



Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 05:12 PM EDT

PDB ID : 8THF
EMDB ID : EMD-41260
Title : SARS-CoV-2 BA.1 S-6P-no-RBD
Authors : Bu, F.; Li, F.; Liu, B.
Deposited on : 2023-07-15
Resolution : 2.83 Å (reported)
Based on initial model : 7TGW

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.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

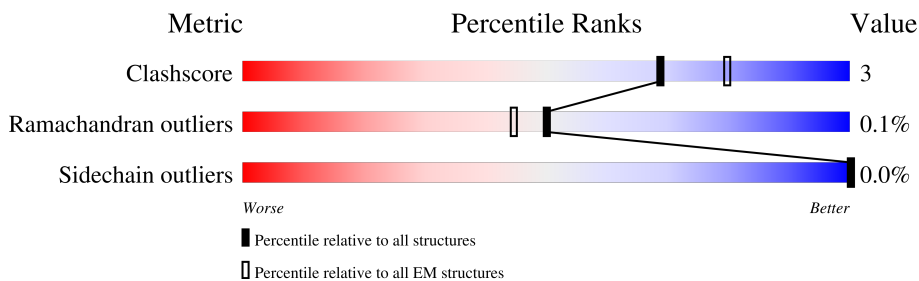
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



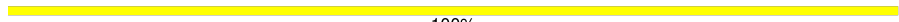
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	1037	
1	B	1037	
1	C	1037	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21515 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 Spike protein S1,Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	900	7041	4499	1172	1338	32	2	0
1	B	890	6955	4445	1155	1323	32	2	0
1	C	892	6973	4456	1162	1323	32	2	0

There are 219 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	325	ARG	-	linker	UNP P0DTC2
A	326	PHE	-	linker	UNP P0DTC2
A	327	PRO	-	linker	UNP P0DTC2
A	350	LYS	THR	conflict	UNP P0DTC2
A	417	GLY	ASP	conflict	UNP P0DTC2
A	458	TYR	HIS	conflict	UNP P0DTC2
A	482	LYS	ASN	conflict	UNP P0DTC2
A	484	HIS	PRO	conflict	UNP P0DTC2
A	485	GLY	ARG	conflict	UNP P0DTC2
A	486	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	488	SER	ARG	conflict	UNP P0DTC2
A	567	LYS	ASN	conflict	UNP P0DTC2
A	599	TYR	ASP	conflict	UNP P0DTC2
A	620	PRO	PHE	conflict	UNP P0DTC2
A	659	LYS	ASN	conflict	UNP P0DTC2
A	695	PRO	ALA	conflict	UNP P0DTC2
A	702	PRO	ALA	conflict	UNP P0DTC2
A	745	PRO	ALA	conflict	UNP P0DTC2
A	757	HIS	GLN	conflict	UNP P0DTC2
A	772	LYS	ASN	conflict	UNP P0DTC2
A	784	PHE	LEU	conflict	UNP P0DTC2
A	789	PRO	LYS	conflict	UNP P0DTC2
A	790	PRO	VAL	conflict	UNP P0DTC2
A	1015	GLY	-	expression tag	UNP P0DTC2
A	1016	SER	-	expression tag	UNP P0DTC2
A	1017	GLY	-	expression tag	UNP P0DTC2
A	1018	TYR	-	expression tag	UNP P0DTC2
A	1019	ILE	-	expression tag	UNP P0DTC2
A	1020	PRO	-	expression tag	UNP P0DTC2
A	1021	GLU	-	expression tag	UNP P0DTC2
A	1022	ALA	-	expression tag	UNP P0DTC2
A	1023	PRO	-	expression tag	UNP P0DTC2
A	1024	ARG	-	expression tag	UNP P0DTC2
A	1025	ASP	-	expression tag	UNP P0DTC2
A	1026	GLY	-	expression tag	UNP P0DTC2
A	1027	GLN	-	expression tag	UNP P0DTC2
A	1028	ALA	-	expression tag	UNP P0DTC2
A	1029	TYR	-	expression tag	UNP P0DTC2
A	1030	VAL	-	expression tag	UNP P0DTC2
A	1031	ARG	-	expression tag	UNP P0DTC2
A	1032	LYS	-	expression tag	UNP P0DTC2
A	1033	ASP	-	expression tag	UNP P0DTC2
A	1034	GLY	-	expression tag	UNP P0DTC2
A	1035	GLU	-	expression tag	UNP P0DTC2
A	1036	TRP	-	expression tag	UNP P0DTC2
A	1037	VAL	-	expression tag	UNP P0DTC2
A	1038	LEU	-	expression tag	UNP P0DTC2
A	1039	LEU	-	expression tag	UNP P0DTC2
A	1040	SER	-	expression tag	UNP P0DTC2
A	1041	THR	-	expression tag	UNP P0DTC2
A	1042	PHE	-	expression tag	UNP P0DTC2
A	1043	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1044	GLY	-	expression tag	UNP P0DTC2
A	1045	HIS	-	expression tag	UNP P0DTC2
A	1046	HIS	-	expression tag	UNP P0DTC2
A	1047	HIS	-	expression tag	UNP P0DTC2
A	1048	HIS	-	expression tag	UNP P0DTC2
A	1049	HIS	-	expression tag	UNP P0DTC2
A	1050	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	conflict	UNP P0DTC2
B	206	ILE	-	insertion	UNP P0DTC2
B	207	VAL	-	insertion	UNP P0DTC2
B	208	ARG	ASN	conflict	UNP P0DTC2
B	209	GLU	LEU	conflict	UNP P0DTC2
B	210	PRO	VAL	conflict	UNP P0DTC2
B	211	GLU	ARG	conflict	UNP P0DTC2
B	325	ARG	-	linker	UNP P0DTC2
B	326	PHE	-	linker	UNP P0DTC2
B	327	PRO	-	linker	UNP P0DTC2
B	350	LYS	THR	conflict	UNP P0DTC2
B	417	GLY	ASP	conflict	UNP P0DTC2
B	458	TYR	HIS	conflict	UNP P0DTC2
B	482	LYS	ASN	conflict	UNP P0DTC2
B	484	HIS	PRO	conflict	UNP P0DTC2
B	485	GLY	ARG	conflict	UNP P0DTC2
B	486	SER	ARG	conflict	UNP P0DTC2
B	488	SER	ARG	conflict	UNP P0DTC2
B	567	LYS	ASN	conflict	UNP P0DTC2
B	599	TYR	ASP	conflict	UNP P0DTC2
B	620	PRO	PHE	conflict	UNP P0DTC2
B	659	LYS	ASN	conflict	UNP P0DTC2
B	695	PRO	ALA	conflict	UNP P0DTC2
B	702	PRO	ALA	conflict	UNP P0DTC2
B	745	PRO	ALA	conflict	UNP P0DTC2
B	757	HIS	GLN	conflict	UNP P0DTC2
B	772	LYS	ASN	conflict	UNP P0DTC2
B	784	PHE	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	789	PRO	LYS	conflict	UNP P0DTC2
B	790	PRO	VAL	conflict	UNP P0DTC2
B	1015	GLY	-	expression tag	UNP P0DTC2
B	1016	SER	-	expression tag	UNP P0DTC2
B	1017	GLY	-	expression tag	UNP P0DTC2
B	1018	TYR	-	expression tag	UNP P0DTC2
B	1019	ILE	-	expression tag	UNP P0DTC2
B	1020	PRO	-	expression tag	UNP P0DTC2
B	1021	GLU	-	expression tag	UNP P0DTC2
B	1022	ALA	-	expression tag	UNP P0DTC2
B	1023	PRO	-	expression tag	UNP P0DTC2
B	1024	ARG	-	expression tag	UNP P0DTC2
B	1025	ASP	-	expression tag	UNP P0DTC2
B	1026	GLY	-	expression tag	UNP P0DTC2
B	1027	GLN	-	expression tag	UNP P0DTC2
B	1028	ALA	-	expression tag	UNP P0DTC2
B	1029	TYR	-	expression tag	UNP P0DTC2
B	1030	VAL	-	expression tag	UNP P0DTC2
B	1031	ARG	-	expression tag	UNP P0DTC2
B	1032	LYS	-	expression tag	UNP P0DTC2
B	1033	ASP	-	expression tag	UNP P0DTC2
B	1034	GLY	-	expression tag	UNP P0DTC2
B	1035	GLU	-	expression tag	UNP P0DTC2
B	1036	TRP	-	expression tag	UNP P0DTC2
B	1037	VAL	-	expression tag	UNP P0DTC2
B	1038	LEU	-	expression tag	UNP P0DTC2
B	1039	LEU	-	expression tag	UNP P0DTC2
B	1040	SER	-	expression tag	UNP P0DTC2
B	1041	THR	-	expression tag	UNP P0DTC2
B	1042	PHE	-	expression tag	UNP P0DTC2
B	1043	LEU	-	expression tag	UNP P0DTC2
B	1044	GLY	-	expression tag	UNP P0DTC2
B	1045	HIS	-	expression tag	UNP P0DTC2
B	1046	HIS	-	expression tag	UNP P0DTC2
B	1047	HIS	-	expression tag	UNP P0DTC2
B	1048	HIS	-	expression tag	UNP P0DTC2
B	1049	HIS	-	expression tag	UNP P0DTC2
B	1050	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	conflict	UNP P0DTC2
C	206	ILE	-	insertion	UNP P0DTC2
C	207	VAL	-	insertion	UNP P0DTC2
C	208	ARG	ASN	conflict	UNP P0DTC2
C	209	GLU	LEU	conflict	UNP P0DTC2
C	210	PRO	VAL	conflict	UNP P0DTC2
C	211	GLU	ARG	conflict	UNP P0DTC2
C	325	ARG	-	linker	UNP P0DTC2
C	326	PHE	-	linker	UNP P0DTC2
C	327	PRO	-	linker	UNP P0DTC2
C	350	LYS	THR	conflict	UNP P0DTC2
C	417	GLY	ASP	conflict	UNP P0DTC2
C	458	TYR	HIS	conflict	UNP P0DTC2
C	482	LYS	ASN	conflict	UNP P0DTC2
C	484	HIS	PRO	conflict	UNP P0DTC2
C	485	GLY	ARG	conflict	UNP P0DTC2
C	486	SER	ARG	conflict	UNP P0DTC2
C	488	SER	ARG	conflict	UNP P0DTC2
C	567	LYS	ASN	conflict	UNP P0DTC2
C	599	TYR	ASP	conflict	UNP P0DTC2
C	620	PRO	PHE	conflict	UNP P0DTC2
C	659	LYS	ASN	conflict	UNP P0DTC2
C	695	PRO	ALA	conflict	UNP P0DTC2
C	702	PRO	ALA	conflict	UNP P0DTC2
C	745	PRO	ALA	conflict	UNP P0DTC2
C	757	HIS	GLN	conflict	UNP P0DTC2
C	772	LYS	ASN	conflict	UNP P0DTC2
C	784	PHE	LEU	conflict	UNP P0DTC2
C	789	PRO	LYS	conflict	UNP P0DTC2
C	790	PRO	VAL	conflict	UNP P0DTC2
C	1015	GLY	-	expression tag	UNP P0DTC2
C	1016	SER	-	expression tag	UNP P0DTC2
C	1017	GLY	-	expression tag	UNP P0DTC2
C	1018	TYR	-	expression tag	UNP P0DTC2
C	1019	ILE	-	expression tag	UNP P0DTC2
C	1020	PRO	-	expression tag	UNP P0DTC2
C	1021	GLU	-	expression tag	UNP P0DTC2
C	1022	ALA	-	expression tag	UNP P0DTC2
C	1023	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1024	ARG	-	expression tag	UNP P0DTC2
C	1025	ASP	-	expression tag	UNP P0DTC2
C	1026	GLY	-	expression tag	UNP P0DTC2
C	1027	GLN	-	expression tag	UNP P0DTC2
C	1028	ALA	-	expression tag	UNP P0DTC2
C	1029	TYR	-	expression tag	UNP P0DTC2
C	1030	VAL	-	expression tag	UNP P0DTC2
C	1031	ARG	-	expression tag	UNP P0DTC2
C	1032	LYS	-	expression tag	UNP P0DTC2
C	1033	ASP	-	expression tag	UNP P0DTC2
C	1034	GLY	-	expression tag	UNP P0DTC2
C	1035	GLU	-	expression tag	UNP P0DTC2
C	1036	TRP	-	expression tag	UNP P0DTC2
C	1037	VAL	-	expression tag	UNP P0DTC2
C	1038	LEU	-	expression tag	UNP P0DTC2
C	1039	LEU	-	expression tag	UNP P0DTC2
C	1040	SER	-	expression tag	UNP P0DTC2
C	1041	THR	-	expression tag	UNP P0DTC2
C	1042	PHE	-	expression tag	UNP P0DTC2
C	1043	LEU	-	expression tag	UNP P0DTC2
C	1044	GLY	-	expression tag	UNP P0DTC2
C	1045	HIS	-	expression tag	UNP P0DTC2
C	1046	HIS	-	expression tag	UNP P0DTC2
C	1047	HIS	-	expression tag	UNP P0DTC2
C	1048	HIS	-	expression tag	UNP P0DTC2
C	1049	HIS	-	expression tag	UNP P0DTC2
C	1050	HIS	-	expression tag	UNP P0DTC2

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



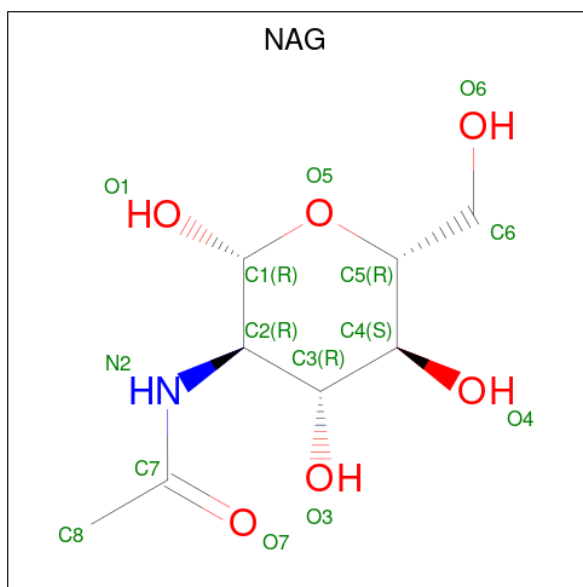
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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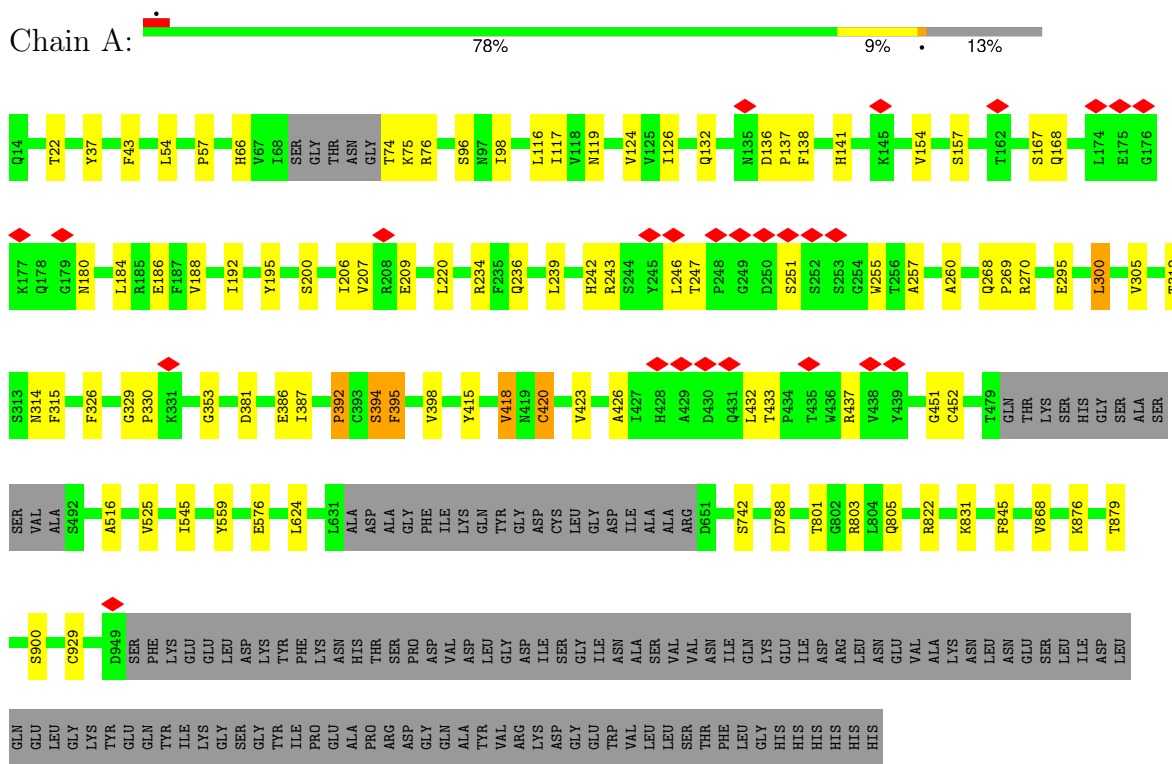
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total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

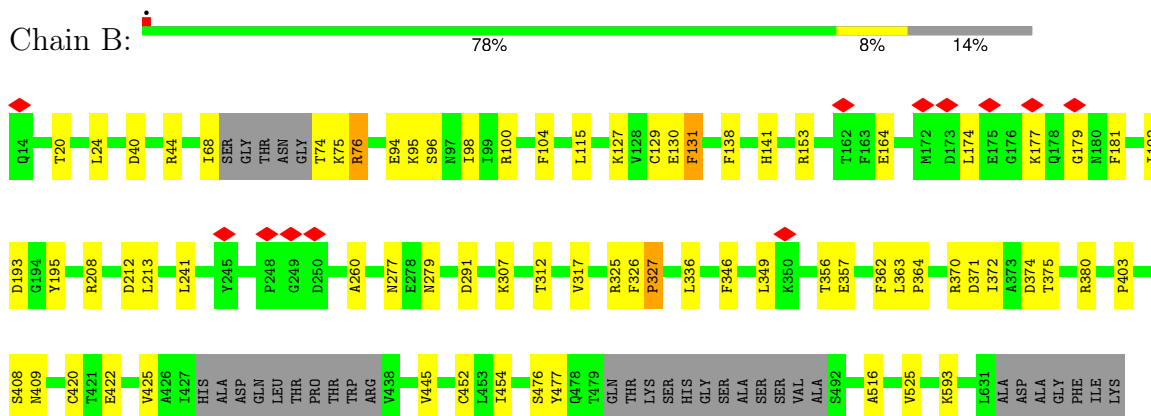
3 Residue-property plots

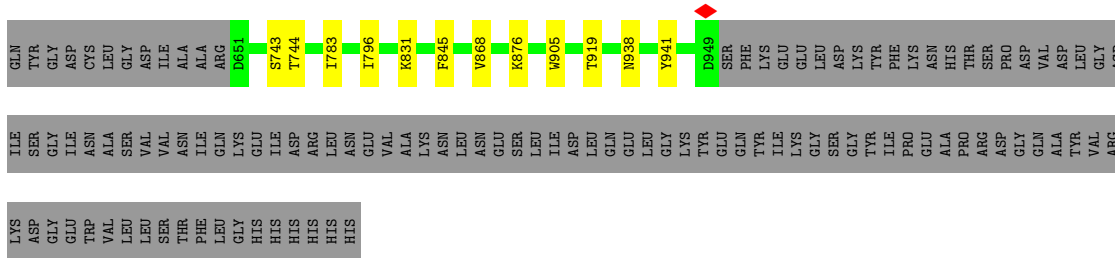
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike protein S1,Spike glycoprotein

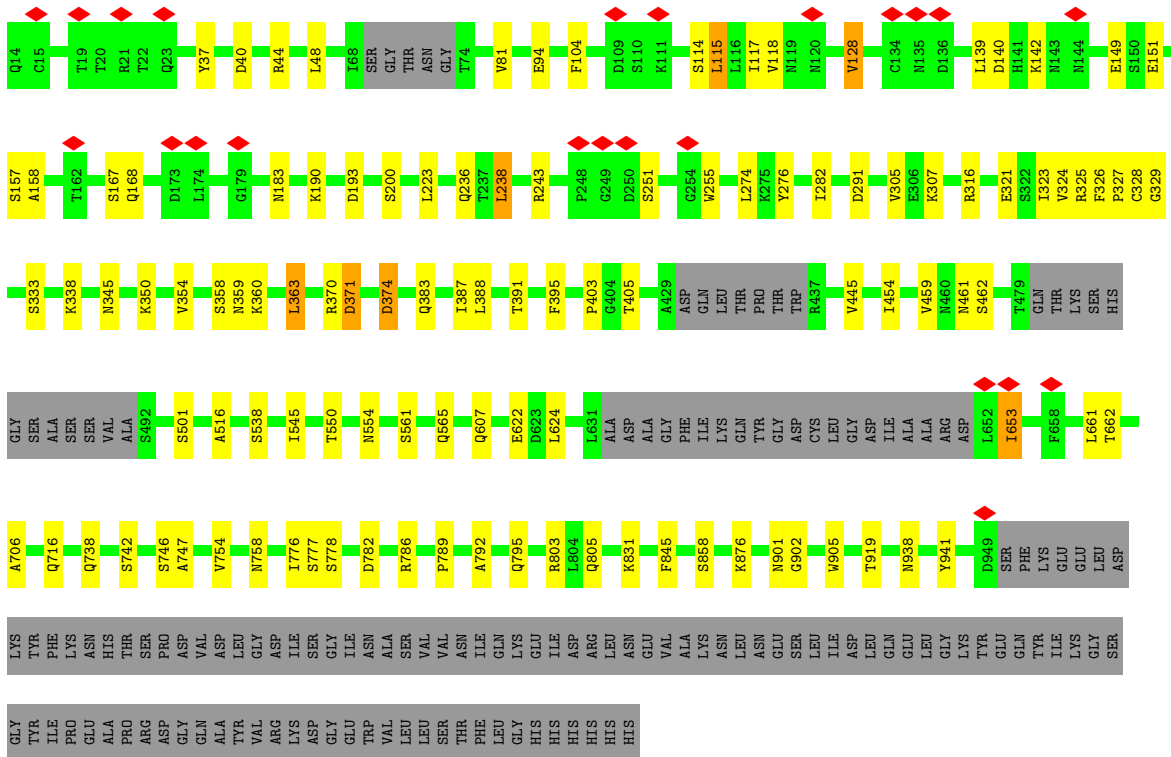
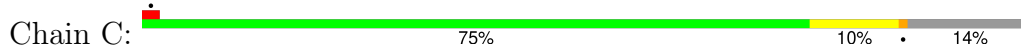


