



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 02:11 AM EST

PDB ID : 6UZ0  
EMDB ID : EMD-20949  
Title : Cardiac sodium channel with flecainide  
Authors : Jiang, D.; Shi, H.; Tonggu, L.; Lenaeus, M.J.; Zheng, N.; Catterall, W.A.  
Deposited on : 2019-11-14  
Resolution : 3.24 Å(reported)  
Based on initial model : 6AGF

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

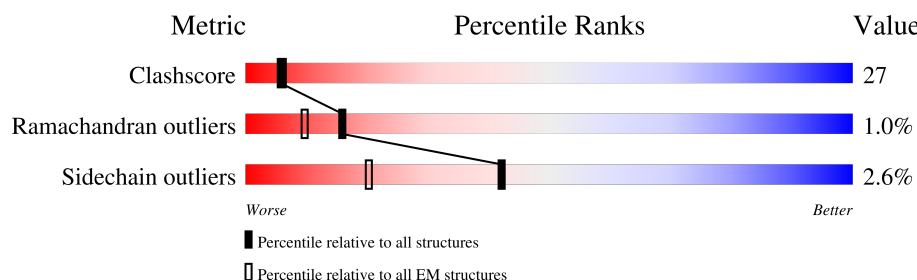
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1838	
2	B	2	
2	D	2	
3	C	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	C	3	X	-	-	-
4	NAG	A	3009	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9557 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	1138	Total	C	N	O	S	0	0
			8970	5942	1426	1534	68		

There are 342 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	THR	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	SER	deletion	UNP P15389
A	?	-	ILE	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	PRO	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	THR	deletion	UNP P15389
A	?	-	SER	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	MET	deletion	UNP P15389
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
A	?	-	GLU	deletion	UNP P15389
A	?	-	GLU	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P15389
A	?	-	GLY	deletion	UNP P15389
A	?	-	SER	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
A	?	-	GLU	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	THR	deletion	UNP P15389
A	?	-	ALA	deletion	UNP P15389

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1899	GLU	-	linker	UNP P15389
A	1900	VAL	-	linker	UNP P15389
A	1901	LEU	-	linker	UNP P15389

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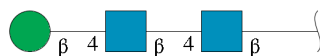
Chain	Residue	Modelled	Actual	Comment	Reference
A	1902	PHE	-	linker	UNP P15389
A	1903	GLN	-	linker	UNP P15389
A	1904	GLY	-	linker	UNP P15389
A	1905	PRO	-	linker	UNP P15389
A	1906	GLY	-	linker	UNP P15389
A	1907	SER	-	linker	UNP P15389
A	1908	MET	-	linker	UNP P15389
A	1909	VAL	-	linker	UNP P15389
A	1972	LEU	PHE	conflict	UNP P42212
A	1973	THR	SER	conflict	UNP P42212
A	2139	LEU	HIS	conflict	UNP P42212
A	2147	GLY	-	expression tag	UNP P42212
A	2148	SER	-	expression tag	UNP P42212
A	2149	ASP	-	expression tag	UNP P42212
A	2150	TYR	-	expression tag	UNP P42212
A	2151	LYS	-	expression tag	UNP P42212
A	2152	ASP	-	expression tag	UNP P42212
A	2153	ASP	-	expression tag	UNP P42212
A	2154	ASP	-	expression tag	UNP P42212
A	2155	ASP	-	expression tag	UNP P42212
A	2156	LYS	-	expression tag	UNP P42212

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	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	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

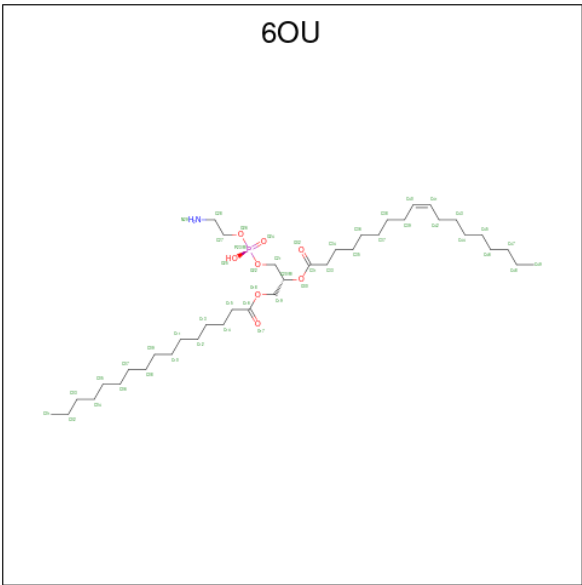


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula:  $C_{34}H_{56}O_5$ ).

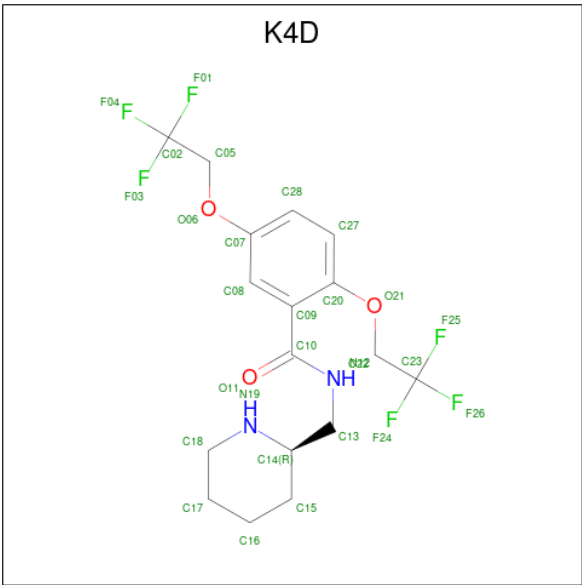


- Molecule 6 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
6	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
6	A	1	Total	C	O			0
			15	12	3			
6	A	1	Total	C	O			0
			26	21	5			
6	A	1	Total	C	O			0
			29	25	4			
6	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
6	A	1	Total	C	N	O	P	0
			26	16	1	8	1	
6	A	1	Total	C	O			0
			27	23	4			
6	A	1	Total	C	O	P		0
			25	16	8	1		
6	A	1	Total	C	O			0
			17	15	2			
6	A	1	Total	C	O			0
			15	13	2			

- Molecule 7 is Flecainide (three-letter code: K4D) (formula: C<sub>17</sub>H<sub>20</sub>F<sub>6</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



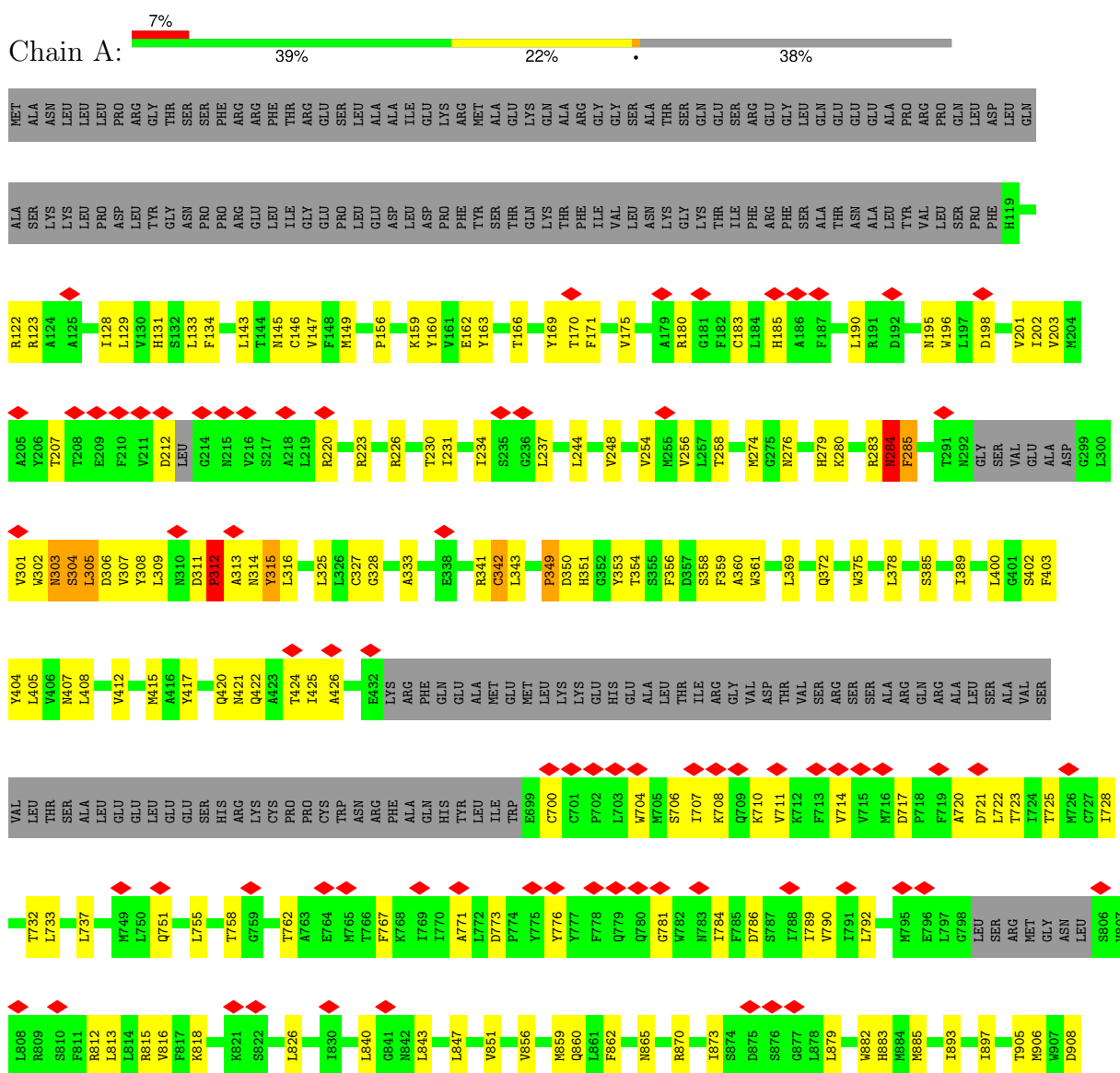
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			28	17	6	2	3	



### 3 Residue-property plots [i](#)

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

- Molecule 1: Sodium channel protein type 5 subunit alpha, Green fluorescent protein






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

Chain B:  50% 50%

MAG1  
MAG2

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

Chain D:  100%

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

Chain C:  100%

MAG1  
MAG2  
BMA3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	513604	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)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.962	Depositor
Minimum map value	-29.432	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.805	Depositor
Recommended contour level	5	Depositor
Map size (Å)	270.336, 270.336, 270.336	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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: 6OU, NAG, BMA, 9Z9, K4D

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	0.40	0/9188	0.55	2/12485 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1373	LEU	C-N-CD	-15.36	86.82	120.60
1	A	312	PRO	N-CA-C	5.06	125.25	112.10

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	8970	0	8990	471	0
2	B	28	0	25	1	0
2	D	28	0	25	1	0
3	C	39	0	34	4	0
4	A	28	0	26	14	0
5	A	146	0	0	22	0
6	A	290	0	0	0	0
7	A	28	0	0	3	0
All	All	9557	0	9100	494	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 27.

