



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:53 AM UTC

PDB ID : 8T6L / pdb_00008t6l
EMDB ID : EMD-41071
Title : Cryo-EM structure of rat cardiac sodium channel NaV1.5 with batrachotoxin analog BTX-B
Authors : Tonggu, L.; Wisedchaisri, G.; Gamal El-Din, T.M.; Zheng, N.; Catterall, W.A.
Deposited on : 2023-06-16
Resolution : 3.30 Å(reported)
Based on initial model : 6UZ0

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

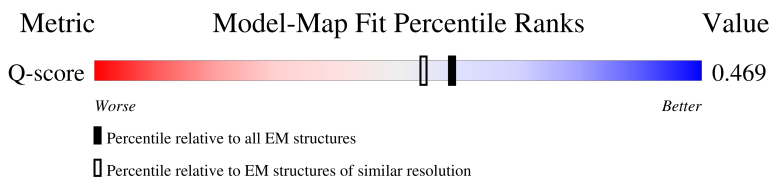
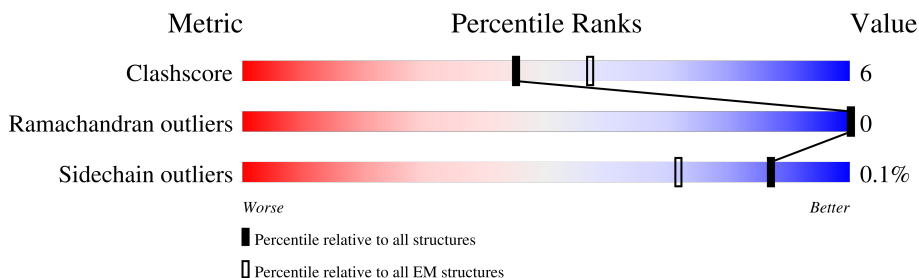
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	A	1874	
2	B	4	
3	C	2	
3	D	2	

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Mol	Chain	Length	Quality of chain
4	E	5	40% 60%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10988 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 Sodium channel protein type 5 subunit alpha, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1237	Total	C	N	O	S	1	0
			9905	6550	1576	1705	74		

There are 347 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	THR	ALA	engineered mutation	UNP P15389
A	214	ASP	GLY	engineered mutation	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
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A	?	-	LEU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	HIS	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	TRP	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	TYR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	ASN	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	LEU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	LYS	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	PHE	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	ARG	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	CYS	deletion	UNP P15389
A	?	-	MET	deletion	UNP P15389
A	?	-	VAL	deletion	UNP P15389
A	?	-	ASP	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	THR	deletion	UNP P15389
A	?	-	GLN	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389
A	?	-	PRO	deletion	UNP P15389
A	1932	VAL	-	linker	UNP P15389

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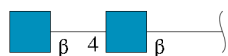
Chain	Residue	Modelled	Actual	Comment	Reference
A	1933	ASP	-	linker	UNP P15389
A	1934	LEU	-	linker	UNP P15389
A	1935	GLU	-	linker	UNP P15389
A	1936	VAL	-	linker	UNP P15389
A	1937	LEU	-	linker	UNP P15389
A	1938	PHE	-	linker	UNP P15389
A	1939	GLN	-	linker	UNP P15389
A	1940	GLY	-	linker	UNP P15389
A	1941	PRO	-	linker	UNP P15389
A	1942	GLY	-	linker	UNP P15389
A	1943	SER	-	linker	UNP P15389
A	1944	MET	-	linker	UNP P15389
A	1945	VAL	-	linker	UNP P15389
A	2008	LEU	PHE	conflict	UNP P42212
A	2009	THR	SER	conflict	UNP P42212
A	2175	LEU	HIS	conflict	UNP P42212
A	2183	GLY	-	expression tag	UNP P42212
A	2184	SER	-	expression tag	UNP P42212
A	2185	ASP	-	expression tag	UNP P42212
A	2186	TYR	-	expression tag	UNP P42212
A	2187	LYS	-	expression tag	UNP P42212
A	2188	ASP	-	expression tag	UNP P42212
A	2189	ASP	-	expression tag	UNP P42212
A	2190	ASP	-	expression tag	UNP P42212
A	2191	ASP	-	expression tag	UNP P42212
A	2192	LYS	-	expression tag	UNP P42212

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4	Total	C	N	O	0	0
			50	28	2	20		

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



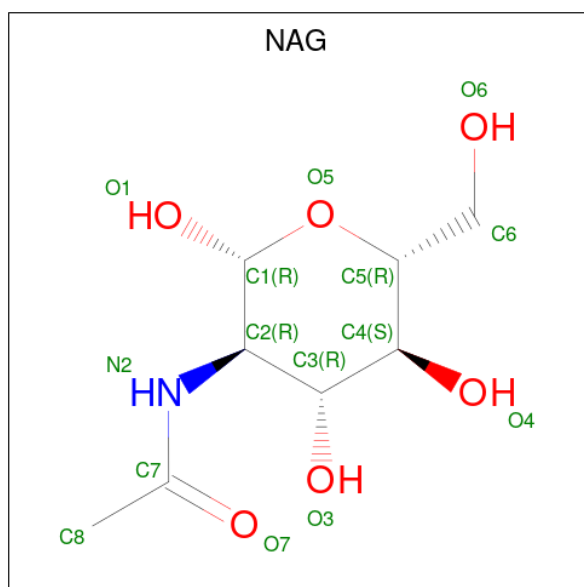
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



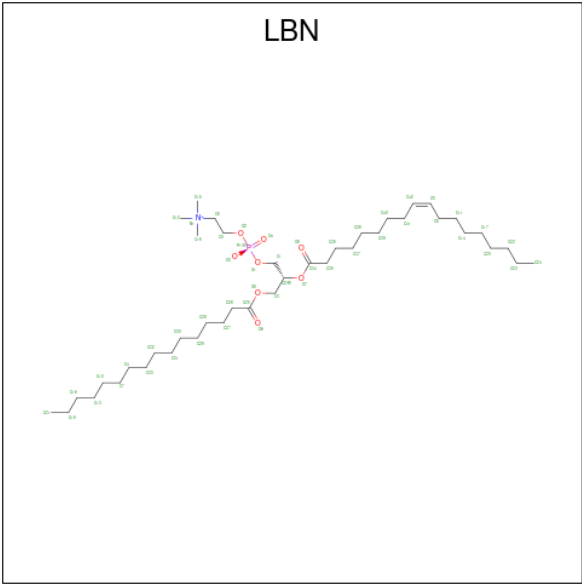
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
6	A	1	Total	C	O	P		0
			30	21	8	1		
6	A	1	Total	C	O	P		0
			28	19	8	1		
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			25	16	1	7	1	
6	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
6	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	A	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total 44	C 34	N 1	O 8	P 1	0
6	A	1	Total 44	C 34	N 1	O 8	P 1	0

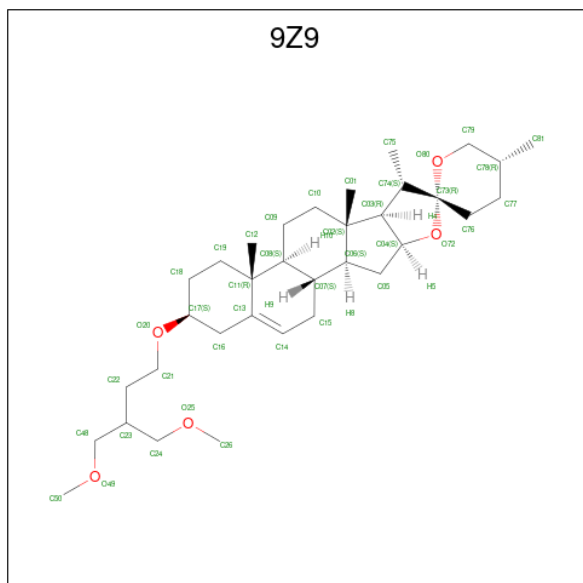
- # Y01

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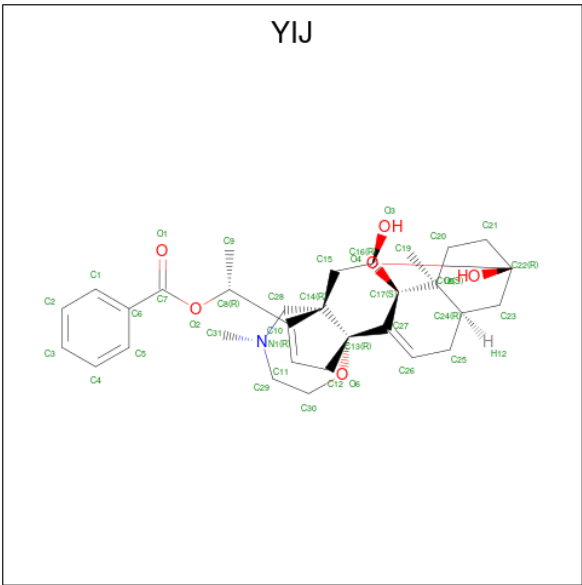
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			35	31	4	
7	A	1	Total	C	O	0
			28	24	4	

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			30	27	3	
8	A	1	Total	C	O	0
			32	29	3	

- Molecule 9 is (1R)-1-[(5aR,7aR,9R,11aS,11bS,12R,13aR)-9,12-dihydroxy-2,11a-dimethyl-1,2,3,4,7a,8,9,10,11,11a,12,13-dodecahydro-7H-9,11b-epoxy-13a,5a-prop[1]enophenanthro[2,1-f][1,4]oxazepin-14-yl]ethyl benzoate (CCD ID: YIJ) (formula: C₃₁H₃₉NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			38	31	1	6	
9	A	1	Total	C	N	O	0
			38	31	1	6	

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	O	0
			1	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.957	Depositor
Minimum map value	-0.691	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	264.16, 264.16, 264.16	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8255, 0.8255, 0.8255	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: YIJ, BMA, NAG, 9Z9, LBN, Y01, MAN

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	0.09	0/10152	0.25	0/13773

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	9905	0	10034	131	0
2	B	50	0	43	1	0
3	C	28	0	25	0	0
3	D	28	0	25	1	0
4	E	61	0	52	2	0
5	A	42	0	39	0	0
6	A	377	0	0	0	0
7	A	358	0	467	13	0
8	A	62	0	0	0	0
9	A	76	0	0	1	0
10	A	1	0	0	0	0
All	All	10988	0	10685	136	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 6.

All (136) 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:A:1730:CYS:SG	1:A:1731:ASP:N	2.55	0.80
1:A:780:GLN:OE1	1:A:781:GLY:N	2.17	0.77
1:A:1724:ASN:HD22	1:A:1729:TYR:HB3	1.56	0.70
1:A:1517:ASN:HB2	1:A:1520:GLN:HB2	1.73	0.70
1:A:1500:MET:HG2	1:A:1654:MET:HE1	1.73	0.69
1:A:258:THR:HA	1:A:405:LEU:HD21	1.76	0.68
1:A:139:MET:HE1	1:A:230:THR:HG23	1.75	0.67
1:A:773:ASP:HB2	1:A:776:TYR:HB3	1.76	0.66
1:A:1549:VAL:HG11	7:A:3024:Y01:HAD2	1.75	0.66
1:A:1584:LEU:HD11	1:A:1587:TYR:HB2	1.77	0.65
1:A:1659:LEU:HD22	1:A:1768:MET:HG2	1.79	0.64
1:A:1591:ASN:ND2	1:A:1594:ASN:OD1	2.30	0.64
1:A:407:ASN:HD21	1:A:1772:ILE:HB	1.64	0.62
1:A:193:PRO:HB2	7:A:3017:Y01:HAI	1.81	0.62
1:A:172:GLU:OE2	1:A:229:LYS:NZ	2.33	0.62
1:A:283:ARG:HH22	1:A:297:ALA:HB1	1.64	0.61
1:A:60:GLN:HB2	1:A:63:LYS:HD2	1.83	0.59
1:A:59:LEU:O	1:A:105:ARG:NH2	2.33	0.59
1:A:1417:VAL:HA	1:A:1423:TRP:HB3	1.86	0.57
1:A:879:LEU:HD22	1:A:885:MET:HE1	1.87	0.57
1:A:92:LYS:HB3	1:A:108:ALA:HB3	1.87	0.56
1:A:823:TRP:HD1	1:A:824:PRO:HD2	1.70	0.56
1:A:1448:MET:HE3	1:A:1448:MET:HA	1.86	0.56
1:A:82:GLU:H	1:A:82:GLU:CD	2.14	0.56
1:A:265:PHE:HB3	1:A:366:LEU:HD11	1.88	0.56
1:A:1224:LEU:HD23	1:A:1675:ILE:HG21	1.87	0.55
1:A:21:LEU:HD11	1:A:92:LYS:HD3	1.88	0.55
1:A:115:LEU:HD12	1:A:122:ARG:HB2	1.89	0.55
1:A:836:SER:HB2	1:A:940:LEU:HD11	1.89	0.55
1:A:880:PRO:HG2	1:A:883:HIS:HB3	1.89	0.54
1:A:277:LEU:HD23	1:A:349:PRO:HG2	1.89	0.54
1:A:146:CYS:HA	1:A:149:MET:HE2	1.89	0.54
1:A:884:MET:HG3	1:A:893:ILE:HD12	1.90	0.54
1:A:183:CYS:O	1:A:191:ARG:NH2	2.41	0.53
1:A:83:ASP:OD1	1:A:105:ARG:NH1	2.41	0.53
1:A:170:THR:HG21	1:A:206:TYR:HE2	1.73	0.53
1:A:303:ASN:OD1	1:A:303:ASN:N	2.42	0.53
1:A:712:LYS:HA	1:A:771:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1709:ILE:HD11	1:A:1718:LEU:HD13	1.91	0.53
1:A:221:THR:HB	7:A:3014:Y01:HAK2	1.91	0.52
1:A:94:PHE:CE1	1:A:106:PHE:HB2	2.43	0.52
1:A:117:PRO:HA	1:A:122:ARG:HD3	1.91	0.50
1:A:237:LEU:HD22	1:A:846:VAL:HG23	1.92	0.50
1:A:807:VAL:O	1:A:810:SER:OG	2.28	0.50
1:A:257:LEU:HD13	1:A:1645:ILE:HG23	1.93	0.50
1:A:755:LEU:HD12	1:A:755:LEU:H	1.77	0.50
1:A:169:TYR:HE2	1:A:226:ARG:HD3	1.77	0.49
1:A:197:LEU:HD21	1:A:228:LEU:HB3	1.95	0.49
1:A:204:MET:HE3	1:A:222:PHE:HB3	1.94	0.49
1:A:869:LEU:HD13	1:A:872:ARG:HH11	1.77	0.49
1:A:262:LEU:HD21	1:A:370:MET:HG3	1.95	0.48
1:A:897:ILE:HG21	1:A:925:VAL:HG13	1.94	0.48
1:A:1730:CYS:O	4:E:5:MAN:O6	2.31	0.48
1:A:1227:GLU:HA	1:A:1231:LEU:HD13	1.94	0.48
1:A:237:LEU:HD11	1:A:845:LEU:HD23	1.94	0.48
1:A:26:LYS:O	1:A:30:GLU:OE1	2.31	0.48
1:A:1450:ILE:HD13	7:A:3018:Y01:HAE1	1.96	0.48
1:A:758:THR:OG1	1:A:812:ARG:NH1	2.47	0.47
1:A:388:LYS:HE2	1:A:1693:MET:HG2	1.97	0.47
1:A:1654:MET:HE2	1:A:1654:MET:HA	1.97	0.47
1:A:1674:SER:O	1:A:1678:MET:HG3	2.15	0.47
1:A:1455:PHE:O	1:A:1459:GLY:N	2.45	0.47
1:A:1443:GLU:HG2	1:A:1446:LEU:HD13	1.96	0.47
1:A:1597:ASP:HA	1:A:1600:VAL:HG12	1.97	0.47
1:A:16:PHE:HB2	1:A:80:PRO:HB2	1.97	0.47
1:A:711:VAL:HG23	1:A:771:ALA:HA	1.96	0.47
1:A:250:LYS:NZ	1:A:419:GLU:OE1	2.33	0.46
1:A:104:PHE:HD2	1:A:130:VAL:HG12	1.81	0.46
1:A:1206:HIS:CD2	1:A:1208:TRP:HB2	2.50	0.46
1:A:396:LEU:HD12	7:A:3022:Y01:HAP2	1.98	0.46
1:A:1234:ARG:HB2	1:A:1237:ILE:HG22	1.98	0.46
1:A:1332:ALA:HB2	1:A:1475:PHE:CE2	2.50	0.46
1:A:22:ALA:O	1:A:26:LYS:HG3	2.15	0.46
1:A:819:LEU:HD21	7:A:3021:Y01:HAQ2	1.98	0.46
1:A:62:SER:O	1:A:62:SER:OG	2.28	0.45
2:B:1:NAG:H61	2:B:2:NAG:H83	1.99	0.45
1:A:1192:VAL:HG12	1:A:1195:ARG:HH21	1.81	0.45
1:A:1377:TYR:HE1	1:A:1441:GLN:HB2	1.82	0.45
1:A:107:SER:HB2	1:A:185:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD13	1:A:103:ILE:HD11	1.99	0.45
1:A:1249:THR:HG21	1:A:1288:LEU:HD22	1.99	0.44
1:A:1502:LYS:HD2	1:A:1502:LYS:C	2.43	0.44
1:A:348:ASN:CB	1:A:352:GLY:HA2	2.48	0.44
1:A:1377:TYR:CE1	1:A:1441:GLN:HB2	2.52	0.44
1:A:1489:MET:HE1	1:A:1497:TYR:HB3	2.00	0.44
1:A:173:SER:O	1:A:177:ILE:HG12	2.18	0.44
1:A:1214:ILE:HG12	1:A:1318:ARG:HG2	2.00	0.43
1:A:1325:VAL:O	1:A:1329:LEU:HD12	2.18	0.43
1:A:1341:LEU:HD13	7:A:3021:Y01:HAS1	2.00	0.43
1:A:1365:CYS:HB2	1:A:1397:TRP:HE3	1.83	0.43
1:A:1517:ASN:O	1:A:1519:TYR:N	2.52	0.43
1:A:1705:CYS:O	1:A:1709:ILE:HG13	2.18	0.43
3:D:1:NAG:H4	3:D:2:NAG:H2	1.74	0.43
1:A:1667[B]:PHE:HE2	7:A:3023:Y01:HAP1	1.82	0.43
1:A:709:GLN:HE22	1:A:710:LYS:HE3	1.84	0.43
1:A:1663:GLY:HA3	9:A:3027:YIJ:C26	2.49	0.43
1:A:185:HIS:O	1:A:188:THR:OG1	2.36	0.43
1:A:924:LEU:HD12	1:A:924:LEU:HA	1.82	0.43
1:A:769:ILE:HG23	1:A:770:ILE:HG23	2.00	0.43
1:A:54:ARG:CZ	1:A:57:LEU:HD21	2.49	0.42
1:A:188:THR:HG22	1:A:189:PHE:H	1.83	0.42
1:A:403:PHE:CZ	1:A:1768:MET:HB3	2.54	0.42
1:A:913:SER:OG	1:A:914:GLY:N	2.51	0.42
1:A:916:SER:HB2	7:A:3015:Y01:HAR1	2.01	0.42
1:A:369:LEU:HD23	1:A:375:TRP:HB2	2.01	0.42
1:A:225:LEU:HD22	1:A:228:LEU:HD22	2.00	0.42
1:A:1201:TYR:HD1	1:A:1262:ALA:HB1	1.84	0.42
1:A:348:ASN:HB3	1:A:352:GLY:HA2	2.02	0.42
1:A:193:PRO:CB	7:A:3017:Y01:HAI	2.49	0.42
1:A:407:ASN:HB2	1:A:1769:TYR:CE1	2.55	0.42
1:A:1570:VAL:HG23	1:A:1604:SER:HB3	2.01	0.42
1:A:26:LYS:O	1:A:29:ALA:HB3	2.20	0.42
1:A:54:ARG:NH1	1:A:57:LEU:HD21	2.34	0.42
1:A:1246:LYS:HB3	1:A:1246:LYS:HE2	1.87	0.42
1:A:1659:LEU:HD11	1:A:1772:ILE:HD11	2.02	0.42
7:A:3019:Y01:HAC1	7:A:3019:Y01:HAP1	1.93	0.42
1:A:1423:TRP:CD1	1:A:1423:TRP:H	2.37	0.41
4:E:4:MAN:H61	4:E:5:MAN:H2	1.68	0.41
1:A:119:HIS:ND1	1:A:121:VAL:HG12	2.36	0.41
1:A:1304:LEU:HD12	1:A:1304:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:LEU:HD23	1:A:1316:LEU:HA	1.94	0.41
1:A:1529:LYS:HG3	1:A:1531:ALA:H	1.85	0.41
1:A:859:MET:HE2	1:A:859:MET:HB3	1.99	0.41
1:A:72:PRO:HA	1:A:73:PRO:HD3	1.95	0.41
7:A:3017:Y01:HAC1	7:A:3017:Y01:HAP1	1.79	0.41
1:A:322:THR:O	1:A:322:THR:OG1	2.37	0.41
1:A:376:GLU:HA	1:A:379:TYR:HB3	2.03	0.41
1:A:254:VAL:HG21	1:A:412:VAL:HG21	2.03	0.41
1:A:782:TRP:CD1	1:A:821:LYS:HE2	2.56	0.41
1:A:1377:TYR:HA	1:A:1380:VAL:O	2.21	0.41
1:A:1453:VAL:O	1:A:1457:ILE:HG13	2.21	0.41
1:A:104:PHE:HB3	1:A:106:PHE:CE2	2.56	0.40
1:A:1285:LEU:HD23	1:A:1285:LEU:HA	1.84	0.40
1:A:129:LEU:HD12	1:A:175:VAL:HG12	2.02	0.40
1:A:724:ILE:HD13	1:A:724:ILE:HA	1.93	0.40
1:A:1406:ASN:HD21	7:A:3019:Y01:HAL2	1.86	0.40