- Molecule 1: Spike protein S1,Spike glycoprotein

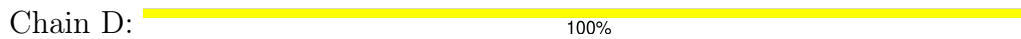




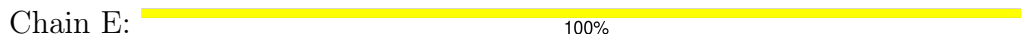
• Molecule 1: Spike protein S1,Spike glycoprotein




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



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

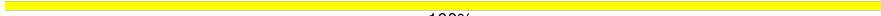


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%


MAG1
MAG2

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

Chain G:  100%

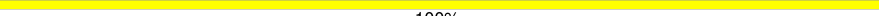
MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2


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

Chain M:  100%MAG1
MAG2

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

Chain N:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	171788	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.633	Depositor
Minimum map value	-0.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	339.968, 339.968, 339.968	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8853333, 0.8853333, 0.8853333	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: NAG

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	0.52	4/7210 (0.1%)	0.77	9/9814 (0.1%)
1	B	0.52	3/7119 (0.0%)	0.76	6/9686 (0.1%)
1	C	0.51	0/7138	0.81	12/9711 (0.1%)
All	All	0.52	7/21467 (0.0%)	0.78	27/29211 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	2
1	C	0	4
All	All	0	15

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	CYS	CB-SG	-7.56	1.69	1.82
1	B	452	CYS	CB-SG	-6.84	1.70	1.82
1	A	420	CYS	CB-SG	-6.65	1.71	1.82
1	A	452	CYS	CB-SG	-5.49	1.72	1.81
1	A	559	TYR	CE2-CZ	-5.48	1.31	1.38
1	B	422	GLU	CD-OE1	-5.43	1.19	1.25
1	A	559	TYR	CZ-OH	-5.25	1.28	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	ASP	CB-CG-OD1	11.79	128.91	118.30
1	B	193	ASP	CB-CG-OD1	10.23	127.50	118.30
1	C	363	LEU	CA-CB-CG	9.44	137.01	115.30
1	A	392	PRO	CA-N-CD	-9.08	98.79	111.50
1	C	115	LEU	CA-CB-CG	8.98	135.96	115.30
1	C	193	ASP	CB-CG-OD1	8.80	126.22	118.30
1	B	76	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	A	300	LEU	CA-CB-CG	7.24	131.94	115.30
1	C	238	LEU	CB-CG-CD1	6.95	122.81	111.00
1	C	238	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	C	238	LEU	CA-CB-CG	6.66	130.61	115.30
1	C	653	ILE	CG1-CB-CG2	6.16	124.95	111.40
1	C	128	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	A	246	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	312	THR	OG1-CB-CG2	-5.47	97.41	110.00
1	A	805	GLN	N-CA-CB	5.47	120.45	110.60
1	C	805	GLN	N-CA-CB	5.45	120.42	110.60
1	C	374	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	336	LEU	CB-CG-CD2	5.17	119.78	111.00
1	B	372	ILE	CG1-CB-CG2	-5.16	100.05	111.40
1	C	350	LYS	CB-CA-C	5.07	120.54	110.40
1	A	929	CYS	CA-CB-SG	5.06	123.10	114.00
1	A	395	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	A	138	PHE	CB-CG-CD2	5.01	124.31	120.80
1	A	116	LEU	CA-CB-CG	5.01	126.81	115.30
1	B	213	LEU	CA-CB-CG	5.01	126.81	115.30
1	A	184	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	HIS	Peptide
1	A	329	GLY	Peptide
1	A	394	SER	Peptide
1	A	418	VAL	Peptide
1	A	420	CYS	Peptide
1	A	423	VAL	Peptide
1	A	426	ALA	Peptide
1	A	432	LEU	Peptide
1	A	801	THR	Mainchain
1	B	131	PHE	Sidechain
1	B	327	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	371	ASP	Peptide
1	C	653	ILE	Peptide
1	C	661	LEU	Peptide
1	C	901	ASN	Peptide

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	7041	0	6931	46	0
1	B	6955	0	6850	43	0
1	C	6973	0	6871	59	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	A	70	0	65	0	0
3	B	84	0	78	0	0
3	C	56	0	52	0	0
All	All	21515	0	21147	147	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 3.

All (147) 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:B:346:PHE:O	1:B:349:LEU:HB2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLU:O	1:C:183:ASN:HB2	1.90	0.71
1:A:22:THR:HG1	1:A:74:THR:N	1.93	0.66
1:B:20:THR:HG1	1:B:74:THR:N	1.93	0.66
1:A:381:ASP:HB2	1:A:386:GLU:H	1.62	0.65
1:C:114:SER:O	1:C:128:VAL:HA	1.99	0.62
1:C:905:TRP:HB2	1:C:938:ASN:HD22	1.65	0.62
1:B:192:ILE:O	1:B:195:TYR:HB3	1.99	0.61
1:C:782:ASP:OD1	1:C:786:ARG:NH1	2.33	0.61
1:C:445:VAL:HG12	1:C:454:ILE:HG12	1.84	0.60
1:B:445:VAL:HG22	1:B:454:ILE:HG12	1.85	0.59
1:B:905:TRP:HB2	1:B:938:ASN:HD22	1.69	0.57
1:C:104:PHE:HB2	1:C:115:LEU:HB2	1.87	0.57
1:A:37:TYR:HA	1:A:220:LEU:H	1.69	0.56
1:A:192:ILE:O	1:A:195:TYR:HB3	2.06	0.56
1:C:328:CYS:SG	1:C:329:GLY:N	2.79	0.56
1:A:66:HIS:HB3	1:A:76:ARG:HH21	1.71	0.55
1:C:459:VAL:HG12	1:C:461:ASN:H	1.71	0.55
1:C:516:ALA:HA	1:C:876:LYS:O	2.06	0.55
1:B:24:LEU:HB2	1:B:76:ARG:HH12	1.71	0.55
1:B:68:ILE:HG12	1:B:76:ARG:HB3	1.89	0.55
1:B:138:PHE:HB2	1:B:153:ARG:HB2	1.89	0.54
1:B:127:LYS:HG2	1:B:164:GLU:HG2	1.89	0.54
1:A:433:THR:O	1:A:437:ARG:NH1	2.41	0.53
1:A:312:THR:O	1:A:398:VAL:HB	2.08	0.53
1:A:326:PHE:HB3	1:A:330:PRO:HD2	1.91	0.53
1:B:370:ARG:NH1	1:B:374:ASP:OD1	2.42	0.53
1:C:44:ARG:HB2	1:C:276:TYR:HD2	1.73	0.53
1:B:362:PHE:HB3	1:B:380:ARG:HH21	1.74	0.52
1:A:243:ARG:NH2	1:A:251:SER:O	2.42	0.52
1:B:208:ARG:NH2	1:B:212:ASP:O	2.42	0.52
1:C:291:ASP:N	1:C:291:ASP:OD1	2.41	0.52
1:C:325:ARG:NH2	1:C:383:GLN:OE1	2.43	0.52
1:C:360:LYS:H	1:C:387:ILE:HD13	1.74	0.52
1:C:831:LYS:NZ	1:C:845:PHE:O	2.43	0.52
1:C:139:LEU:HD12	1:C:149:GLU:HG3	1.91	0.51
1:C:561:SER:O	1:C:565:GLN:NE2	2.43	0.51
1:B:96:SER:HB3	1:B:177:LYS:HB3	1.92	0.51
1:C:118:VAL:HG22	1:C:238:LEU:HD21	1.92	0.51
1:C:325:ARG:HH22	1:C:383:GLN:HB2	1.76	0.51
1:C:550:THR:O	1:C:554:ASN:ND2	2.44	0.51
1:C:140:ASP:OD2	1:C:142:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HA	1:C:345:ASN:HB2	1.92	0.51
1:C:776:ILE:HG12	1:C:795:GLN:HG2	1.92	0.51
1:C:243:ARG:NH2	1:C:251:SER:OG	2.44	0.51
1:B:743:SER:OG	1:B:744:THR:N	2.45	0.50
1:C:338:LYS:HE2	1:C:388:LEU:HD11	1.94	0.50
1:B:40:ASP:OD2	1:B:44:ARG:NH2	2.44	0.50
1:C:746:SER:OG	1:C:747:ALA:N	2.41	0.50
1:C:274:LEU:HD12	1:C:282:ILE:HD13	1.94	0.49
1:C:140:ASP:HB3	1:C:151:GLU:HB3	1.95	0.49
1:A:98:ILE:HG22	1:A:239:LEU:HD12	1.93	0.49
1:B:141:HIS:ND1	1:B:241:LEU:O	2.44	0.49
1:B:476:SER:OG	1:B:477:TYR:N	2.46	0.49
1:B:831:LYS:NZ	1:B:845:PHE:O	2.45	0.49
1:A:180:ASN:HD21	1:A:206:ILE:HG23	1.78	0.49
1:A:624:LEU:HD11	1:A:742:SER:HB2	1.95	0.49
1:C:371:ASP:O	1:C:374:ASP:N	2.46	0.49
1:B:95:LYS:HB3	1:B:181:PHE:HA	1.94	0.48
1:C:81:VAL:HG22	1:C:236:GLN:HG3	1.94	0.48
1:A:98:ILE:HD13	1:A:260:ALA:HB2	1.96	0.48
1:C:706:ALA:HB1	1:C:716:GLN:HB2	1.95	0.48
1:C:157:SER:OG	1:C:158:ALA:N	2.45	0.48
1:A:295:GLU:OE1	1:A:314:ASN:ND2	2.47	0.47
1:A:353:GLY:HA2	1:A:392:PRO:HA	1.96	0.47
1:A:268:GLN:OE1	1:A:270:ARG:NH2	2.46	0.47
1:B:371:ASP:OD1	1:B:375:THR:OG1	2.32	0.47
1:A:516:ALA:HA	1:A:876:LYS:O	2.14	0.47
1:A:831:LYS:NZ	1:A:845:PHE:O	2.46	0.47
1:C:754:VAL:O	1:C:758:ASN:ND2	2.46	0.47
1:B:74:THR:OG1	1:B:75:LYS:N	2.47	0.47
1:A:545:ILE:O	1:A:803:ARG:NH1	2.47	0.47
1:B:20:THR:O	1:B:74:THR:N	2.47	0.47
1:A:247:THR:HB	1:A:255:TRP:HA	1.97	0.47
1:B:516:ALA:HA	1:B:876:LYS:O	2.15	0.47
1:A:132:GLN:OE1	1:A:157:SER:OG	2.25	0.47
1:C:243:ARG:HG2	1:C:255:TRP:HB3	1.97	0.47
1:C:305:VAL:HG12	1:C:405:THR:HG23	1.97	0.46
1:B:363:LEU:HD12	1:B:364:PRO:HD2	1.97	0.46
1:C:326:PHE:O	1:C:333:SER:OG	2.34	0.46
1:A:525:VAL:HG22	1:A:868:VAL:HG22	1.98	0.46
1:C:316:ARG:HG2	1:C:395:PHE:HD1	1.80	0.46
1:A:117:ILE:HG12	1:A:126:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.44	0.45
1:B:291:ASP:N	1:B:291:ASP:OD1	2.49	0.45
1:A:576:GLU:OE2	1:A:822[A]:ARG:NH1	2.44	0.45
1:A:167:SER:OG	1:A:168:GLN:OE1	2.35	0.45
1:B:919:THR:HG22	1:B:941:TYR:HB3	1.99	0.45
1:C:140:ASP:OD2	1:C:243:ARG:NH2	2.51	0.44
1:C:789:PRO:HA	1:C:792:ALA:HB3	1.99	0.44
1:C:919:THR:HG22	1:C:941:TYR:HB3	2.00	0.44
1:C:622:GLU:OE2	1:C:858:SER:OG	2.34	0.44
1:C:624:LEU:HD11	1:C:742:SER:HB2	2.00	0.44
1:C:354:VAL:HB	1:C:391:THR:O	2.16	0.44
1:A:57:PRO:HG3	1:A:270:ARG:HE	1.83	0.44
1:C:327:PRO:O	1:C:383:GLN:NE2	2.51	0.44
1:A:167:SER:OG	1:A:168:GLN:N	2.51	0.43
1:A:315:PHE:HE1	1:A:418:VAL:HG11	1.84	0.43
1:A:137:PRO:HB3	1:A:154:VAL:HG13	2.00	0.43
1:B:593:LYS:HE3	1:B:593:LYS:HB3	1.91	0.43
1:C:37:TYR:OH	1:C:190:LYS:NZ	2.44	0.43
1:B:94:GLU:OE2	1:B:98:ILE:N	2.51	0.43
1:C:325:ARG:HG2	1:C:333:SER:HB3	2.00	0.43
1:B:129:CYS:SG	1:B:130:GLU:N	2.92	0.43
1:B:783:ILE:HG21	1:B:796:ILE:HG23	2.01	0.43
1:A:75:LYS:HB2	1:A:255:TRP:HZ3	1.82	0.42
1:A:242:HIS:HB3	1:A:257:ALA:HA	2.01	0.42
1:A:136:ASP:N	1:A:136:ASP:OD1	2.52	0.42
1:A:879:THR:HB	1:A:900:SER:HB3	2.01	0.42
1:A:54:LEU:HA	1:A:269:PRO:HA	2.02	0.42
1:A:234:ARG:HH21	1:A:236:GLN:HB2	1.85	0.42
1:B:325:ARG:HD2	1:B:346:PHE:HE1	1.84	0.42
1:C:200:SER:HB3	1:C:223:LEU:HD23	2.02	0.42
1:A:394:SER:OG	1:A:395:PHE:N	2.52	0.42
1:B:100:ARG:HH22	1:B:174:LEU:HD13	1.84	0.42
1:C:48:LEU:HA	1:C:274:LEU:O	2.20	0.42
1:C:307:LYS:HG3	1:C:403:PRO:HA	2.00	0.42
1:B:307:LYS:HG3	1:B:403:PRO:HA	2.01	0.42
1:C:607:GLN:OE1	1:C:738:GLN:NE2	2.49	0.42
1:A:387:ILE:HD12	1:A:387:ILE:HA	1.87	0.42
1:A:415:TYR:O	1:A:451:GLY:HA3	2.20	0.42
1:A:188:VAL:HG23	1:A:220:LEU:HD12	2.02	0.41
1:A:207:VAL:HG22	1:A:209:GLU:HB2	2.02	0.41
1:A:186:GLU:O	1:A:200:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LYS:HG2	1:B:179:GLY:H	1.85	0.41
1:B:129:CYS:HB3	1:B:131:PHE:CE2	2.55	0.41
1:B:277:ASN:HD21	1:B:279:ASN:HB2	1.85	0.41
1:B:408:SER:OG	1:B:409:ASN:N	2.53	0.41
1:C:115:LEU:HD12	1:C:117:ILE:HD11	2.02	0.41
1:B:104:PHE:HB2	1:B:115:LEU:HB3	2.02	0.41
1:C:167:SER:OG	1:C:168:GLN:N	2.52	0.41
1:C:321:GLU:HG3	1:C:323:ILE:HG12	2.02	0.41
1:C:545:ILE:O	1:C:803:ARG:NH1	2.53	0.41
1:C:777:SER:OG	1:C:778:SER:N	2.54	0.41
1:A:788:ASP:OD1	1:A:788:ASP:N	2.54	0.41
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.95	0.41
1:A:300:LEU:HD21	1:A:305:VAL:HG12	2.03	0.41
1:A:43:PHE:HA	1:C:363:LEU:HD21	2.03	0.41
1:B:317:VAL:HG13	1:B:425:VAL:HG21	2.03	0.41
1:B:356:THR:OG1	1:B:357:GLU:N	2.52	0.41
1:C:462:SER:HB3	1:C:501:SER:HB3	2.02	0.41
1:A:96:SER:O	1:A:96:SER:OG	2.37	0.40
1:C:538:SER:OG	1:C:662:THR:OG1	2.38	0.40
1:A:119:ASN:HA	1:A:124:VAL:HG12	2.02	0.40
1:B:98:ILE:HD13	1:B:260:ALA:HB2	2.02	0.40
1:B:525:VAL:HG22	1:B:868:VAL:HG22	2.03	0.40
1:C:358:SER:OG	1:C:359:ASN:N	2.54	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	894/1037 (86%)	840 (94%)	54 (6%)	0	100 100
1	B	882/1037 (85%)	825 (94%)	55 (6%)	2 (0%)	44 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	884/1037 (85%)	817 (92%)	66 (8%)	1 (0%)	48 69
All	All	2660/3111 (86%)	2482 (93%)	175 (7%)	3 (0%)	50 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	PRO
1	C	902	GLY
1	B	326	PHE

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	794/905 (88%)	794 (100%)	0	100 100
1	B	785/905 (87%)	785 (100%)	0	100 100
1	C	786/905 (87%)	785 (100%)	1 (0%)	92 98
All	All	2365/2715 (87%)	2364 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
1	C	370	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 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	D	1	2,1	14,14,15	0.92	2 (14%)	17,19,21	0.75	0
2	NAG	D	2	2	14,14,15	0.85	1 (7%)	17,19,21	0.61	0
2	NAG	E	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	E	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	F	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	G	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
2	NAG	H	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	I	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.74	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	J	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.38	0	17,19,21	0.84	1 (5%)
2	NAG	K	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.72	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.38	0	17,19,21	0.84	1 (5%)
2	NAG	L	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	M	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.74	1 (5%)
2	NAG	N	1	2,1	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
2	NAG	N	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	1	2,1	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
2	NAG	O	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.73	1 (5%)

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	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	NAG	O5-C1	2.46	1.47	1.43
2	M	2	NAG	O5-C1	2.46	1.47	1.43
2	I	2	NAG	O5-C1	2.43	1.47	1.43
2	G	2	NAG	O5-C1	2.43	1.47	1.43
2	O	2	NAG	O5-C1	2.43	1.47	1.43
2	N	2	NAG	O5-C1	2.42	1.47	1.43
2	E	2	NAG	O5-C1	2.42	1.47	1.43
2	H	2	NAG	O5-C1	2.41	1.47	1.43
2	L	2	NAG	O5-C1	2.41	1.47	1.43
2	K	2	NAG	O5-C1	2.40	1.47	1.43
2	F	2	NAG	O5-C1	2.40	1.47	1.43
2	D	1	NAG	C1-C2	2.40	1.55	1.52
2	D	2	NAG	C1-C2	2.18	1.55	1.52
2	D	1	NAG	O5-C1	2.17	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1	NAG	C1-O5-C5	2.92	116.10	112.19
2	K	1	NAG	C1-O5-C5	2.89	116.06	112.19
2	L	1	NAG	C1-O5-C5	2.89	116.06	112.19
2	J	1	NAG	C1-O5-C5	2.89	116.06	112.19
2	H	1	NAG	C1-O5-C5	2.88	116.05	112.19
2	M	1	NAG	C1-O5-C5	2.87	116.03	112.19
2	I	1	NAG	C1-O5-C5	2.86	116.03	112.19
2	O	1	NAG	C1-O5-C5	2.86	116.02	112.19
2	F	1	NAG	C1-O5-C5	2.86	116.02	112.19
2	E	1	NAG	C1-O5-C5	2.86	116.02	112.19
2	G	1	NAG	C1-O5-C5	2.85	116.00	112.19
2	I	2	NAG	C1-O5-C5	2.65	115.74	112.19
2	L	2	NAG	C1-O5-C5	2.65	115.73	112.19
2	H	2	NAG	C1-O5-C5	2.64	115.72	112.19
2	M	2	NAG	C1-O5-C5	2.63	115.71	112.19
2	N	2	NAG	C1-O5-C5	2.63	115.71	112.19
2	O	2	NAG	C1-O5-C5	2.62	115.70	112.19
2	E	2	NAG	C1-O5-C5	2.62	115.69	112.19
2	F	2	NAG	C1-O5-C5	2.61	115.68	112.19
2	G	2	NAG	C1-O5-C5	2.60	115.67	112.19
2	J	2	NAG	C1-O5-C5	2.60	115.67	112.19
2	K	2	NAG	C1-O5-C5	2.60	115.67	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