All (494) 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:840:LEU:CD1	1:A:940:LEU:HD12	1.24	1.66
5:A:3010:9Z9:C11	5:A:3010:9Z9:C08	1.74	1.65
5:A:3014:9Z9:C08	5:A:3014:9Z9:C11	1.75	1.58
1:A:284:ASN:HD21	4:A:3009:NAG:C1	0.95	1.55
5:A:3011:9Z9:C04	5:A:3011:9Z9:C05	1.77	1.51
5:A:3013:9Z9:C04	5:A:3013:9Z9:C05	1.78	1.50
5:A:3012:9Z9:C04	5:A:3012:9Z9:C05	1.77	1.48
1:A:302:TRP:HB3	1:A:307:VAL:CB	1.41	1.48
1:A:1734:LEU:CD2	1:A:1735:PRO:HD2	1.44	1.48
1:A:840:LEU:CD1	1:A:940:LEU:CD1	1.90	1.46
1:A:284:ASN:CG	4:A:3009:NAG:C8	1.79	1.46
5:A:3014:9Z9:C05	5:A:3014:9Z9:C04	1.77	1.46
5:A:3010:9Z9:C04	5:A:3010:9Z9:C05	1.77	1.44
1:A:1377:TYR:CB	1:A:1441:GLN:NE2	1.79	1.44
1:A:284:ASN:ND2	4:A:3009:NAG:C1	1.76	1.44
1:A:840:LEU:HD12	1:A:940:LEU:CD1	1.43	1.42
1:A:284:ASN:CG	4:A:3009:NAG:H83	1.31	1.42
1:A:1364:ARG:HH11	1:A:1429:ALA:CB	1.33	1.40
1:A:303:ASN:ND2	1:A:306:ASP:HB3	1.36	1.36
1:A:1580:LYS:CB	1:A:1588:TYR:HE1	1.39	1.36
1:A:1734:LEU:HD22	1:A:1735:PRO:CD	1.56	1.35
1:A:1343:CYS:SG	1:A:1467:PHE:HE1	1.53	1.32
1:A:1364:ARG:NH1	1:A:1429:ALA:HB2	1.50	1.25
1:A:1580:LYS:CB	1:A:1588:TYR:CE1	2.19	1.25
1:A:420:GLN:O	1:A:424:THR:CG2	1.86	1.23
1:A:303:ASN:ND2	1:A:306:ASP:CB	2.05	1.20
1:A:1448:MET:HE3	5:A:3014:9Z9:C09	1.72	1.19
1:A:302:TRP:CB	1:A:307:VAL:CB	2.21	1.18
1:A:1365:CYS:HB2	1:A:1397:TRP:CD1	1.79	1.17
1:A:284:ASN:OD1	4:A:3009:NAG:C7	1.92	1.15
1:A:1364:ARG:NH1	1:A:1429:ALA:CB	2.04	1.14
1:A:1448:MET:CE	5:A:3014:9Z9:C09	2.26	1.14
1:A:840:LEU:HD13	1:A:940:LEU:CD1	1.76	1.12
1:A:302:TRP:CE3	1:A:308:TYR:HE1	1.70	1.09
1:A:1339:VAL:HG11	1:A:1470:VAL:HG11	1.32	1.09
1:A:284:ASN:OD1	4:A:3009:NAG:H81	1.33	1.08
1:A:420:GLN:O	1:A:424:THR:HG23	0.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1746:SER:HB3	1:A:1749:VAL:HG12	1.41	1.01
1:A:303:ASN:HD22	1:A:306:ASP:CB	1.70	1.00
1:A:1364:ARG:HH11	1:A:1429:ALA:HB1	1.25	1.00
1:A:1490:THR:HG22	1:A:1491:GLU:H	1.22	1.00
1:A:1380:VAL:O	1:A:1439:GLN:HG3	1.62	0.99
1:A:302:TRP:CZ3	1:A:308:TYR:HE1	1.83	0.96
1:A:870:ARG:HD3	1:A:879:LEU:HD23	1.48	0.95
1:A:283:ARG:O	1:A:284:ASN:O	1.85	0.94
1:A:1423:TRP:HZ3	1:A:1456:ILE:CD1	1.81	0.94
1:A:302:TRP:CZ3	1:A:308:TYR:CE1	2.56	0.93
1:A:1466:LEU:O	1:A:1470:VAL:HG12	1.68	0.93
1:A:840:LEU:HD13	1:A:940:LEU:HD13	1.50	0.93
1:A:1365:CYS:HB2	1:A:1397:TRP:HD1	1.18	0.92
1:A:1365:CYS:HG	1:A:1386:CYS:CB	1.82	0.92
1:A:1377:TYR:CB	1:A:1441:GLN:HE21	1.75	0.92
1:A:1364:ARG:HH21	1:A:1364:ARG:HG2	1.33	0.91
1:A:1423:TRP:CZ3	1:A:1456:ILE:CD1	2.52	0.91
1:A:303:ASN:HD22	1:A:306:ASP:HB3	0.96	0.91
1:A:420:GLN:C	1:A:424:THR:HG23	1.89	0.91
1:A:1377:TYR:CB	1:A:1441:GLN:HE22	1.60	0.91
1:A:840:LEU:HD11	1:A:940:LEU:HD12	1.49	0.91
1:A:1381:ASN:OD1	1:A:1434:ARG:NH2	2.05	0.89
1:A:284:ASN:OD1	4:A:3009:NAG:C8	0.58	0.88
1:A:1490:THR:HG22	1:A:1491:GLU:N	1.87	0.88
1:A:1683:TYR:CG	1:A:1736:ASN:ND2	2.41	0.88
1:A:1448:MET:HE1	5:A:3014:9Z9:C10	2.04	0.88
1:A:1464:LEU:O	1:A:1468:ILE:HG12	1.72	0.88
1:A:1768:MET:O	1:A:1772:ILE:HG12	1.73	0.87
1:A:1448:MET:O	1:A:1450:ILE:N	2.07	0.87
1:A:1448:MET:CE	5:A:3014:9Z9:C10	2.53	0.87
1:A:840:LEU:HD12	1:A:940:LEU:HD11	1.52	0.86
1:A:1278:PHE:CE1	1:A:1282:ASP:OD2	2.29	0.86
1:A:341:ARG:NH2	3:C:2:NAG:O7	2.09	0.86
1:A:1423:TRP:CZ3	1:A:1456:ILE:HD11	2.11	0.86
1:A:1448:MET:HE1	5:A:3014:9Z9:C09	2.03	0.85
1:A:302:TRP:CE3	1:A:308:TYR:CE1	2.62	0.85
1:A:1683:TYR:CD1	1:A:1736:ASN:ND2	2.43	0.85
1:A:303:ASN:HD21	1:A:306:ASP:CB	1.87	0.84
1:A:1365:CYS:HA	1:A:1397:TRP:HA	1.59	0.83
1:A:305:LEU:HD12	1:A:305:LEU:O	1.79	0.83
1:A:284:ASN:CG	4:A:3009:NAG:C1	2.47	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HG23	1:A:175:VAL:HG11	1.61	0.82
1:A:1316:LEU:HD23	1:A:1326:VAL:HG21	1.61	0.82
1:A:284:ASN:OD1	4:A:3009:NAG:H82	1.01	0.82
1:A:840:LEU:HD12	1:A:940:LEU:HD12	0.83	0.82
1:A:180:ARG:HB3	1:A:185:HIS:CB	2.10	0.81
1:A:1373:LEU:HB3	1:A:1374:PRO:HD3	1.61	0.80
1:A:1220:SER:HB2	1:A:1311:ARG:HD3	1.63	0.80
1:A:302:TRP:CG	1:A:307:VAL:CB	2.64	0.80
1:A:1448:MET:O	1:A:1451:TYR:N	2.14	0.80
1:A:284:ASN:CG	4:A:3009:NAG:H82	1.67	0.79
1:A:1424:MET:HA	1:A:1424:MET:CE	2.12	0.79
1:A:882:TRP:HE1	1:A:1428:TYR:HH	1.28	0.78
1:A:303:ASN:HD21	1:A:306:ASP:CG	1.86	0.78
1:A:1766:VAL:O	1:A:1770:ILE:HG22	1.84	0.77
1:A:1365:CYS:SG	1:A:1386:CYS:CB	2.72	0.77
5:A:3010:9Z9:C08	5:A:3010:9Z9:C12	2.63	0.76
1:A:128:ILE:HG23	1:A:175:VAL:CG1	2.16	0.76
1:A:1362:PHE:O	1:A:1364:ARG:HD2	1.85	0.76
1:A:1374:PRO:HG3	1:A:1439:GLN:OE1	1.84	0.76
1:A:1490:THR:CG2	1:A:1491:GLU:H	1.96	0.75
1:A:725:THR:HA	1:A:728:ILE:HD12	1.67	0.75
1:A:1577:CYS:HA	1:A:1588:TYR:OH	1.86	0.75
1:A:309:LEU:O	1:A:309:LEU:HD23	1.86	0.74
1:A:122:ARG:CZ	1:A:180:ARG:O	2.34	0.74
1:A:1365:CYS:CB	1:A:1397:TRP:HD1	1.98	0.74
1:A:1578:ILE:HA	1:A:1581:MET:HE2	1.69	0.73
1:A:870:ARG:CD	1:A:879:LEU:HD23	2.19	0.73
1:A:1373:LEU:HB3	1:A:1374:PRO:CD	2.17	0.73
1:A:1580:LYS:CB	1:A:1588:TYR:CZ	2.72	0.73
1:A:1434:ARG:NH1	1:A:1441:GLN:OE1	2.22	0.73
1:A:341:ARG:HH21	1:A:343:LEU:HD11	1.55	0.72
1:A:1423:TRP:CE3	1:A:1456:ILE:HD11	2.25	0.71
5:A:3010:9Z9:C11	5:A:3010:9Z9:C09	2.68	0.71
1:A:1448:MET:O	1:A:1449:TYR:C	2.27	0.71
1:A:1767:ASN:O	1:A:1770:ILE:HG23	1.90	0.71
5:A:3014:9Z9:C08	5:A:3014:9Z9:C12	2.68	0.71
1:A:1517:ASN:HB3	1:A:1520:GLN:HB2	1.73	0.71
1:A:1364:ARG:HD2	1:A:1364:ARG:N	2.06	0.70
1:A:1373:LEU:HD22	1:A:1373:LEU:H	1.55	0.70
1:A:128:ILE:CG2	1:A:175:VAL:HG13	2.22	0.70
1:A:1543:ASN:HD21	1:A:1634:ARG:HH11	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ARG:NH1	1:A:1429:ALA:CA	2.54	0.70
1:A:1366:ILE:HG22	1:A:1373:LEU:HA	1.72	0.69
5:A:3010:9Z9:C08	5:A:3010:9Z9:C13	2.45	0.69
1:A:1365:CYS:HG	1:A:1386:CYS:HB2	1.56	0.69
1:A:1365:CYS:HB3	1:A:1439:GLN:HE21	1.57	0.69
1:A:1459:GLY:O	1:A:1463:THR:OG1	2.11	0.69
1:A:128:ILE:CG2	1:A:175:VAL:CG1	2.72	0.68
1:A:302:TRP:HZ3	1:A:308:TYR:CE1	2.11	0.68
1:A:1655:SER:HB3	1:A:1775:GLU:HG3	1.76	0.68
1:A:415:MET:CB	1:A:1777:PHE:CZ	2.77	0.68
1:A:1746:SER:HB3	1:A:1749:VAL:CG1	2.21	0.67
1:A:1620:SER:OG	1:A:1623:LEU:HB2	1.95	0.67
1:A:873:ILE:HD11	1:A:908:ASP:HB3	1.75	0.67
1:A:882:TRP:HB3	1:A:893:ILE:HD11	1.77	0.67
1:A:1343:CYS:SG	1:A:1467:PHE:CE1	2.44	0.67
1:A:1768:MET:O	1:A:1772:ILE:CG1	2.41	0.66
1:A:905:THR:HG23	1:A:922:PHE:HE2	1.59	0.66
1:A:1482:LEU:C	1:A:1484:GLY:H	1.99	0.66
1:A:1365:CYS:CB	1:A:1397:TRP:CD1	2.69	0.66
1:A:1423:TRP:CZ3	1:A:1456:ILE:HD13	2.31	0.66
1:A:1373:LEU:HD22	1:A:1373:LEU:N	2.11	0.65
1:A:312:PRO:O	1:A:315:TYR:HB2	1.96	0.65
1:A:732:THR:HG22	1:A:816:VAL:HG22	1.78	0.65
1:A:1217:ILE:HD13	1:A:1314:ARG:HD2	1.77	0.65
1:A:1351:SER:O	1:A:1355:VAL:HG23	1.96	0.65
1:A:244:LEU:HD11	1:A:932:VAL:HG12	1.78	0.65
1:A:1365:CYS:SG	1:A:1386:CYS:HB3	2.37	0.65
1:A:407:ASN:ND2	1:A:1769:TYR:HB2	2.12	0.64
1:A:1234:ARG:HD3	1:A:1237:ILE:HD12	1.79	0.64
1:A:327:CYS:SG	1:A:328:GLY:N	2.70	0.64
1:A:1214:ILE:HD11	1:A:1318:ARG:HB3	1.79	0.64
1:A:1767:ASN:HA	1:A:1770:ILE:CG2	2.27	0.64
1:A:1606:VAL:O	1:A:1610:LEU:HG	1.97	0.63
1:A:1362:PHE:O	1:A:1364:ARG:CD	2.46	0.63
1:A:190:LEU:O	1:A:196:TRP:NE1	2.31	0.63
1:A:1366:ILE:HB	1:A:1372:ASP:O	1.98	0.63
1:A:897:ILE:HG21	1:A:925:VAL:HG13	1.81	0.62
1:A:1221:SER:HB3	1:A:1671:PHE:HE2	1.64	0.62
1:A:1775:GLU:OE2	1:A:1775:GLU:HA	1.99	0.62
1:A:1458:PHE:HA	1:A:1462:PHE:HD2	1.62	0.62
5:A:3014:9Z9:C08	5:A:3014:9Z9:C19	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ARG:HG2	1:A:1364:ARG:NH2	2.10	0.62
1:A:1420:PHE:HZ	7:A:3026:K4D:O06	1.83	0.62
1:A:1607:GLY:HA2	1:A:1627:ILE:HD11	1.82	0.62
1:A:311:ASP:N	1:A:312:PRO:HD2	2.14	0.62
1:A:1554:GLN:HB2	1:A:1558:LYS:HD3	1.81	0.62
1:A:1278:PHE:CZ	1:A:1282:ASP:OD2	2.52	0.62
1:A:122:ARG:NH2	1:A:180:ARG:O	2.33	0.62
1:A:1767:ASN:O	1:A:1770:ILE:CG2	2.47	0.62
1:A:1419:THR:HG21	1:A:1715:TRP:HE1	1.65	0.62
1:A:1310:LEU:HB3	1:A:1313:LEU:HD12	1.82	0.62
1:A:276:ASN:O	1:A:279:HIS:ND1	2.30	0.61
1:A:1698:THR:HG22	1:A:1699:PHE:H	1.66	0.61
1:A:856:VAL:HA	1:A:859:MET:HG2	1.83	0.61
1:A:1373:LEU:H	1:A:1373:LEU:CD2	2.13	0.61
1:A:1365:CYS:HA	1:A:1396:TYR:O	2.00	0.61
1:A:309:LEU:HD23	1:A:309:LEU:C	2.20	0.61
1:A:1373:LEU:CB	1:A:1374:PRO:CD	2.72	0.61
1:A:1779:VAL:O	1:A:1779:VAL:HG12	1.99	0.60
5:A:3014:9Z9:C11	5:A:3014:9Z9:C09	2.76	0.60
1:A:1374:PRO:HG3	1:A:1439:GLN:CD	2.22	0.60
1:A:1580:LYS:CB	1:A:1588:TYR:OH	2.50	0.60
1:A:403:PHE:CZ	1:A:1711:THR:HG22	2.36	0.60
1:A:1365:CYS:HB3	1:A:1439:GLN:NE2	2.17	0.60
1:A:1448:MET:CE	1:A:1448:MET:HA	2.31	0.60
1:A:1683:TYR:CD2	1:A:1736:ASN:ND2	2.64	0.60
1:A:1482:LEU:O	1:A:1484:GLY:N	2.34	0.59
1:A:1364:ARG:HH21	1:A:1364:ARG:CG	2.11	0.59
1:A:1734:LEU:CD2	1:A:1735:PRO:CD	2.38	0.59
1:A:1380:VAL:O	1:A:1380:VAL:HG12	2.01	0.59
1:A:1687:GLU:HB2	1:A:1721:PRO:HB3	1.85	0.59
5:A:3010:9Z9:C08	5:A:3010:9Z9:C19	2.78	0.59
1:A:882:TRP:NE1	1:A:1428:TYR:OH	2.29	0.59
3:C:1:NAG:O7	3:C:1:NAG:O3	2.17	0.59
1:A:1445:ASN:ND2	1:A:1448:MET:SD	2.76	0.58
1:A:145:ASN:HD21	1:A:226:ARG:HH11	1.51	0.58
1:A:201:VAL:HG21	1:A:226:ARG:HG2	1.85	0.58
1:A:862:PHE:HA	1:A:865:ASN:HD22	1.67	0.58
1:A:1364:ARG:HG2	1:A:1373:LEU:CD1	2.33	0.58
1:A:305:LEU:HD12	1:A:305:LEU:C	2.24	0.58
1:A:1364:ARG:NH1	1:A:1429:ALA:HA	2.18	0.58
1:A:1400:VAL:O	1:A:1403:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1751:ILE:O	1:A:1755:THR:OG1	2.18	0.58
1:A:1445:ASN:O	1:A:1448:MET:HG2	2.04	0.58
1:A:1539:LEU:HD23	1:A:1572:ILE:HG21	1.85	0.58
1:A:870:ARG:HD3	1:A:879:LEU:HA	1.83	0.58
1:A:1363:GLY:HA2	1:A:1399:LYS:HA	1.85	0.58
1:A:1365:CYS:SG	1:A:1386:CYS:HB2	2.41	0.58
1:A:1398:THR:OG1	1:A:1729:TYR:OH	2.21	0.58
1:A:254:VAL:HG21	1:A:412:VAL:HG21	1.86	0.58
1:A:302:TRP:HE3	1:A:308:TYR:HE1	1.39	0.58
1:A:1380:VAL:O	1:A:1439:GLN:CG	2.45	0.58
1:A:1489:MET:CE	1:A:1657:PRO:HG2	2.34	0.58
1:A:162:GLU:OE1	1:A:223:ARG:NH1	2.37	0.57
1:A:1332:ALA:CB	1:A:1474:ASN:HD21	2.16	0.57
1:A:1715:TRP:CD2	1:A:1758:ILE:HD11	2.39	0.57
1:A:1727:PRO:HG3	1:A:1732:PRO:HD3	1.86	0.57
1:A:1379:ILE:HG22	1:A:1380:VAL:HG23	1.87	0.57
1:A:1364:ARG:HH12	1:A:1429:ALA:HB2	1.63	0.57
1:A:1683:TYR:CE1	1:A:1736:ASN:ND2	2.72	0.57
1:A:758:THR:O	1:A:762:THR:HG23	2.04	0.57
1:A:1448:MET:HE3	1:A:1448:MET:HA	1.86	0.57
1:A:369:LEU:HD21	1:A:378:LEU:HD23	1.85	0.57
1:A:1448:MET:C	1:A:1450:ILE:N	2.56	0.57
1:A:1774:LEU:C	1:A:1774:LEU:HD23	2.24	0.56
1:A:1364:ARG:HH11	1:A:1429:ALA:CA	2.09	0.56
1:A:160:TYR:HA	1:A:163:TYR:HD2	1.67	0.56
1:A:1368:GLN:HA	1:A:1368:GLN:HE21	1.69	0.56
1:A:786:ASP:O	1:A:790:VAL:HG23	2.06	0.56
1:A:1347:TRP:HE1	1:A:1463:THR:HG21	1.71	0.56
1:A:1417:VAL:HA	1:A:1423:TRP:HB3	1.88	0.56
1:A:407:ASN:HD21	1:A:1769:TYR:HB2	1.69	0.56
1:A:417:TYR:CE2	1:A:421:ASN:OD1	2.59	0.55
1:A:1730:CYS:SG	1:A:1744:CYS:HB3	2.46	0.55
1:A:710:LYS:O	1:A:714:VAL:HG23	2.06	0.55
1:A:358:SER:O	1:A:360:ALA:N	2.39	0.55
1:A:1424:MET:HA	1:A:1424:MET:HE2	1.86	0.55
1:A:1709:ILE:HD11	1:A:1718:LEU:HD22	1.87	0.55
5:A:3010:9Z9:C12	5:A:3010:9Z9:C09	2.85	0.55
1:A:274:MET:HG2	1:A:1552:ASP:HB3	1.87	0.55
1:A:1278:PHE:O	1:A:1282:ASP:CG	2.45	0.55
1:A:1195:ARG:O	1:A:1199:THR:HG23	2.06	0.55
1:A:1332:ALA:HB2	1:A:1474:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1677:GLY:O	1:A:1681:PHE:N	2.38	0.55
1:A:1332:ALA:CB	1:A:1474:ASN:ND2	2.71	0.54
1:A:1366:ILE:HG22	1:A:1373:LEU:CA	2.37	0.54
1:A:1685:LYS:NZ	1:A:1729:TYR:O	2.29	0.54
1:A:400:LEU:O	1:A:404:TYR:HB3	2.07	0.54
1:A:1399:LYS:HD3	1:A:1403:ASN:HD21	1.71	0.54
1:A:284:ASN:OD1	4:A:3009:NAG:C1	2.55	0.54
4:A:3009:NAG:C1	4:A:3009:NAG:C8	2.85	0.54
1:A:1364:ARG:NH2	1:A:1373:LEU:HD11	2.23	0.54
1:A:166:THR:O	1:A:170:THR:HG23	2.07	0.54
7:A:3026:K4D:C02	7:A:3026:K4D:C28	2.85	0.54
1:A:162:GLU:O	1:A:166:THR:HG23	2.07	0.53
1:A:284:ASN:ND2	4:A:3009:NAG:O5	2.28	0.53
1:A:372:GLN:NE2	1:A:402:SER:OG	2.28	0.53
1:A:1769:TYR:O	1:A:1769:TYR:HD1	1.91	0.53
1:A:131:HIS:CD2	1:A:133:LEU:HB3	2.44	0.53
1:A:812:ARG:HB3	1:A:815:ARG:HH21	1.73	0.53
1:A:1366:ILE:HG22	1:A:1372:ASP:O	2.08	0.53
1:A:1774:LEU:HD23	1:A:1774:LEU:O	2.08	0.53
1:A:1634:ARG:HG2	1:A:1637:ARG:HH22	1.74	0.52
1:A:843:LEU:HD22	1:A:936:LEU:HB2	1.91	0.52
1:A:1436:TYR:CD2	1:A:1437:GLU:HG3	2.45	0.52
1:A:1490:THR:CG2	1:A:1491:GLU:N	2.58	0.52
1:A:767:PHE:O	1:A:771:ALA:HB2	2.09	0.52
1:A:284:ASN:CB	4:A:3009:NAG:C8	2.84	0.52
1:A:1366:ILE:CB	1:A:1372:ASP:O	2.58	0.52
1:A:1424:MET:HE2	1:A:1424:MET:CA	2.39	0.52
1:A:1725:THR:CG2	1:A:1747:PRO:CG	2.87	0.52
1:A:1364:ARG:N	1:A:1364:ARG:CD	2.73	0.51
1:A:1676:PHE:O	1:A:1680:ASN:HB2	2.10	0.51
1:A:1424:MET:CE	1:A:1424:MET:CA	2.87	0.51
1:A:1769:TYR:CD1	1:A:1769:TYR:C	2.84	0.51
1:A:840:LEU:HD21	1:A:939:ALA:HB1	1.92	0.51
1:A:358:SER:HA	1:A:1551:THR:HG22	1.93	0.51
1:A:1282:ASP:O	1:A:1286:VAL:HG13	2.10	0.51
1:A:316:LEU:HD23	1:A:325:LEU:HD23	1.91	0.51
1:A:1254:LEU:O	1:A:1258:LEU:HG	2.11	0.51
1:A:1596:PHE:O	1:A:1600:VAL:HG23	2.11	0.50
1:A:1602:ILE:O	1:A:1606:VAL:HG23	2.11	0.50
1:A:1734:LEU:HD22	1:A:1735:PRO:HD2	0.60	0.50
1:A:422:GLN:O	1:A:426:ALA:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:ASN:HD22	2:B:1:NAG:H61	1.77	0.50
1:A:1424:MET:HA	1:A:1424:MET:HE1	1.92	0.50
1:A:1523:ILE:O	1:A:1526:ILE:HG22	2.11	0.50
1:A:1568:LEU:O	1:A:1572:ILE:HG13	2.12	0.50
1:A:1380:VAL:HG11	1:A:1386:CYS:HB3	1.94	0.50
1:A:1555:SER:O	1:A:1559:VAL:HG23	2.12	0.50
1:A:1531:ALA:O	1:A:1535:THR:HG23	2.12	0.49
5:A:3014:9Z9:C09	5:A:3014:9Z9:C12	2.89	0.49
1:A:304:SER:O	1:A:305:LEU:C	2.50	0.49
1:A:1420:PHE:CZ	7:A:3026:K4D:O06	2.63	0.49
1:A:327:CYS:O	1:A:385:SER:HA	2.12	0.49
1:A:1640:ARG:O	1:A:1646:ARG:NH1	2.46	0.49
1:A:1692:ASP:OD1	1:A:1693:MET:N	2.46	0.49
1:A:1338:ASN:O	1:A:1342:VAL:HG23	2.12	0.49
3:C:1:NAG:HO3	3:C:1:NAG:C7	2.24	0.49
1:A:248:VAL:HG22	1:A:931:LEU:HD11	1.94	0.49
1:A:1366:ILE:CG2	1:A:1372:ASP:O	2.60	0.49
1:A:1364:ARG:NH2	1:A:1364:ARG:CG	2.72	0.48
1:A:129:LEU:O	1:A:134:PHE:CE1	2.66	0.48
1:A:403:PHE:HZ	1:A:1711:THR:HG22	1.79	0.48
1:A:1365:CYS:CA	1:A:1397:TRP:HA	2.38	0.48
1:A:1725:THR:HG21	1:A:1747:PRO:HG2	1.96	0.48
1:A:1368:GLN:HE21	1:A:1368:GLN:CA	2.23	0.48
1:A:1725:THR:HG21	1:A:1747:PRO:CG	2.43	0.48
1:A:308:TYR:N	1:A:308:TYR:HD1	2.10	0.48
1:A:1308:ARG:HD2	1:A:1311:ARG:NH1	2.27	0.48
1:A:1373:LEU:HB3	1:A:1374:PRO:HD2	1.96	0.48
1:A:314:ASN:O	1:A:315:TYR:C	2.52	0.48
1:A:1482:LEU:C	1:A:1484:GLY:N	2.65	0.48
1:A:1517:ASN:OD1	1:A:1518:LYS:N	2.46	0.48
3:C:1:NAG:H61	3:C:2:NAG:C7	2.44	0.48
1:A:1373:LEU:N	1:A:1373:LEU:CD2	2.76	0.48
2:D:1:NAG:O3	2:D:2:NAG:O5	2.26	0.48
1:A:169:TYR:CE2	1:A:226:ARG:HD3	2.49	0.47
1:A:1471:ILE:HG21	1:A:1766:VAL:HG11	1.96	0.47
1:A:717:ASP:OD1	1:A:717:ASP:N	2.47	0.47
1:A:1206:HIS:CE1	1:A:1208:TRP:HD1	2.32	0.47
1:A:283:ARG:C	1:A:284:ASN:O	2.52	0.47
1:A:302:TRP:HZ3	1:A:308:TYR:CZ	2.32	0.47
1:A:1358:PHE:HA	1:A:1361:LYS:HD2	1.96	0.47
1:A:1532:PHE:O	1:A:1536:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:PHE:O	1:A:1219:LEU:HG	2.15	0.47
1:A:1364:ARG:HD2	1:A:1364:ARG:H	1.79	0.47
1:A:1366:ILE:HG22	1:A:1372:ASP:C	2.35	0.47
1:A:1368:GLN:HA	1:A:1368:GLN:NE2	2.30	0.47
1:A:1375:LEU:CB	1:A:1379:ILE:HD12	2.44	0.47
1:A:1767:ASN:HA	1:A:1770:ILE:HG22	1.97	0.47
1:A:706:SER:O	1:A:710:LYS:HG2	2.15	0.47
1:A:1373:LEU:CB	1:A:1374:PRO:HD2	2.44	0.47
1:A:906:MET:SD	1:A:910:MET:HE2	2.55	0.47
1:A:1365:CYS:HB2	1:A:1397:TRP:CG	2.43	0.47
1:A:1301:ILE:O	1:A:1302:LYS:HB3	2.14	0.47
1:A:201:VAL:HG21	1:A:226:ARG:CG	2.44	0.46
1:A:1427:MET:HE3	1:A:1449:TYR:CE1	2.51	0.46
1:A:1729:TYR:CD1	1:A:1729:TYR:N	2.73	0.46
1:A:279:HIS:HB3	1:A:327:CYS:SG	2.55	0.46
1:A:351:HIS:HB3	1:A:353:TYR:HE1	1.80	0.46
1:A:1247:MET:O	1:A:1251:VAL:HG12	2.15	0.46
1:A:1588:TYR:HD2	1:A:1598:PHE:HB2	1.79	0.46
1:A:1605:ILE:O	1:A:1609:VAL:HG13	2.15	0.46
5:A:3014:9Z9:C11	5:A:3014:9Z9:C07	2.56	0.46
1:A:1527:VAL:HG11	1:A:1579:VAL:CG1	2.46	0.46
1:A:1764:ILE:O	1:A:1767:ASN:HB2	2.15	0.46
1:A:156:PRO:O	1:A:159:LYS:HG3	2.16	0.46
1:A:389:ILE:HD12	1:A:389:ILE:H	1.81	0.46
1:A:1761:SER:O	1:A:1765:VAL:HG13	2.16	0.46
1:A:361:TRP:HA	1:A:361:TRP:CE3	2.51	0.46
1:A:751:GLN:O	1:A:755:LEU:HG	2.16	0.46
1:A:1336:ILE:HD13	1:A:1763:LEU:HD11	1.97	0.46
1:A:1358:PHE:HE2	1:A:1451:TYR:CE2	2.34	0.46
1:A:1597:ASP:OD2	1:A:1640:ARG:NH1	2.49	0.46
1:A:815:ARG:O	1:A:818:LYS:HG2	2.16	0.45
1:A:308:TYR:N	1:A:308:TYR:CD1	2.83	0.45
1:A:1278:PHE:CE1	1:A:1282:ASP:CG	2.88	0.45
1:A:1344:LEU:HA	1:A:1344:LEU:HD23	1.78	0.45
1:A:1364:ARG:CD	1:A:1364:ARG:H	2.30	0.45
1:A:1278:PHE:O	1:A:1282:ASP:OD1	2.34	0.45
1:A:1301:ILE:HG13	1:A:1302:LYS:H	1.81	0.45
1:A:1767:ASN:CA	1:A:1770:ILE:HG22	2.46	0.45
1:A:1443:GLU:OE1	1:A:1446:LEU:HG	2.15	0.45
1:A:1525:ASP:O	1:A:1529:LYS:HG3	2.17	0.45
1:A:707:ILE:O	1:A:711:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:MET:CB	1:A:1777:PHE:HZ	2.27	0.45
1:A:1577:CYS:SG	1:A:1588:TYR:CE2	3.06	0.45
1:A:280:LYS:HD2	1:A:315:TYR:CE2	2.52	0.45
1:A:1730:CYS:CB	1:A:1744:CYS:HB3	2.46	0.45
1:A:826:LEU:HD13	1:A:1342:VAL:HG13	1.99	0.45
1:A:940:LEU:HB3	1:A:1465:ASN:HD21	1.82	0.45
1:A:1364:ARG:CG	1:A:1373:LEU:CD1	2.95	0.45
1:A:1489:MET:HE2	1:A:1657:PRO:HG2	1.98	0.45
1:A:1769:TYR:O	1:A:1769:TYR:CD1	2.70	0.45
1:A:1774:LEU:C	1:A:1774:LEU:CD2	2.85	0.45
1:A:195:ASN:HA	1:A:198:ASP:OD2	2.18	0.44
1:A:314:ASN:O	1:A:315:TYR:O	2.36	0.44
1:A:789:ILE:HG21	1:A:815:ARG:HG3	1.98	0.44
1:A:1502:LYS:HE2	1:A:1502:LYS:HB3	1.70	0.44
1:A:1535:THR:O	1:A:1539:LEU:HD13	2.17	0.44
1:A:720:ALA:HB1	1:A:723:THR:OG1	2.17	0.44
1:A:1606:VAL:HA	1:A:1609:VAL:HG22	1.99	0.44
1:A:1772:ILE:HG12	1:A:1772:ILE:H	1.62	0.44
1:A:1362:PHE:O	1:A:1364:ARG:NE	2.51	0.44
1:A:198:ASP:HA	1:A:201:VAL:HG12	1.99	0.44
1:A:285:PHE:HZ	1:A:304:SER:HG	1.63	0.44
1:A:704:TRP:NE1	1:A:708:LYS:HE2	2.33	0.44
1:A:1431:VAL:HG21	1:A:1449:TYR:CE2	2.52	0.44
1:A:1655:SER:CB	1:A:1775:GLU:HG3	2.47	0.44
1:A:143:LEU:O	1:A:147:VAL:HG23	2.18	0.44
1:A:258:THR:HG23	1:A:405:LEU:HD13	1.99	0.44
1:A:375:TRP:HZ2	1:A:1711:THR:HG1	1.66	0.44
1:A:1272:ALA:HA	1:A:1275:TRP:HD1	1.83	0.44
1:A:254:VAL:O	1:A:258:THR:OG1	2.20	0.44
1:A:350:ASP:OD1	1:A:351:HIS:N	2.48	0.44
1:A:231:ILE:HG23	1:A:237:LEU:HB3	2.00	0.43
1:A:1459:GLY:HA2	1:A:1463:THR:HG23	1.99	0.43
1:A:309:LEU:C	1:A:309:LEU:CD2	2.86	0.43
1:A:1194:TRP:HD1	1:A:1197:ARG:HH21	1.65	0.43
1:A:1364:ARG:HG2	1:A:1373:LEU:HD13	2.00	0.43
1:A:773:ASP:HB3	1:A:776:TYR:CD2	2.54	0.43
1:A:781:GLY:HA2	1:A:784:ILE:HB	2.00	0.43
1:A:1368:GLN:HB2	1:A:1396:TYR:HE1	1.83	0.43
1:A:1681:PHE:HE2	1:A:1753:PHE:CD1	2.36	0.43
1:A:171:PHE:O	1:A:175:VAL:HG23	2.18	0.43
1:A:1673:TYR:HD2	1:A:1753:PHE:CE2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:CYS:HB3	1:A:1744:CYS:HB3	1.99	0.43
1:A:328:GLY:HA3	1:A:333:ALA:HB3	2.00	0.43
1:A:1200:CYS:HB3	1:A:1262:ALA:HB2	2.01	0.43
1:A:1308:ARG:HE	1:A:1308:ARG:HB3	1.69	0.43
1:A:1561:ILE:O	1:A:1565:ILE:HG13	2.19	0.43
1:A:1654:MET:SD	1:A:1779:VAL:HG21	2.58	0.43
1:A:700:CYS:O	1:A:704:TRP:HB2	2.18	0.43
1:A:1586:HIS:O	1:A:1590:THR:OG1	2.34	0.43
1:A:231:ILE:HG12	1:A:237:LEU:HD12	2.01	0.43
1:A:762:THR:HG22	1:A:790:VAL:HG13	1.99	0.43
1:A:1427:MET:HE3	1:A:1427:MET:HB3	1.86	0.43
1:A:280:LYS:O	1:A:342:CYS:HB2	2.19	0.43
1:A:1230:TYR:O	1:A:1234:ARG:HG3	2.19	0.43
1:A:1272:ALA:O	1:A:1275:TRP:HB2	2.18	0.43
1:A:1332:ALA:HB1	1:A:1474:ASN:ND2	2.33	0.43
1:A:1431:VAL:HG11	1:A:1449:TYR:CD2	2.54	0.43
1:A:1366:ILE:O	1:A:1366:ILE:HG13	2.17	0.43
1:A:203:VAL:O	1:A:207:THR:HG23	2.18	0.42
1:A:1445:ASN:O	1:A:1448:MET:CG	2.66	0.42
1:A:341:ARG:NH2	1:A:343:LEU:HD11	2.29	0.42
1:A:883:HIS:CD2	1:A:885:MET:HG2	2.54	0.42
1:A:1224:LEU:HB3	1:A:1675:ILE:HD13	2.00	0.42
1:A:1368:GLN:CA	1:A:1368:GLN:NE2	2.81	0.42
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.77	0.42
1:A:369:LEU:CD2	1:A:375:TRP:HB2	2.49	0.42
1:A:408:LEU:HD21	1:A:1648:LEU:HB3	2.01	0.42
1:A:1671:PHE:CZ	1:A:1675:ILE:HD11	2.54	0.42
1:A:1217:ILE:HD12	1:A:1220:SER:OG	2.20	0.42
1:A:1300:PRO:HA	1:A:1301:ILE:HA	1.62	0.42
1:A:256:VAL:HG12	1:A:1645:ILE:HD11	2.02	0.42
1:A:1460:SER:O	1:A:1464:LEU:HB2	2.20	0.42
1:A:859:MET:HG3	1:A:860:GLN:N	2.35	0.42
1:A:1365:CYS:SG	1:A:1365:CYS:O	2.78	0.42
1:A:1674:SER:HB3	1:A:1706:LEU:HD22	2.02	0.42
1:A:1705:CYS:HB3	1:A:1718:LEU:HD21	2.01	0.42
1:A:276:ASN:O	1:A:385:SER:OG	2.35	0.42
1:A:1203:ILE:HD12	1:A:1203:ILE:HA	1.87	0.42
1:A:1613:ILE:HG13	1:A:1616:LYS:HD2	2.01	0.42
1:A:160:TYR:HA	1:A:163:TYR:CD2	2.52	0.42
1:A:781:GLY:HA2	1:A:784:ILE:HD12	2.02	0.42
1:A:1214:ILE:HD11	1:A:1318:ARG:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:MET:SD	1:A:1268:TYR:OH	2.71	0.42
1:A:1529:LYS:HB3	1:A:1529:LYS:HE2	1.71	0.42
1:A:1532:PHE:CE1	1:A:1536:ILE:HD11	2.55	0.42
1:A:1554:GLN:H	1:A:1554:GLN:HG2	1.61	0.42
1:A:721:ASP:OD1	1:A:722:LEU:N	2.53	0.41
1:A:230:THR:O	1:A:234:ILE:HG12	2.21	0.41
1:A:733:LEU:O	1:A:737:LEU:HG	2.20	0.41
1:A:198:ASP:O	1:A:202:ILE:HG12	2.21	0.41
1:A:349:PRO:HB2	1:A:354:THR:OG1	2.20	0.41
1:A:361:TRP:HA	1:A:361:TRP:HE3	1.85	0.41
1:A:1359:ALA:C	1:A:1361:LYS:H	2.23	0.41
1:A:1364:ARG:O	1:A:1365:CYS:HB3	2.21	0.41
1:A:1418:ALA:HB2	1:A:1455:PHE:CZ	2.56	0.41
1:A:1629:LEU:O	1:A:1632:ILE:HG12	2.21	0.41
1:A:1767:ASN:C	1:A:1770:ILE:HG22	2.41	0.41
1:A:302:TRP:HE3	1:A:308:TYR:CE1	2.25	0.41
1:A:311:ASP:O	1:A:313:ALA:N	2.54	0.41
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.94	0.41
1:A:1245:ASP:O	1:A:1249:THR:HG22	2.21	0.41
1:A:1253:VAL:O	1:A:1257:LEU:HG	2.21	0.41
1:A:408:LEU:O	1:A:412:VAL:HG23	2.21	0.41
1:A:422:GLN:O	1:A:426:ALA:HB2	2.21	0.41
1:A:1344:LEU:HD22	1:A:1411:TYR:CZ	2.56	0.41
1:A:1422:GLY:HA3	1:A:1716:ASP:HB3	2.03	0.41
1:A:1448:MET:C	1:A:1450:ILE:H	2.23	0.41
1:A:1458:PHE:HA	1:A:1462:PHE:CD2	2.48	0.41
1:A:1543:ASN:HD21	1:A:1634:ARG:HD2	1.85	0.41
1:A:1725:THR:CG2	1:A:1747:PRO:HG3	2.50	0.41
1:A:303:ASN:ND2	1:A:306:ASP:HB2	2.23	0.41
1:A:847:LEU:O	1:A:851:VAL:HG23	2.20	0.41
1:A:1345:ILE:O	1:A:1348:LEU:HB3	2.21	0.41
1:A:1554:GLN:HG3	1:A:1555:SER:H	1.86	0.41
1:A:1734:LEU:HD23	1:A:1734:LEU:HA	1.89	0.41
1:A:212:ASP:OD2	1:A:220:ARG:NH2	2.47	0.40
1:A:1439:GLN:HA	1:A:1440:PRO:HD3	1.89	0.40
1:A:146:CYS:HA	1:A:149:MET:HE3	2.04	0.40
1:A:407:ASN:ND2	1:A:1769:TYR:CB	2.82	0.40
1:A:422:GLN:O	1:A:426:ALA:N	2.45	0.40
1:A:1380:VAL:CG1	1:A:1386:CYS:HB3	2.52	0.40
1:A:1545:VAL:O	1:A:1549:VAL:HG13	2.21	0.40
1:A:421:ASN:O	1:A:425:ILE:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:LEU:HD13	1:A:1353:MET:HG3	2.03	0.40
1:A:781:GLY:O	1:A:784:ILE:HB	2.22	0.40
1:A:1278:PHE:CD1	1:A:1282:ASP:OD1	2.75	0.40
1:A:1308:ARG:HD2	1:A:1311:ARG:HH11	1.87	0.40
1:A:1311:ARG:HG3	1:A:1314:ARG:HH12	1.86	0.40
1:A:1489:MET:HE1	1:A:1657:PRO:HG2	2.02	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	1126/1838 (61%)	1030 (92%)	85 (8%)	11 (1%)	13	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	A	304	SER
1	A	312	PRO
1	A	1374	PRO
1	A	1449	TYR
1	A	315	TYR
1	A	359	PHE
1	A	1483	GLY
1	A	1733	ASN
1	A	349	PRO
1	A	301	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	954/1612 (59%)	929 (97%)	25 (3%)	41 67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	183	CYS
1	A	284	ASN
1	A	285	PHE
1	A	303	ASN
1	A	305	LEU
1	A	342	CYS
1	A	356	PHE
1	A	1194	TRP
1	A	1364	ARG
1	A	1367	ASN
1	A	1376	ASN
1	A	1421	LYS
1	A	1423	TRP
1	A	1425	ASP
1	A	1448	MET
1	A	1473	ASP
1	A	1487	ILE
1	A	1729	TYR
1	A	1733	ASN
1	A	1734	LEU
1	A	1744	CYS
1	A	1769	TYR
1	A	1772	ILE
1	A	1777	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	151	GLN
1	A	284	ASN
1	A	303	ASN
1	A	407	ASN
1	A	420	GLN
1	A	421	ASN
1	A	865	ASN
1	A	930	ASN
1	A	1206	HIS
1	A	1368	GLN
1	A	1403	ASN
1	A	1474	ASN
1	A	1493	GLN
1	A	1543	ASN
1	A	1586	HIS
1	A	1661	ASN
1	A	1701	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 ⓘ