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	1228/1874 (66%)	1174 (96%)	54 (4%)	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	1077/1648 (65%)	1076 (100%)	1 (0%)	88 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	865	ASN
1	A	1368	GLN
1	A	1543	ASN
1	A	1680	ASN
1	A	1724	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	B	1	2,1	14,14,15	0.34	0	17,19,21	0.78	0
2	NAG	B	2	2	14,14,15	0.30	0	17,19,21	0.84	0
2	BMA	B	3	2	11,11,12	0.23	0	15,15,17	0.85	1 (6%)
2	MAN	B	4	2	11,11,12	0.22	0	15,15,17	0.50	0
3	NAG	C	1	3,1	14,14,15	0.38	0	17,19,21	1.33	1 (5%)
3	NAG	C	2	3	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
3	NAG	D	2	3	14,14,15	0.39	0	17,19,21	0.60	0
4	NAG	E	1	4,1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	0.66	0
4	BMA	E	3	4	11,11,12	0.23	0	15,15,17	0.78	1 (6%)
4	MAN	E	4	4	11,11,12	0.25	0	15,15,17	0.63	0
4	MAN	E	5	4	11,11,12	0.24	0	15,15,17	0.62	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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	1/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	4.18	117.79	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	2.47	115.49	112.19
4	E	3	BMA	C1-O5-C5	2.22	115.16	112.19
3	D	1	NAG	C1-O5-C5	2.15	115.06	112.19
2	B	3	BMA	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
4	E	4	MAN	O5-C5-C6-O6
4	E	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7

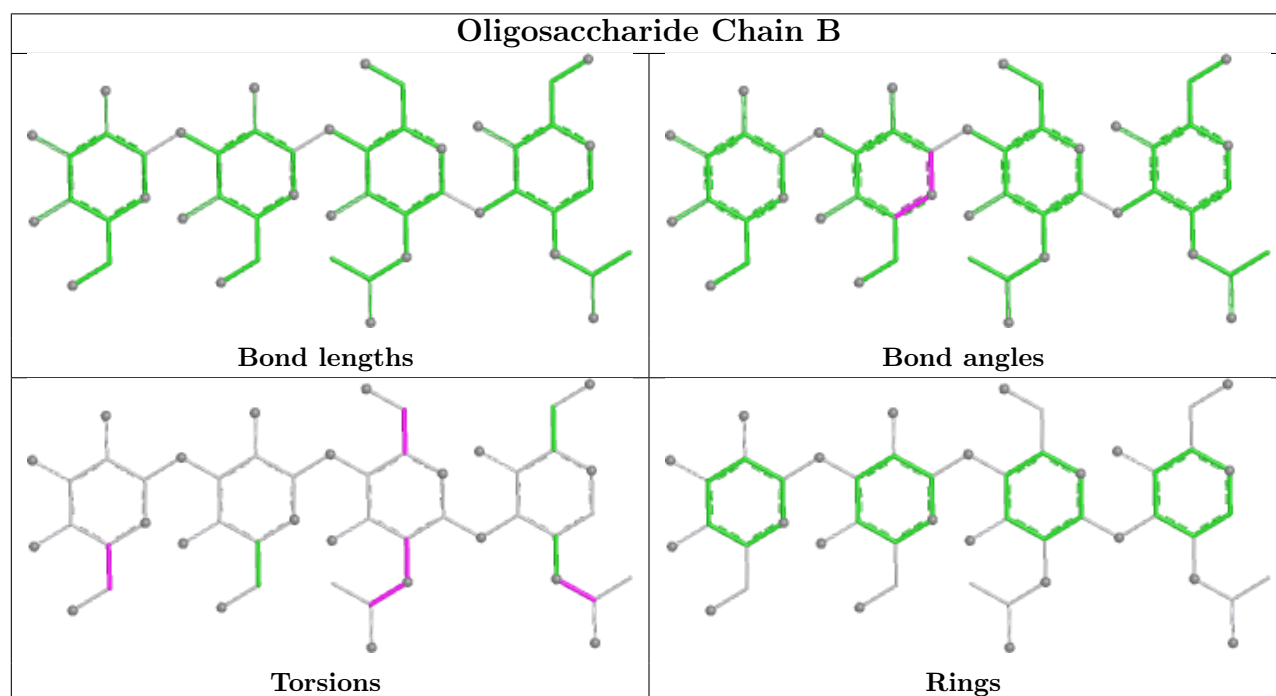
All (1) ring outliers are listed below:

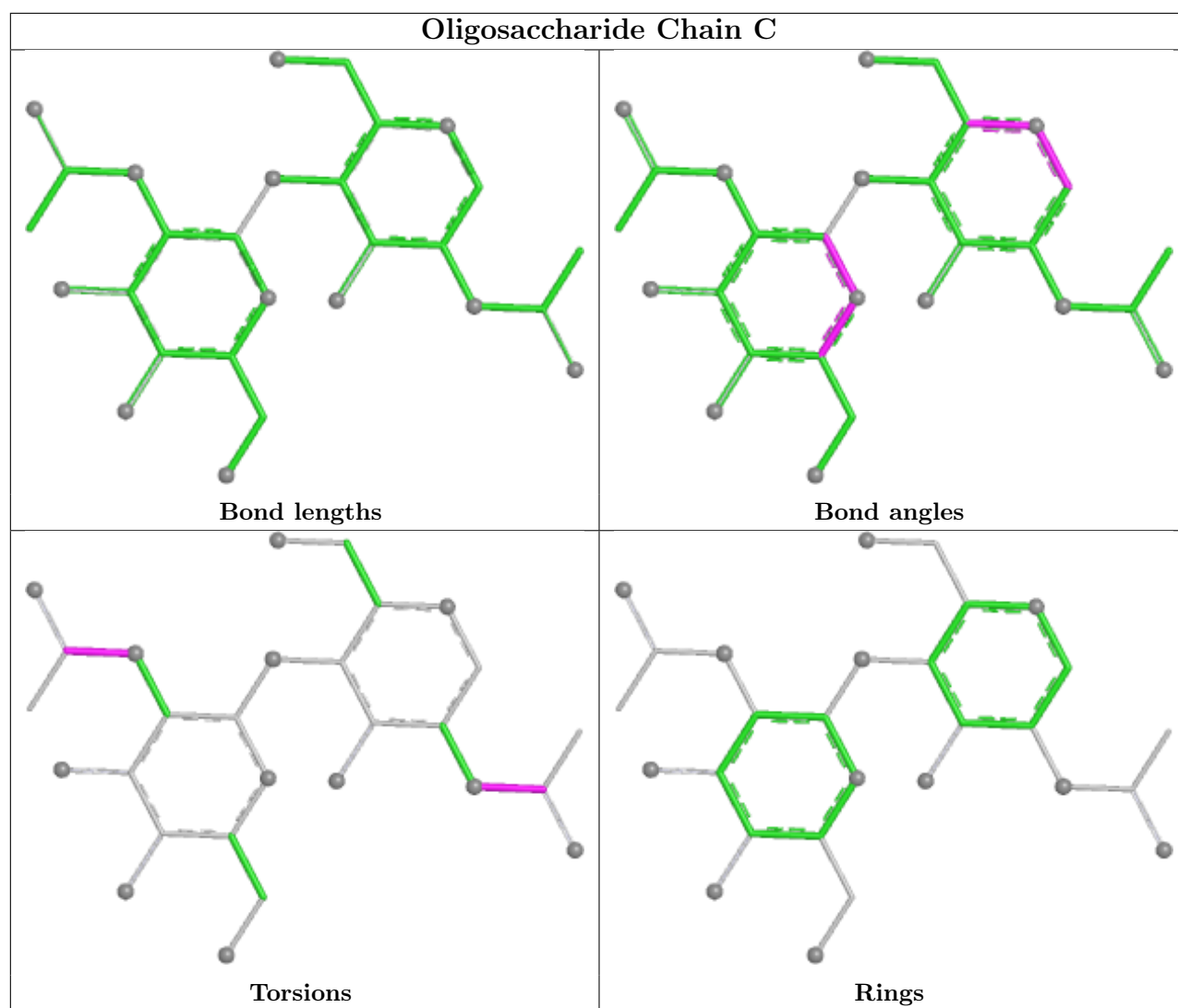
Mol	Chain	Res	Type	Atoms
4	E	4	MAN	C1-C2-C3-C4-C5-O5

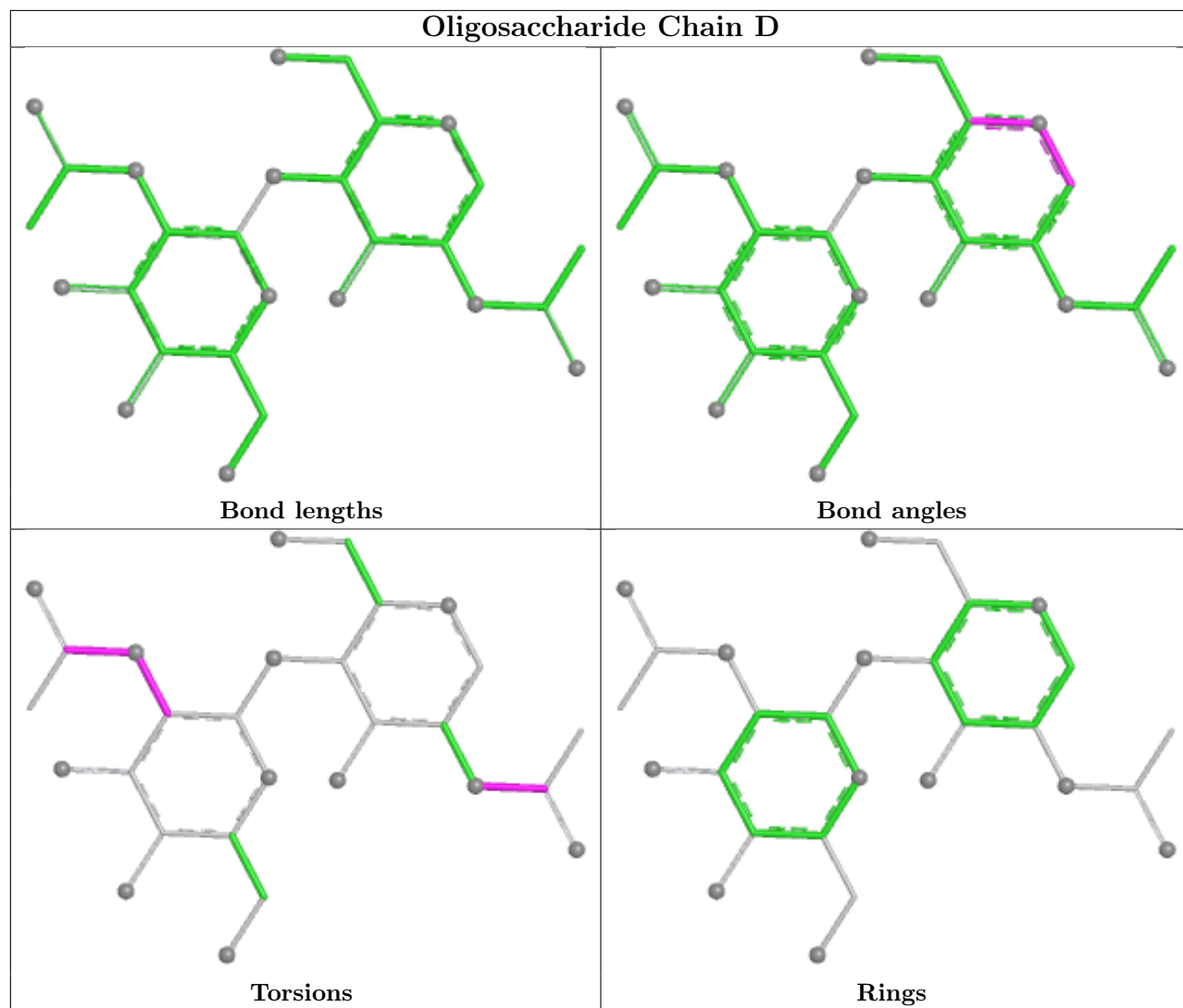
6 monomers are involved in 4 short contacts:

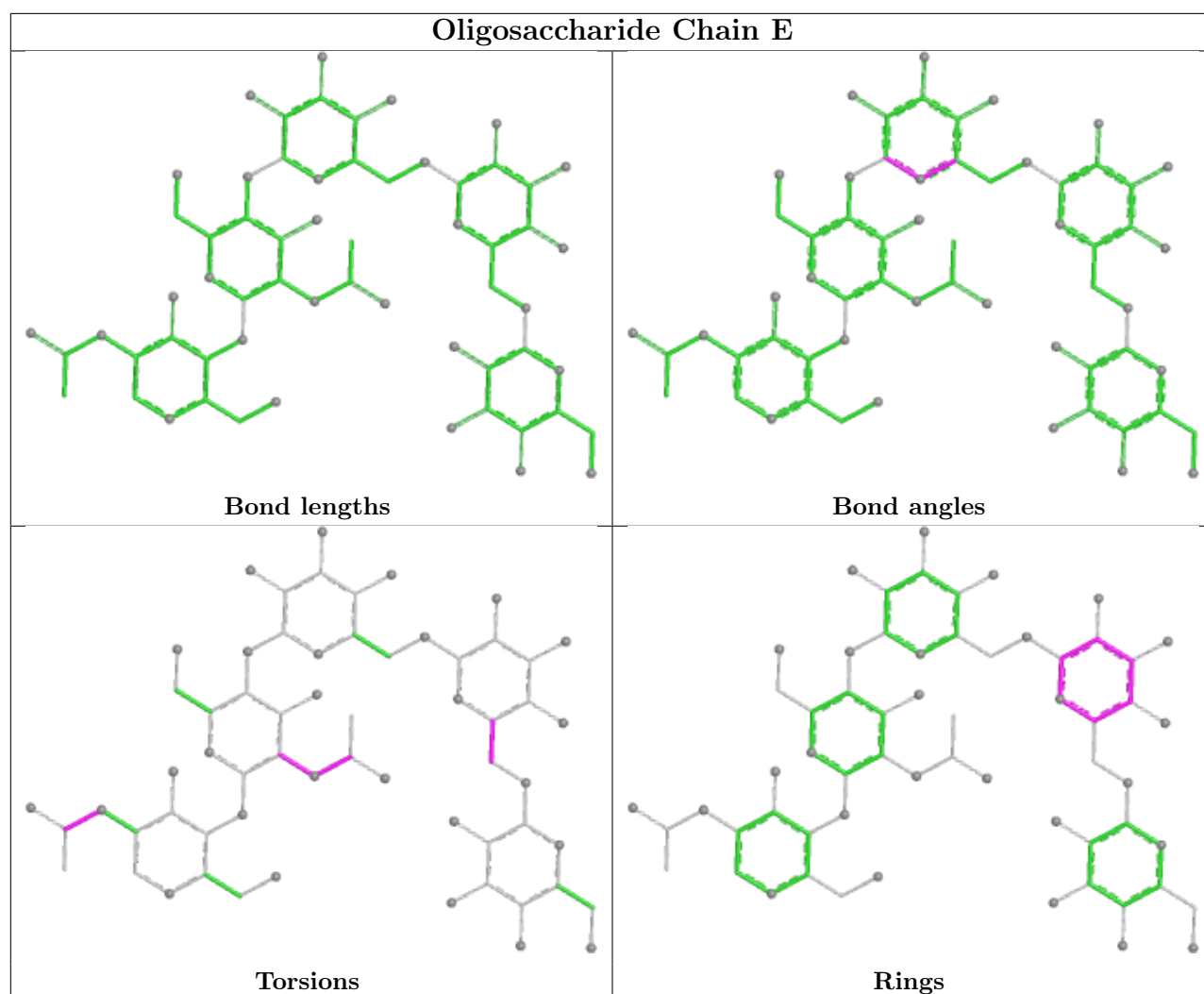
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	1	0
3	D	2	NAG	1	0
3	D	1	NAG	1	0
4	E	5	MAN	2	0
4	E	4	MAN	1	0

