



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 06:50 PM EST

PDB ID : 7UGN
EMDB ID : EMD-26490
Title : Cryo-EM structure of BG24 inferred germline Fabs with germline CDR3s and 10-1074 Fabs in complex with HIV-1 Env immunogen BG505-SOSIPv4.1-GT1 - Class 1
Authors : Dam, K.A.; Bjorkman, P.J.
Deposited on : 2022-03-25
Resolution : 3.40 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

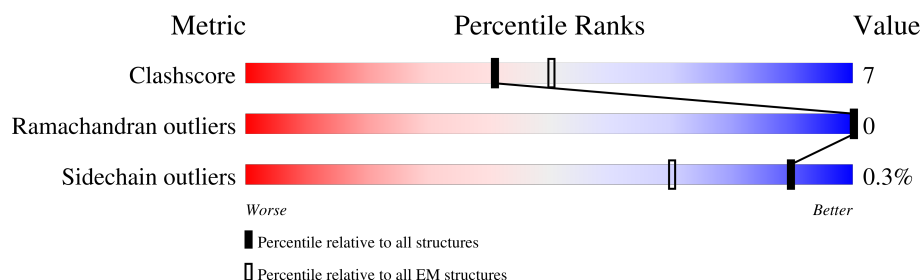
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	451	
1	B	451	
1	C	451	
2	D	129	
2	E	129	
2	F	129	
3	G	125	
3	H	125	

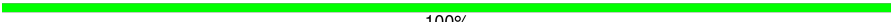
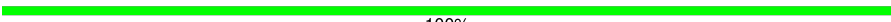







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Mol	Chain	Length	Quality of chain
3	I	125	
4	J	106	
4	K	106	
4	L	106	
5	M	133	
5	N	133	
5	O	133	
6	P	107	
6	Q	107	
6	R	107	
7	S	2	
7	T	2	
7	V	2	
7	W	2	
7	Y	2	
7	Z	2	
7	a	2	
7	b	2	
7	d	2	
7	e	2	
7	g	2	
7	h	2	
7	i	2	
7	j	2	
7	l	2	

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Mol	Chain	Length	Quality of chain
7	m	2	 100%
7	o	2	 100%
7	p	2	 100%
8	U	5	 60% 40%
8	c	5	 60% 40%
8	k	5	 60% 40%
9	X	7	 14% 57% 29%
9	n	7	 43% 57%
10	f	6	 67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	f	4	X	-	-	-
10	MAN	f	5	X	-	-	-
7	NAG	S	2	X	-	-	-
7	NAG	W	2	X	-	-	-
7	NAG	Y	2	X	-	-	-
7	NAG	a	2	X	-	-	-
7	NAG	e	2	X	-	-	-
7	NAG	g	2	X	-	-	-
7	NAG	m	2	X	-	-	-
7	NAG	o	2	X	-	-	-
7	NAG	p	1	X	-	-	-
8	MAN	U	4	X	-	-	-
8	MAN	U	5	X	-	-	-
8	MAN	c	4	X	-	-	-
8	MAN	c	5	X	-	-	-
8	MAN	k	4	X	-	-	-
9	MAN	X	6	X	-	-	-
9	MAN	X	7	X	-	-	-
9	MAN	n	6	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25698 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total	C	N	O	S	0	0
			3552	2234	627	663	28		
1	B	451	Total	C	N	O	S	0	0
			3552	2234	627	663	28		
1	C	451	Total	C	N	O	S	0	0
			3552	2234	627	663	28		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	64	LYS	GLU	conflict	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	169	ARG	LYS	conflict	UNP Q2N0S5
A	173	HIS	TYR	conflict	UNP Q2N0S5
A	174	ALA	SER	conflict	UNP Q2N0S5
A	178	LYS	ARG	conflict	UNP Q2N0S5
A	181	ILE	VAL	conflict	UNP Q2N0S5
A	183	PRO	GLN	conflict	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ARG	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	189	THR	LYS	conflict	UNP Q2N0S5
A	190	SER	GLU	conflict	UNP Q2N0S5
A	199	ALA	SER	conflict	UNP Q2N0S5
A	276	ASP	ASN	conflict	UNP Q2N0S5
A	278	ARG	THR	conflict	UNP Q2N0S5
A	316	TRP	ALA	conflict	UNP Q2N0S5
A	332	ASN	THR	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	386	ASP	ASN	conflict	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	VAL	deletion	UNP Q2N0S5
A	?	-	GLN	deletion	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	462	ASP	ASN	conflict	UNP Q2N0S5
A	471	SER	GLY	conflict	UNP Q2N0S5
A	501	CYS	ALA	conflict	UNP Q2N0S5
B	?	-	GLU	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	64	LYS	GLU	conflict	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	169	ARG	LYS	conflict	UNP Q2N0S5
B	173	HIS	TYR	conflict	UNP Q2N0S5
B	174	ALA	SER	conflict	UNP Q2N0S5
B	178	LYS	ARG	conflict	UNP Q2N0S5
B	181	ILE	VAL	conflict	UNP Q2N0S5
B	183	PRO	GLN	conflict	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	ARG	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	189	THR	LYS	conflict	UNP Q2N0S5
B	190	SER	GLU	conflict	UNP Q2N0S5
B	199	ALA	SER	conflict	UNP Q2N0S5
B	276	ASP	ASN	conflict	UNP Q2N0S5
B	278	ARG	THR	conflict	UNP Q2N0S5
B	316	TRP	ALA	conflict	UNP Q2N0S5
B	332	ASN	THR	conflict	UNP Q2N0S5
B	386	ASP	ASN	conflict	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	VAL	deletion	UNP Q2N0S5
B	?	-	GLN	deletion	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	462	ASP	ASN	conflict	UNP Q2N0S5
B	471	SER	GLY	conflict	UNP Q2N0S5
B	501	CYS	ALA	conflict	UNP Q2N0S5
C	?	-	GLU	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	64	LYS	GLU	conflict	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	169	ARG	LYS	conflict	UNP Q2N0S5
C	173	HIS	TYR	conflict	UNP Q2N0S5
C	174	ALA	SER	conflict	UNP Q2N0S5
C	178	LYS	ARG	conflict	UNP Q2N0S5
C	181	ILE	VAL	conflict	UNP Q2N0S5
C	183	PRO	GLN	conflict	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ARG	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	189	THR	LYS	conflict	UNP Q2N0S5
C	190	SER	GLU	conflict	UNP Q2N0S5
C	199	ALA	SER	conflict	UNP Q2N0S5
C	276	ASP	ASN	conflict	UNP Q2N0S5
C	278	ARG	THR	conflict	UNP Q2N0S5
C	316	TRP	ALA	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	386	ASP	ASN	conflict	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	VAL	deletion	UNP Q2N0S5
C	?	-	GLN	deletion	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	462	ASP	ASN	conflict	UNP Q2N0S5
C	471	SER	GLY	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total 1030	C 655	N 176	O 193	S 6	0	0
2	E	129	Total 1030	C 655	N 176	O 193	S 6	0	0
2	F	129	Total 1030	C 655	N 176	O 193	S 6	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP Q2N0S5
D	?	-	ILE	deletion	UNP Q2N0S5
D	?	-	VAL	deletion	UNP Q2N0S5
D	?	-	GLN	deletion	UNP Q2N0S5
D	?	-	GLN	deletion	UNP Q2N0S5
D	?	-	GLN	deletion	UNP Q2N0S5
D	?	-	SER	deletion	UNP Q2N0S5
D	?	-	ASN	deletion	UNP Q2N0S5
D	?	-	LEU	deletion	UNP Q2N0S5
D	?	-	LEU	deletion	UNP Q2N0S5
D	?	-	ARG	deletion	UNP Q2N0S5
D	?	-	ALA	deletion	UNP Q2N0S5
D	?	-	ILE	deletion	UNP Q2N0S5
D	?	-	GLU	deletion	UNP Q2N0S5
D	?	-	ALA	deletion	UNP Q2N0S5
D	?	-	GLN	deletion	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLN	deletion	UNP Q2N0S5
D	?	-	HIS	deletion	UNP Q2N0S5
D	605	CYS	THR	conflict	UNP Q2N0S5
E	?	-	GLY	deletion	UNP Q2N0S5
E	?	-	ILE	deletion	UNP Q2N0S5
E	?	-	VAL	deletion	UNP Q2N0S5
E	?	-	GLN	deletion	UNP Q2N0S5
E	?	-	GLN	deletion	UNP Q2N0S5
E	?	-	GLN	deletion	UNP Q2N0S5
E	?	-	SER	deletion	UNP Q2N0S5
E	?	-	ASN	deletion	UNP Q2N0S5
E	?	-	LEU	deletion	UNP Q2N0S5
E	?	-	LEU	deletion	UNP Q2N0S5
E	?	-	ARG	deletion	UNP Q2N0S5
E	?	-	ALA	deletion	UNP Q2N0S5
E	?	-	ILE	deletion	UNP Q2N0S5
E	?	-	GLU	deletion	UNP Q2N0S5
E	?	-	ALA	deletion	UNP Q2N0S5
E	?	-	GLN	deletion	UNP Q2N0S5
E	?	-	GLN	deletion	UNP Q2N0S5
E	?	-	HIS	deletion	UNP Q2N0S5
E	605	CYS	THR	conflict	UNP Q2N0S5
F	?	-	GLY	deletion	UNP Q2N0S5
F	?	-	ILE	deletion	UNP Q2N0S5
F	?	-	VAL	deletion	UNP Q2N0S5
F	?	-	GLN	deletion	UNP Q2N0S5
F	?	-	GLN	deletion	UNP Q2N0S5
F	?	-	GLN	deletion	UNP Q2N0S5
F	?	-	SER	deletion	UNP Q2N0S5
F	?	-	ASN	deletion	UNP Q2N0S5
F	?	-	LEU	deletion	UNP Q2N0S5
F	?	-	LEU	deletion	UNP Q2N0S5
F	?	-	ARG	deletion	UNP Q2N0S5
F	?	-	ALA	deletion	UNP Q2N0S5
F	?	-	ILE	deletion	UNP Q2N0S5
F	?	-	GLU	deletion	UNP Q2N0S5
F	?	-	ALA	deletion	UNP Q2N0S5
F	?	-	GLN	deletion	UNP Q2N0S5
F	?	-	GLN	deletion	UNP Q2N0S5
F	?	-	HIS	deletion	UNP Q2N0S5
F	605	CYS	THR	conflict	UNP Q2N0S5

- Molecule 3 is a protein called BG24 inferred germline Fab with germline CDR3s heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	125	Total	C	N	O	S	0	0
			959	601	163	188	7		
3	H	125	Total	C	N	O	S	0	0
			959	601	163	188	7		
3	I	125	Total	C	N	O	S	0	0
			959	601	163	188	7		

- Molecule 4 is a protein called BG24 inferred germline Fab with germline CDR3s light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	105	Total	C	N	O	S	0	0
			778	483	129	163	3		
4	K	105	Total	C	N	O	S	0	0
			778	483	129	163	3		
4	L	105	Total	C	N	O	S	0	0
			778	483	129	163	3		

- Molecule 5 is a protein called 10-1074 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	N	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 6 is a protein called 10-1074 Fab light chain.

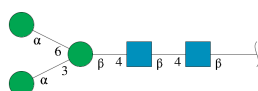
Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	Q	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



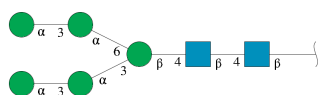
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called 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.



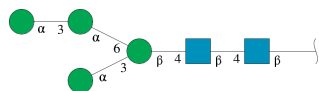
Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	5	Total	C	N	O	0	0
			61	34	2	25		
8	c	5	Total	C	N	O	0	0
			61	34	2	25		
8	k	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[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
9	X	7	Total	C	N	O	0	0
			83	46	2	35		
9	n	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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
10	f	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



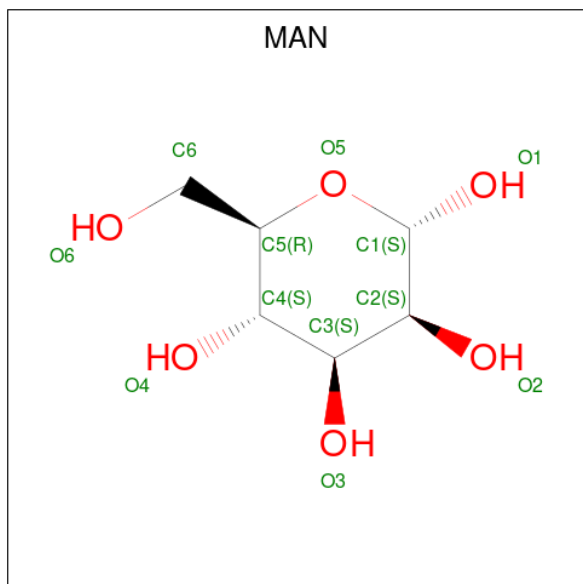
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	A	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14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

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

- Molecule 12 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

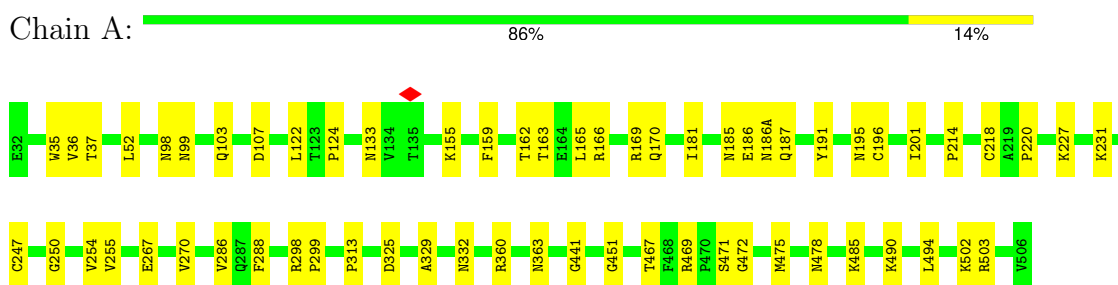


Mol	Chain	Residues	Atoms			AltConf
12	Q	1	Total	C	O	0
			11	6	5	

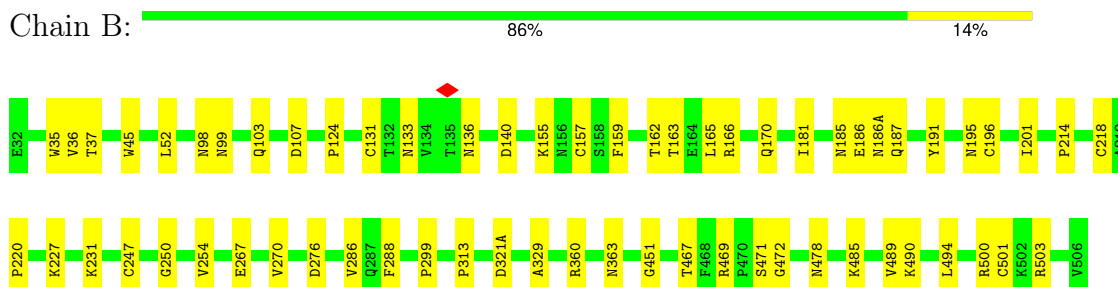
3 Residue-property plots

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.