7 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	0.17	0	17,19,21	0.46	0
2	NAG	B	2	2	14,14,15	0.24	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.51	0
3	BMA	C	3	3	11,11,12	0.32	0	15,15,17	0.91	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.26	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.49	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	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	1/1/4/5	0/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	2.61	115.68	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1
3	C	3	BMA	C1

All (12) torsion outliers are listed below:

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

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

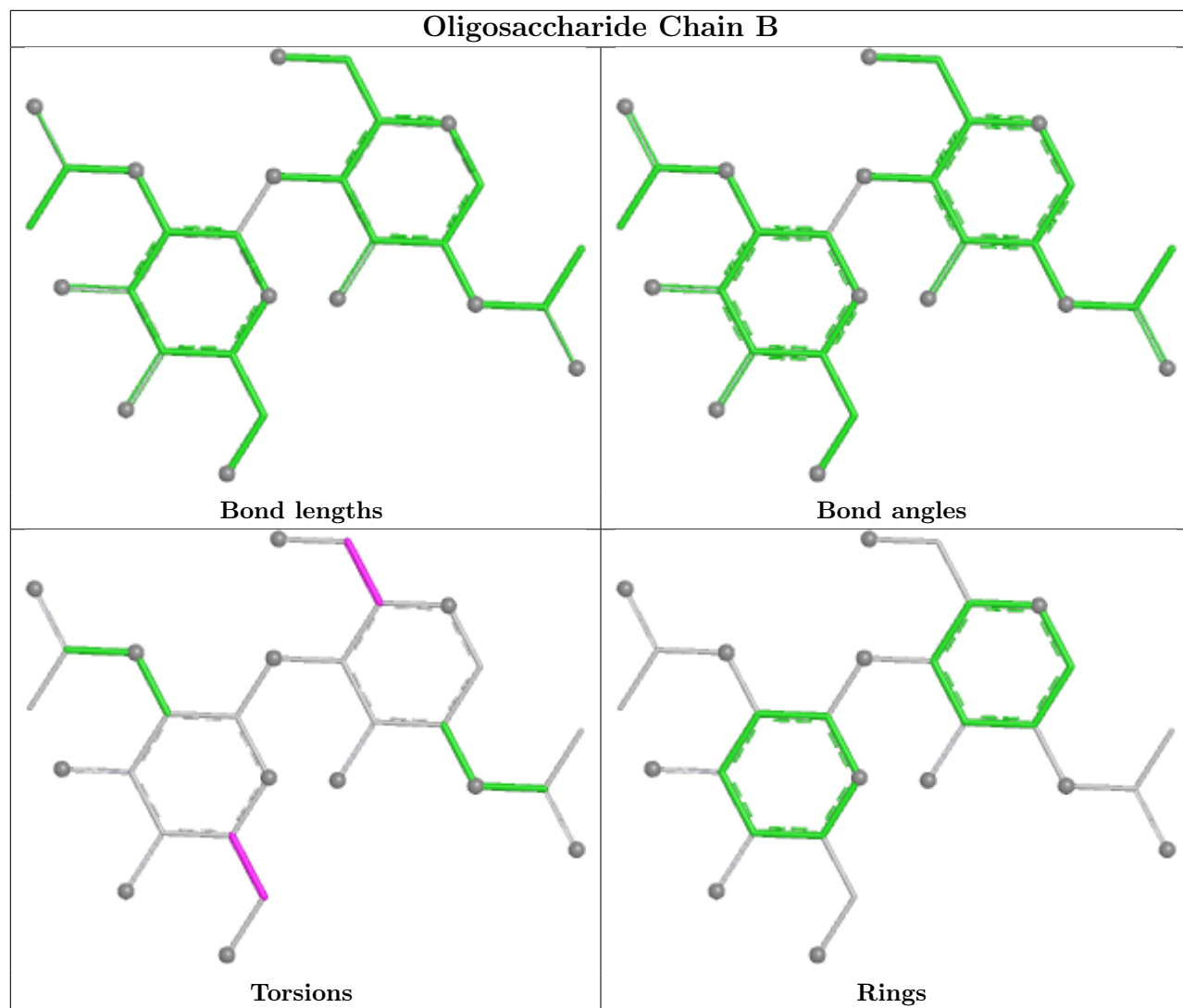
All (1) ring outliers are listed below:

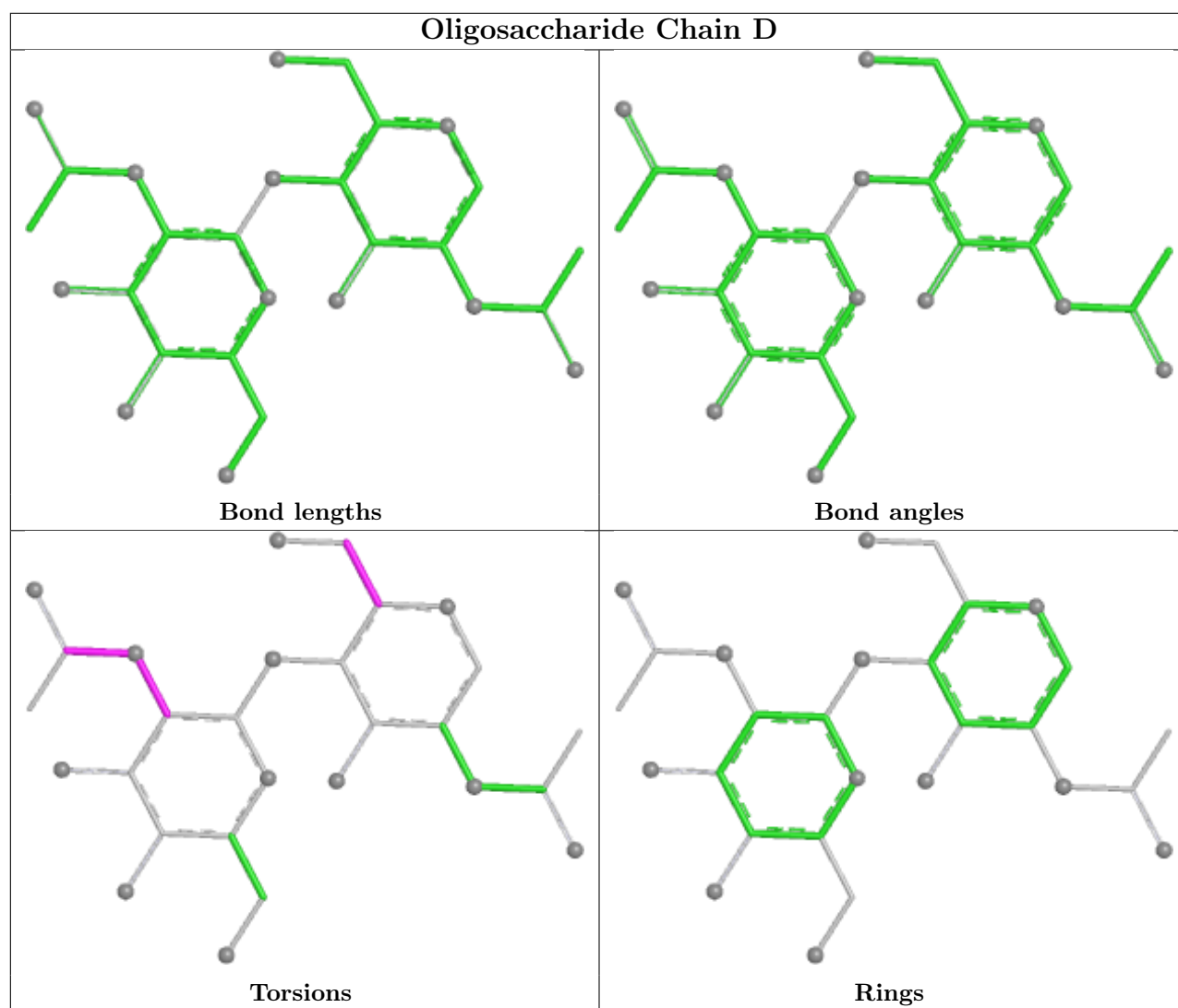
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C1-C2-C3-C4-C5-O5

5 monomers are involved in 6 short contacts:

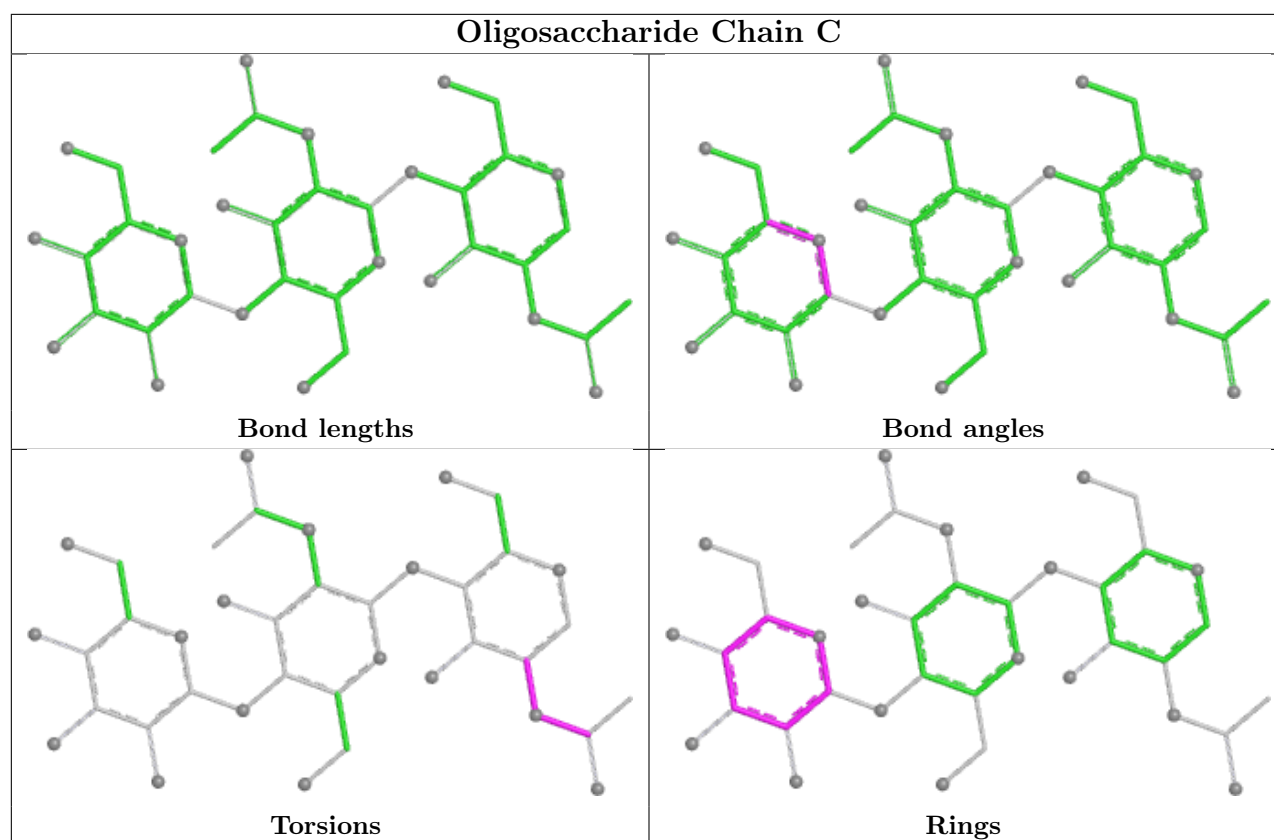
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
3	C	2	NAG	2	0
2	D	1	NAG	1	0
3	C	1	NAG	3	0
2	B	1	NAG	1	0

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](#)

19 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$
4	NAG	A	3009	-	14,14,15	0.43	0	17,19,21	0.67	0
6	6OU	A	3023	-	24,24,48	1.29	5 (20%)	27,29,53	1.36	2 (7%)
4	NAG	A	3003	1	14,14,15	0.30	0	17,19,21	0.41	0
6	6OU	A	3019	-	28,28,48	1.15	4 (14%)	30,30,53	1.35	3 (10%)
5	9Z9	A	3010	-	36,36,44	8.40	25 (69%)	59,59,68	2.45	24 (40%)
5	9Z9	A	3013	-	34,34,44	8.53	22 (64%)	56,56,68	2.30	20 (35%)
5	9Z9	A	3012	-	42,42,44	7.69	23 (54%)	63,66,68	2.13	22 (34%)
6	6OU	A	3024	-	16,16,48	1.35	3 (18%)	16,16,53	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	6OU	A	3015	-	34,34,48	1.02	2 (5%)	37,39,53	1.13	3 (8%)
6	6OU	A	3018	-	25,25,48	1.10	4 (16%)	27,27,53	1.25	2 (7%)
6	6OU	A	3021	-	25,25,48	1.23	4 (16%)	28,30,53	1.20	2 (7%)
6	6OU	A	3016	-	34,34,48	1.05	3 (8%)	37,39,53	1.15	2 (5%)
6	6OU	A	3017	-	14,14,48	0.96	1 (7%)	14,14,53	1.08	1 (7%)
6	6OU	A	3020	-	39,39,48	0.99	4 (10%)	42,44,53	1.07	2 (4%)
5	9Z9	A	3011	-	23,23,44	6.79	13 (56%)	35,37,68	2.17	13 (37%)
6	6OU	A	3022	-	26,26,48	0.97	2 (7%)	27,27,53	1.17	2 (7%)
6	6OU	A	3025	-	14,14,48	1.45	3 (21%)	14,14,53	1.06	1 (7%)
7	K4D	A	3026	-	29,29,29	1.61	3 (10%)	37,41,41	1.71	7 (18%)
5	9Z9	A	3014	-	34,34,44	8.56	22 (64%)	56,56,68	2.20	20 (35%)

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
4	NAG	A	3009	-	-	3/6/23/26	0/1/1/1
6	6OU	A	3023	-	-	4/26/26/52	-
4	NAG	A	3003	1	-	2/6/23/26	0/1/1/1
6	6OU	A	3019	-	-	16/29/29/52	-
5	9Z9	A	3010	-	-	0/2/90/100	0/6/6/6
5	9Z9	A	3013	-	-	-	0/6/6/6
5	9Z9	A	3012	-	-	3/9/97/100	0/6/6/6
6	6OU	A	3024	-	-	4/15/15/52	-
6	6OU	A	3015	-	-	16/38/38/52	-
6	6OU	A	3018	-	-	13/27/27/52	-
6	6OU	A	3021	-	-	9/29/29/52	-
6	6OU	A	3016	-	-	18/38/38/52	-
6	6OU	A	3017	-	-	5/13/13/52	-
6	6OU	A	3020	-	-	16/43/43/52	-
5	9Z9	A	3011	-	-	-	0/4/4/6
6	6OU	A	3022	-	-	8/26/26/52	-
6	6OU	A	3025	-	-	3/13/13/52	-
7	K4D	A	3026	-	-	9/21/29/29	0/2/2/2
5	9Z9	A	3014	-	-	-	0/6/6/6

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3010	9Z9	C15-C07	-22.07	1.17	1.53
5	A	3014	9Z9	C15-C07	-21.94	1.17	1.53
5	A	3012	9Z9	C15-C07	-21.43	1.18	1.53
5	A	3013	9Z9	C15-C07	-21.30	1.18	1.53
5	A	3010	9Z9	C07-C06	-21.10	1.14	1.53
5	A	3014	9Z9	C07-C06	-20.95	1.14	1.53
5	A	3012	9Z9	C07-C06	-20.83	1.14	1.53
5	A	3013	9Z9	C07-C06	-20.61	1.14	1.53
5	A	3010	9Z9	C11-C13	-18.60	1.17	1.52
5	A	3013	9Z9	C11-C13	-18.57	1.17	1.52
5	A	3012	9Z9	C11-C13	-18.39	1.17	1.52
5	A	3014	9Z9	C11-C13	-18.27	1.18	1.52
5	A	3012	9Z9	C10-C02	-18.05	1.22	1.54
5	A	3013	9Z9	C10-C02	-17.98	1.22	1.54
5	A	3011	9Z9	C10-C02	-17.92	1.22	1.54
5	A	3010	9Z9	C10-C02	-17.71	1.23	1.54
5	A	3014	9Z9	C10-C02	-17.71	1.23	1.54
5	A	3011	9Z9	C07-C06	-16.12	1.14	1.53
5	A	3014	9Z9	C11-C08	12.47	1.75	1.56
5	A	3013	9Z9	C10-C09	-12.38	1.28	1.53
5	A	3012	9Z9	C10-C09	-12.16	1.29	1.53
5	A	3010	9Z9	C10-C09	-12.14	1.29	1.53
5	A	3014	9Z9	C10-C09	-11.98	1.29	1.53
5	A	3013	9Z9	C05-C04	11.87	1.78	1.52
5	A	3014	9Z9	C05-C04	11.75	1.77	1.52
5	A	3010	9Z9	C05-C04	11.69	1.77	1.52
5	A	3011	9Z9	C05-C04	11.65	1.77	1.52
5	A	3010	9Z9	C11-C08	11.59	1.74	1.56
5	A	3013	9Z9	C11-C08	11.51	1.74	1.56
5	A	3012	9Z9	C05-C04	11.39	1.77	1.52
5	A	3012	9Z9	C11-C08	11.35	1.74	1.56
5	A	3010	9Z9	C07-C08	-10.96	1.33	1.53
5	A	3014	9Z9	C07-C08	-10.80	1.33	1.53
5	A	3012	9Z9	C07-C08	-10.76	1.33	1.53
5	A	3013	9Z9	C07-C08	-10.59	1.33	1.53
5	A	3011	9Z9	C10-C09	-9.78	1.29	1.52
5	A	3010	9Z9	C19-C11	9.45	1.71	1.54
5	A	3014	9Z9	C19-C11	9.39	1.71	1.54
5	A	3013	9Z9	C19-C11	9.32	1.71	1.54
5	A	3012	9Z9	C19-C11	9.23	1.71	1.54
5	A	3011	9Z9	C08-C07	-7.96	1.33	1.53
5	A	3012	9Z9	C18-C17	-7.81	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3010	9Z9	C18-C17	-7.65	1.30	1.51
5	A	3011	9Z9	C02-C03	7.09	1.69	1.56
5	A	3012	9Z9	C02-C03	6.92	1.68	1.56
5	A	3010	9Z9	C02-C03	6.71	1.68	1.56
5	A	3014	9Z9	C02-C03	6.67	1.68	1.56
7	A	3026	K4D	C10-N12	6.56	1.48	1.33
5	A	3013	9Z9	C02-C03	6.35	1.67	1.56
5	A	3014	9Z9	C16-C13	6.25	1.60	1.50
5	A	3013	9Z9	C16-C13	6.17	1.60	1.50
5	A	3013	9Z9	C15-C14	6.15	1.62	1.50
5	A	3010	9Z9	C15-C14	5.87	1.62	1.50
5	A	3013	9Z9	C18-C17	-5.76	1.30	1.51
5	A	3012	9Z9	C15-C14	5.72	1.61	1.50
5	A	3014	9Z9	C18-C17	-5.71	1.30	1.51
5	A	3014	9Z9	C15-C14	5.68	1.61	1.50
5	A	3013	9Z9	C03-C04	-5.64	1.43	1.54
5	A	3012	9Z9	C03-C04	-5.47	1.44	1.54
5	A	3011	9Z9	C03-C04	-5.44	1.44	1.54
5	A	3010	9Z9	C03-C04	-5.40	1.44	1.54
5	A	3014	9Z9	C03-C04	-5.30	1.44	1.54
5	A	3010	9Z9	C03-C74	-4.91	1.40	1.54
5	A	3012	9Z9	C03-C74	-4.82	1.40	1.54
5	A	3013	9Z9	C03-C74	-4.80	1.40	1.54
5	A	3014	9Z9	C03-C74	-4.79	1.40	1.54
5	A	3011	9Z9	C03-C74	-4.78	1.40	1.54
5	A	3010	9Z9	C16-C13	4.57	1.60	1.51
5	A	3012	9Z9	O72-C73	-4.50	1.33	1.42
5	A	3014	9Z9	O72-C73	-4.50	1.33	1.42
5	A	3012	9Z9	C16-C13	4.33	1.60	1.51
5	A	3011	9Z9	O72-C73	-4.33	1.33	1.42
5	A	3013	9Z9	O72-C73	-4.22	1.33	1.42
5	A	3010	9Z9	O72-C73	-4.21	1.33	1.42
6	A	3019	6OU	O30-C20	-4.06	1.40	1.47
5	A	3011	9Z9	O80-C73	4.05	1.48	1.42
6	A	3025	6OU	C08-C07	-3.96	1.32	1.51
6	A	3024	6OU	C08-C07	-3.91	1.32	1.51
5	A	3013	9Z9	O80-C73	3.89	1.48	1.42
5	A	3012	9Z9	O80-C73	3.62	1.47	1.42
5	A	3011	9Z9	C76-C77	-3.55	1.46	1.53
5	A	3010	9Z9	O80-C73	3.51	1.47	1.42
5	A	3012	9Z9	C76-C77	-3.42	1.46	1.53
5	A	3014	9Z9	O80-C73	3.22	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3013	9Z9	C76-C73	3.22	1.56	1.51
5	A	3014	9Z9	C76-C77	-3.14	1.47	1.53
5	A	3010	9Z9	O20-C17	3.14	1.51	1.43
5	A	3010	9Z9	C16-C17	3.08	1.58	1.52
5	A	3013	9Z9	C05-C06	3.06	1.60	1.54
5	A	3010	9Z9	C76-C77	-3.04	1.47	1.53
5	A	3012	9Z9	C76-C73	2.89	1.56	1.51
6	A	3018	6OU	O30-C20	-2.89	1.39	1.46
5	A	3012	9Z9	C16-C17	2.88	1.58	1.52
5	A	3013	9Z9	C76-C77	-2.87	1.47	1.53
5	A	3010	9Z9	C76-C73	2.81	1.56	1.51
5	A	3014	9Z9	C05-C06	2.81	1.60	1.54
6	A	3015	6OU	O30-C20	-2.79	1.40	1.46
5	A	3011	9Z9	C76-C73	2.78	1.56	1.51
5	A	3010	9Z9	C05-C06	2.78	1.60	1.54
6	A	3020	6OU	O30-C20	-2.77	1.40	1.46
6	A	3023	6OU	P23-O26	2.76	1.65	1.54
5	A	3011	9Z9	C05-C06	2.75	1.59	1.53
6	A	3021	6OU	O30-C20	-2.71	1.40	1.46
5	A	3012	9Z9	C05-C06	2.69	1.59	1.54
6	A	3023	6OU	O30-C20	-2.65	1.40	1.46
5	A	3012	9Z9	O20-C17	2.61	1.51	1.43
7	A	3026	K4D	O11-C10	-2.52	1.17	1.23
6	A	3016	6OU	O30-C20	-2.51	1.40	1.46
6	A	3016	6OU	O18-C16	2.50	1.40	1.33
6	A	3020	6OU	O18-C16	2.50	1.40	1.33
6	A	3022	6OU	O18-C16	2.47	1.40	1.33
6	A	3021	6OU	O18-C16	2.45	1.40	1.33
7	A	3026	K4D	O21-C20	2.44	1.42	1.37
5	A	3014	9Z9	C76-C73	2.41	1.55	1.51
6	A	3024	6OU	O18-C16	2.40	1.40	1.33
6	A	3015	6OU	O18-C16	2.40	1.40	1.33
6	A	3017	6OU	O30-C31	2.39	1.40	1.33
6	A	3025	6OU	O18-C16	2.39	1.40	1.33
6	A	3018	6OU	O18-C19	-2.38	1.39	1.45
6	A	3019	6OU	O18-C19	-2.37	1.39	1.45
6	A	3022	6OU	O30-C31	2.31	1.40	1.33
6	A	3023	6OU	O18-C16	2.29	1.40	1.33
5	A	3012	9Z9	C19-C18	-2.26	1.48	1.53
6	A	3018	6OU	O18-C16	2.25	1.39	1.33
6	A	3024	6OU	O18-C19	-2.25	1.40	1.45
6	A	3025	6OU	O18-C19	-2.24	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3016	6OU	O30-C31	2.23	1.40	1.34
6	A	3021	6OU	O18-C19	-2.18	1.40	1.45
6	A	3021	6OU	O30-C31	2.17	1.40	1.34
5	A	3010	9Z9	C19-C18	-2.17	1.49	1.53
6	A	3019	6OU	O30-C31	2.14	1.40	1.34
5	A	3014	9Z9	C17-C16	2.14	1.59	1.52
6	A	3023	6OU	O18-C19	-2.13	1.40	1.45
6	A	3020	6OU	O30-C31	2.12	1.40	1.34
6	A	3019	6OU	O18-C16	2.08	1.39	1.33
5	A	3013	9Z9	C17-C16	2.07	1.58	1.52
6	A	3023	6OU	O30-C31	2.07	1.40	1.34
5	A	3013	9Z9	C73-C74	2.07	1.57	1.53
5	A	3010	9Z9	C14-C13	-2.07	1.28	1.33
6	A	3018	6OU	O30-C31	2.07	1.40	1.34
5	A	3010	9Z9	C79-C78	2.03	1.55	1.51
5	A	3014	9Z9	C79-C78	2.02	1.55	1.51
6	A	3020	6OU	O18-C19	-2.01	1.40	1.45