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









5.6 Ligand geometry [i](#)

28 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	$\# Z > 2$
5	NAG	A	3002	1	14,14,15	0.31	0	17,19,21	0.59	0
6	LBN	A	3007	-	39,39,51	0.32	0	45,47,59	0.39	0
7	Y01	A	3017	-	34,34,38	0.49	0	52,52,57	0.69	1 (1%)
5	NAG	A	3003	1	14,14,15	0.33	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	Y01	A	3020	-	34,34,38	0.48	0	52,52,57	0.55	0
7	Y01	A	3014	-	38,38,38	0.45	0	57,57,57	0.49	0
6	LBN	A	3006	-	27,27,51	0.46	0	30,32,59	0.60	1 (3%)
7	Y01	A	3023	-	38,38,38	0.45	0	57,57,57	0.54	0
7	Y01	A	3018	-	34,34,38	0.48	0	52,52,57	0.61	0
8	9Z9	A	3025	-	35,35,44	0.29	0	58,58,68	0.51	0
9	YIJ	A	3028	-	35,44,44	0.53	0	34,73,73	1.09	3 (8%)
6	LBN	A	3009	-	33,33,51	0.33	0	39,41,59	0.42	0
7	Y01	A	3024	-	31,31,38	0.51	0	47,48,57	0.64	1 (2%)
6	LBN	A	3004	-	47,47,51	0.30	0	53,55,59	0.32	0
6	LBN	A	3013	-	43,43,51	0.30	0	49,51,59	0.35	0
6	LBN	A	3010	-	35,35,51	0.31	0	41,43,59	0.39	0
7	Y01	A	3016	-	38,38,38	0.44	0	57,57,57	0.51	0
7	Y01	A	3022	-	38,38,38	0.45	0	57,57,57	0.55	0
6	LBN	A	3008	-	24,24,51	0.36	0	29,31,59	0.51	0
5	NAG	A	3001	1	14,14,15	0.28	0	17,19,21	0.60	0
6	LBN	A	3005	-	29,29,51	0.45	0	32,34,59	0.59	1 (3%)
7	Y01	A	3019	-	38,38,38	0.46	0	57,57,57	0.74	1 (1%)
7	Y01	A	3015	-	34,34,38	0.48	0	52,52,57	0.59	0
9	YIJ	A	3027	-	35,44,44	0.52	0	34,73,73	0.96	2 (5%)
7	Y01	A	3021	-	34,34,38	0.46	0	52,52,57	0.57	0
6	LBN	A	3012	-	43,43,51	0.31	0	49,51,59	0.39	0
6	LBN	A	3011	-	47,47,51	0.31	0	53,55,59	0.33	0
8	9Z9	A	3026	-	37,37,44	0.28	0	58,60,68	0.48	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
5	NAG	A	3002	1	-	2/6/23/26	0/1/1/1
6	LBN	A	3007	-	-	12/43/43/55	-
7	Y01	A	3017	-	-	9/15/73/77	0/4/4/4
5	NAG	A	3003	1	-	3/6/23/26	0/1/1/1
7	Y01	A	3020	-	-	4/15/73/77	0/4/4/4
7	Y01	A	3014	-	-	6/19/77/77	0/4/4/4
6	LBN	A	3006	-	-	4/29/29/55	-
7	Y01	A	3023	-	-	4/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	Y01	A	3018	-	-	4/15/73/77	0/4/4/4
9	YIJ	A	3028	-	-	5/12/106/106	0/1/7/7
8	9Z9	A	3025	-	-	-	0/6/6/6
6	LBN	A	3009	-	-	7/37/37/55	-
7	Y01	A	3024	-	-	0/9/67/77	0/4/4/4
6	LBN	A	3004	-	-	4/51/51/55	-
6	LBN	A	3013	-	-	7/47/47/55	-
6	LBN	A	3010	-	-	9/39/39/55	-
7	Y01	A	3016	-	-	2/19/77/77	0/4/4/4
7	Y01	A	3022	-	-	4/19/77/77	0/4/4/4
6	LBN	A	3008	-	-	0/27/27/55	-
5	NAG	A	3001	1	-	3/6/23/26	0/1/1/1
6	LBN	A	3005	-	-	0/31/31/55	-
7	Y01	A	3019	-	-	8/19/77/77	0/4/4/4
7	Y01	A	3015	-	-	4/15/73/77	0/4/4/4
9	YIJ	A	3027	-	-	6/12/106/106	0/1/7/7
7	Y01	A	3021	-	-	8/15/73/77	0/4/4/4
6	LBN	A	3012	-	-	6/47/47/55	-
6	LBN	A	3011	-	-	13/51/51/55	-
8	9Z9	A	3026	-	-	0/3/91/100	0/6/6/6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	3028	YIJ	C12-C11-C10	-3.59	110.40	113.19
9	A	3027	YIJ	C8-C10-C11	-3.30	122.90	128.39
7	A	3019	Y01	CBI-CBE-CBB	3.05	124.20	119.50
7	A	3017	Y01	CBI-CBE-CBB	2.76	123.77	119.50
9	A	3028	YIJ	C14-C10-C11	-2.59	107.00	110.75
6	A	3006	LBN	O3-P1-O4	2.41	120.23	110.83
9	A	3028	YIJ	C21-C20-C18	-2.39	109.72	113.73
7	A	3024	Y01	CBB-CBE-CBI	2.36	120.26	116.20
6	A	3005	LBN	O3-P1-O4	2.34	119.94	110.83
9	A	3027	YIJ	C21-C20-C18	-2.29	109.89	113.73

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3001	NAG	C8-C7-N2-C2
5	A	3001	NAG	O7-C7-N2-C2
5	A	3003	NAG	C3-C2-N2-C7
5	A	3003	NAG	O7-C7-N2-C2
6	A	3006	LBN	C2-C1-O1-P1
6	A	3007	LBN	C2-C1-O1-P1
6	A	3007	LBN	C1-O1-P1-O4
6	A	3007	LBN	C9-O2-P1-O1
6	A	3007	LBN	C9-O2-P1-O4
6	A	3007	LBN	C6-C9-O2-P1
6	A	3007	LBN	C26-C25-O5-C3
6	A	3007	LBN	O6-C25-O5-C3
6	A	3007	LBN	C35-C34-O7-C2
6	A	3010	LBN	C2-C1-O1-P1
6	A	3010	LBN	C1-O1-P1-O2
6	A	3010	LBN	C1-O1-P1-O4
6	A	3010	LBN	C9-O2-P1-O4
6	A	3010	LBN	C26-C25-O5-C3
6	A	3010	LBN	O6-C25-O5-C3
6	A	3011	LBN	C1-O1-P1-O4
6	A	3011	LBN	C9-O2-P1-O4
6	A	3011	LBN	C6-C9-O2-P1
6	A	3012	LBN	C35-C34-O7-C2
6	A	3012	LBN	O8-C34-O7-C2
6	A	3013	LBN	C1-O1-P1-O4
6	A	3013	LBN	C9-O2-P1-O4
7	A	3014	Y01	OAG-CAY-OAW-CBC
7	A	3014	Y01	CAM-CAY-OAW-CBC
7	A	3017	Y01	CAO-CBB-CBE-CBI
7	A	3020	Y01	OAG-CAY-OAW-CBC
7	A	3020	Y01	CAM-CAY-OAW-CBC
9	A	3027	YIJ	C6-C7-O2-C8
9	A	3027	YIJ	O1-C7-O2-C8
9	A	3027	YIJ	C14-C10-C8-C9
9	A	3027	YIJ	C14-C10-C8-O2
9	A	3028	YIJ	C6-C7-O2-C8
9	A	3028	YIJ	C14-C10-C8-C9
9	A	3028	YIJ	C9-C8-O2-C7
6	A	3007	LBN	O8-C34-O7-C2
5	A	3003	NAG	C8-C7-N2-C2
9	A	3028	YIJ	O1-C7-O2-C8
7	A	3021	Y01	CAV-CBC-OAW-CAY
7	A	3015	Y01	CAR-CBC-OAW-CAY

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Mol	Chain	Res	Type	Atoms
7	A	3019	Y01	CAM-CAY-OAW-CBC
7	A	3017	Y01	CAC-CBB-CBE-CAP
7	A	3021	Y01	CAR-CBC-OAW-CAY
7	A	3019	Y01	CAO-CBB-CBE-CBI
7	A	3019	Y01	OAG-CAY-OAW-CBC
7	A	3022	Y01	CAR-CBC-OAW-CAY
7	A	3022	Y01	CAV-CBC-OAW-CAY
7	A	3019	Y01	CAO-CBB-CBE-CAP
7	A	3017	Y01	CAO-CBB-CBE-CAP
6	A	3013	LBN	C35-C34-O7-C2
7	A	3018	Y01	CAM-CAY-OAW-CBC
7	A	3019	Y01	CAC-CBB-CBE-CAP
6	A	3004	LBN	C28-C29-C30-C31
7	A	3015	Y01	CAV-CBC-OAW-CAY
6	A	3013	LBN	O8-C34-O7-C2
5	A	3001	NAG	O5-C5-C6-O6
6	A	3011	LBN	C26-C25-O5-C3
7	A	3017	Y01	CAC-CBB-CBE-CBI
6	A	3009	LBN	C35-C34-O7-C2
6	A	3012	LBN	C2-C1-O1-P1
6	A	3009	LBN	O5-C25-C26-C27
7	A	3018	Y01	OAG-CAY-OAW-CBC
6	A	3006	LBN	O7-C2-C3-O5
6	A	3011	LBN	O7-C2-C3-O5
6	A	3004	LBN	C7-C10-C13-C16
6	A	3013	LBN	C42-C5-C8-C11
9	A	3027	YIJ	C11-C10-C8-C9
9	A	3028	YIJ	C11-C10-C8-C9
6	A	3009	LBN	O8-C34-O7-C2
6	A	3011	LBN	O6-C25-O5-C3
6	A	3010	LBN	C6-C9-O2-P1
5	A	3002	NAG	C8-C7-N2-C2
6	A	3004	LBN	N1-C6-C9-O2
6	A	3007	LBN	N1-C6-C9-O2
6	A	3010	LBN	N1-C6-C9-O2
6	A	3011	LBN	N1-C6-C9-O2
6	A	3012	LBN	N1-C6-C9-O2
6	A	3013	LBN	N1-C6-C9-O2
7	A	3023	Y01	CAC-CBB-CBE-CBI
9	A	3027	YIJ	C11-C10-C8-O2
6	A	3011	LBN	C40-C41-C42-C5
7	A	3023	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
6	A	3011	LBN	C2-C3-O5-C25
6	A	3009	LBN	C1-O1-P1-O4
6	A	3009	LBN	C9-O2-P1-O4
6	A	3012	LBN	C9-O2-P1-O4
7	A	3023	Y01	CAO-CBB-CBE-CAP
6	A	3004	LBN	C42-C5-C8-C11
6	A	3011	LBN	C35-C36-C37-C38
6	A	3007	LBN	C1-C2-O7-C34
7	A	3021	Y01	CAO-CBB-CBE-CBI
6	A	3012	LBN	C42-C5-C8-C11
6	A	3006	LBN	C26-C25-O5-C3
7	A	3023	Y01	CAC-CBB-CBE-CAP
6	A	3013	LBN	C40-C41-C42-C5
5	A	3002	NAG	O7-C7-N2-C2
7	A	3017	Y01	CAR-CBC-OAW-CAY
6	A	3009	LBN	O6-C25-C26-C27
6	A	3011	LBN	C1-C2-C3-O5
7	A	3021	Y01	CAO-CBB-CBE-CAP
7	A	3021	Y01	CAC-CBB-CBE-CBI
6	A	3009	LBN	C3-C2-O7-C34
6	A	3010	LBN	C3-C2-O7-C34
7	A	3019	Y01	CAC-CBB-CBE-CBI
7	A	3016	Y01	CAM-CAL-CAX-OAH
7	A	3021	Y01	CAM-CAL-CAX-OAH
7	A	3015	Y01	CAM-CAL-CAX-OAH
7	A	3020	Y01	CAM-CAL-CAX-OAH
7	A	3016	Y01	CAM-CAL-CAX-OAF
7	A	3017	Y01	CAM-CAL-CAX-OAH
7	A	3014	Y01	CAM-CAL-CAX-OAH
7	A	3018	Y01	CAM-CAL-CAX-OAH
7	A	3019	Y01	CAM-CAL-CAX-OAH
7	A	3015	Y01	CAM-CAL-CAX-OAF
6	A	3011	LBN	C42-C5-C8-C11
7	A	3021	Y01	CAM-CAL-CAX-OAF
7	A	3022	Y01	CAM-CAL-CAX-OAH
7	A	3014	Y01	CAM-CAL-CAX-OAF
7	A	3017	Y01	CAM-CAL-CAX-OAF
7	A	3018	Y01	CAM-CAL-CAX-OAF
7	A	3019	Y01	CAM-CAL-CAX-OAF
7	A	3020	Y01	CAM-CAL-CAX-OAF
7	A	3022	Y01	CAM-CAL-CAX-OAF
6	A	3006	LBN	O6-C25-O5-C3

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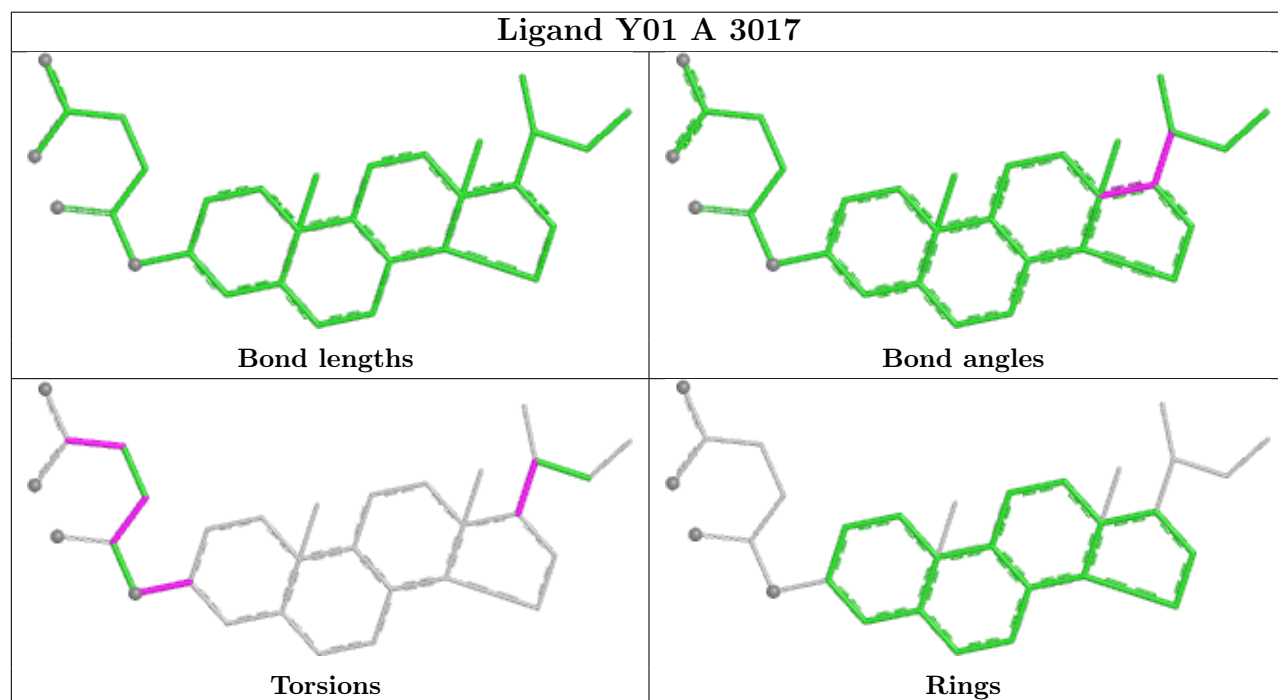
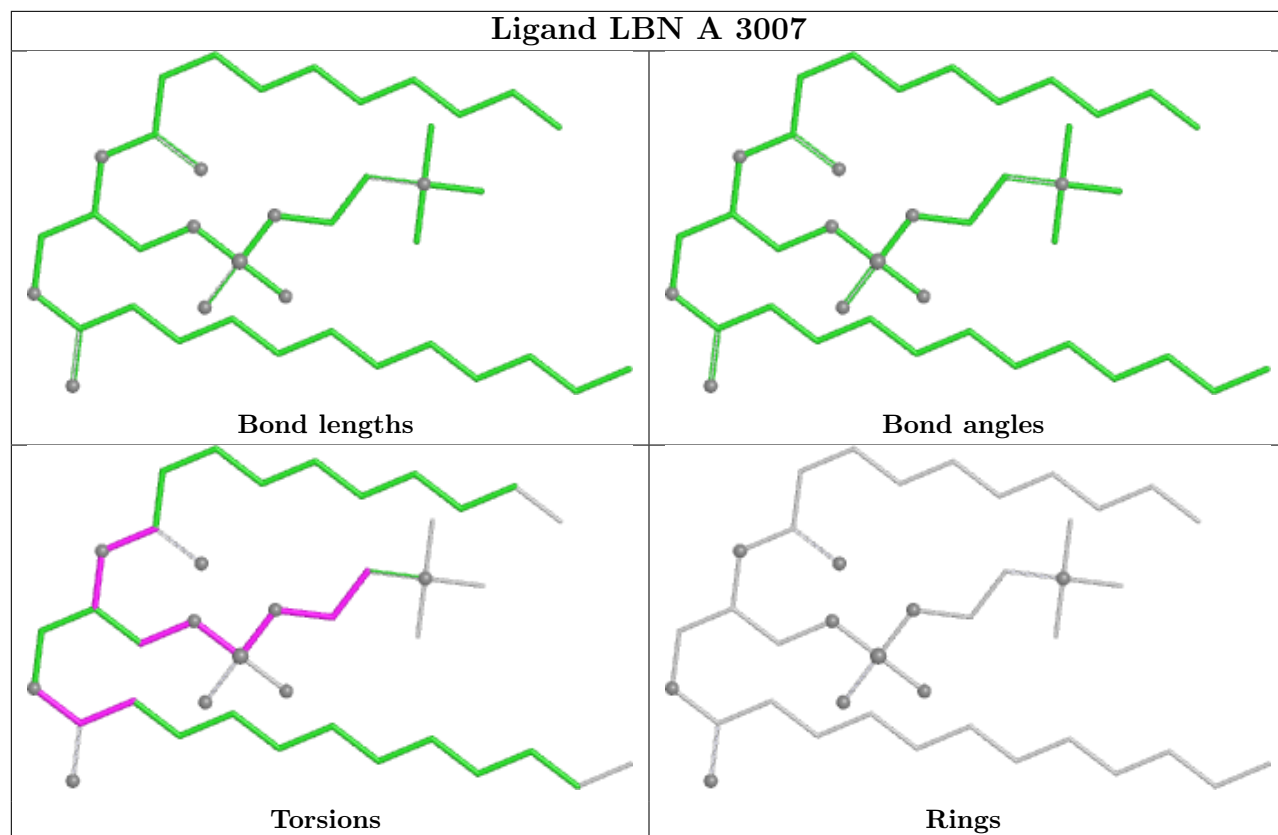
Mol	Chain	Res	Type	Atoms
7	A	3014	Y01	CAC-CBB-CBE-CBI
6	A	3011	LBN	C37-C38-C39-C40
7	A	3017	Y01	CAV-CBC-OAW-CAY
7	A	3021	Y01	CAM-CAY-OAW-CBC
6	A	3007	LBN	O5-C25-C26-C27
7	A	3017	Y01	CAL-CAM-CAY-OAW
7	A	3014	Y01	CAO-CBB-CBE-CAP