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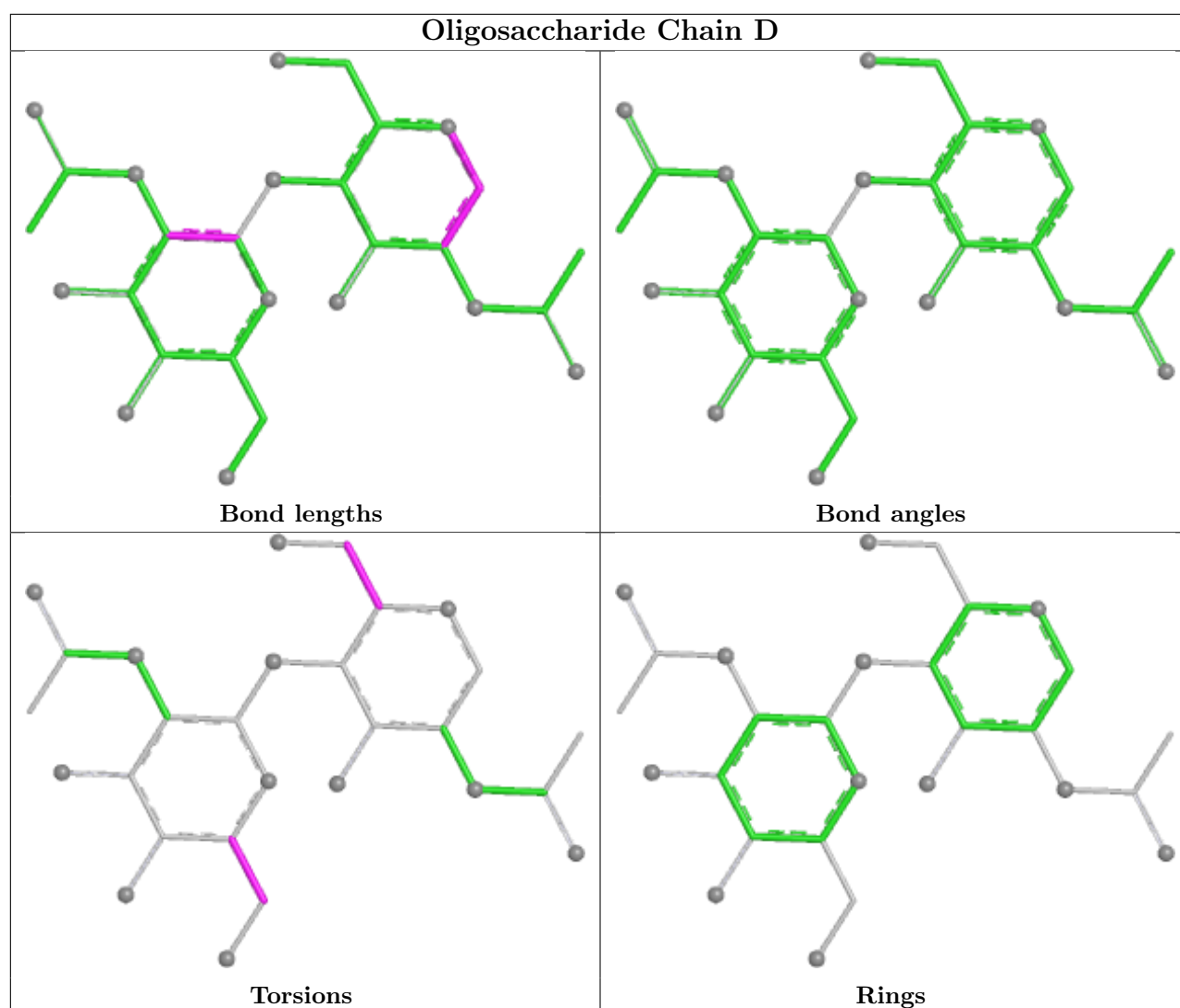
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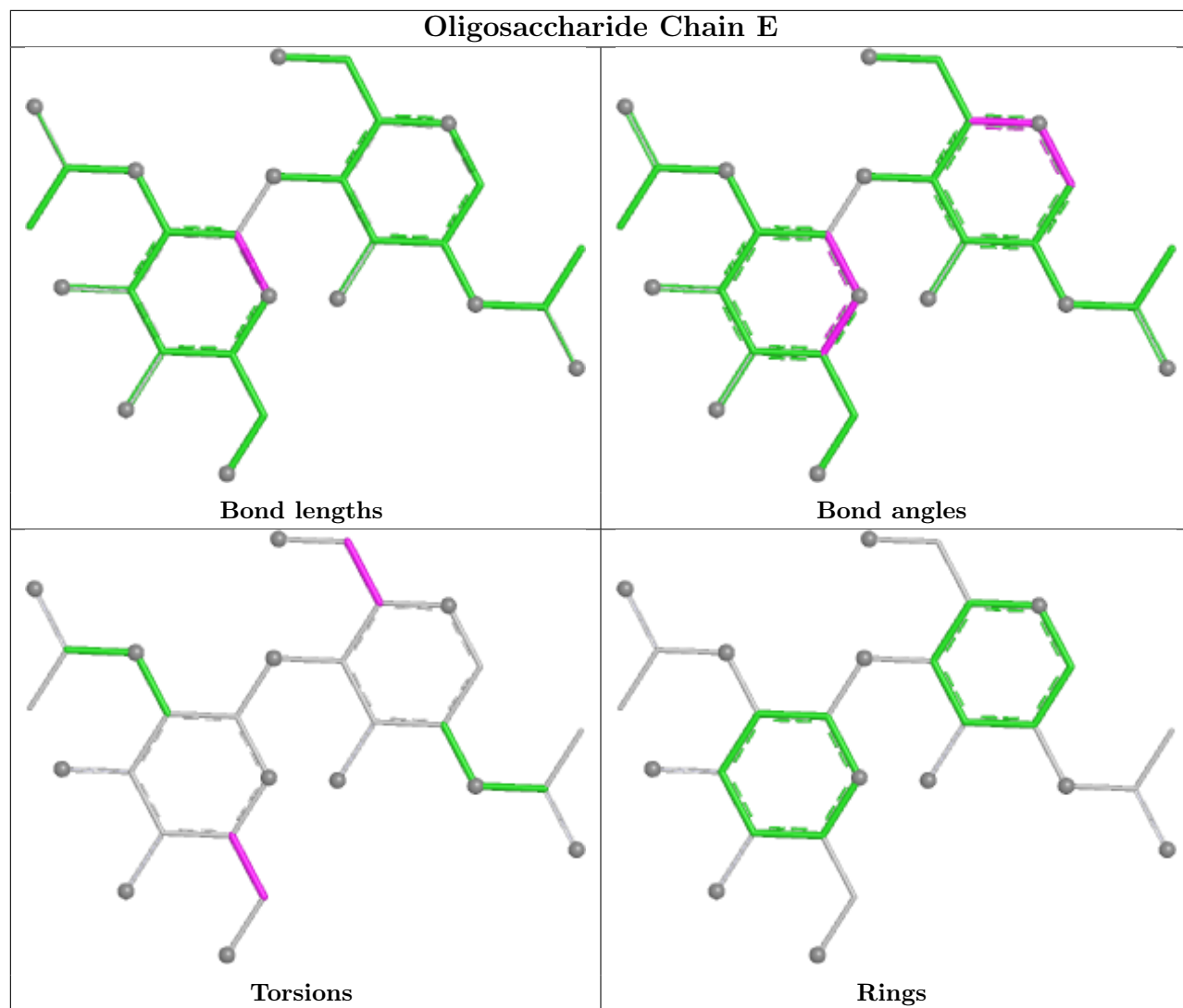
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6

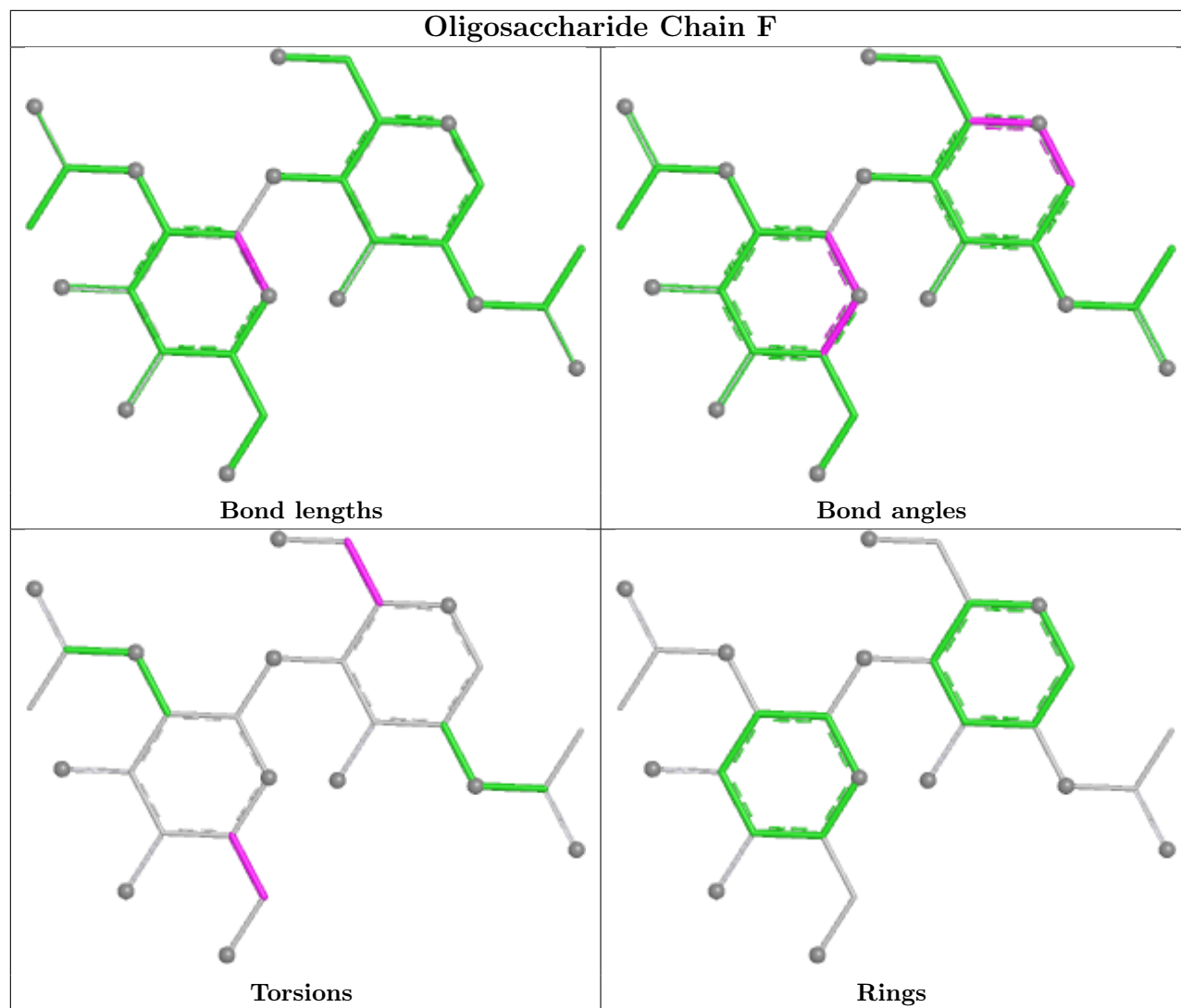
There are no ring outliers.

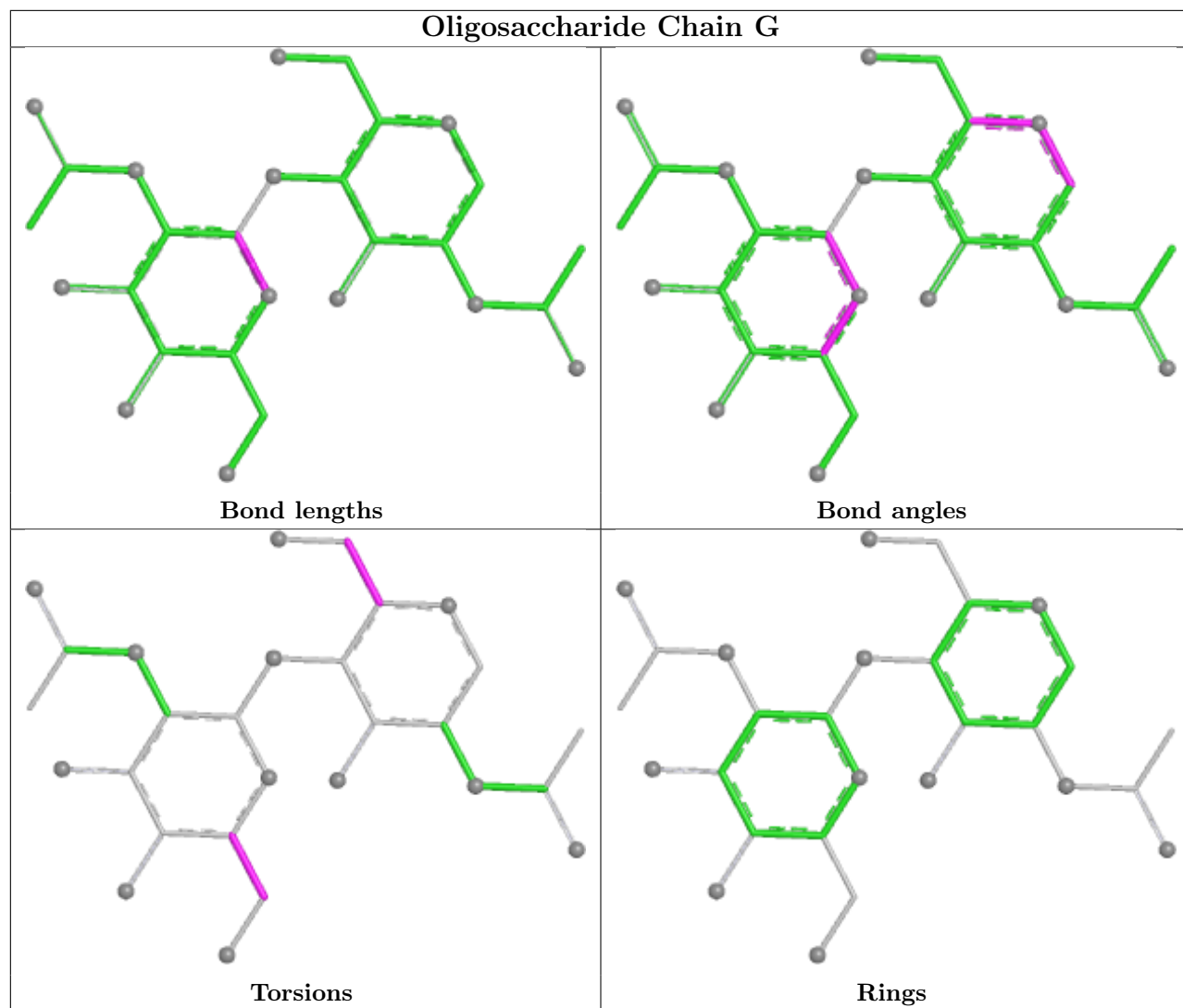
No monomer is involved in short contacts.

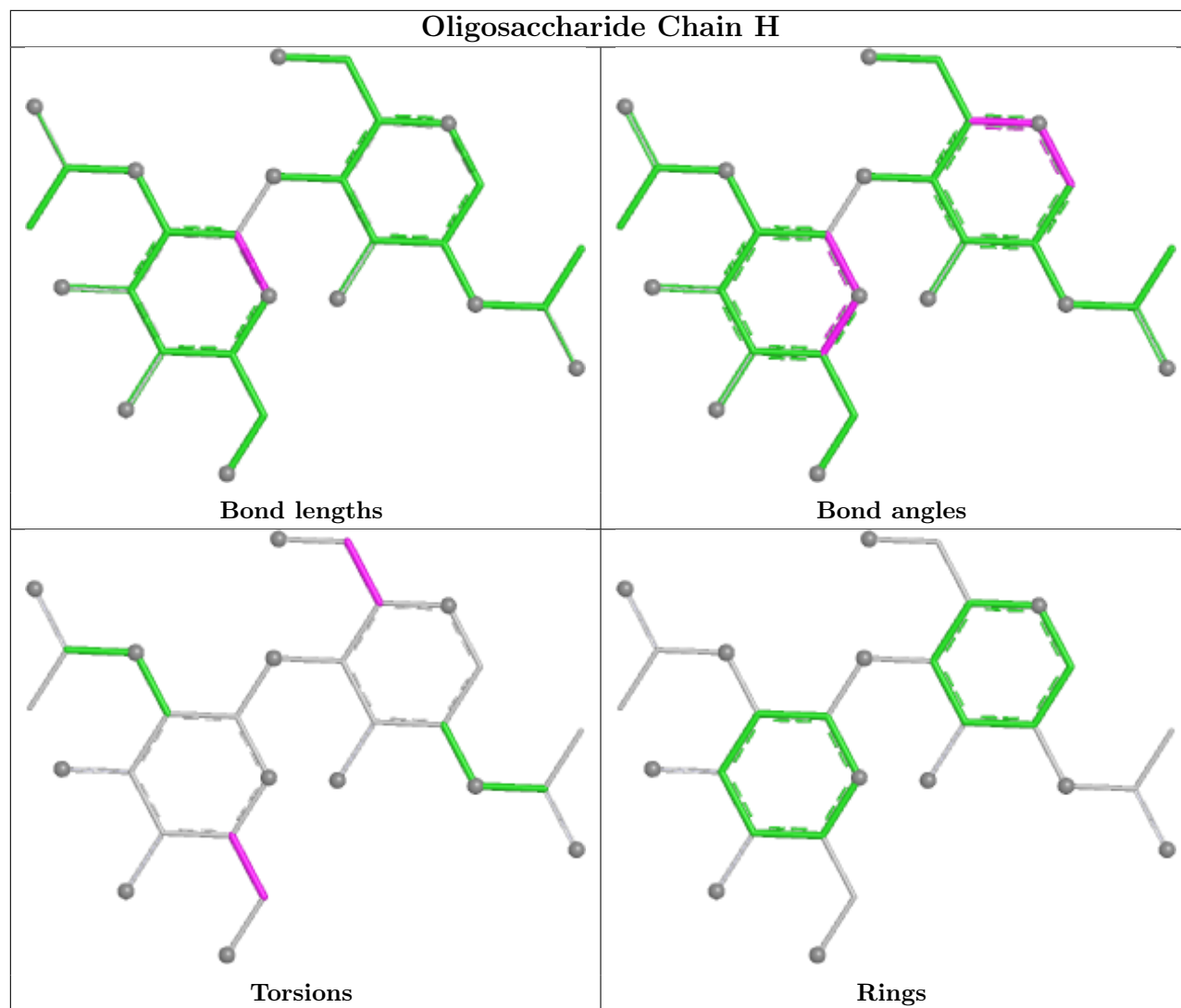
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

