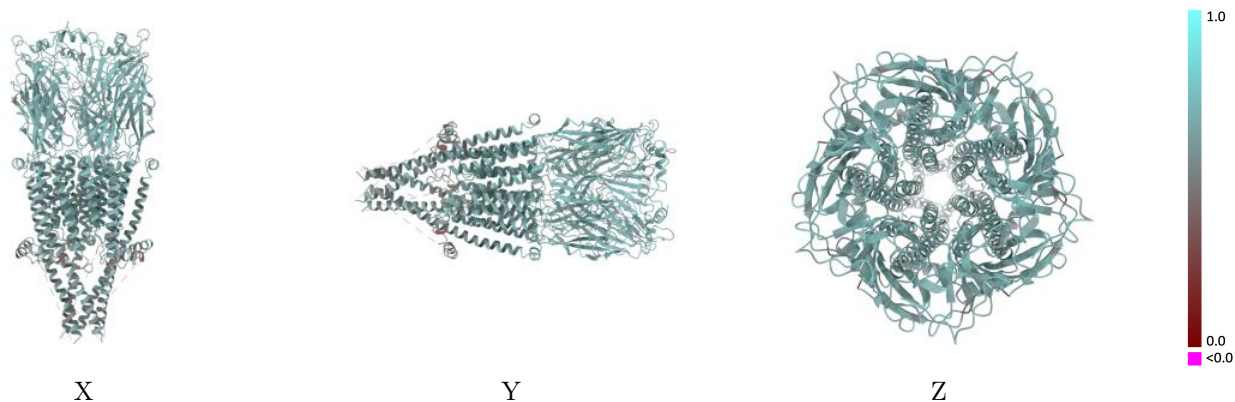
This section contains information regarding the fit between EMDB map EMD-43015 and PDB model 8V82. Per-residue inclusion information can be found in section 3 on page 22.

### 9.1 Map-model overlay [i](#)



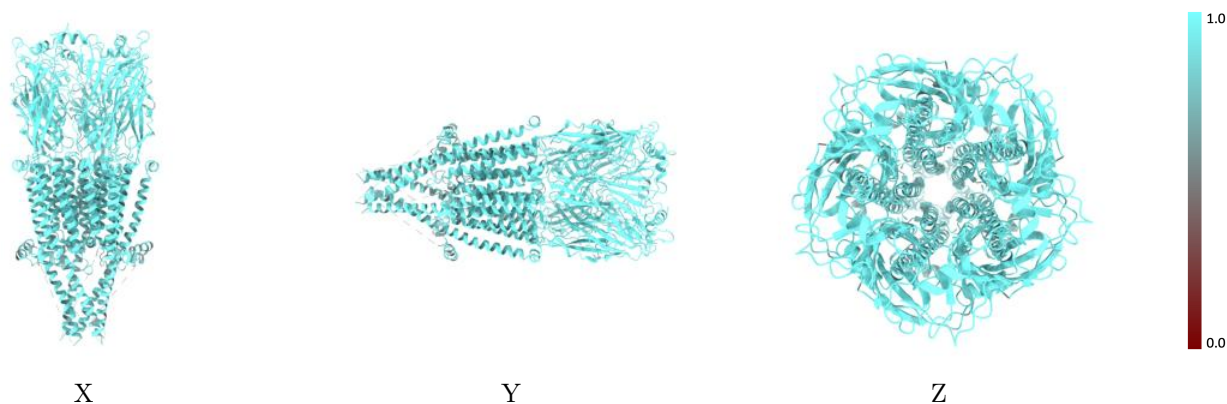
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