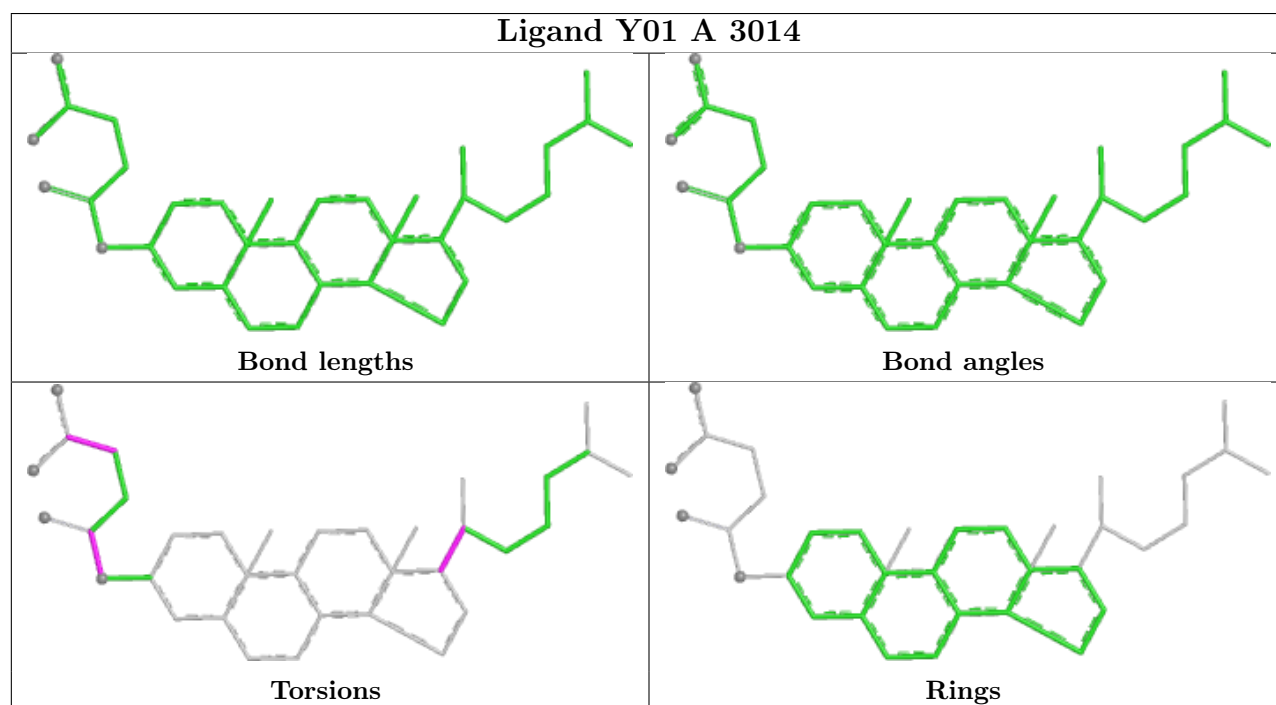
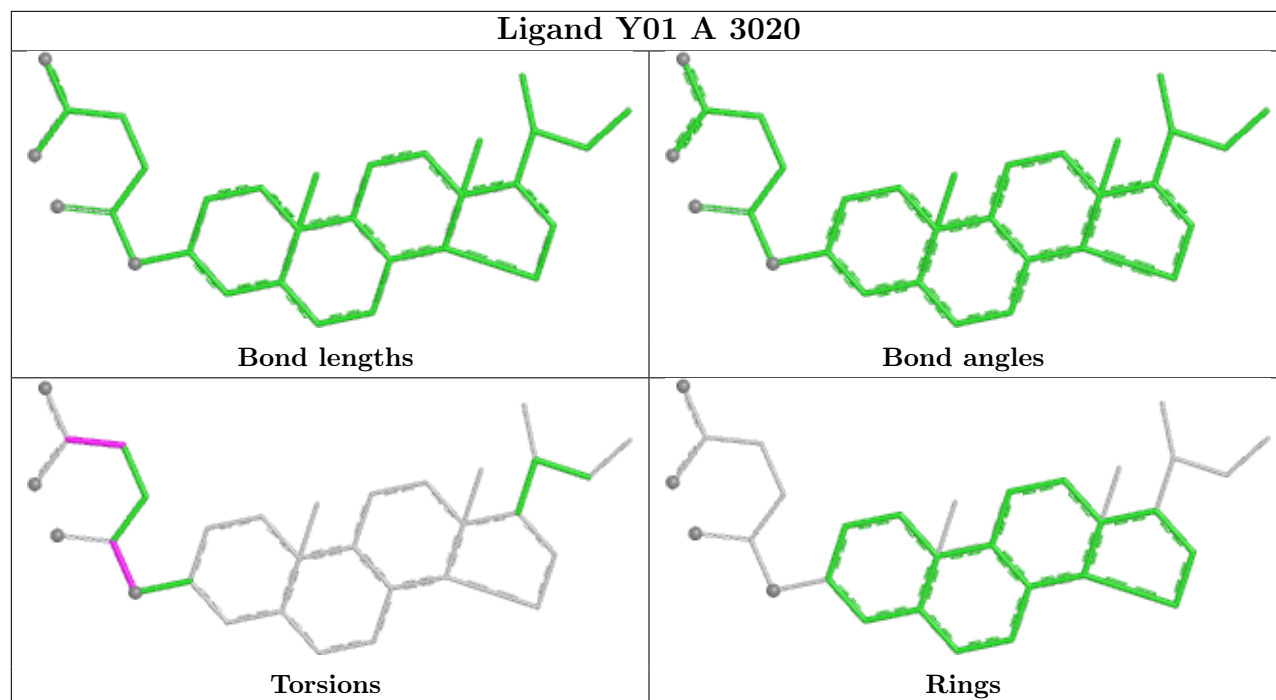
There are no ring outliers.

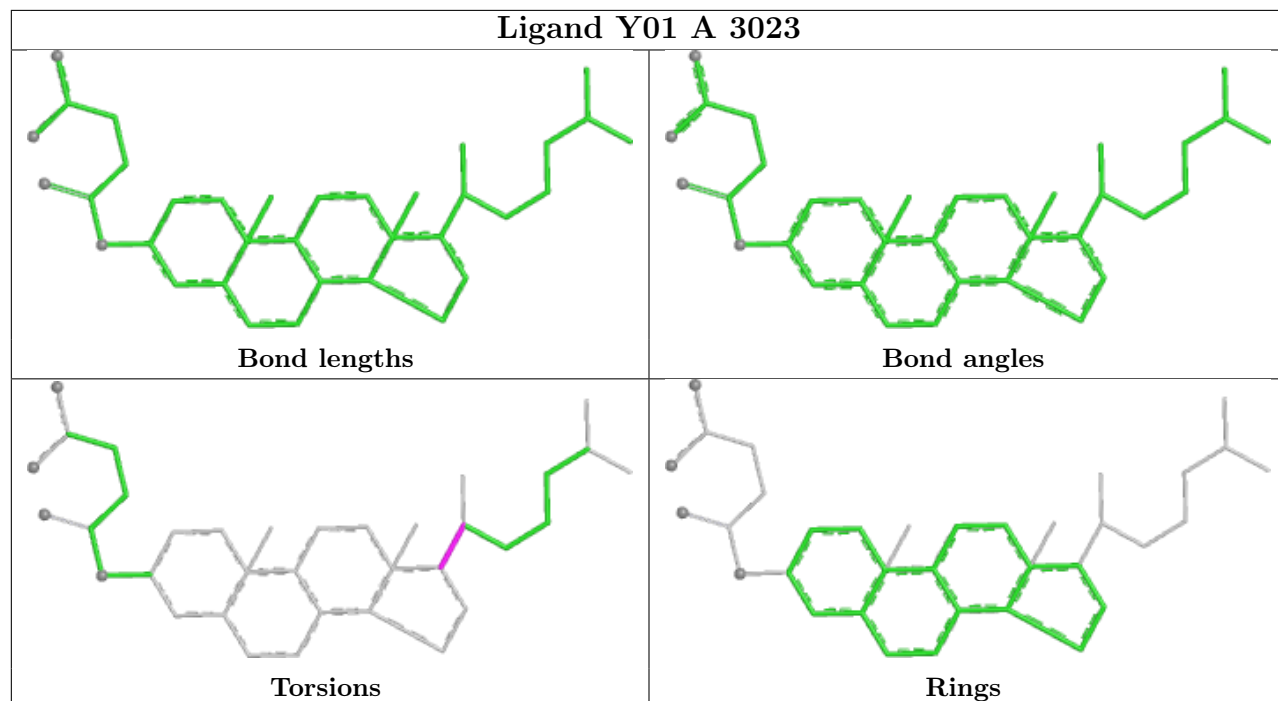
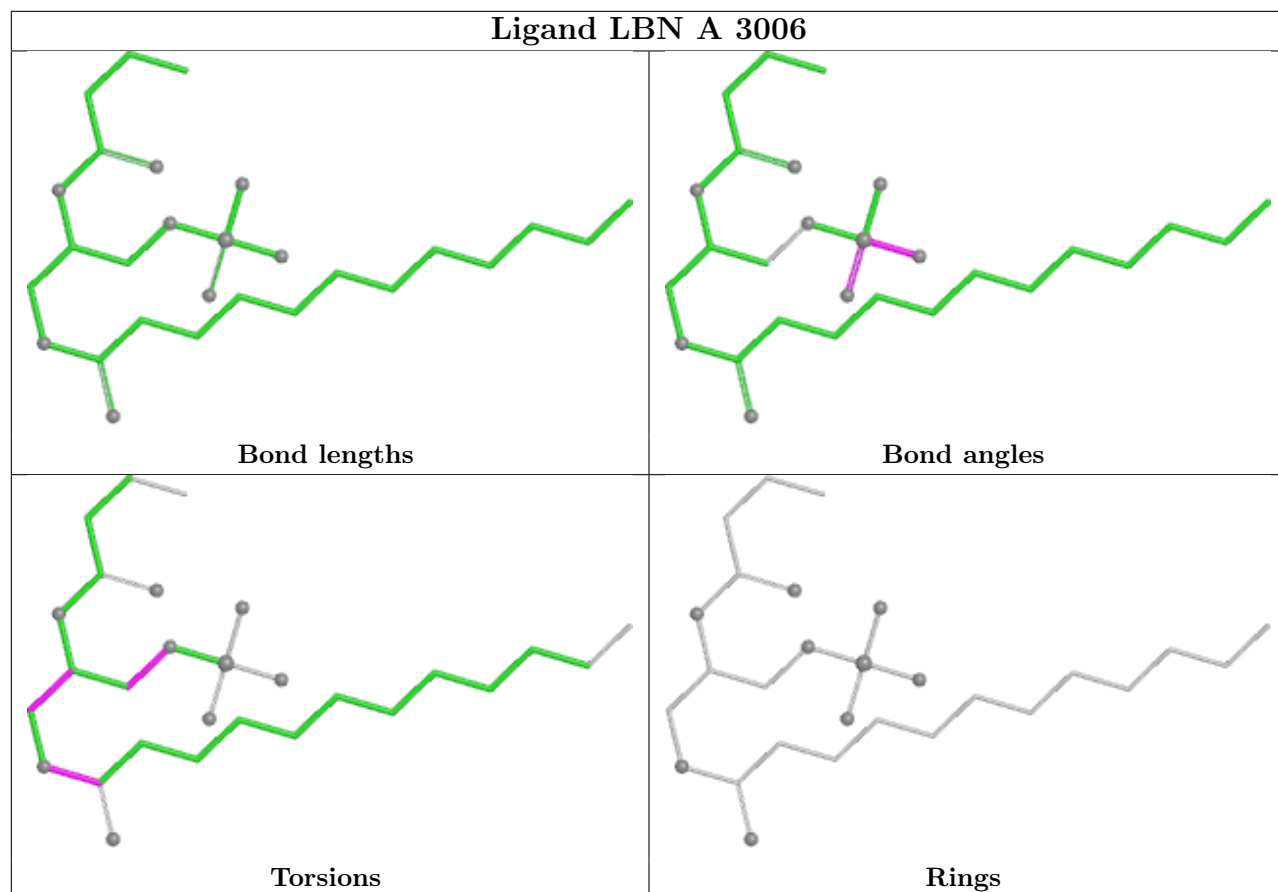
10 monomers are involved in 14 short contacts:

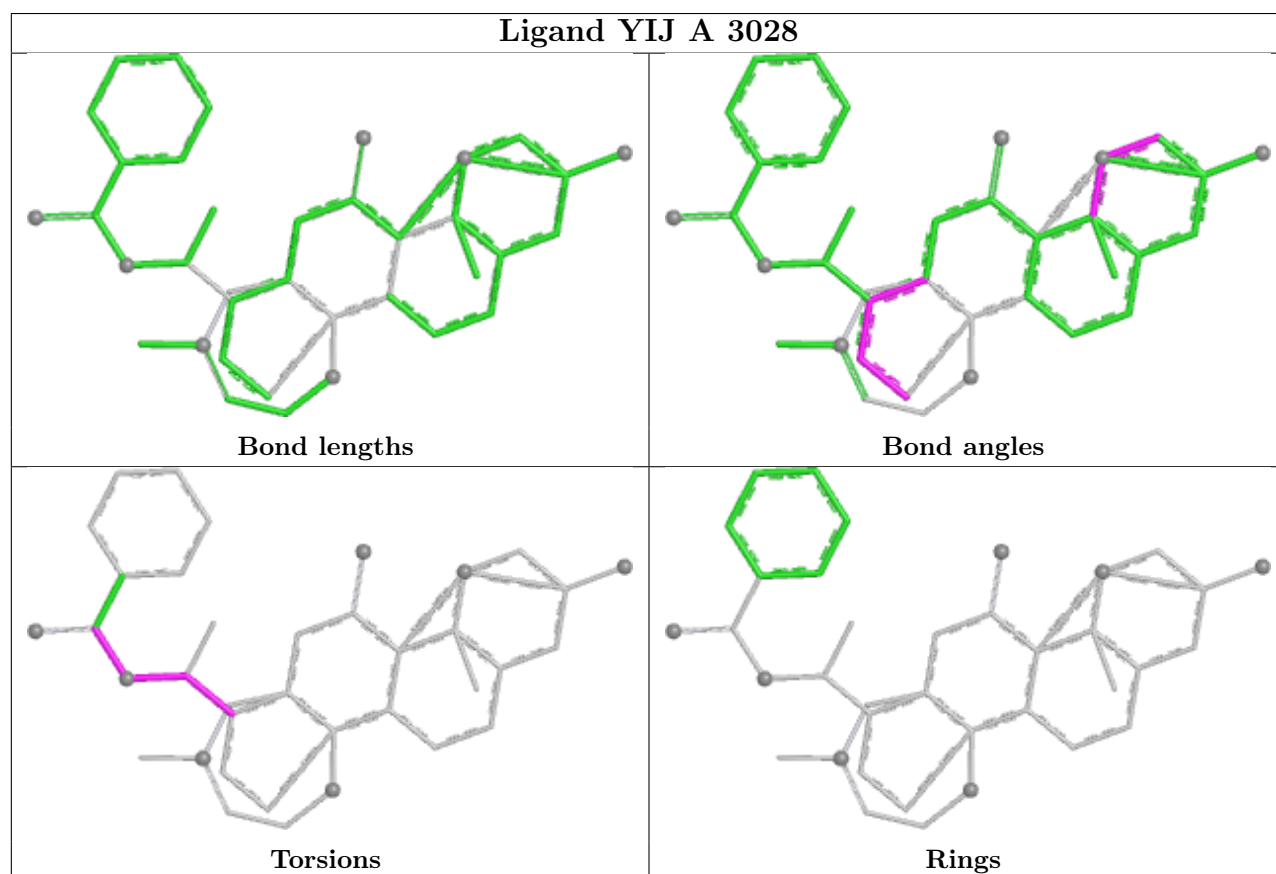
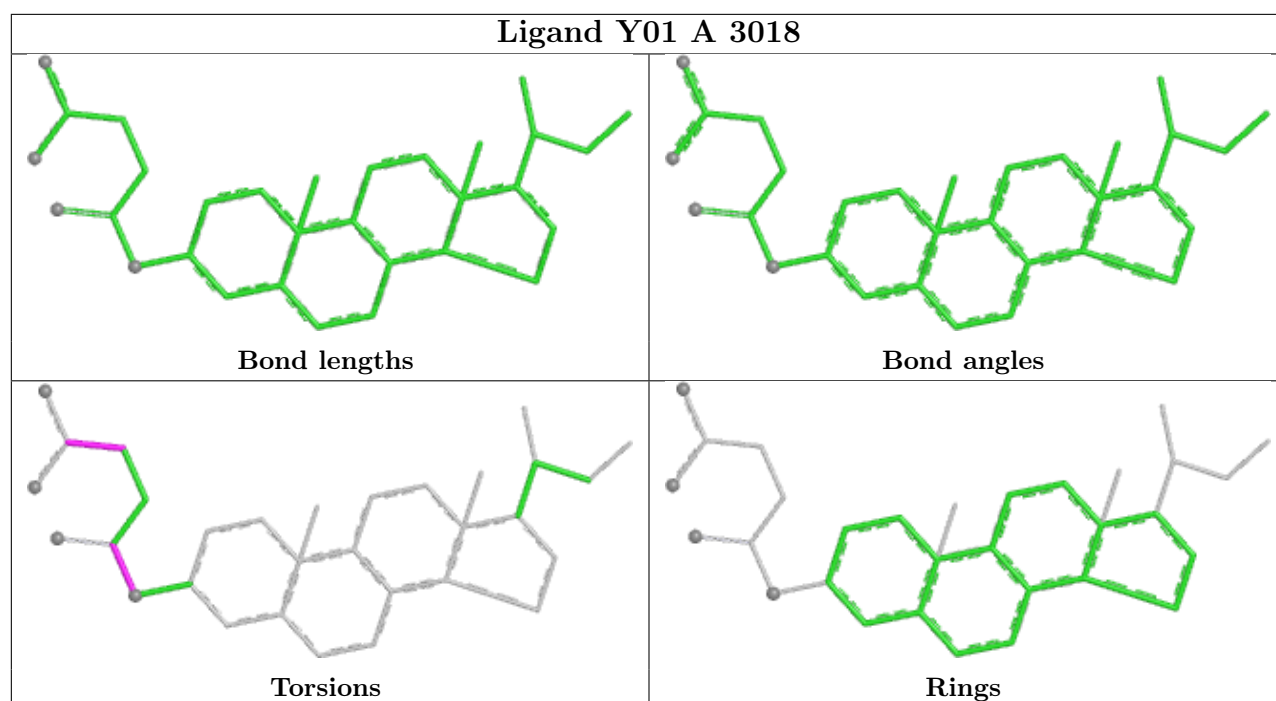
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3017	Y01	3	0
7	A	3014	Y01	1	0
7	A	3023	Y01	1	0
7	A	3018	Y01	1	0
7	A	3024	Y01	1	0
7	A	3022	Y01	1	0
7	A	3019	Y01	2	0
7	A	3015	Y01	1	0
9	A	3027	YIJ	1	0
7	A	3021	Y01	2	0