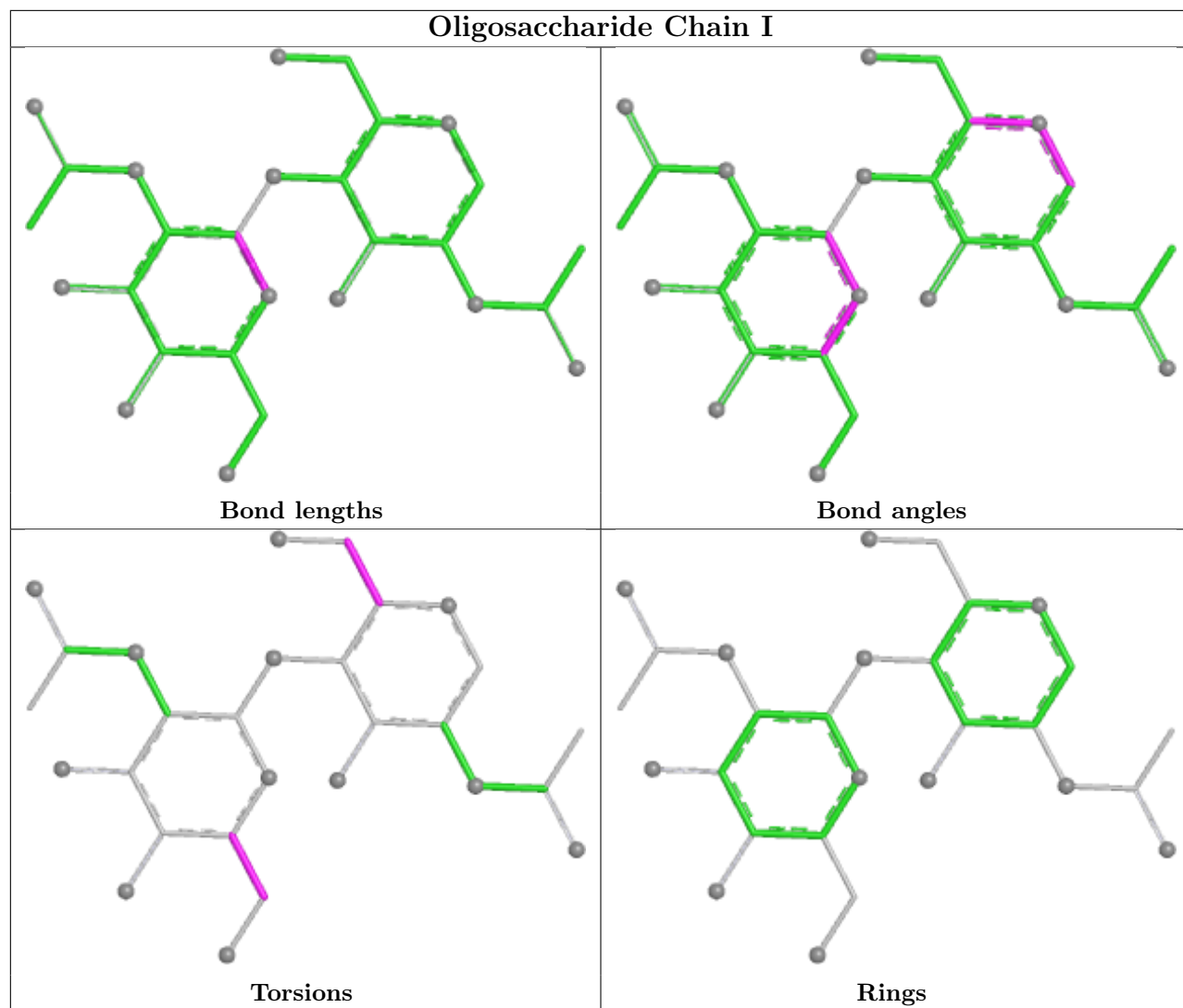


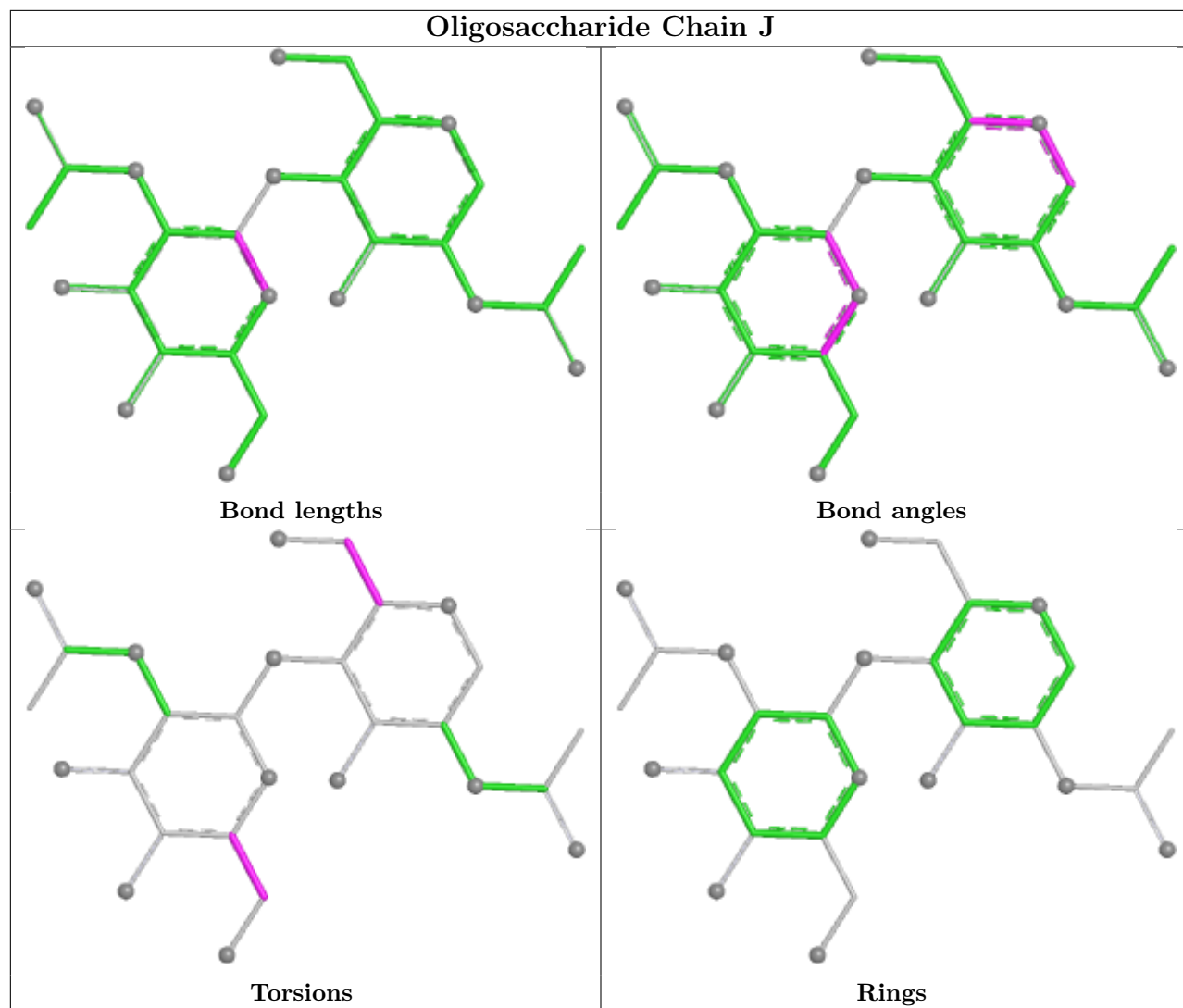


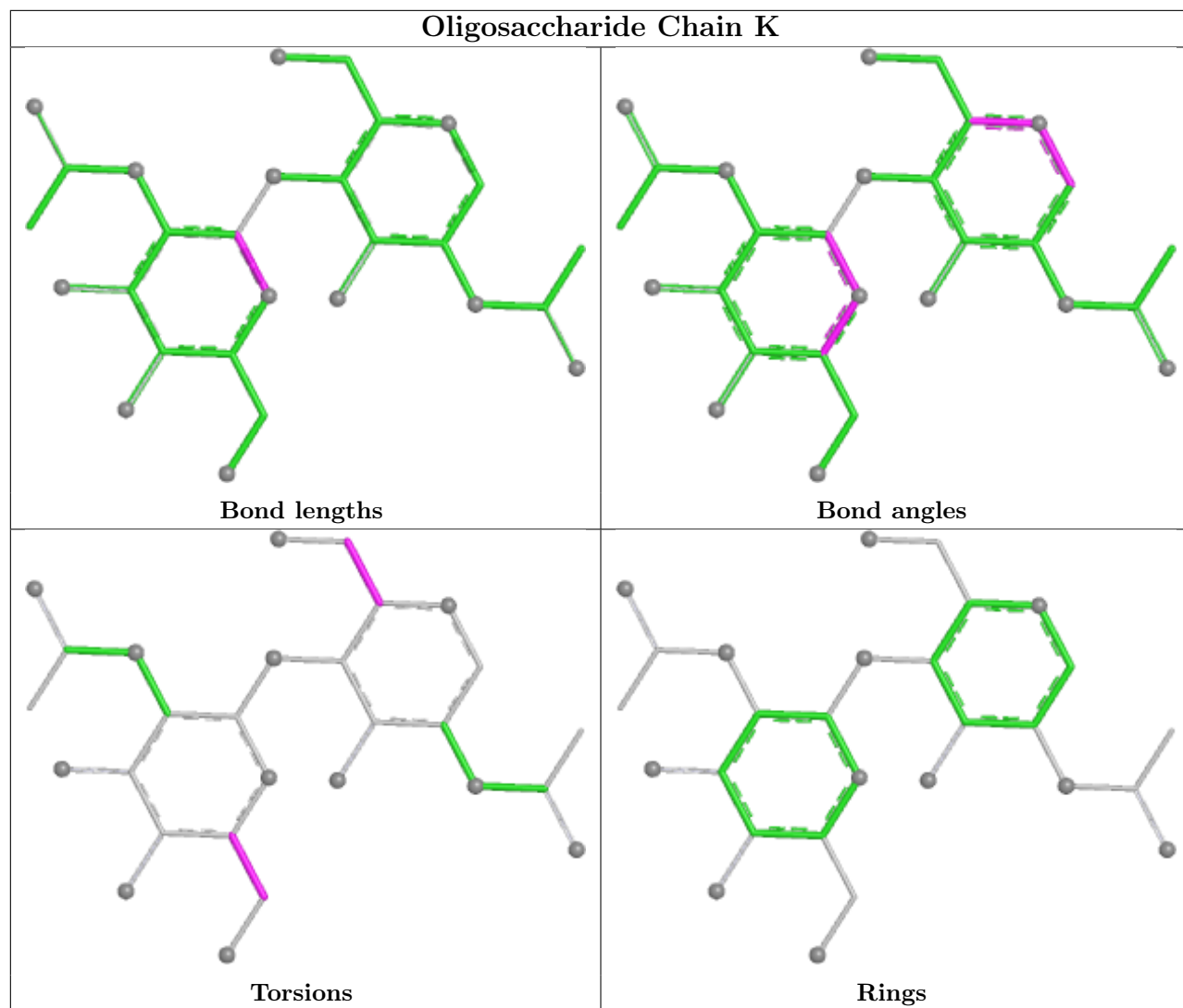


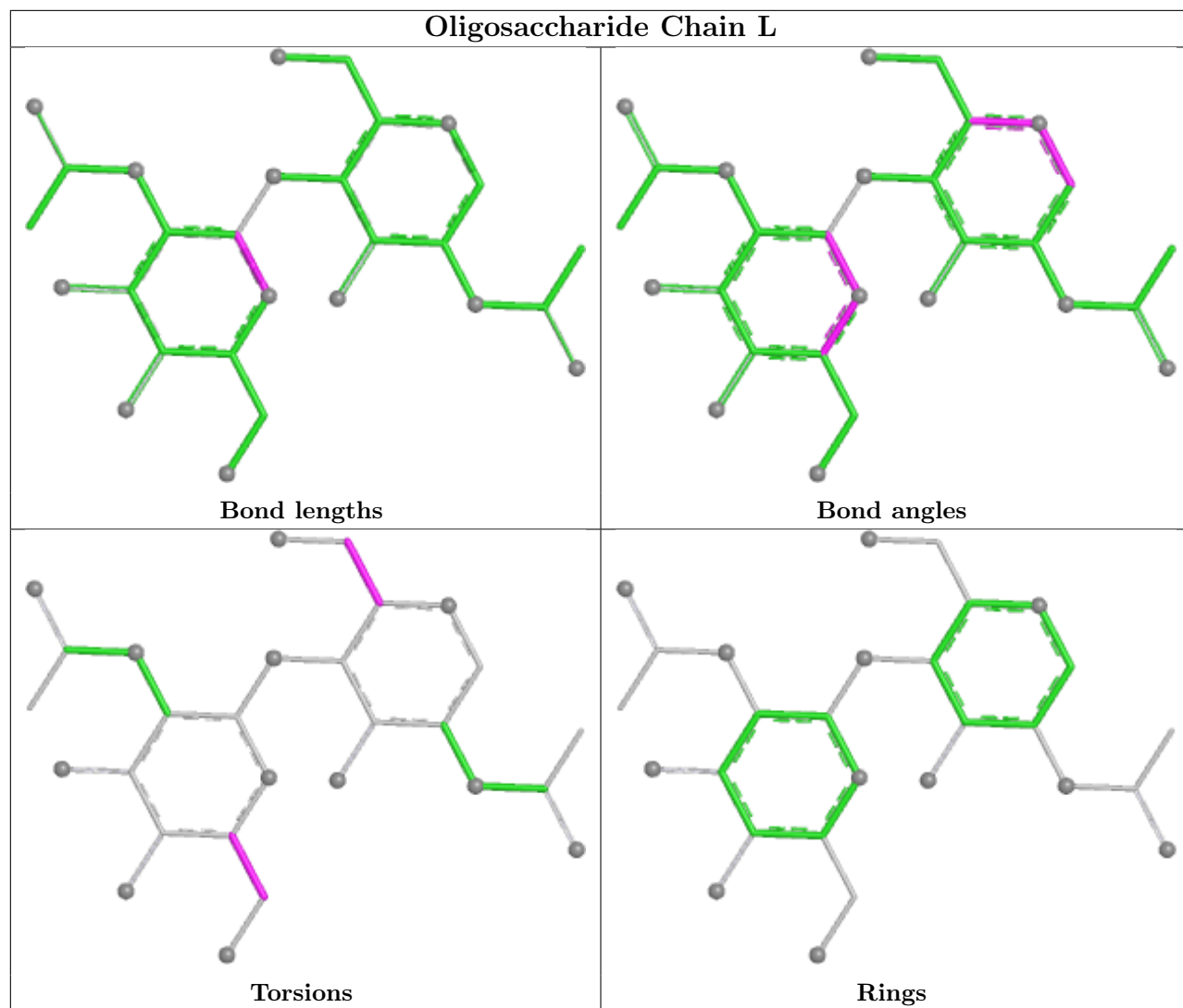


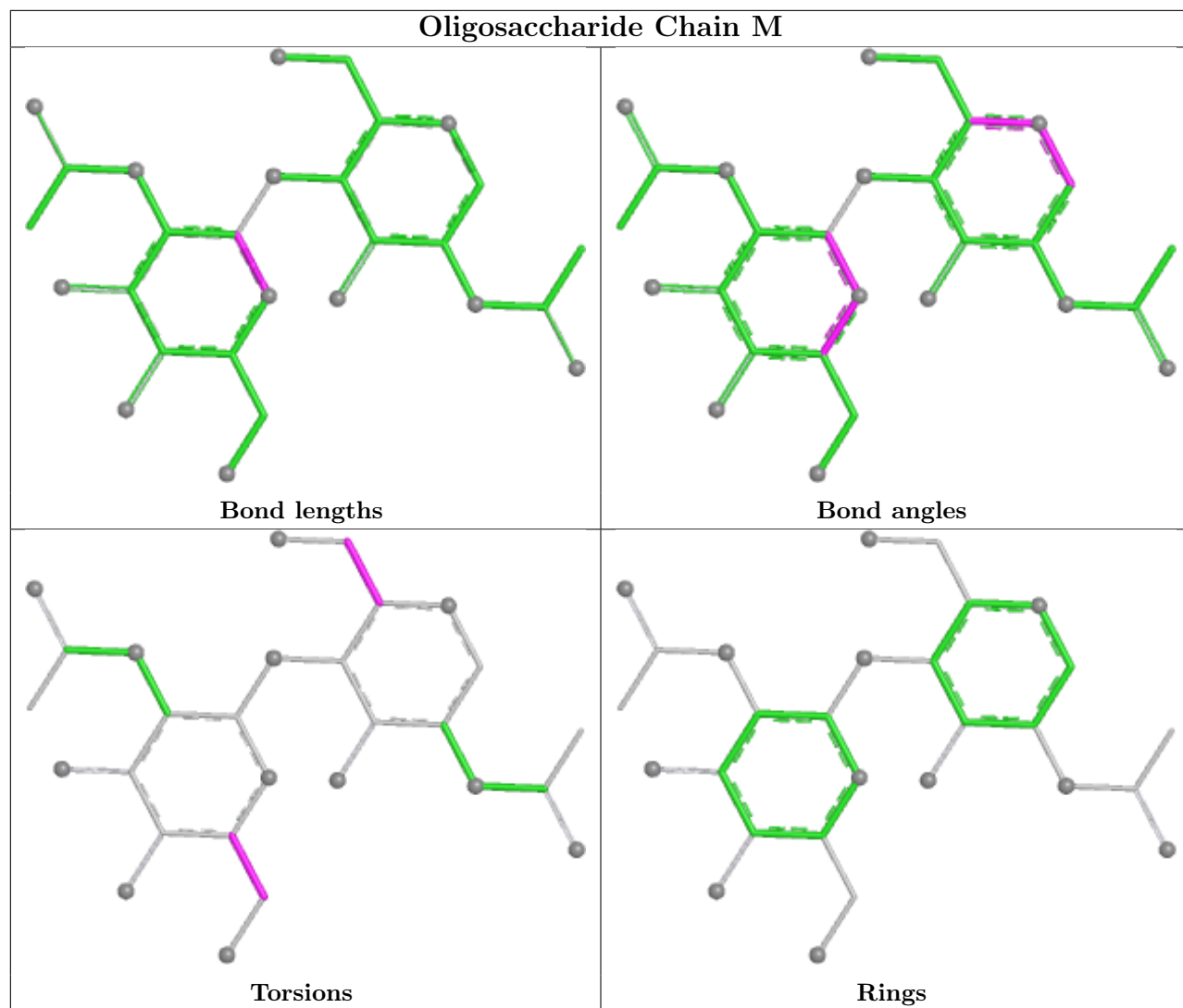


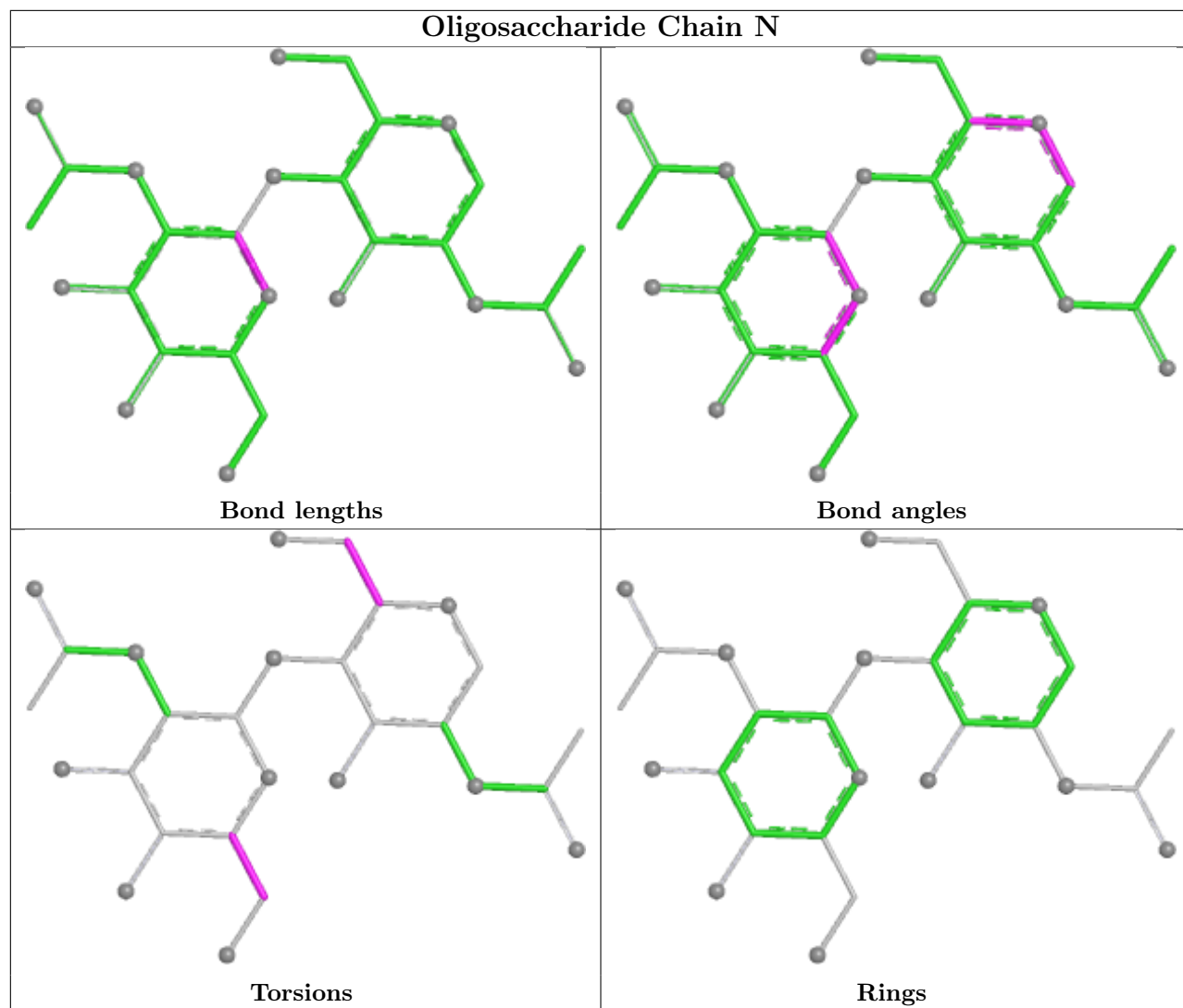


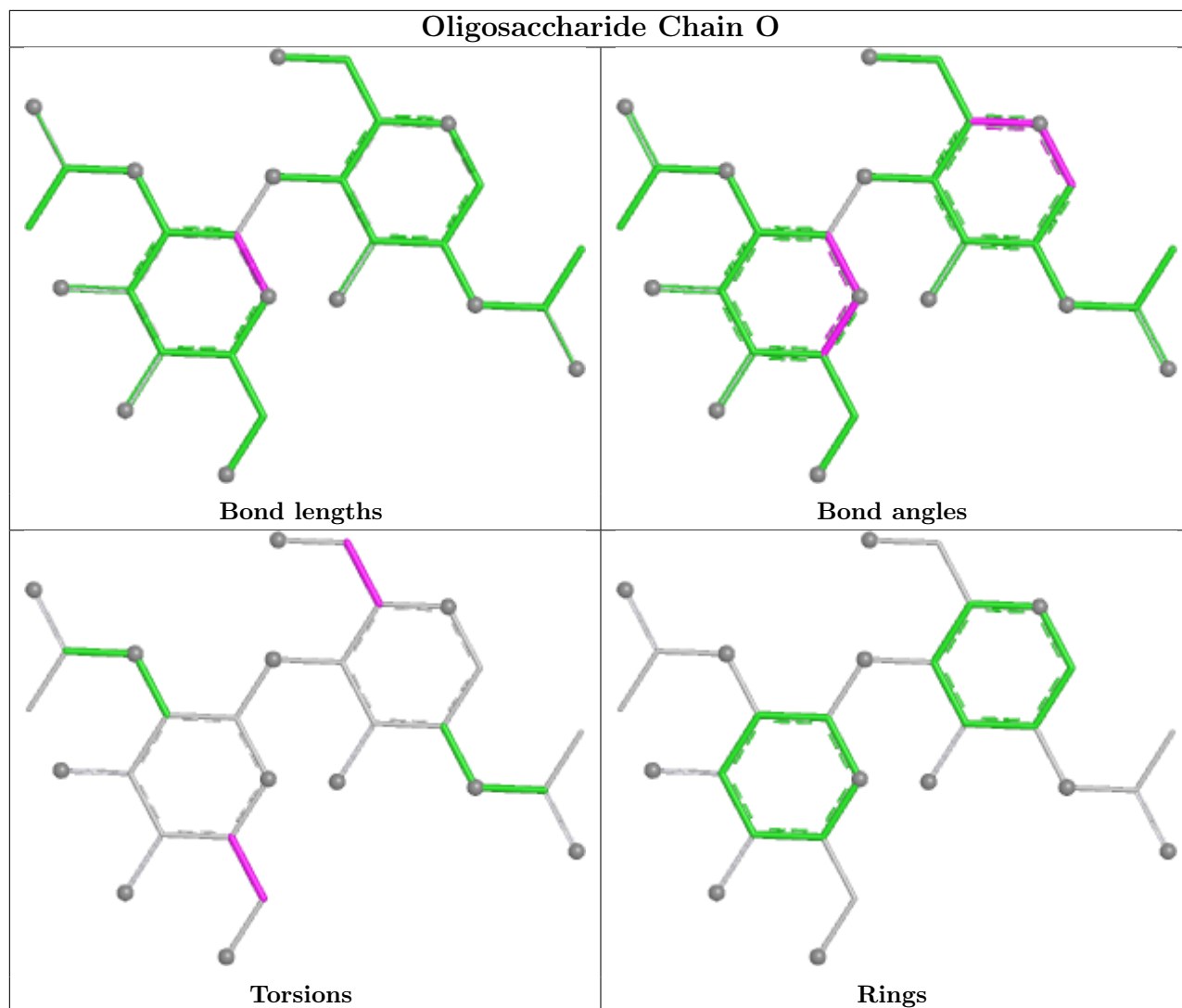












5.6 Ligand geometry [i](#)

15 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$
3	NAG	A	1301	1	14,14,15	0.87	1 (7%)	17,19,21	1.46	3 (17%)
3	NAG	A	1300	1	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
3	NAG	A	1304	1	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1104	1	14,14,15	0.70	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	C	1102	1	14,14,15	0.87	1 (7%)	17,19,21	0.92	2 (11%)
3	NAG	B	1304	1	14,14,15	1.37	2 (14%)	17,19,21	2.95	5 (29%)
3	NAG	C	1103	1	14,14,15	0.79	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	A	1303	1	14,14,15	0.92	2 (14%)	17,19,21	1.26	1 (5%)
3	NAG	B	1300	1	14,14,15	0.83	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	B	1302	1	14,14,15	0.86	1 (7%)	17,19,21	1.57	3 (17%)
3	NAG	C	1101	1	14,14,15	0.71	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	A	1302	1	14,14,15	0.95	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	B	1301	1	14,14,15	0.65	0	17,19,21	0.70	1 (5%)
3	NAG	B	1303	1	14,14,15	0.64	0	17,19,21	0.80	1 (5%)
3	NAG	B	1305	1	14,14,15	0.84	1 (7%)	17,19,21	1.03	1 (5%)

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
3	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1300	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1104	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1102	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1103	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1300	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1101	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1304	NAG	C1-C2	3.67	1.57	1.52
3	A	1302	NAG	O5-C1	3.08	1.48	1.43
3	B	1300	NAG	O5-C1	2.70	1.48	1.43
3	B	1305	NAG	O5-C1	2.55	1.48	1.43
3	A	1303	NAG	C1-C2	2.41	1.55	1.52
3	C	1102	NAG	C1-C2	2.37	1.55	1.52
3	A	1303	NAG	O5-C1	2.36	1.47	1.43
3	B	1302	NAG	C1-C2	2.33	1.55	1.52
3	A	1301	NAG	O5-C1	2.33	1.47	1.43
3	A	1304	NAG	O5-C1	2.30	1.47	1.43
3	C	1104	NAG	O5-C1	2.27	1.47	1.43
3	B	1304	NAG	C3-C2	2.24	1.57	1.52
3	C	1103	NAG	O5-C1	2.21	1.47	1.43
3	C	1101	NAG	O5-C1	2.15	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1304	NAG	C2-N2-C7	9.70	135.90	122.90
3	B	1304	NAG	C1-C2-N2	5.02	118.34	110.43
3	A	1303	NAG	C1-O5-C5	4.91	118.76	112.19
3	A	1301	NAG	C2-N2-C7	4.71	129.22	122.90
3	B	1302	NAG	C2-N2-C7	4.40	128.80	122.90
3	B	1305	NAG	C1-O5-C5	3.96	117.49	112.19
3	C	1104	NAG	C1-O5-C5	3.58	116.98	112.19
3	A	1304	NAG	C1-O5-C5	3.57	116.98	112.19
3	C	1103	NAG	C1-O5-C5	3.53	116.92	112.19
3	A	1300	NAG	C1-O5-C5	3.25	116.54	112.19
3	B	1304	NAG	C4-C3-C2	3.12	115.58	111.02
3	B	1300	NAG	C1-O5-C5	3.09	116.32	112.19
3	C	1101	NAG	C1-O5-C5	2.91	116.09	112.19
3	B	1303	NAG	C1-O5-C5	2.88	116.04	112.19
3	B	1302	NAG	C4-C3-C2	2.82	115.15	111.02
3	A	1302	NAG	C1-O5-C5	2.76	115.89	112.19
3	B	1304	NAG	C3-C4-C5	2.62	114.98	110.23
3	B	1304	NAG	C8-C7-N2	2.58	120.41	116.12
3	B	1301	NAG	C1-O5-C5	2.52	115.56	112.19
3	C	1102	NAG	C2-N2-C7	2.44	126.17	122.90
3	B	1302	NAG	C1-C2-N2	2.42	114.24	110.43
3	A	1301	NAG	C1-C2-N2	2.35	114.13	110.43
3	A	1301	NAG	C1-O5-C5	2.29	115.26	112.19
3	C	1102	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