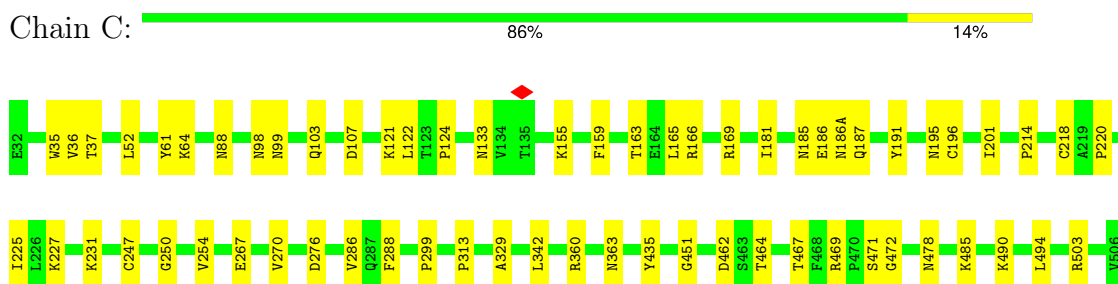
• Molecule 1: Envelope glycoprotein gp120



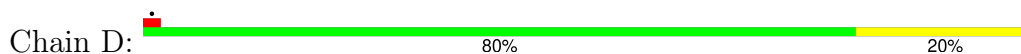
• Molecule 1: Envelope glycoprotein gp120



• Molecule 1: Envelope glycoprotein gp120

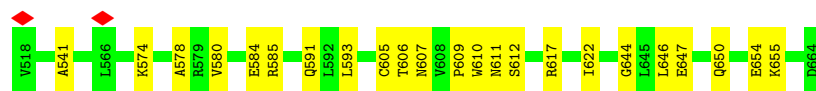
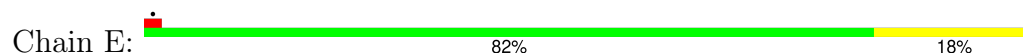


• Molecule 2: Envelope glycoprotein gp41

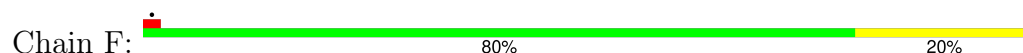




- Molecule 2: Envelope glycoprotein gp41



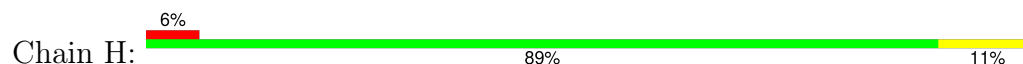
- Molecule 2: Envelope glycoprotein gp41



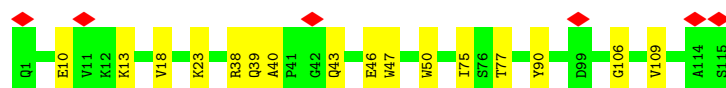
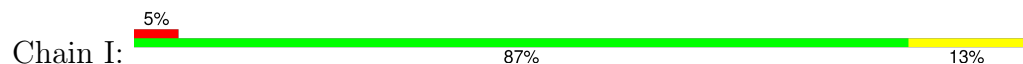
- Molecule 3: BG24 inferred germline Fab with germline CDR3s heavy chain



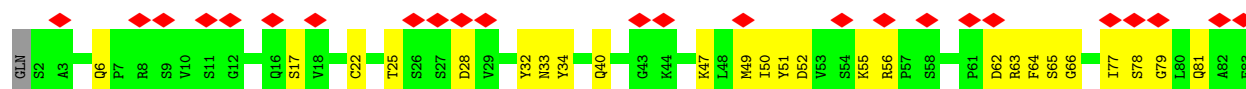
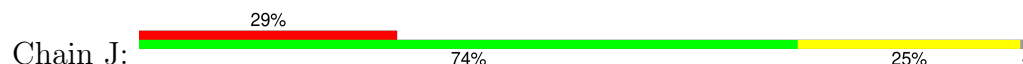
- Molecule 3: BG24 inferred germline Fab with germline CDR3s heavy chain

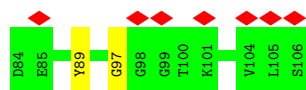


- Molecule 3: BG24 inferred germline Fab with germline CDR3s heavy chain

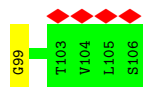
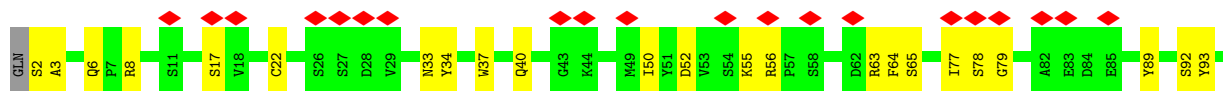
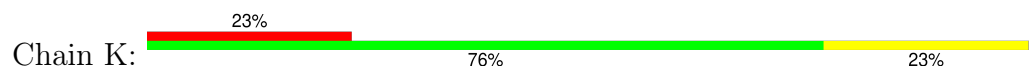


- Molecule 4: BG24 inferred germline Fab with germline CDR3s light chain

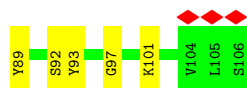
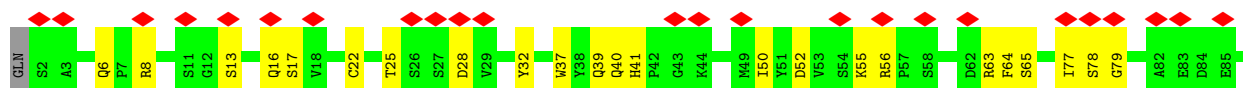




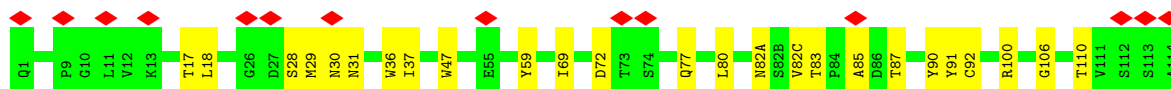
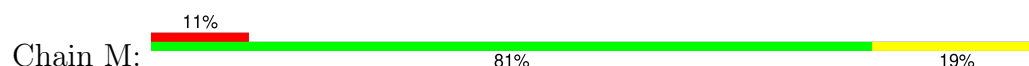
- Molecule 4: BG24 inferred germline Fab with germline CDR3s light chain



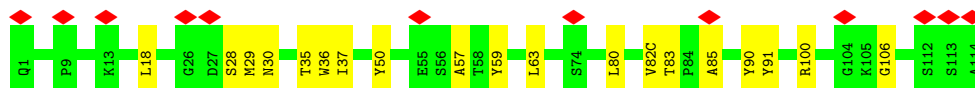
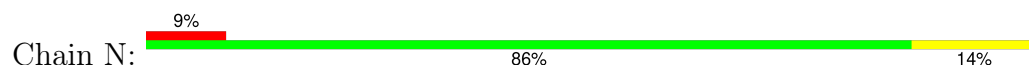
- Molecule 4: BG24 inferred germline Fab with germline CDR3s light chain



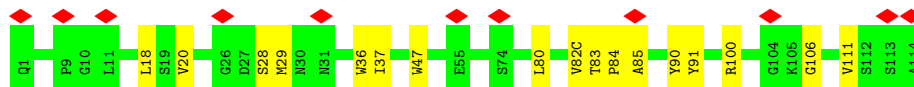
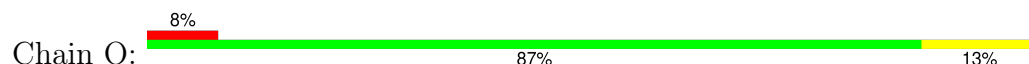
- Molecule 5: 10-1074 Fab heavy chain




- Molecule 5: 10-1074 Fab heavy chain

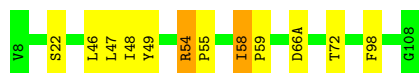


- Molecule 5: 10-1074 Fab heavy chain




- Molecule 6: 10-1074 Fab light chain

Chain P:  89% 9%




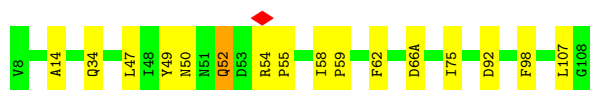
- Molecule 6: 10-1074 Fab light chain

Chain Q:  89% 10%



- Molecule 6: 10-1074 Fab light chain

Chain R:  85% 14%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 50%
100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50%
100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  50%
100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  50%
100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%

NAG1
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

NAG1
NAG2

- Molecule 8: 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

Chain U:  60% 40%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 8: 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

Chain c:  60% 40%


NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 8: 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

Chain k:  60% 40%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[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

Chain X:  14% 57% 29%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[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

Chain n:  43% 57%

MAN1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 10: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain f:  67% 33%

MAN1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0081	Depositor
Map size (Å)	290.7744, 290.7744, 290.7744	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8654, 0.8654, 0.8654	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3628	0.45	0/4927
1	B	0.25	0/3628	0.45	0/4927
1	C	0.25	0/3628	0.45	0/4927
2	D	0.24	0/1048	0.41	0/1421
2	E	0.23	0/1048	0.42	0/1421
2	F	0.23	0/1048	0.42	0/1421
3	G	0.24	0/981	0.47	0/1330
3	H	0.24	0/981	0.47	0/1330
3	I	0.24	0/981	0.47	0/1330
4	J	0.25	0/796	0.46	0/1080
4	K	0.25	0/796	0.45	0/1080
4	L	0.25	0/796	0.44	0/1080
5	M	0.24	0/1066	0.46	0/1451
5	N	0.24	0/1066	0.45	0/1451
5	O	0.24	0/1066	0.46	0/1451
6	P	0.25	0/845	0.47	0/1148
6	Q	0.25	0/845	0.45	0/1148
6	R	0.25	0/845	0.44	0/1148
All	All	0.25	0/25092	0.45	0/34071

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
6	Q	0	1
6	R	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Q	54	ARG	Peptide
6	R	54	ARG	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	3552	0	3485	46	0
1	B	3552	0	3485	43	0
1	C	3552	0	3483	48	0
2	D	1030	0	1020	22	0
2	E	1030	0	1020	18	0
2	F	1030	0	1020	25	0
3	G	959	0	916	7	0
3	H	959	0	916	8	0
3	I	959	0	916	9	0
4	J	778	0	738	18	0
4	K	778	0	738	16	0
4	L	778	0	738	19	0
5	M	1041	0	1005	16	0
5	N	1041	0	1005	11	0
5	O	1041	0	1005	10	0
6	P	824	0	788	26	0
6	Q	824	0	788	18	0
6	R	824	0	788	14	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	Y	28	0	25	1	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	d	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	e	28	0	25	0	0
7	g	28	0	25	0	0
7	h	28	0	25	0	0
7	i	28	0	25	0	0
7	j	28	0	25	0	0
7	l	28	0	25	0	0
7	m	28	0	25	0	0
7	o	28	0	25	0	0
7	p	28	0	22	0	0
8	U	61	0	52	0	0
8	c	61	0	52	0	0
8	k	61	0	52	0	0
9	X	83	0	69	3	0
9	n	83	0	69	0	0
10	f	72	0	59	0	0
11	A	56	0	52	1	0
11	B	56	0	52	1	0
11	C	56	0	52	2	0
11	D	14	0	13	0	0
11	E	14	0	13	0	0
11	F	14	0	13	0	0
12	Q	11	0	10	0	0
All	All	25698	0	24859	322	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 7.