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

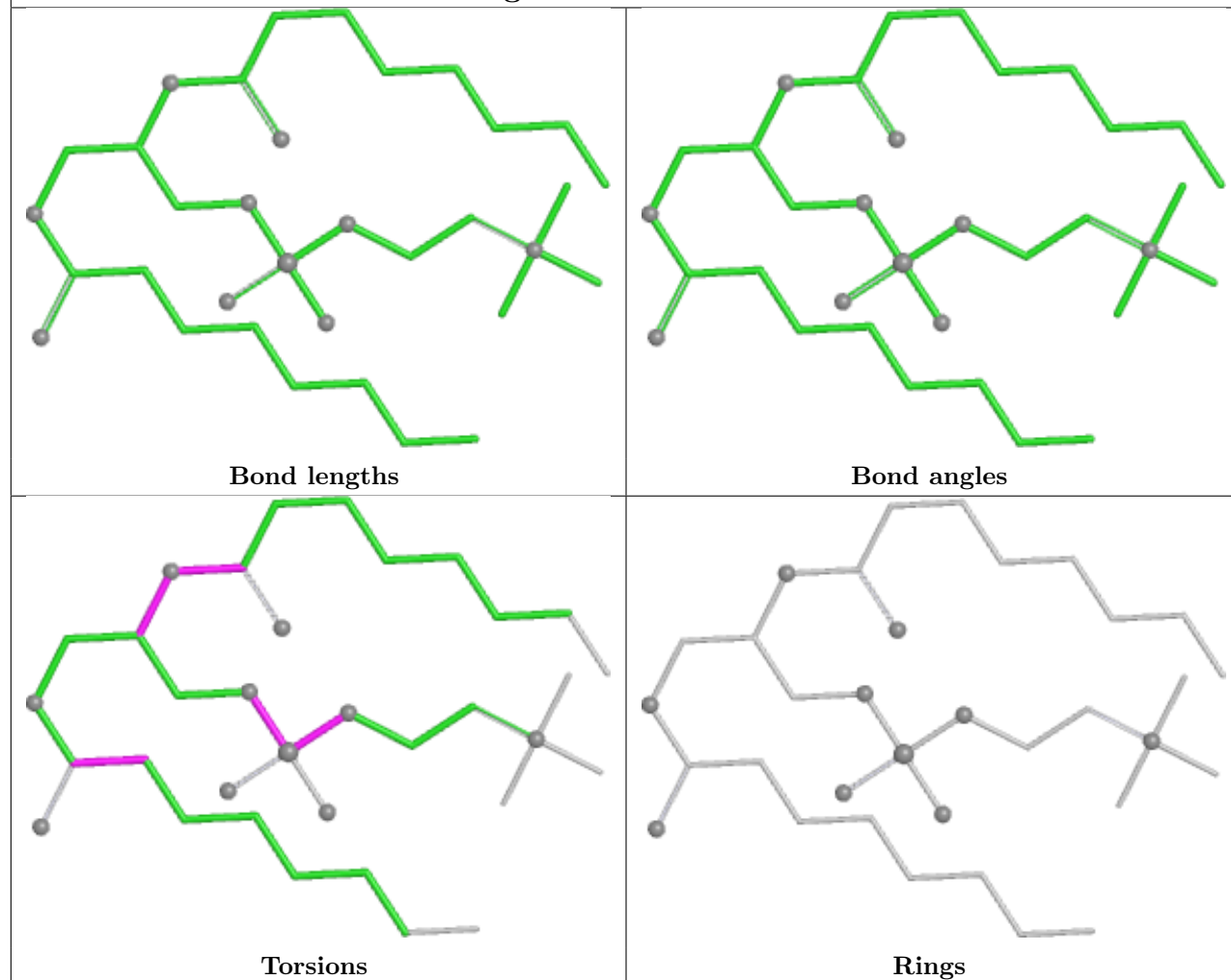




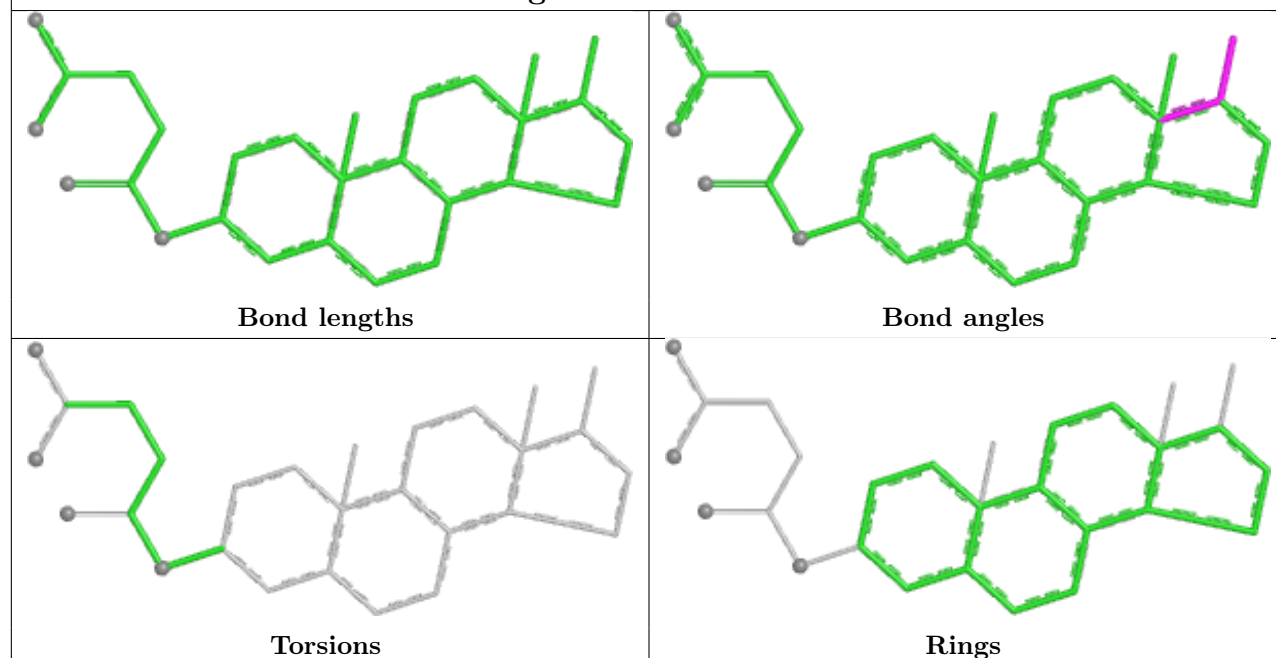


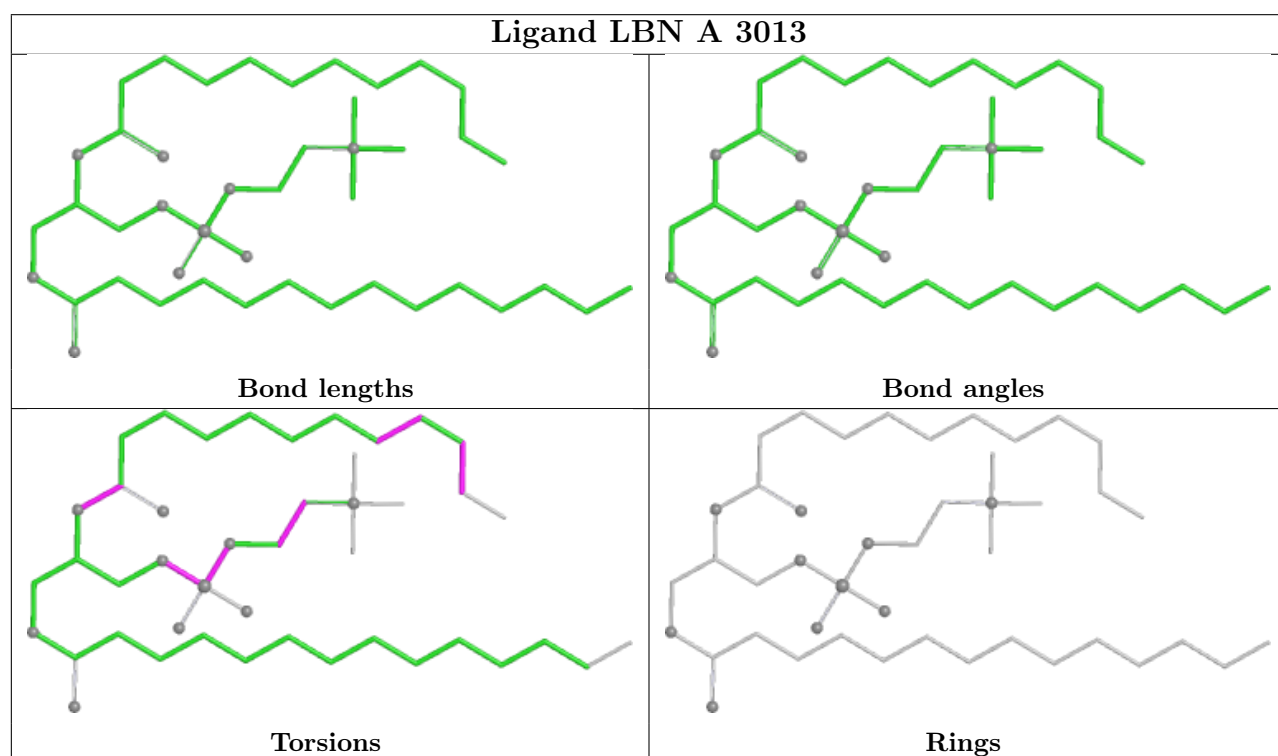
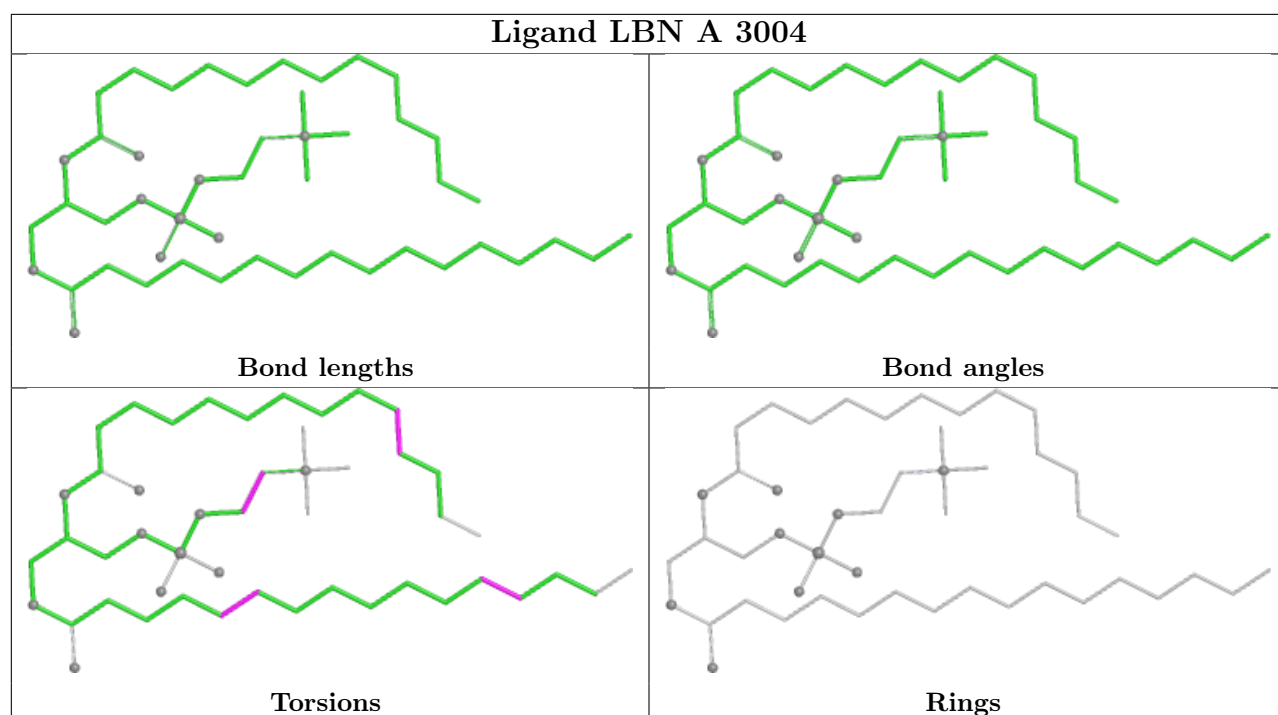


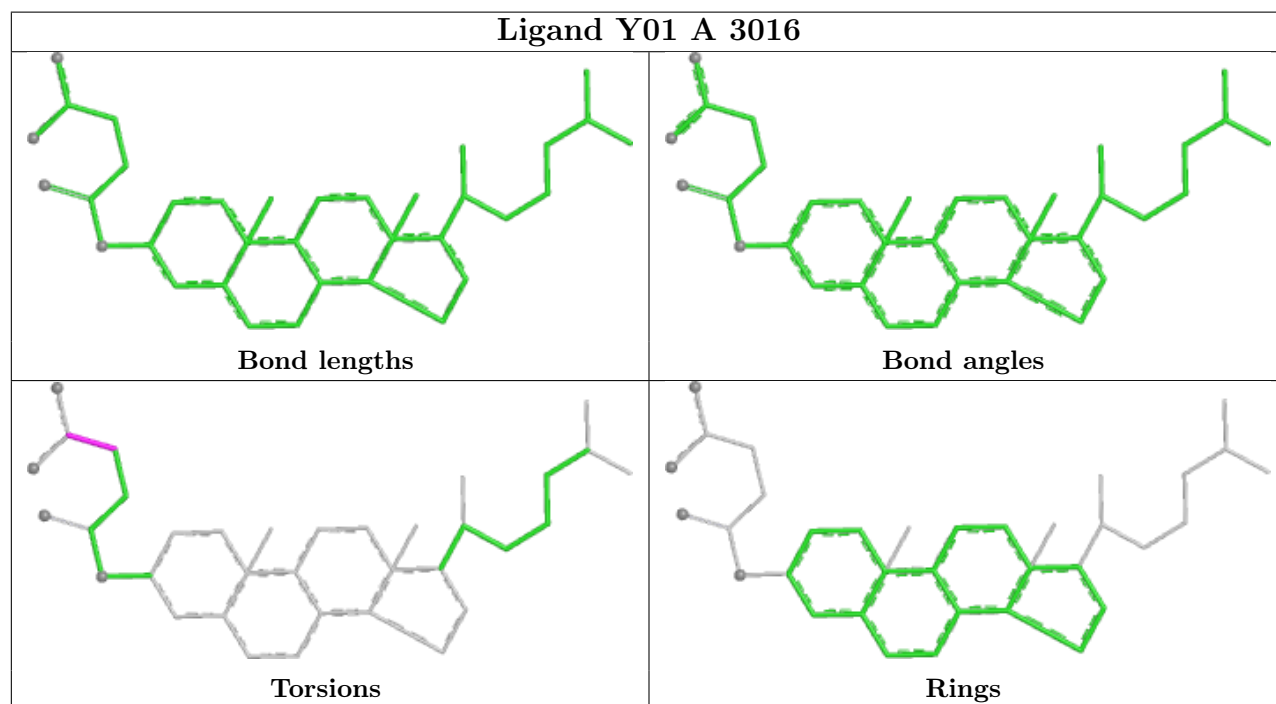
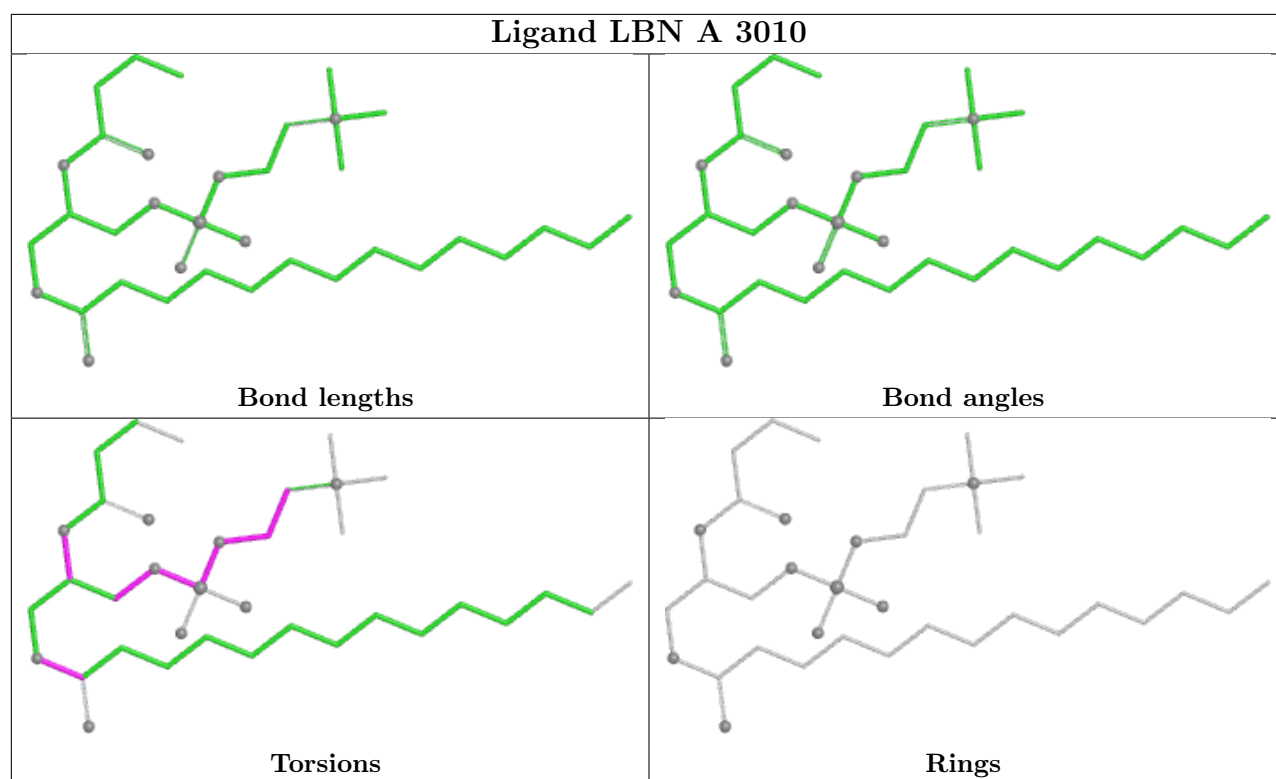
Ligand LBN A 3009

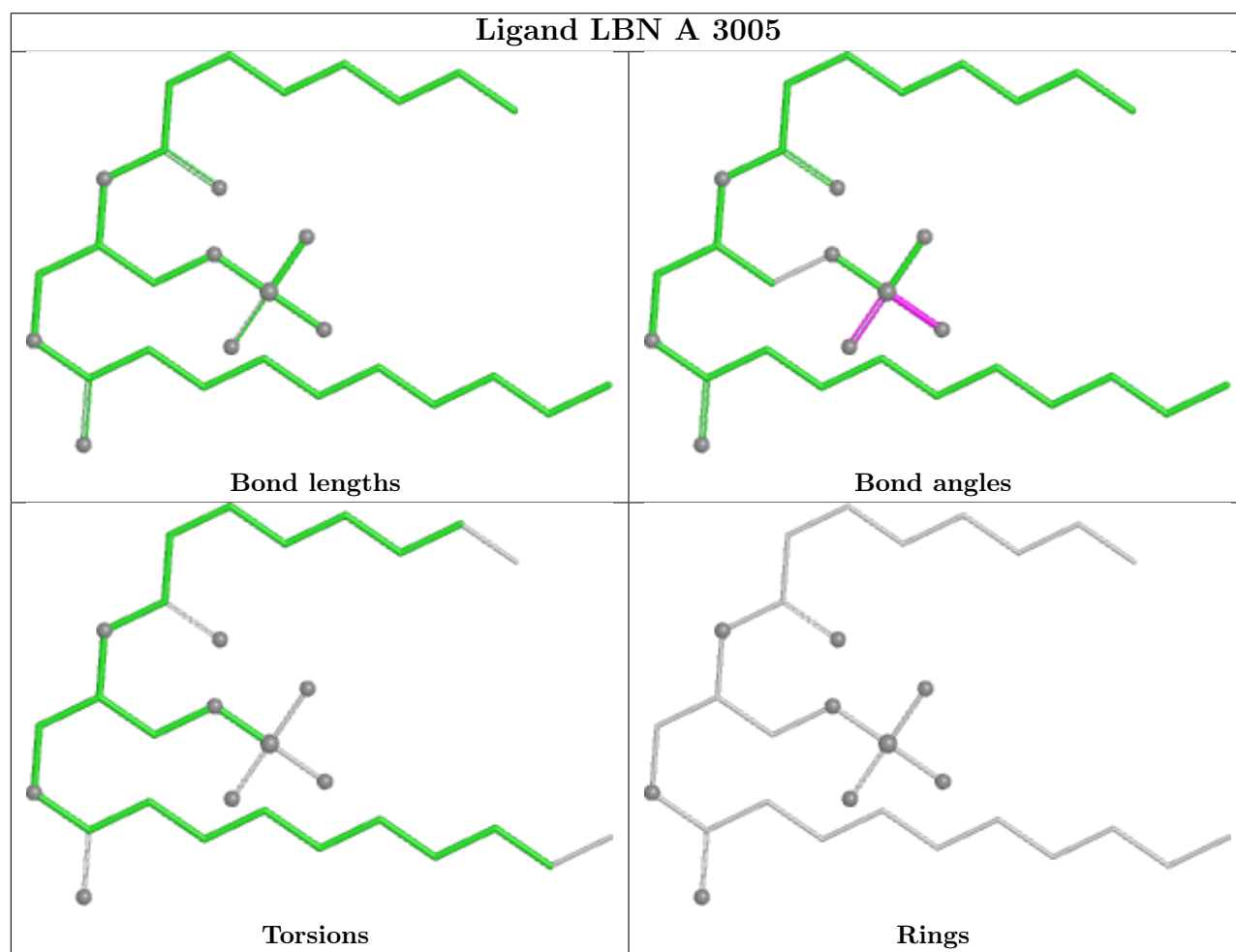
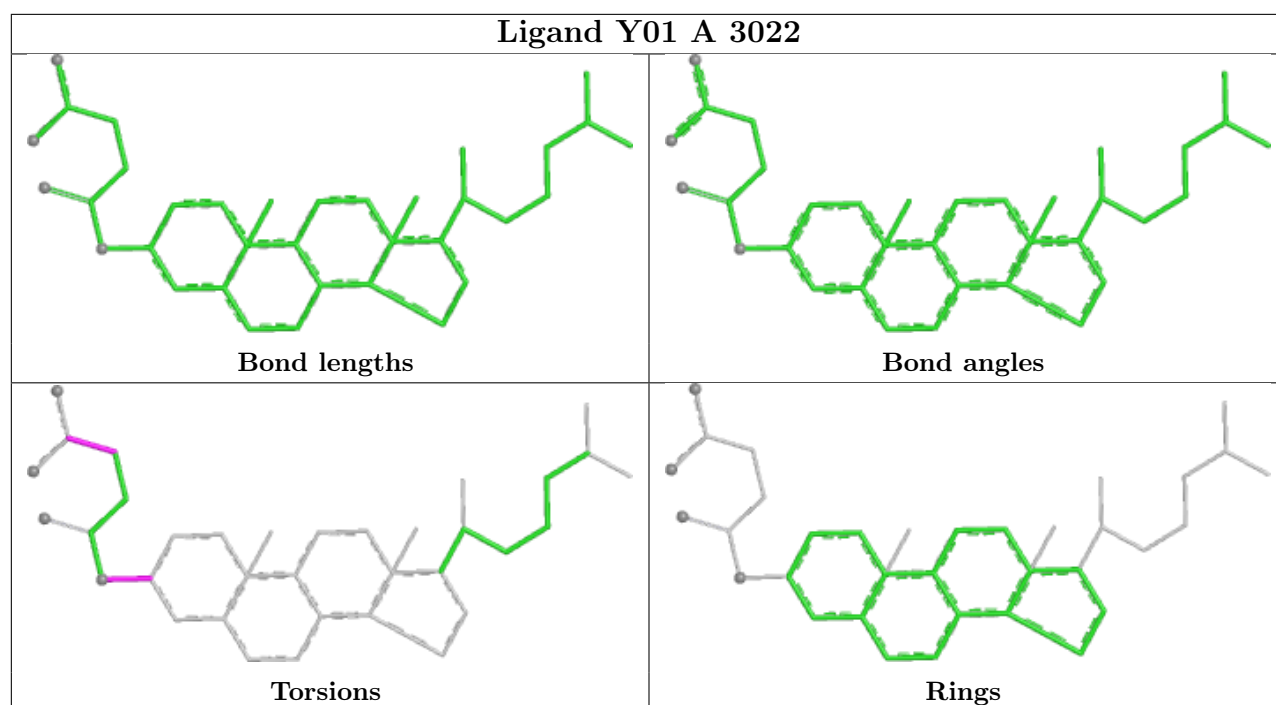