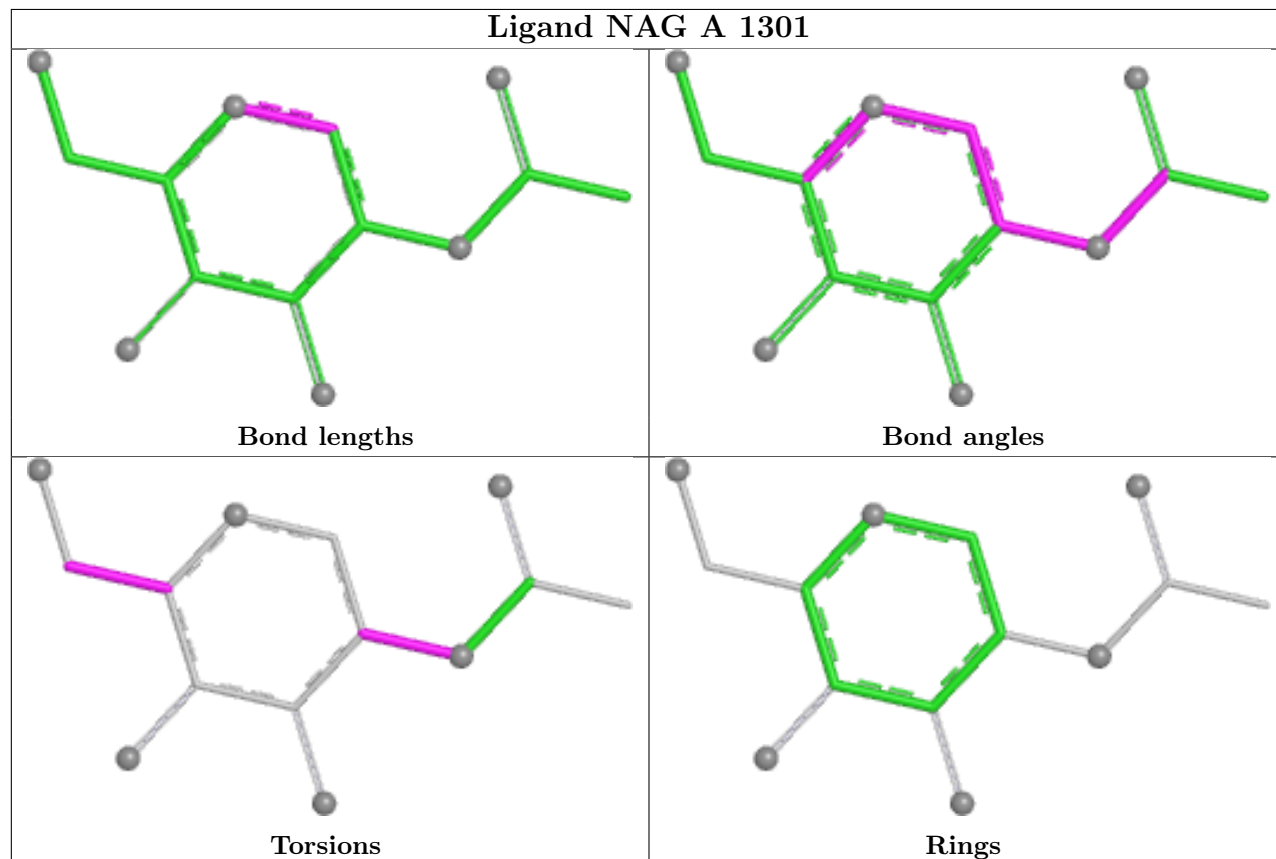
Mol	Chain	Res	Type	Atoms
3	A	1304	NAG	O5-C5-C6-O6
3	C	1104	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1300	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1101	NAG	O5-C5-C6-O6
3	C	1104	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	C	1102	NAG	C8-C7-N2-C2
3	C	1102	NAG	O7-C7-N2-C2
3	B	1300	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1101	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1301	NAG	C1-C2-N2-C7
3	B	1302	NAG	C1-C2-N2-C7
3	B	1304	NAG	C1-C2-N2-C7
3	A	1301	NAG	C3-C2-N2-C7
3	B	1302	NAG	C3-C2-N2-C7
3	A	1300	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6

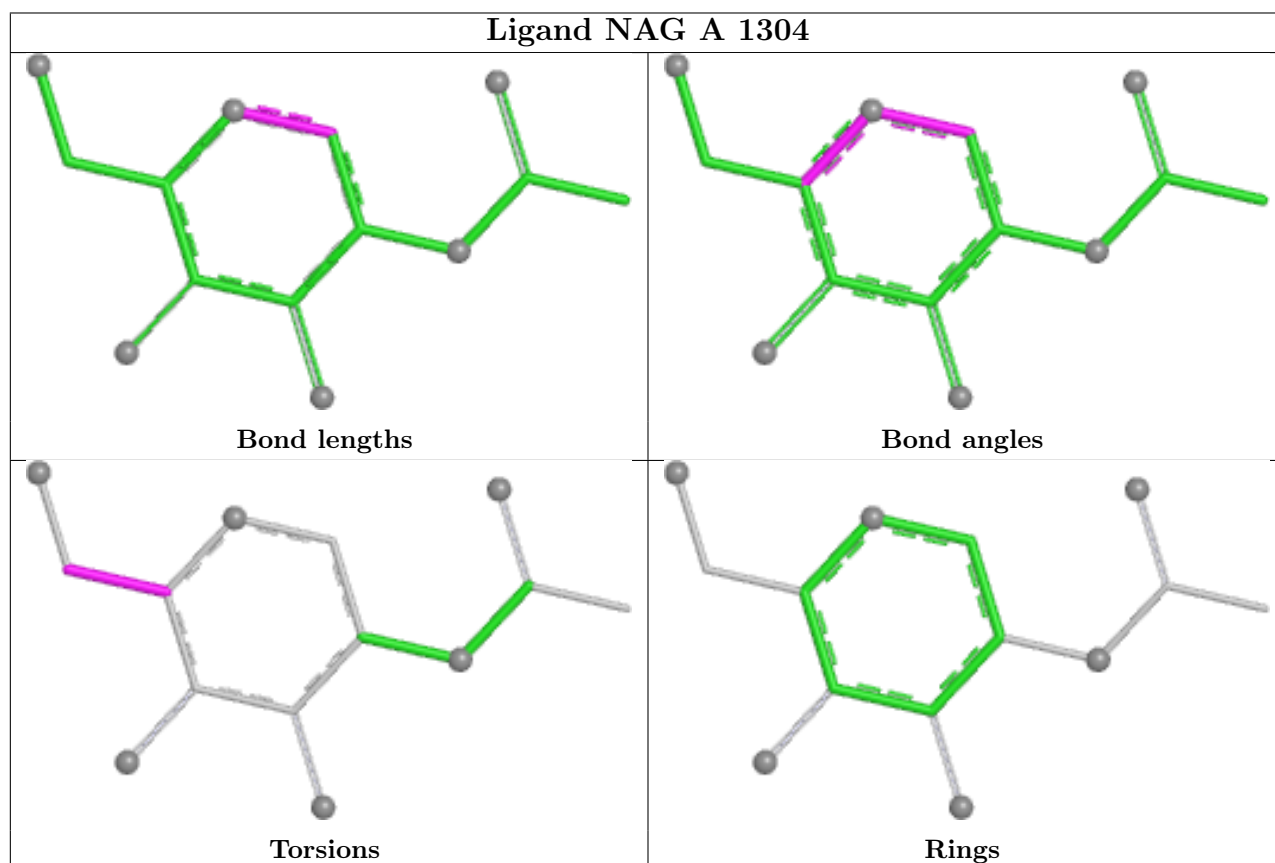
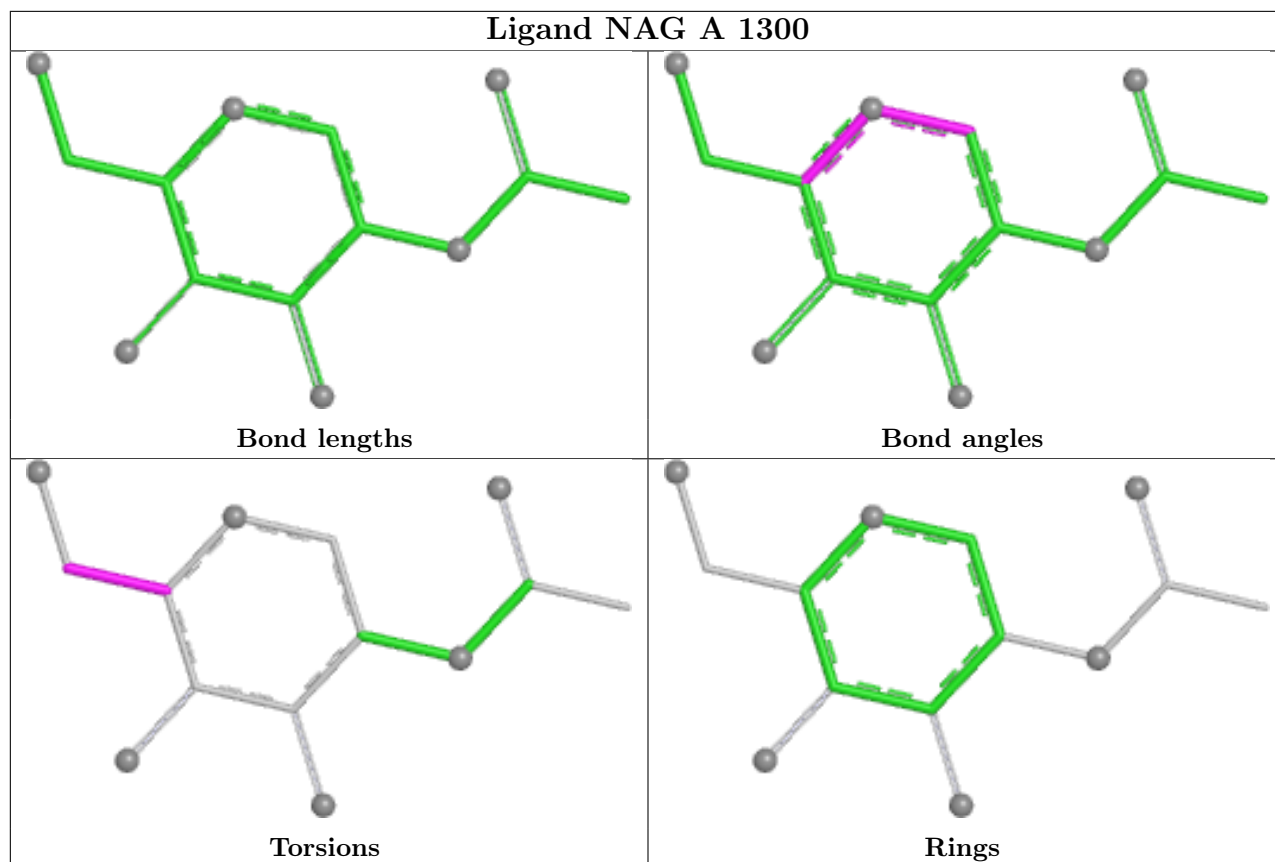
There are no ring outliers.

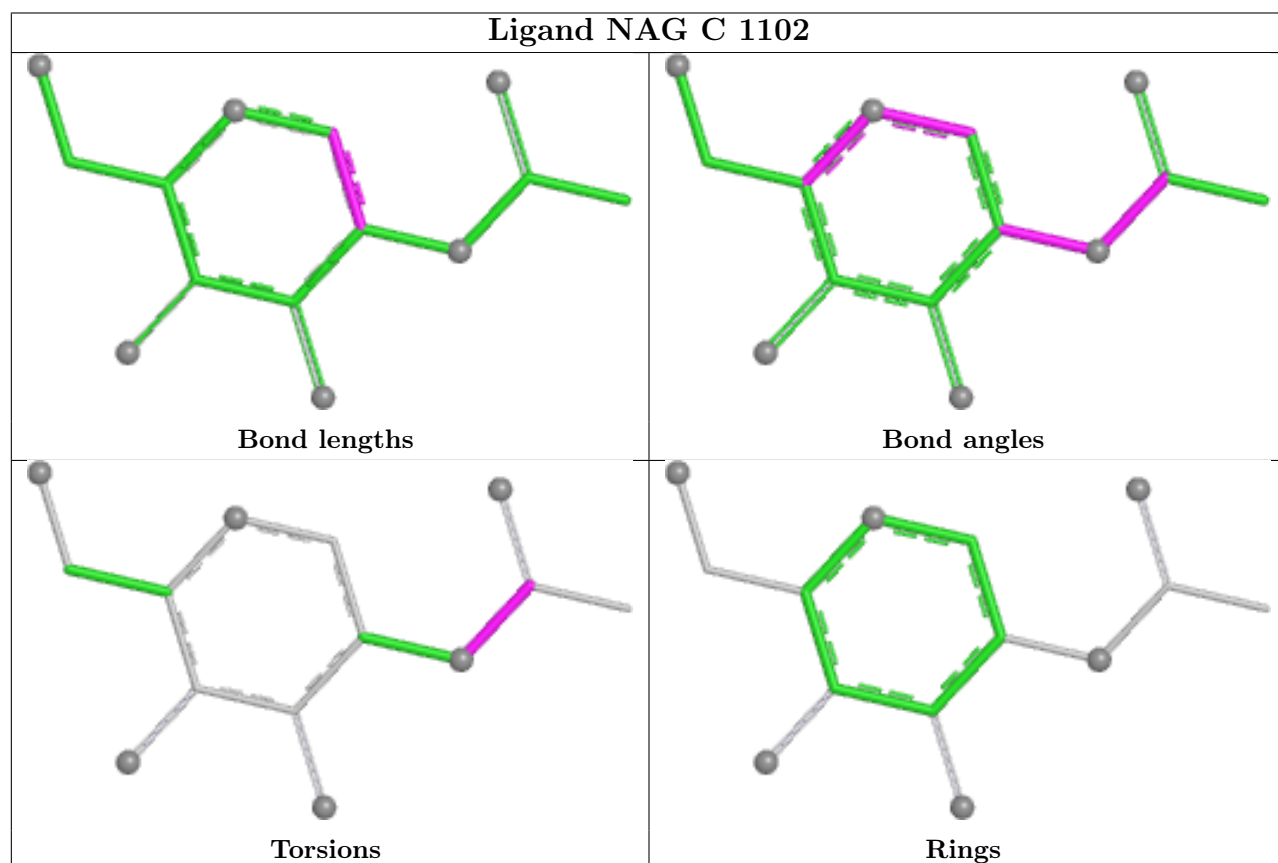
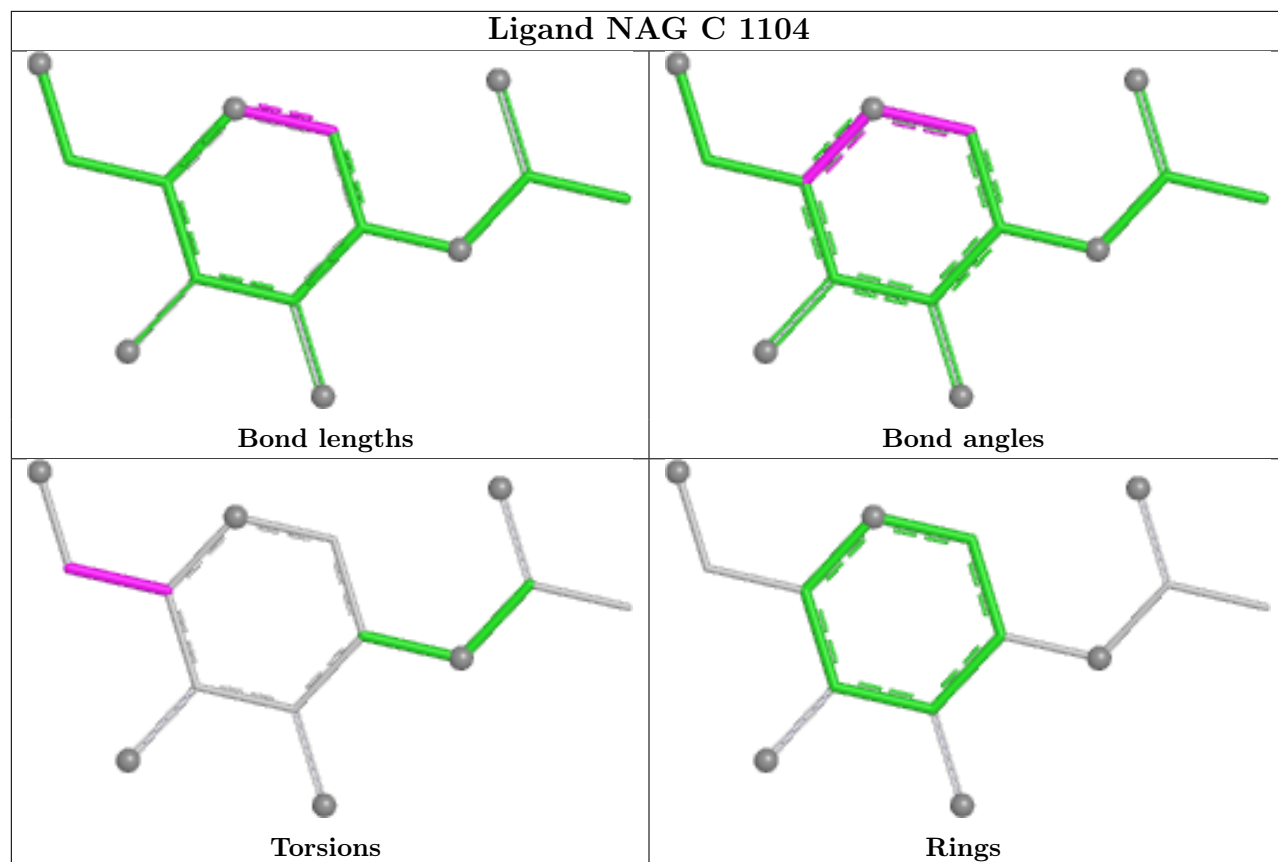
No monomer is involved in short contacts.

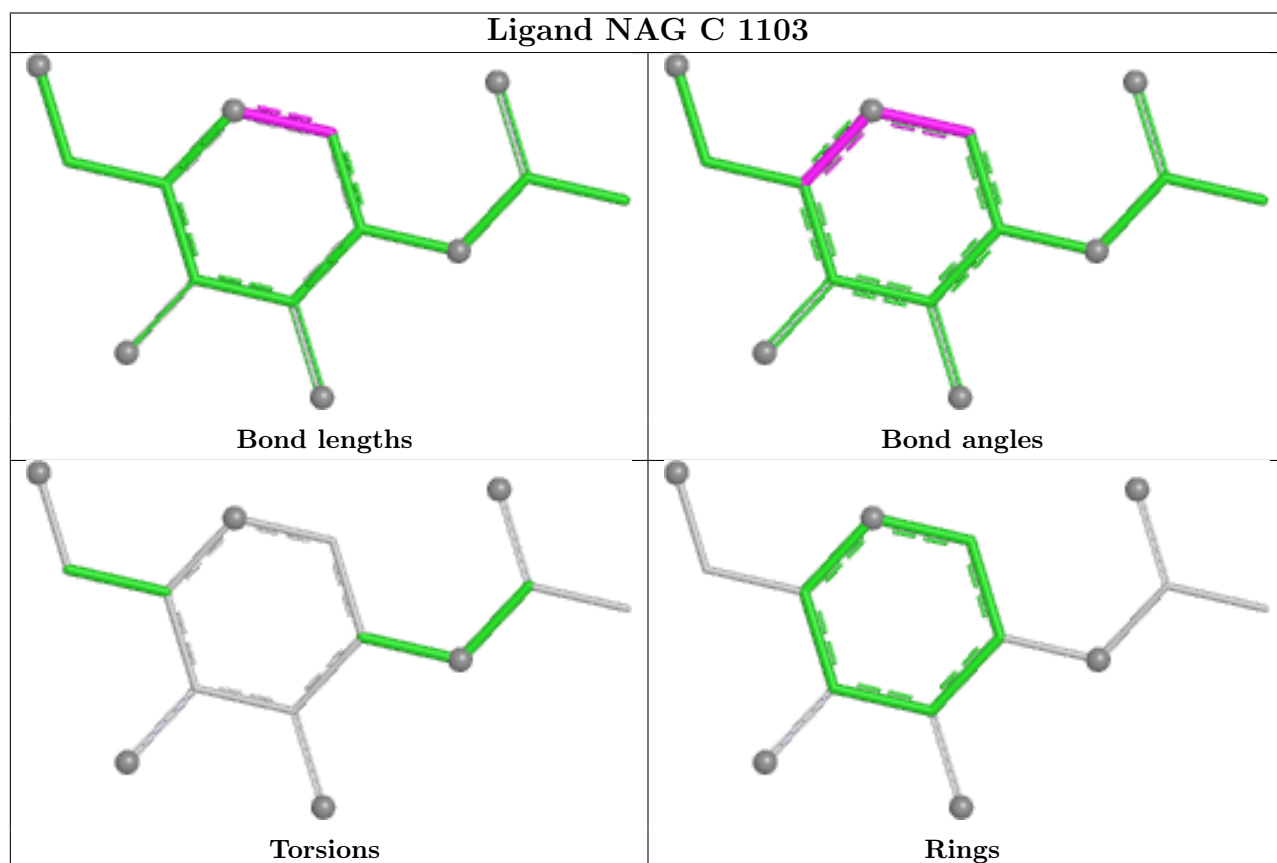
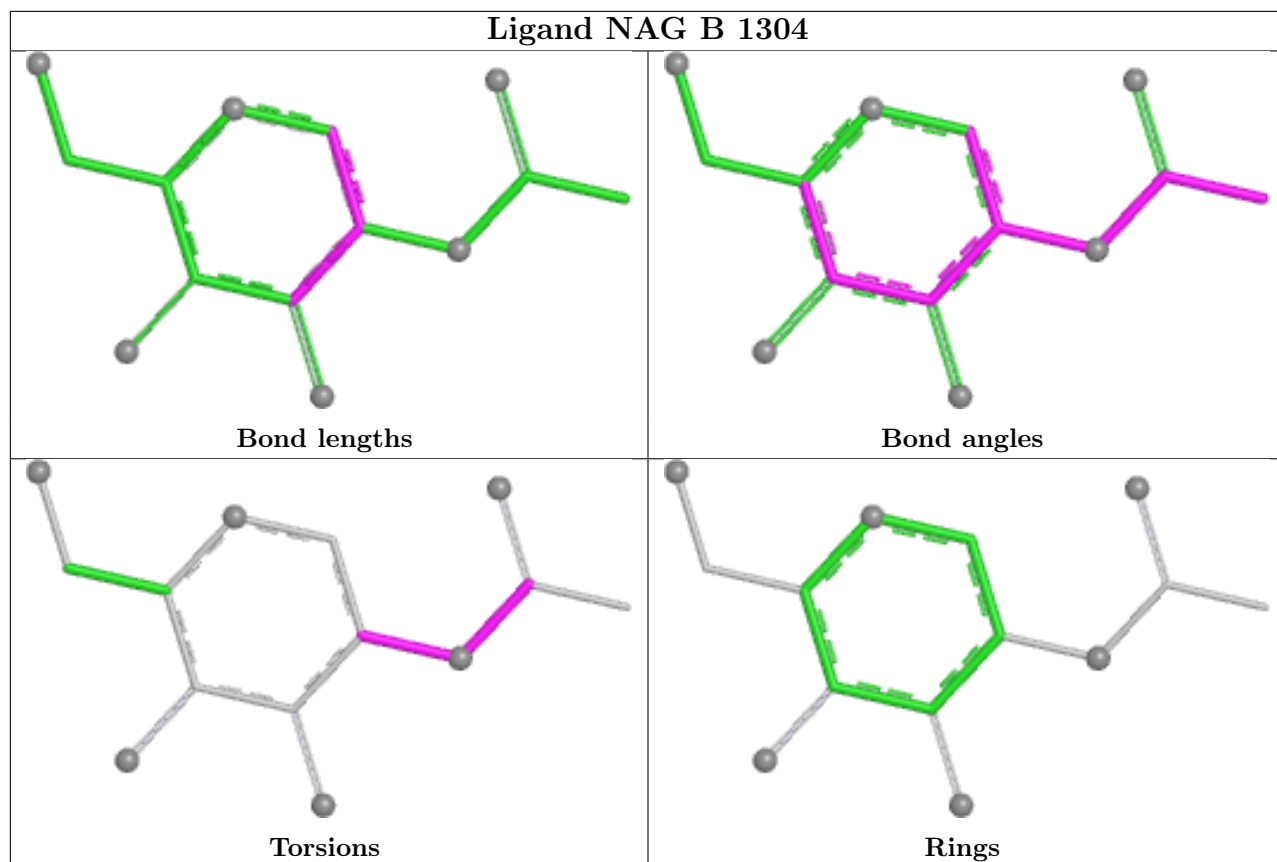
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

