



Full wwPDB EM Validation Report ⓘ

Aug 20, 2026 – 02:59 PM EDT

PDB ID : 9YMK / pdb_00009ymk
EMDB ID : EMD-73109
Title : RVz20_wk72_08 Fab in complex with BG505 MD39 SOSIP and RM20A3 Fab
Authors : Sewall, L.M.; Ozorowski, G.; Ward, A.B.
Deposited on : 2025-10-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

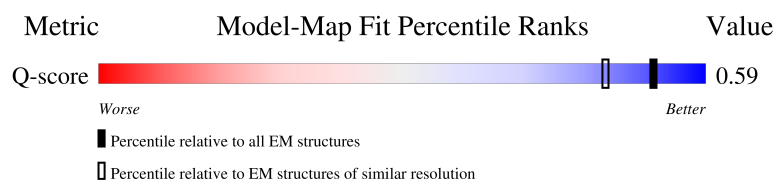
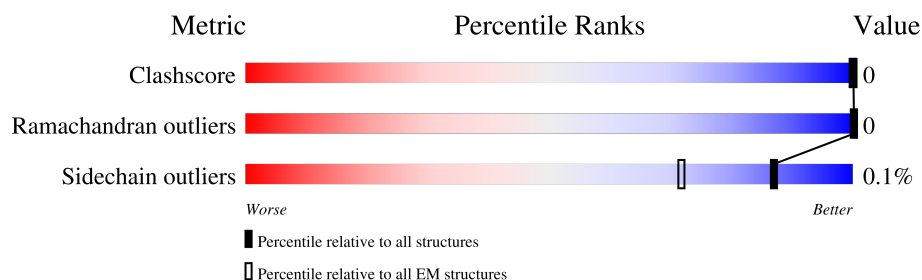
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	G	229	8% 54% 46%
1	J	229	7% 54% 46%
1	O	229	9% 54% 46%
2	I	215	9% 50% 50%

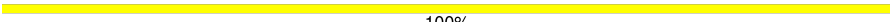
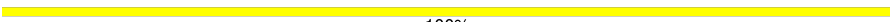
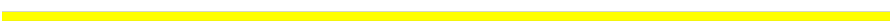
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Mol	Chain	Length	Quality of chain
2	M	215	
2	Q	215	
3	A	513	
3	C	513	
3	E	513	
4	B	153	
4	D	153	
4	F	153	
5	H	230	
5	K	230	
5	P	230	
6	L	217	
6	N	217	
6	R	217	
7	S	7	
7	X	7	
7	c	7	
8	T	9	
8	Y	9	
8	d	9	
9	U	2	
9	W	2	
9	Z	2	
9	b	2	
9	e	2	

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Mol	Chain	Length	Quality of chain
9	g	2	 100%
10	V	3	 100%
10	a	3	 100%
10	f	3	 100%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 25272 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 RM20A3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	123	Total	C	N	O	S	0	0
			934	590	160	179	5		
1	J	123	Total	C	N	O	S	0	0
			934	590	160	179	5		
1	O	123	Total	C	N	O	S	0	0
			934	590	160	179	5		

- Molecule 2 is a protein called RM20A3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	108	Total	C	N	O	S	0	0
			803	499	135	166	3		
2	M	108	Total	C	N	O	S	0	0
			803	499	135	166	3		
2	Q	108	Total	C	N	O	S	0	0
			803	499	135	166	3		

- Molecule 3 is a protein called BG505 MD39 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	438	Total	C	N	O	S	0	0
			3457	2177	608	645	27		
3	C	438	Total	C	N	O	S	0	0
			3457	2177	608	645	27		
3	E	438	Total	C	N	O	S	0	0
			3457	2177	608	645	27		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q2N0S6
A	0	LYS	-	expression tag	UNP Q2N0S6
A	1	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP Q2N0S6
A	3	LEU	-	expression tag	UNP Q2N0S6
A	4	CYS	-	expression tag	UNP Q2N0S6
A	5	CYS	-	expression tag	UNP Q2N0S6
A	6	VAL	-	expression tag	UNP Q2N0S6
A	7	LEU	-	expression tag	UNP Q2N0S6
A	8	LEU	-	expression tag	UNP Q2N0S6
A	9	LEU	-	expression tag	UNP Q2N0S6
A	10	CYS	-	expression tag	UNP Q2N0S6
A	11	GLY	-	expression tag	UNP Q2N0S6
A	12	ALA	-	expression tag	UNP Q2N0S6
A	13	VAL	-	expression tag	UNP Q2N0S6
A	14	PHE	-	expression tag	UNP Q2N0S6
A	15	VAL	-	expression tag	UNP Q2N0S6
A	16	SER	-	expression tag	UNP Q2N0S6
A	17	PRO	-	expression tag	UNP Q2N0S6
A	18	SER	-	expression tag	UNP Q2N0S6
A	19	GLN	-	expression tag	UNP Q2N0S6
A	20	GLU	-	expression tag	UNP Q2N0S6
A	21	ILE	-	expression tag	UNP Q2N0S6
A	22	HIS	-	expression tag	UNP Q2N0S6
A	23	ALA	-	expression tag	UNP Q2N0S6
A	24	ARG	-	expression tag	UNP Q2N0S6
A	25	PHE	-	expression tag	UNP Q2N0S6
A	26	ARG	-	expression tag	UNP Q2N0S6
A	27	ARG	-	expression tag	UNP Q2N0S6
A	28	GLY	-	expression tag	UNP Q2N0S6
A	29	ALA	-	expression tag	UNP Q2N0S6
A	30	ARG	-	expression tag	UNP Q2N0S6
A	106	GLU	THR	conflict	UNP Q2N0S6
A	271	ILE	MET	conflict	UNP Q2N0S6
A	288	LEU	PHE	conflict	UNP Q2N0S6
A	304	VAL	ARG	conflict	UNP Q2N0S6
A	319	TYR	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	363	GLN	ASN	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP Q2N0S6
C	0	LYS	-	expression tag	UNP Q2N0S6
C	1	ARG	-	expression tag	UNP Q2N0S6
C	2	GLY	-	expression tag	UNP Q2N0S6
C	3	LEU	-	expression tag	UNP Q2N0S6
C	4	CYS	-	expression tag	UNP Q2N0S6
C	5	CYS	-	expression tag	UNP Q2N0S6
C	6	VAL	-	expression tag	UNP Q2N0S6
C	7	LEU	-	expression tag	UNP Q2N0S6
C	8	LEU	-	expression tag	UNP Q2N0S6
C	9	LEU	-	expression tag	UNP Q2N0S6
C	10	CYS	-	expression tag	UNP Q2N0S6
C	11	GLY	-	expression tag	UNP Q2N0S6
C	12	ALA	-	expression tag	UNP Q2N0S6
C	13	VAL	-	expression tag	UNP Q2N0S6
C	14	PHE	-	expression tag	UNP Q2N0S6
C	15	VAL	-	expression tag	UNP Q2N0S6
C	16	SER	-	expression tag	UNP Q2N0S6
C	17	PRO	-	expression tag	UNP Q2N0S6
C	18	SER	-	expression tag	UNP Q2N0S6
C	19	GLN	-	expression tag	UNP Q2N0S6
C	20	GLU	-	expression tag	UNP Q2N0S6
C	21	ILE	-	expression tag	UNP Q2N0S6
C	22	HIS	-	expression tag	UNP Q2N0S6
C	23	ALA	-	expression tag	UNP Q2N0S6
C	24	ARG	-	expression tag	UNP Q2N0S6
C	25	PHE	-	expression tag	UNP Q2N0S6
C	26	ARG	-	expression tag	UNP Q2N0S6
C	27	ARG	-	expression tag	UNP Q2N0S6
C	28	GLY	-	expression tag	UNP Q2N0S6
C	29	ALA	-	expression tag	UNP Q2N0S6
C	30	ARG	-	expression tag	UNP Q2N0S6
C	106	GLU	THR	conflict	UNP Q2N0S6
C	271	ILE	MET	conflict	UNP Q2N0S6
C	288	LEU	PHE	conflict	UNP Q2N0S6
C	304	VAL	ARG	conflict	UNP Q2N0S6
C	319	TYR	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	363	GLN	ASN	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
E	-1	MET	-	expression tag	UNP Q2N0S6
E	0	LYS	-	expression tag	UNP Q2N0S6
E	1	ARG	-	expression tag	UNP Q2N0S6
E	2	GLY	-	expression tag	UNP Q2N0S6
E	3	LEU	-	expression tag	UNP Q2N0S6
E	4	CYS	-	expression tag	UNP Q2N0S6
E	5	CYS	-	expression tag	UNP Q2N0S6
E	6	VAL	-	expression tag	UNP Q2N0S6
E	7	LEU	-	expression tag	UNP Q2N0S6
E	8	LEU	-	expression tag	UNP Q2N0S6
E	9	LEU	-	expression tag	UNP Q2N0S6
E	10	CYS	-	expression tag	UNP Q2N0S6
E	11	GLY	-	expression tag	UNP Q2N0S6
E	12	ALA	-	expression tag	UNP Q2N0S6
E	13	VAL	-	expression tag	UNP Q2N0S6
E	14	PHE	-	expression tag	UNP Q2N0S6
E	15	VAL	-	expression tag	UNP Q2N0S6
E	16	SER	-	expression tag	UNP Q2N0S6
E	17	PRO	-	expression tag	UNP Q2N0S6
E	18	SER	-	expression tag	UNP Q2N0S6
E	19	GLN	-	expression tag	UNP Q2N0S6
E	20	GLU	-	expression tag	UNP Q2N0S6
E	21	ILE	-	expression tag	UNP Q2N0S6
E	22	HIS	-	expression tag	UNP Q2N0S6
E	23	ALA	-	expression tag	UNP Q2N0S6
E	24	ARG	-	expression tag	UNP Q2N0S6
E	25	PHE	-	expression tag	UNP Q2N0S6
E	26	ARG	-	expression tag	UNP Q2N0S6
E	27	ARG	-	expression tag	UNP Q2N0S6
E	28	GLY	-	expression tag	UNP Q2N0S6
E	29	ALA	-	expression tag	UNP Q2N0S6
E	30	ARG	-	expression tag	UNP Q2N0S6
E	106	GLU	THR	conflict	UNP Q2N0S6
E	271	ILE	MET	conflict	UNP Q2N0S6
E	288	LEU	PHE	conflict	UNP Q2N0S6
E	304	VAL	ARG	conflict	UNP Q2N0S6
E	319	TYR	ALA	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	363	GLN	ASN	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 4 is a protein called BG505 MD39 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	121	Total	C	N	O	S	0	0
			956	600	165	185	6		
4	D	121	Total	C	N	O	S	0	0
			956	600	165	185	6		
4	F	121	Total	C	N	O	S	0	0
			956	600	165	185	6		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	PRO	ALA	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	519	SER	PHE	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	561	PRO	ALA	conflict	UNP Q2N0S6
D	568	ASP	LEU	conflict	UNP Q2N0S6
D	570	HIS	VAL	conflict	UNP Q2N0S6
D	585	HIS	ARG	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
F	519	SER	PHE	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	PRO	ALA	conflict	UNP Q2N0S6
F	568	ASP	LEU	conflict	UNP Q2N0S6
F	570	HIS	VAL	conflict	UNP Q2N0S6
F	585	HIS	ARG	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

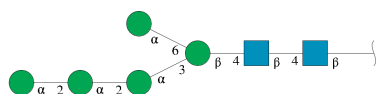
- Molecule 5 is a protein called RVz20_wk72_08 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	126	Total	C	N	O	S	0	0
			976	617	168	188	3		
5	K	126	Total	C	N	O	S	0	0
			976	617	168	188	3		
5	P	126	Total	C	N	O	S	0	0
			976	617	168	188	3		

- Molecule 6 is a protein called RVz20_wk72_08 light chain.

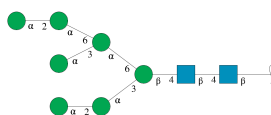
Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	111	Total	C	N	O	S	0	0
			847	529	145	170	3		
6	N	111	Total	C	N	O	S	0	0
			847	529	145	170	3		
6	R	111	Total	C	N	O	S	0	0
			847	529	145	170	3		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	7	Total	C	N	O	0	0
			83	46	2	35		
7	X	7	Total	C	N	O	0	0
			83	46	2	35		
7	c	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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
8	T	9	Total	C	N	O	0	0
			105	58	2	45		
8	Y	9	Total	C	N	O	0	0
			105	58	2	45		
8	d	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 9 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
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	W	2	Total	C	N	O	0	0
			28	16	2	10		
9	Z	2	Total	C	N	O	0	0
			28	16	2	10		
9	b	2	Total	C	N	O	0	0
			28	16	2	10		
9	e	2	Total	C	N	O	0	0
			28	16	2	10		
9	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 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.



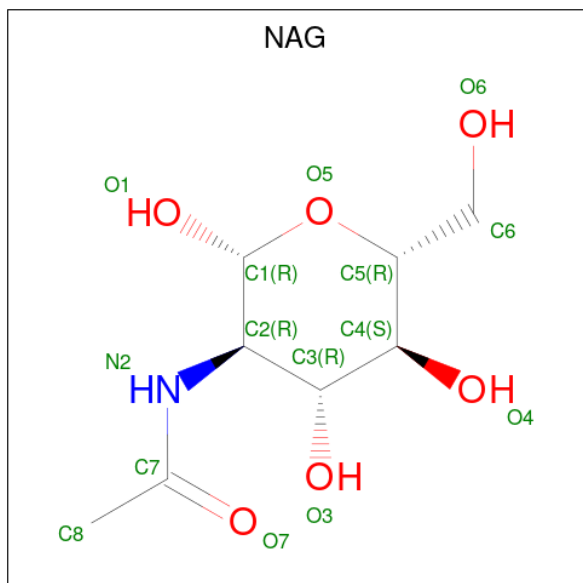
Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	3	Total	C	N	O	0	0
			39	22	2	15		
10	f	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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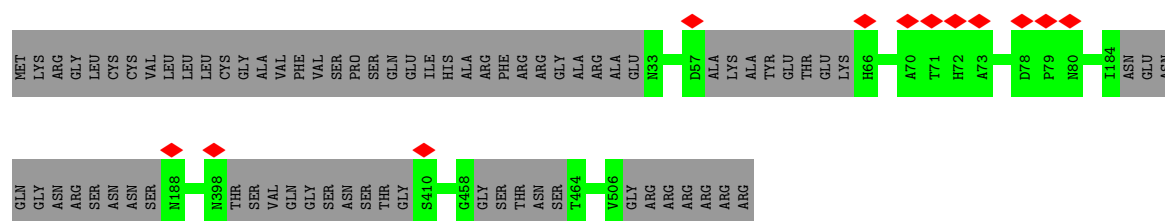
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	B	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O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

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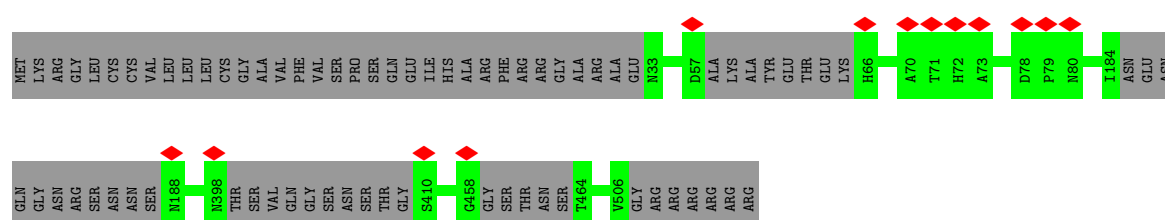
Mol	Chain	Residues	Atoms				AltConf
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	E	1	Total	C	N	O	0
			14	8	1	5	
11	F	1	Total	C	N	O	0
			14	8	1	5	
11	F	1	Total	C	N	O	0
			14	8	1	5	

Chain C: 



- Molecule 3: BG505 MD39 SOSIP gp120

Chain E: 



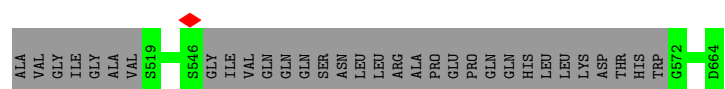
- Molecule 4: BG505 MD39 SOSIP gp41

Chain B: 



- Molecule 4: BG505 MD39 SOSIP gp41

Chain D: 



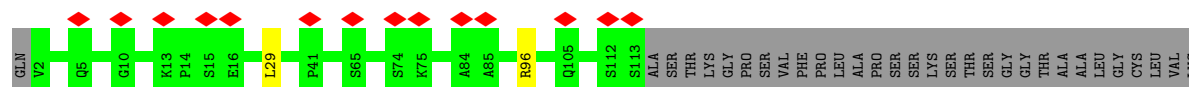
- Molecule 4: BG505 MD39 SOSIP gp41

Chain F: 

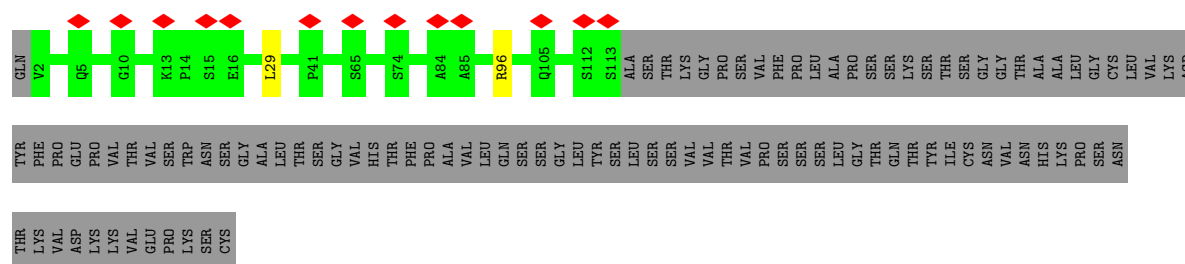


- Molecule 5: RVz20_wk72_08 Fab heavy chain

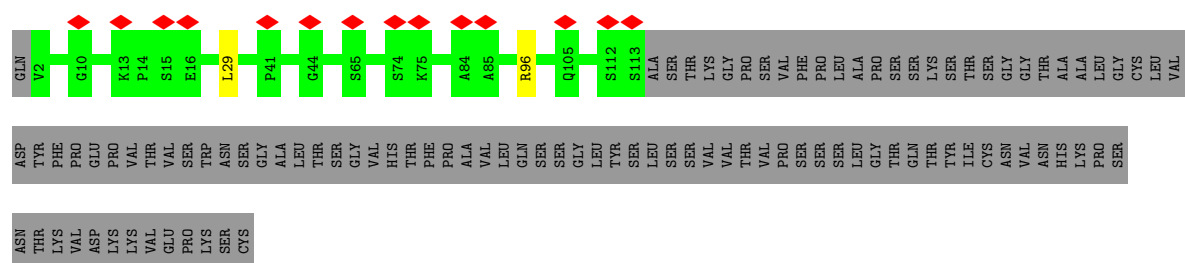
Chain H: 



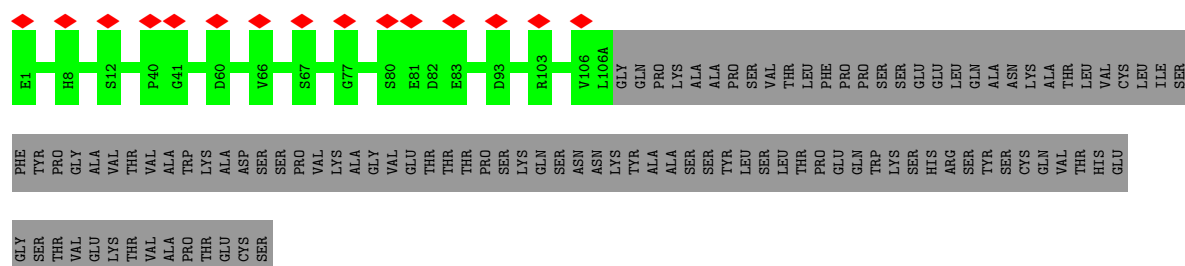
- Molecule 5: RVz20 wk72 08 Fab heavy chain



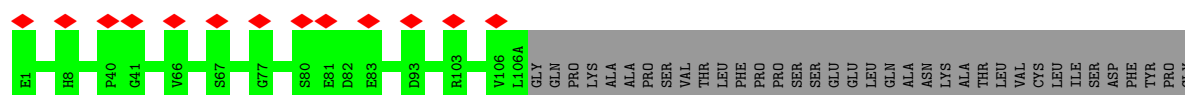
- Molecule 5: RVz20 wk72 08 Fab heavy chain