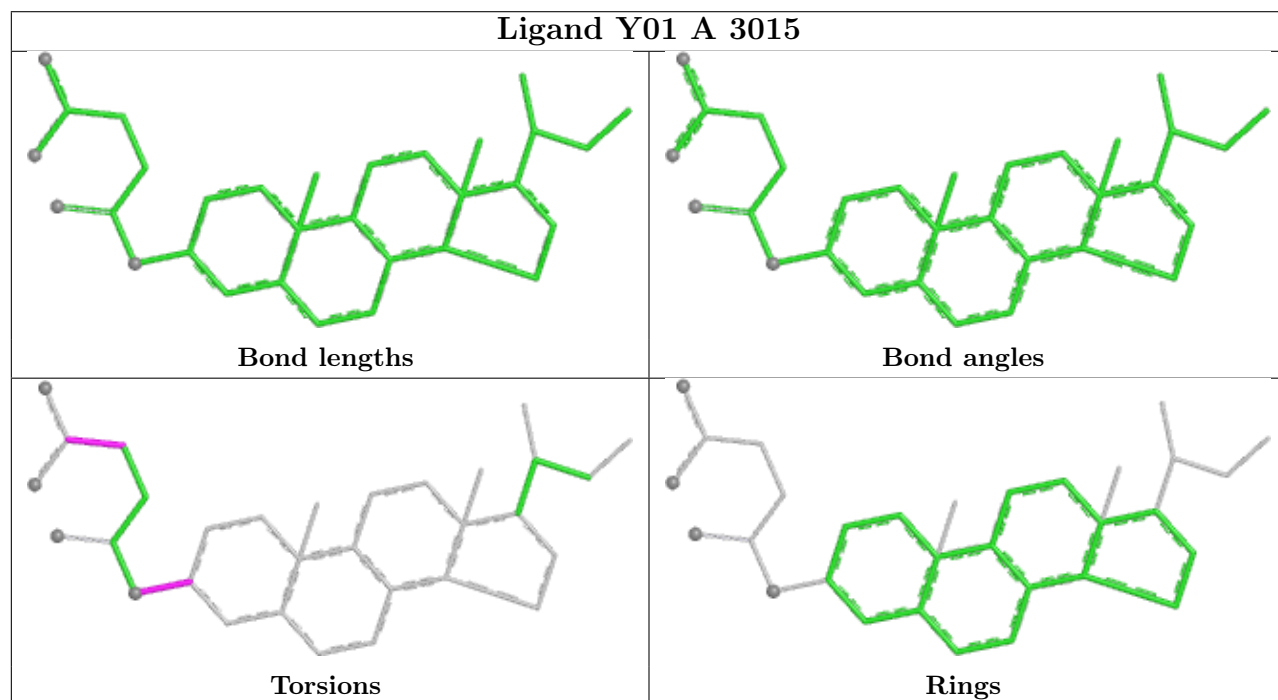
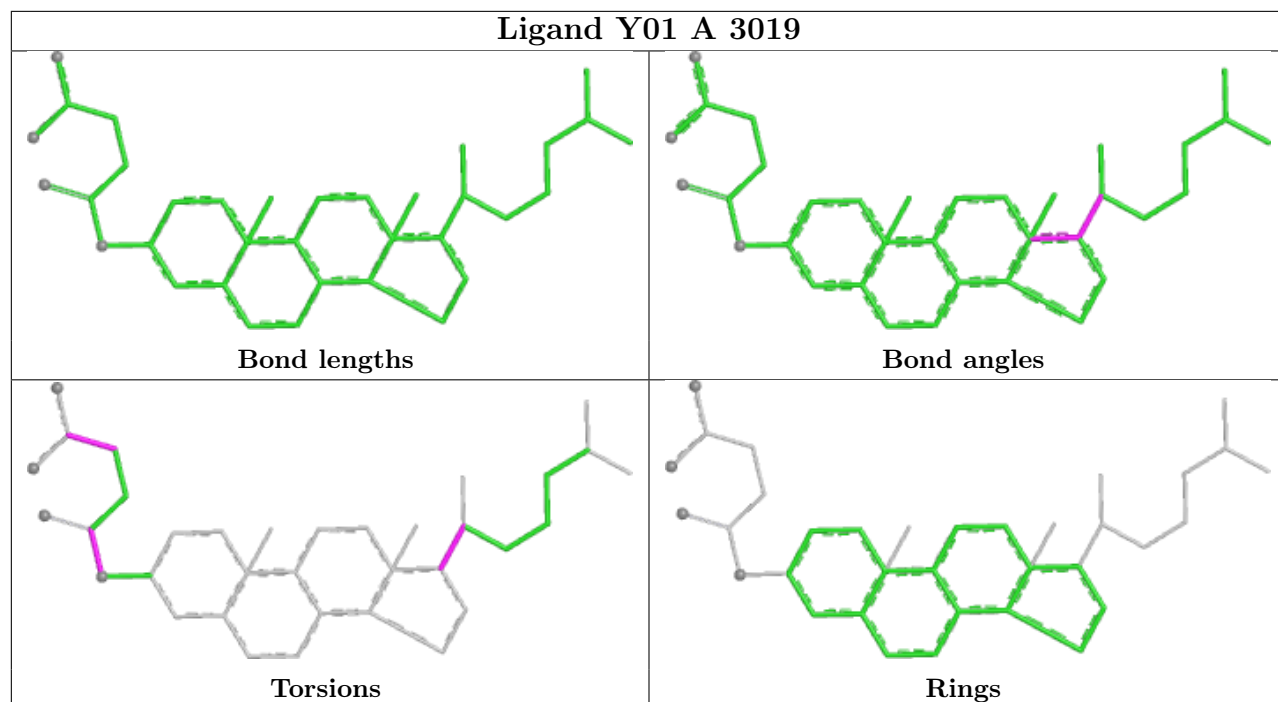
Ligand Y01 A 3024

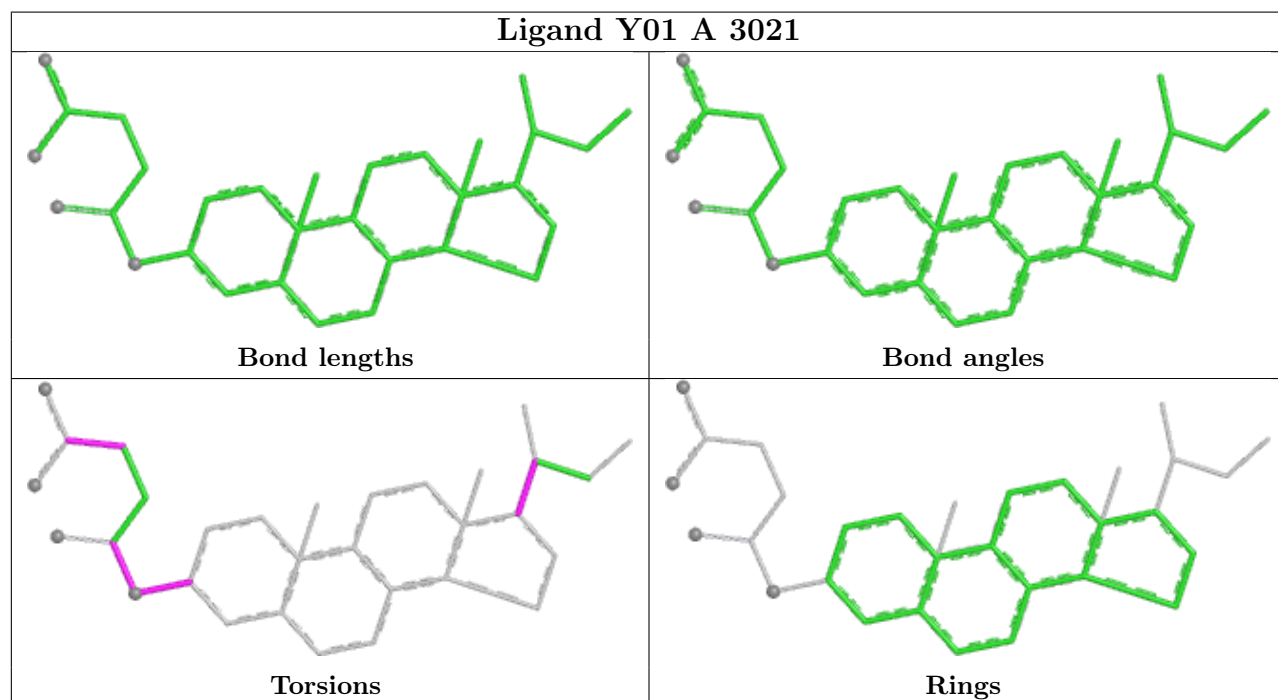
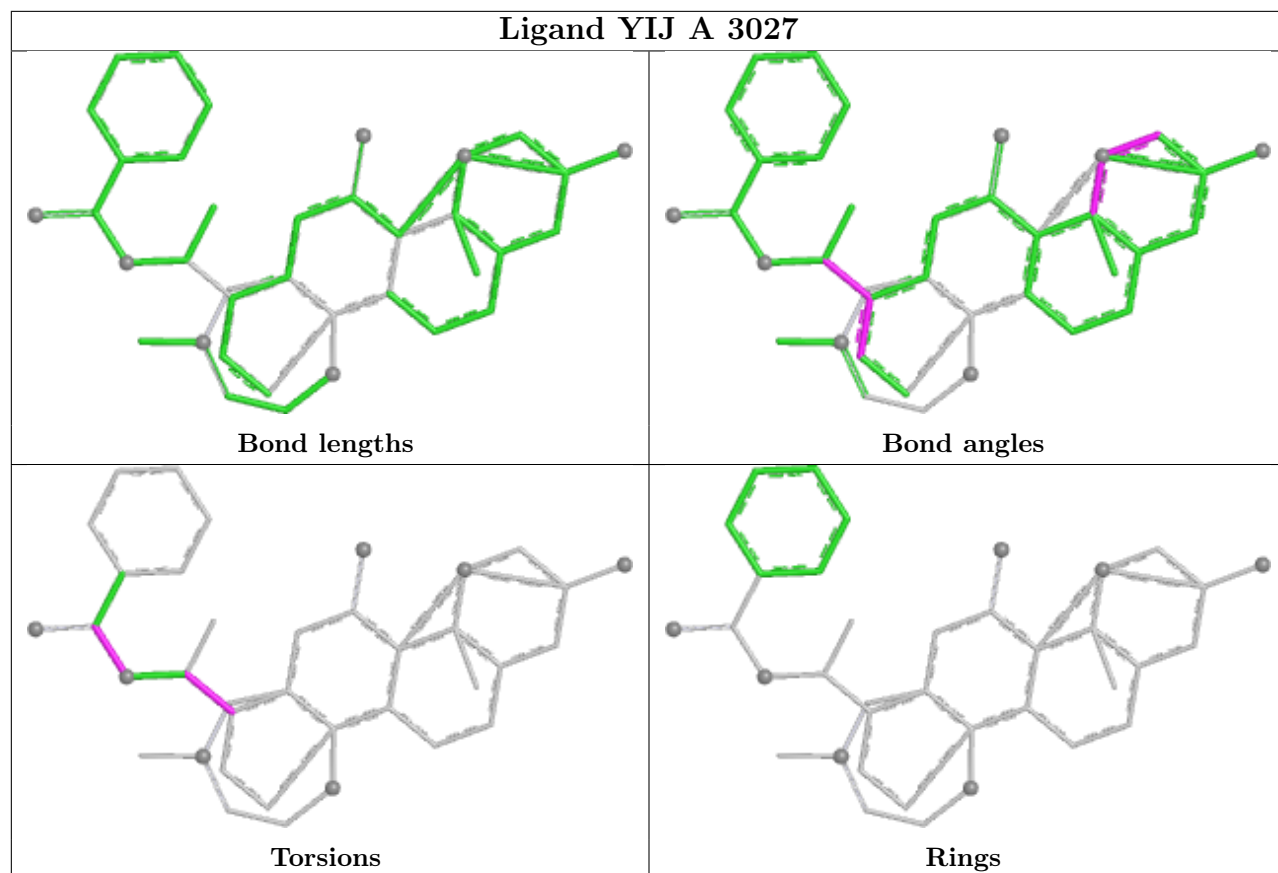


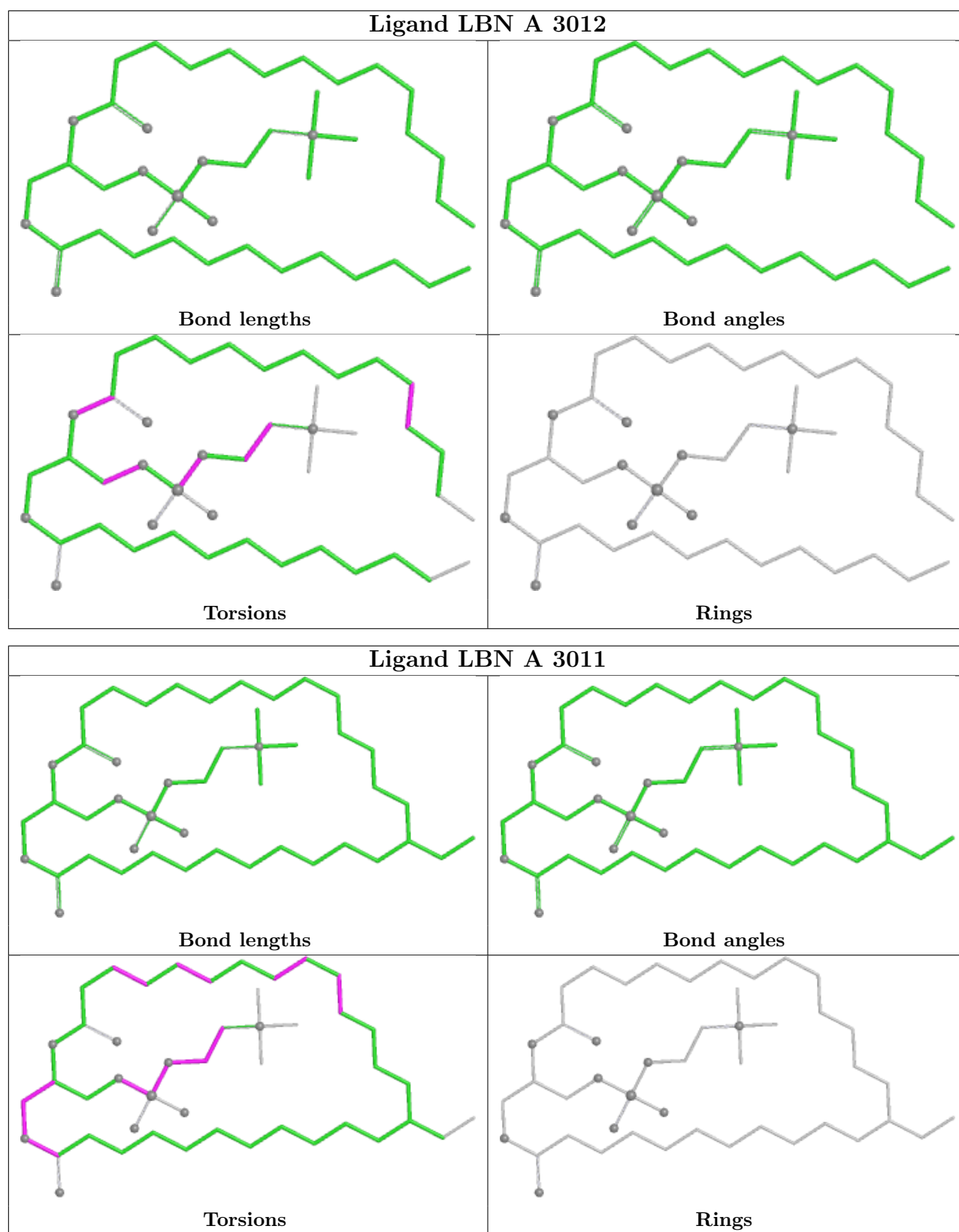












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

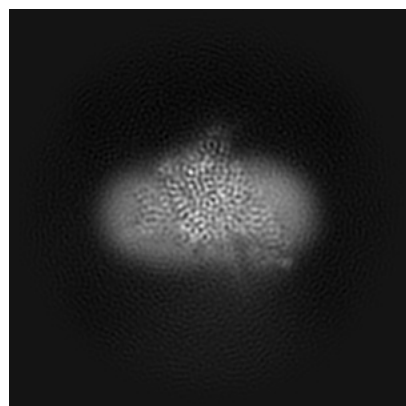
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41071. These allow visual inspection of the internal detail of the map and identification of artifacts.