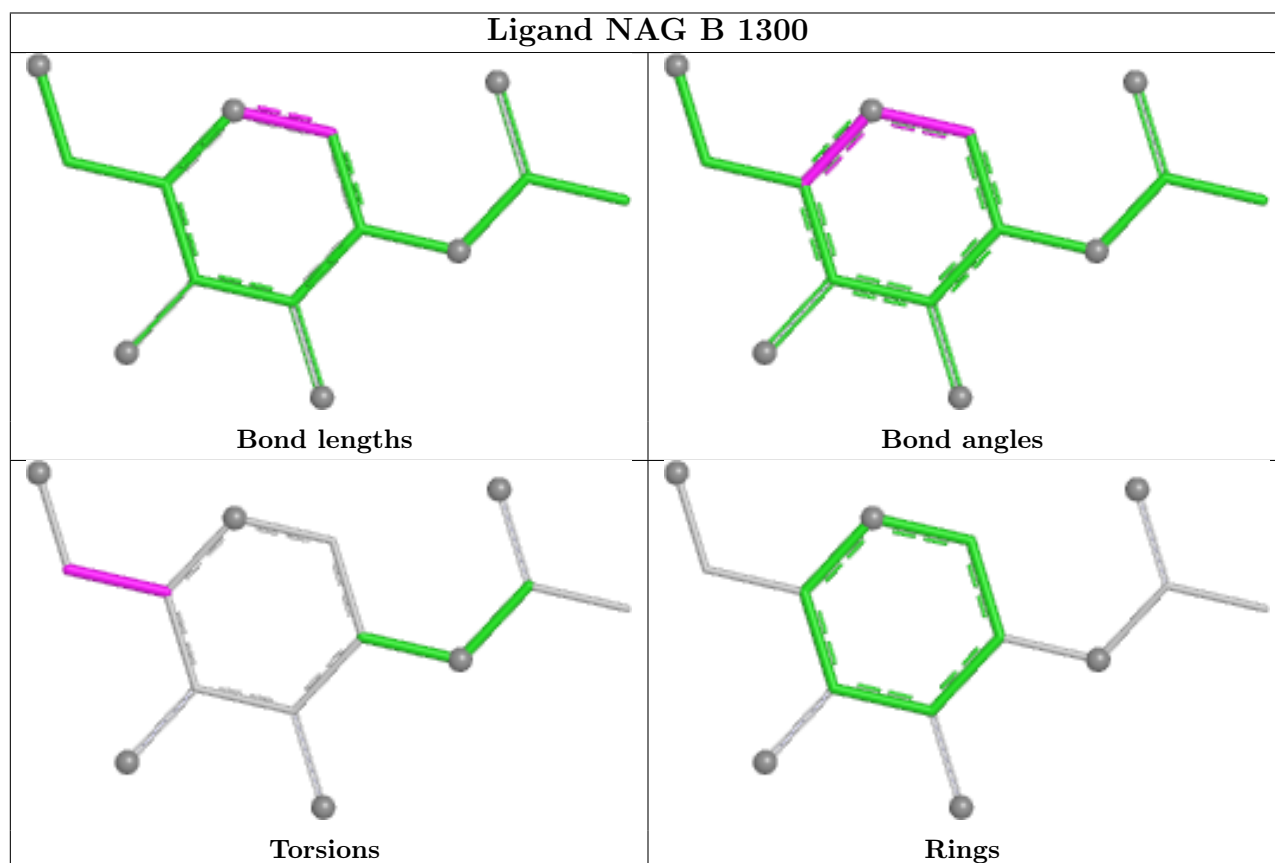
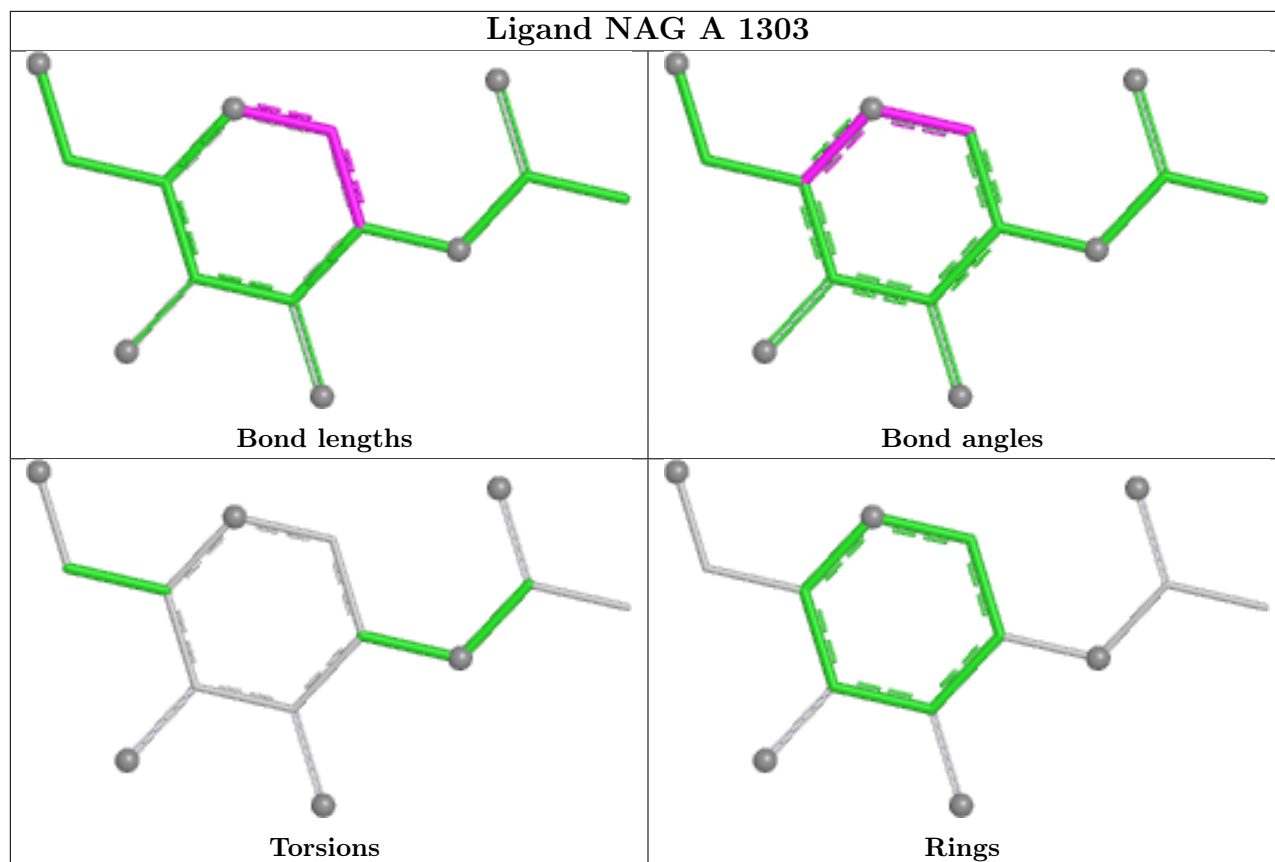
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

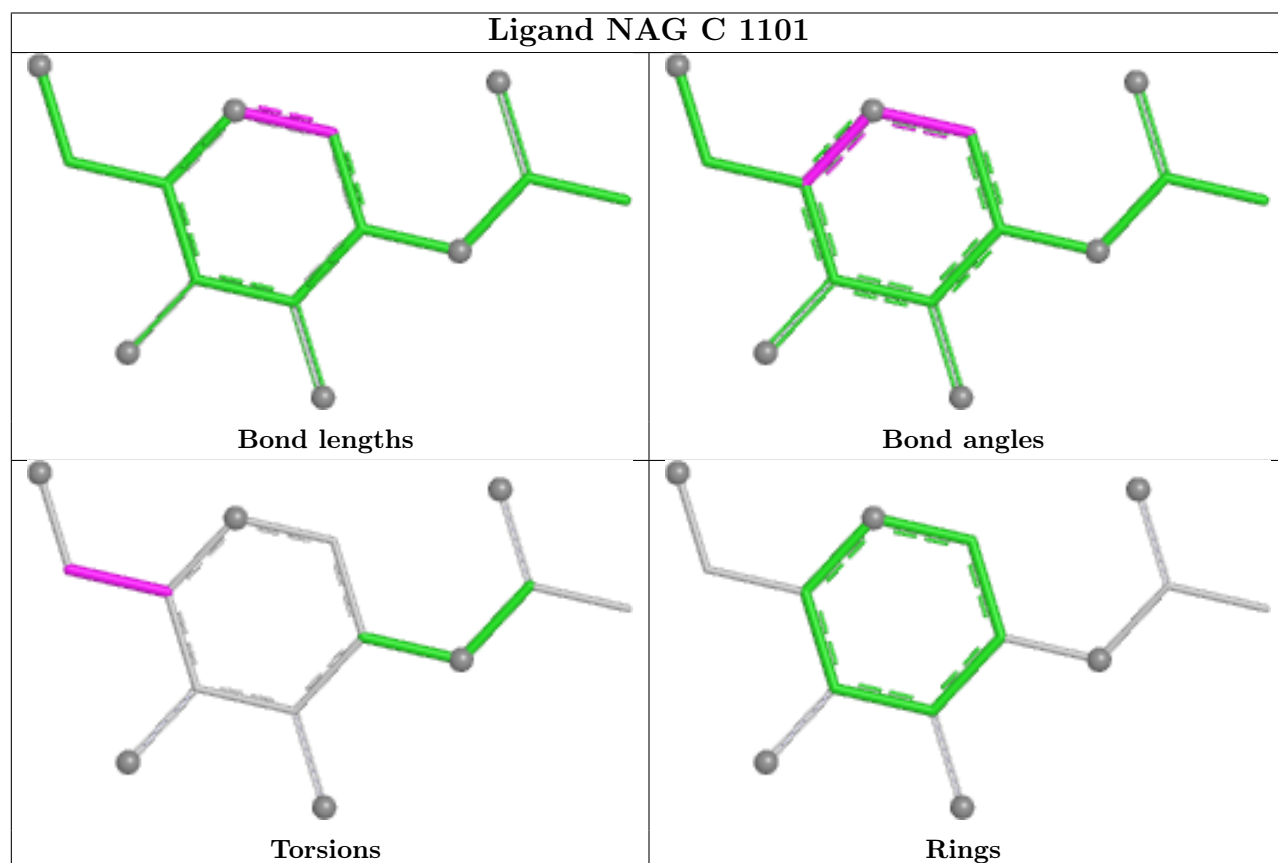
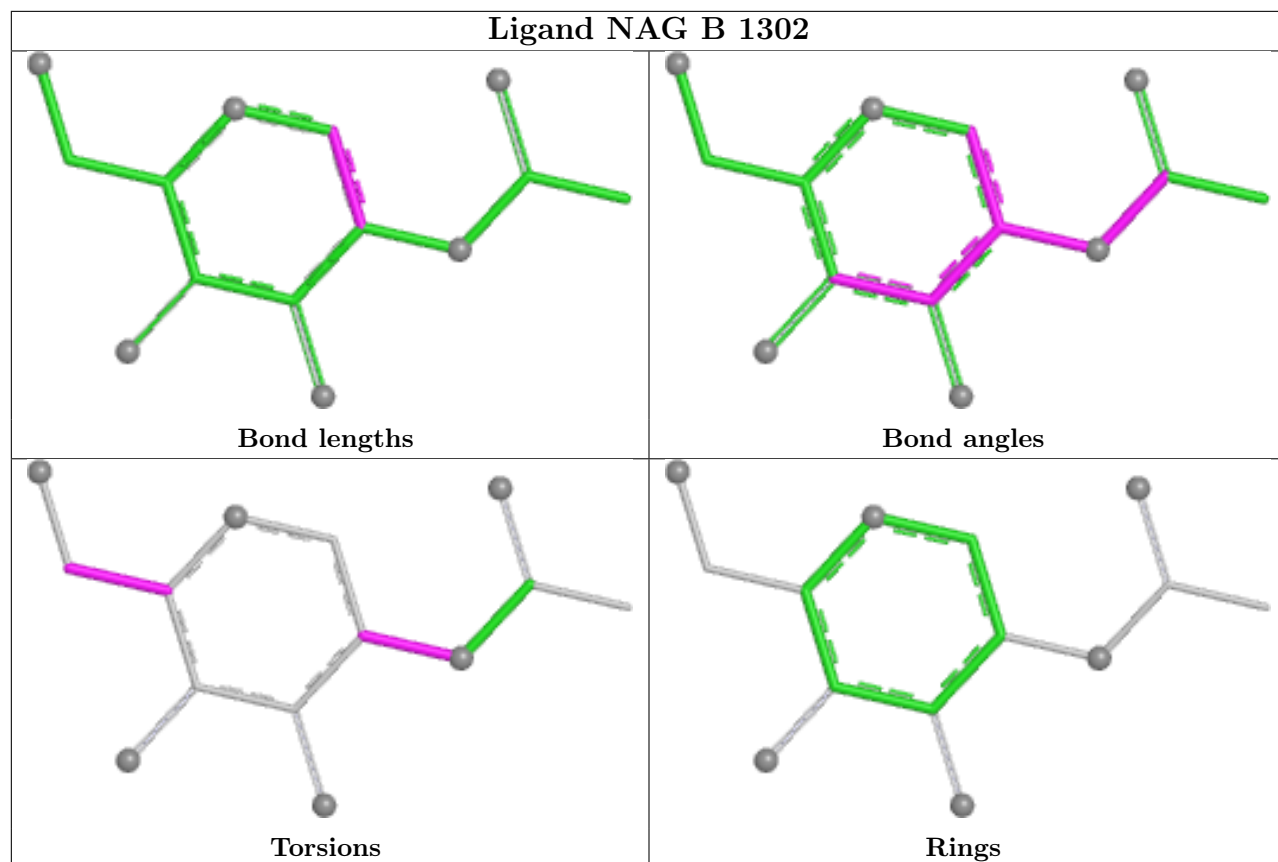


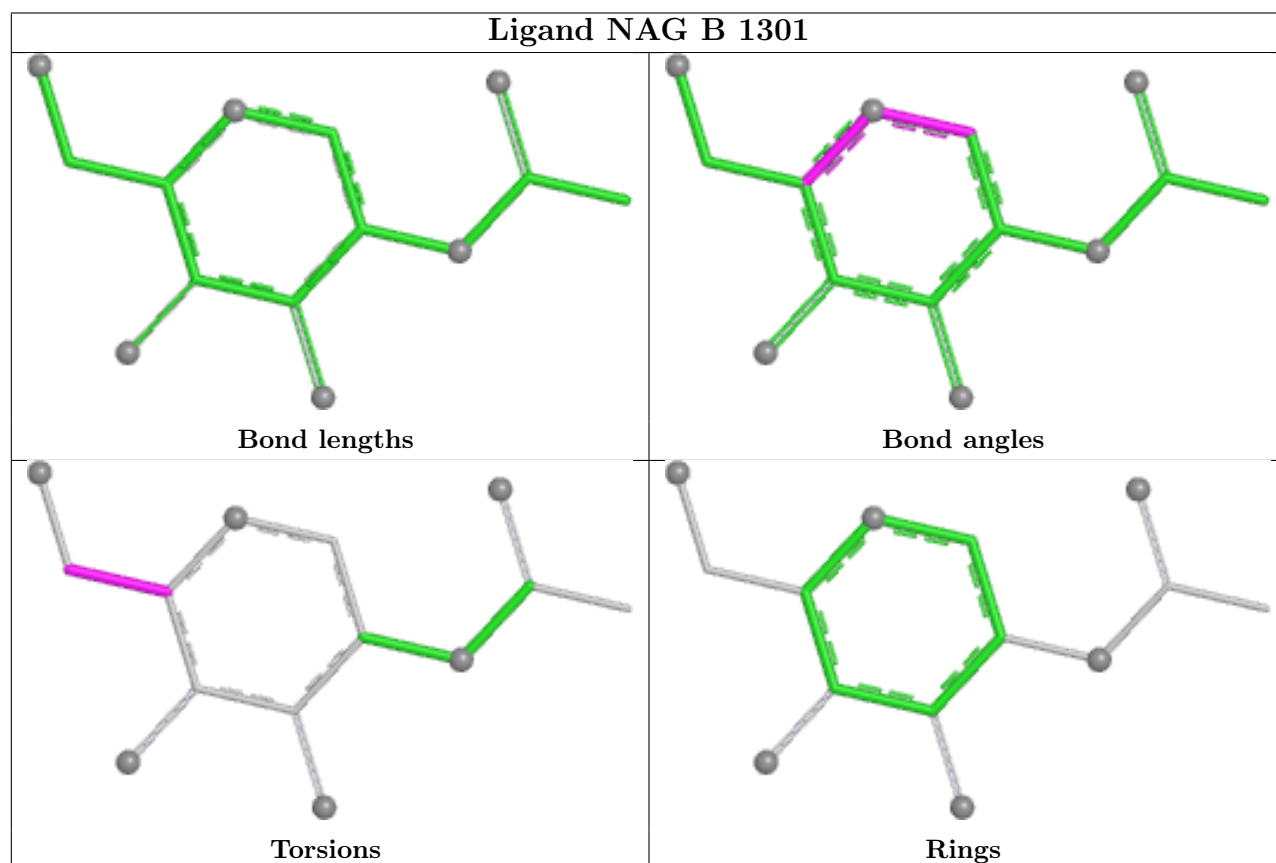
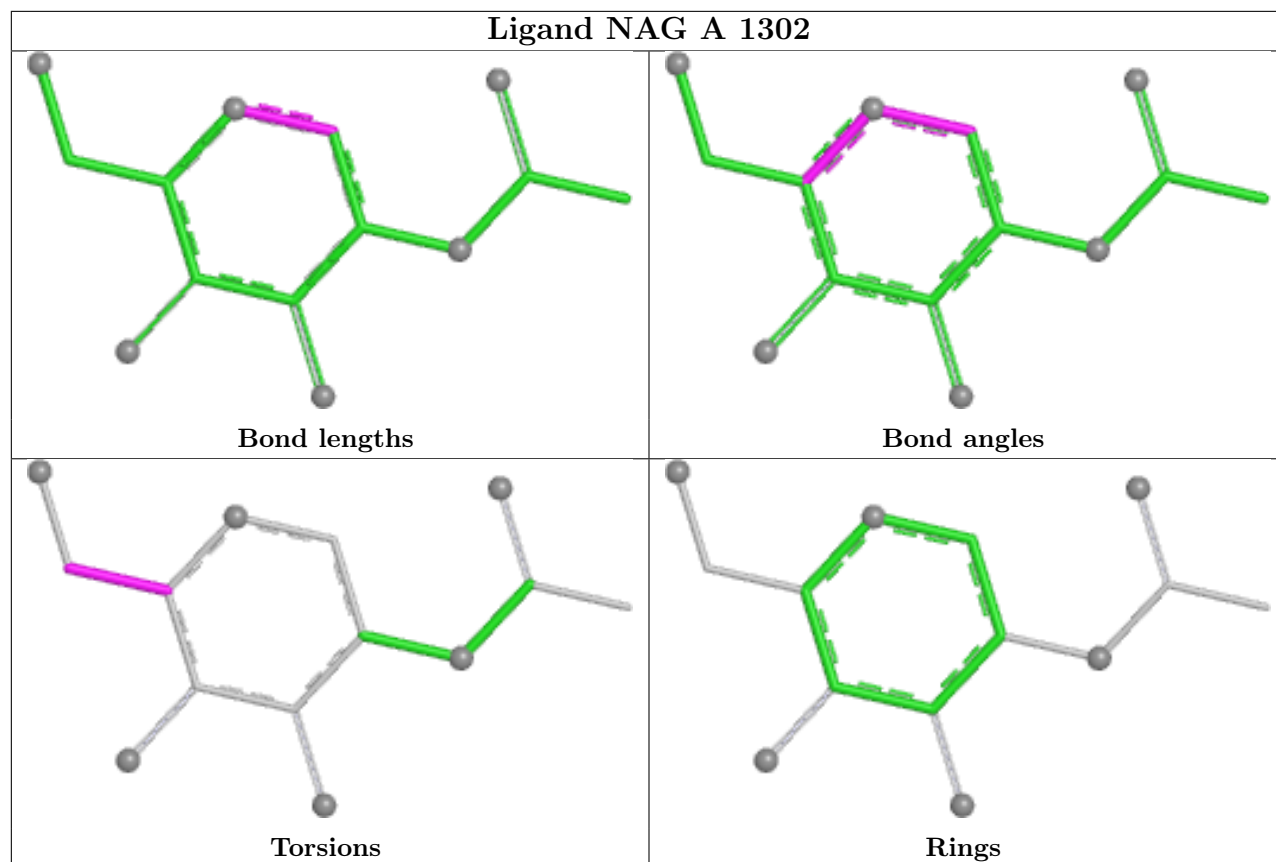