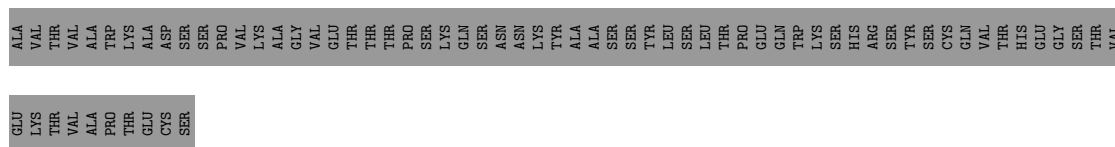


- Molecule 6: RVz20 wk72 08 light chain

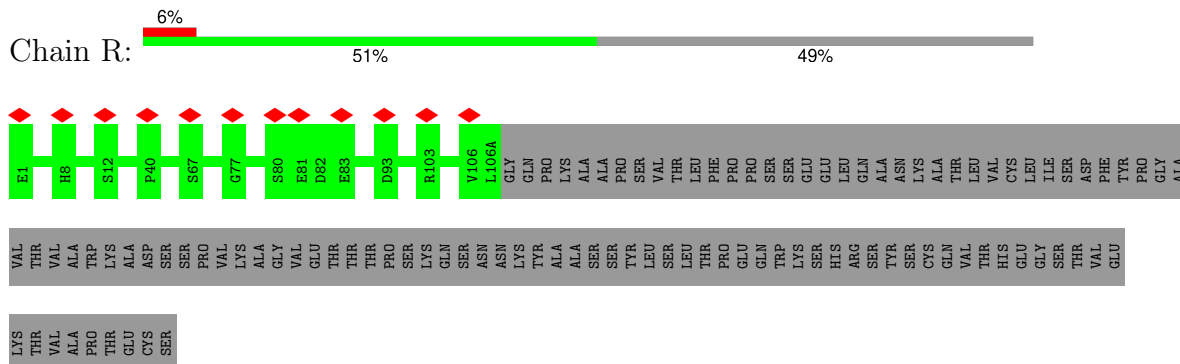


- Molecule 6: RVz20 wk72 08 light chain

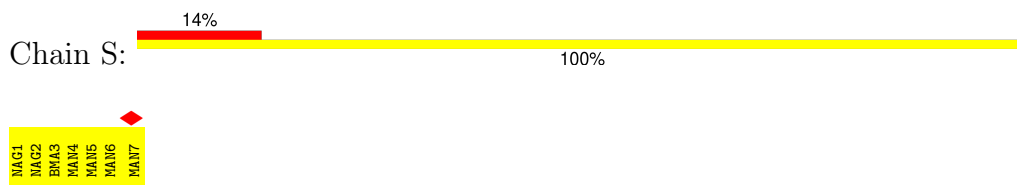




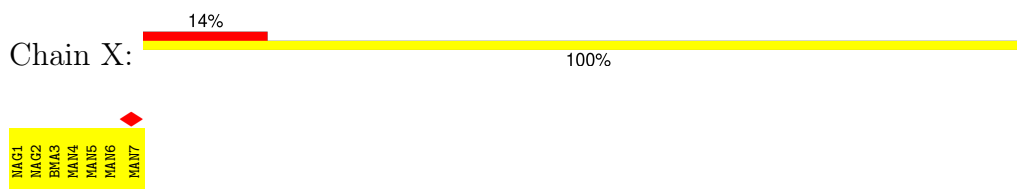
- Molecule 6: RVz20_wk72_08 light chain



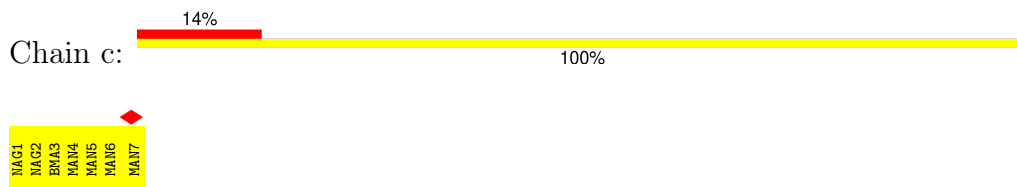
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(

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

Chain T:  100%

MAG1
MAG2
EM43
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1
MAG2
EM43
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1
MAG2
EM43
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

● Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1
MAG2

● Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1
MAG2

● Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

MAG1
MAG2

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

MAG1
MAG2
EMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1
MAG2
EMA3

- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

MAG1
MAG2
EMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	252448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.191	Depositor
Minimum map value	-1.573	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	413.56, 413.56, 413.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0339, 1.0339, 1.0339	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.21	0/954	0.49	0/1288
1	J	0.21	0/954	0.49	0/1288
1	O	0.21	0/954	0.49	0/1288
2	I	0.25	0/822	0.52	0/1118
2	M	0.25	0/822	0.52	0/1118
2	Q	0.25	0/822	0.52	0/1118
3	A	0.22	0/3528	0.50	0/4791
3	C	0.23	0/3528	0.50	0/4791
3	E	0.23	0/3528	0.50	0/4791
4	B	0.20	0/972	0.42	0/1317
4	D	0.20	0/972	0.42	0/1317
4	F	0.20	0/972	0.42	0/1317
5	H	0.22	0/1001	0.54	0/1363
5	K	0.22	0/1001	0.54	0/1363
5	P	0.22	0/1001	0.54	0/1363
6	L	0.21	0/868	0.49	0/1181
6	N	0.21	0/868	0.49	0/1181
6	R	0.21	0/868	0.49	0/1181
All	All	0.22	0/24435	0.50	0/33174

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
5	H	0	1
5	K	0	1
5	P	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	96	ARG	Sidechain
5	K	96	ARG	Sidechain
5	P	96	ARG	Sidechain

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	G	934	0	906	0	0
1	J	934	0	906	0	0
1	O	934	0	906	0	0
2	I	803	0	756	0	0
2	M	803	0	756	0	0
2	Q	803	0	756	0	0
3	A	3457	0	3403	0	0
3	C	3457	0	3403	0	0
3	E	3457	0	3403	0	0
4	B	956	0	928	0	0
4	D	956	0	928	0	0
4	F	956	0	928	0	0
5	H	976	0	937	0	0
5	K	976	0	937	0	0
5	P	976	0	937	0	0
6	L	847	0	801	0	0
6	N	847	0	801	0	0
6	R	847	0	801	0	0
7	S	83	0	70	0	0
7	X	83	0	70	0	0
7	c	83	0	70	0	0
8	T	105	0	88	0	0
8	Y	105	0	88	0	0
8	d	105	0	88	0	0
9	U	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	28	0	25	0	0
9	Z	28	0	25	0	0
9	b	28	0	25	0	0
9	e	28	0	25	0	0
9	g	28	0	25	0	0
10	V	39	0	34	0	0
10	a	39	0	34	0	0
10	f	39	0	34	0	0
11	A	140	0	130	0	0
11	B	28	0	26	0	0
11	C	140	0	130	0	0
11	D	28	0	26	0	0
11	E	140	0	130	0	0
11	F	28	0	26	0	0
All	All	25272	0	24387	0	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 0.

There are no clashes within the asymmetric unit.

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	G	121/229 (53%)	114 (94%)	7 (6%)	0	100	100
1	J	121/229 (53%)	114 (94%)	7 (6%)	0	100	100
1	O	121/229 (53%)	114 (94%)	7 (6%)	0	100	100
2	I	106/215 (49%)	98 (92%)	8 (8%)	0	100	100
2	M	106/215 (49%)	98 (92%)	8 (8%)	0	100	100
2	Q	106/215 (49%)	98 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	428/513 (83%)	413 (96%)	15 (4%)	0	100	100
3	C	428/513 (83%)	413 (96%)	15 (4%)	0	100	100
3	E	428/513 (83%)	413 (96%)	15 (4%)	0	100	100
4	B	117/153 (76%)	114 (97%)	3 (3%)	0	100	100
4	D	117/153 (76%)	114 (97%)	3 (3%)	0	100	100
4	F	117/153 (76%)	114 (97%)	3 (3%)	0	100	100
5	H	124/230 (54%)	117 (94%)	7 (6%)	0	100	100
5	K	124/230 (54%)	117 (94%)	7 (6%)	0	100	100
5	P	124/230 (54%)	117 (94%)	7 (6%)	0	100	100
6	L	109/217 (50%)	101 (93%)	8 (7%)	0	100	100
6	N	109/217 (50%)	101 (93%)	8 (7%)	0	100	100
6	R	109/217 (50%)	101 (93%)	8 (7%)	0	100	100
All	All	3015/4671 (64%)	2871 (95%)	144 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	G	100/192 (52%)	100 (100%)	0	100	100
1	J	100/192 (52%)	100 (100%)	0	100	100
1	O	100/192 (52%)	100 (100%)	0	100	100
2	I	88/180 (49%)	88 (100%)	0	100	100
2	M	88/180 (49%)	88 (100%)	0	100	100
2	Q	88/180 (49%)	88 (100%)	0	100	100
3	A	394/455 (87%)	394 (100%)	0	100	100
3	C	394/455 (87%)	394 (100%)	0	100	100
3	E	394/455 (87%)	394 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	104/130 (80%)	104 (100%)	0	100	100
4	D	104/130 (80%)	104 (100%)	0	100	100
4	F	104/130 (80%)	104 (100%)	0	100	100
5	H	108/198 (54%)	107 (99%)	1 (1%)	70	87
5	K	108/198 (54%)	107 (99%)	1 (1%)	70	87
5	P	108/198 (54%)	107 (99%)	1 (1%)	70	87
6	L	96/187 (51%)	96 (100%)	0	100	100
6	N	96/187 (51%)	96 (100%)	0	100	100
6	R	96/187 (51%)	96 (100%)	0	100	100
All	All	2670/4026 (66%)	2667 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	29	LEU
5	K	29	LEU
5	P	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	105	GLN
2	I	37	GLN
3	A	363	GLN
4	B	590	GLN
4	B	658	GLN
5	H	32	HIS
5	H	58	HIS
6	L	37	GLN
6	L	52	ASN
2	M	37	GLN
3	C	363	GLN
4	D	590	GLN
4	D	658	GLN
5	K	32	HIS
6	N	37	GLN
6	N	52	ASN
1	O	105	GLN

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Mol	Chain	Res	Type
2	Q	37	GLN
3	E	363	GLN
3	E	398	ASN
4	F	590	GLN
4	F	658	GLN
5	P	32	HIS
6	R	37	GLN
6	R	52	ASN

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](#)

69 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	$\# Z > 2$
7	NAG	S	1	3,7	14,14,15	0.74	0	17,19,21	1.71	3 (17%)
7	NAG	S	2	7	14,14,15	0.79	1 (7%)	17,19,21	1.61	2 (11%)
7	BMA	S	3	7	11,11,12	0.87	0	15,15,17	1.27	2 (13%)
7	MAN	S	4	7	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
7	MAN	S	5	7	11,11,12	0.79	0	15,15,17	1.03	1 (6%)
7	MAN	S	6	7	11,11,12	0.83	1 (9%)	15,15,17	1.09	2 (13%)
7	MAN	S	7	7	11,11,12	0.68	0	15,15,17	1.25	1 (6%)
8	NAG	T	1	8,3	14,14,15	0.74	0	17,19,21	1.90	3 (17%)
8	NAG	T	2	8	14,14,15	0.77	0	17,19,21	2.03	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	T	3	8	11,11,12	0.81	0	15,15,17	1.22	1 (6%)
8	MAN	T	4	8	11,11,12	0.80	0	15,15,17	0.92	1 (6%)
8	MAN	T	5	8	11,11,12	0.77	0	15,15,17	1.05	1 (6%)
8	MAN	T	6	8	11,11,12	0.78	0	15,15,17	1.01	1 (6%)
8	MAN	T	7	8	11,11,12	0.72	0	15,15,17	1.04	1 (6%)
8	MAN	T	8	8	11,11,12	0.72	0	15,15,17	1.13	1 (6%)
8	MAN	T	9	8	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
9	NAG	U	1	9,3	14,14,15	0.75	0	17,19,21	1.59	2 (11%)
9	NAG	U	2	9	14,14,15	0.72	0	17,19,21	1.72	2 (11%)
10	NAG	V	1	3,10	14,14,15	0.72	0	17,19,21	1.99	3 (17%)
10	NAG	V	2	10	14,14,15	0.74	1 (7%)	17,19,21	1.57	4 (23%)
10	BMA	V	3	10	11,11,12	1.31	2 (18%)	15,15,17	2.04	5 (33%)
9	NAG	W	1	9,3	14,14,15	0.92	1 (7%)	17,19,21	1.37	3 (17%)
9	NAG	W	2	9	14,14,15	0.69	0	17,19,21	1.81	3 (17%)
7	NAG	X	1	3,7	14,14,15	0.74	0	17,19,21	1.71	3 (17%)
7	NAG	X	2	7	14,14,15	0.79	1 (7%)	17,19,21	1.61	2 (11%)
7	BMA	X	3	7	11,11,12	0.87	0	15,15,17	1.28	2 (13%)
7	MAN	X	4	7	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
7	MAN	X	5	7	11,11,12	0.78	0	15,15,17	1.02	1 (6%)
7	MAN	X	6	7	11,11,12	0.83	1 (9%)	15,15,17	1.09	2 (13%)
7	MAN	X	7	7	11,11,12	0.69	0	15,15,17	1.24	1 (6%)
8	NAG	Y	1	8,3	14,14,15	0.74	0	17,19,21	1.90	3 (17%)
8	NAG	Y	2	8	14,14,15	0.78	0	17,19,21	2.03	3 (17%)
8	BMA	Y	3	8	11,11,12	0.81	0	15,15,17	1.23	1 (6%)
8	MAN	Y	4	8	11,11,12	0.80	0	15,15,17	0.92	1 (6%)
8	MAN	Y	5	8	11,11,12	0.78	0	15,15,17	1.06	1 (6%)
8	MAN	Y	6	8	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
8	MAN	Y	7	8	11,11,12	0.71	0	15,15,17	1.04	1 (6%)
8	MAN	Y	8	8	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
8	MAN	Y	9	8	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
9	NAG	Z	1	9,3	14,14,15	0.75	0	17,19,21	1.59	2 (11%)
9	NAG	Z	2	9	14,14,15	0.72	0	17,19,21	1.72	2 (11%)
10	NAG	a	1	3,10	14,14,15	0.72	0	17,19,21	1.99	3 (17%)
10	NAG	a	2	10	14,14,15	0.75	1 (7%)	17,19,21	1.57	4 (23%)
10	BMA	a	3	10	11,11,12	1.31	2 (18%)	15,15,17	2.04	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	b	1	9,3	14,14,15	0.92	1 (7%)	17,19,21	1.37	3 (17%)
9	NAG	b	2	9	14,14,15	0.69	0	17,19,21	1.81	3 (17%)
7	NAG	c	1	3,7	14,14,15	0.74	0	17,19,21	1.71	3 (17%)
7	NAG	c	2	7	14,14,15	0.79	1 (7%)	17,19,21	1.61	2 (11%)
7	BMA	c	3	7	11,11,12	0.87	0	15,15,17	1.28	2 (13%)
7	MAN	c	4	7	11,11,12	0.77	0	15,15,17	1.04	1 (6%)
7	MAN	c	5	7	11,11,12	0.79	0	15,15,17	1.02	1 (6%)
7	MAN	c	6	7	11,11,12	0.83	1 (9%)	15,15,17	1.09	2 (13%)
7	MAN	c	7	7	11,11,12	0.69	0	15,15,17	1.25	1 (6%)
8	NAG	d	1	8,3	14,14,15	0.74	0	17,19,21	1.90	3 (17%)
8	NAG	d	2	8	14,14,15	0.77	0	17,19,21	2.03	3 (17%)
8	BMA	d	3	8	11,11,12	0.80	0	15,15,17	1.23	1 (6%)
8	MAN	d	4	8	11,11,12	0.80	0	15,15,17	0.92	1 (6%)
8	MAN	d	5	8	11,11,12	0.77	0	15,15,17	1.06	1 (6%)
8	MAN	d	6	8	11,11,12	0.78	0	15,15,17	1.01	1 (6%)
8	MAN	d	7	8	11,11,12	0.70	0	15,15,17	1.04	1 (6%)
8	MAN	d	8	8	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
8	MAN	d	9	8	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
9	NAG	e	1	9,3	14,14,15	0.75	0	17,19,21	1.59	2 (11%)
9	NAG	e	2	9	14,14,15	0.72	0	17,19,21	1.71	2 (11%)
10	NAG	f	1	3,10	14,14,15	0.72	0	17,19,21	2.00	3 (17%)
10	NAG	f	2	10	14,14,15	0.74	1 (7%)	17,19,21	1.57	4 (23%)
10	BMA	f	3	10	11,11,12	1.31	2 (18%)	15,15,17	2.04	5 (33%)
9	NAG	g	1	9,3	14,14,15	0.93	1 (7%)	17,19,21	1.37	3 (17%)
9	NAG	g	2	9	14,14,15	0.69	0	17,19,21	1.81	3 (17%)