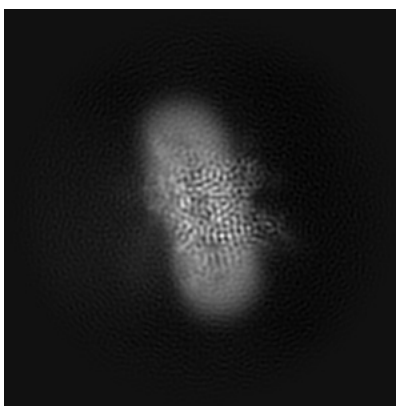
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

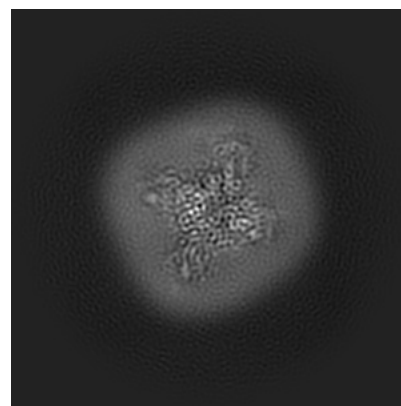
6.1.1 Primary map



X

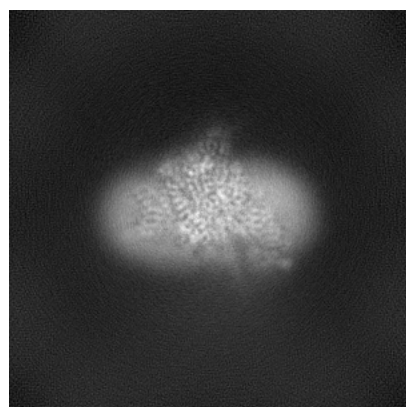


Y

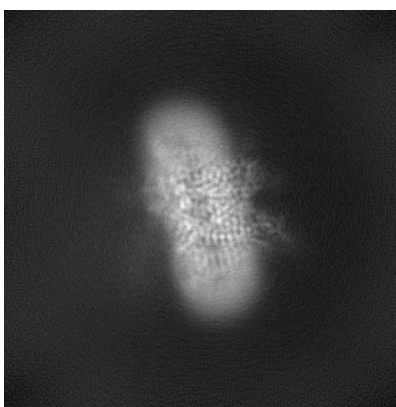


Z

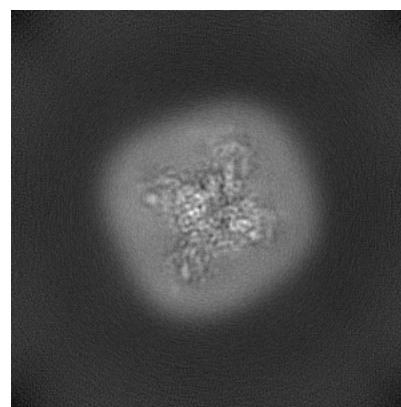
6.1.2 Raw map



X



Y

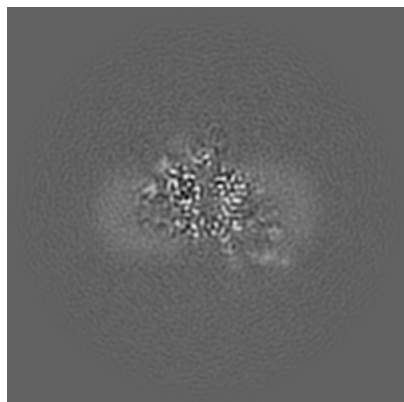


Z

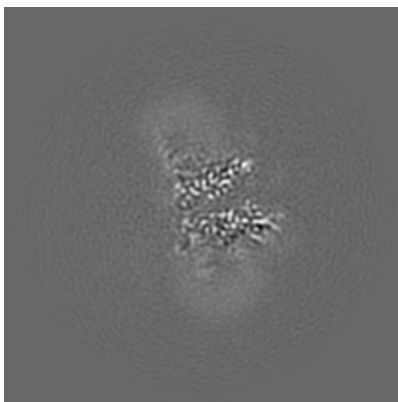
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

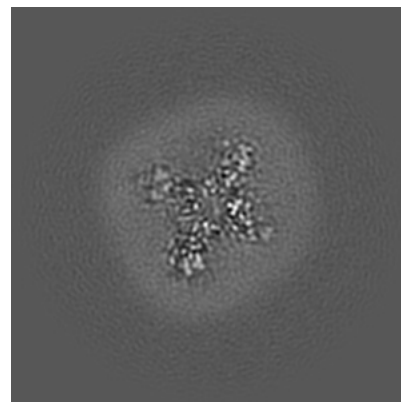
6.2.1 Primary map



X Index: 160

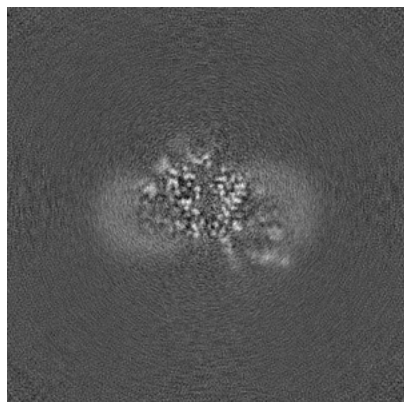


Y Index: 160

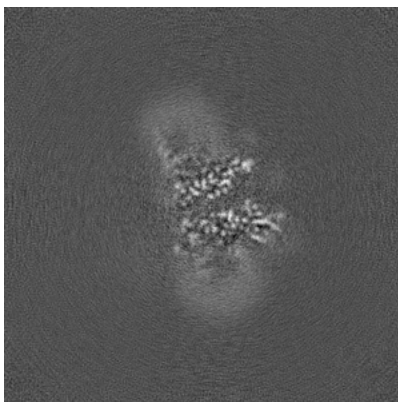


Z Index: 160

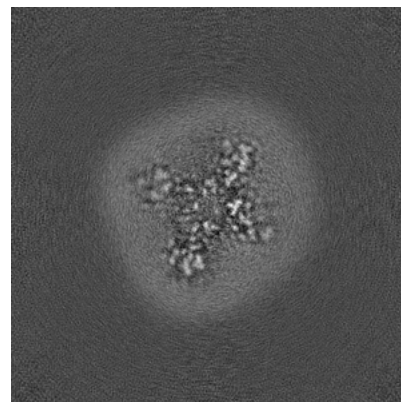
6.2.2 Raw map



X Index: 160



Y Index: 160

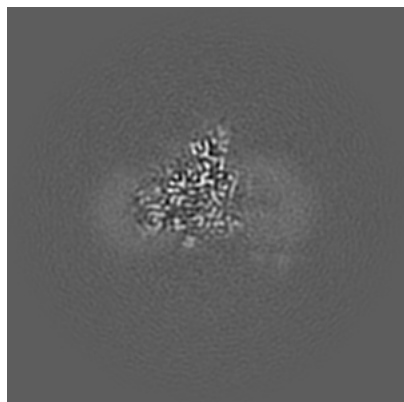


Z Index: 160

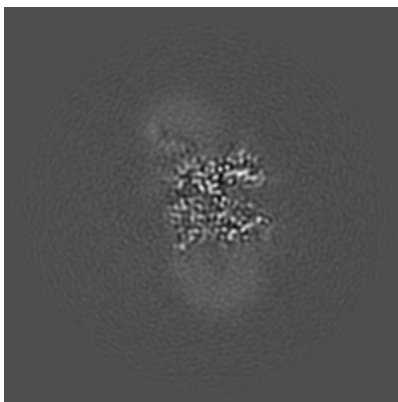
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

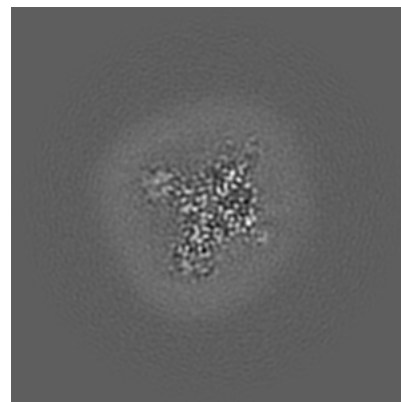
6.3.1 Primary map



X Index: 149

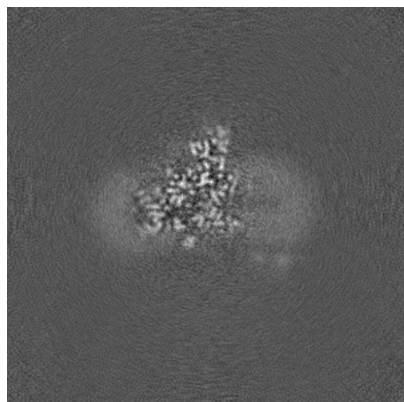


Y Index: 150

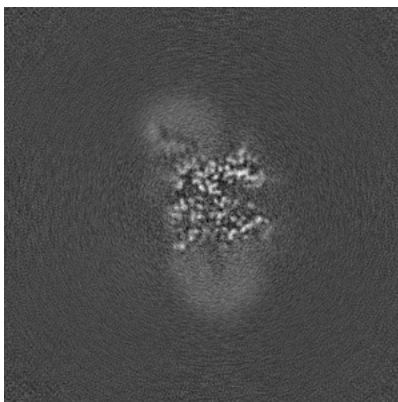


Z Index: 167

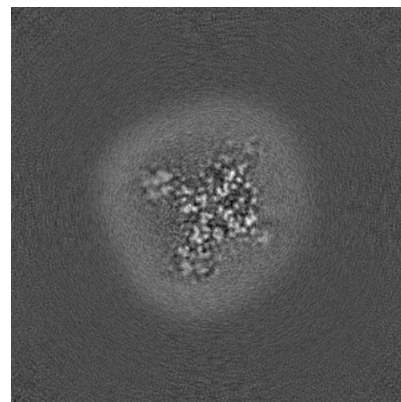
6.3.2 Raw map



X Index: 149



Y Index: 150

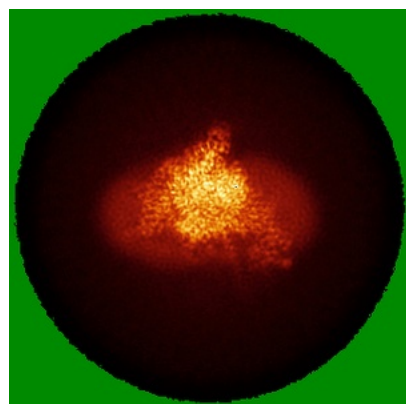


Z Index: 167

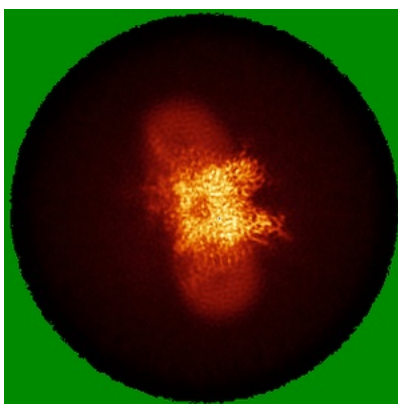
The images above show the largest variance slices of the map in three orthogonal directions.

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

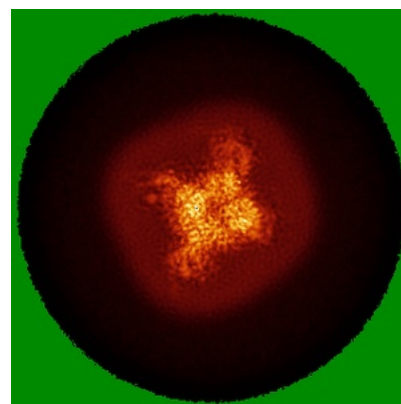
6.4.1 Primary map



X

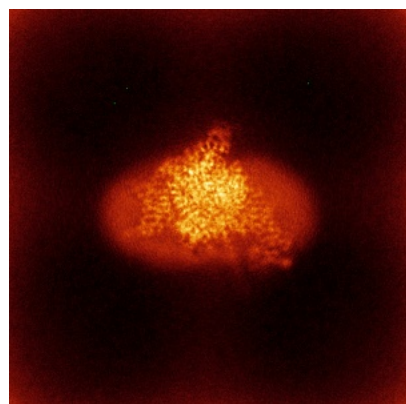


Y

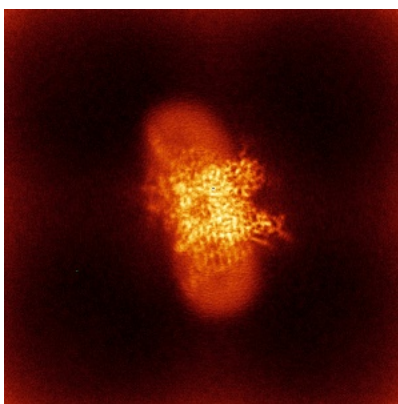


Z

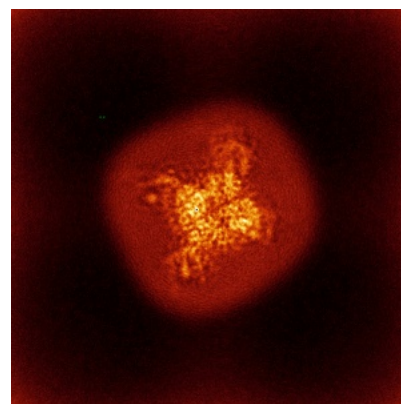
6.4.2 Raw map



X



Y

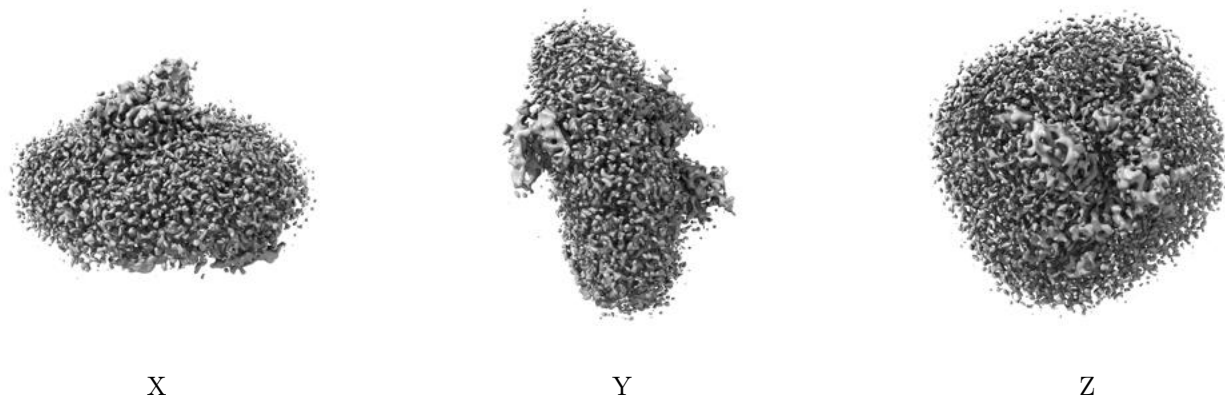


Z

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.

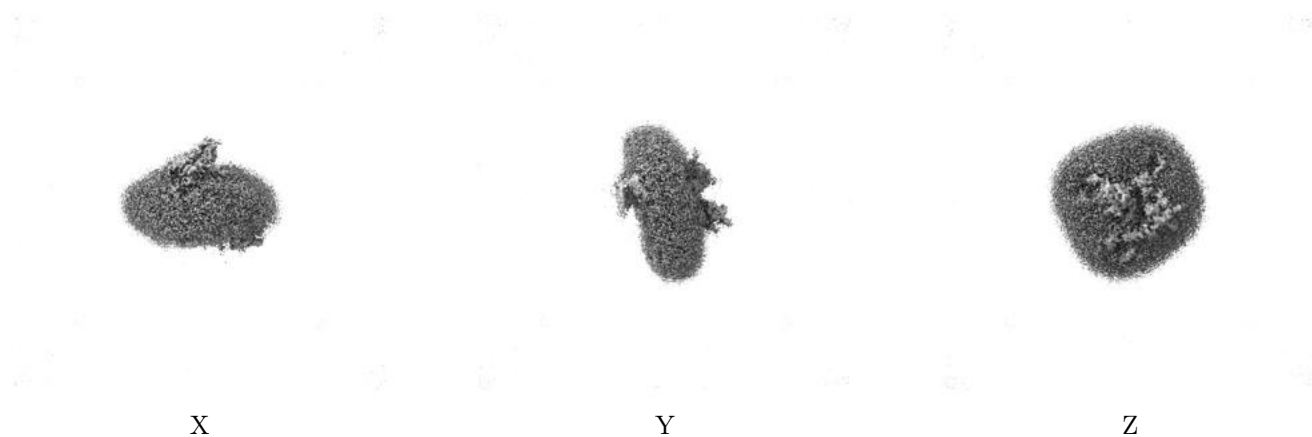
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

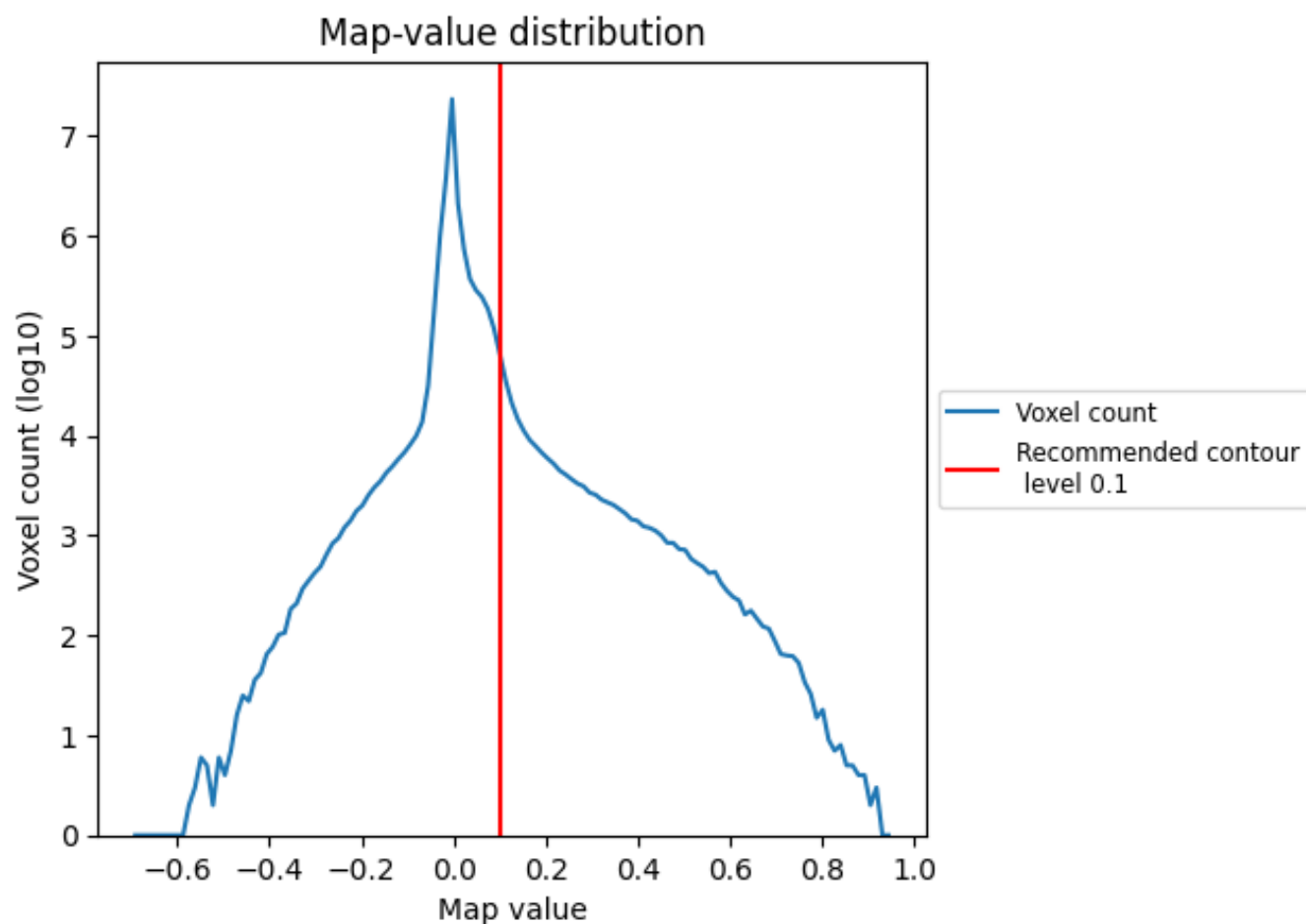
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