All (322) 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)
6:Q:47:LEU:O	6:Q:55:PRO:CG	1.69	1.41
6:Q:47:LEU:O	6:Q:55:PRO:HG3	1.12	1.23
6:P:47:LEU:O	6:P:55:PRO:HD2	1.44	1.16
6:P:58:ILE:HG22	6:P:59:PRO:CD	1.79	1.12
6:P:58:ILE:HG22	6:P:59:PRO:HD2	1.12	1.09
6:P:49:TYR:CE1	6:P:55:PRO:HA	1.96	1.00
6:P:49:TYR:HE1	6:P:55:PRO:HA	1.29	0.96
6:P:49:TYR:CD1	6:P:55:PRO:HB3	2.04	0.92
6:P:47:LEU:O	6:P:55:PRO:CD	2.17	0.91
6:Q:47:LEU:O	6:Q:55:PRO:CD	2.19	0.89
6:R:47:LEU:O	6:R:55:PRO:CG	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:54:ARG:O	6:Q:54:ARG:NE	2.12	0.82
6:R:47:LEU:O	6:R:55:PRO:HG3	1.78	0.82
1:B:37:THR:HG22	2:E:605:CYS:HB3	1.60	0.80
6:P:49:TYR:CE1	6:P:55:PRO:CA	2.64	0.79
6:P:46:LEU:HG	6:P:55:PRO:HG3	1.67	0.77
6:P:49:TYR:HE1	6:P:55:PRO:CA	2.00	0.75
6:P:54:ARG:HD3	6:P:54:ARG:N	2.05	0.72
6:Q:54:ARG:HE	6:Q:54:ARG:C	1.92	0.71
3:G:23:LYS:HG3	3:G:77:THR:HG22	1.71	0.71
6:Q:47:LEU:C	6:Q:55:PRO:HG3	2.08	0.71
6:P:49:TYR:HD1	6:P:55:PRO:HB3	1.53	0.70
6:P:58:ILE:CG2	6:P:59:PRO:CD	2.66	0.69
5:O:83:THR:HG22	5:O:85:ALA:H	1.58	0.68
3:I:23:LYS:HG3	3:I:77:THR:HG22	1.76	0.68
1:C:159:PHE:HA	11:C:603:NAG:H82	1.77	0.67
3:H:23:LYS:HG3	3:H:77:THR:HG22	1.76	0.67
6:R:47:LEU:O	6:R:55:PRO:CD	2.43	0.67
1:B:159:PHE:HA	11:B:603:NAG:H82	1.77	0.67
1:C:36:VAL:HG12	2:F:610:TRP:HE3	1.60	0.66
4:J:52:ASP:HB2	4:J:55:LYS:HB2	1.78	0.66
6:P:49:TYR:CD1	6:P:55:PRO:CB	2.78	0.66
5:M:100:ARG:NH2	6:P:66(A):ASP:OD2	2.29	0.66
5:N:100:ARG:NH2	6:Q:66(A):ASP:OD2	2.28	0.66
6:Q:22:SER:HB2	6:Q:72:THR:HG22	1.78	0.65
4:J:6:GLN:HE22	4:J:89:TYR:HA	1.62	0.65
1:A:159:PHE:HA	11:A:603:NAG:H82	1.78	0.65
4:K:56:ARG:NH2	4:K:65:SER:OG	2.31	0.64
5:N:83:THR:HG22	5:N:85:ALA:H	1.63	0.64
5:M:83:THR:HG22	5:M:85:ALA:H	1.62	0.64
1:B:218:CYS:HA	1:B:247:CYS:HB3	1.80	0.63
1:C:218:CYS:HA	1:C:247:CYS:HB3	1.80	0.63
1:B:36:VAL:HG12	2:E:610:TRP:HE3	1.64	0.63
4:L:56:ARG:NH2	4:L:65:SER:OG	2.32	0.62
4:K:6:GLN:HE22	4:K:89:TYR:HA	1.62	0.62
1:A:218:CYS:HA	1:A:247:CYS:HB3	1.82	0.62
4:L:6:GLN:HE22	4:L:89:TYR:HA	1.64	0.61
1:A:36:VAL:HG12	2:D:610:TRP:HE3	1.65	0.61
1:C:494:LEU:HD21	2:F:593:LEU:HD21	1.84	0.60
1:A:133:ASN:OD1	1:A:155:LYS:NZ	2.34	0.60
1:A:254:VAL:O	1:A:478:ASN:ND2	2.35	0.59
1:B:133:ASN:OD1	1:B:155:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG22	2:D:605:CYS:HB3	1.83	0.59
1:A:494:LEU:HD21	2:D:593:LEU:HD21	1.83	0.59
1:B:254:VAL:O	1:B:478:ASN:ND2	2.36	0.59
1:B:136:ASN:ND2	1:B:140:ASP:OD2	2.36	0.59
6:P:22:SER:HB2	6:P:72:THR:HG22	1.85	0.58
1:B:494:LEU:HD21	2:E:593:LEU:HD21	1.86	0.58
2:D:580:VAL:O	2:D:584:GLU:HG2	2.04	0.58
2:F:580:VAL:O	2:F:584:GLU:HG2	2.04	0.57
5:O:100:ARG:NH2	6:R:66(A):ASP:OD2	2.36	0.57
1:A:270:VAL:HG12	1:A:288:PHE:HA	1.87	0.57
2:E:580:VAL:O	2:E:584:GLU:HG2	2.04	0.57
1:B:270:VAL:HG12	1:B:288:PHE:HA	1.87	0.57
1:C:270:VAL:HG12	1:C:288:PHE:HA	1.87	0.57
6:P:54:ARG:HD3	6:P:54:ARG:H	1.67	0.57
6:Q:54:ARG:NH1	6:Q:60:GLU:HG2	2.20	0.57
1:B:186(A):ASN:N	1:B:187:GLN:HA	2.20	0.57
4:L:63:ARG:NH1	4:L:79:GLY:O	2.38	0.56
6:P:48:ILE:HA	6:P:55:PRO:HD3	1.87	0.56
1:C:186(A):ASN:N	1:C:187:GLN:HA	2.19	0.56
1:C:254:VAL:O	1:C:478:ASN:ND2	2.38	0.56
5:O:47:TRP:HB2	6:R:98:PHE:HE1	1.71	0.56
6:R:49:TYR:HE1	6:R:55:PRO:HB3	1.71	0.56
4:J:6:GLN:HG2	4:J:22:CYS:SG	2.46	0.56
1:A:231:LYS:NZ	1:A:267:GLU:OE2	2.38	0.55
4:L:6:GLN:HG3	4:L:97:GLY:HA3	1.87	0.55
3:I:39:GLN:HE22	4:L:40:GLN:HE22	1.53	0.55
1:C:231:LYS:NZ	1:C:267:GLU:OE2	2.37	0.55
2:D:606:THR:HG21	2:D:646:LEU:HD11	1.89	0.55
5:M:36:TRP:CE2	5:M:80:LEU:HD22	2.42	0.55
1:B:503:ARG:NH1	2:E:654:GLU:OE1	2.39	0.55
4:K:64:PHE:HB3	4:K:77:ILE:HA	1.89	0.54
1:A:186(A):ASN:N	1:A:187:GLN:HA	2.21	0.54
1:C:360:ARG:HB2	1:C:467:THR:HG22	1.89	0.54
1:B:195:ASN:ND2	1:B:201:ILE:HB	2.21	0.54
3:G:39:GLN:HE22	4:J:40:GLN:HE22	1.54	0.54
3:H:75:ILE:HG13	3:H:77:THR:HG23	1.90	0.54
3:I:75:ILE:HG13	3:I:77:THR:HG23	1.90	0.54
1:B:231:LYS:NZ	1:B:267:GLU:OE1	2.37	0.53
2:D:541:ALA:O	2:E:591:GLN:NE2	2.41	0.53
4:J:63:ARG:NH1	4:J:79:GLY:O	2.41	0.53
1:C:276:ASP:OD1	1:C:276:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:NH1	2:D:654:GLU:OE1	2.41	0.53
3:H:39:GLN:HE22	4:K:40:GLN:HE22	1.56	0.53
1:B:360:ARG:HB2	1:B:467:THR:HG22	1.90	0.53
1:C:133:ASN:OD1	1:C:155:LYS:NZ	2.41	0.53
3:G:75:ILE:HG13	3:G:77:THR:HG23	1.91	0.53
4:L:25:THR:O	4:L:32:TYR:OH	2.23	0.53
5:O:36:TRP:CE2	5:O:80:LEU:HD22	2.44	0.53
1:A:360:ARG:HB2	1:A:467:THR:HG22	1.91	0.52
6:Q:54:ARG:HH12	6:Q:60:GLU:HG2	1.75	0.52
4:K:6:GLN:HG2	4:K:22:CYS:SG	2.49	0.52
6:Q:54:ARG:HE	6:Q:54:ARG:CA	2.22	0.52
1:C:88:ASN:HB2	11:C:601:NAG:O5	2.10	0.52
4:J:6:GLN:HG3	4:J:97:GLY:HA3	1.92	0.52
6:P:49:TYR:HD1	6:P:55:PRO:CB	2.20	0.52
4:J:63:ARG:O	4:J:78:SER:OG	2.26	0.52
5:O:28:SER:OG	5:O:29:MET:N	2.44	0.51
1:C:220:PRO:HB3	2:F:578:ALA:HB1	1.93	0.51
4:L:6:GLN:HG2	4:L:22:CYS:SG	2.51	0.51
2:E:541:ALA:O	2:F:591:GLN:NE2	2.44	0.51
1:C:363:ASN:O	1:C:469:ARG:NH1	2.45	0.51
5:N:37:ILE:HG23	5:N:91:TYR:HB2	1.92	0.51
5:M:17:THR:OG1	5:M:82(A):ASN:ND2	2.44	0.50
1:A:490:LYS:HE2	2:D:585:ARG:HH21	1.76	0.50
4:K:52:ASP:HB2	4:K:55:LYS:HB2	1.93	0.50
1:A:124:PRO:O	1:C:166:ARG:NH1	2.45	0.50
1:C:503:ARG:NH1	2:F:654:GLU:OE1	2.44	0.50
1:C:490:LYS:HE2	2:F:585:ARG:HH21	1.76	0.50
6:R:52:GLN:O	6:R:52:GLN:HG3	2.12	0.50
1:C:195:ASN:ND2	1:C:201:ILE:HB	2.26	0.50
2:D:591:GLN:NE2	2:F:541:ALA:O	2.44	0.50
5:M:18:LEU:HB2	5:M:82(C):VAL:HG11	1.92	0.50
1:B:490:LYS:HE2	2:E:585:ARG:HH21	1.76	0.50
4:L:63:ARG:O	4:L:78:SER:OG	2.26	0.50
6:P:58:ILE:CG2	6:P:59:PRO:HD2	2.08	0.50
5:N:36:TRP:CE2	5:N:80:LEU:HD22	2.46	0.50
4:K:63:ARG:NH1	4:K:79:GLY:O	2.45	0.49
1:A:166:ARG:NH1	1:B:124:PRO:O	2.45	0.49
1:B:166:ARG:NH1	1:C:124:PRO:O	2.45	0.49
1:B:471:SER:OG	1:B:472:GLY:N	2.46	0.49
5:N:28:SER:OG	5:N:29:MET:N	2.45	0.49
1:B:363:ASN:O	1:B:469:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:47:LYS:NZ	4:J:49:MET:SD	2.86	0.49
4:L:52:ASP:HB2	4:L:55:LYS:HB2	1.94	0.49
1:A:286:VAL:O	1:A:451:GLY:HA2	2.12	0.49
1:B:276:ASP:OD1	1:B:276:ASP:N	2.42	0.49
5:O:18:LEU:HB2	5:O:82(C):VAL:HG11	1.94	0.49
4:J:50:ILE:HD13	4:J:66:GLY:H	1.77	0.49
1:C:286:VAL:O	1:C:451:GLY:HA2	2.13	0.49
4:L:64:PHE:HB3	4:L:77:ILE:HA	1.95	0.49
1:B:286:VAL:O	1:B:451:GLY:HA2	2.12	0.49
1:C:37:THR:HG22	2:F:605:CYS:HB3	1.95	0.49
2:F:606:THR:OG1	2:F:607:ASN:N	2.46	0.49
5:M:59:TYR:HE1	5:M:69:ILE:HD12	1.78	0.49
5:O:37:ILE:HG23	5:O:91:TYR:HB2	1.95	0.48
5:M:90:TYR:O	5:M:106:GLY:CA	2.61	0.48
6:R:49:TYR:CE1	6:R:55:PRO:HB3	2.48	0.48
5:M:28:SER:OG	5:M:29:MET:N	2.46	0.48
1:A:471:SER:OG	1:A:472:GLY:N	2.46	0.48
5:O:90:TYR:O	5:O:106:GLY:CA	2.61	0.48
2:F:644:GLY:O	2:F:647:GLU:HG3	2.14	0.48
1:A:163:THR:HG23	1:A:165:LEU:H	1.78	0.48
1:A:195:ASN:ND2	1:A:201:ILE:HB	2.29	0.48
2:E:606:THR:HG21	2:E:646:LEU:HD11	1.96	0.48
5:N:90:TYR:O	5:N:106:GLY:CA	2.61	0.48
6:R:50:ASN:C	6:R:52:GLN:H	2.17	0.48
4:K:92:SER:OG	4:K:93:TYR:N	2.47	0.47
6:P:58:ILE:HG22	6:P:59:PRO:HD3	1.88	0.47
1:B:220:PRO:HB3	2:E:578:ALA:HB1	1.95	0.47
1:C:185:ASN:O	1:C:186:GLU:HG3	2.15	0.47
1:A:196:CYS:HB2	1:C:313:PRO:HB3	1.96	0.47
1:C:462:ASP:OD2	1:C:464:THR:OG1	2.29	0.47
1:A:363:ASN:O	1:A:469:ARG:NH1	2.47	0.47
4:K:63:ARG:O	4:K:78:SER:OG	2.24	0.47
5:M:37:ILE:HG23	5:M:91:TYR:HB2	1.97	0.47
1:A:220:PRO:HB3	2:D:578:ALA:HB1	1.95	0.47
2:D:607:ASN:HB2	2:D:650:GLN:NE2	2.30	0.47
2:E:607:ASN:HB2	2:E:650:GLN:HE22	1.79	0.47
6:Q:54:ARG:NE	6:Q:54:ARG:CA	2.78	0.47
3:H:40:ALA:HB3	3:H:43:GLN:HB2	1.97	0.47
1:A:185:ASN:O	1:A:186:GLU:HG3	2.14	0.46
5:M:72:ASP:OD1	5:M:77:GLN:NE2	2.49	0.46
6:Q:47:LEU:O	6:Q:55:PRO:HG2	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:28:ASP:N	4:L:28:ASP:OD1	2.46	0.46
1:C:471:SER:OG	1:C:472:GLY:N	2.47	0.46
4:J:25:THR:O	4:J:32:TYR:OH	2.27	0.46
4:J:56:ARG:NH1	4:J:62:ASP:OD2	2.48	0.46
3:H:47:TRP:HZ2	3:H:50:TRP:HD1	1.64	0.46
6:R:92:ASP:OD1	6:R:92:ASP:N	2.48	0.46
2:F:617:ARG:HB2	2:F:622:ILE:HD11	1.98	0.46
1:B:35:TRP:CD1	2:E:609:PRO:HA	2.50	0.46
3:I:10:GLU:HG3	3:I:18:VAL:HG23	1.98	0.46
3:I:40:ALA:HB3	3:I:43:GLN:HB2	1.98	0.45
6:P:66(A):ASP:HB3	9:X:5:MAN:H2	1.98	0.45
6:R:14:ALA:HA	6:R:107:LEU:HB2	1.98	0.45
1:B:98:ASN:OD1	1:B:99:ASN:N	2.50	0.45
1:B:131:CYS:HA	1:B:157:CYS:HA	1.98	0.45
1:C:98:ASN:OD1	1:C:99:ASN:N	2.50	0.45
2:D:617:ARG:HB2	2:D:622:ILE:HD11	1.99	0.45
4:L:92:SER:OG	4:L:93:TYR:N	2.49	0.45
1:A:502:LYS:HD3	1:A:502:LYS:HA	1.73	0.45
3:I:47:TRP:HZ2	3:I:50:TRP:HD1	1.64	0.45
1:B:185:ASN:O	1:B:186:GLU:HG3	2.16	0.45
3:G:47:TRP:HZ2	3:G:50:TRP:HD1	1.64	0.45
6:P:46:LEU:HD21	6:P:49:TYR:HB3	1.99	0.45
6:P:49:TYR:CD1	6:P:55:PRO:CA	2.98	0.45
4:J:33:ASN:OD1	4:J:34:TYR:N	2.50	0.45
1:B:181:ILE:HG23	1:B:191:TYR:HB3	1.99	0.45
4:L:101:LYS:HD2	4:L:101:LYS:HA	1.73	0.45
6:Q:46:LEU:HD21	6:Q:49:TYR:HB3	1.99	0.45
1:A:181:ILE:HG23	1:A:191:TYR:HB3	1.99	0.45
2:E:617:ARG:HB2	2:E:622:ILE:HD11	1.99	0.45
1:A:107:ASP:OD2	2:D:574:LYS:NZ	2.50	0.44
2:E:644:GLY:O	2:E:647:GLU:HG3	2.17	0.44
4:L:39:GLN:HE22	4:L:41:HIS:CE1	2.34	0.44
1:B:299:PRO:HD3	1:B:329:ALA:HA	1.98	0.44
1:C:181:ILE:HG23	1:C:191:TYR:HB3	1.99	0.44
3:I:90:TYR:O	3:I:106:GLY:HA2	2.16	0.44
4:K:2:SER:OG	4:K:3:ALA:N	2.49	0.44
1:B:166:ARG:HH21	1:C:169:ARG:HH12	1.64	0.44
2:F:655:LYS:HA	2:F:655:LYS:HD3	1.78	0.44
3:G:40:ALA:HB3	3:G:43:GLN:HB2	1.99	0.44
4:K:50:ILE:HG13	4:K:55:LYS:O	2.16	0.44
4:L:50:ILE:HG13	4:L:55:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB2	1:A:201:ILE:HG23	2.00	0.44
6:R:34:GLN:HG3	6:R:49:TYR:HA	1.99	0.44
1:C:503:ARG:HB3	2:F:607:ASN:OD1	2.17	0.44
1:A:299:PRO:HD3	1:A:329:ALA:HA	1.99	0.44
4:J:79:GLY:O	4:J:81:GLN:NE2	2.48	0.44
6:Q:52:GLN:O	6:Q:52:GLN:HG2	2.17	0.44
1:B:186:GLU:C	1:B:187:GLN:HA	2.38	0.44
1:C:107:ASP:OD2	2:F:574:LYS:NZ	2.50	0.44
5:N:18:LEU:HB2	5:N:82(C):VAL:HG21	1.99	0.44
6:Q:50:ASN:C	6:Q:52:GLN:H	2.19	0.44
3:H:90:TYR:O	3:H:106:GLY:HA2	2.18	0.43
1:C:299:PRO:HD3	1:C:329:ALA:HA	1.99	0.43
4:J:64:PHE:HB3	4:J:77:ILE:HA	1.99	0.43
4:K:6:GLN:NE2	4:K:89:TYR:HA	2.33	0.43
1:B:227:LYS:HE3	1:B:485:LYS:HE2	2.00	0.43
1:B:500:ARG:O	2:F:663:LEU:HD23	2.19	0.43
5:M:90:TYR:O	5:M:106:GLY:HA3	2.18	0.43
1:B:107:ASP:OD2	2:E:574:LYS:NZ	2.52	0.43
1:C:214:PRO:HB3	1:C:250:GLY:HA3	2.01	0.43
2:F:660:LEU:HA	2:F:663:LEU:HD12	2.01	0.43
4:L:37:TRP:HD1	4:L:50:ILE:HG23	1.82	0.43
1:C:122:LEU:HB2	1:C:201:ILE:HG23	2.00	0.43
9:X:3:BMA:H62	9:X:6:MAN:H2	1.85	0.43
3:H:98:LEU:H	3:H:98:LEU:HD12	1.83	0.43
5:N:57:ALA:HB1	5:N:59:TYR:CZ	2.54	0.43
1:A:98:ASN:OD1	1:A:99:ASN:N	2.51	0.43
1:A:313:PRO:HB3	1:B:196:CYS:HB2	2.01	0.43
1:C:186:GLU:C	1:C:187:GLN:HA	2.39	0.43
1:C:227:LYS:HE3	1:C:485:LYS:HE2	2.00	0.43
2:D:655:LYS:NZ	2:F:601:LYS:HG3	2.34	0.43
2:E:655:LYS:HA	2:E:655:LYS:HD3	1.66	0.43
1:A:35:TRP:CD1	2:D:609:PRO:HA	2.54	0.42
1:A:227:LYS:HE3	1:A:485:LYS:HE2	2.00	0.42
4:K:6:GLN:NE2	4:K:99:GLY:H	2.17	0.42
1:A:162:THR:O	1:A:170:GLN:NE2	2.53	0.42
1:B:103:GLN:HE21	2:E:574:LYS:NZ	2.17	0.42
4:L:13:SER:HB2	4:L:16:GLN:HE21	1.84	0.42
5:M:87:THR:HG22	5:M:110:THR:HA	2.00	0.42
5:O:84:PRO:HA	5:O:111:VAL:HB	2.00	0.42
1:A:52:LEU:H	1:A:103:GLN:HE22	1.68	0.42
1:A:503:ARG:HB3	2:D:607:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PRO:HB3	1:B:250:GLY:HA3	2.01	0.42
1:B:321(A):ASP:OD1	1:B:321(A):ASP:N	2.53	0.42
2:D:644:GLY:O	2:D:647:GLU:HG3	2.20	0.42
2:F:596:TRP:NE1	2:F:647:GLU:HB3	2.35	0.42
4:K:37:TRP:HD1	4:K:50:ILE:HG23	1.83	0.42
5:M:36:TRP:CH2	5:M:92:CYS:HB2	2.54	0.42
4:J:17:SER:HA	4:J:77:ILE:O	2.19	0.42
1:A:169:ARG:HH12	1:C:166:ARG:HH21	1.66	0.42
2:E:611:ASN:OD1	2:E:612:SER:N	2.53	0.42
3:H:38:ARG:HG2	3:H:46:GLU:HB3	2.02	0.42
7:Y:1:NAG:H61	7:Y:2:NAG:HN2	1.84	0.42
1:C:163:THR:HG23	1:C:165:LEU:H	1.84	0.42
1:C:490:LYS:HE2	2:F:585:ARG:NH2	2.35	0.42
1:A:186:GLU:O	1:A:186(A):ASN:ND2	2.49	0.42
1:A:214:PRO:HB3	1:A:250:GLY:HA3	2.02	0.42
5:M:30:ASN:OD1	5:M:30:ASN:N	2.53	0.42
1:A:298:ARG:NH2	1:A:441:GLY:O	2.53	0.42
1:C:201:ILE:HD11	1:C:435:TYR:HB2	2.01	0.42
1:A:490:LYS:HE2	2:D:585:ARG:NH2	2.35	0.42
5:M:30:ASN:ND2	5:M:31:ASN:OD1	2.53	0.42
5:N:63:LEU:HD23	5:N:63:LEU:HA	1.91	0.42
1:C:61:TYR:HD2	1:C:64:LYS:HB3	1.85	0.41
1:A:103:GLN:HE21	2:D:574:LYS:NZ	2.17	0.41
1:A:186:GLU:C	1:A:187:GLN:HA	2.40	0.41
1:C:35:TRP:CD1	2:F:609:PRO:HA	2.55	0.41
5:M:47:TRP:HB2	6:P:98:PHE:HE1	1.86	0.41
1:A:255:VAL:HG13	1:A:475:MET:SD	2.61	0.41
2:D:592:LEU:HD23	2:D:592:LEU:HA	1.90	0.41
6:Q:92:ASP:OD1	6:Q:92:ASP:N	2.48	0.41
1:B:313:PRO:HB3	1:C:196:CYS:HB2	2.01	0.41
2:D:653:GLN:O	2:D:657:GLU:HG2	2.21	0.41
4:J:56:ARG:NH2	4:J:65:SER:HB2	2.36	0.41
4:K:17:SER:HA	4:K:77:ILE:O	2.20	0.41
4:K:33:ASN:OD1	4:K:34:TYR:N	2.53	0.41
2:F:607:ASN:HB2	2:F:650:GLN:NE2	2.35	0.41
3:G:98:LEU:HD11	4:J:51:TYR:CE1	2.56	0.41
1:C:52:LEU:H	1:C:103:GLN:HE22	1.68	0.41
1:C:103:GLN:HE21	2:F:574:LYS:NZ	2.17	0.41
4:J:28:ASP:N	4:J:28:ASP:OD1	2.53	0.41
5:O:20:VAL:HB	5:O:80:LEU:HD21	2.03	0.41
2:F:545:LEU:HD12	2:F:545:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:38:ARG:HG2	3:I:46:GLU:HB3	2.02	0.41
2:F:637:ASN:OD1	2:F:637:ASN:N	2.53	0.41
3:G:38:ARG:HG2	3:G:46:GLU:HB3	2.03	0.41
6:R:58:ILE:CG2	6:R:59:PRO:HD2	2.50	0.41
6:R:62:PHE:HD1	6:R:75:ILE:HG12	1.86	0.41
1:B:163:THR:HG23	1:B:165:LEU:H	1.86	0.41
1:C:121:LYS:HE2	1:C:121:LYS:HB3	1.93	0.41
4:L:6:GLN:NE2	4:L:89:TYR:HA	2.34	0.41
5:N:30:ASN:OD1	5:N:30:ASN:N	2.54	0.41
6:Q:54:ARG:NE	6:Q:54:ARG:HA	2.36	0.41
1:A:332:ASN:HD22	9:X:1:NAG:H83	1.86	0.40
1:B:131:CYS:HB2	1:B:191:TYR:CD2	2.56	0.40
2:D:611:ASN:OD1	2:D:612:SER:N	2.55	0.40
1:A:124:PRO:HA	1:C:166:ARG:HD3	2.03	0.40
3:I:10:GLU:HB2	3:I:109:VAL:HG12	2.02	0.40
6:P:54:ARG:H	6:P:54:ARG:CD	2.33	0.40
1:A:325:ASP:OD1	1:A:325:ASP:N	2.52	0.40
1:B:45:TRP:HB2	1:B:489:VAL:HG22	2.03	0.40
1:B:162:THR:O	1:B:170:GLN:NE2	2.54	0.40
5:N:35:THR:HA	5:N:50:TYR:HA	2.04	0.40
1:B:52:LEU:H	1:B:103:GLN:HE22	1.69	0.40
1:C:225:ILE:HD12	1:C:247:CYS:HA	2.03	0.40
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.93	0.40
4:L:17:SER:HA	4:L:77:ILE:O	2.22	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	443/451 (98%)	426 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	443/451 (98%)	424 (96%)	19 (4%)	0	100	100
1	C	443/451 (98%)	424 (96%)	19 (4%)	0	100	100
2	D	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
2	E	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
2	F	125/129 (97%)	121 (97%)	4 (3%)	0	100	100
3	G	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
3	H	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
3	I	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
4	J	103/106 (97%)	92 (89%)	11 (11%)	0	100	100
4	K	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
4	L	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
5	M	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
5	N	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
5	O	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
6	P	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
6	Q	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
6	R	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	3090/3153 (98%)	2951 (96%)	139 (4%)	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	A	401/403 (100%)	401 (100%)	0	100	100
1	B	401/403 (100%)	400 (100%)	1 (0%)	92	96
1	C	401/403 (100%)	401 (100%)	0	100	100
2	D	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	112/112 (100%)	112 (100%)	0	100	100
2	F	112/112 (100%)	112 (100%)	0	100	100
3	G	101/101 (100%)	100 (99%)	1 (1%)	73	83
3	H	101/101 (100%)	100 (99%)	1 (1%)	73	83
3	I	101/101 (100%)	100 (99%)	1 (1%)	73	83
4	J	87/88 (99%)	87 (100%)	0	100	100
4	K	87/88 (99%)	86 (99%)	1 (1%)	70	81
4	L	87/88 (99%)	86 (99%)	1 (1%)	70	81
5	M	116/116 (100%)	116 (100%)	0	100	100
5	N	116/116 (100%)	116 (100%)	0	100	100
5	O	116/116 (100%)	116 (100%)	0	100	100
6	P	85/85 (100%)	83 (98%)	2 (2%)	44	66
6	Q	85/85 (100%)	85 (100%)	0	100	100
6	R	85/85 (100%)	84 (99%)	1 (1%)	67	80
All	All	2706/2715 (100%)	2697 (100%)	9 (0%)	90	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	501	CYS
3	G	13	LYS
3	H	13	LYS
3	I	13	LYS
4	K	8	ARG
4	L	8	ARG
6	P	54	ARG
6	P	58	ILE
6	R	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	105	HIS
1	A	186(A)	ASN
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	280	ASN
1	A	411	ASN
1	A	428	GLN
1	B	103	GLN
1	B	105	HIS
1	B	258	GLN
1	B	280	ASN
1	B	411	ASN
1	B	428	GLN
1	C	103	GLN
1	C	105	HIS
1	C	258	GLN
1	C	280	ASN
1	C	411	ASN
1	C	428	GLN
2	D	625	ASN
2	D	650	GLN
2	E	650	GLN
2	F	625	ASN
2	F	650	GLN
3	H	39	GLN
3	H	105	GLN
3	I	1	GLN
4	J	6	GLN
4	J	16	GLN
4	J	40	GLN
4	J	41	HIS
4	K	6	GLN
4	K	16	GLN
4	K	40	GLN
4	L	6	GLN
4	L	16	GLN
4	L	40	GLN
4	L	41	HIS
5	M	82(A)	ASN
5	O	64	ASN
6	P	52	GLN
6	P	66(C)	ASN
6	Q	66(C)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