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
7	NAG	S	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	0/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	2/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	1/2/19/22	0/1/1/1
8	MAN	T	6	8	-	0/2/19/22	0/1/1/1
8	MAN	T	7	8	-	1/2/19/22	0/1/1/1
8	MAN	T	8	8	-	2/2/19/22	0/1/1/1
8	MAN	T	9	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
10	NAG	V	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	V	2	10	-	1/6/23/26	0/1/1/1
10	BMA	V	3	10	-	1/2/19/22	0/1/1/1
9	NAG	W	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
7	NAG	X	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	2/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
7	MAN	X	4	7	-	2/2/19/22	0/1/1/1
7	MAN	X	5	7	-	2/2/19/22	0/1/1/1
7	MAN	X	6	7	-	0/2/19/22	0/1/1/1
7	MAN	X	7	7	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	5	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	6	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	7	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	8	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	9	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
10	NAG	a	1	3,10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	a	2	10	-	1/6/23/26	0/1/1/1
10	BMA	a	3	10	-	1/2/19/22	0/1/1/1
9	NAG	b	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	b	2	9	-	2/6/23/26	0/1/1/1
7	NAG	c	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	MAN	c	4	7	-	2/2/19/22	0/1/1/1
7	MAN	c	5	7	-	2/2/19/22	0/1/1/1
7	MAN	c	6	7	-	0/2/19/22	0/1/1/1
7	MAN	c	7	7	-	0/2/19/22	0/1/1/1
8	NAG	d	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	BMA	d	3	8	-	0/2/19/22	0/1/1/1
8	MAN	d	4	8	-	0/2/19/22	0/1/1/1
8	MAN	d	5	8	-	1/2/19/22	0/1/1/1
8	MAN	d	6	8	-	0/2/19/22	0/1/1/1
8	MAN	d	7	8	-	1/2/19/22	0/1/1/1
8	MAN	d	8	8	-	2/2/19/22	0/1/1/1
8	MAN	d	9	8	-	0/2/19/22	0/1/1/1
9	NAG	e	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	e	2	9	-	2/6/23/26	0/1/1/1
10	NAG	f	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	1/6/23/26	0/1/1/1
10	BMA	f	3	10	-	1/2/19/22	0/1/1/1
9	NAG	g	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	3	BMA	C2-C3	3.06	1.57	1.52
10	f	3	BMA	C2-C3	3.05	1.57	1.52
10	V	3	BMA	C2-C3	3.05	1.57	1.52
10	a	3	BMA	C1-C2	2.56	1.58	1.52
10	V	3	BMA	C1-C2	2.55	1.58	1.52
10	f	3	BMA	C1-C2	2.55	1.58	1.52
9	g	1	NAG	O5-C1	-2.32	1.39	1.43
9	W	1	NAG	O5-C1	-2.28	1.39	1.43
9	b	1	NAG	O5-C1	-2.28	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	2	NAG	O5-C1	-2.17	1.40	1.43
10	f	2	NAG	O5-C1	-2.15	1.40	1.43
10	V	2	NAG	O5-C1	-2.13	1.40	1.43
7	S	6	MAN	O5-C1	-2.13	1.40	1.43
7	X	6	MAN	O5-C1	-2.13	1.40	1.43
7	c	6	MAN	O5-C1	-2.12	1.40	1.43
7	c	2	NAG	C1-C2	2.03	1.55	1.52
7	X	2	NAG	C1-C2	2.01	1.55	1.52
7	S	2	NAG	C1-C2	2.00	1.55	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	2	NAG	C2-N2-C7	7.03	132.32	122.90
8	d	2	NAG	C2-N2-C7	7.03	132.32	122.90
8	T	2	NAG	C2-N2-C7	7.02	132.31	122.90
8	Y	1	NAG	C2-N2-C7	6.00	130.94	122.90
8	d	1	NAG	C2-N2-C7	6.00	130.94	122.90
8	T	1	NAG	C2-N2-C7	5.99	130.92	122.90
9	b	2	NAG	C2-N2-C7	5.84	130.73	122.90
9	W	2	NAG	C2-N2-C7	5.83	130.71	122.90
9	g	2	NAG	C2-N2-C7	5.83	130.71	122.90
10	f	1	NAG	C2-N2-C7	5.80	130.67	122.90
10	V	1	NAG	C2-N2-C7	5.80	130.67	122.90
10	a	1	NAG	C2-N2-C7	5.78	130.65	122.90
9	Z	2	NAG	C2-N2-C7	5.64	130.45	122.90
9	U	2	NAG	C2-N2-C7	5.62	130.44	122.90
9	e	2	NAG	C2-N2-C7	5.61	130.41	122.90
7	X	1	NAG	C2-N2-C7	5.46	130.22	122.90
7	c	1	NAG	C2-N2-C7	5.46	130.21	122.90
7	S	1	NAG	C2-N2-C7	5.44	130.20	122.90
10	f	3	BMA	C1-O5-C5	5.43	119.46	112.19
10	a	3	BMA	C1-O5-C5	5.42	119.46	112.19
10	V	3	BMA	C1-O5-C5	5.41	119.44	112.19
9	e	1	NAG	C2-N2-C7	5.11	129.75	122.90
9	U	1	NAG	C2-N2-C7	5.10	129.74	122.90
9	Z	1	NAG	C2-N2-C7	5.10	129.73	122.90
10	f	1	NAG	C1-O5-C5	4.36	118.03	112.19
10	a	1	NAG	C1-O5-C5	4.36	118.02	112.19
10	V	1	NAG	C1-O5-C5	4.35	118.01	112.19
7	S	2	NAG	C2-N2-C7	4.19	128.51	122.90
7	c	2	NAG	C2-N2-C7	4.17	128.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	2	NAG	C2-N2-C7	4.16	128.48	122.90
7	X	3	BMA	C1-O5-C5	3.97	117.50	112.19
7	c	3	BMA	C1-O5-C5	3.95	117.47	112.19
7	S	3	BMA	C1-O5-C5	3.94	117.47	112.19
7	S	7	MAN	C1-O5-C5	3.74	117.19	112.19
7	c	7	MAN	C1-O5-C5	3.73	117.19	112.19
7	X	7	MAN	C1-O5-C5	3.72	117.18	112.19
8	Y	3	BMA	C1-O5-C5	3.53	116.92	112.19
8	d	3	BMA	C1-O5-C5	3.52	116.91	112.19
8	T	3	BMA	C1-O5-C5	3.51	116.89	112.19
10	f	3	BMA	C2-C3-C4	3.44	116.92	110.86
10	V	3	BMA	C2-C3-C4	3.44	116.92	110.86
10	a	3	BMA	C2-C3-C4	3.44	116.91	110.86
8	d	8	MAN	C1-O5-C5	3.40	116.74	112.19
8	Y	8	MAN	C1-O5-C5	3.39	116.73	112.19
8	T	8	MAN	C1-O5-C5	3.38	116.72	112.19
7	X	2	NAG	C1-C2-N2	3.36	115.72	110.43
7	c	2	NAG	C1-C2-N2	3.35	115.72	110.43
7	S	2	NAG	C1-C2-N2	3.35	115.72	110.43
10	f	2	NAG	O5-C1-C2	-3.35	106.11	111.29
10	V	2	NAG	O5-C1-C2	-3.34	106.13	111.29
10	a	2	NAG	O5-C1-C2	-3.34	106.13	111.29
10	a	2	NAG	O4-C4-C3	-2.88	103.59	110.38
10	V	2	NAG	O4-C4-C3	-2.87	103.60	110.38
10	f	2	NAG	O4-C4-C3	-2.87	103.60	110.38
8	Y	7	MAN	C1-O5-C5	2.85	116.01	112.19
8	d	7	MAN	C1-O5-C5	2.85	116.00	112.19
8	T	7	MAN	C1-O5-C5	2.85	116.00	112.19
9	g	1	NAG	O5-C1-C2	-2.80	106.96	111.29
9	W	1	NAG	O5-C1-C2	-2.80	106.96	111.29
10	f	2	NAG	C1-O5-C5	2.80	115.93	112.19
9	b	1	NAG	O5-C1-C2	-2.79	106.98	111.29
8	Y	5	MAN	C1-O5-C5	2.77	115.89	112.19
10	V	2	NAG	C1-O5-C5	2.77	115.89	112.19
8	T	5	MAN	C1-O5-C5	2.76	115.89	112.19
8	d	5	MAN	C1-O5-C5	2.76	115.89	112.19
10	a	2	NAG	C1-O5-C5	2.76	115.89	112.19
7	S	5	MAN	C1-O5-C5	2.68	115.77	112.19
7	c	5	MAN	C1-O5-C5	2.64	115.73	112.19
7	X	5	MAN	C1-O5-C5	2.63	115.72	112.19
10	V	2	NAG	C2-N2-C7	2.62	126.41	122.90
10	a	2	NAG	C2-N2-C7	2.60	126.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	f	2	NAG	C2-N2-C7	2.60	126.38	122.90
7	S	4	MAN	C1-O5-C5	2.58	115.65	112.19
7	X	4	MAN	C1-O5-C5	2.56	115.62	112.19
7	c	4	MAN	C1-O5-C5	2.56	115.62	112.19
8	T	6	MAN	C1-O5-C5	2.52	115.57	112.19
8	Y	6	MAN	C1-O5-C5	2.52	115.56	112.19
8	d	6	MAN	C1-O5-C5	2.50	115.53	112.19
8	T	2	NAG	C8-C7-N2	2.42	120.12	116.12
8	d	9	MAN	C1-O5-C5	2.41	115.42	112.19
8	d	2	NAG	C8-C7-N2	2.41	120.12	116.12
8	Y	2	NAG	C8-C7-N2	2.40	120.10	116.12
8	T	9	MAN	C1-O5-C5	2.40	115.40	112.19
8	Y	9	MAN	C1-O5-C5	2.39	115.39	112.19
9	g	2	NAG	C1-O5-C5	2.36	115.34	112.19
9	b	2	NAG	C1-O5-C5	2.35	115.34	112.19
9	W	2	NAG	C1-O5-C5	2.34	115.33	112.19
8	d	1	NAG	O3-C3-C2	-2.33	104.55	109.40
8	Y	1	NAG	O3-C3-C2	-2.33	104.57	109.40
9	W	2	NAG	C8-C7-N2	2.32	119.97	116.12
8	T	1	NAG	O3-C3-C2	-2.32	104.59	109.40
9	b	2	NAG	C8-C7-N2	2.31	119.95	116.12
9	g	2	NAG	C8-C7-N2	2.30	119.94	116.12
8	Y	2	NAG	C1-O5-C5	2.29	115.26	112.19
8	d	2	NAG	C1-O5-C5	2.29	115.25	112.19
8	T	2	NAG	C1-O5-C5	2.27	115.23	112.19
9	W	1	NAG	C2-N2-C7	2.27	125.95	122.90
8	T	1	NAG	C8-C7-N2	2.27	119.89	116.12
9	g	1	NAG	C2-N2-C7	2.27	125.94	122.90
9	b	1	NAG	C2-N2-C7	2.26	125.93	122.90
8	d	1	NAG	C8-C7-N2	2.26	119.86	116.12
8	Y	1	NAG	C8-C7-N2	2.25	119.85	116.12
10	a	3	BMA	C3-C4-C5	2.23	114.27	110.23
10	V	3	BMA	C3-C4-C5	2.22	114.26	110.23
10	f	3	BMA	C3-C4-C5	2.22	114.25	110.23
8	Y	4	MAN	C1-O5-C5	2.22	115.16	112.19
8	T	4	MAN	C1-O5-C5	2.21	115.15	112.19
7	X	1	NAG	C1-O5-C5	2.21	115.15	112.19
8	d	4	MAN	C1-O5-C5	2.21	115.15	112.19
7	c	1	NAG	C1-O5-C5	2.20	115.13	112.19
7	S	1	NAG	C1-O5-C5	2.20	115.13	112.19
9	b	1	NAG	C1-O5-C5	-2.18	109.27	112.19
10	a	3	BMA	C1-C2-C3	2.17	112.80	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	6	MAN	C1-O5-C5	2.17	115.09	112.19
7	c	6	MAN	C1-O5-C5	2.16	115.08	112.19
10	f	3	BMA	C1-C2-C3	2.16	112.79	109.64
9	g	1	NAG	C1-O5-C5	-2.16	109.29	112.19
10	V	3	BMA	C1-C2-C3	2.16	112.79	109.64
7	S	6	MAN	C1-O5-C5	2.16	115.08	112.19
9	W	1	NAG	C1-O5-C5	-2.15	109.30	112.19
7	S	6	MAN	O4-C4-C3	-2.15	105.30	110.38
7	c	6	MAN	O4-C4-C3	-2.15	105.30	110.38
7	X	6	MAN	O4-C4-C3	-2.15	105.31	110.38
7	c	3	BMA	O3-C3-C2	-2.12	105.72	110.05
7	c	1	NAG	C8-C7-N2	2.12	119.64	116.12
7	X	1	NAG	C8-C7-N2	2.12	119.63	116.12
7	S	1	NAG	C8-C7-N2	2.12	119.63	116.12
7	S	3	BMA	O3-C3-C2	-2.11	105.74	110.05
7	X	3	BMA	O3-C3-C2	-2.10	105.77	110.05
9	e	2	NAG	C8-C7-N2	2.07	119.55	116.12
9	U	2	NAG	C8-C7-N2	2.06	119.54	116.12
10	V	1	NAG	C8-C7-N2	2.06	119.53	116.12
9	Z	2	NAG	C8-C7-N2	2.05	119.52	116.12
10	f	1	NAG	C8-C7-N2	2.05	119.52	116.12
10	a	1	NAG	C8-C7-N2	2.05	119.51	116.12
10	f	3	BMA	O4-C4-C3	-2.05	105.55	110.38
10	V	3	BMA	O4-C4-C3	-2.04	105.56	110.38
10	a	3	BMA	O4-C4-C3	-2.04	105.57	110.38
9	e	1	NAG	C8-C7-N2	2.04	119.50	116.12
9	U	1	NAG	C8-C7-N2	2.03	119.49	116.12
9	Z	1	NAG	C8-C7-N2	2.03	119.49	116.12

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	T	8	MAN	O5-C5-C6-O6
8	Y	8	MAN	O5-C5-C6-O6
8	d	8	MAN	O5-C5-C6-O6
7	S	4	MAN	O5-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6
7	c	4	MAN	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
7	X	5	MAN	O5-C5-C6-O6
7	c	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	S	4	MAN	C4-C5-C6-O6
7	S	5	MAN	C4-C5-C6-O6
7	X	4	MAN	C4-C5-C6-O6
7	X	5	MAN	C4-C5-C6-O6
7	c	4	MAN	C4-C5-C6-O6
7	c	5	MAN	C4-C5-C6-O6
8	T	8	MAN	C4-C5-C6-O6
8	Y	8	MAN	C4-C5-C6-O6
8	d	8	MAN	C4-C5-C6-O6
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	c	1	NAG	C8-C7-N2-C2
7	c	1	NAG	O7-C7-N2-C2
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
8	T	2	NAG	C8-C7-N2-C2
8	T	2	NAG	O7-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
8	Y	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
8	d	1	NAG	C8-C7-N2-C2
8	d	1	NAG	O7-C7-N2-C2
8	d	2	NAG	C8-C7-N2-C2
8	d	2	NAG	O7-C7-N2-C2
9	U	1	NAG	C8-C7-N2-C2
9	U	1	NAG	O7-C7-N2-C2
9	U	2	NAG	C8-C7-N2-C2
9	U	2	NAG	O7-C7-N2-C2
9	W	2	NAG	C8-C7-N2-C2
9	W	2	NAG	O7-C7-N2-C2
9	Z	1	NAG	C8-C7-N2-C2
9	Z	1	NAG	O7-C7-N2-C2
9	Z	2	NAG	C8-C7-N2-C2
9	Z	2	NAG	O7-C7-N2-C2
9	b	2	NAG	C8-C7-N2-C2
9	b	2	NAG	O7-C7-N2-C2
9	e	1	NAG	C8-C7-N2-C2
9	e	1	NAG	O7-C7-N2-C2
9	e	2	NAG	C8-C7-N2-C2

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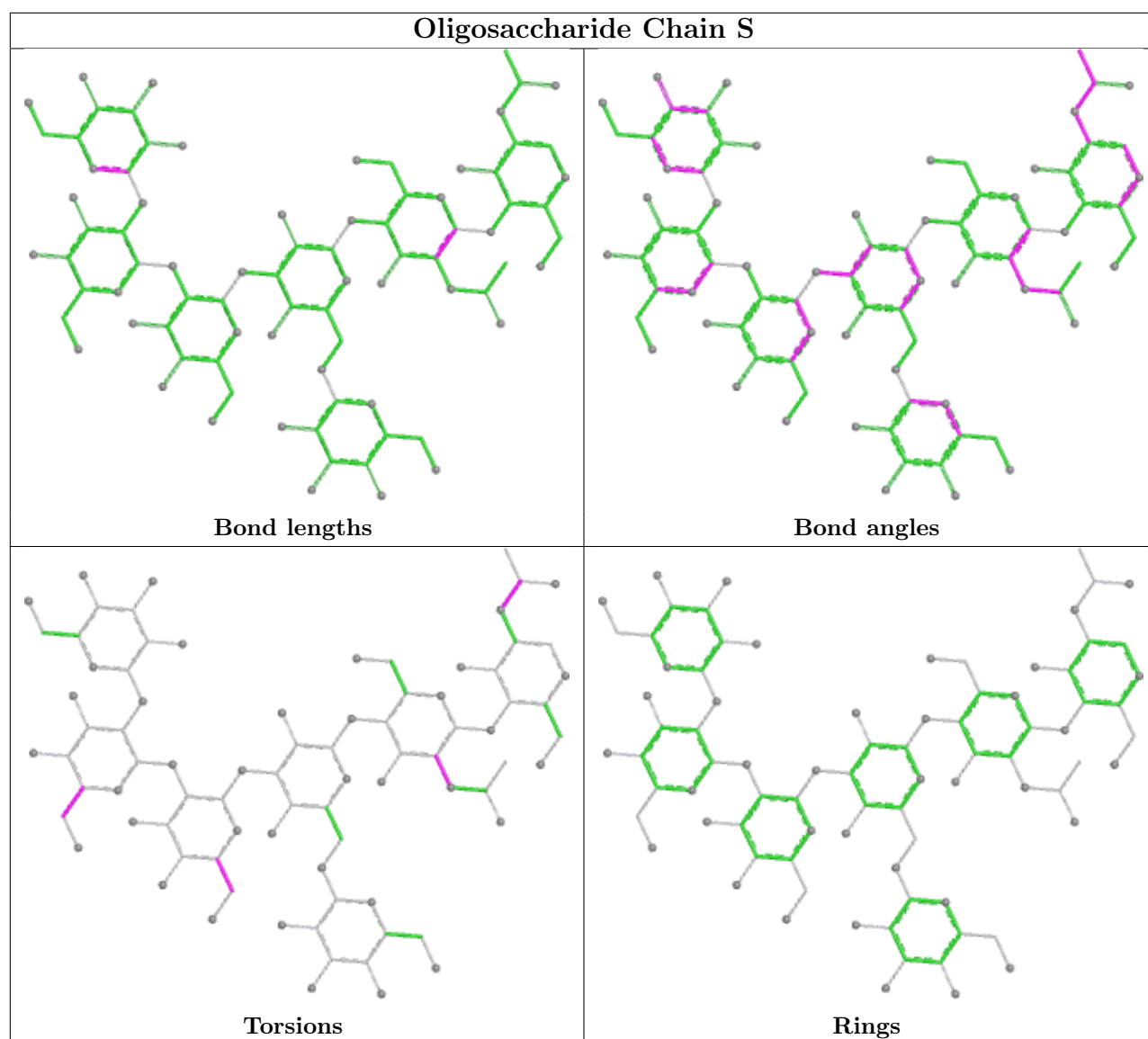
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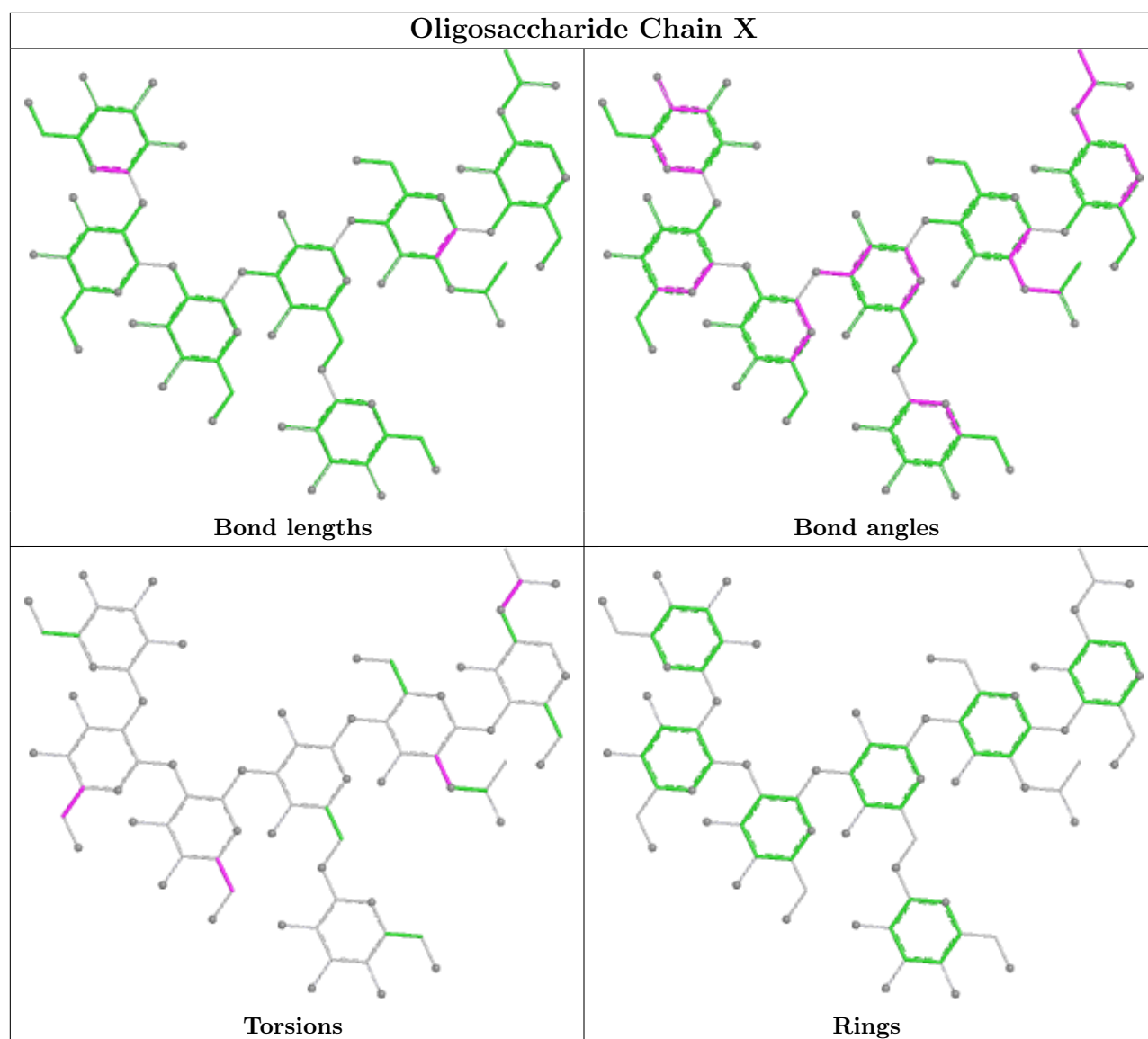
Mol	Chain	Res	Type	Atoms
9	e	2	NAG	O7-C7-N2-C2
9	g	2	NAG	C8-C7-N2-C2
9	g	2	NAG	O7-C7-N2-C2
10	V	1	NAG	C8-C7-N2-C2
10	V	1	NAG	O7-C7-N2-C2
10	a	1	NAG	C8-C7-N2-C2
10	a	1	NAG	O7-C7-N2-C2
10	f	1	NAG	C8-C7-N2-C2
10	f	1	NAG	O7-C7-N2-C2
10	V	3	BMA	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
10	f	3	BMA	O5-C5-C6-O6
7	S	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	c	2	NAG	C3-C2-N2-C7
10	V	2	NAG	C3-C2-N2-C7
10	a	2	NAG	C3-C2-N2-C7
10	f	2	NAG	C3-C2-N2-C7
7	S	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C1-C2-N2-C7
7	c	2	NAG	C1-C2-N2-C7
8	T	5	MAN	O5-C5-C6-O6
8	Y	5	MAN	O5-C5-C6-O6
8	d	5	MAN	O5-C5-C6-O6
8	T	7	MAN	O5-C5-C6-O6
8	Y	7	MAN	O5-C5-C6-O6
8	d	7	MAN	O5-C5-C6-O6