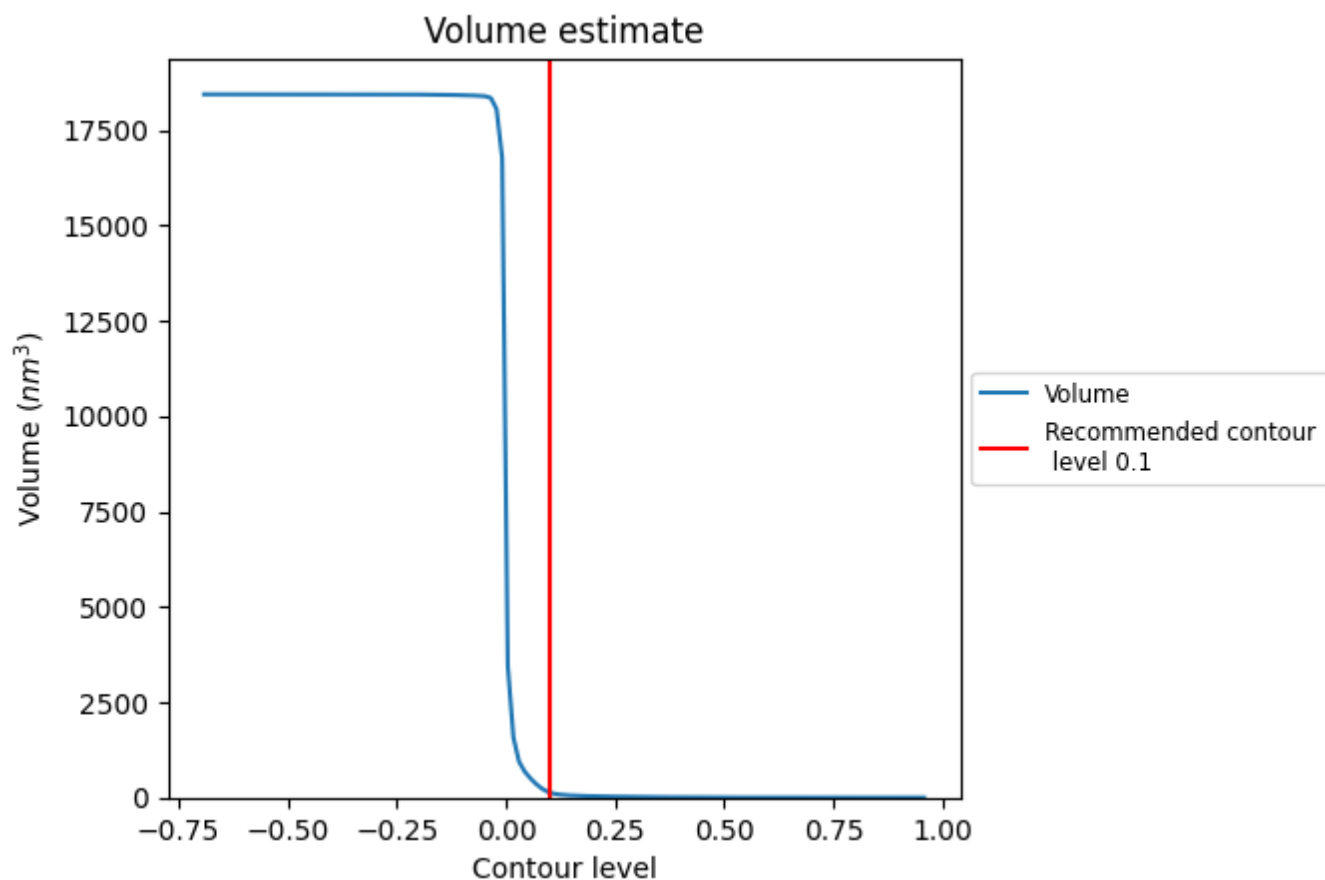
This section contains the results of statistical analysis of the map.

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.

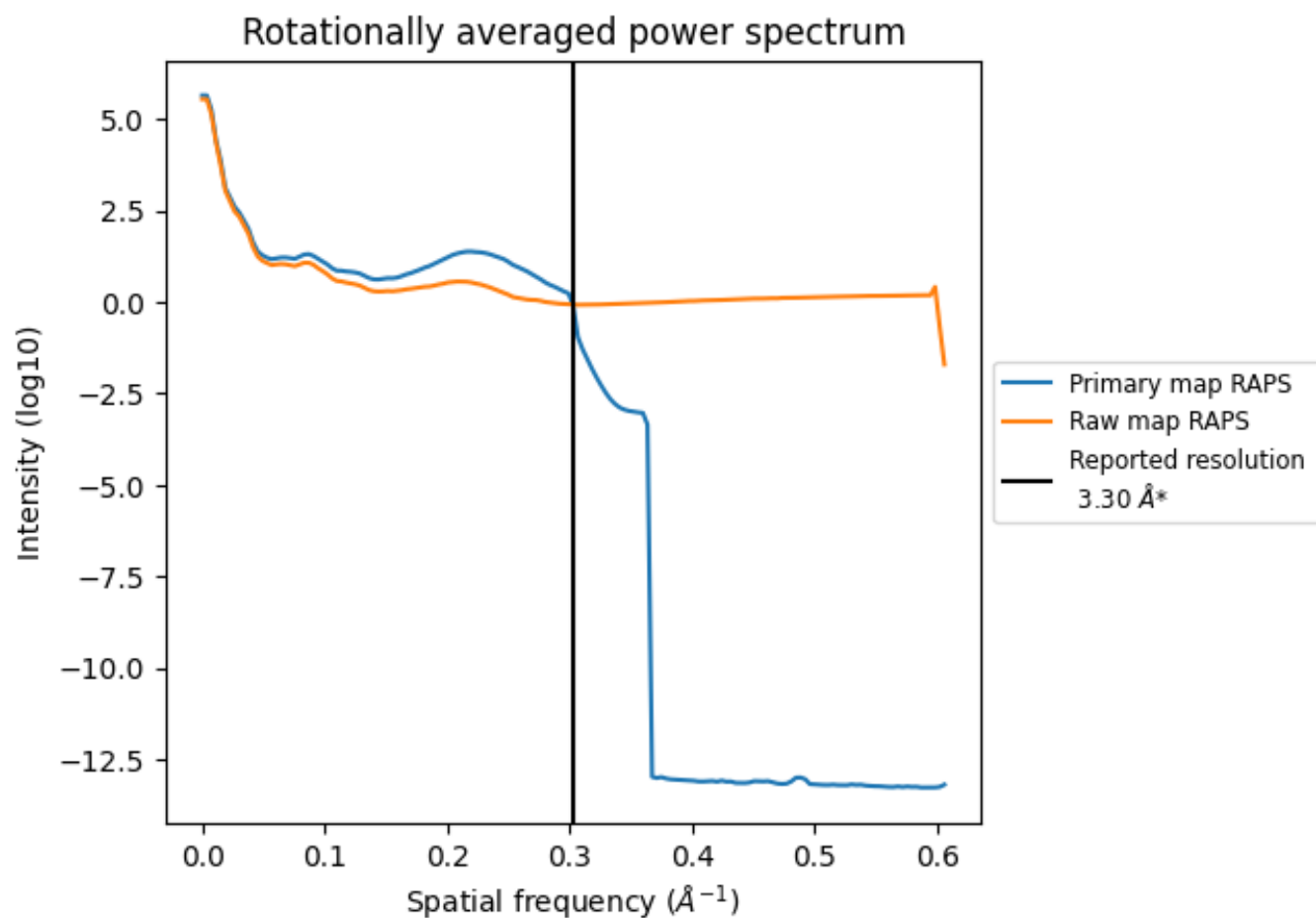
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

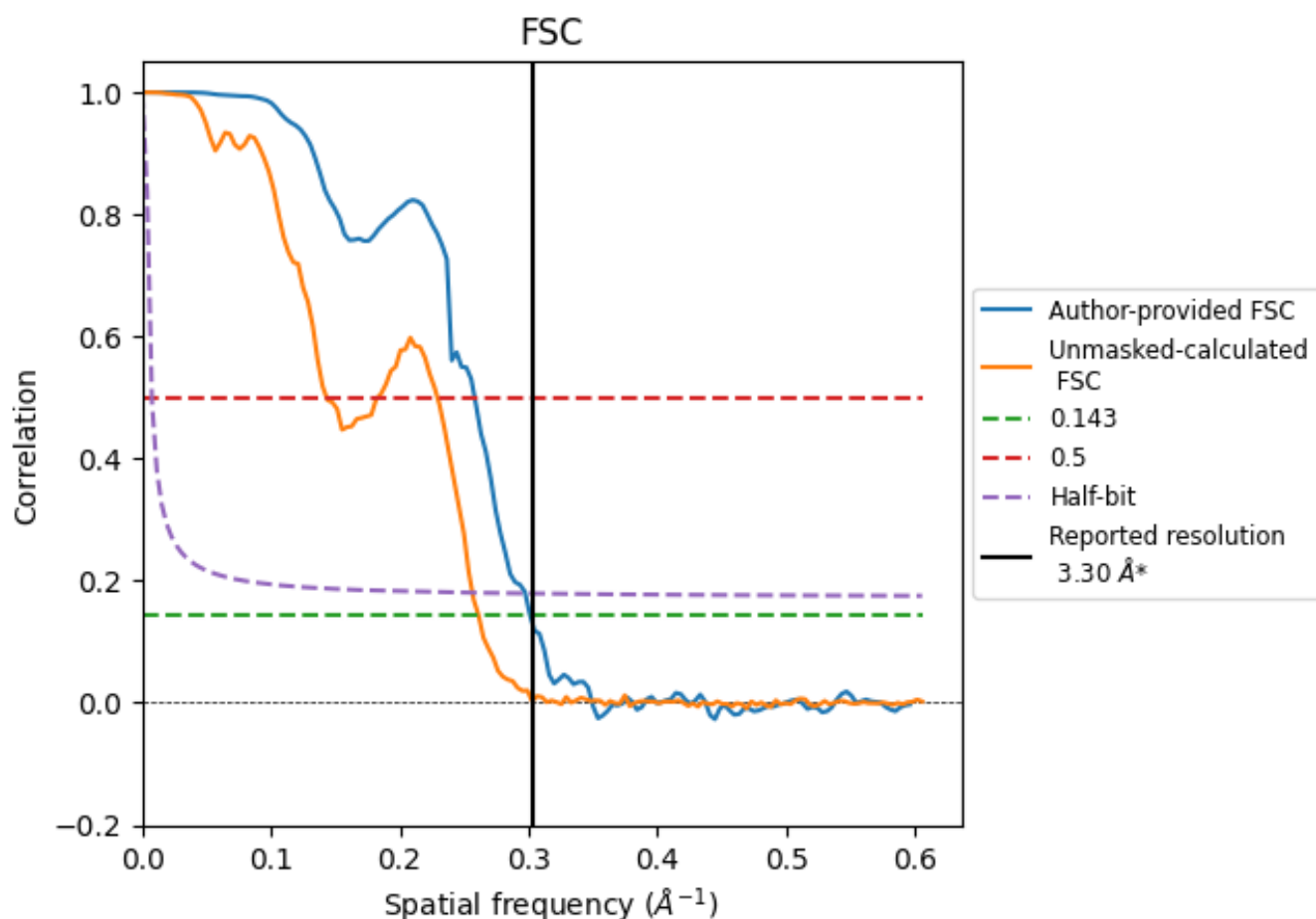


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

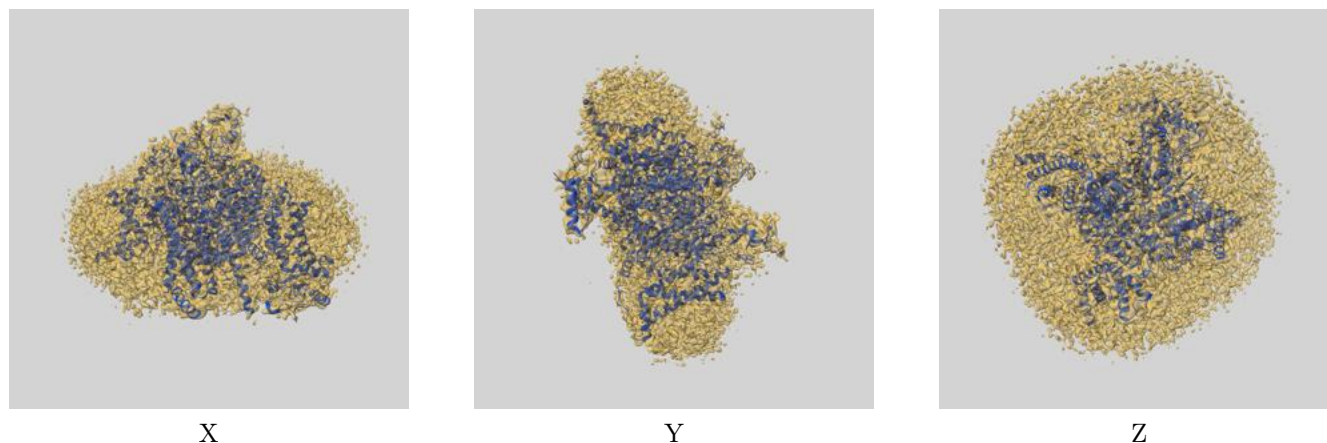
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.87	3.36
Unmasked-calculated*	3.83	6.98	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

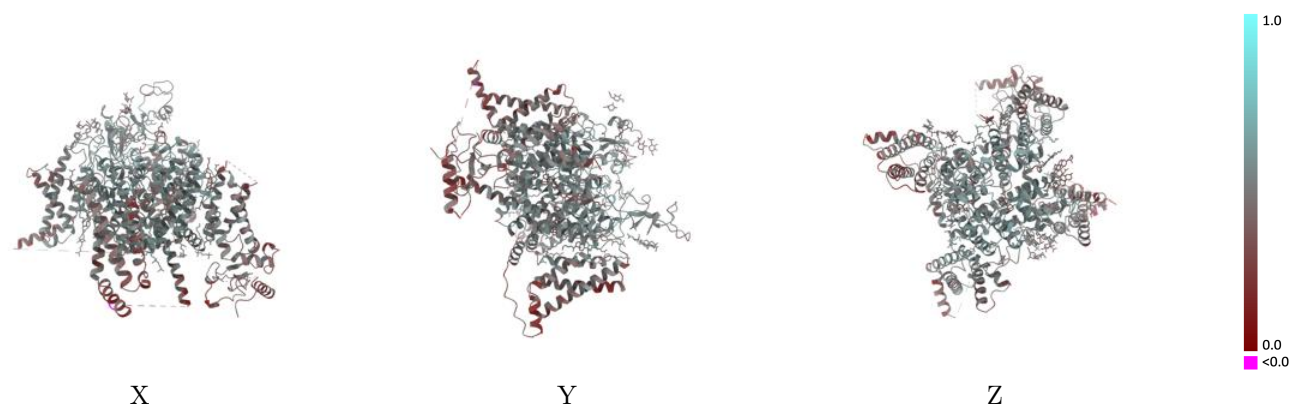
This section contains information regarding the fit between EMDB map EMD-41071 and PDB model 8T6L. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



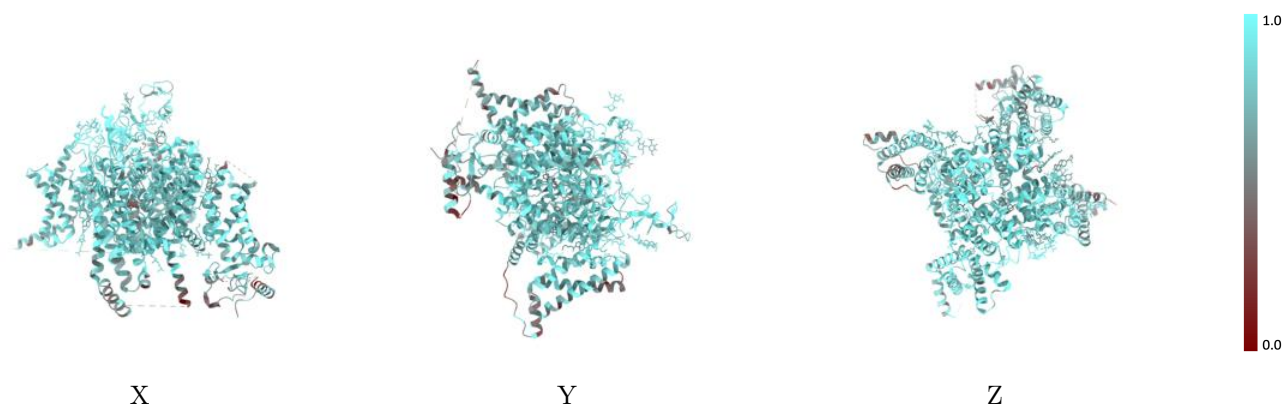
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



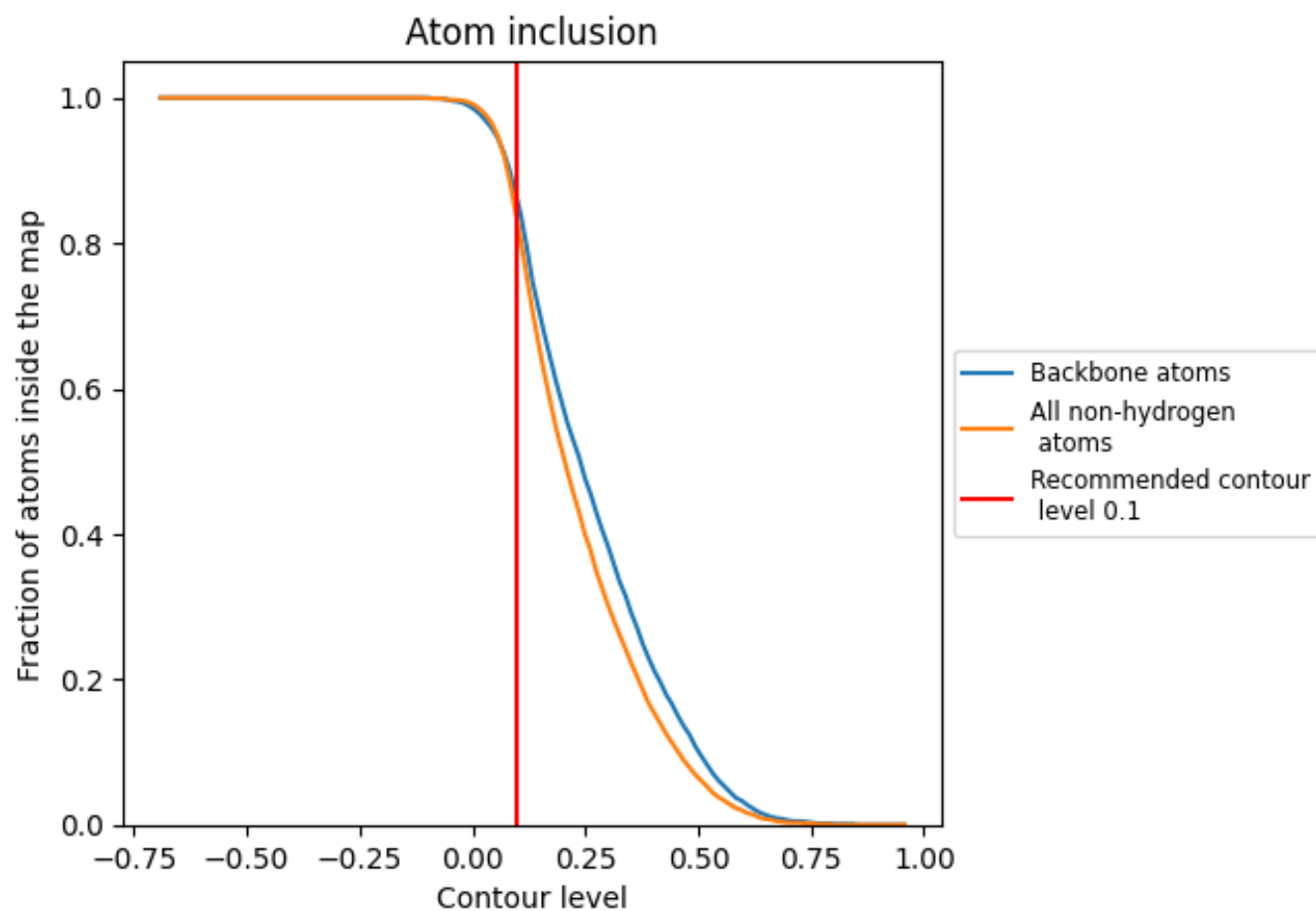
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.4690
A	0.8280	0.4690
B	0.8600	0.4710
C	0.6790	0.3980
D	0.8210	0.4220
E	0.8690	0.4490