71 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	7,1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	S	2	7	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	T	1	7,1	14,14,15	0.18	0	17,19,21	0.42	0
7	NAG	T	2	7	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	U	1	8,1	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	U	2	8	14,14,15	0.23	0	17,19,21	0.43	0
8	BMA	U	3	8	11,11,12	0.58	0	15,15,17	0.72	0
8	MAN	U	4	8	11,11,12	0.63	0	15,15,17	1.01	2 (13%)
8	MAN	U	5	8	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
7	NAG	V	1	7,1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	V	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	W	1	7,1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	W	2	7	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	X	1	9,1	14,14,15	0.15	0	17,19,21	0.43	0
9	NAG	X	2	9	14,14,15	0.22	0	17,19,21	0.43	0
9	BMA	X	3	9	11,11,12	0.55	0	15,15,17	0.74	0
9	MAN	X	4	9	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
9	MAN	X	5	9	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
9	MAN	X	6	9	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
9	MAN	X	7	9	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
7	NAG	Y	1	7,1	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Y	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	Z	1	7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	Z	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	a	1	7,1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	a	2	7	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	b	1	7,1	14,14,15	0.19	0	17,19,21	0.42	0
7	NAG	b	2	7	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	c	1	8,1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	c	2	8	14,14,15	0.22	0	17,19,21	0.43	0
8	BMA	c	3	8	11,11,12	0.58	0	15,15,17	0.72	0
8	MAN	c	4	8	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
8	MAN	c	5	8	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
7	NAG	d	1	7,1	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	d	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	e	1	7,1	14,14,15	0.23	0	17,19,21	0.47	0
7	NAG	e	2	7	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	f	1	10,1	14,14,15	0.16	0	17,19,21	0.43	0
10	NAG	f	2	10	14,14,15	0.22	0	17,19,21	0.44	0
10	BMA	f	3	10	11,11,12	0.55	0	15,15,17	0.74	0
10	MAN	f	4	10	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
10	MAN	f	5	10	11,11,12	0.68	0	15,15,17	1.01	2 (13%)
10	MAN	f	6	10	11,11,12	0.23	0	15,15,17	0.47	0
7	NAG	g	1	7,1	14,14,15	0.26	0	17,19,21	0.47	0
7	NAG	g	2	7	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	h	1	7	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	h	2	7	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	i	1	7,1	14,14,15	0.25	0	17,19,21	0.45	0
7	NAG	i	2	7	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	j	1	7,1	14,14,15	0.18	0	17,19,21	0.42	0
7	NAG	j	2	7	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	k	1	8,1	14,14,15	0.23	0	17,19,21	0.46	0
8	NAG	k	2	8	14,14,15	0.22	0	17,19,21	0.43	0
8	BMA	k	3	8	11,11,12	0.59	0	15,15,17	0.73	0
8	MAN	k	4	8	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
8	MAN	k	5	8	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
7	NAG	l	1	7,1	14,14,15	0.23	0	17,19,21	0.48	0
7	NAG	l	2	7	14,14,15	0.20	0	17,19,21	0.45	0
7	NAG	m	1	7,1	14,14,15	0.23	0	17,19,21	0.48	0
7	NAG	m	2	7	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	n	1	9,1	14,14,15	0.18	0	17,19,21	0.43	0
9	NAG	n	2	9	14,14,15	0.21	0	17,19,21	0.43	0
9	BMA	n	3	9	11,11,12	0.53	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	n	4	9	11,11,12	0.66	0	15,15,17	0.94	2 (13%)
9	MAN	n	5	9	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
9	MAN	n	6	9	11,11,12	0.57	0	15,15,17	1.04	2 (13%)
9	MAN	n	7	9	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
7	NAG	o	1	7,1	14,14,15	0.25	0	17,19,21	0.46	0
7	NAG	o	2	7	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	p	1	7,1	14,14,15	0.28	0	17,19,21	0.47	0
7	NAG	p	2	7	14,14,15	0.28	0	17,19,21	0.51	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
7	NAG	S	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	T	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
8	NAG	U	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	2/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	U	5	8	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	V	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	NAG	W	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	1/1/5/7	2/6/23/26	0/1/1/1
9	NAG	X	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	1/2/19/22	0/1/1/1
9	MAN	X	4	9	-	0/2/19/22	0/1/1/1
9	MAN	X	5	9	-	1/2/19/22	0/1/1/1
9	MAN	X	6	9	1/1/4/5	0/2/19/22	0/1/1/1
9	MAN	X	7	9	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	Y	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	Z	1	7	-	4/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	n	3	9	-	1/2/19/22	0/1/1/1
9	MAN	n	4	9	-	0/2/19/22	0/1/1/1
9	MAN	n	5	9	-	1/2/19/22	0/1/1/1
9	MAN	n	6	9	1/1/4/5	2/2/19/22	0/1/1/1
9	MAN	n	7	9	-	0/2/19/22	0/1/1/1
7	NAG	o	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	p	1	7,1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	p	2	7	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	6	MAN	C1-O5-C5	2.63	115.70	112.19
9	n	7	MAN	C1-O5-C5	2.47	115.50	112.19
8	k	5	MAN	C1-O5-C5	2.46	115.48	112.19
9	n	5	MAN	C1-O5-C5	2.44	115.46	112.19
10	f	5	MAN	C1-O5-C5	2.40	115.41	112.19
9	X	7	MAN	C1-O5-C5	2.39	115.39	112.19
8	U	5	MAN	C1-O5-C5	2.36	115.36	112.19
8	k	4	MAN	C1-O5-C5	2.36	115.34	112.19
8	c	4	MAN	C1-O5-C5	2.35	115.34	112.19
8	U	4	MAN	C1-O5-C5	2.34	115.33	112.19
8	c	5	MAN	C1-O5-C5	2.33	115.30	112.19
9	X	5	MAN	C1-O5-C5	2.32	115.29	112.19
9	n	4	MAN	C1-O5-C5	2.25	115.20	112.19
10	f	4	MAN	C1-O5-C5	2.25	115.20	112.19
8	U	4	MAN	O2-C2-C3	-2.24	105.51	110.15
8	c	4	MAN	O2-C2-C3	-2.24	105.51	110.15
9	X	4	MAN	C1-O5-C5	2.24	115.19	112.19
9	X	4	MAN	O2-C2-C3	-2.24	105.52	110.15
9	n	6	MAN	O2-C2-C3	-2.22	105.55	110.15
9	n	4	MAN	O2-C2-C3	-2.22	105.55	110.15
8	k	4	MAN	O2-C2-C3	-2.21	105.57	110.15
9	X	6	MAN	C1-O5-C5	2.21	115.14	112.19
10	f	5	MAN	O2-C2-C3	-2.19	105.61	110.15
9	X	7	MAN	O2-C2-C3	-2.19	105.61	110.15
9	X	5	MAN	O2-C2-C3	-2.19	105.62	110.15
9	n	7	MAN	O2-C2-C3	-2.19	105.62	110.15
9	X	6	MAN	O2-C2-C3	-2.18	105.63	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	n	5	MAN	O2-C2-C3	-2.17	105.66	110.15
8	k	5	MAN	O2-C2-C3	-2.16	105.68	110.15
8	U	5	MAN	O2-C2-C3	-2.15	105.69	110.15
10	f	4	MAN	O2-C2-C3	-2.15	105.69	110.15
8	c	5	MAN	O2-C2-C3	-2.15	105.71	110.15

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	S	2	NAG	C1
7	W	2	NAG	C1
7	Y	2	NAG	C1
7	a	2	NAG	C1
7	e	2	NAG	C1
7	g	2	NAG	C1
7	m	2	NAG	C1
7	o	2	NAG	C1
7	p	1	NAG	C1
8	U	4	MAN	C1
8	U	5	MAN	C1
8	c	4	MAN	C1
8	c	5	MAN	C1
8	k	4	MAN	C1
9	X	6	MAN	C1
9	X	7	MAN	C1
9	n	6	MAN	C1
10	f	4	MAN	C1
10	f	5	MAN	C1

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	p	1	NAG	C3-C2-N2-C7
7	p	1	NAG	C8-C7-N2-C2
7	p	1	NAG	O7-C7-N2-C2
7	p	2	NAG	C3-C2-N2-C7
7	i	1	NAG	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	T	2	NAG	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
10	f	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
9	n	6	MAN	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	h	1	NAG	C8-C7-N2-C2
7	h	1	NAG	O7-C7-N2-C2
7	p	2	NAG	C8-C7-N2-C2
9	X	1	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
9	n	1	NAG	C8-C7-N2-C2
9	n	1	NAG	O7-C7-N2-C2
10	f	1	NAG	C8-C7-N2-C2
10	f	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6

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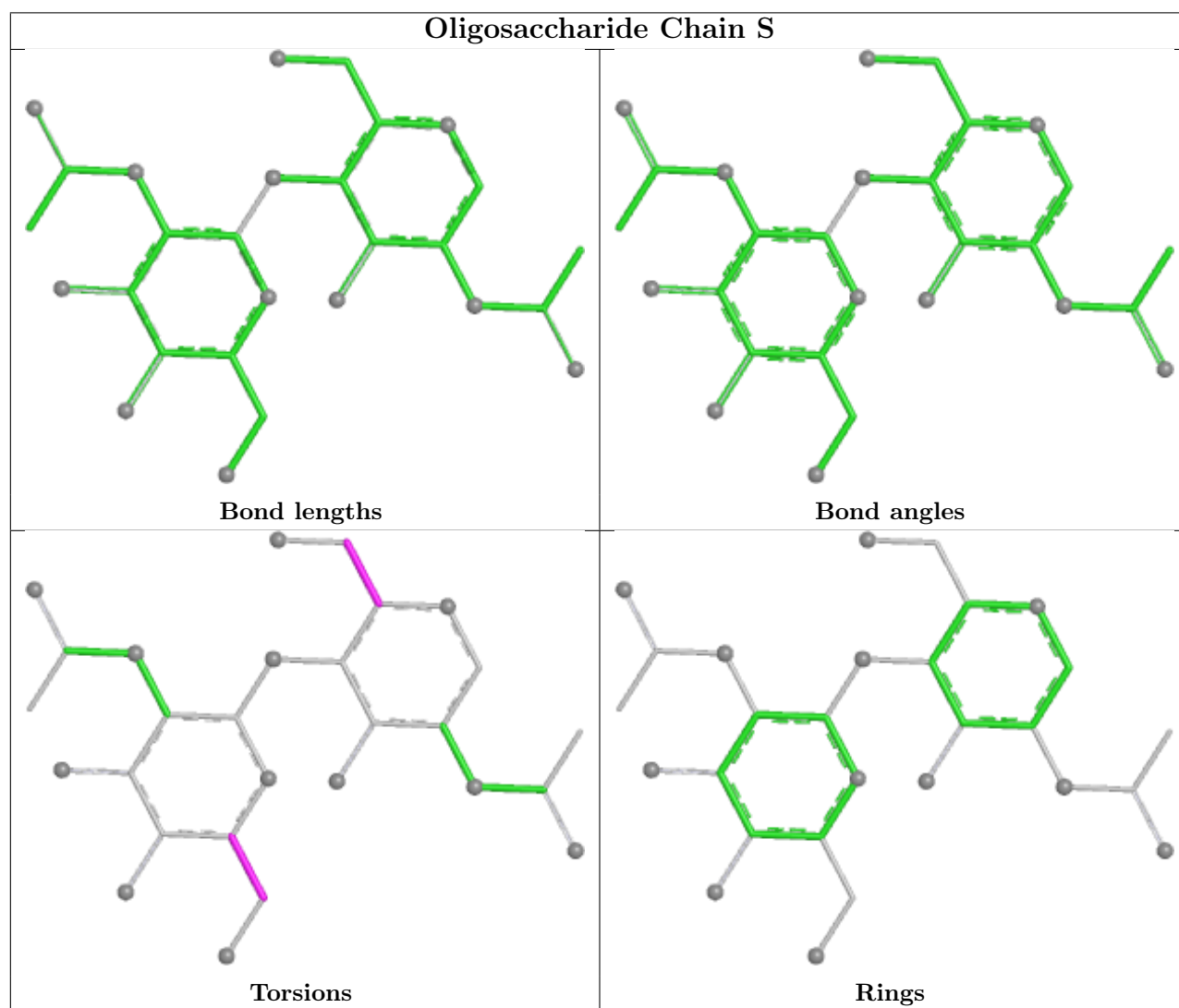
Mol	Chain	Res	Type	Atoms
9	n	5	MAN	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
7	p	2	NAG	O7-C7-N2-C2
7	e	2	NAG	O5-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
10	f	3	BMA	O5-C5-C6-O6
10	f	2	NAG	C4-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
9	X	5	MAN	O5-C5-C6-O6
9	n	3	BMA	O5-C5-C6-O6
10	f	1	NAG	C4-C5-C6-O6
8	c	2	NAG	C4-C5-C6-O6
9	X	1	NAG	C4-C5-C6-O6
10	f	1	NAG	O5-C5-C6-O6
9	X	1	NAG	O5-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
9	n	2	NAG	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
9	n	6	MAN	C4-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
7	a	2	NAG	C1-C2-N2-C7
7	W	2	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6