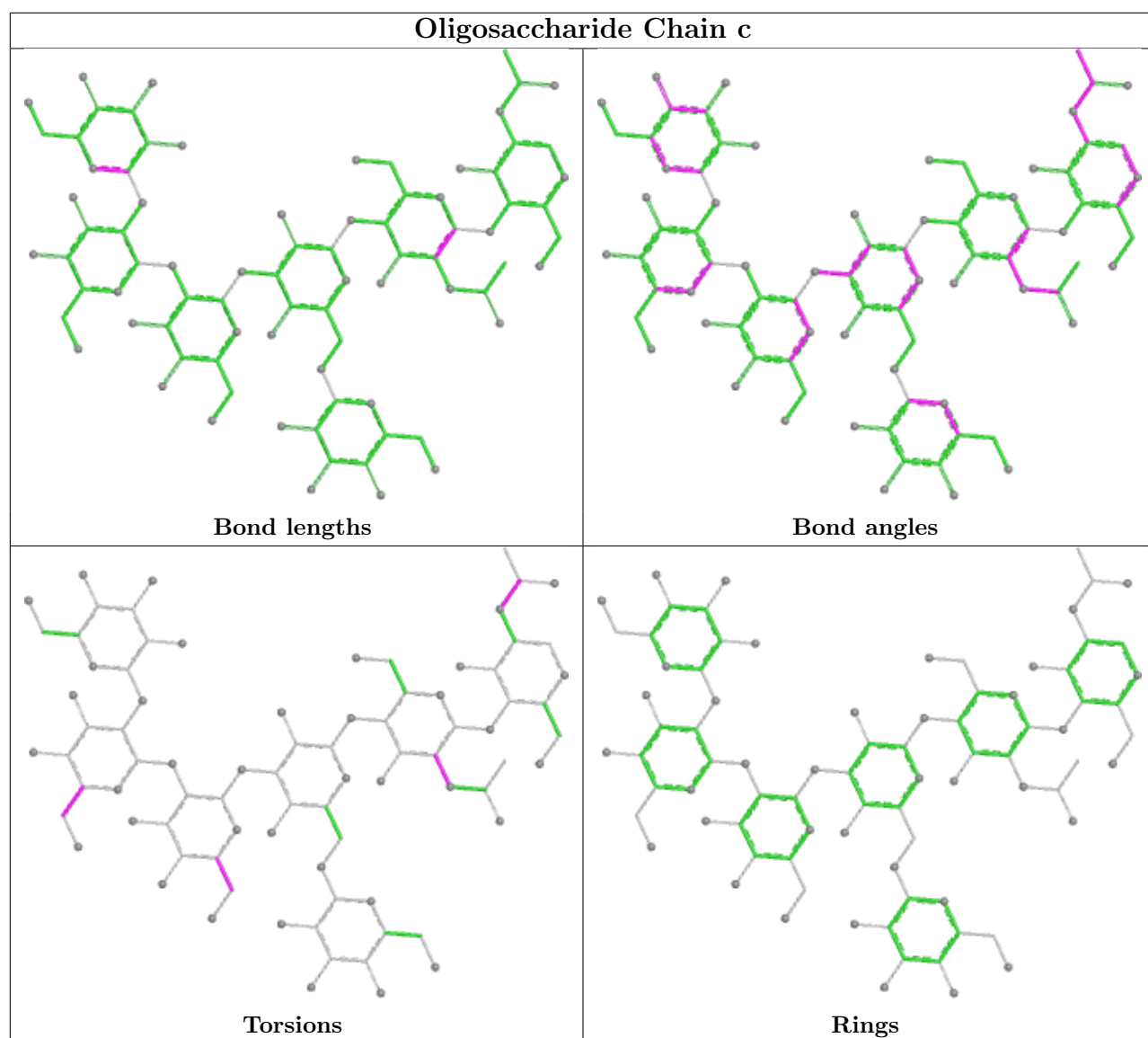
There are no ring outliers.

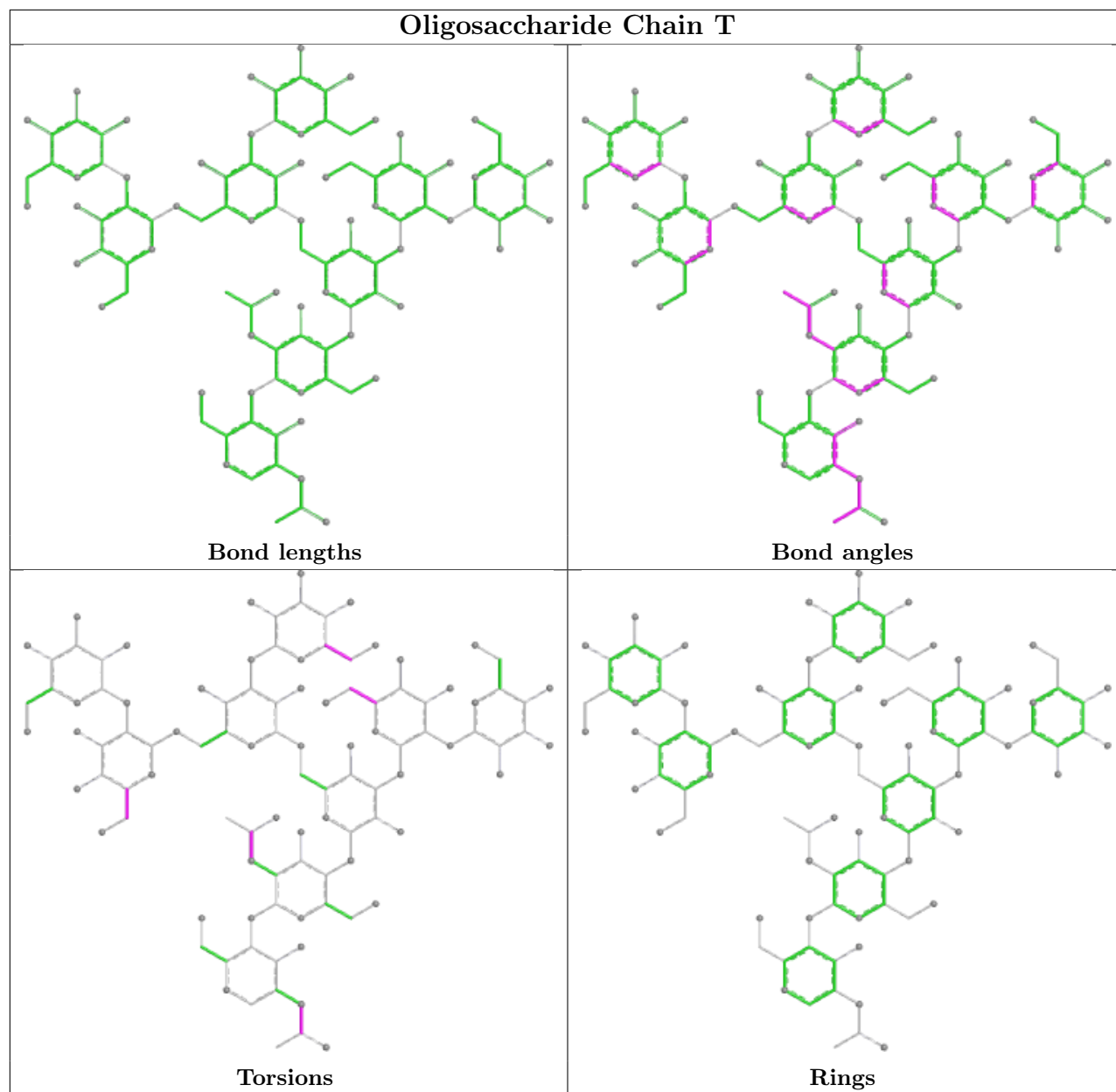
No monomer is involved in short contacts.

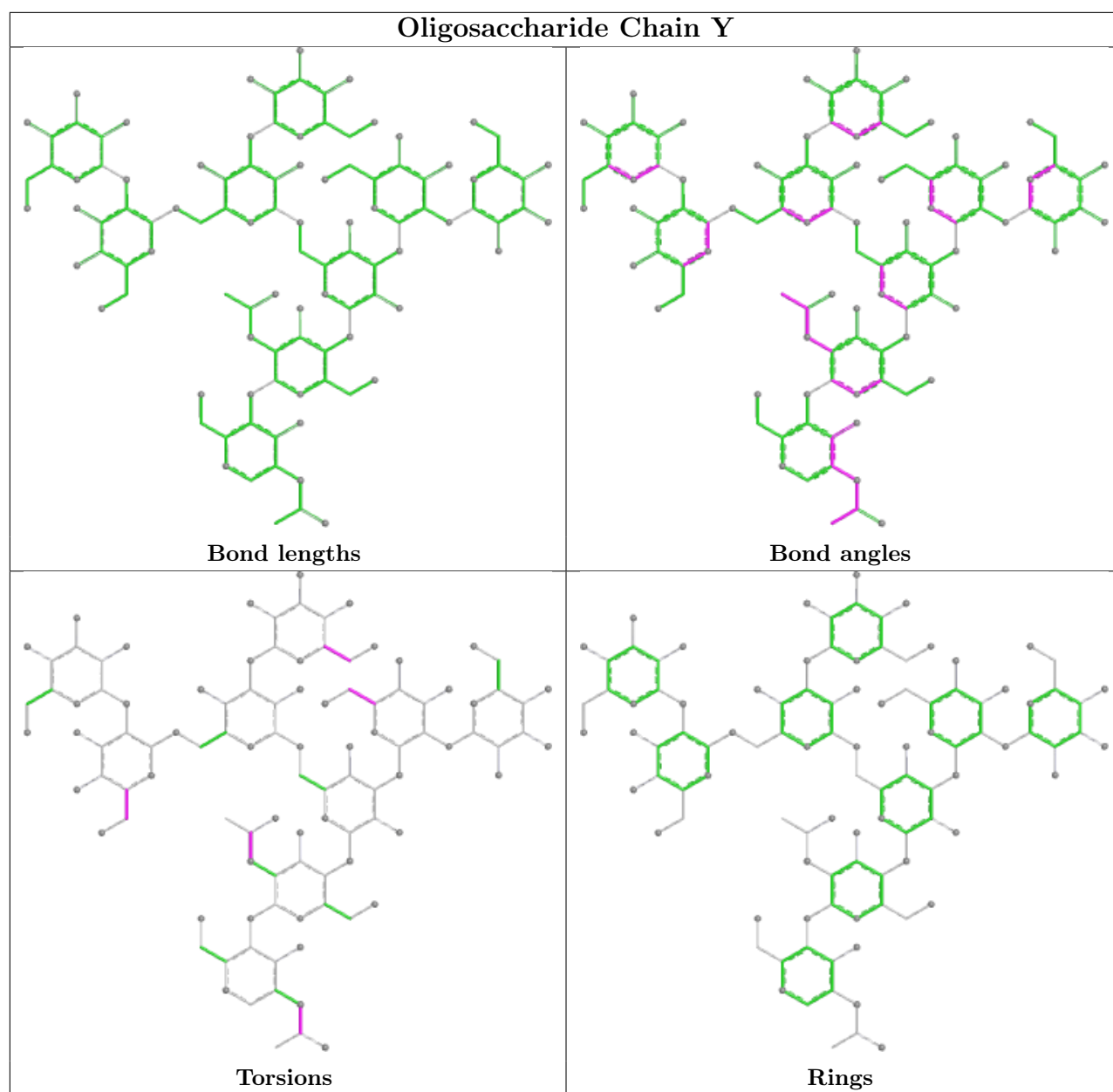
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