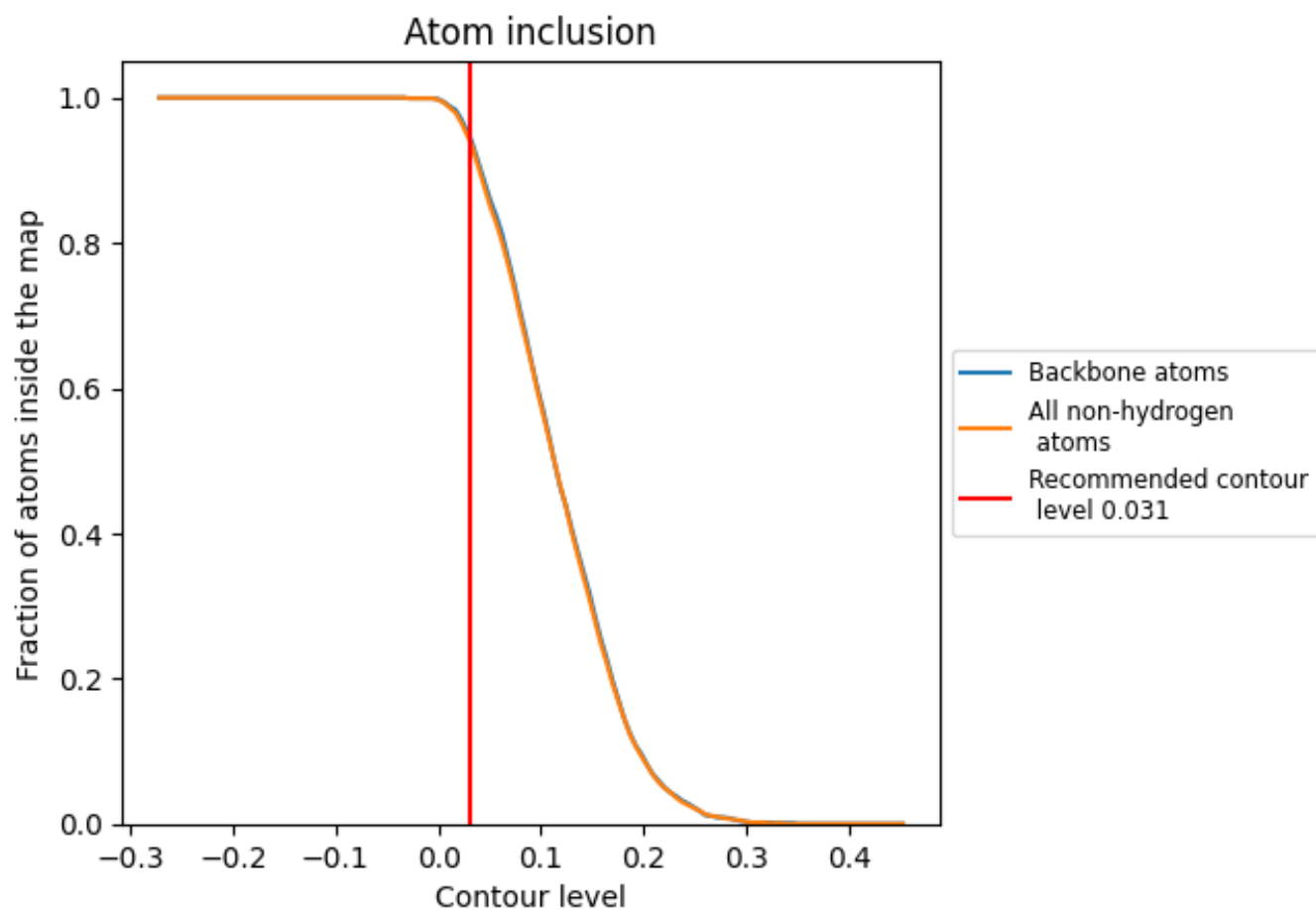
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.031).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.6040
A	 0.9400	 0.6060
B	 0.9420	 0.6080
C	 0.9440	 0.6080
D	 0.9430	 0.6060
E	 0.9470	 0.6080
F	 0.5710	 0.4020
G	 0.7690	 0.5180
H	 0.5710	 0.4050
I	 0.7690	 0.5140
J	 0.5710	 0.3890
K	 0.7180	 0.5140
L	 0.5710	 0.3830
M	 0.7690	 0.5190
N	 0.5710	 0.3850
O	 0.7690	 0.5050