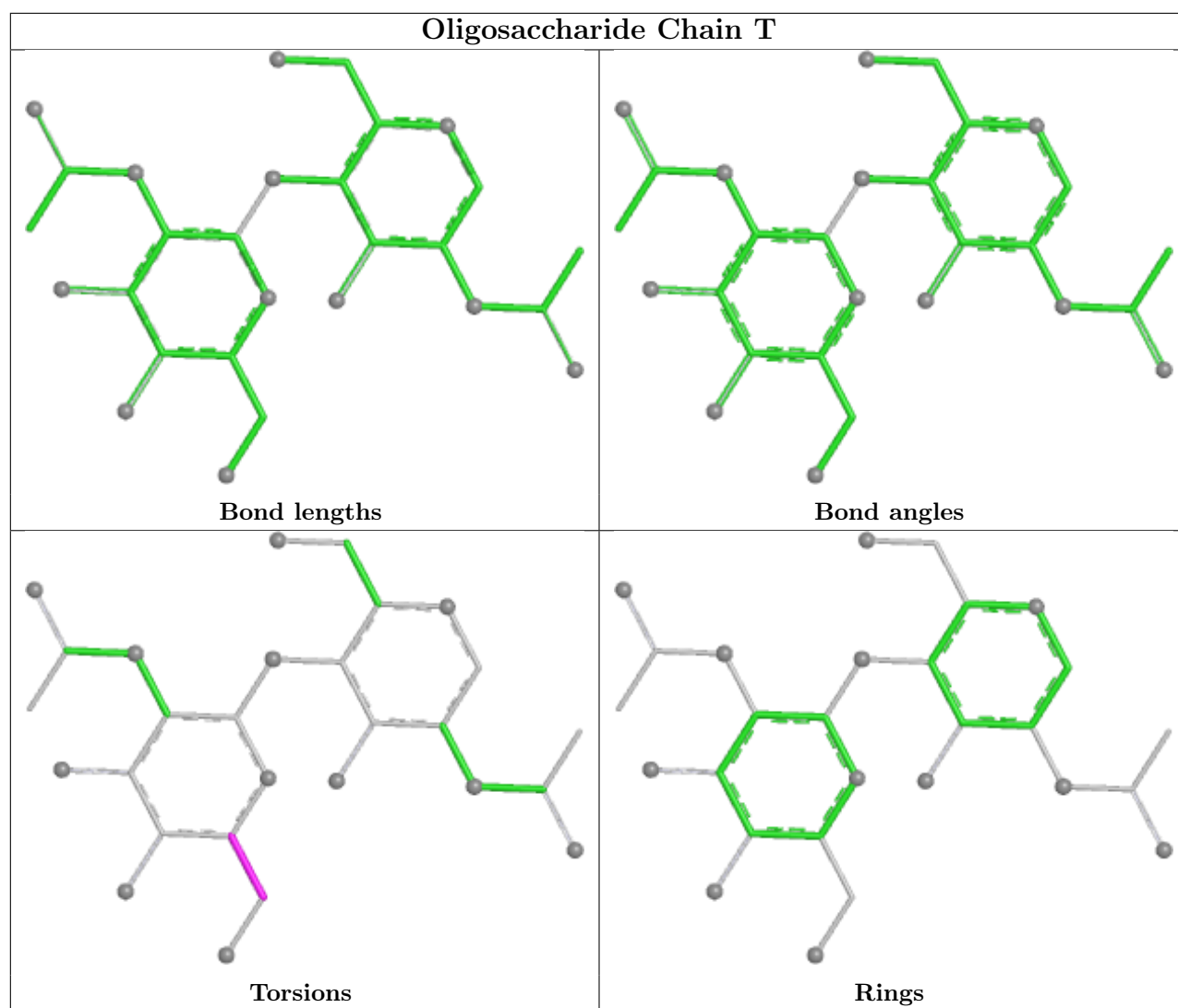
There are no ring outliers.

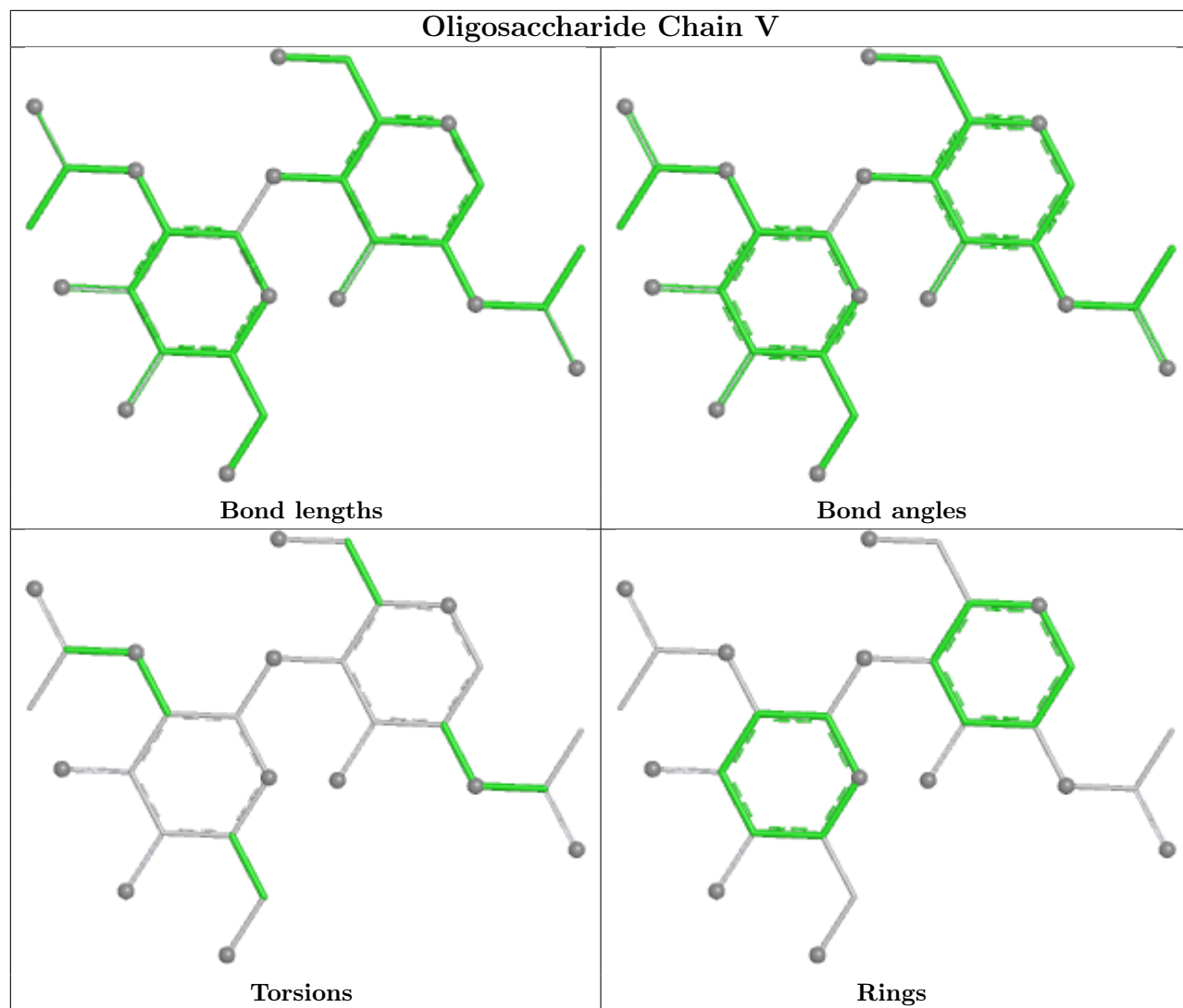
6 monomers are involved in 4 short contacts:

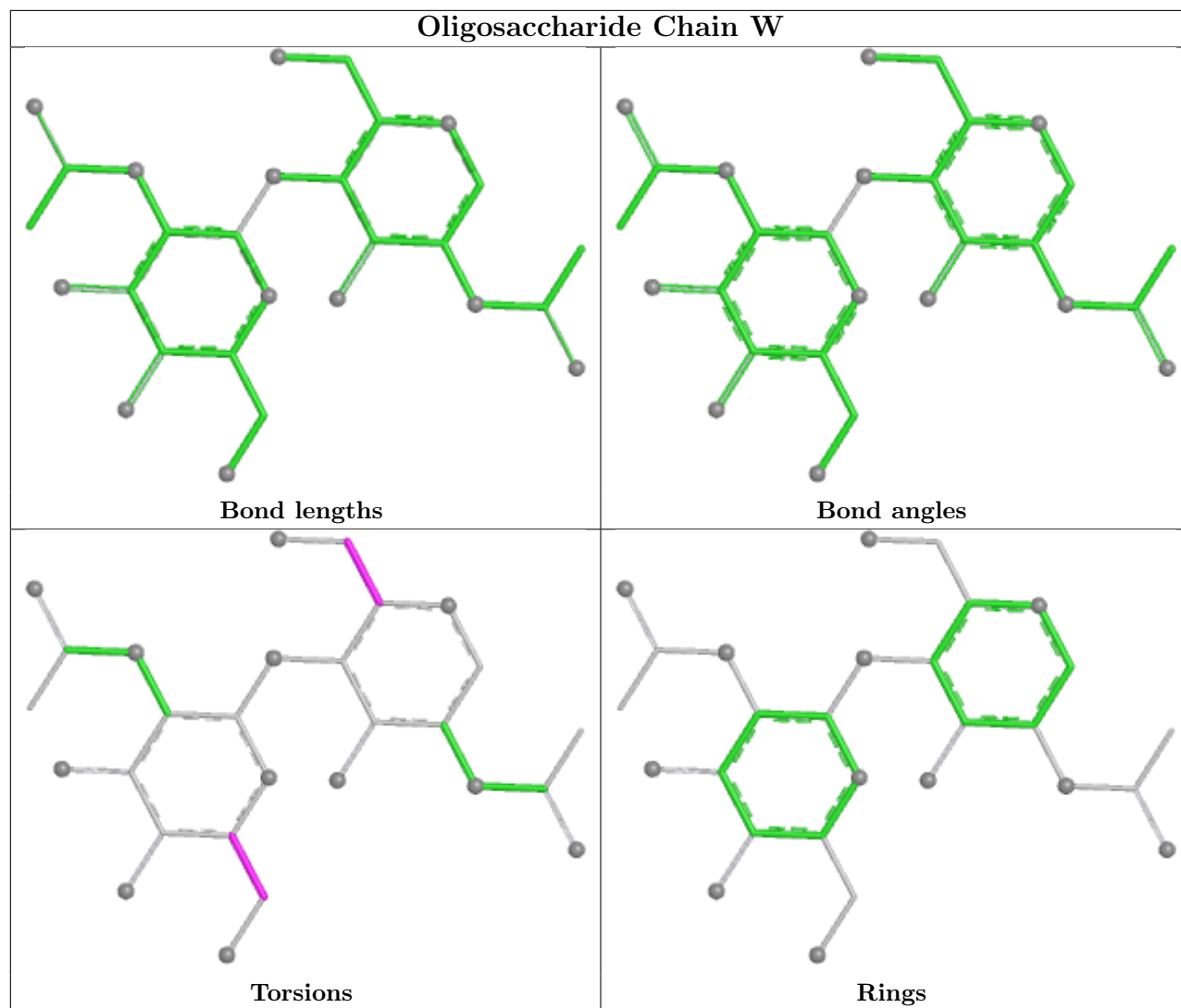
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	5	MAN	1	0
7	Y	1	NAG	1	0
9	X	3	BMA	1	0
7	Y	2	NAG	1	0
9	X	1	NAG	1	0
9	X	6	MAN	1	0

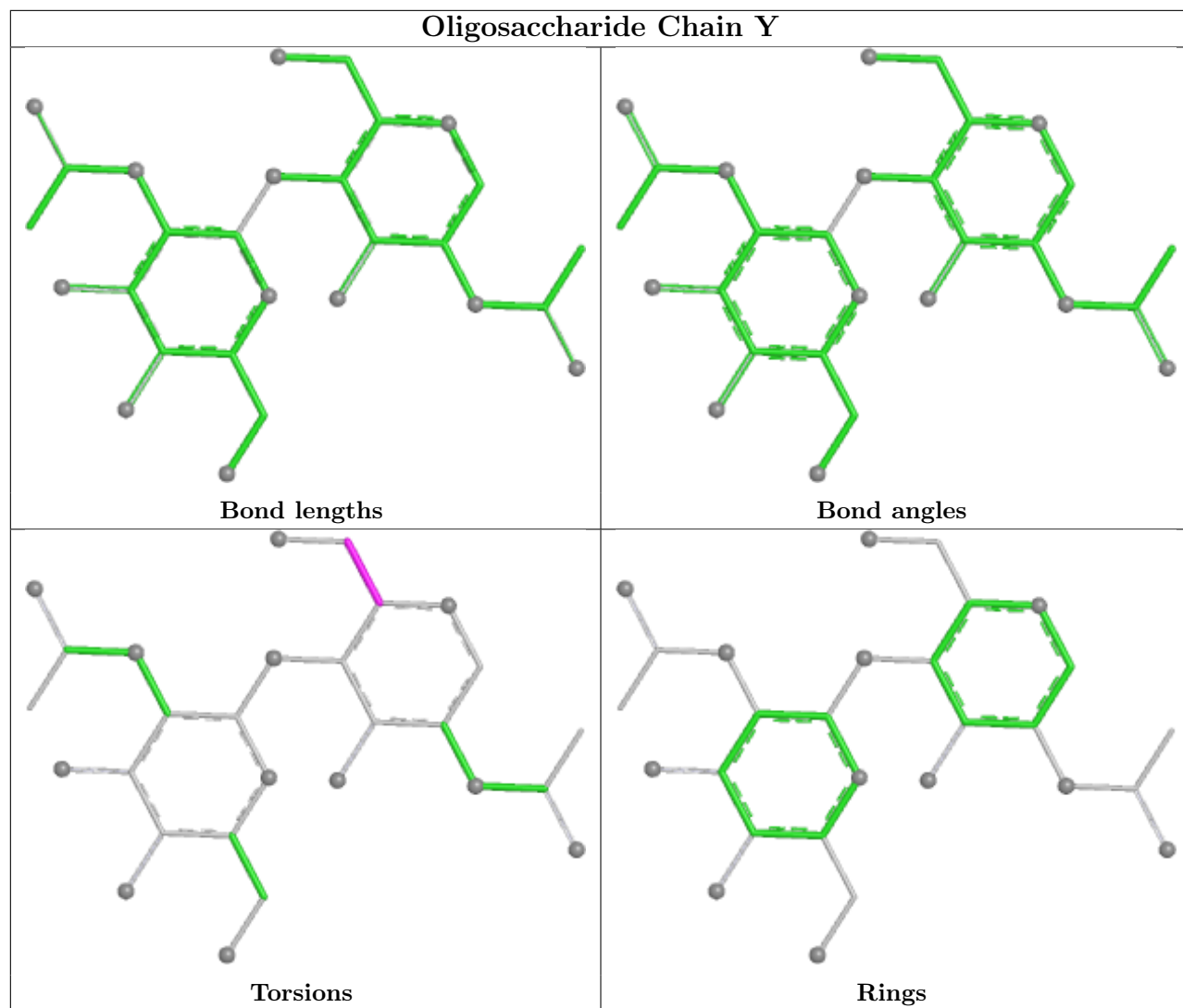
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