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3026	K4D	C20-C09-C10	-6.38	114.74	126.24
5	A	3010	9Z9	C15-C07-C08	5.96	116.61	109.72
5	A	3013	9Z9	C10-C02-C06	5.87	116.03	107.25
5	A	3014	9Z9	C10-C02-C06	5.65	115.71	107.25
5	A	3010	9Z9	C10-C02-C06	5.43	115.37	107.25
5	A	3013	9Z9	O80-C73-C76	5.20	115.29	110.76
5	A	3012	9Z9	O80-C73-C76	5.09	115.20	110.76
5	A	3012	9Z9	C15-C14-C13	-5.06	116.47	125.02
5	A	3011	9Z9	O80-C73-C76	5.02	115.13	110.76
5	A	3014	9Z9	C08-C11-C13	4.71	116.55	109.65
5	A	3010	9Z9	C15-C14-C13	-4.68	117.12	125.02
5	A	3014	9Z9	C10-C02-C03	4.61	121.92	115.36
5	A	3013	9Z9	C15-C14-C13	-4.49	117.44	125.02
5	A	3013	9Z9	C10-C02-C03	4.32	121.52	115.36
5	A	3010	9Z9	O80-C73-C76	4.32	114.52	110.76
5	A	3010	9Z9	C05-C06-C07	4.26	127.78	119.53
5	A	3010	9Z9	C09-C08-C07	-4.17	105.97	111.78
5	A	3011	9Z9	C10-C02-C03	4.10	121.19	115.36
6	A	3023	6OU	O30-C31-C33	4.04	120.22	111.48
5	A	3012	9Z9	C10-C02-C03	4.04	121.11	115.36
5	A	3010	9Z9	C10-C02-C03	4.03	121.09	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3012	9Z9	C75-C74-C73	-4.02	108.45	114.94
5	A	3010	9Z9	C01-C02-C10	-3.98	104.73	110.61
6	A	3021	6OU	O30-C31-C33	3.96	120.04	111.48
5	A	3014	9Z9	C15-C14-C13	-3.95	118.35	125.02
7	A	3026	K4D	C09-C10-N12	3.93	124.96	117.32
6	A	3019	6OU	O30-C31-C33	3.91	119.93	111.48
5	A	3012	9Z9	C15-C07-C08	3.90	114.23	109.72
5	A	3010	9Z9	C02-C03-C04	3.88	108.40	104.20
5	A	3013	9Z9	C01-C02-C10	-3.88	104.88	110.61
5	A	3010	9Z9	C12-C11-C08	-3.88	107.31	111.66
5	A	3014	9Z9	C01-C02-C03	-3.85	103.21	111.58
6	A	3020	6OU	O30-C31-C33	3.85	119.80	111.48
6	A	3016	6OU	O30-C31-C33	3.83	119.77	111.48
5	A	3012	9Z9	C01-C02-C03	-3.75	103.43	111.58
5	A	3013	9Z9	C11-C13-C14	-3.75	117.46	122.93
5	A	3012	9Z9	C03-C02-C06	3.72	105.06	100.18
5	A	3012	9Z9	C10-C02-C06	3.72	112.81	107.25
5	A	3013	9Z9	C15-C07-C08	3.71	114.01	109.72
5	A	3012	9Z9	C12-C11-C08	-3.68	107.53	111.66
5	A	3011	9Z9	C01-C02-C03	-3.65	103.66	111.58
5	A	3014	9Z9	C05-C06-C02	-3.51	99.68	103.85
6	A	3018	6OU	O30-C31-C33	3.50	119.06	111.48
5	A	3013	9Z9	C01-C02-C03	-3.48	104.01	111.58
5	A	3010	9Z9	C11-C13-C14	-3.43	117.93	122.93
5	A	3011	9Z9	C02-C03-C04	3.42	107.89	104.20
5	A	3010	9Z9	C01-C02-C03	-3.42	104.15	111.58
5	A	3013	9Z9	O80-C79-C78	-3.42	107.78	112.17
5	A	3011	9Z9	C75-C74-C73	-3.38	109.48	114.94
6	A	3015	6OU	O30-C31-C33	3.37	118.77	111.48
5	A	3013	9Z9	C05-C06-C02	-3.37	99.86	103.85
5	A	3011	9Z9	C01-C02-C10	-3.34	105.69	110.61
5	A	3014	9Z9	C01-C02-C10	-3.30	105.74	110.61
5	A	3014	9Z9	C75-C74-C73	-3.29	109.63	114.94
5	A	3013	9Z9	O72-C73-C74	-3.28	100.20	104.56
5	A	3010	9Z9	C02-C03-C74	-3.25	110.90	120.50
5	A	3012	9Z9	C02-C03-C04	3.23	107.69	104.20
5	A	3011	9Z9	C76-C73-C74	-3.23	109.82	115.66
7	A	3026	K4D	C08-C09-C10	3.21	126.31	117.21
5	A	3011	9Z9	C01-C02-C06	-3.19	107.25	112.07
5	A	3013	9Z9	C02-C03-C74	-3.19	111.07	120.50
5	A	3013	9Z9	C05-C06-C07	3.18	125.70	119.53
5	A	3010	9Z9	C77-C76-C73	3.18	116.92	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3013	9Z9	C75-C74-C03	-3.17	108.16	114.50
5	A	3012	9Z9	C01-C02-C10	-3.11	106.02	110.61
5	A	3011	9Z9	C03-C02-C06	3.10	104.26	100.19
5	A	3010	9Z9	C76-C73-C74	-3.10	110.05	115.66
6	A	3022	6OU	O30-C31-C33	3.08	121.24	111.83
5	A	3010	9Z9	C08-C07-C06	-3.08	105.06	109.09
5	A	3012	9Z9	C76-C73-C74	-3.07	110.10	115.66
5	A	3013	9Z9	C77-C76-C73	3.06	116.72	111.93
5	A	3014	9Z9	C01-C02-C06	-2.99	106.25	111.68
5	A	3014	9Z9	C77-C78-C79	2.99	112.21	108.59
7	A	3026	K4D	O06-C05-C02	2.97	114.94	108.00
6	A	3016	6OU	O18-C16-C15	2.95	120.84	111.83
6	A	3023	6OU	O18-C16-C15	2.89	120.64	111.83
5	A	3011	9Z9	C02-C03-C74	-2.89	111.96	120.50
5	A	3014	9Z9	C05-C06-C07	2.88	125.11	119.53
5	A	3012	9Z9	C05-C06-C07	2.82	125.00	119.53
5	A	3013	9Z9	C12-C11-C08	-2.79	108.53	111.66
6	A	3021	6OU	O18-C16-C15	2.75	120.22	111.83
5	A	3012	9Z9	C02-C03-C74	-2.75	112.38	120.50
5	A	3014	9Z9	C15-C07-C08	2.73	112.87	109.72
5	A	3013	9Z9	C76-C73-C74	-2.72	110.73	115.66
5	A	3010	9Z9	C01-C02-C06	-2.72	106.74	111.68
7	A	3026	K4D	O21-C20-C27	-2.71	118.05	123.95
5	A	3012	9Z9	O80-C79-C78	-2.70	108.70	112.17
6	A	3018	6OU	O18-C16-C15	2.70	120.06	111.83
5	A	3014	9Z9	C02-C03-C74	-2.68	112.57	120.50
5	A	3013	9Z9	C19-C11-C13	2.66	113.33	108.74
5	A	3010	9Z9	C05-C06-C02	-2.64	100.72	103.85
6	A	3017	6OU	O30-C31-C33	2.63	119.84	111.83
5	A	3012	9Z9	C05-C06-C02	-2.61	100.75	103.85
7	A	3026	K4D	O11-C10-N12	-2.59	117.54	122.59
5	A	3012	9Z9	C09-C08-C11	-2.59	109.89	113.08
5	A	3012	9Z9	C08-C11-C13	2.56	113.40	109.65
5	A	3010	9Z9	C77-C78-C79	2.54	111.68	108.59
6	A	3022	6OU	O18-C16-C15	2.54	119.58	111.83
5	A	3010	9Z9	C03-C02-C06	2.53	103.50	100.18
5	A	3010	9Z9	C08-C11-C13	2.52	113.34	109.65
5	A	3014	9Z9	C19-C11-C08	-2.51	105.41	108.74
5	A	3014	9Z9	O72-C73-C74	-2.49	101.25	104.56
6	A	3020	6OU	O18-C16-C15	2.47	119.37	111.83
5	A	3010	9Z9	C75-C74-C03	-2.44	109.63	114.50
5	A	3011	9Z9	O72-C04-C03	2.43	108.42	105.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3012	9Z9	O72-C04-C03	2.38	108.35	105.12
5	A	3012	9Z9	C01-C02-C06	-2.37	107.37	111.68
6	A	3015	6OU	C20-O30-C31	-2.37	112.12	117.80
6	A	3019	6OU	C20-O30-C31	-2.35	114.40	117.78
5	A	3011	9Z9	C75-C74-C03	-2.30	109.91	114.50
5	A	3013	9Z9	C02-C03-C04	2.29	106.67	104.20
6	A	3019	6OU	O18-C16-C15	2.28	118.80	111.83
5	A	3011	9Z9	C05-C06-C07	2.27	124.63	114.87
5	A	3012	9Z9	C11-C08-C07	-2.22	109.47	112.71
5	A	3014	9Z9	C12-C11-C08	-2.19	109.21	111.66
5	A	3014	9Z9	C73-O72-C04	-2.18	102.11	108.14
5	A	3012	9Z9	C11-C13-C14	-2.16	119.77	122.93
5	A	3014	9Z9	C09-C08-C07	-2.16	108.76	111.78
6	A	3025	6OU	O18-C16-C15	2.14	120.21	112.14
5	A	3014	9Z9	O80-C73-C76	2.12	112.61	110.76
5	A	3010	9Z9	O72-C73-C74	-2.11	101.76	104.56
6	A	3015	6OU	O18-C16-C15	2.11	118.25	111.83
6	A	3024	6OU	O18-C16-C15	2.10	120.06	112.14
5	A	3010	9Z9	C09-C10-C02	2.08	116.25	112.74
5	A	3014	9Z9	C02-C03-C04	2.02	106.38	104.20
5	A	3013	9Z9	C09-C08-C11	-2.00	110.61	113.08
7	A	3026	K4D	O21-C20-C09	2.00	121.37	116.97

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3009	NAG	C8-C7-N2-C2
4	A	3009	NAG	O7-C7-N2-C2
5	A	3012	9Z9	C22-C21-O20-C17
5	A	3012	9Z9	C21-C22-C23-C48
6	A	3015	6OU	C15-C16-O18-C19
6	A	3015	6OU	O17-C16-O18-C19
6	A	3015	6OU	O32-C31-O30-C20
6	A	3015	6OU	C33-C31-O30-C20
6	A	3016	6OU	C21-O22-P23-O24
6	A	3016	6OU	C21-O22-P23-O25
6	A	3016	6OU	C21-O22-P23-O26
6	A	3016	6OU	O26-C27-C28-N29
6	A	3018	6OU	C33-C31-O30-C20
6	A	3019	6OU	O18-C19-C20-O30
6	A	3020	6OU	C27-O26-P23-O22

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Mol	Chain	Res	Type	Atoms
6	A	3020	6OU	C27-O26-P23-O24
6	A	3020	6OU	C27-O26-P23-O25
6	A	3020	6OU	O26-C27-C28-N29
6	A	3021	6OU	O26-C27-C28-N29
7	A	3026	K4D	F01-C02-C05-O06
7	A	3026	K4D	F04-C02-C05-O06
6	A	3021	6OU	O17-C16-O18-C19
6	A	3021	6OU	C15-C16-O18-C19
6	A	3018	6OU	O32-C31-O30-C20
6	A	3023	6OU	O32-C31-O30-C20
7	A	3026	K4D	F03-C02-C05-O06
6	A	3023	6OU	C33-C31-O30-C20
6	A	3018	6OU	O17-C16-O18-C19
6	A	3024	6OU	C06-C07-C08-C09
7	A	3026	K4D	C09-C10-N12-C13
6	A	3018	6OU	C15-C16-O18-C19
4	A	3003	NAG	O5-C5-C6-O6
7	A	3026	K4D	O11-C10-N12-C13
6	A	3015	6OU	C11-C12-C13-C14
6	A	3019	6OU	C15-C16-O18-C19
6	A	3017	6OU	C33-C34-C35-C36
6	A	3018	6OU	C13-C14-C15-C16
4	A	3003	NAG	C4-C5-C6-O6
4	A	3009	NAG	O5-C5-C6-O6
6	A	3019	6OU	O17-C16-O18-C19
6	A	3021	6OU	O32-C31-O30-C20
6	A	3024	6OU	C04-C05-C06-C07
6	A	3016	6OU	C33-C31-O30-C20
6	A	3021	6OU	C33-C31-O30-C20
6	A	3016	6OU	O32-C31-O30-C20
6	A	3025	6OU	C12-C13-C14-C15
6	A	3016	6OU	C13-C14-C15-C16
6	A	3020	6OU	C31-C33-C34-C35
7	A	3026	K4D	C20-C09-C10-N12
6	A	3020	6OU	C10-C11-C12-C13
6	A	3015	6OU	C31-C33-C34-C35
6	A	3019	6OU	C31-C33-C34-C35
6	A	3017	6OU	C34-C35-C36-C37
6	A	3018	6OU	C34-C35-C36-C37
6	A	3020	6OU	C33-C31-O30-C20
6	A	3015	6OU	C37-C38-C39-C40
6	A	3020	6OU	O32-C31-O30-C20

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Mol	Chain	Res	Type	Atoms
7	A	3026	K4D	C20-C09-C10-O11
6	A	3019	6OU	C12-C13-C14-C15
6	A	3015	6OU	C10-C11-C12-C13
7	A	3026	K4D	C02-C05-O06-C07
6	A	3018	6OU	O18-C19-C20-C21
6	A	3017	6OU	C37-C38-C39-C40
6	A	3025	6OU	C11-C12-C13-C14
6	A	3022	6OU	C15-C16-O18-C19
6	A	3015	6OU	O30-C20-C21-O22
6	A	3020	6OU	C15-C16-O18-C19
6	A	3018	6OU	C09-C10-C11-C12
6	A	3018	6OU	C33-C34-C35-C36
6	A	3020	6OU	C35-C36-C37-C38
6	A	3022	6OU	C13-C14-C15-C16
6	A	3025	6OU	C13-C14-C15-C16
6	A	3016	6OU	C08-C09-C10-C11
6	A	3020	6OU	C08-C09-C10-C11
6	A	3019	6OU	O18-C19-C20-C21
6	A	3019	6OU	C06-C07-C08-C09
6	A	3021	6OU	C11-C12-C13-C14
6	A	3016	6OU	C09-C10-C11-C12
6	A	3022	6OU	O17-C16-O18-C19
6	A	3020	6OU	C36-C37-C38-C39
6	A	3015	6OU	C08-C09-C10-C11
6	A	3015	6OU	C35-C36-C37-C38
6	A	3018	6OU	C10-C11-C12-C13
6	A	3020	6OU	O17-C16-O18-C19
6	A	3015	6OU	C19-C20-C21-O22
6	A	3019	6OU	C14-C15-C16-O18
6	A	3022	6OU	C11-C12-C13-C14
6	A	3018	6OU	O18-C19-C20-O30
6	A	3016	6OU	C33-C34-C35-C36
6	A	3016	6OU	C11-C12-C13-C14
6	A	3019	6OU	C10-C11-C12-C13
6	A	3016	6OU	C37-C38-C39-C40
6	A	3024	6OU	C08-C09-C10-C11
6	A	3016	6OU	C19-C20-C21-O22
6	A	3021	6OU	O18-C19-C20-O30
6	A	3021	6OU	O18-C19-C20-C21
6	A	3021	6OU	C21-O22-P23-O24
6	A	3022	6OU	C10-C11-C12-C13
6	A	3019	6OU	C34-C35-C36-C37

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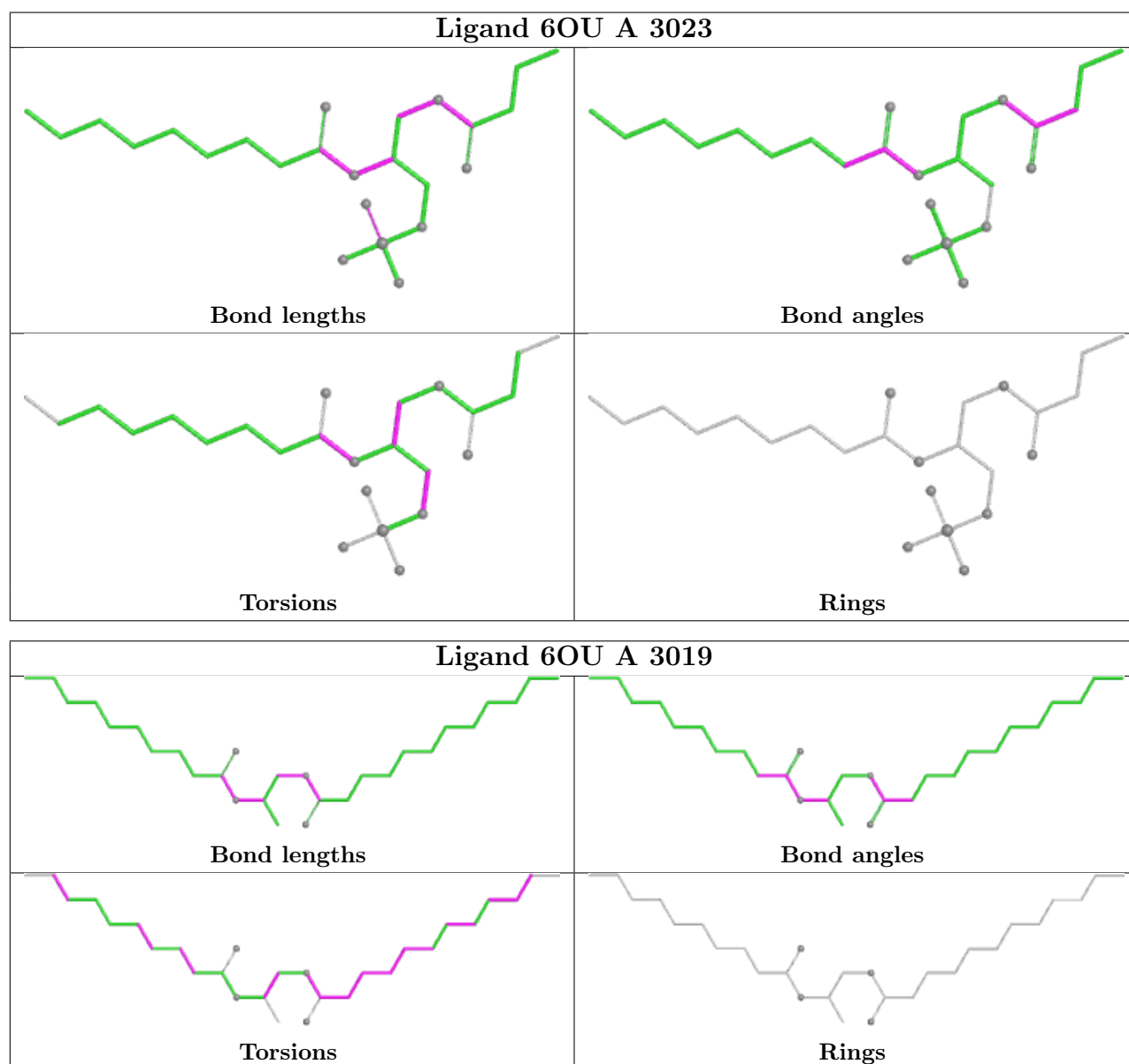
Mol	Chain	Res	Type	Atoms
6	A	3018	6OU	C38-C39-C40-C41
6	A	3022	6OU	C14-C15-C16-O18
6	A	3019	6OU	C08-C09-C10-C11
5	A	3012	9Z9	C21-C22-C23-C24
6	A	3016	6OU	O18-C19-C20-O30
6	A	3023	6OU	O18-C19-C20-O30
6	A	3019	6OU	C11-C12-C13-C14
6	A	3019	6OU	C38-C39-C40-C41
6	A	3023	6OU	C20-C21-O22-P23
6	A	3015	6OU	C34-C35-C36-C37
6	A	3017	6OU	C31-C33-C34-C35
6	A	3016	6OU	C38-C39-C40-C41
6	A	3016	6OU	C36-C37-C38-C39
7	A	3026	K4D	C14-C13-N12-C10
6	A	3017	6OU	C38-C39-C40-C41
6	A	3018	6OU	O30-C20-C21-O22
6	A	3016	6OU	O30-C20-C21-O22
6	A	3020	6OU	C12-C13-C14-C15
6	A	3020	6OU	C38-C39-C40-C41
6	A	3022	6OU	C38-C39-C40-C41
6	A	3020	6OU	O30-C20-C21-O22
6	A	3019	6OU	C05-C06-C07-C08
6	A	3022	6OU	C40-C41-C42-C43
6	A	3016	6OU	C07-C08-C09-C10
6	A	3024	6OU	C11-C12-C13-C14
6	A	3019	6OU	C13-C14-C15-C16
6	A	3015	6OU	C38-C39-C40-C41
6	A	3015	6OU	C14-C15-C16-O18
6	A	3019	6OU	C14-C15-C16-O17
6	A	3015	6OU	C14-C15-C16-O17

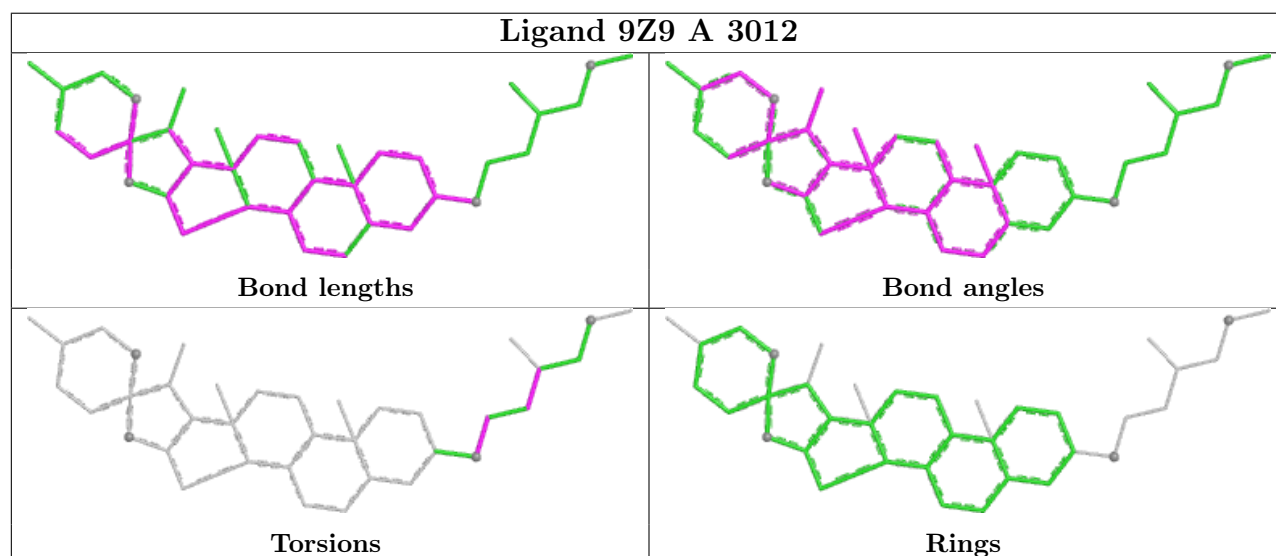
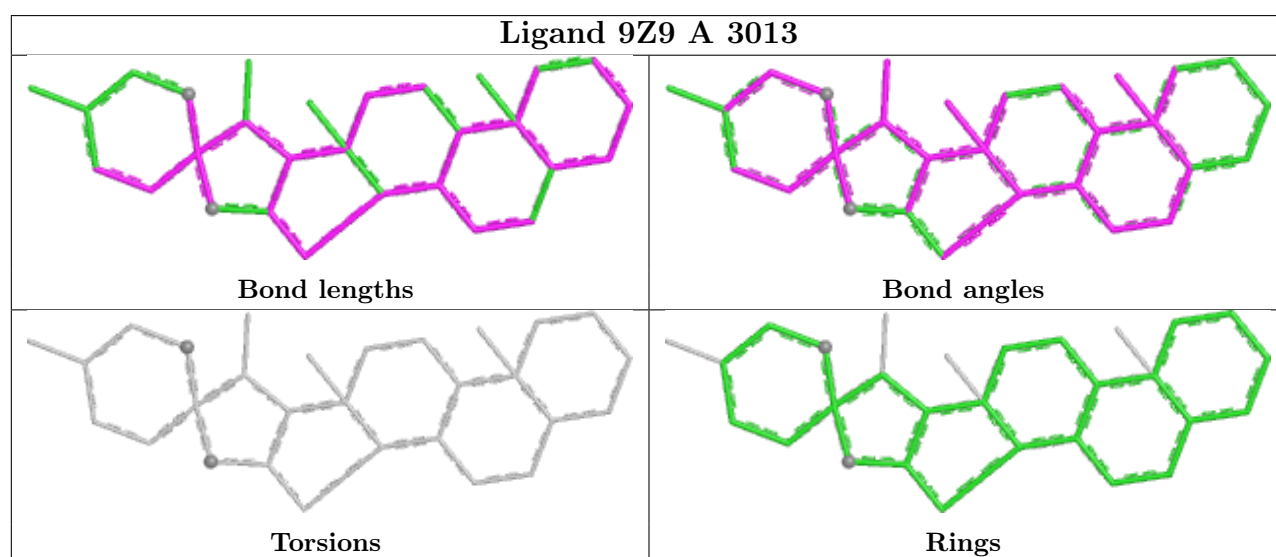
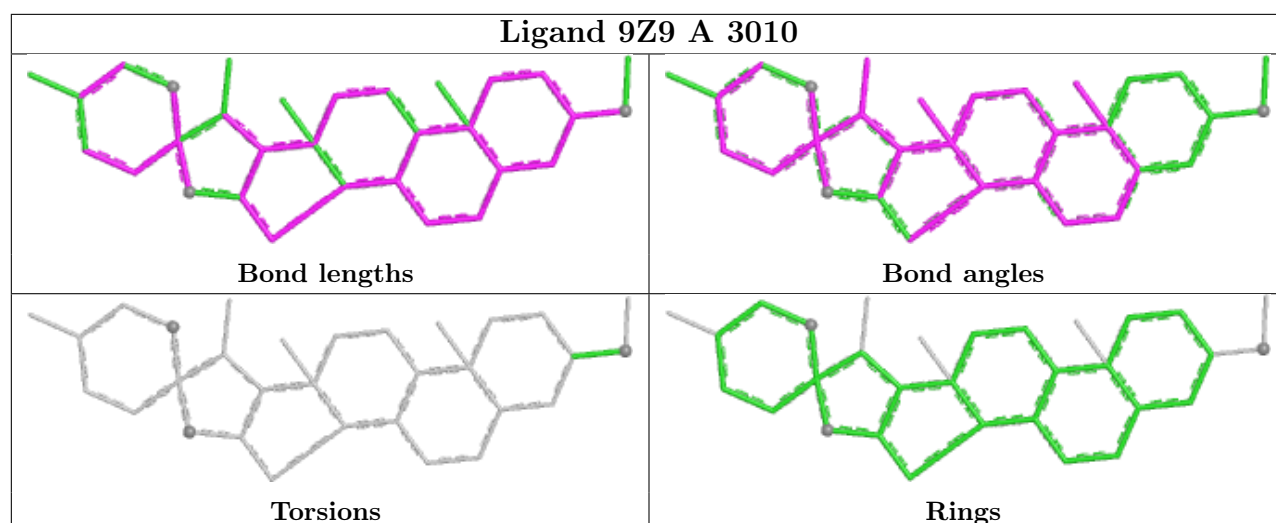
There are no ring outliers.