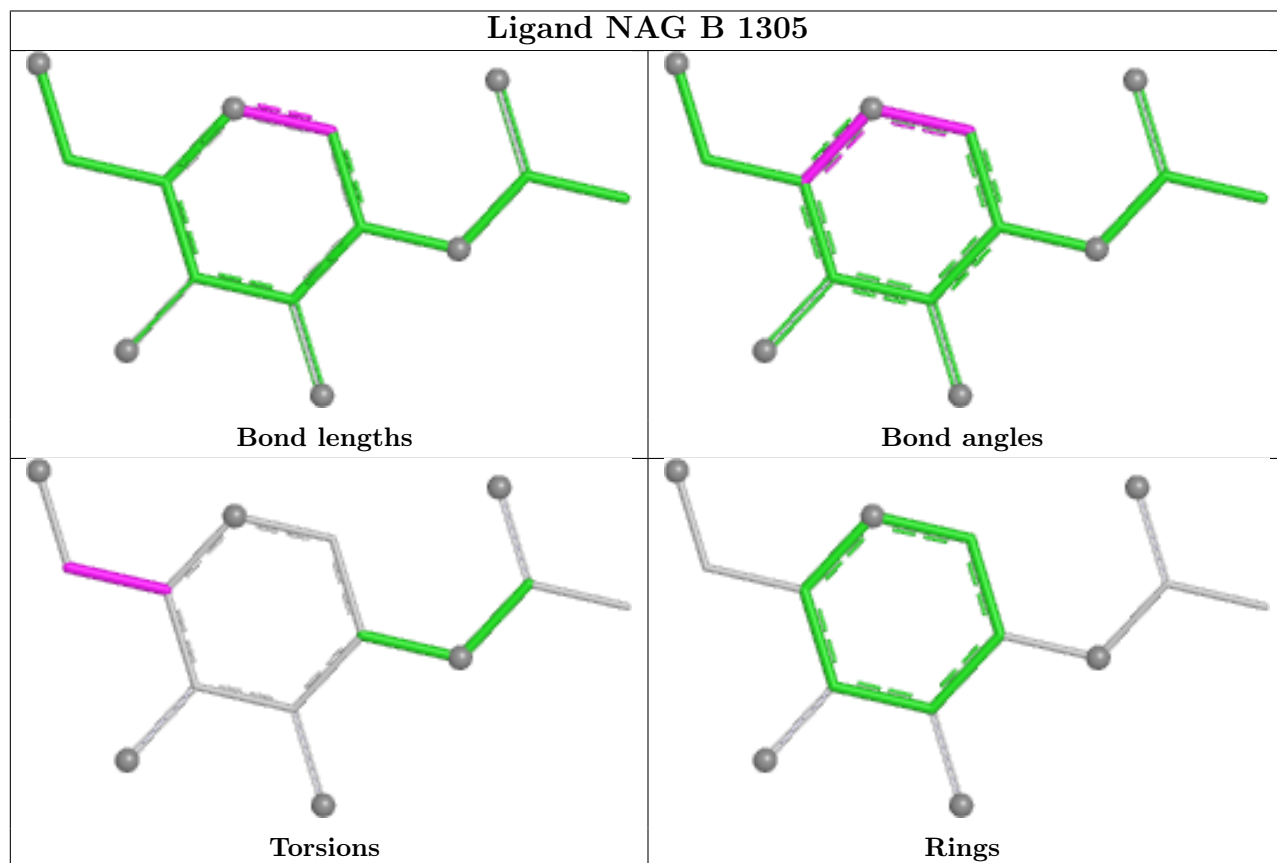
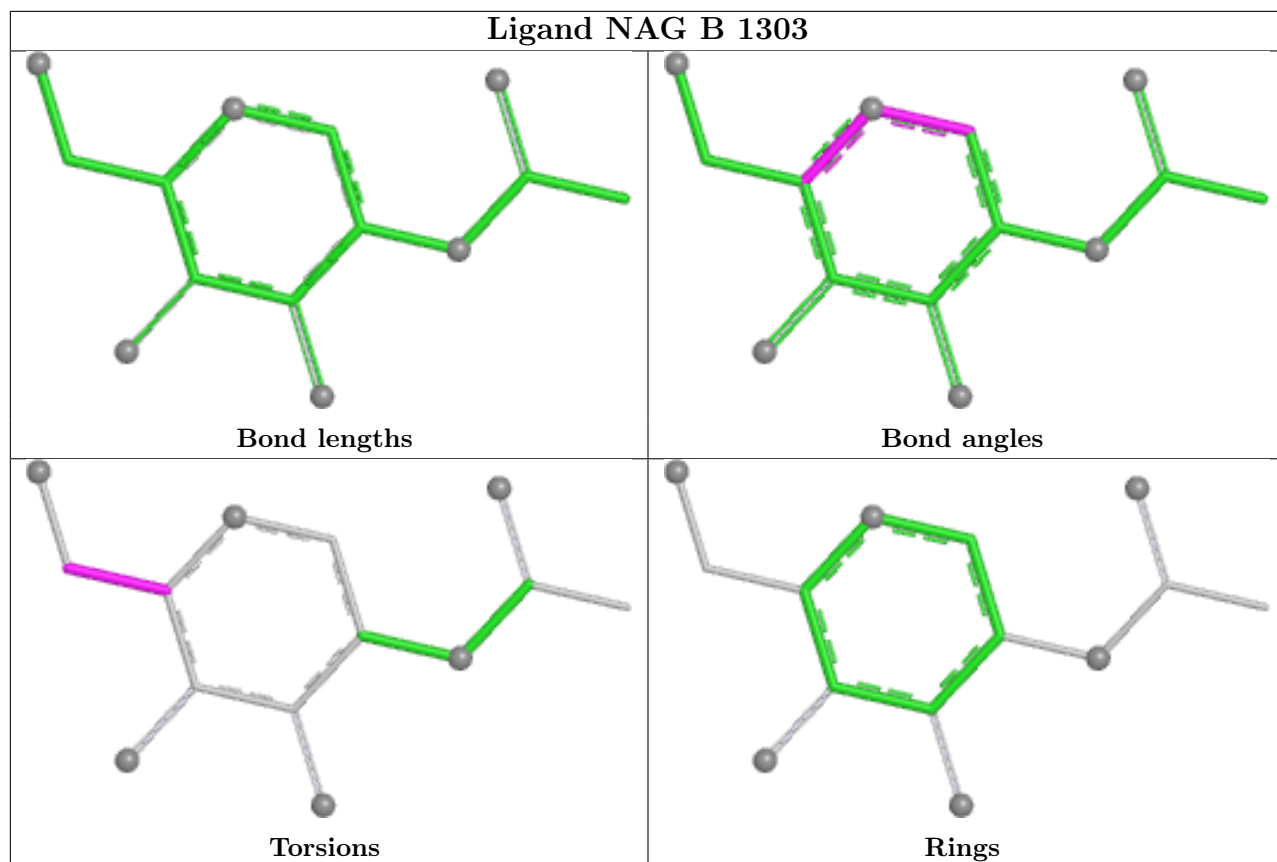












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

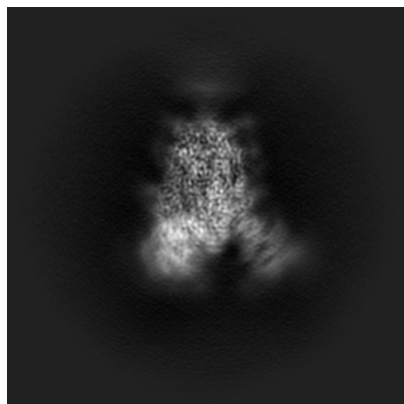
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41260. These allow visual inspection of the internal detail of the map and identification of artifacts.

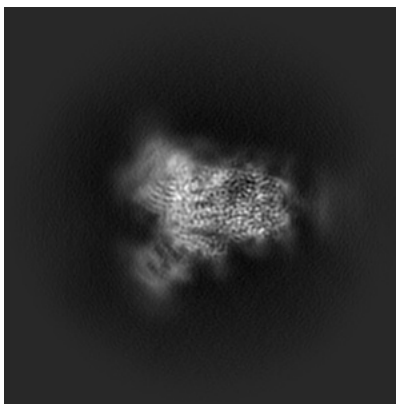
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

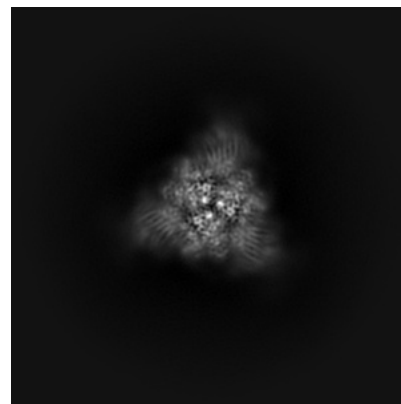
6.1.1 Primary map



X

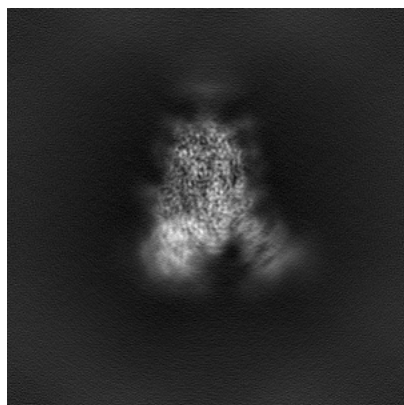


Y

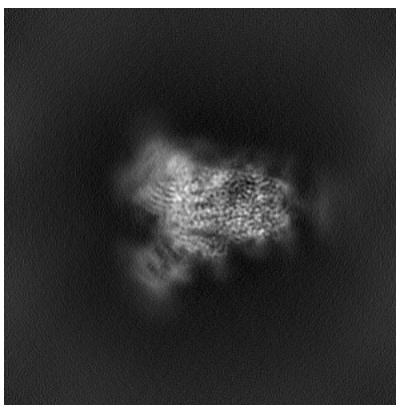


Z

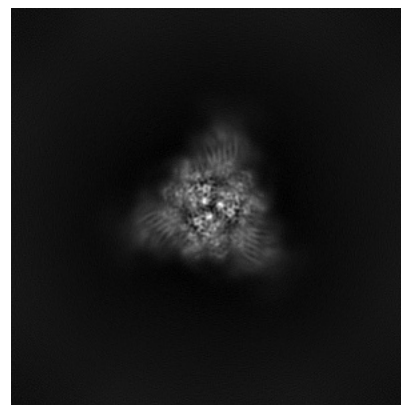
6.1.2 Raw map



X



Y

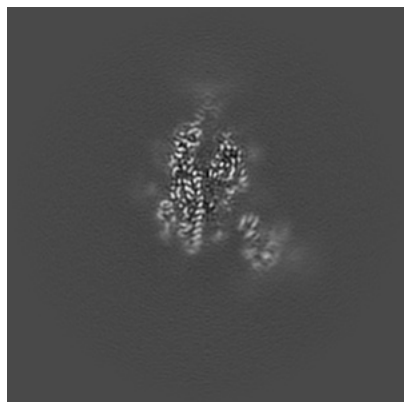


Z

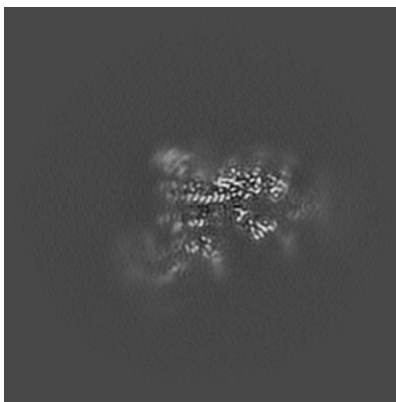
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

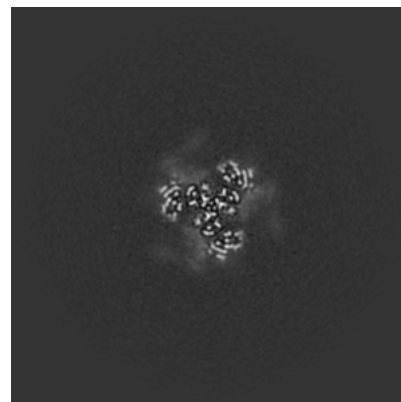
6.2.1 Primary map



X Index: 192

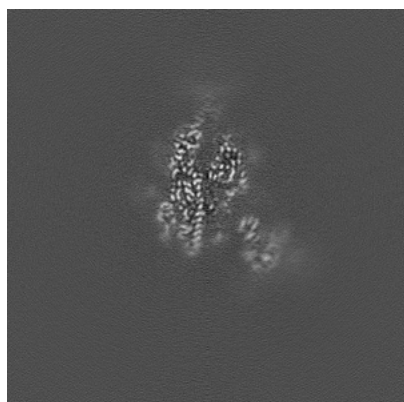


Y Index: 192

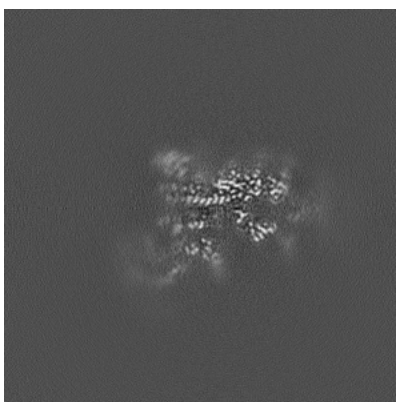


Z Index: 192

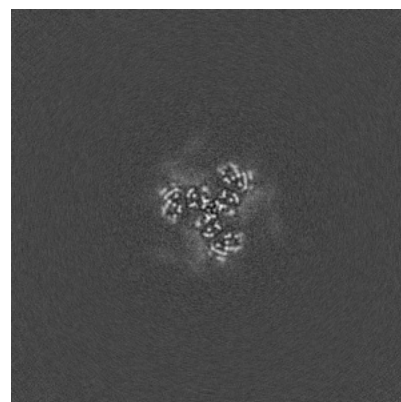
6.2.2 Raw map



X Index: 192



Y Index: 192

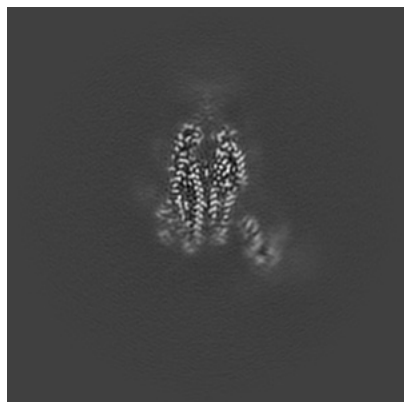


Z Index: 192

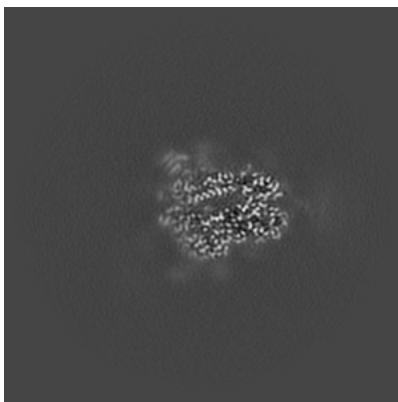
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

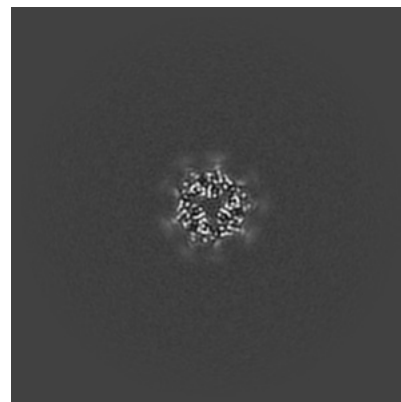
6.3.1 Primary map



X Index: 189

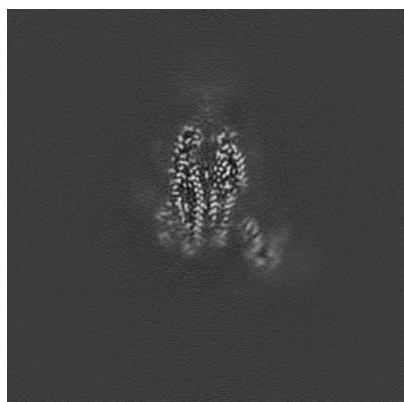


Y Index: 205

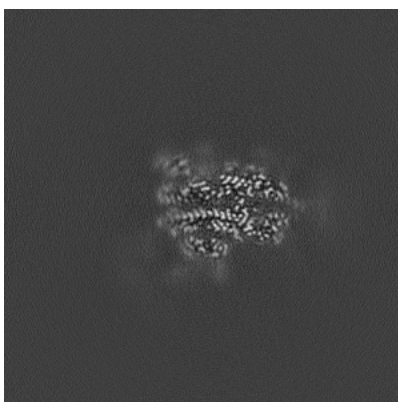


Z Index: 243

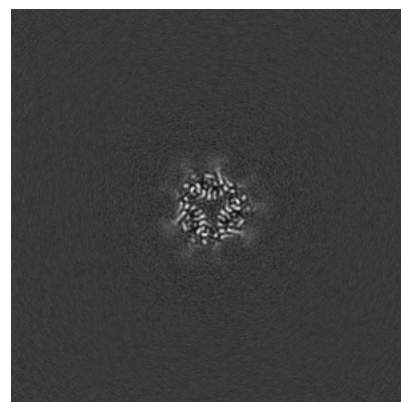
6.3.2 Raw map



X Index: 189



Y Index: 200

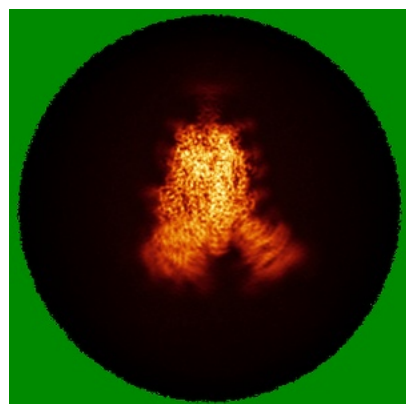


Z Index: 244

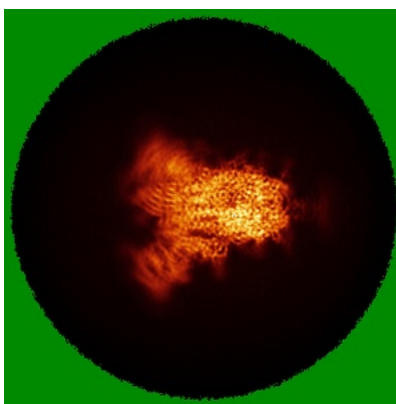
The images above show the largest variance slices of the map in three orthogonal directions.

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

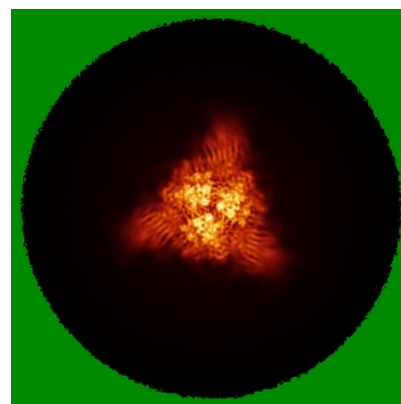
6.4.1 Primary map



X

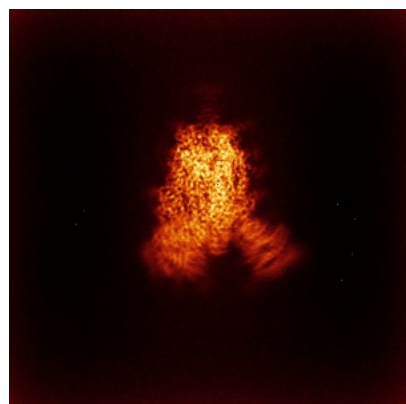


Y

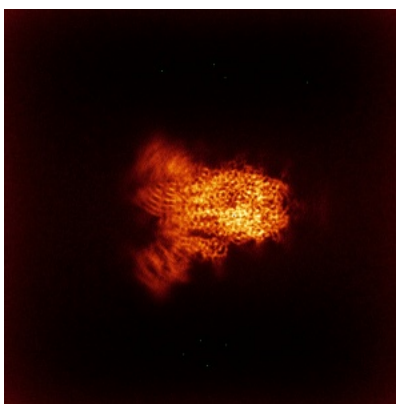


Z

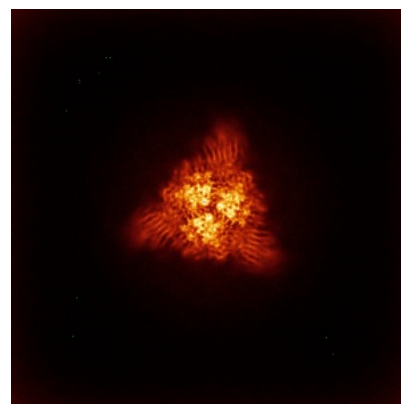
6.4.2 Raw map



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.