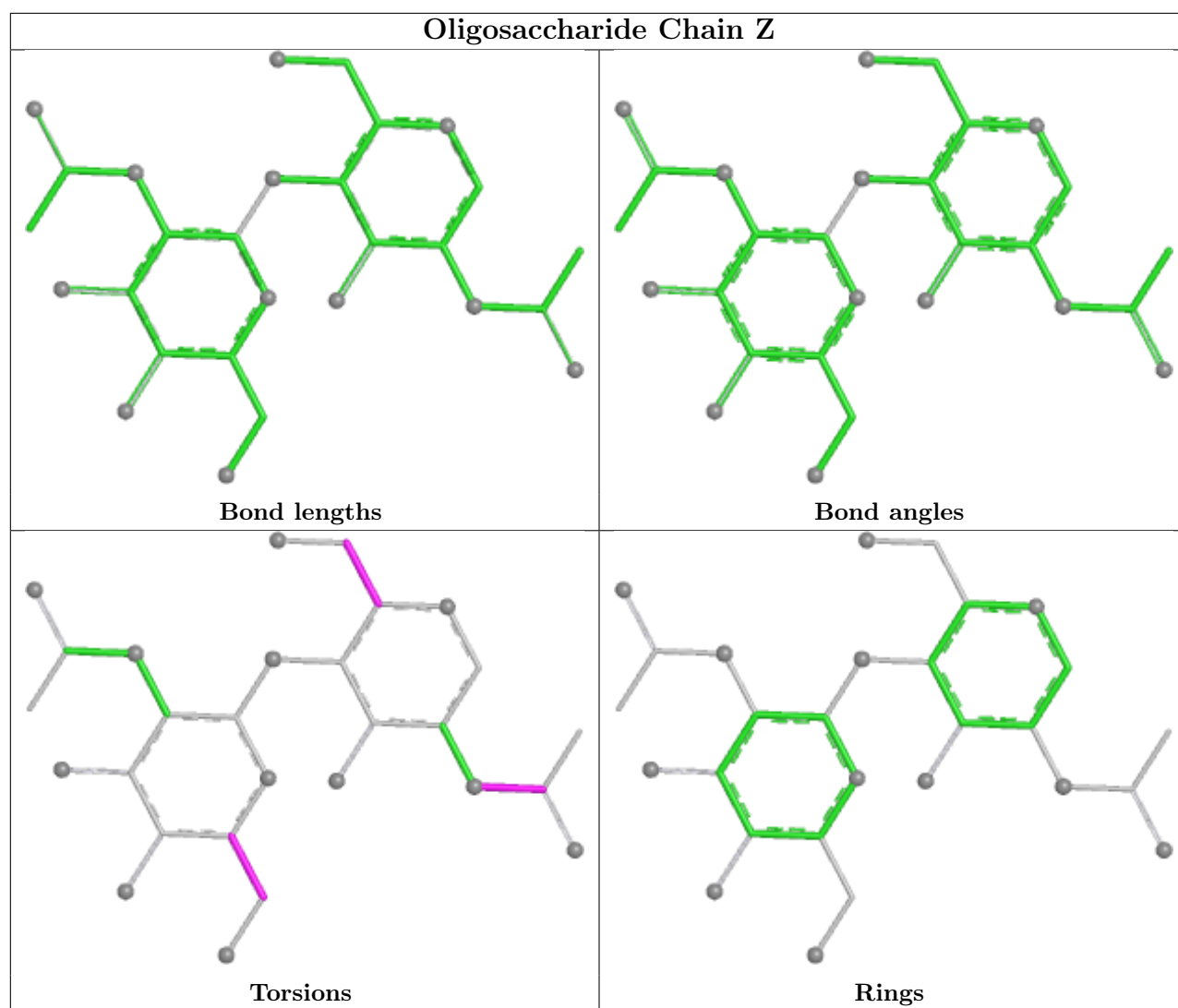


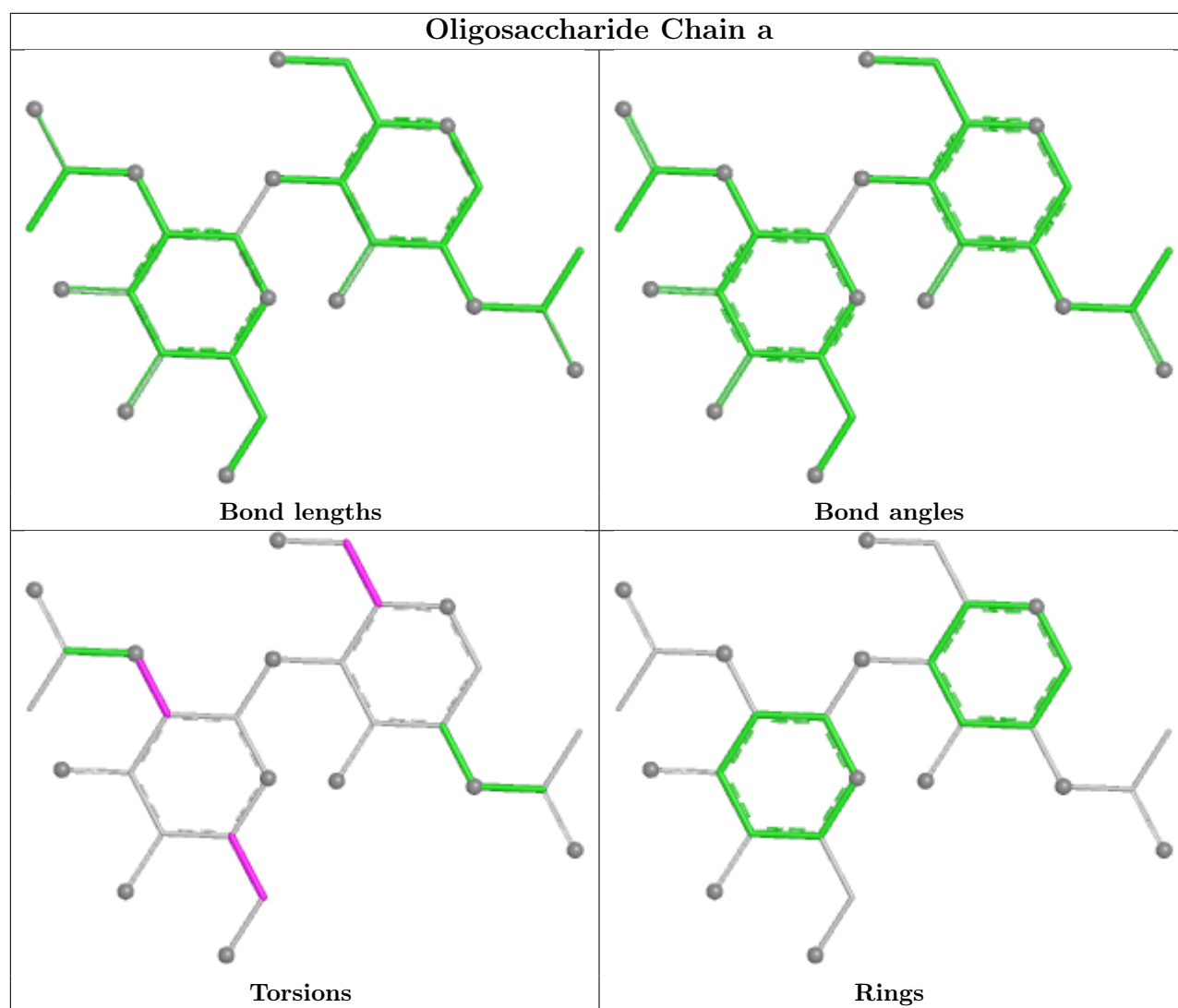


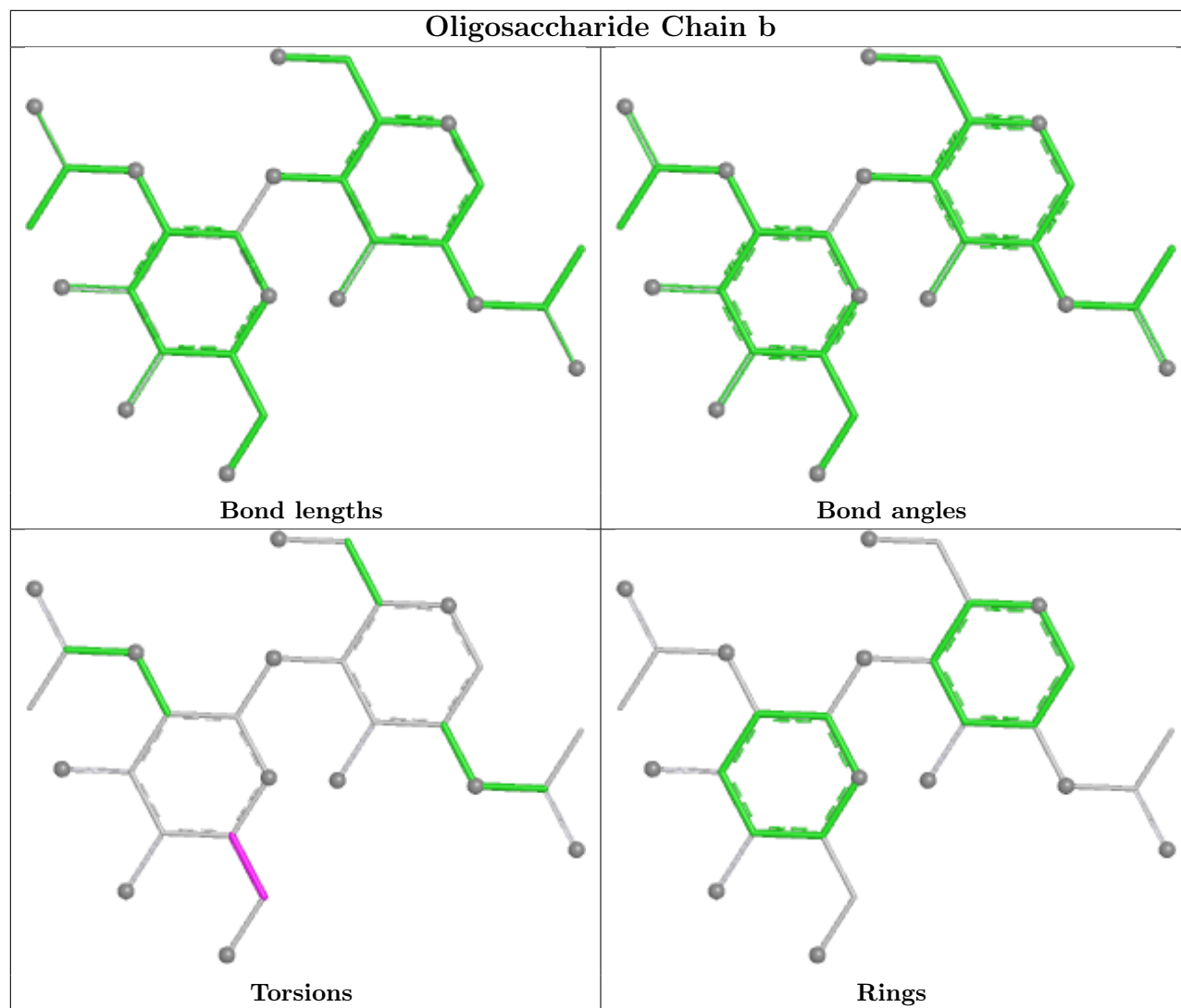


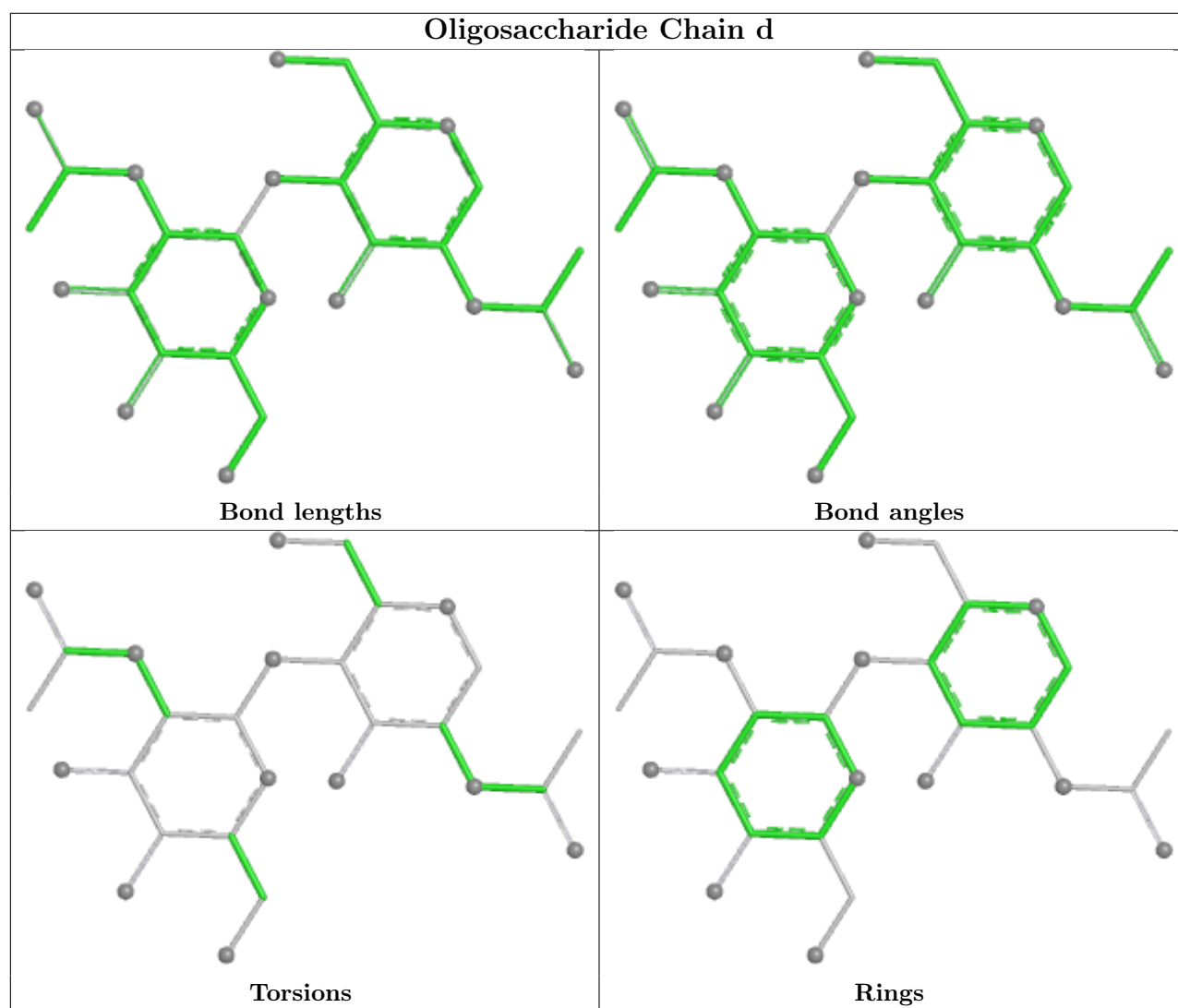


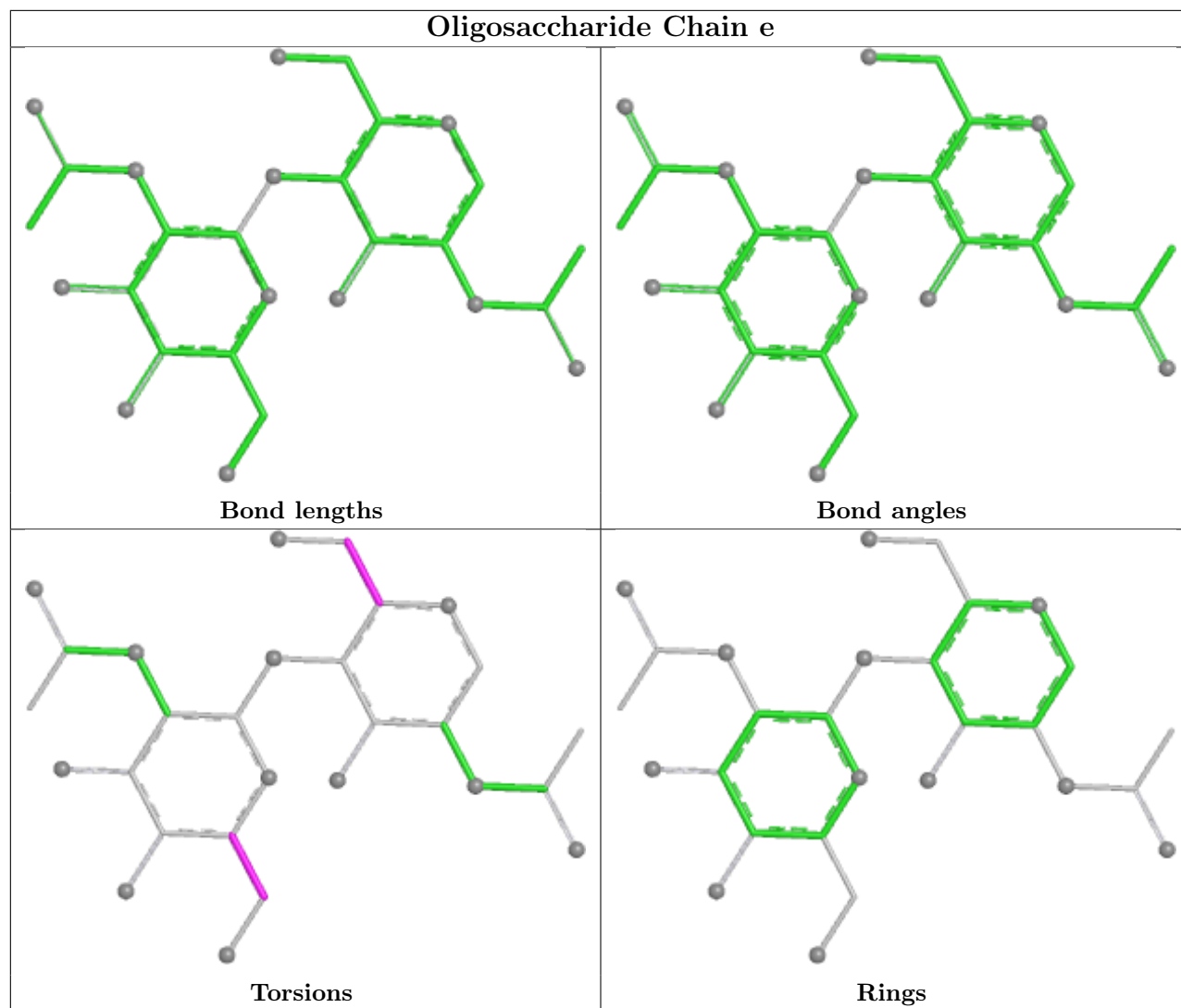