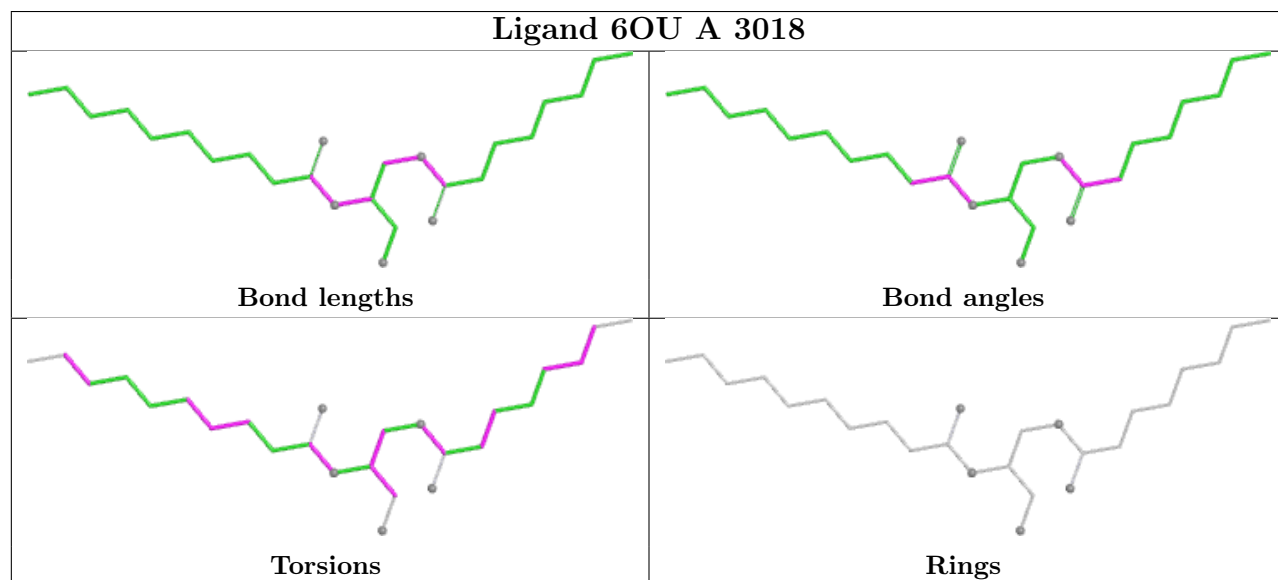
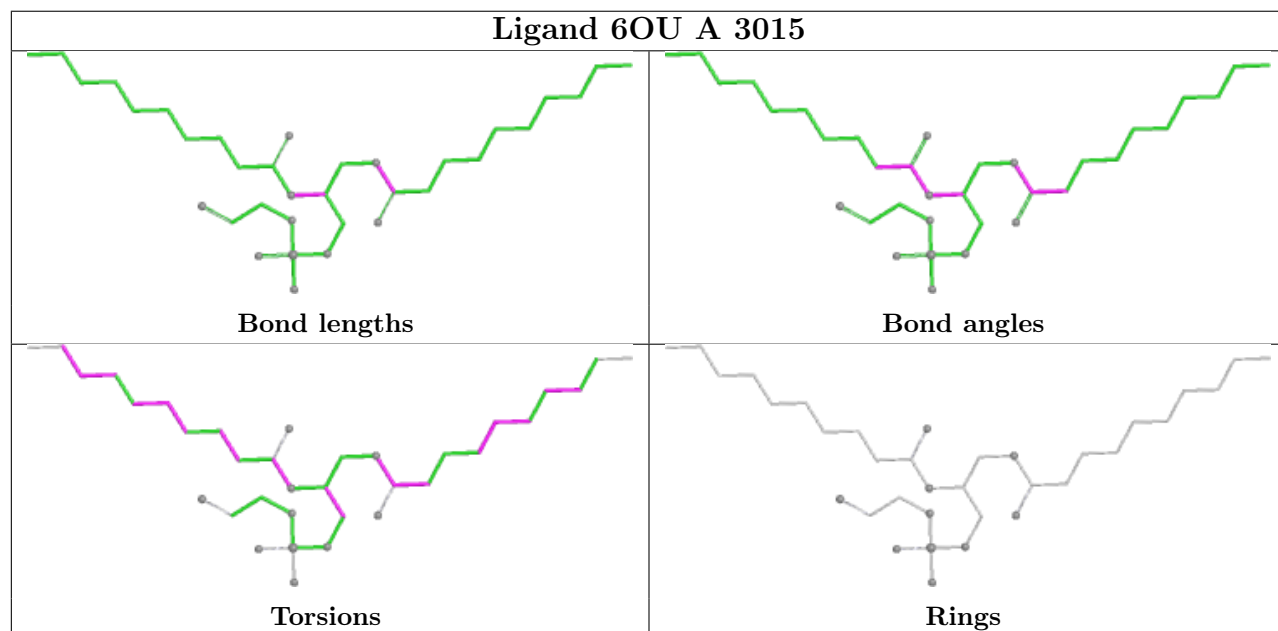
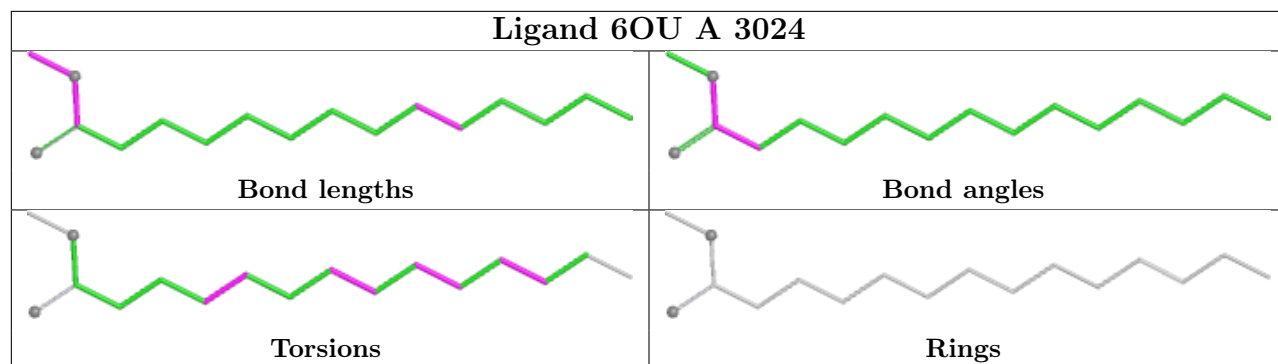
7 monomers are involved in 39 short contacts:

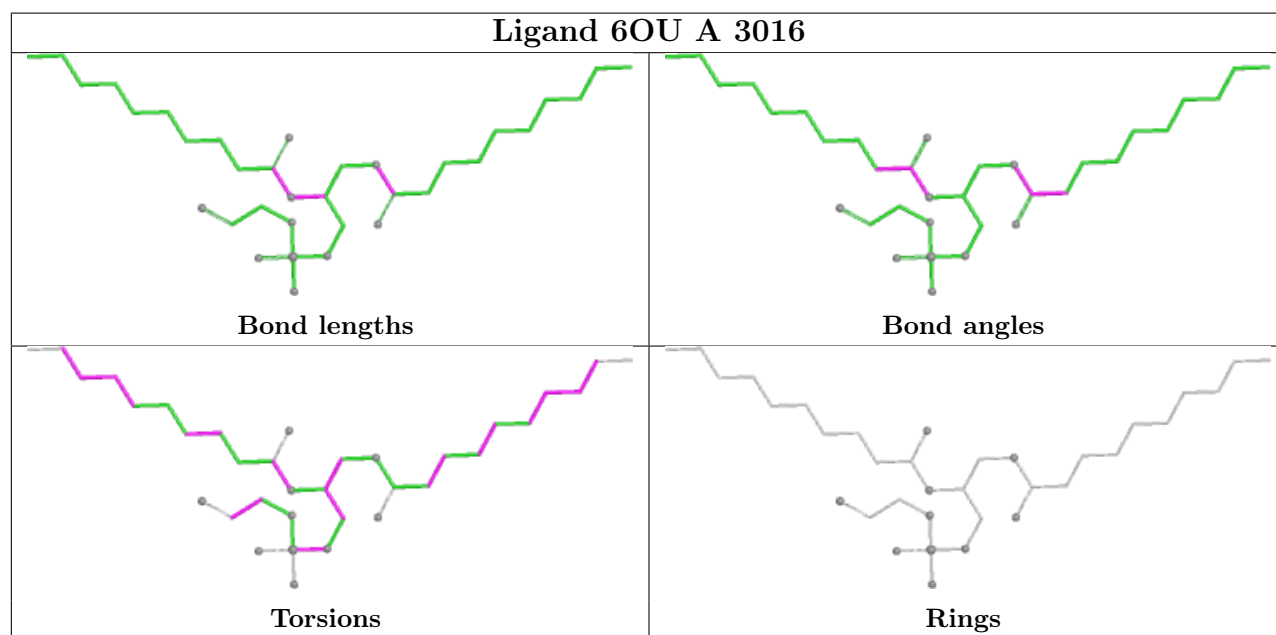
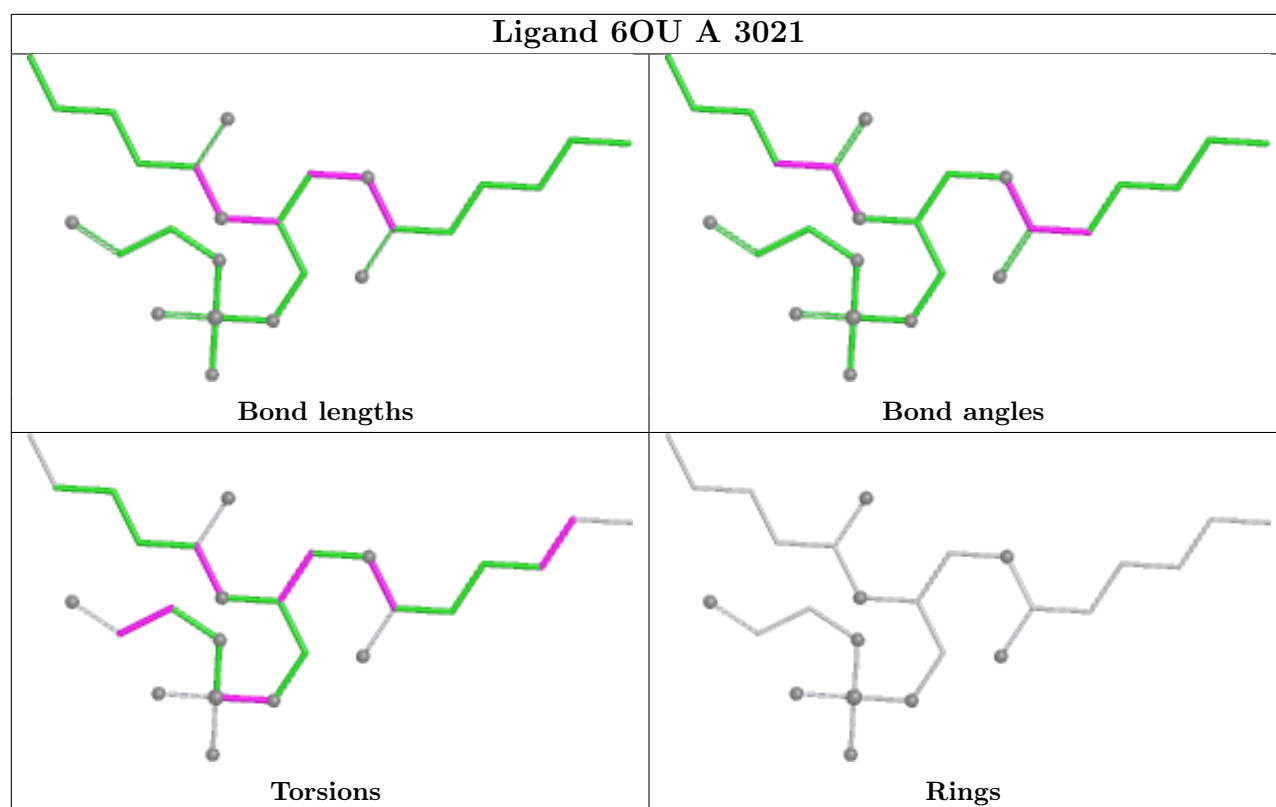
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3009	NAG	14	0
5	A	3010	9Z9	7	0
5	A	3013	9Z9	1	0
5	A	3012	9Z9	1	0
5	A	3011	9Z9	1	0
7	A	3026	K4D	3	0
5	A	3014	9Z9	12	0

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.

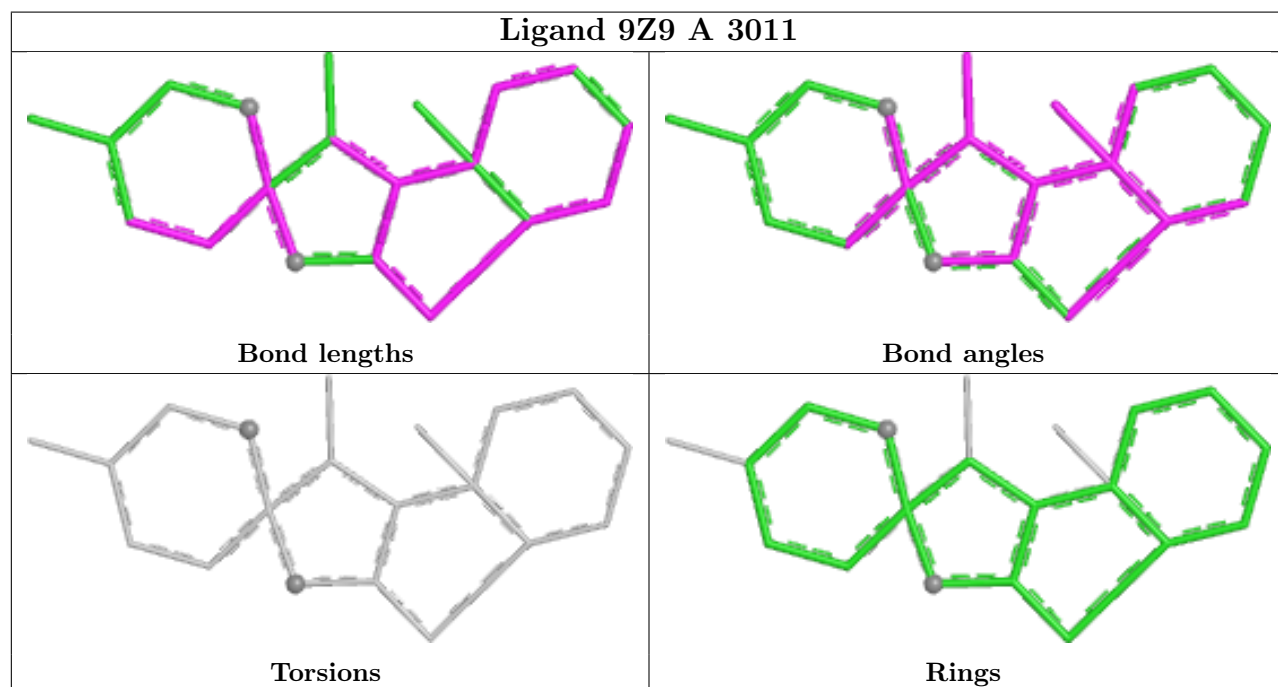
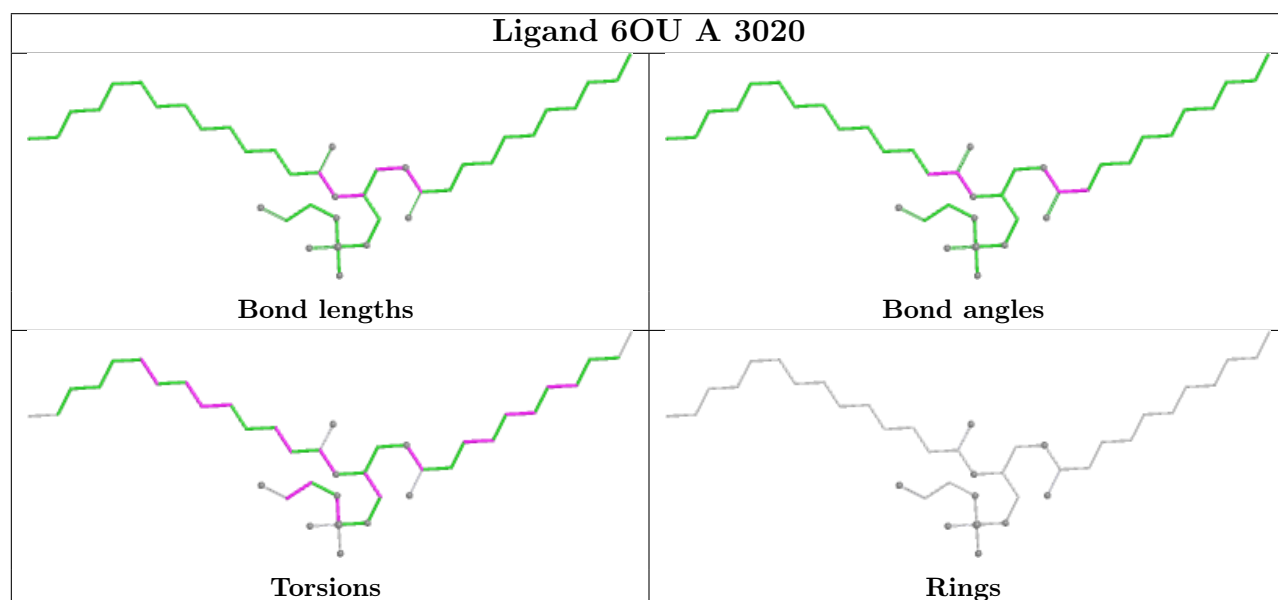
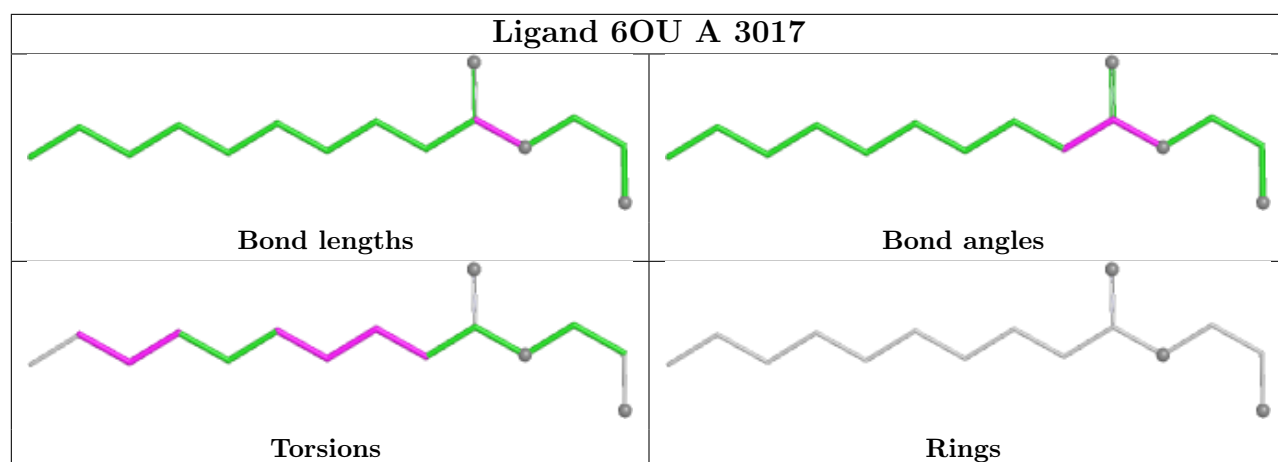