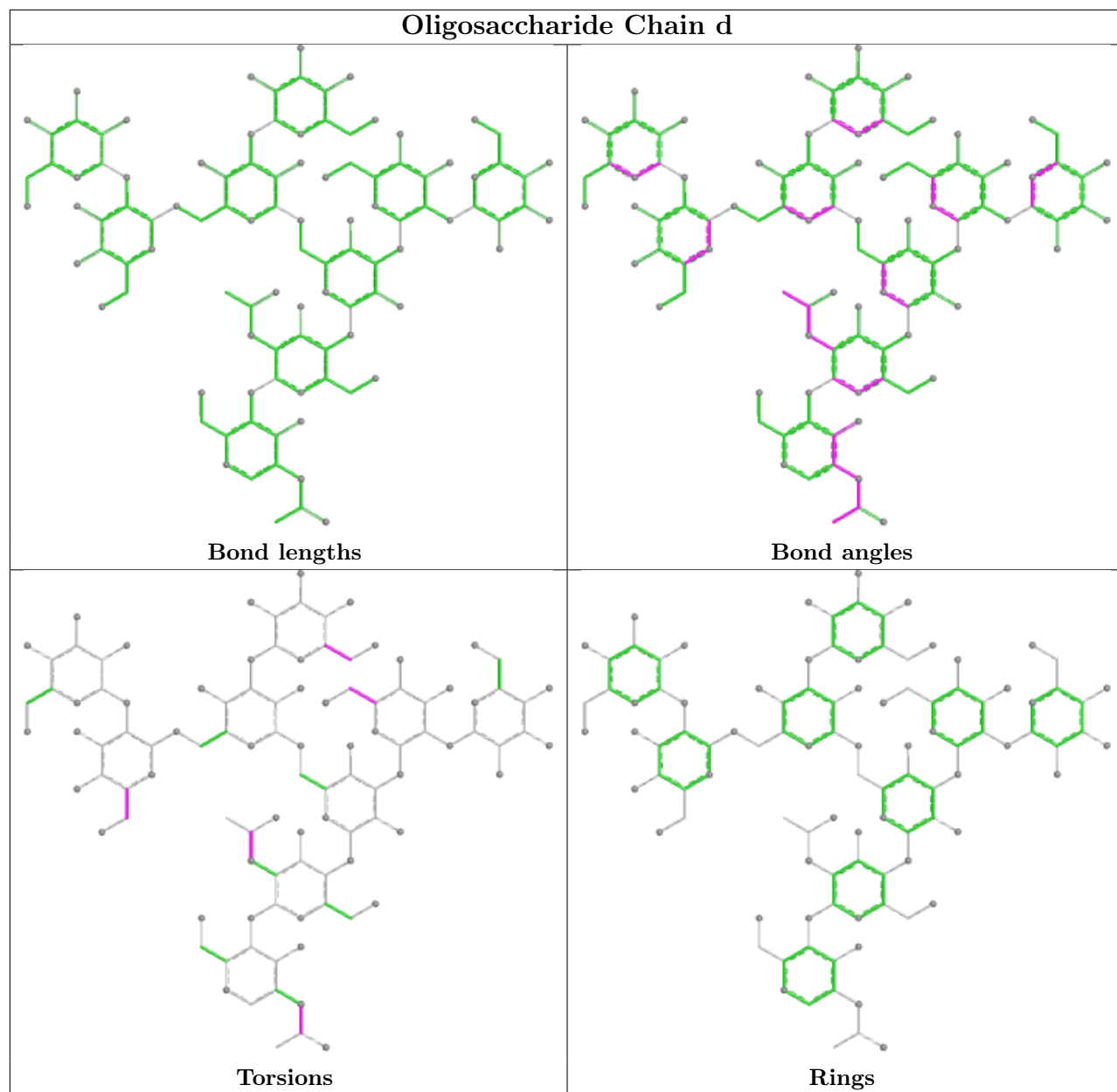


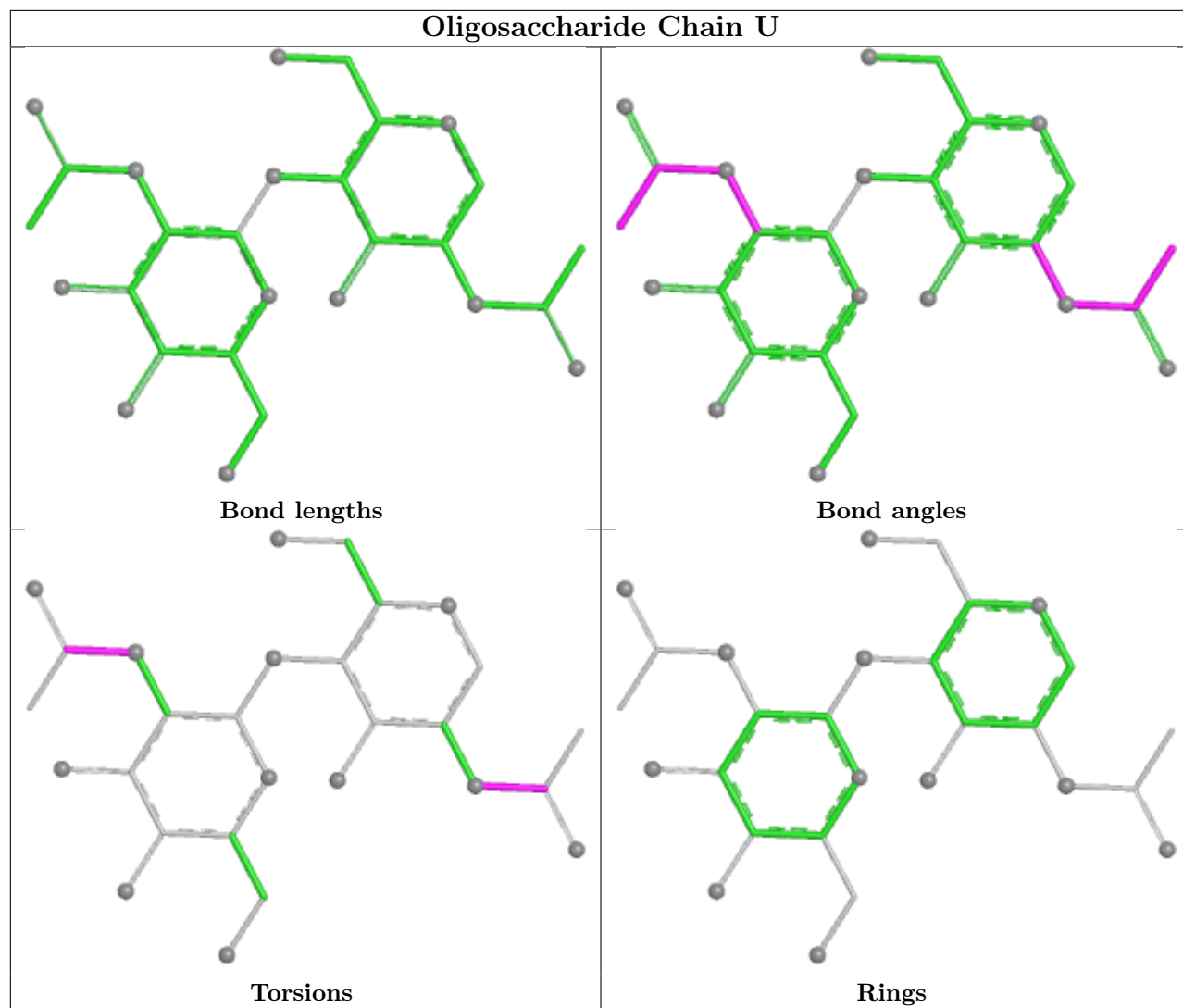


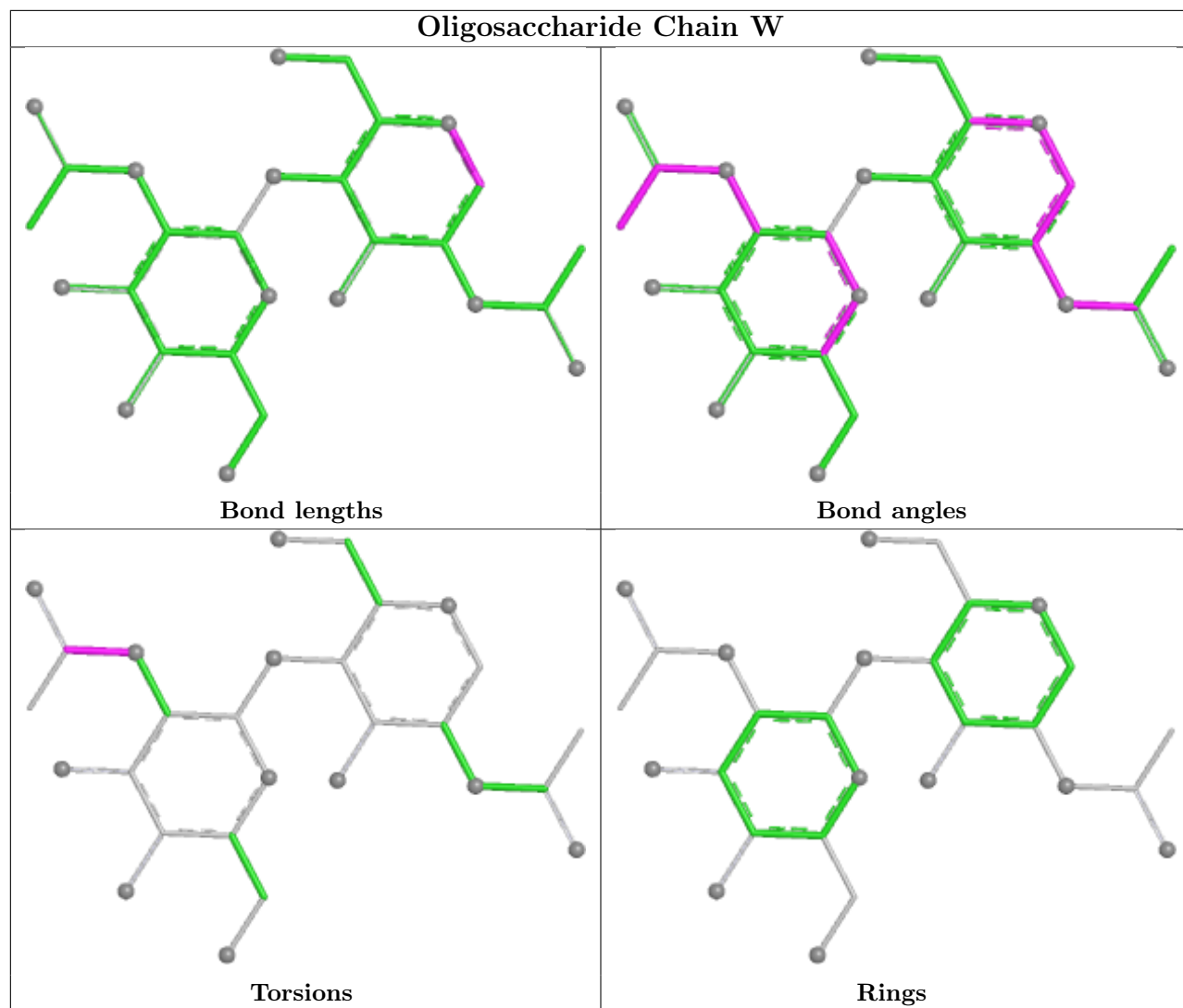


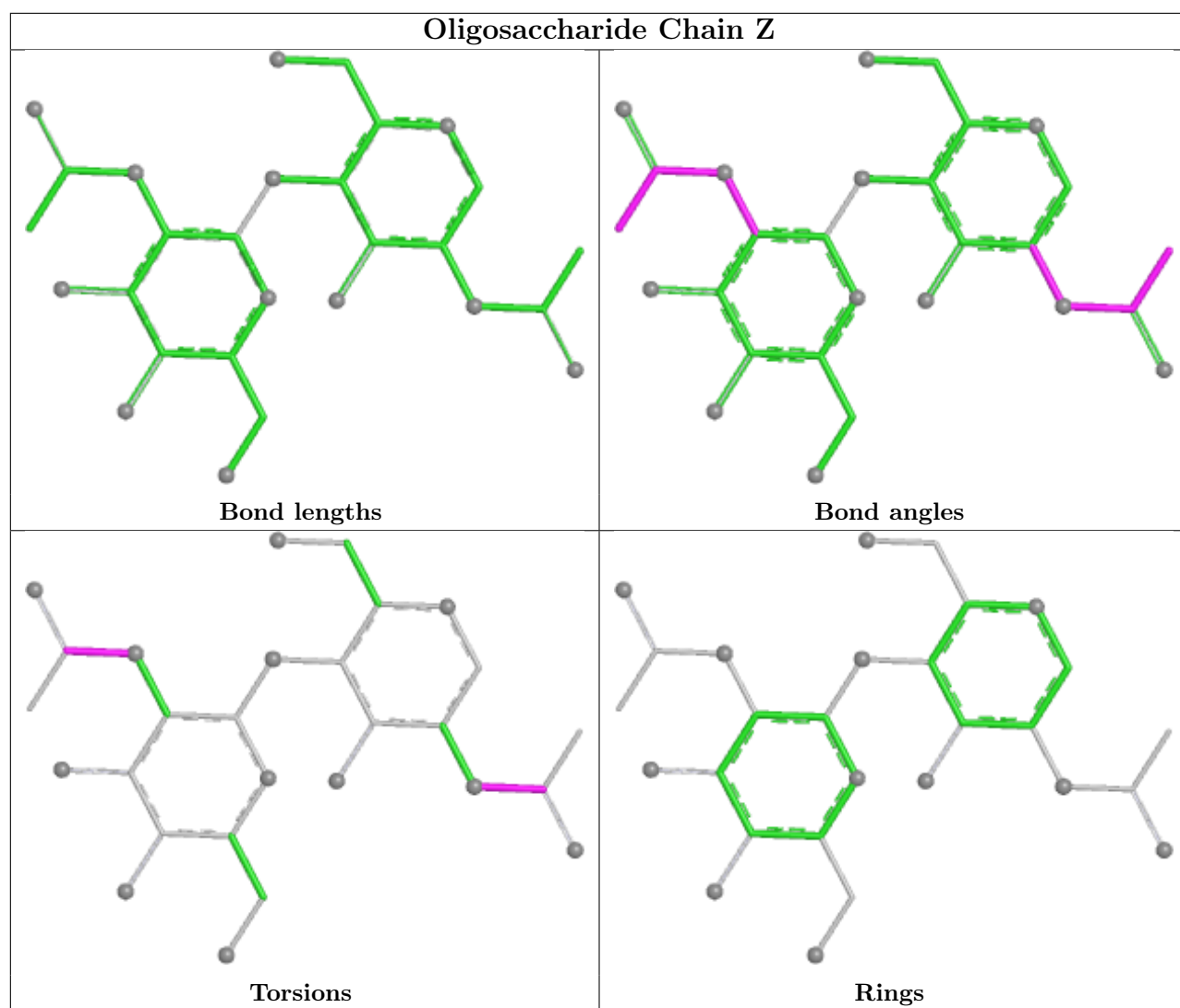


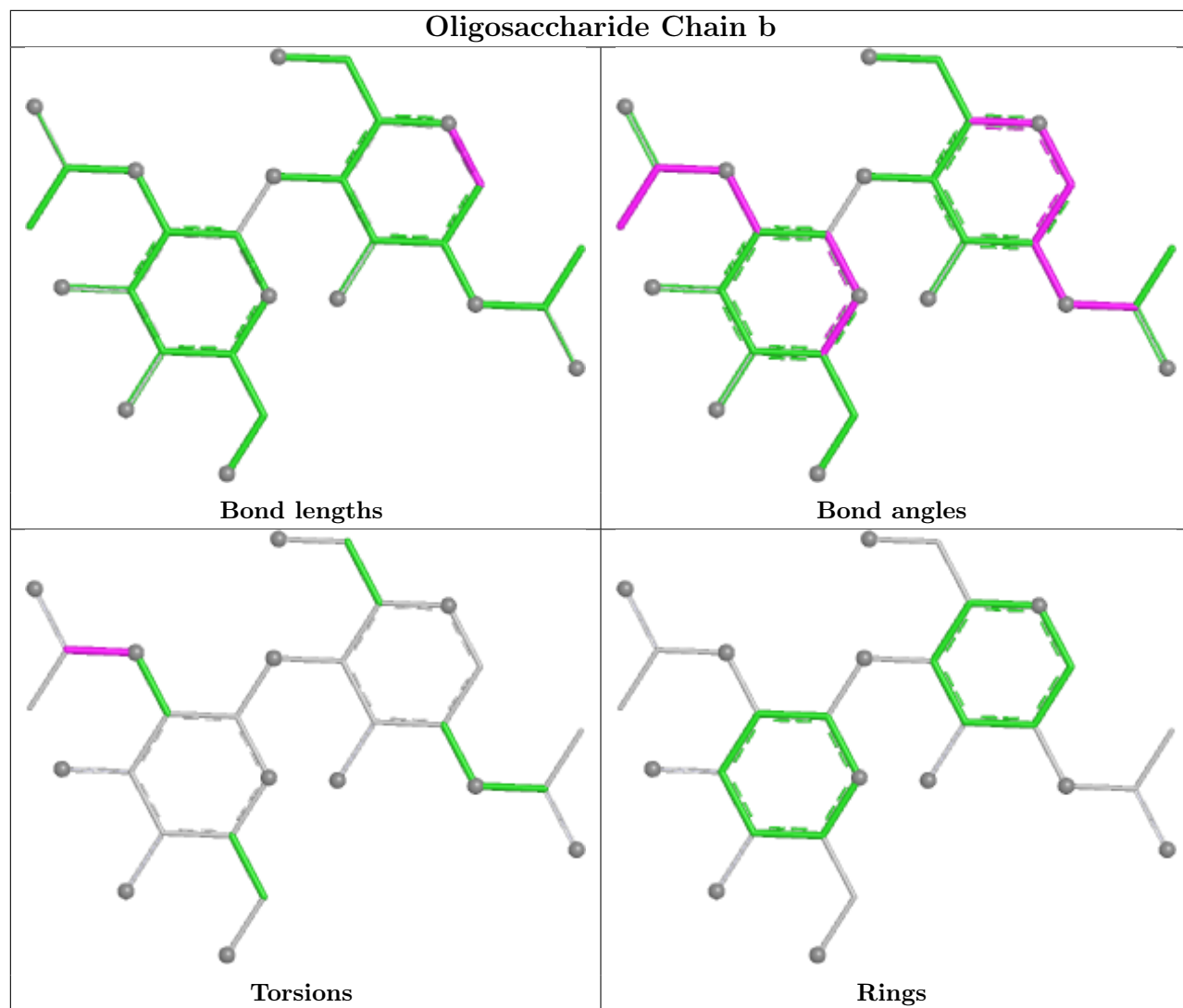


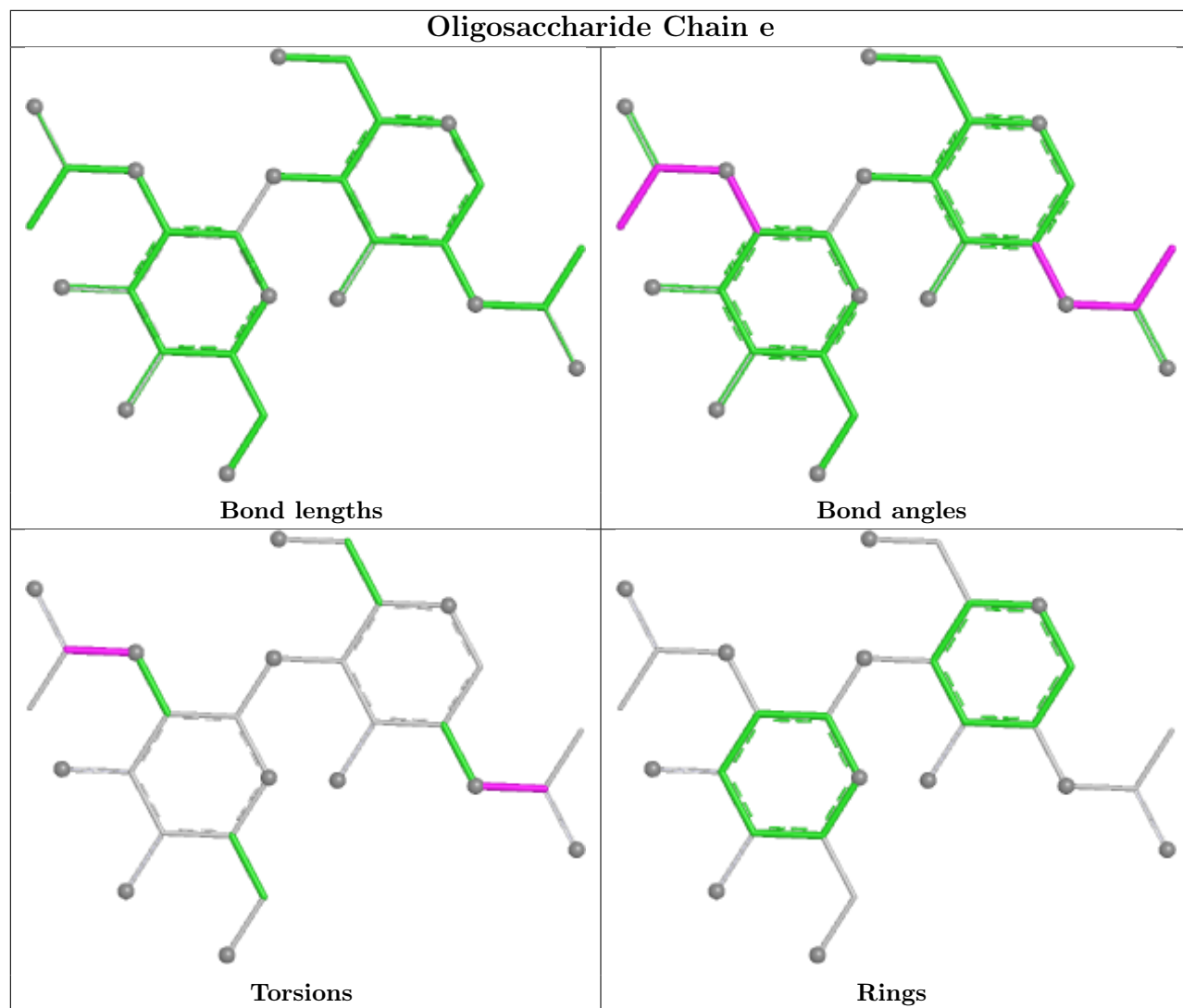


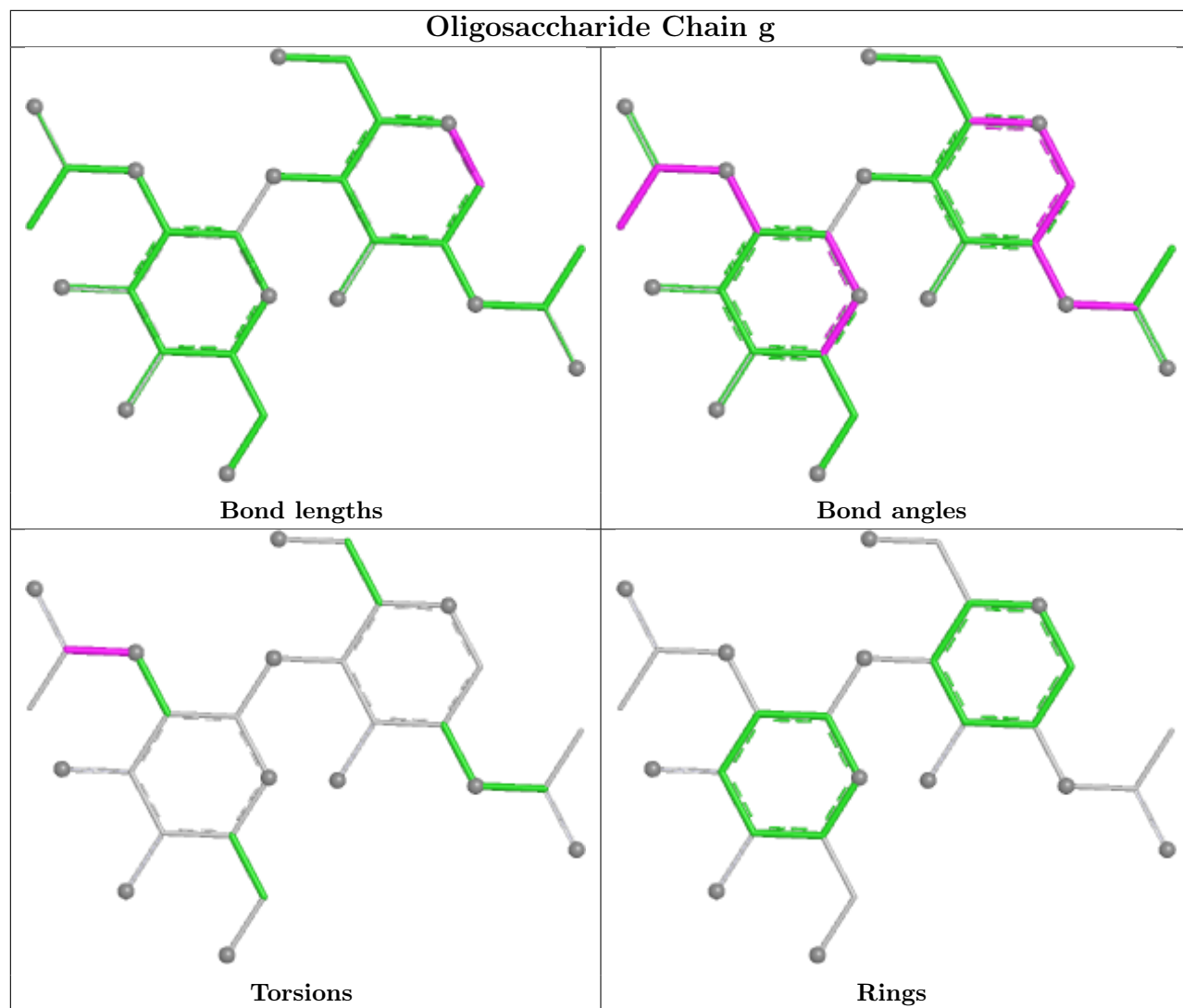


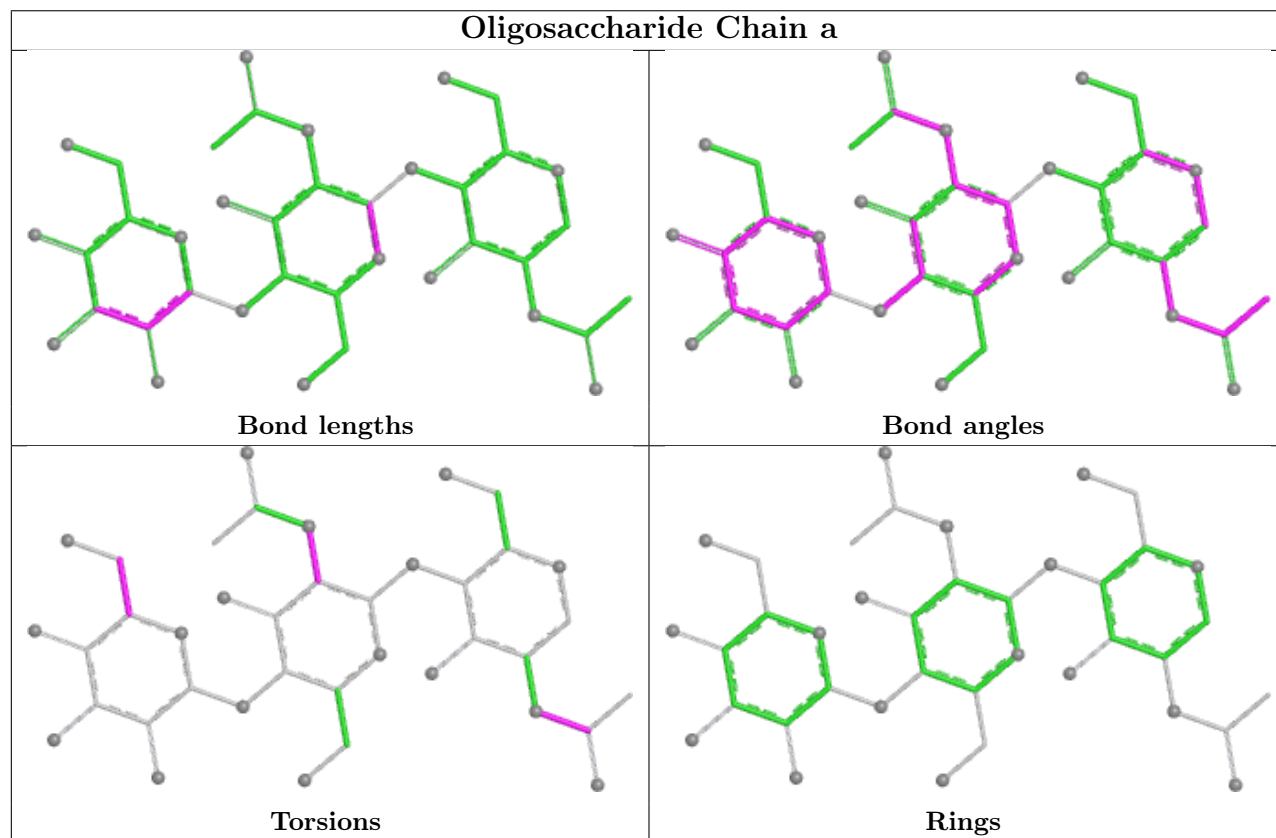
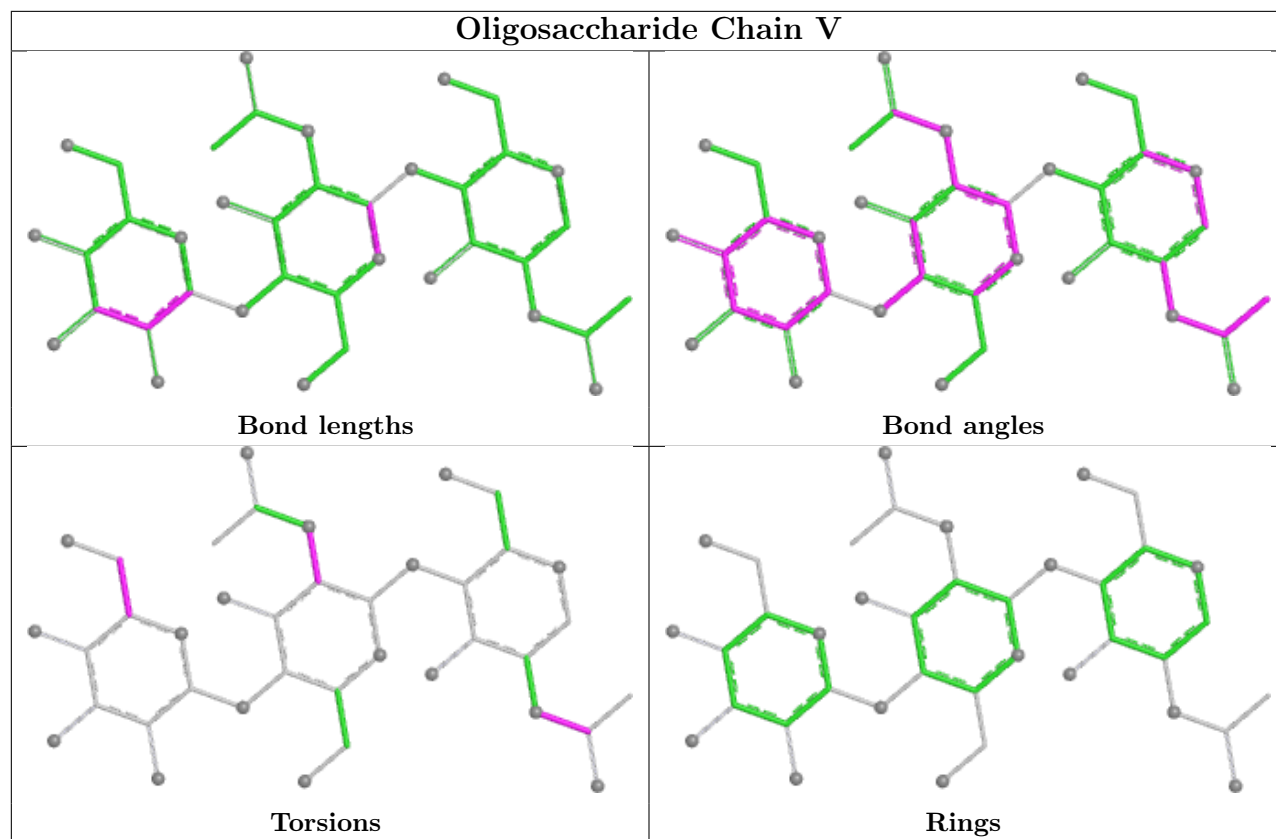


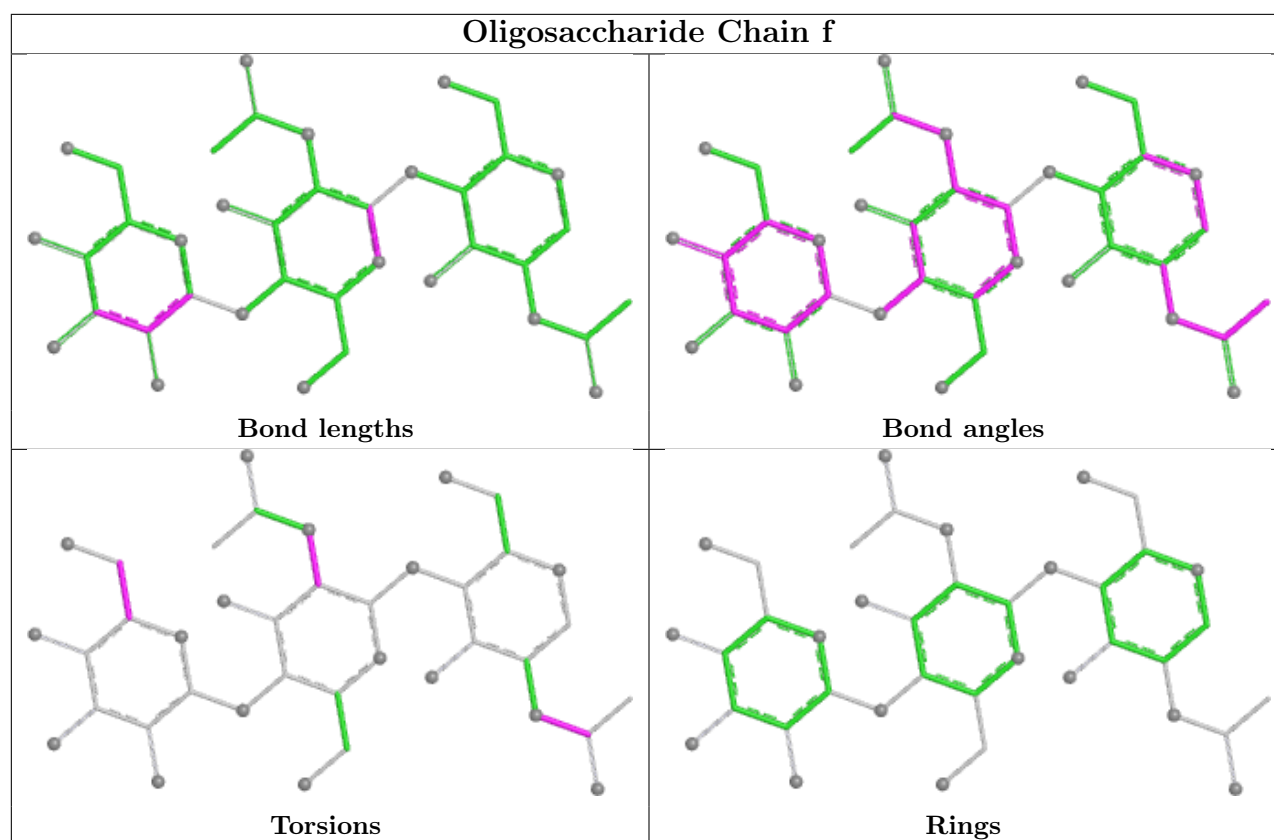












5.6 Ligand geometry [i](#)

36 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	$\# Z > 2$
11	NAG	A	610	3	14,14,15	0.73	0	17,19,21	1.61	4 (23%)
11	NAG	E	610	3	14,14,15	0.72	0	17,19,21	1.61	4 (23%)
11	NAG	F	701	4	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
11	NAG	F	702	4	14,14,15	0.73	0	17,19,21	1.23	2 (11%)
11	NAG	E	607	3	14,14,15	0.77	0	17,19,21	1.29	1 (5%)
11	NAG	C	608	3	14,14,15	0.79	0	17,19,21	1.05	0
11	NAG	A	601	3	14,14,15	0.67	0	17,19,21	1.13	0
11	NAG	C	607	3	14,14,15	0.78	0	17,19,21	1.29	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	D	701	4	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
11	NAG	C	601	3	14,14,15	0.66	0	17,19,21	1.13	0
11	NAG	C	602	3	14,14,15	0.84	0	17,19,21	1.21	1 (5%)
11	NAG	A	607	3	14,14,15	0.78	0	17,19,21	1.28	1 (5%)
11	NAG	C	606	3	14,14,15	0.71	0	17,19,21	1.00	0
11	NAG	C	610	3	14,14,15	0.73	0	17,19,21	1.61	4 (23%)
11	NAG	E	603	3	14,14,15	0.70	0	17,19,21	1.82	2 (11%)
11	NAG	B	701	4	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
11	NAG	E	609	3	14,14,15	0.88	1 (7%)	17,19,21	1.44	2 (11%)
11	NAG	C	609	3	14,14,15	0.89	1 (7%)	17,19,21	1.44	2 (11%)
11	NAG	A	606	3	14,14,15	0.72	0	17,19,21	1.00	0
11	NAG	A	608	3	14,14,15	0.80	0	17,19,21	1.04	0
11	NAG	C	603	3	14,14,15	0.70	0	17,19,21	1.82	2 (11%)
11	NAG	A	604	3	14,14,15	0.74	0	17,19,21	0.91	0
11	NAG	A	609	3	14,14,15	0.89	1 (7%)	17,19,21	1.44	2 (11%)
11	NAG	E	606	3	14,14,15	0.72	0	17,19,21	1.00	0
11	NAG	E	608	3	14,14,15	0.79	0	17,19,21	1.05	0
11	NAG	D	702	4	14,14,15	0.73	0	17,19,21	1.23	2 (11%)
11	NAG	C	605	3	14,14,15	0.72	0	17,19,21	1.07	0
11	NAG	E	601	3	14,14,15	0.67	0	17,19,21	1.13	0
11	NAG	E	604	3	14,14,15	0.75	0	17,19,21	0.91	0
11	NAG	B	702	4	14,14,15	0.73	0	17,19,21	1.23	2 (11%)
11	NAG	C	604	3	14,14,15	0.75	0	17,19,21	0.90	0
11	NAG	E	605	3	14,14,15	0.73	0	17,19,21	1.08	0
11	NAG	E	602	3	14,14,15	0.83	0	17,19,21	1.20	1 (5%)
11	NAG	A	603	3	14,14,15	0.70	0	17,19,21	1.82	2 (11%)
11	NAG	A	602	3	14,14,15	0.83	0	17,19,21	1.21	1 (5%)
11	NAG	A	605	3	14,14,15	0.73	0	17,19,21	1.08	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
11	NAG	A	610	3	-	1/6/23/26	0/1/1/1
11	NAG	E	610	3	-	1/6/23/26	0/1/1/1
11	NAG	F	701	4	-	0/6/23/26	0/1/1/1
11	NAG	F	702	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	E	607	3	-	0/6/23/26	0/1/1/1
11	NAG	C	608	3	-	0/6/23/26	0/1/1/1
11	NAG	A	601	3	-	2/6/23/26	0/1/1/1
11	NAG	C	607	3	-	0/6/23/26	0/1/1/1
11	NAG	D	701	4	-	0/6/23/26	0/1/1/1
11	NAG	C	601	3	-	2/6/23/26	0/1/1/1
11	NAG	C	602	3	-	0/6/23/26	0/1/1/1
11	NAG	A	607	3	-	0/6/23/26	0/1/1/1
11	NAG	C	606	3	-	1/6/23/26	0/1/1/1
11	NAG	C	610	3	-	1/6/23/26	0/1/1/1
11	NAG	E	603	3	-	2/6/23/26	0/1/1/1
11	NAG	B	701	4	-	0/6/23/26	0/1/1/1
11	NAG	E	609	3	-	0/6/23/26	0/1/1/1
11	NAG	C	609	3	-	0/6/23/26	0/1/1/1
11	NAG	A	606	3	-	1/6/23/26	0/1/1/1
11	NAG	A	608	3	-	0/6/23/26	0/1/1/1
11	NAG	C	603	3	-	2/6/23/26	0/1/1/1