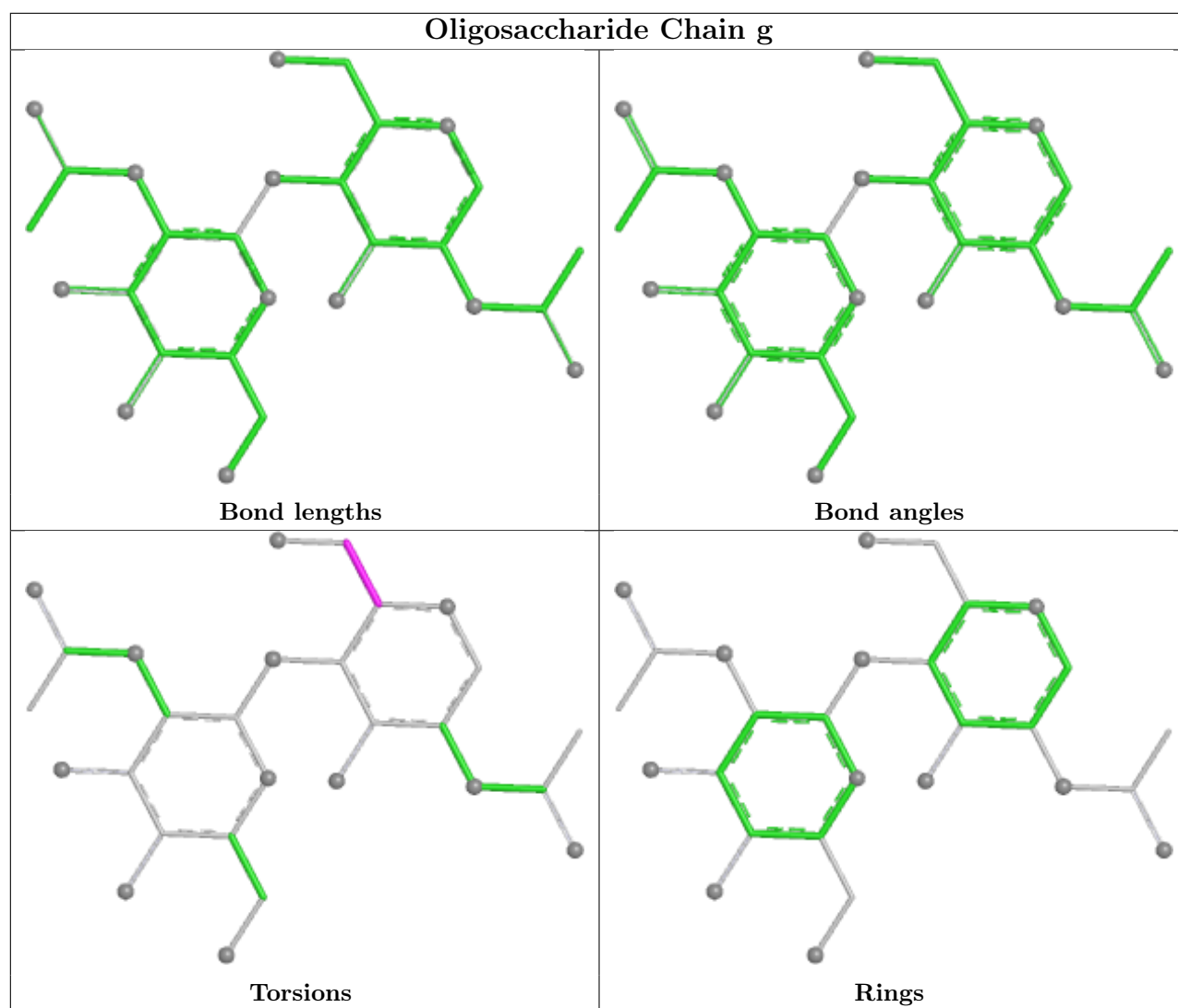


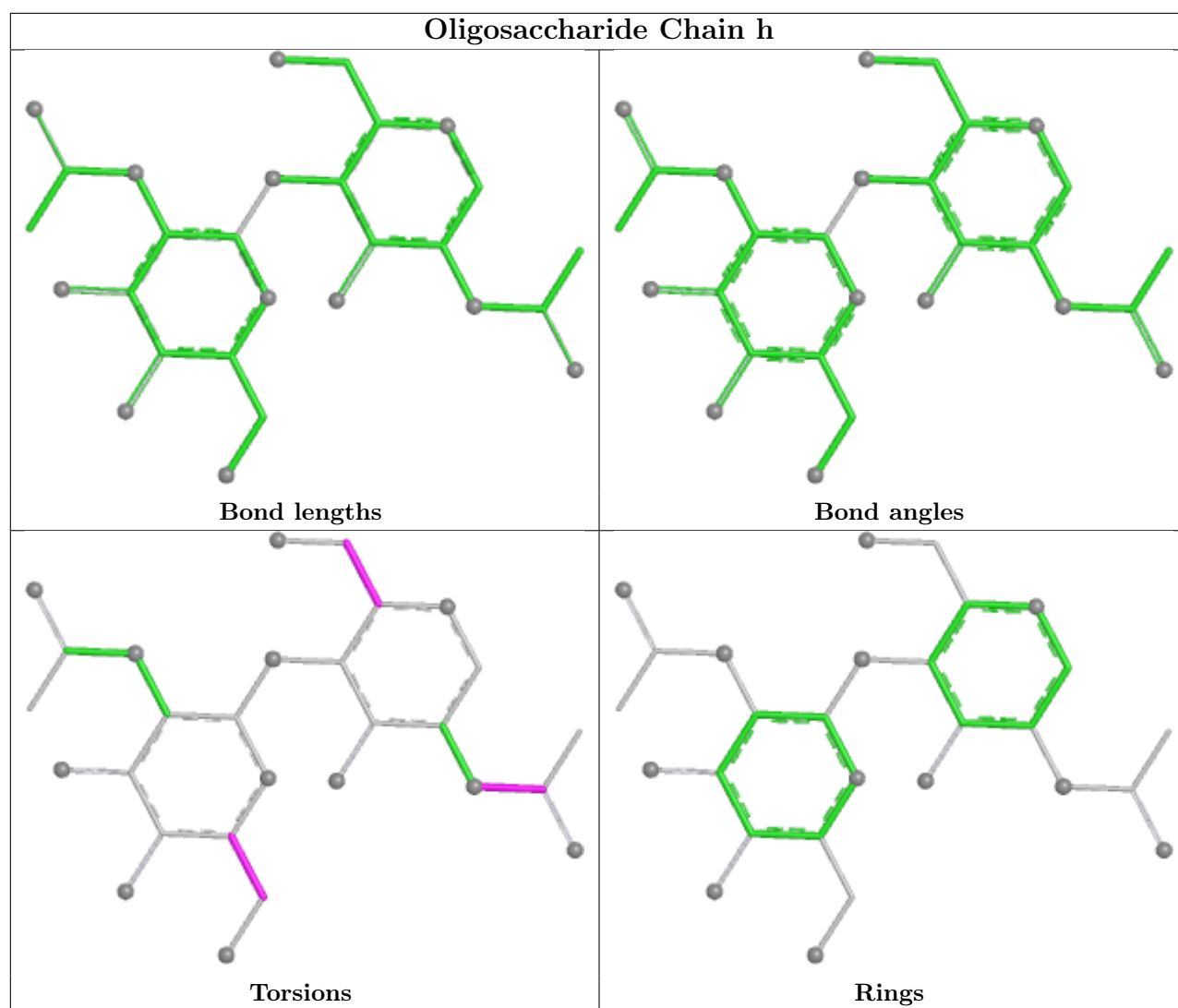


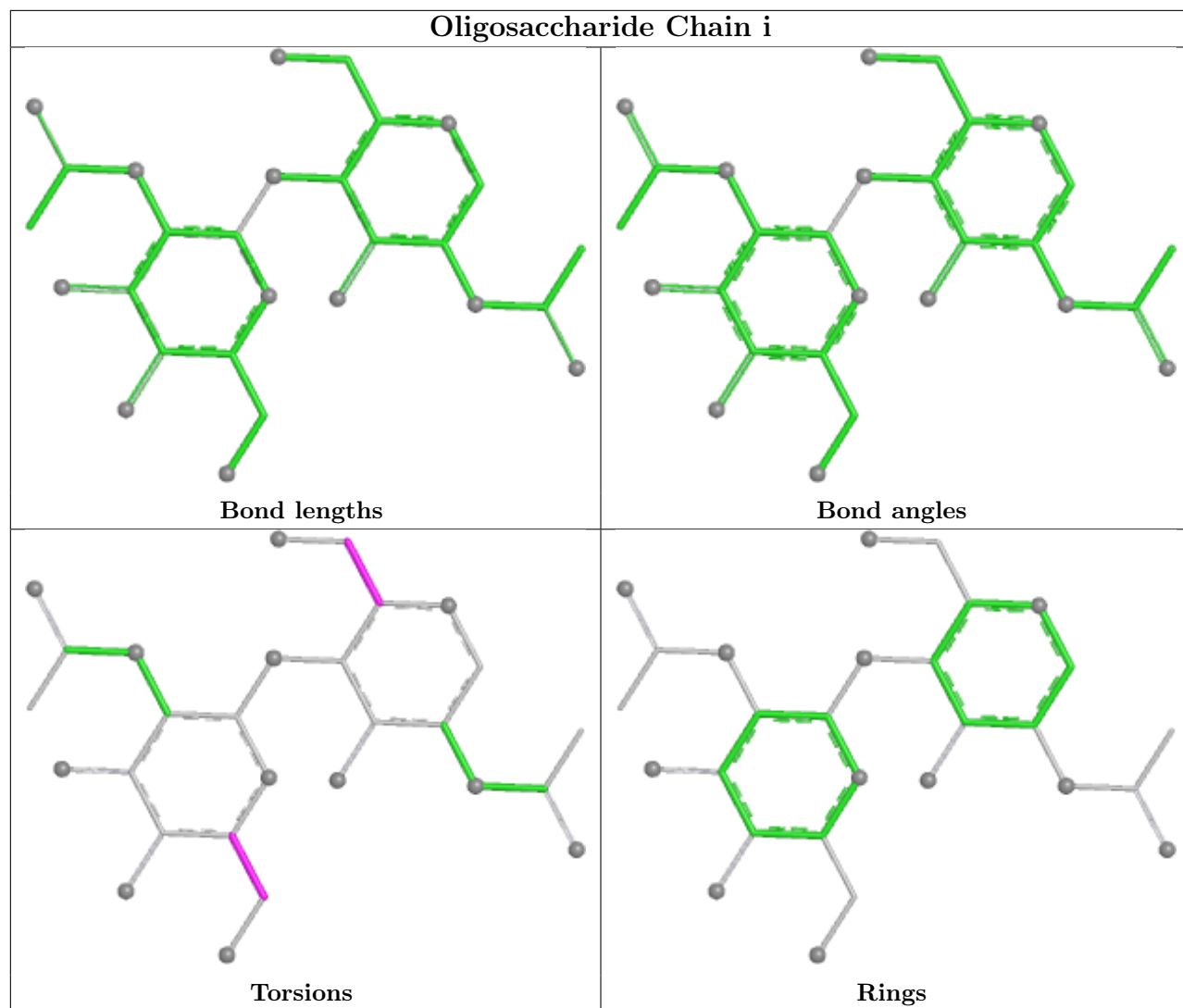


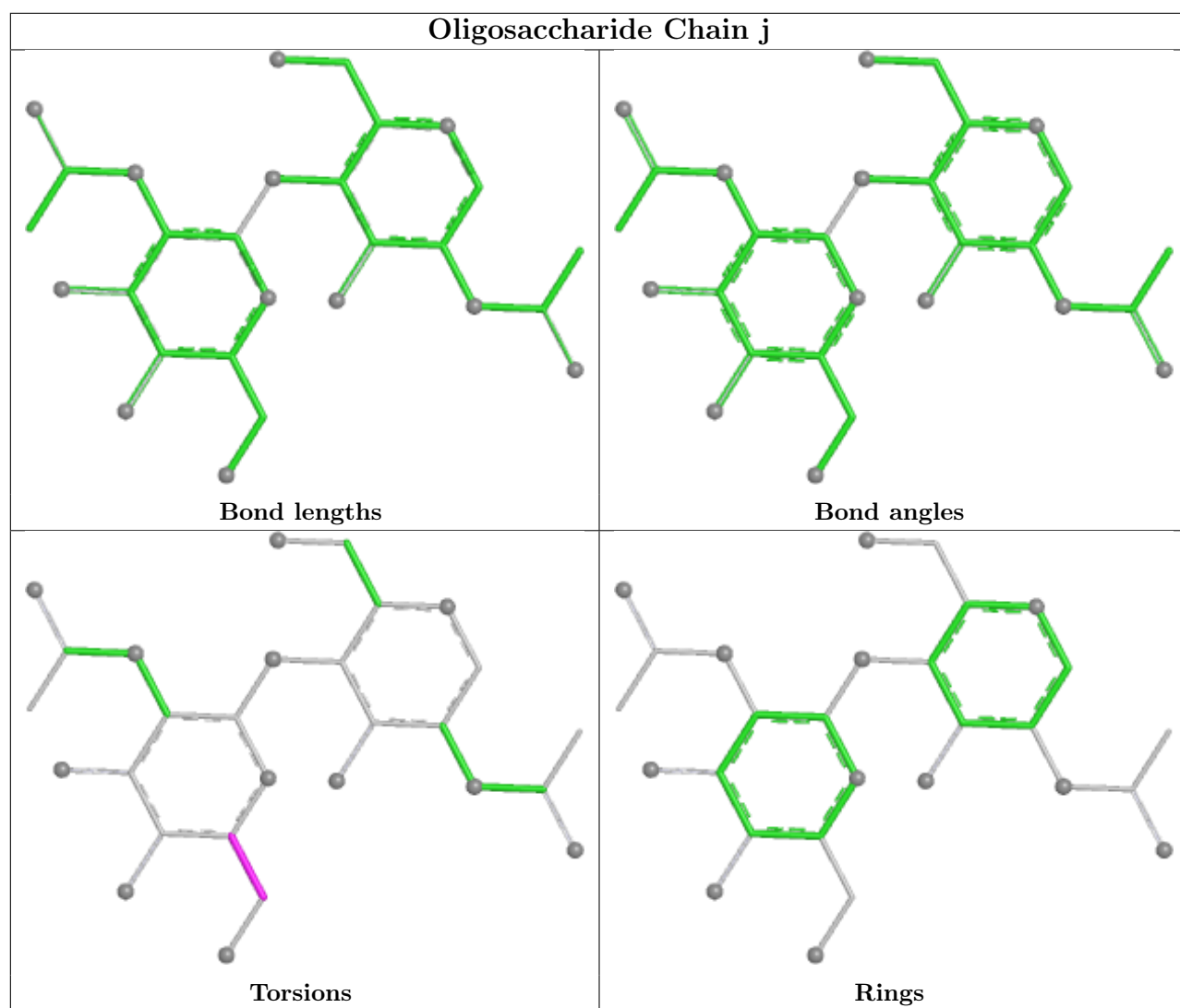