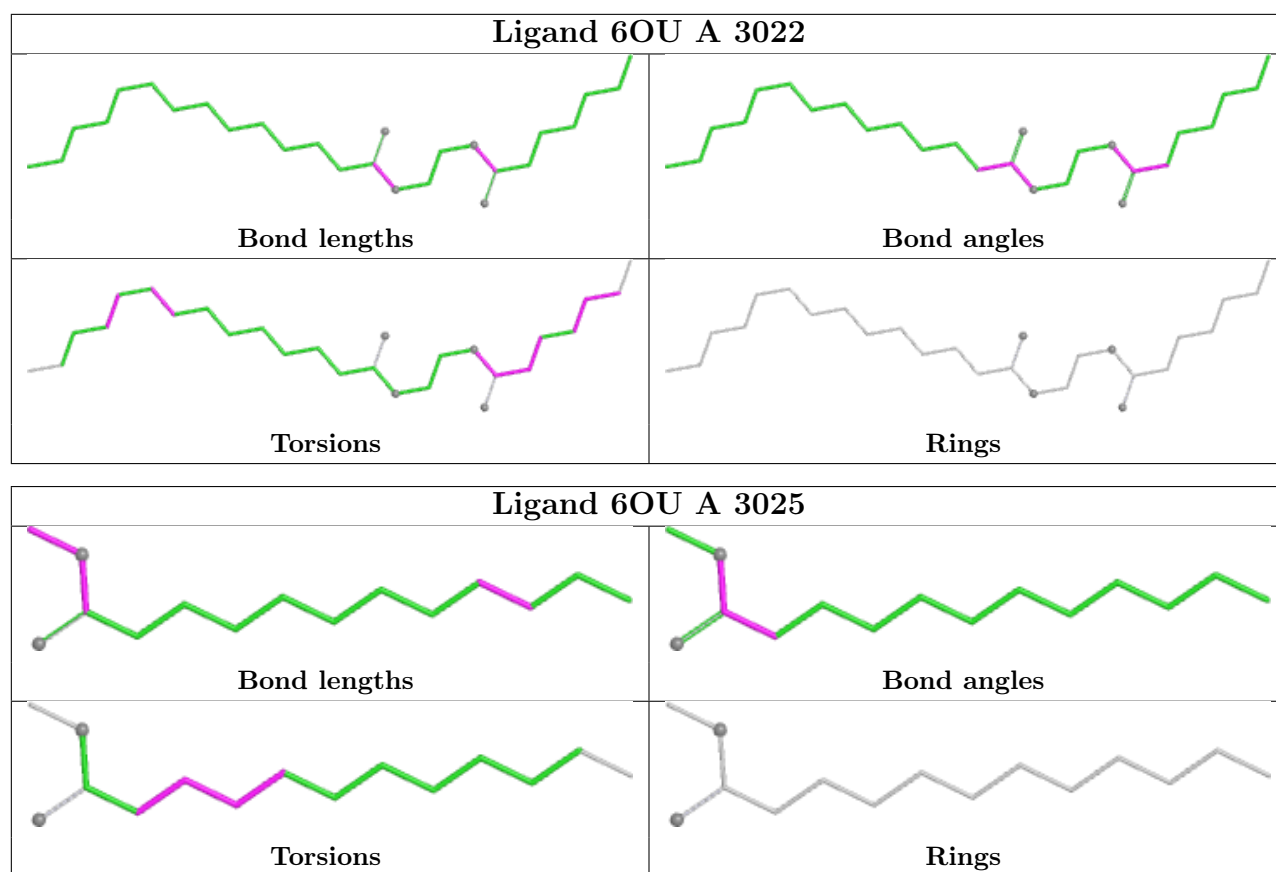




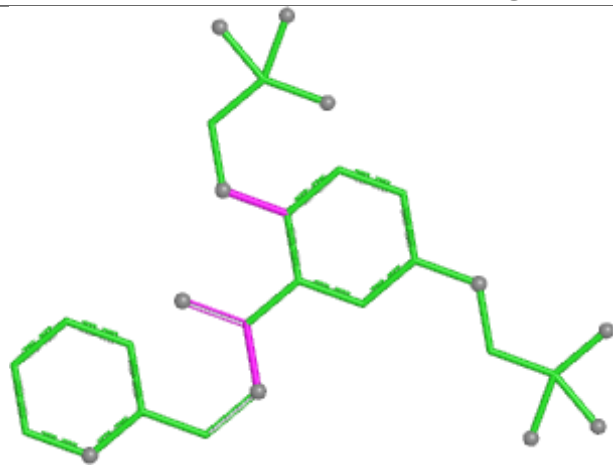




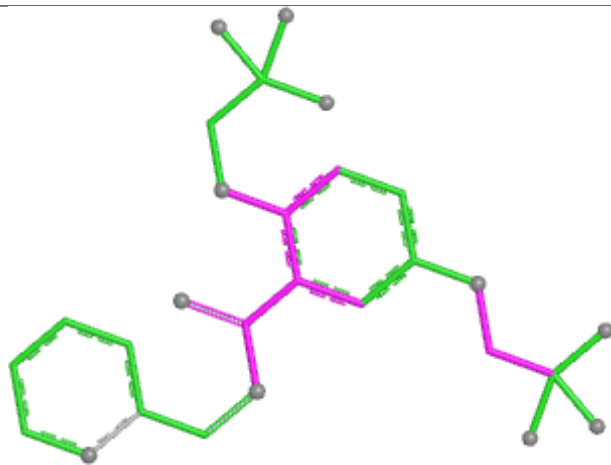




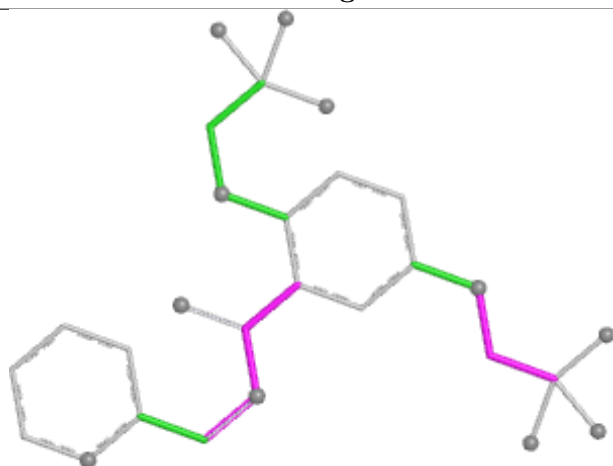
## Ligand K4D A 3026



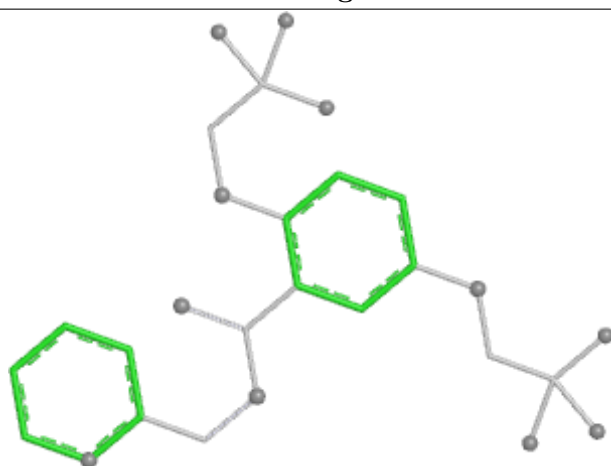
Bond lengths



Bond angles

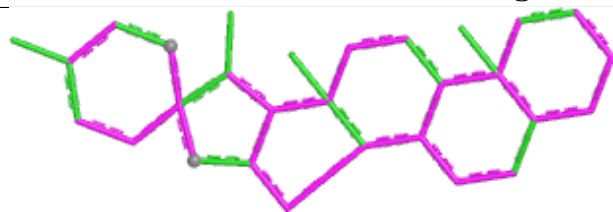


Torsions

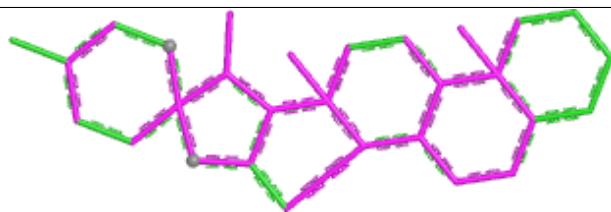


Rings

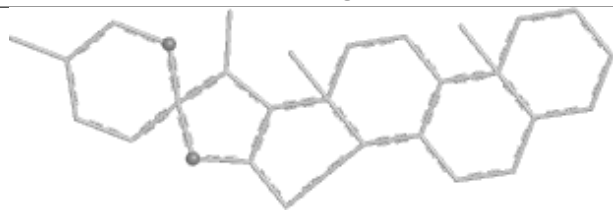
## Ligand 9Z9 A 3014



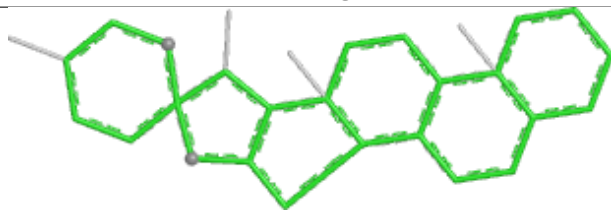
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

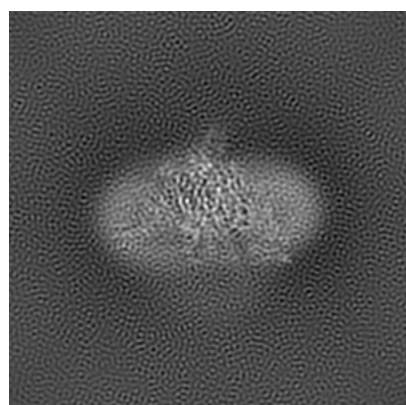
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20949. These allow visual inspection of the internal detail of the map and identification of artifacts.

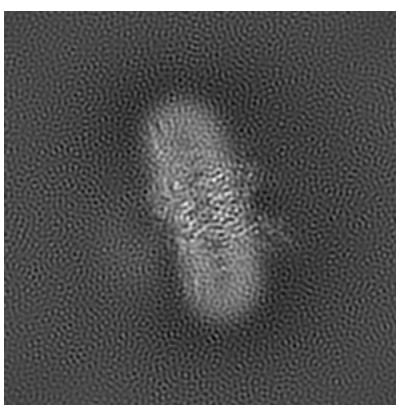
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

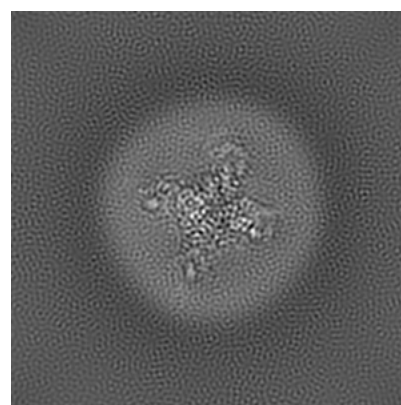
#### 6.1.1 Primary map



X



Y

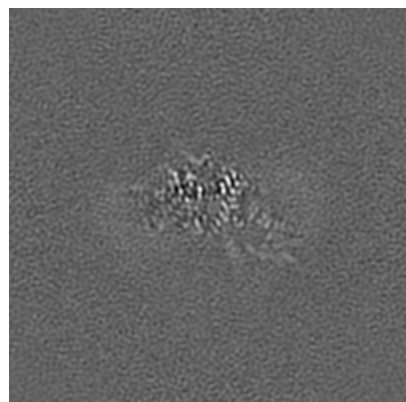


Z

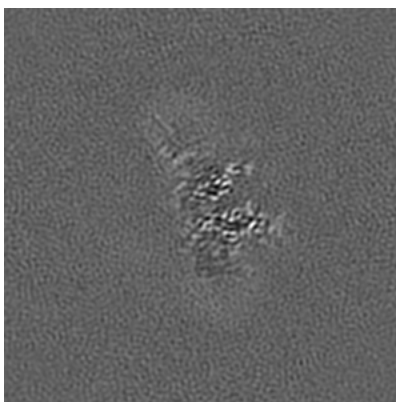
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

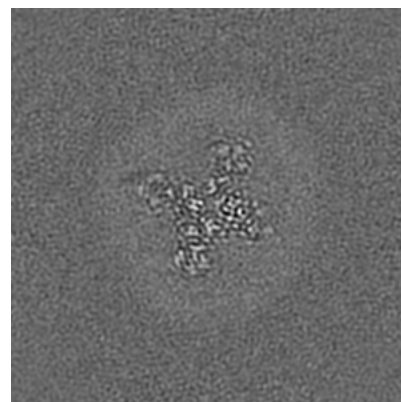
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

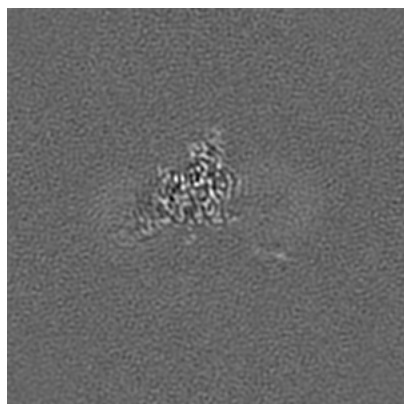


Z Index: 128

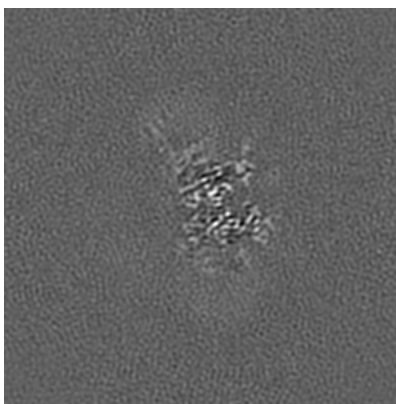
The images above show central slices of the map in three orthogonal directions.

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

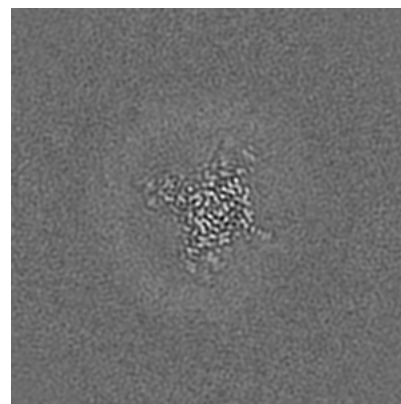
### 6.3.1 Primary map



X Index: 119



Y Index: 125

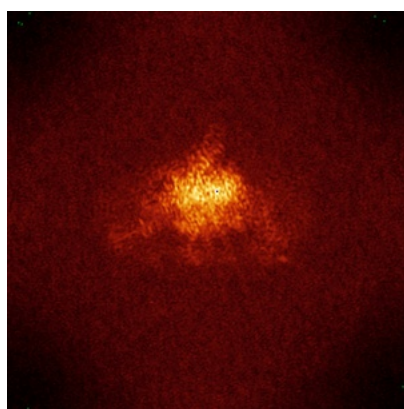


Z Index: 138

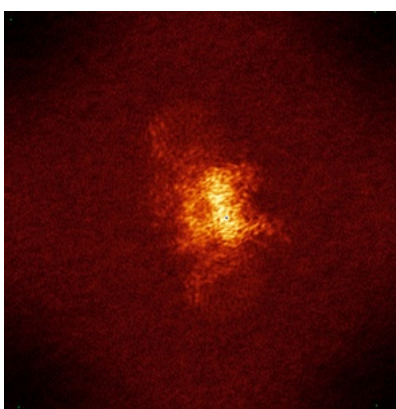
The images above show the largest variance slices of the map in three orthogonal directions.

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

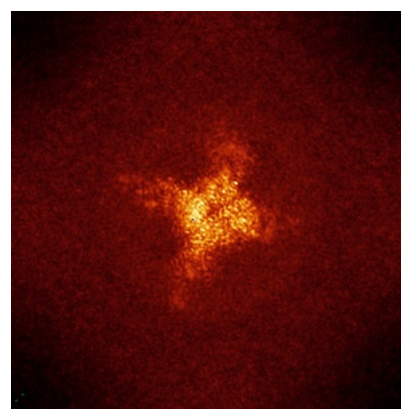
### 6.4.1 Primary map



X



Y

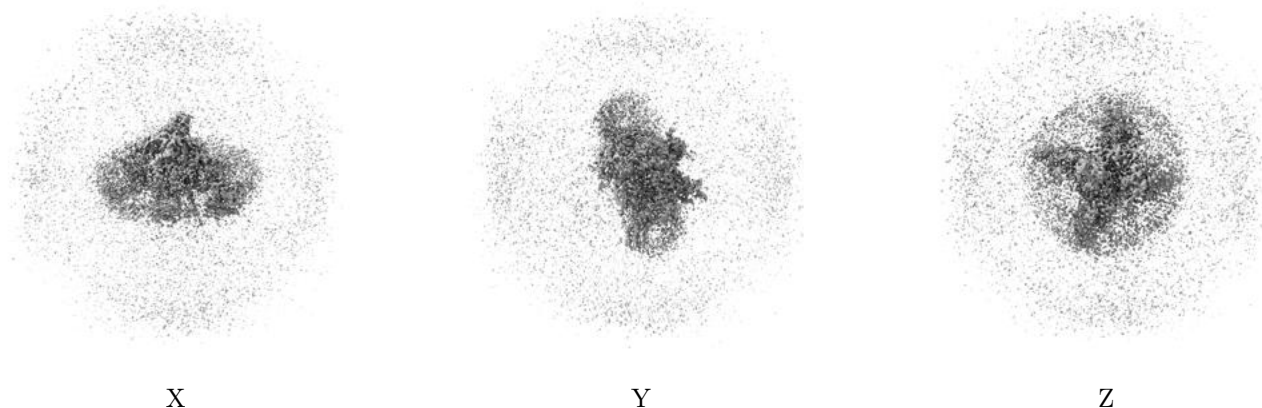


Z

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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

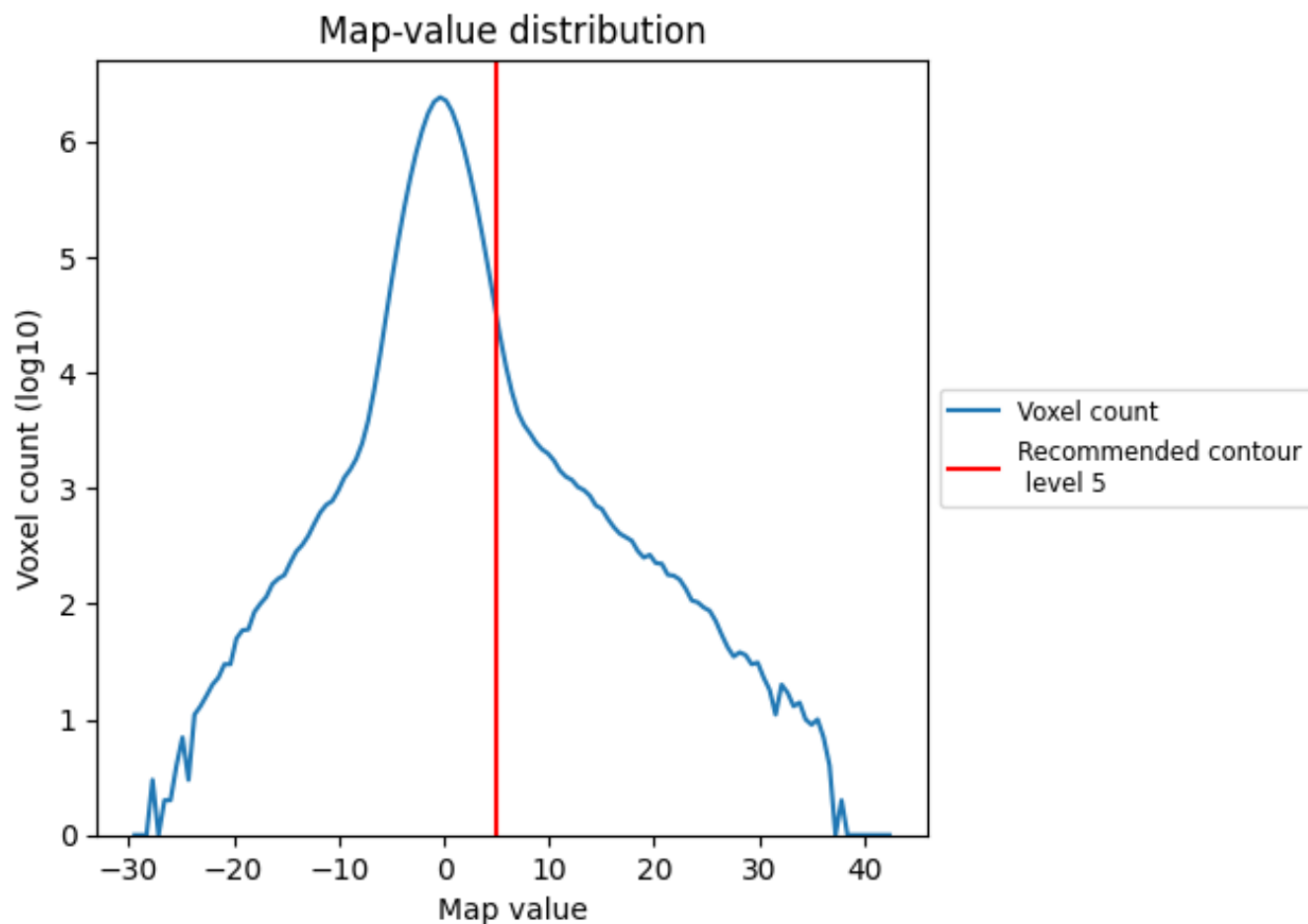
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