11	NAG	A	604	3	-	1/6/23/26	0/1/1/1
11	NAG	A	609	3	-	0/6/23/26	0/1/1/1
11	NAG	E	606	3	-	1/6/23/26	0/1/1/1
11	NAG	E	608	3	-	0/6/23/26	0/1/1/1
11	NAG	D	702	4	-	0/6/23/26	0/1/1/1
11	NAG	C	605	3	-	2/6/23/26	0/1/1/1
11	NAG	E	601	3	-	2/6/23/26	0/1/1/1
11	NAG	E	604	3	-	1/6/23/26	0/1/1/1
11	NAG	B	702	4	-	0/6/23/26	0/1/1/1
11	NAG	C	604	3	-	1/6/23/26	0/1/1/1
11	NAG	E	605	3	-	2/6/23/26	0/1/1/1
11	NAG	E	602	3	-	0/6/23/26	0/1/1/1
11	NAG	A	603	3	-	2/6/23/26	0/1/1/1
11	NAG	A	602	3	-	0/6/23/26	0/1/1/1
11	NAG	A	605	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	609	NAG	C1-C2	2.06	1.55	1.52
11	A	609	NAG	C1-C2	2.06	1.55	1.52
11	E	609	NAG	C1-C2	2.06	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	603	NAG	C2-N2-C7	5.76	130.62	122.90
11	E	603	NAG	C2-N2-C7	5.75	130.61	122.90
11	A	603	NAG	C2-N2-C7	5.74	130.60	122.90
11	C	610	NAG	C1-O5-C5	3.96	117.50	112.19
11	E	610	NAG	C1-O5-C5	3.96	117.50	112.19
11	A	610	NAG	C1-O5-C5	3.96	117.50	112.19
11	A	609	NAG	C1-O5-C5	3.46	116.82	112.19
11	E	609	NAG	C1-O5-C5	3.45	116.81	112.19
11	C	609	NAG	C1-O5-C5	3.44	116.79	112.19
11	E	607	NAG	C1-O5-C5	3.21	116.48	112.19
11	C	607	NAG	C1-O5-C5	3.20	116.47	112.19
11	A	607	NAG	C1-O5-C5	3.20	116.47	112.19
11	E	609	NAG	O3-C3-C2	-3.04	103.09	109.40
11	C	609	NAG	O3-C3-C2	-3.03	103.10	109.40
11	A	609	NAG	O3-C3-C2	-3.03	103.10	109.40
11	C	610	NAG	O5-C1-C2	-3.03	106.60	111.29
11	E	610	NAG	O5-C1-C2	-3.03	106.61	111.29
11	A	610	NAG	O5-C1-C2	-3.02	106.62	111.29
11	B	702	NAG	O5-C1-C2	-2.73	107.07	111.29
11	D	702	NAG	O5-C1-C2	-2.72	107.08	111.29
11	F	702	NAG	O5-C1-C2	-2.71	107.10	111.29
11	D	702	NAG	C1-O5-C5	2.47	115.50	112.19
11	B	702	NAG	C1-O5-C5	2.46	115.48	112.19
11	F	702	NAG	C1-O5-C5	2.45	115.47	112.19
11	C	602	NAG	C1-C2-N2	-2.43	106.60	110.43
11	A	602	NAG	C1-C2-N2	-2.43	106.61	110.43
11	E	602	NAG	C1-C2-N2	-2.43	106.61	110.43
11	A	610	NAG	C2-N2-C7	2.35	126.05	122.90
11	C	610	NAG	C2-N2-C7	2.34	126.04	122.90
11	E	610	NAG	C2-N2-C7	2.32	126.02	122.90
11	A	603	NAG	C8-C7-N2	2.26	119.87	116.12
11	C	603	NAG	C8-C7-N2	2.26	119.87	116.12
11	E	603	NAG	C8-C7-N2	2.25	119.85	116.12
11	A	610	NAG	C1-C2-N2	2.10	113.75	110.43
11	E	610	NAG	C1-C2-N2	2.09	113.73	110.43
11	C	610	NAG	C1-C2-N2	2.08	113.71	110.43
11	B	701	NAG	C1-O5-C5	2.07	114.96	112.19
11	D	701	NAG	C1-O5-C5	2.07	114.95	112.19
11	F	701	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	610	NAG	C1-C2-N2-C7
11	C	610	NAG	C1-C2-N2-C7
11	E	610	NAG	C1-C2-N2-C7
11	A	601	NAG	C4-C5-C6-O6
11	C	601	NAG	C4-C5-C6-O6
11	E	601	NAG	C4-C5-C6-O6
11	A	601	NAG	O5-C5-C6-O6
11	C	601	NAG	O5-C5-C6-O6
11	E	601	NAG	O5-C5-C6-O6
11	A	603	NAG	C8-C7-N2-C2
11	A	603	NAG	O7-C7-N2-C2
11	C	603	NAG	C8-C7-N2-C2
11	C	603	NAG	O7-C7-N2-C2
11	E	603	NAG	C8-C7-N2-C2
11	E	603	NAG	O7-C7-N2-C2
11	A	606	NAG	O5-C5-C6-O6
11	C	606	NAG	O5-C5-C6-O6
11	E	606	NAG	O5-C5-C6-O6
11	A	604	NAG	C1-C2-N2-C7
11	A	605	NAG	C1-C2-N2-C7
11	C	604	NAG	C1-C2-N2-C7
11	C	605	NAG	C1-C2-N2-C7
11	E	604	NAG	C1-C2-N2-C7
11	E	605	NAG	C1-C2-N2-C7
11	A	605	NAG	C4-C5-C6-O6
11	C	605	NAG	C4-C5-C6-O6
11	E	605	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

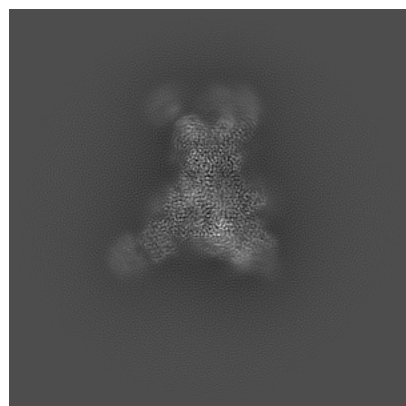
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73109. These allow visual inspection of the internal detail of the map and identification of artifacts.