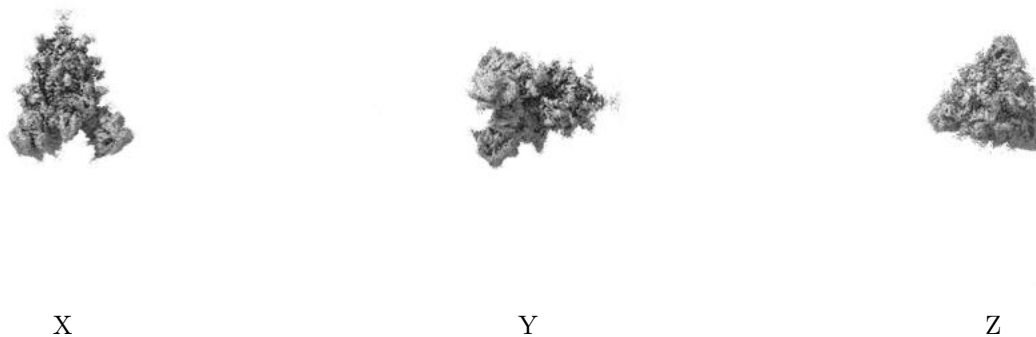
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

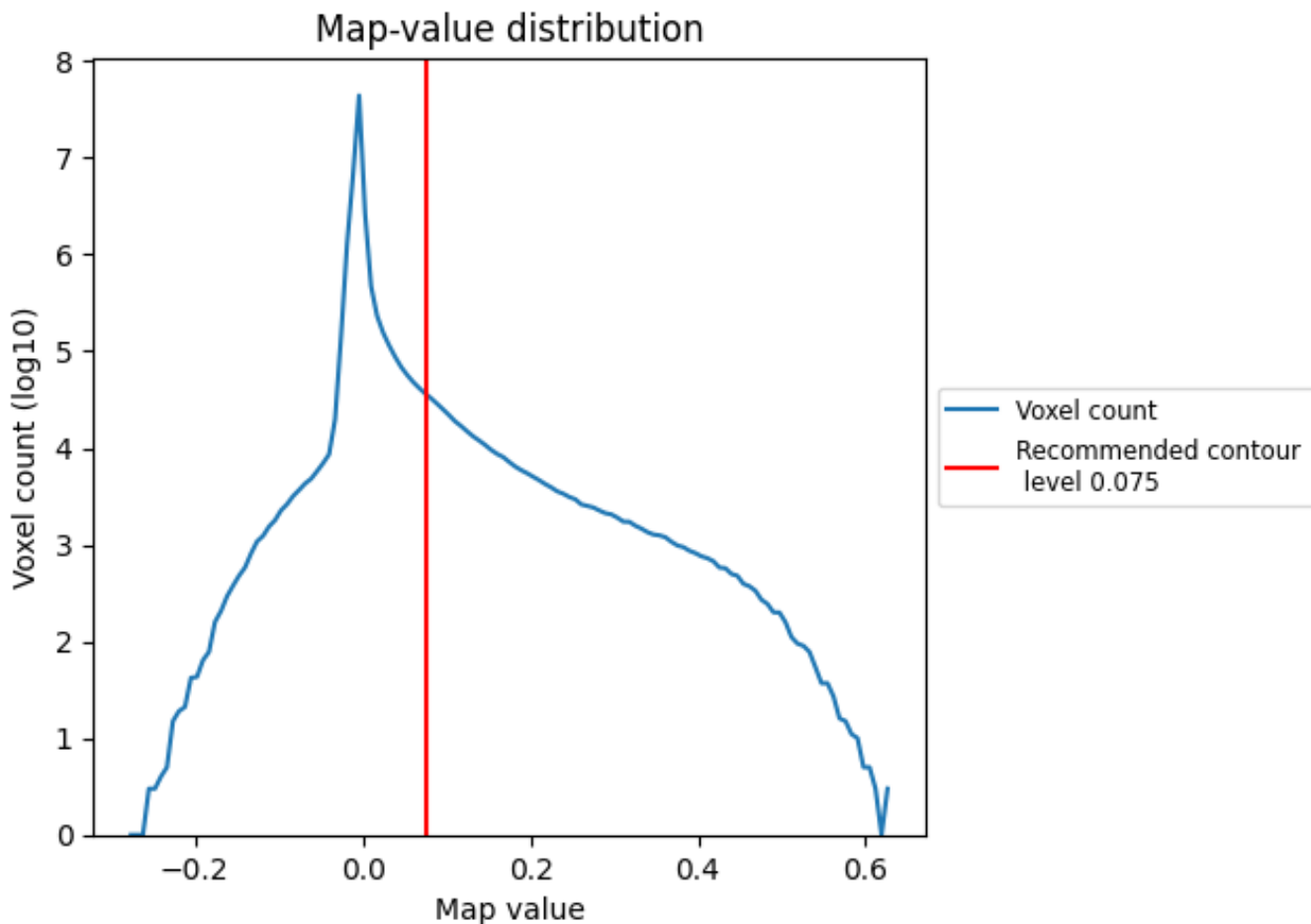
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

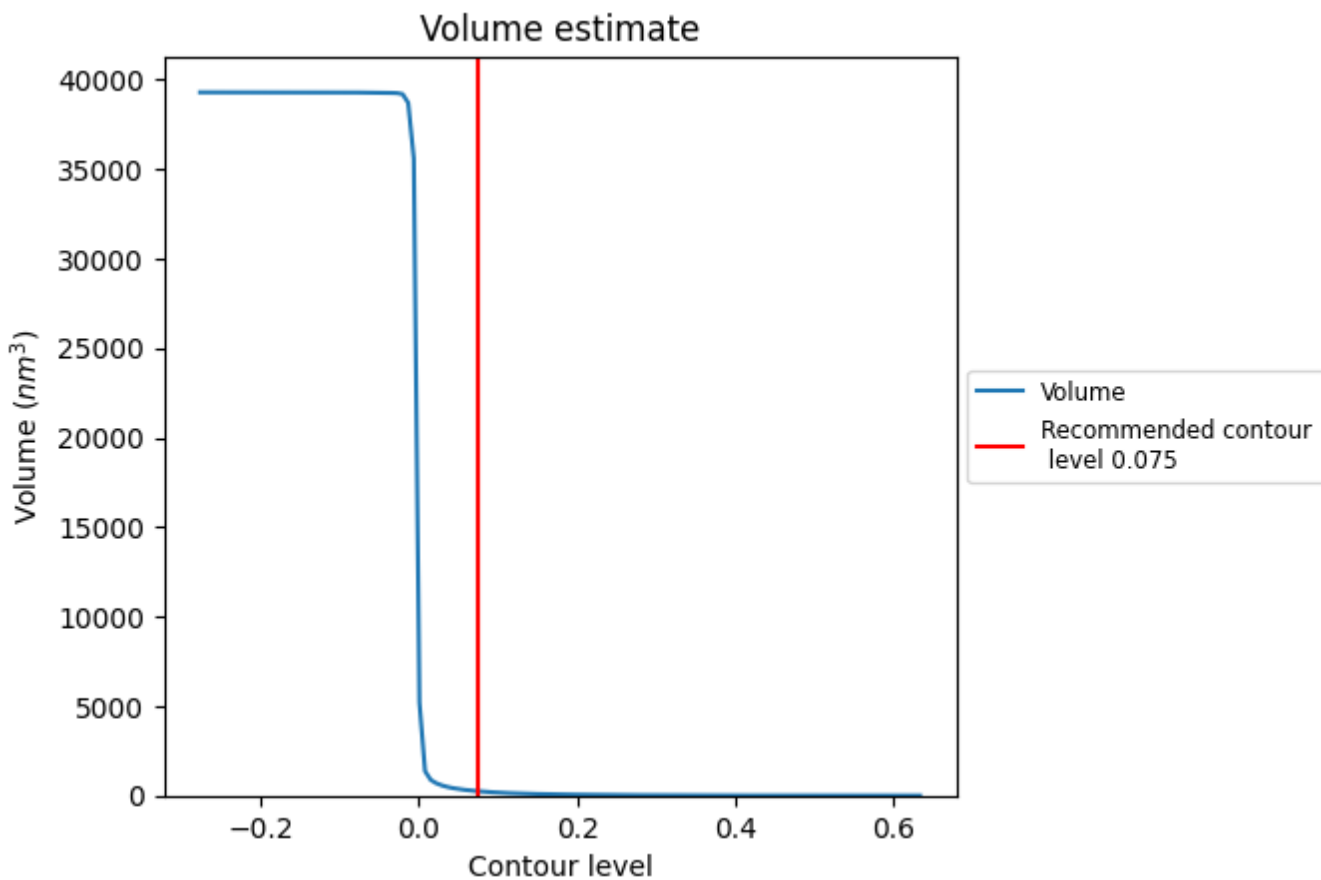
This section contains the results of statistical analysis of the map.

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.

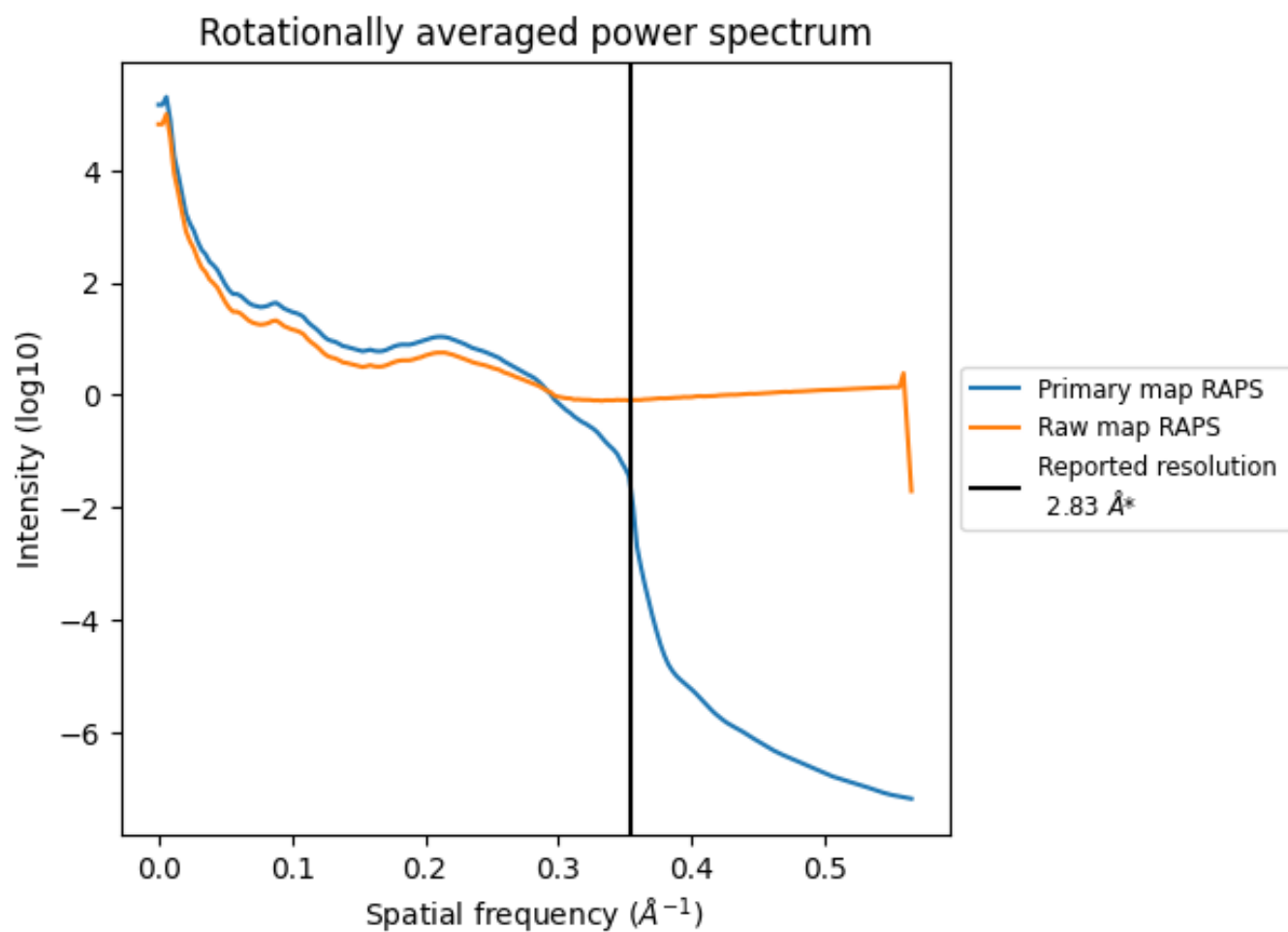
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm^3 ; this corresponds to an approximate mass of 220 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

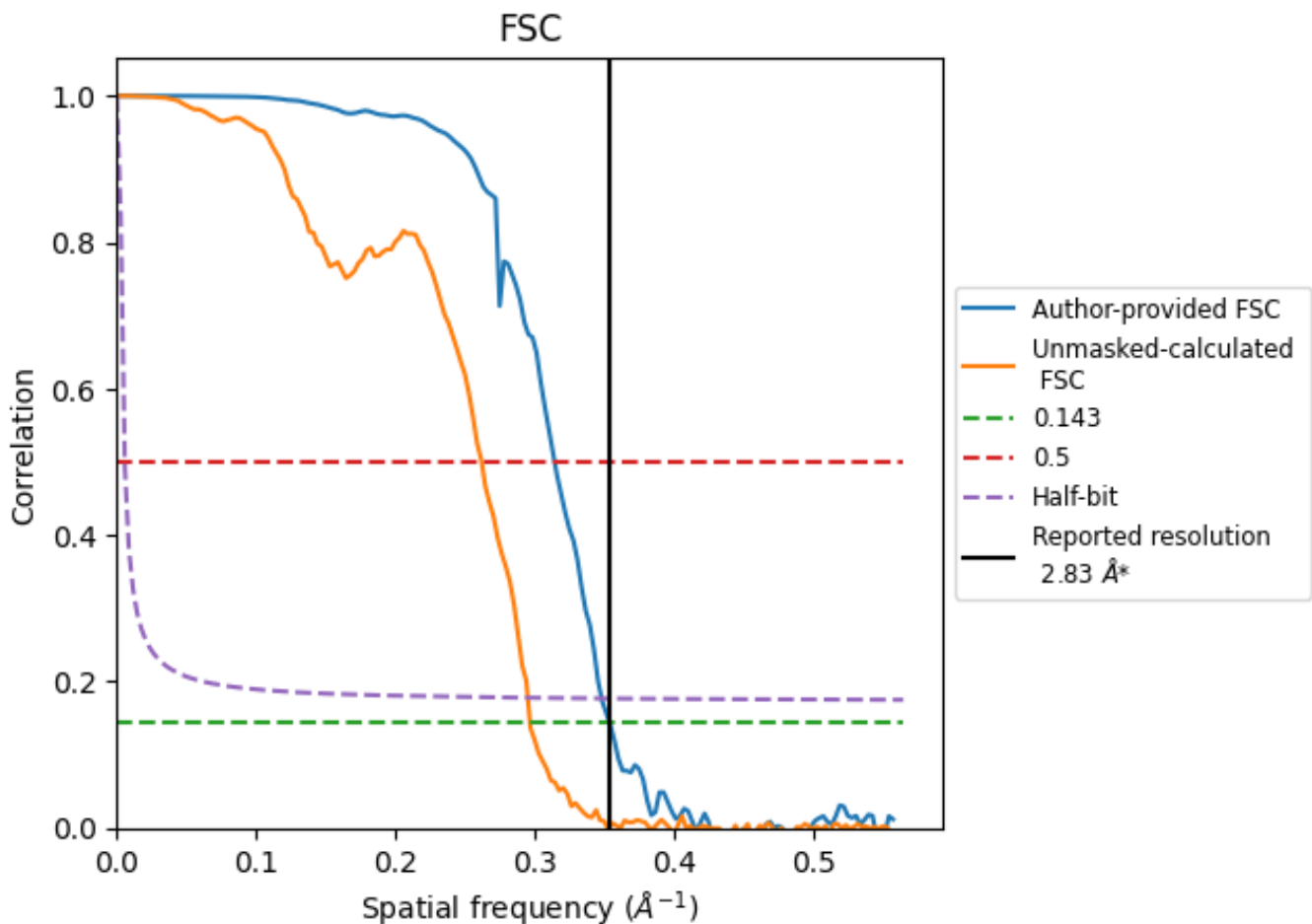


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353\AA^{-1}

8.2 Resolution estimates [i](#)

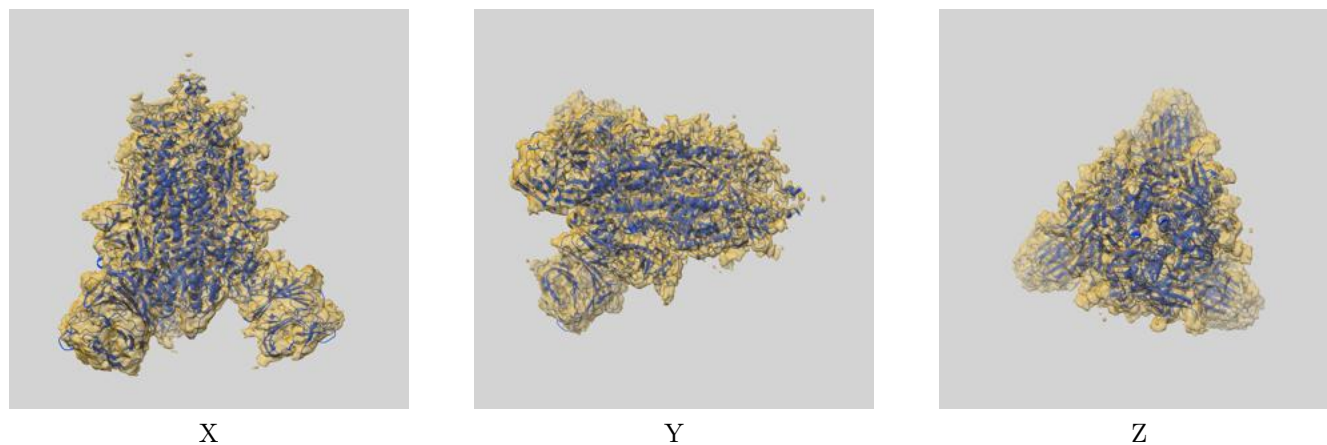
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.82	3.18	2.87
Unmasked-calculated*	3.37	3.82	3.39

*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 3.37 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41260 and PDB model 8THF. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



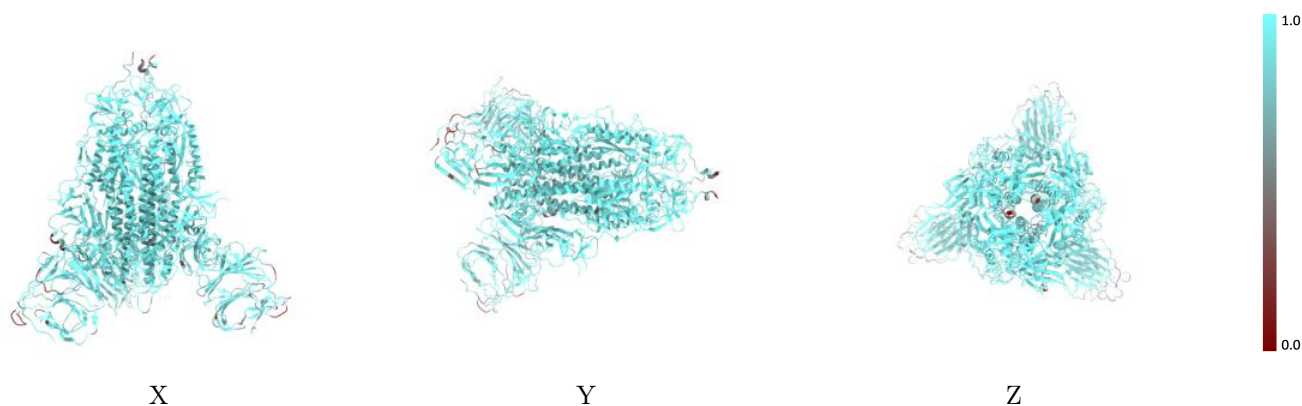
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



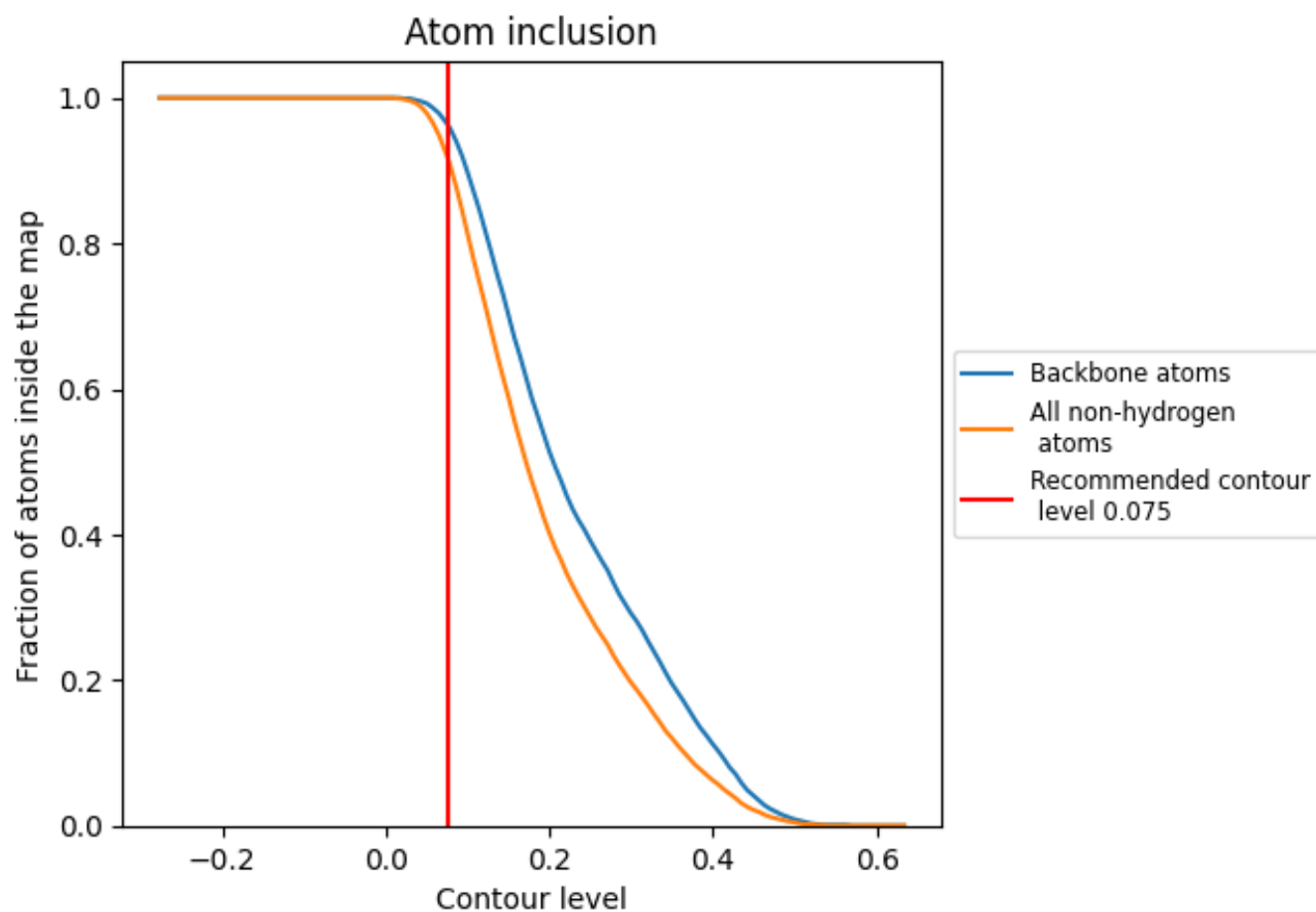
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.4610
A	 0.9150	 0.4590
B	 0.9270	 0.4660
C	 0.9190	 0.4580
D	 0.8930	 0.4460
E	 0.9290	 0.5010
F	 0.9290	 0.4750
G	 0.8930	 0.4420
H	 0.7140	 0.4440
I	 0.9290	 0.5000
J	 0.8930	 0.4680
K	 0.8930	 0.4450
L	 0.6790	 0.4210
M	 0.9290	 0.4810
N	 0.8570	 0.4460
O	 0.7500	 0.4270