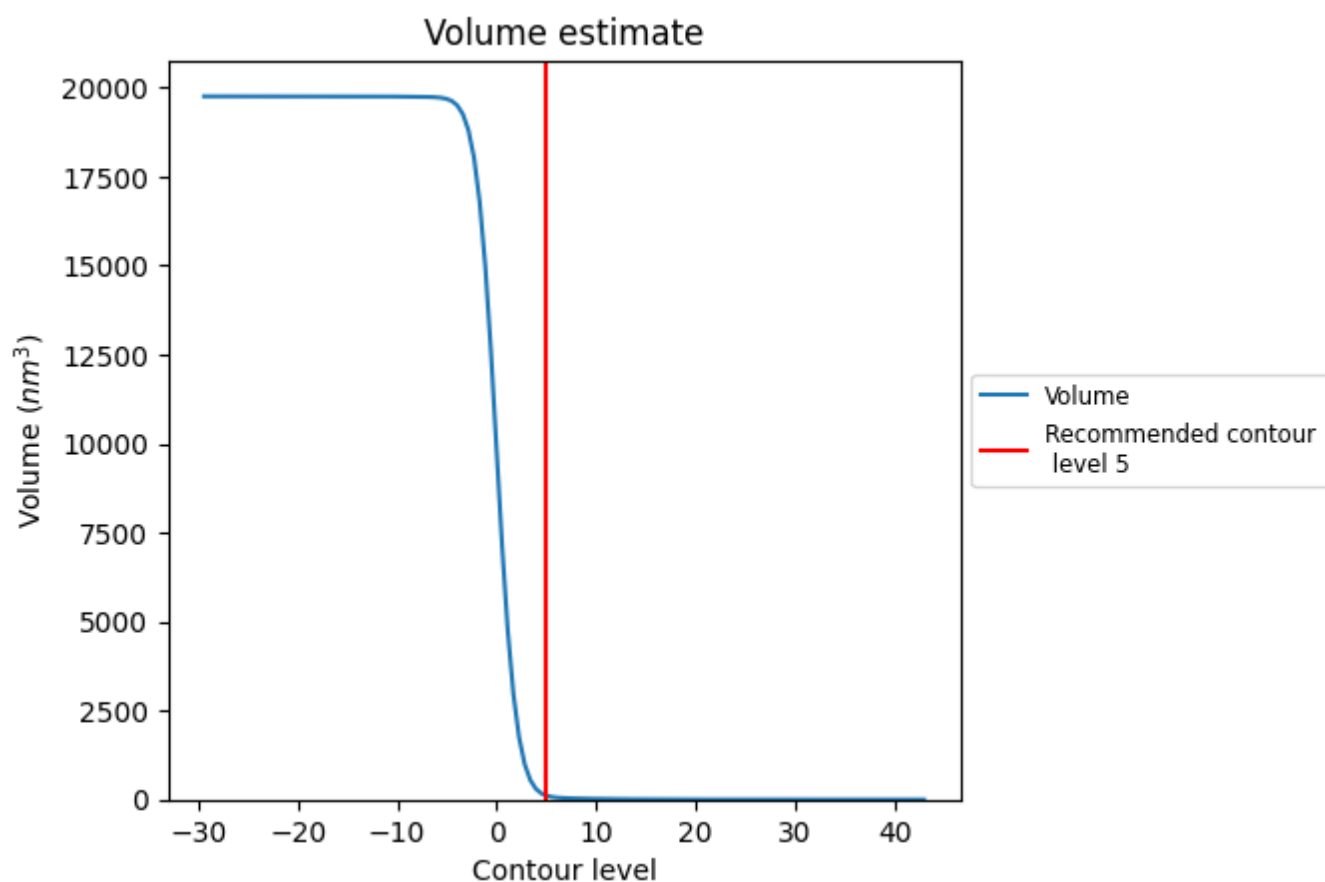
### 7.1 Map-value distribution [i](#)



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.



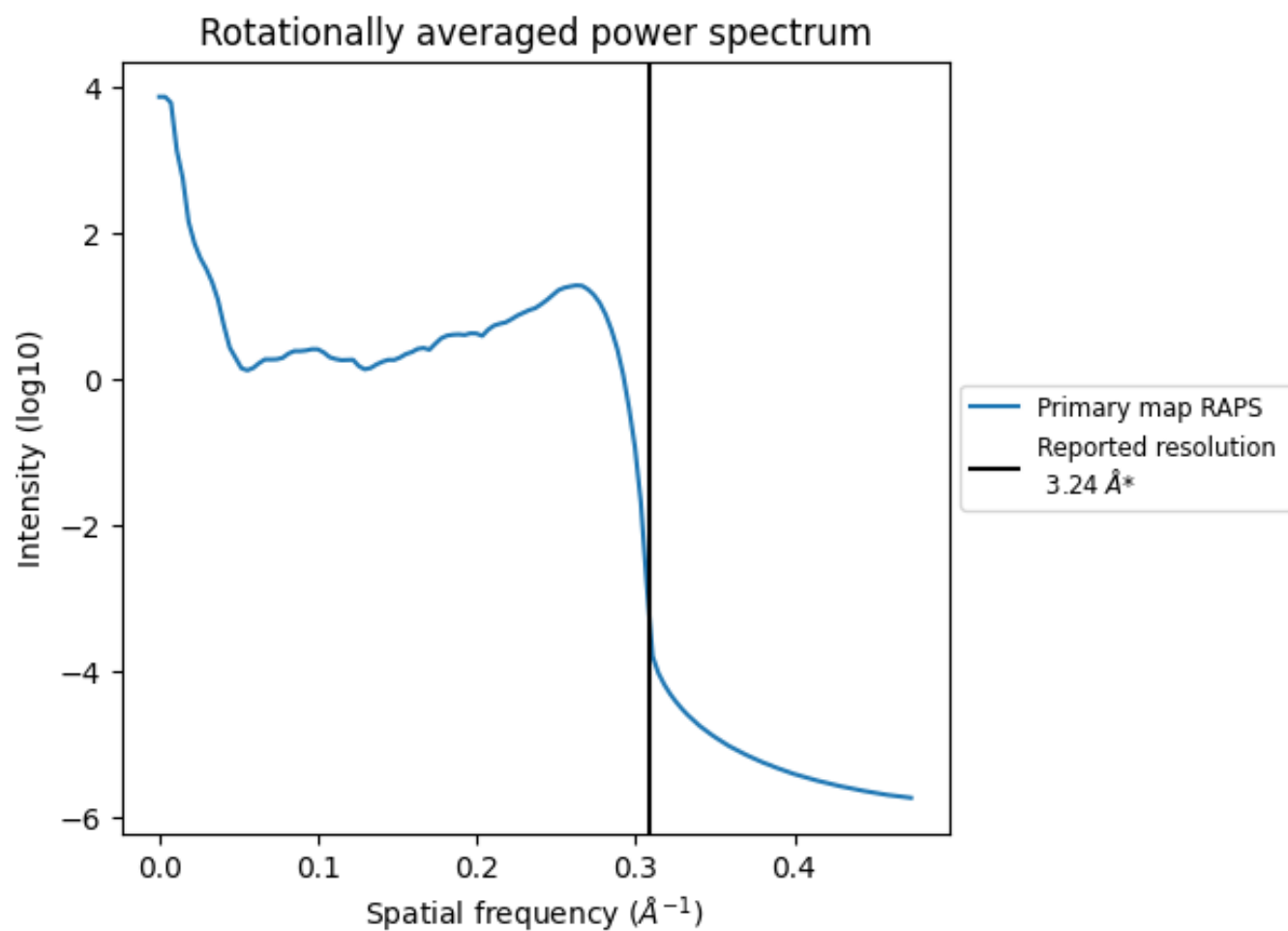
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111  $\text{nm}^3$ ; this corresponds to an approximate mass of 100 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 ⓘ

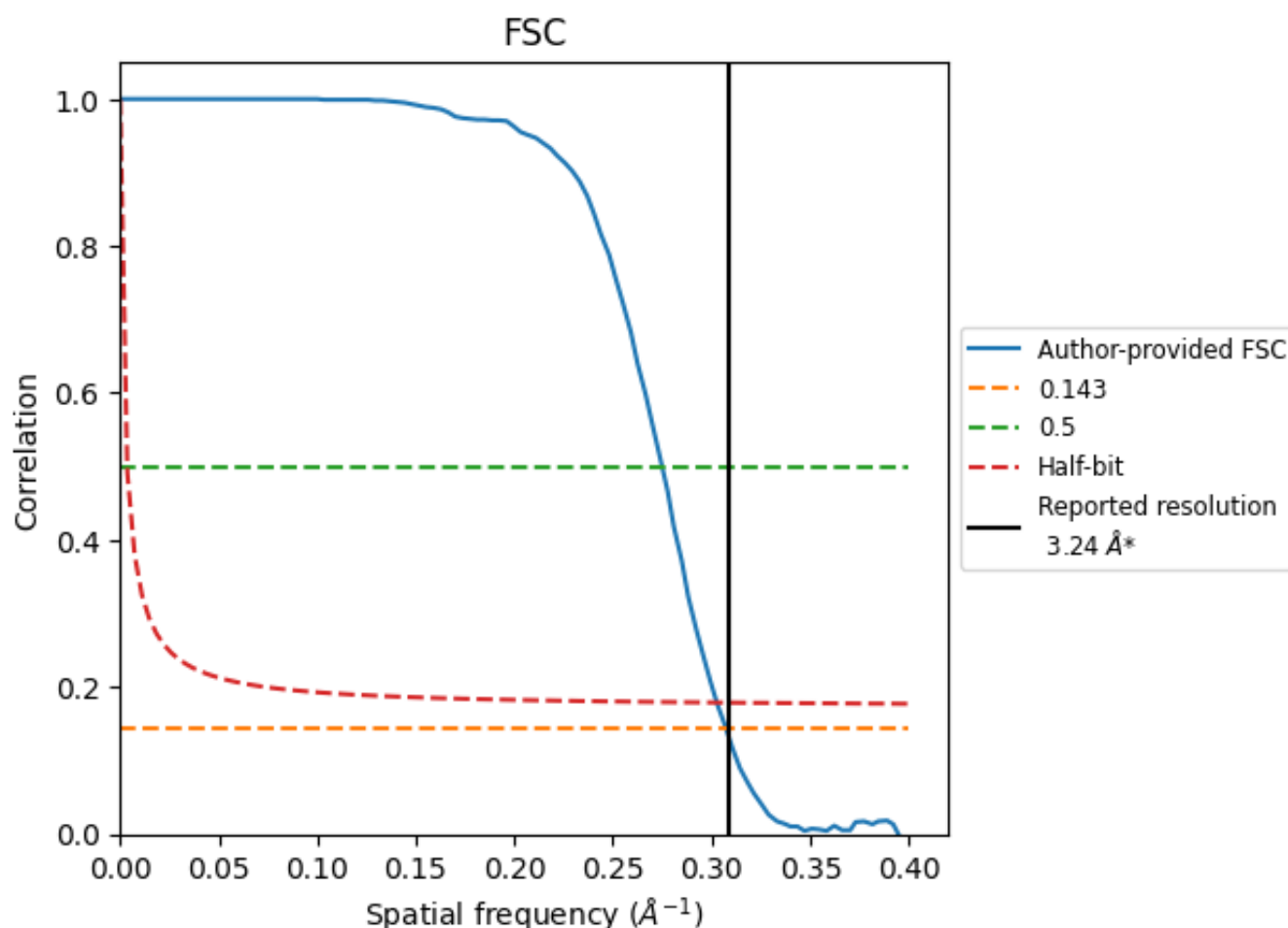


\*Reported resolution corresponds to spatial frequency of 0.309 Å<sup>-1</sup>

## 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  $0.309 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

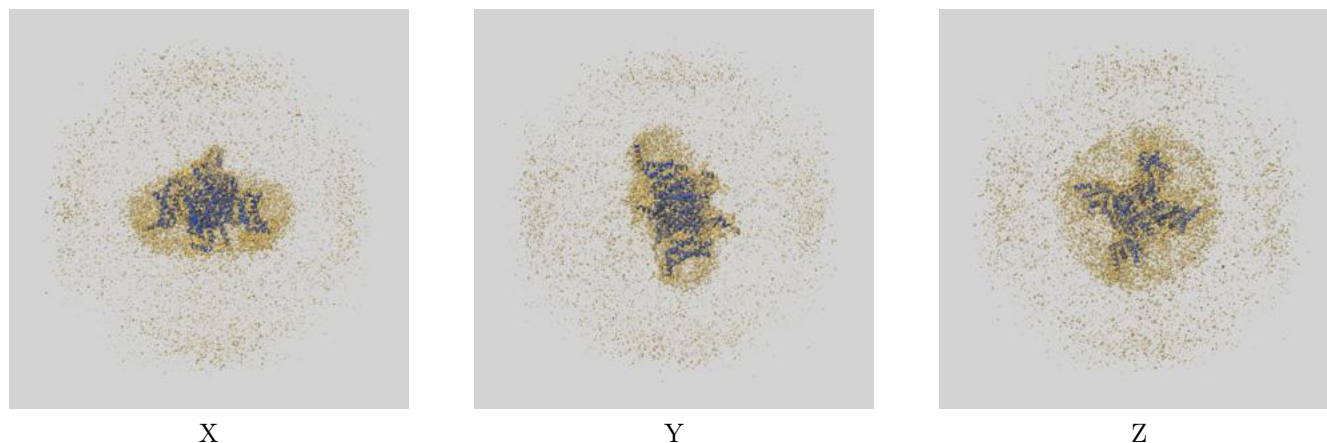
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.25	3.64	3.30
Unmasked-calculated*	-	-	-

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

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

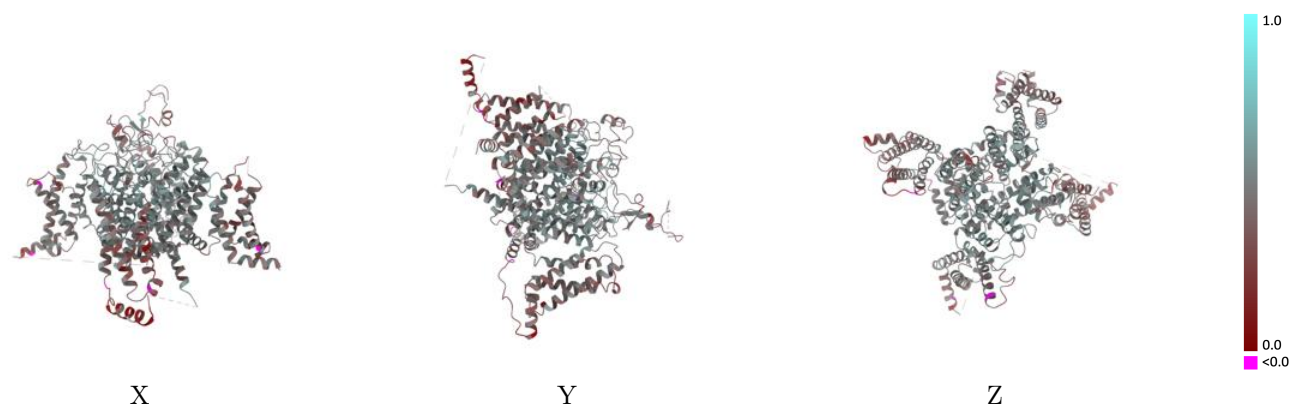
This section contains information regarding the fit between EMDB map EMD-20949 and PDB model 6UZ0. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



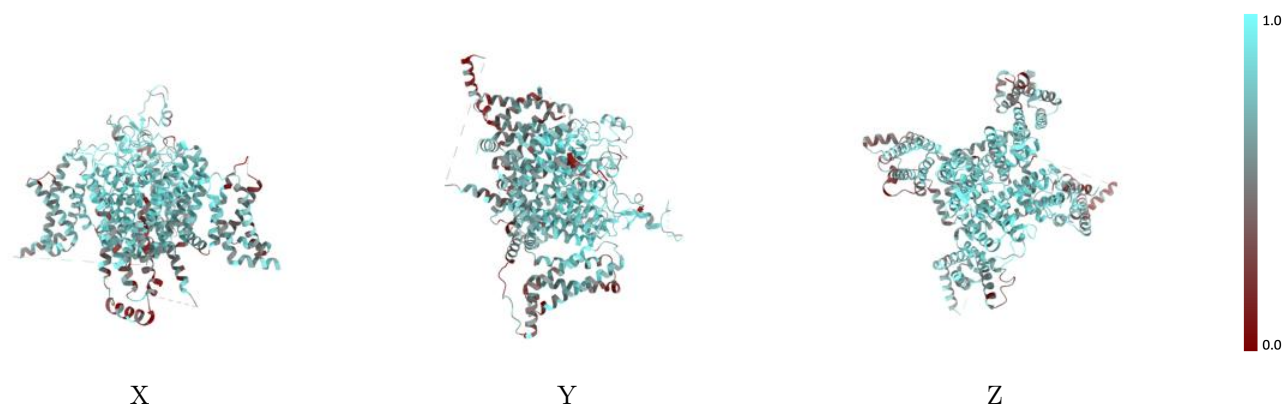
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



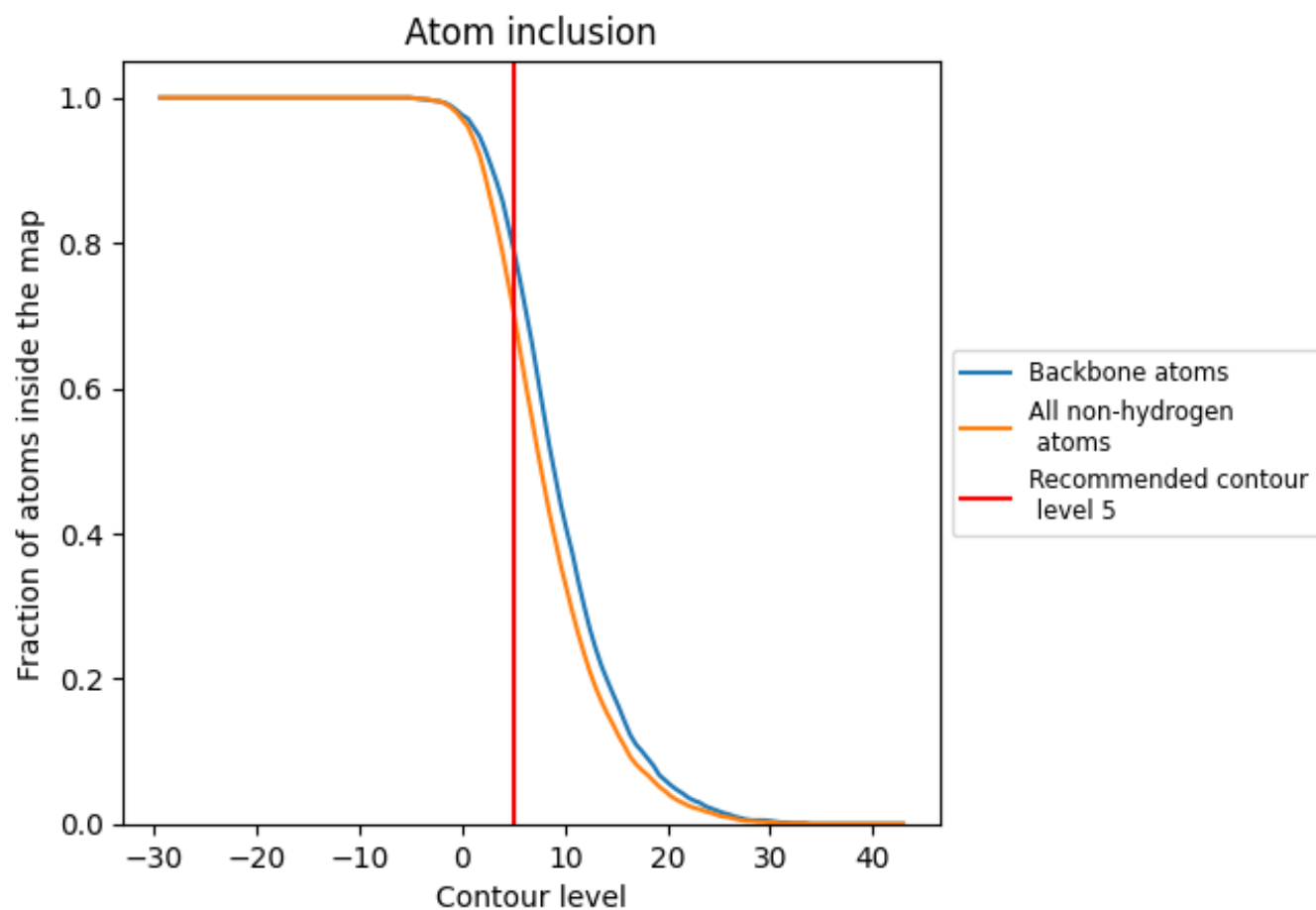
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7060	<div></div> 0.4590
A	<div></div> 0.7060	<div></div> 0.4590
B	<div></div> 0.6430	<div></div> 0.4370
C	<div></div> 0.7440	<div></div> 0.4520
D	<div></div> 0.6430	<div></div> 0.3460