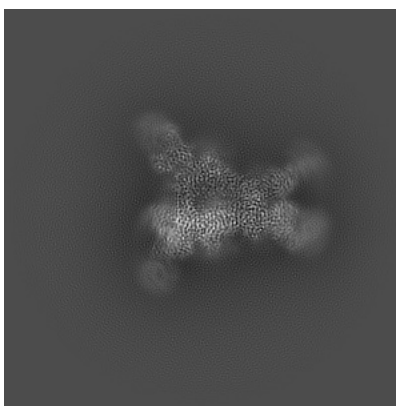
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

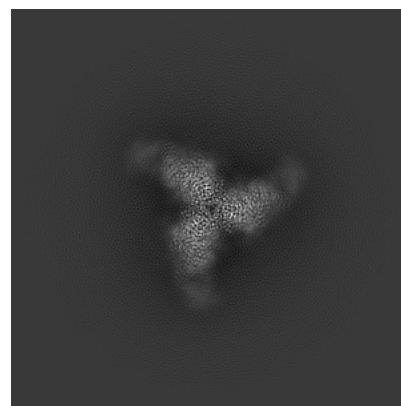
6.1.1 Primary map



X

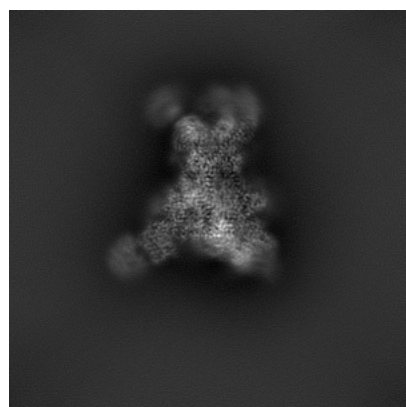


Y

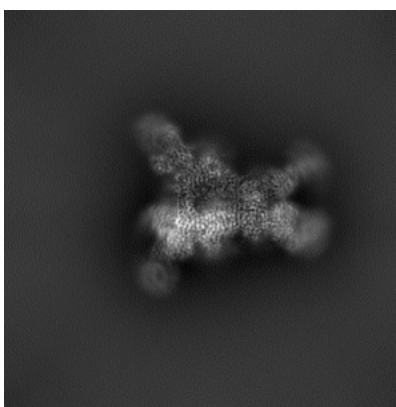


Z

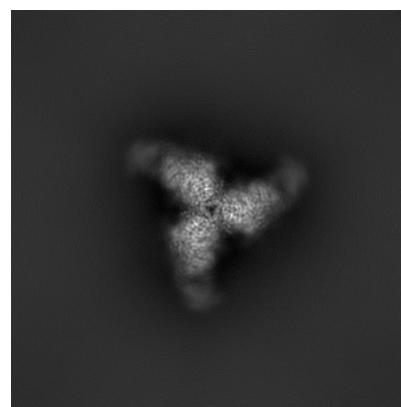
6.1.2 Raw map



X



Y

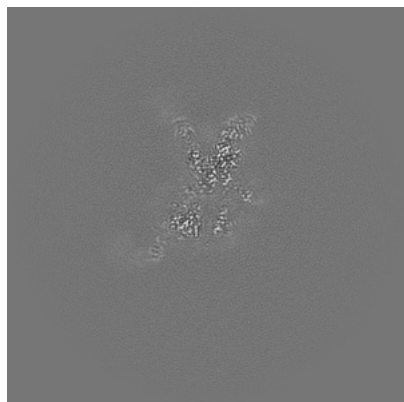


Z

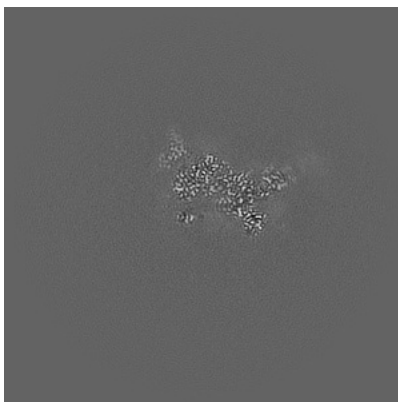
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

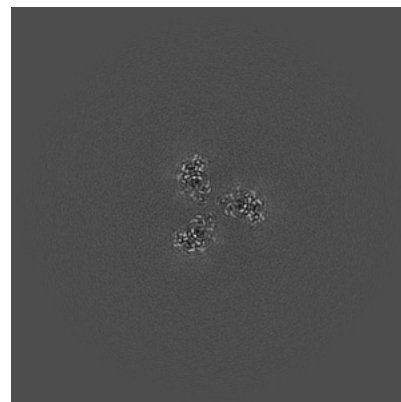
6.2.1 Primary map



X Index: 200

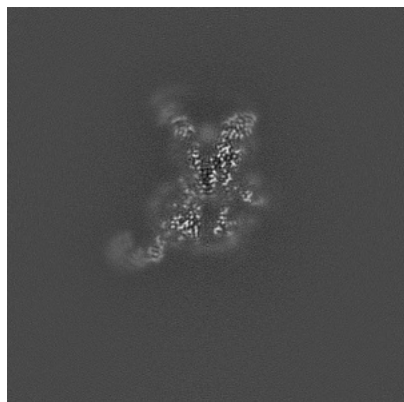


Y Index: 200

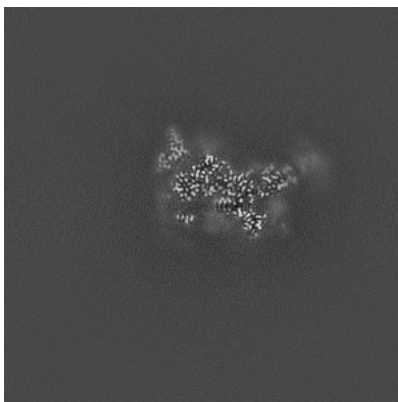


Z Index: 200

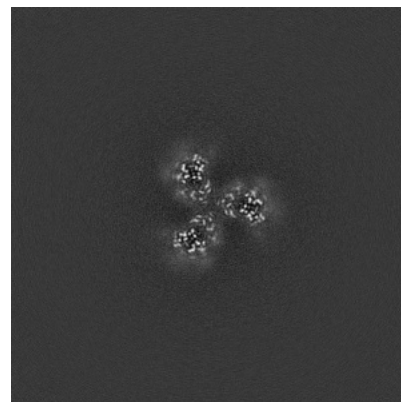
6.2.2 Raw map



X Index: 200



Y Index: 200

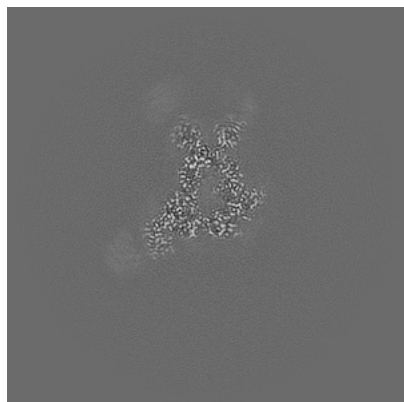


Z Index: 200

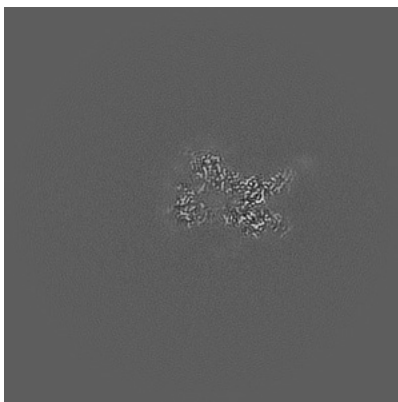
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

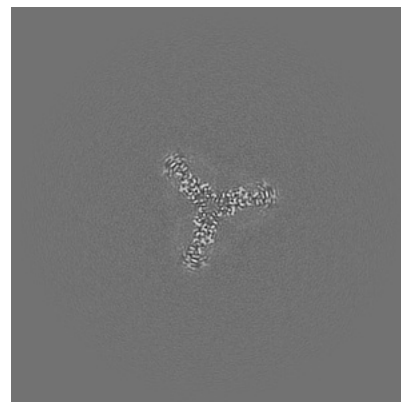
6.3.1 Primary map



X Index: 187

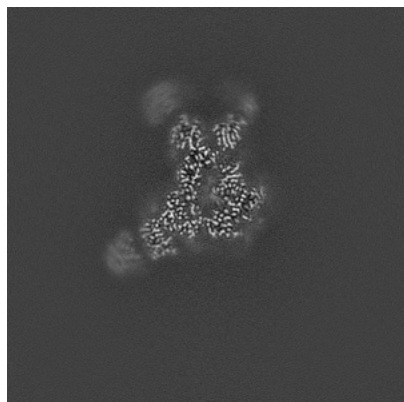


Y Index: 191

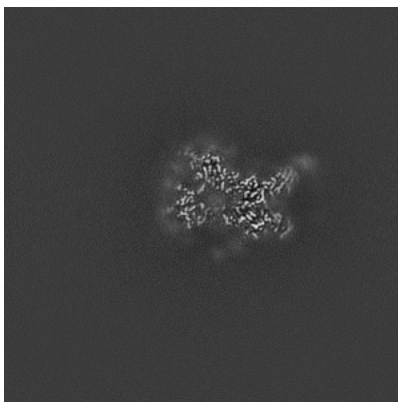


Z Index: 180

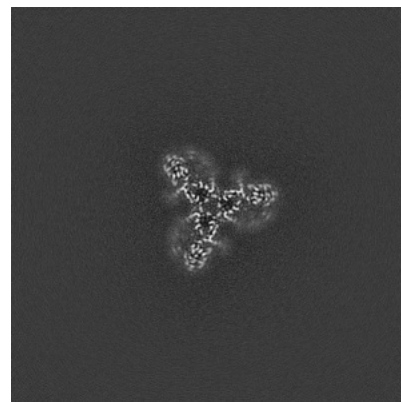
6.3.2 Raw map



X Index: 186



Y Index: 191

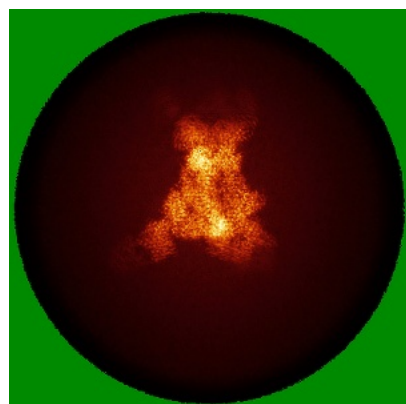


Z Index: 184

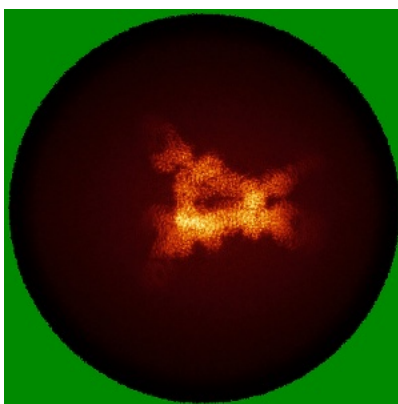
The images above show the largest variance slices of the map in three orthogonal directions.

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

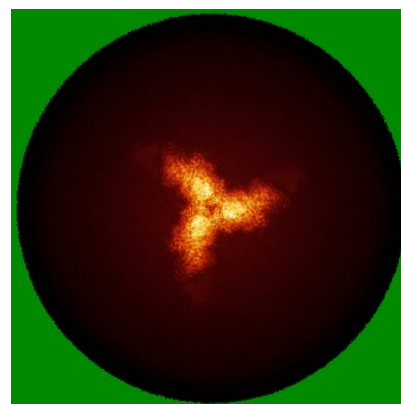
6.4.1 Primary map



X

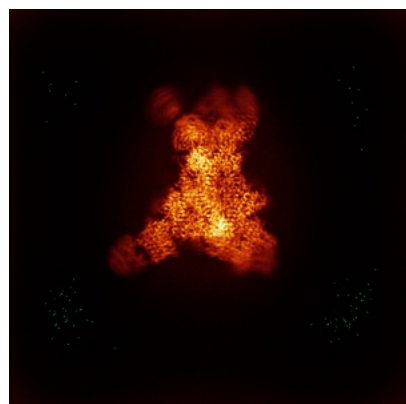


Y

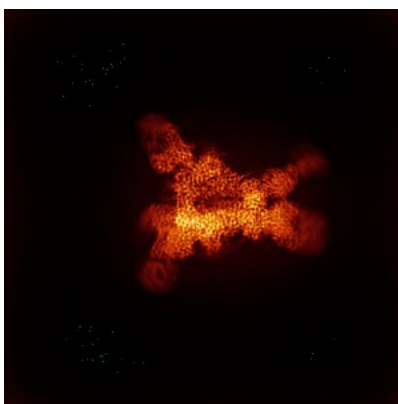


Z

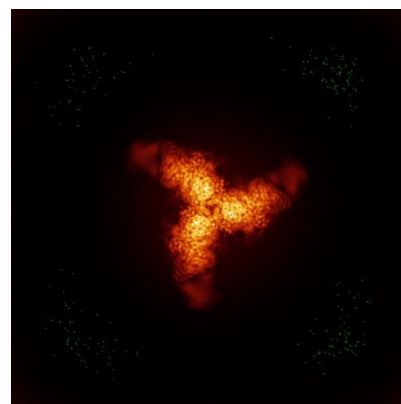
6.4.2 Raw map



X



Y

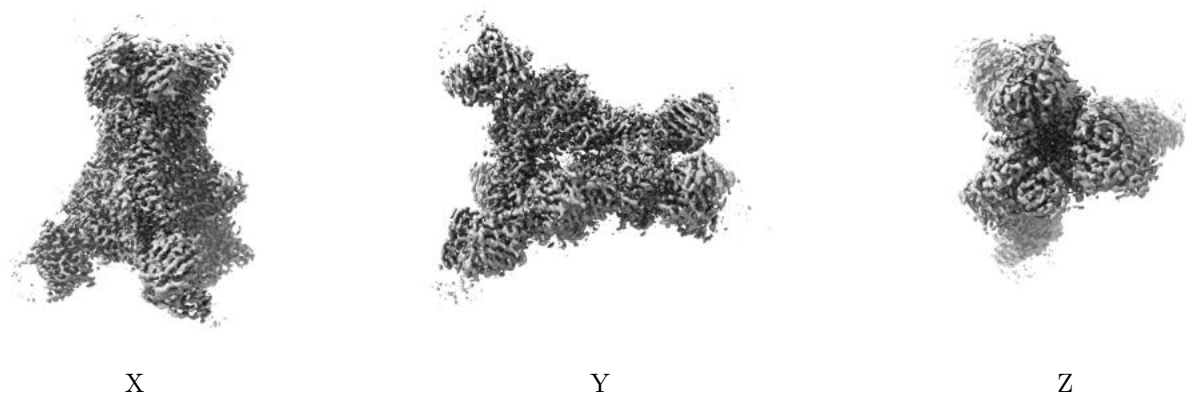


Z

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 0.25. 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.

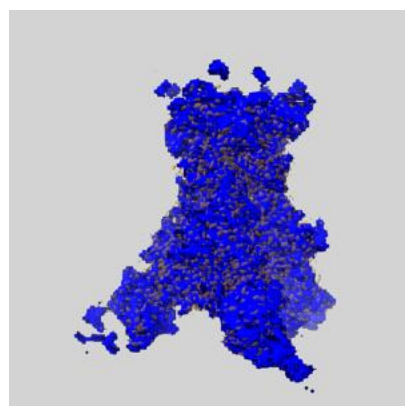
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

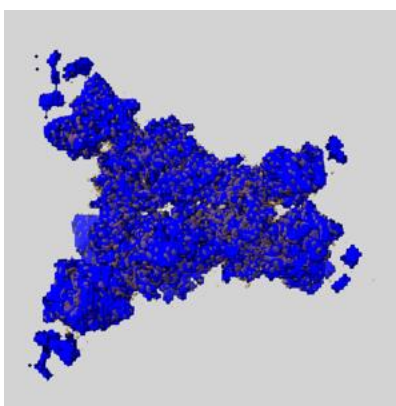
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

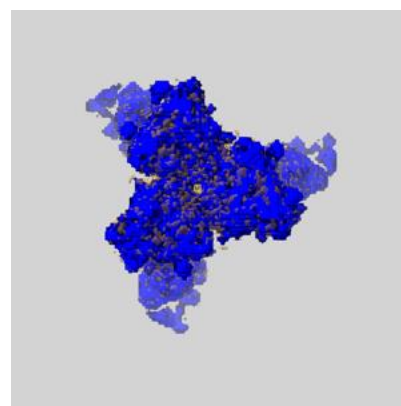
6.6.1 emd_73109_msk_1.map [i](#)



X



Y

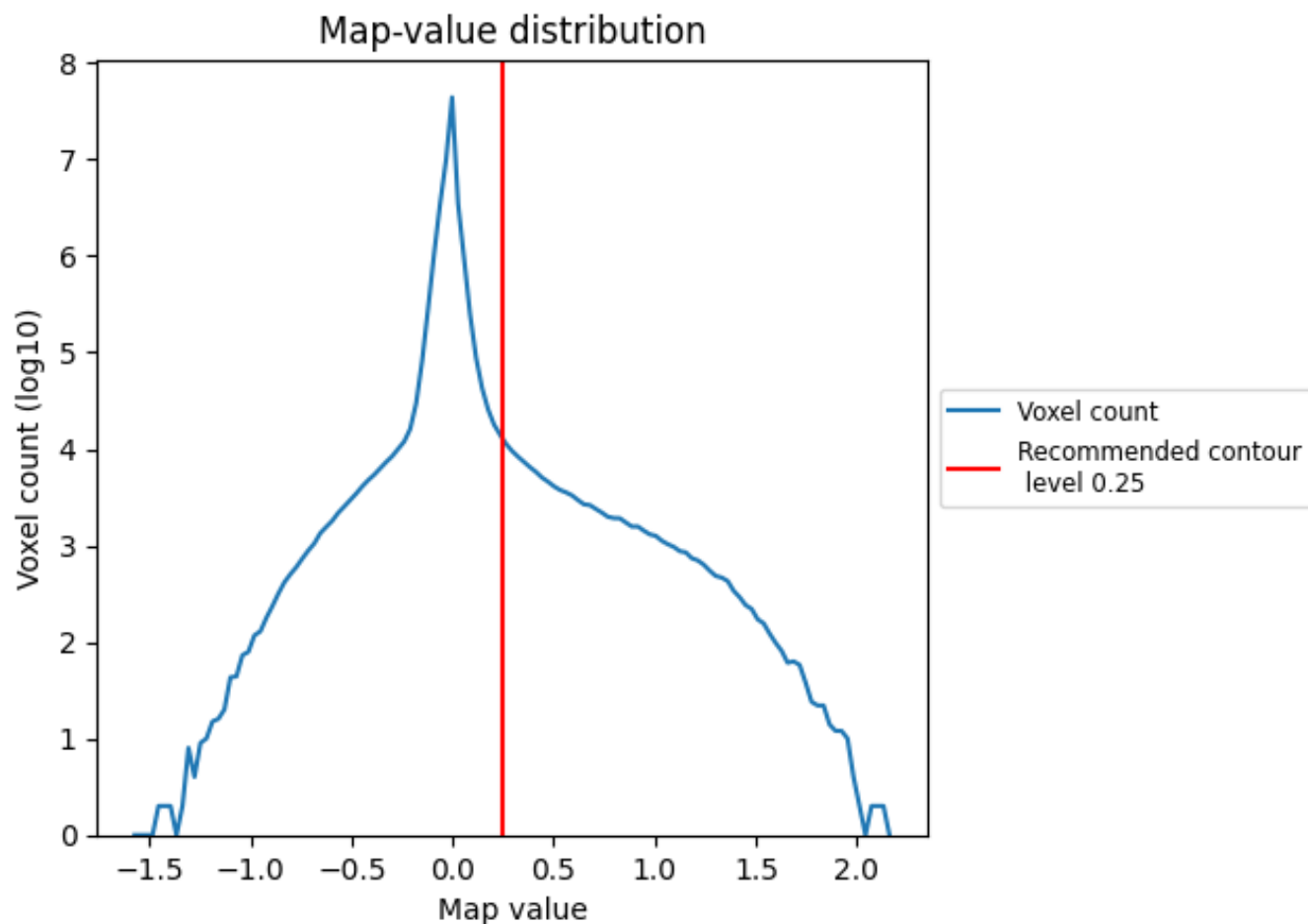


Z

7 Map analysis [i](#)

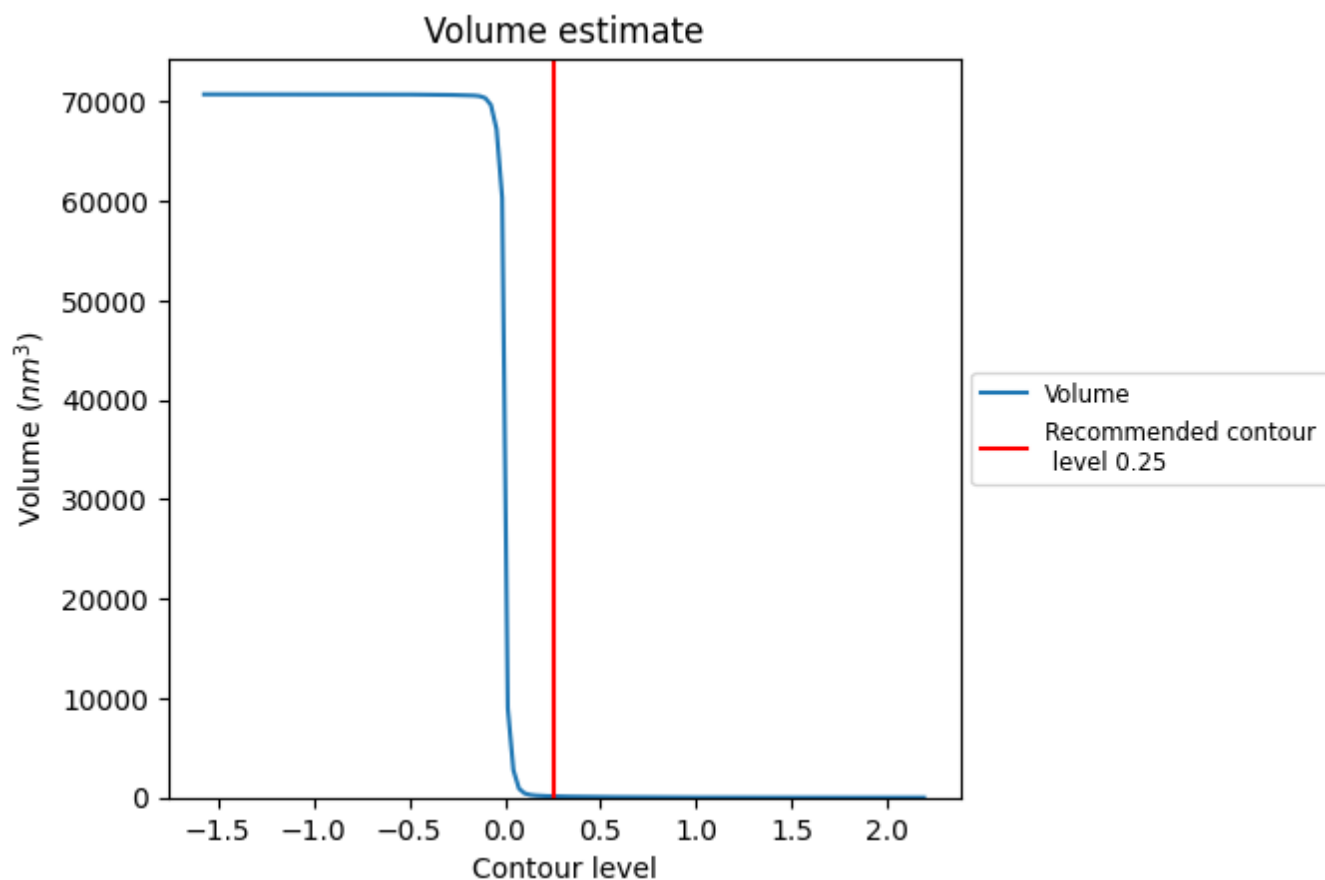
This section contains the results of statistical analysis of the map.

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.

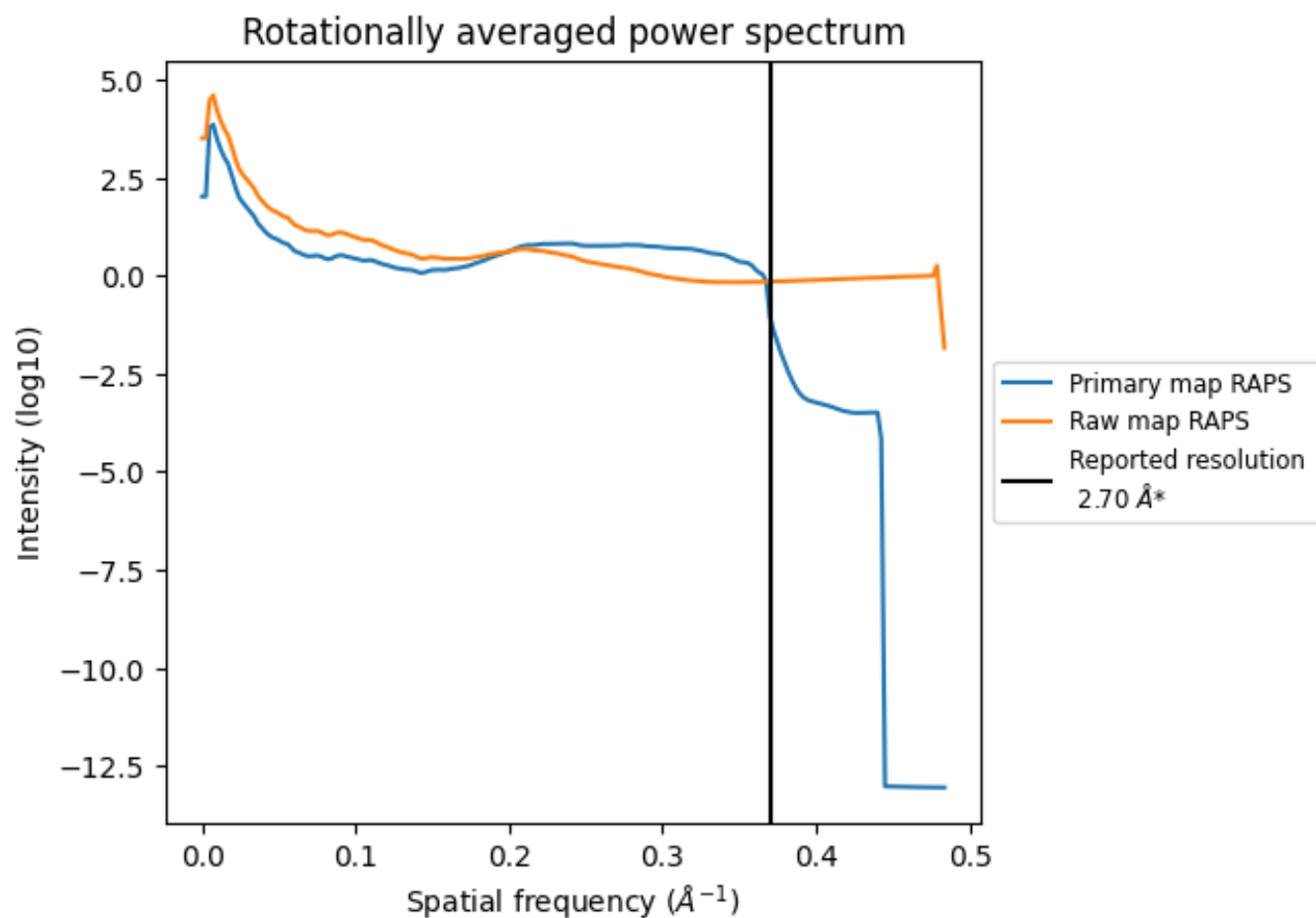
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 118 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 ⓘ

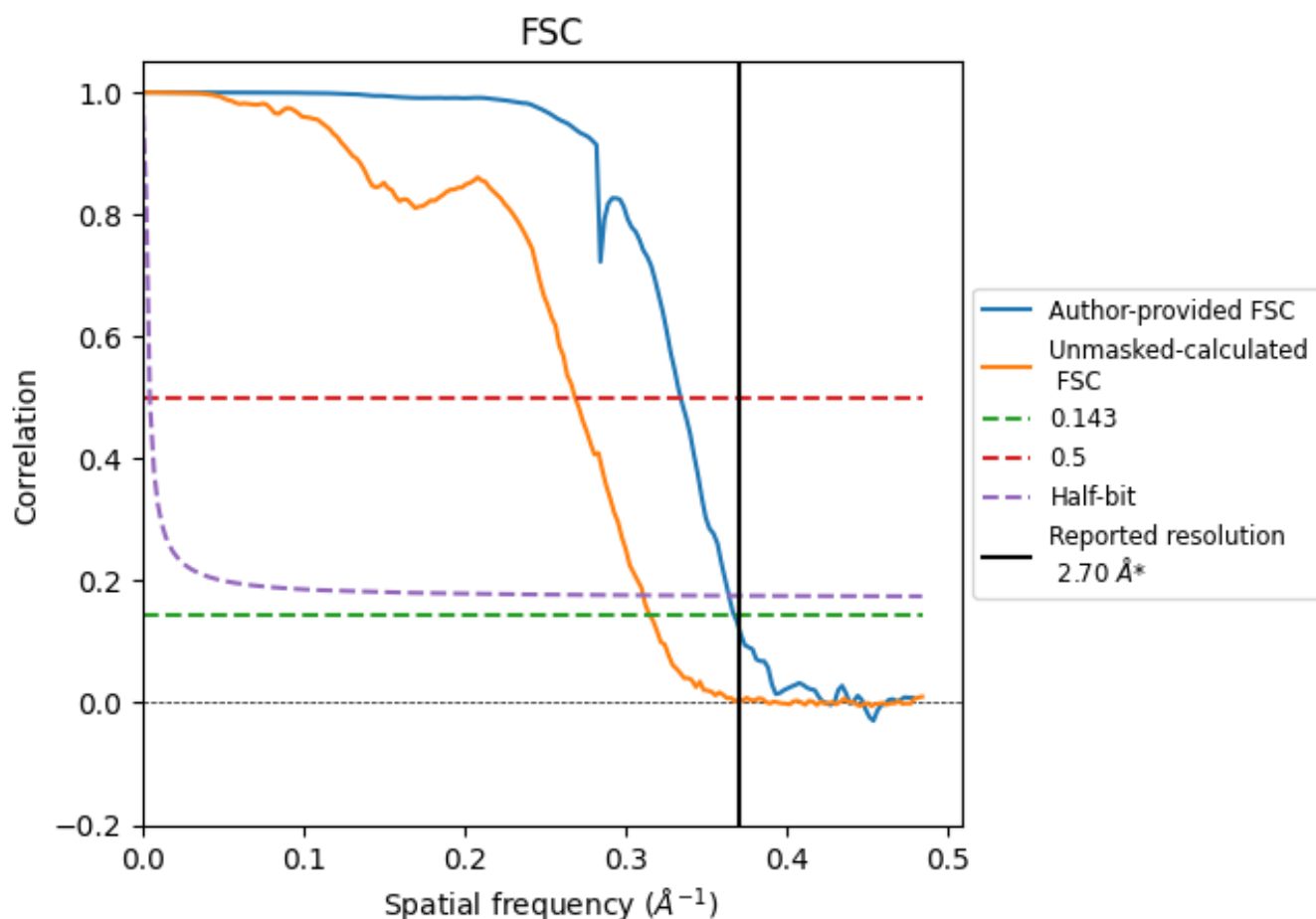


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

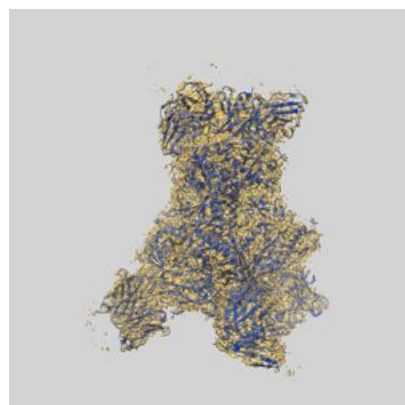
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	2.99	2.75
Unmasked-calculated*	3.18	3.73	3.22

*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 3.18 differs from the reported value 2.7 by more than 10 %

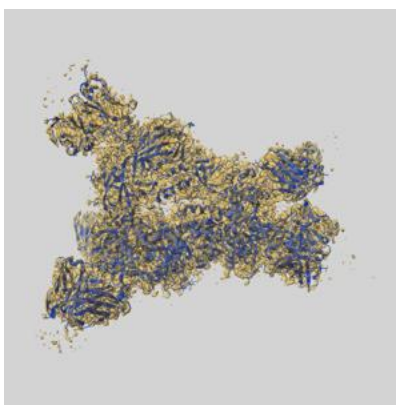
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73109 and PDB model 9YMK. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

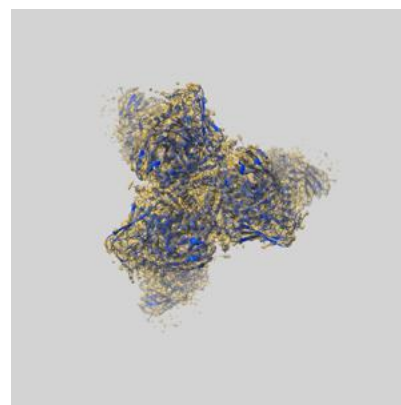
9.1 Map-model overlay [i](#)



X



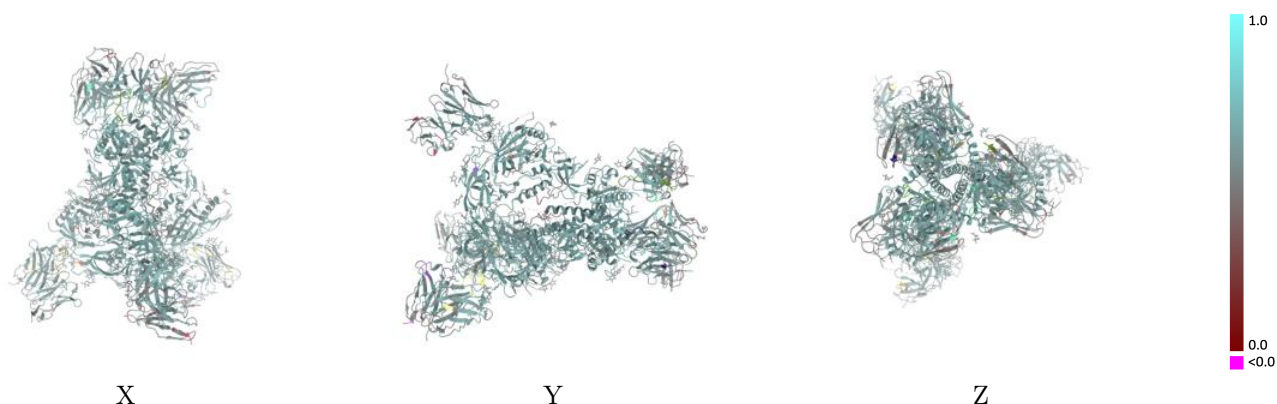
Y



Z

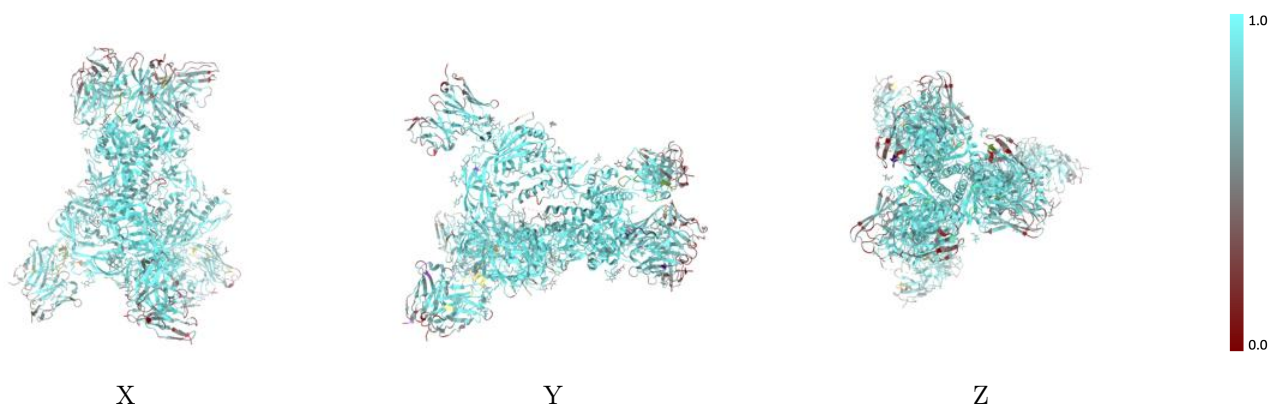
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



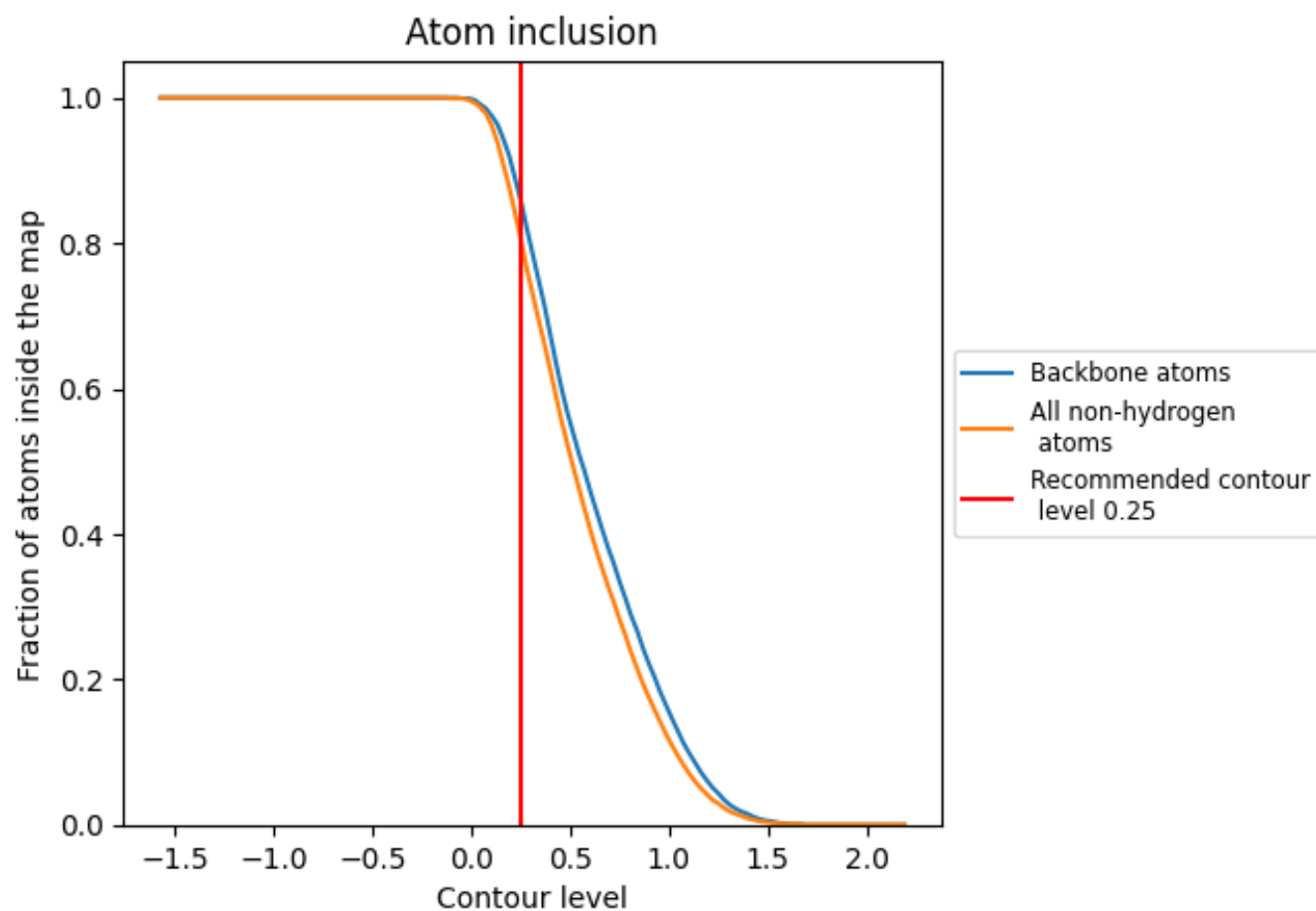
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.5900
A	 0.8800	 0.6150
B	 0.9010	 0.6250
C	 0.8800	 0.6120
D	 0.8980	 0.6240
E	 0.8800	 0.6130
F	 0.8980	 0.6240
G	 0.7330	 0.5720
H	 0.7390	 0.5690
I	 0.6370	 0.5450
J	 0.7350	 0.5700
K	 0.7340	 0.5710
L	 0.7010	 0.5480
M	 0.6340	 0.5440
N	 0.7010	 0.5490
O	 0.7190	 0.5680
P	 0.7370	 0.5710
Q	 0.6310	 0.5430
R	 0.7080	 0.5470
S	 0.6750	 0.5510
T	 0.8570	 0.5900
U	 0.7860	 0.5750
V	 0.8460	 0.5410
W	 0.7860	 0.5700
X	 0.6750	 0.5460
Y	 0.8480	 0.5920
Z	 0.7860	 0.5750
a	 0.8720	 0.5480
b	 0.8210	 0.5620
c	 0.6750	 0.5520
d	 0.8570	 0.5920
e	 0.8210	 0.5730
f	 0.8460	 0.5390
g	 0.7860	 0.5510