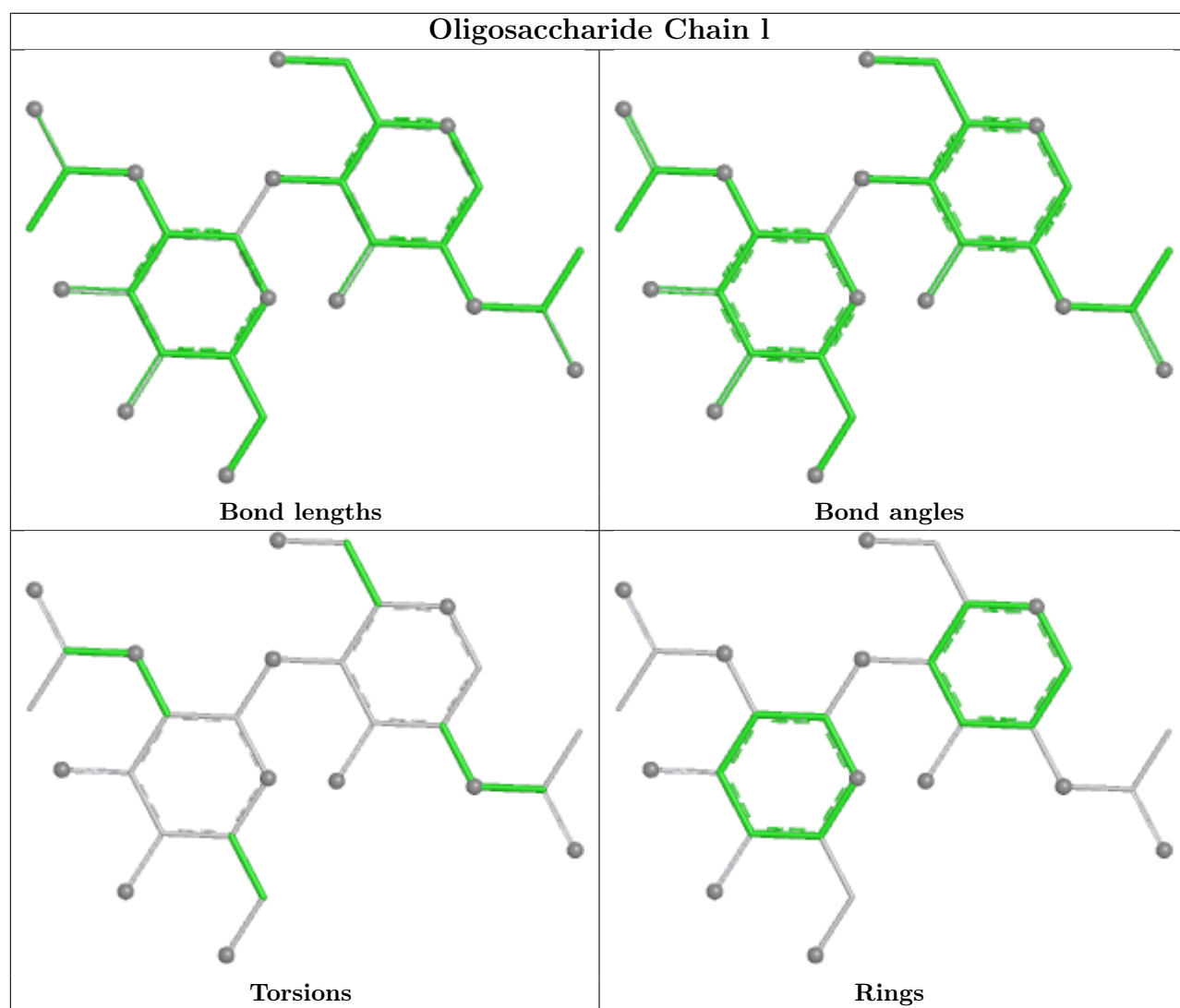


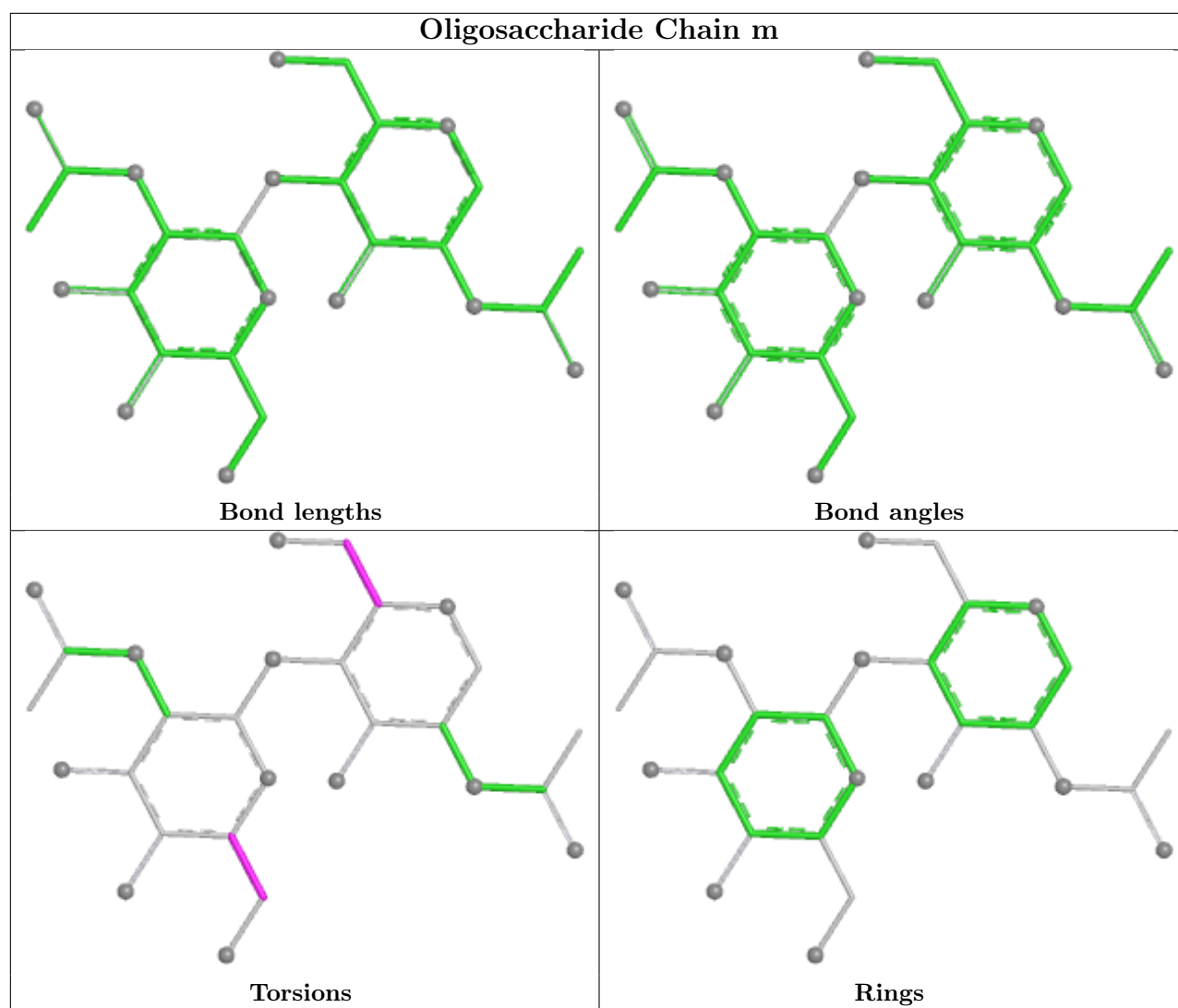


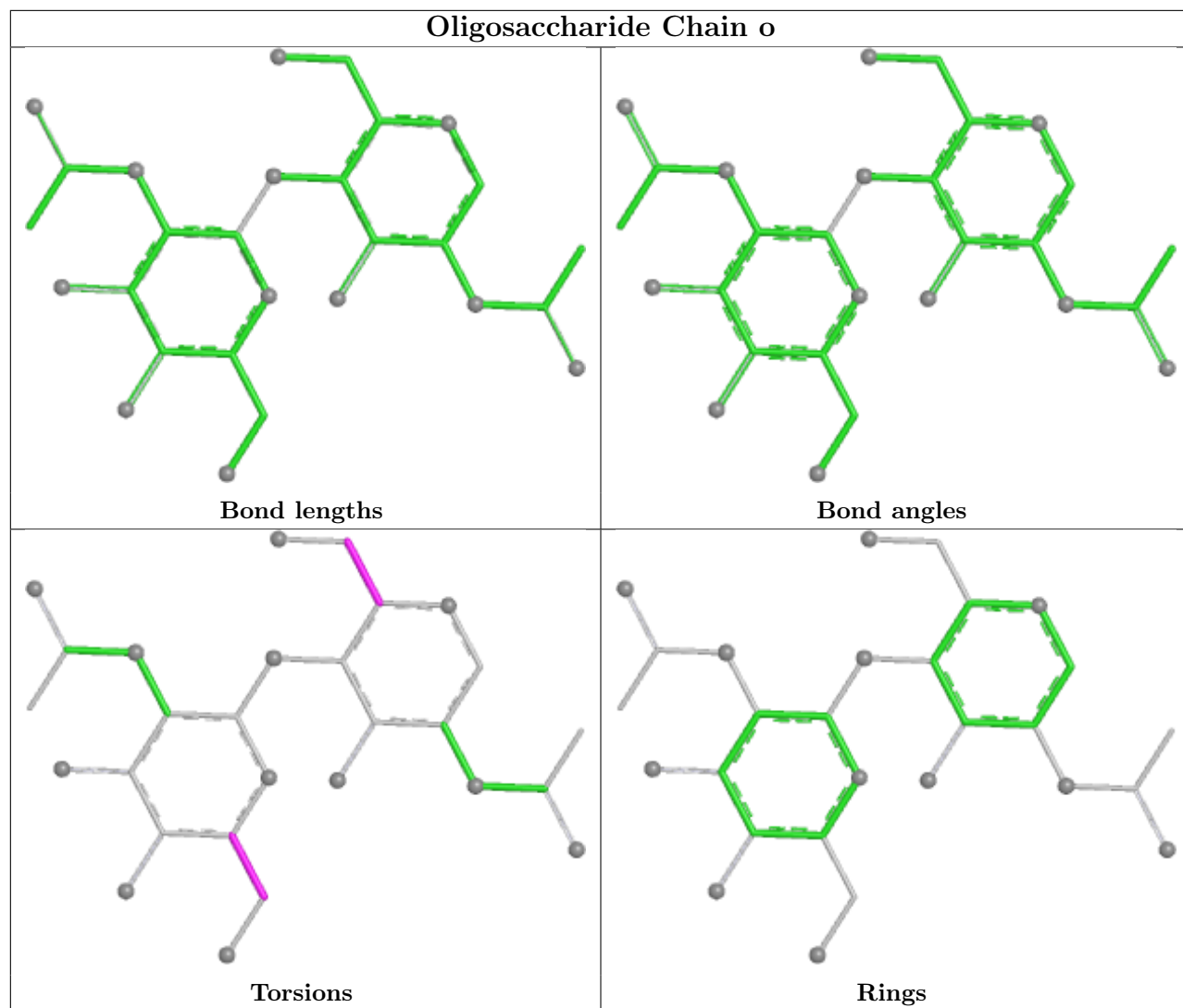


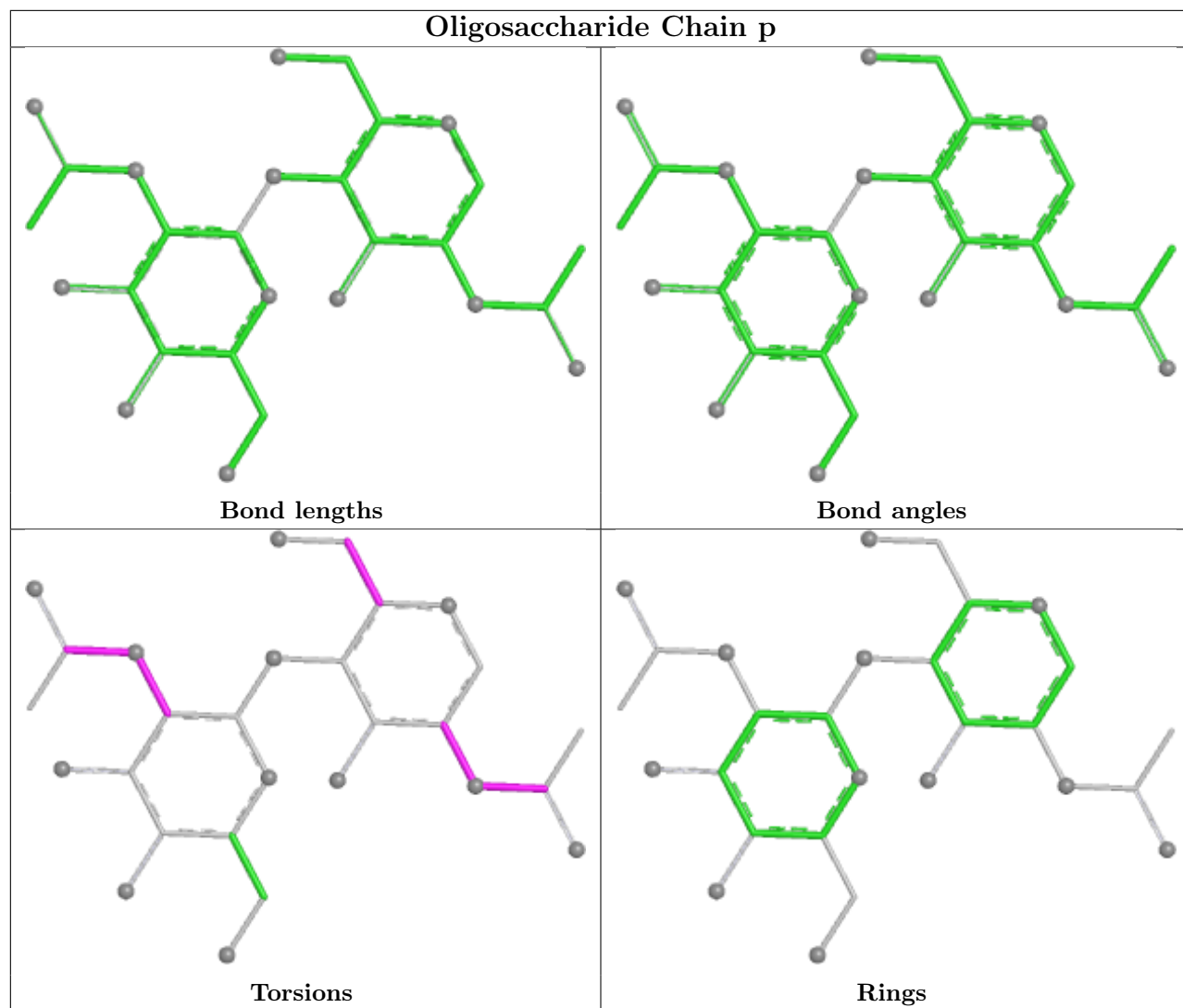


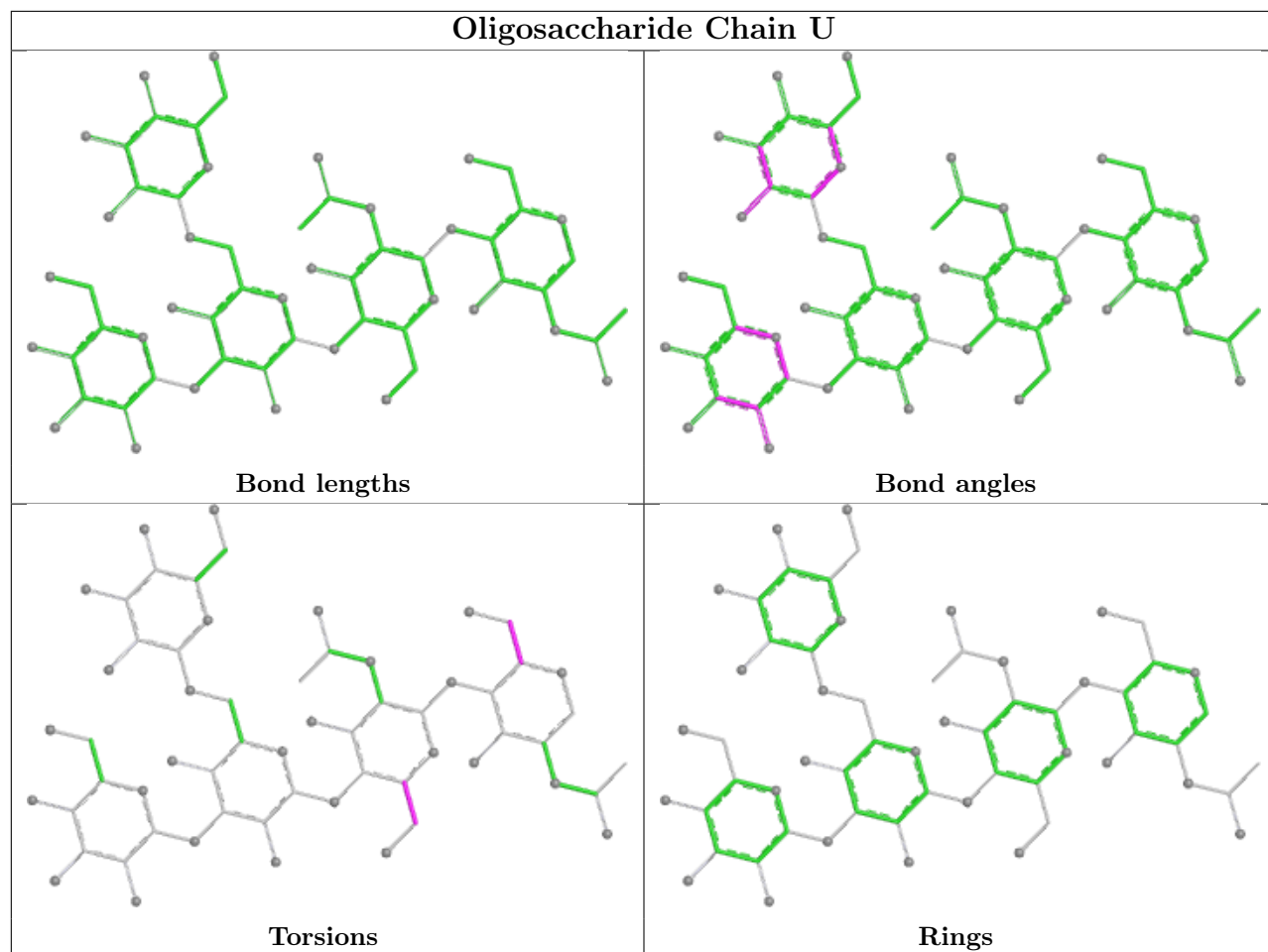


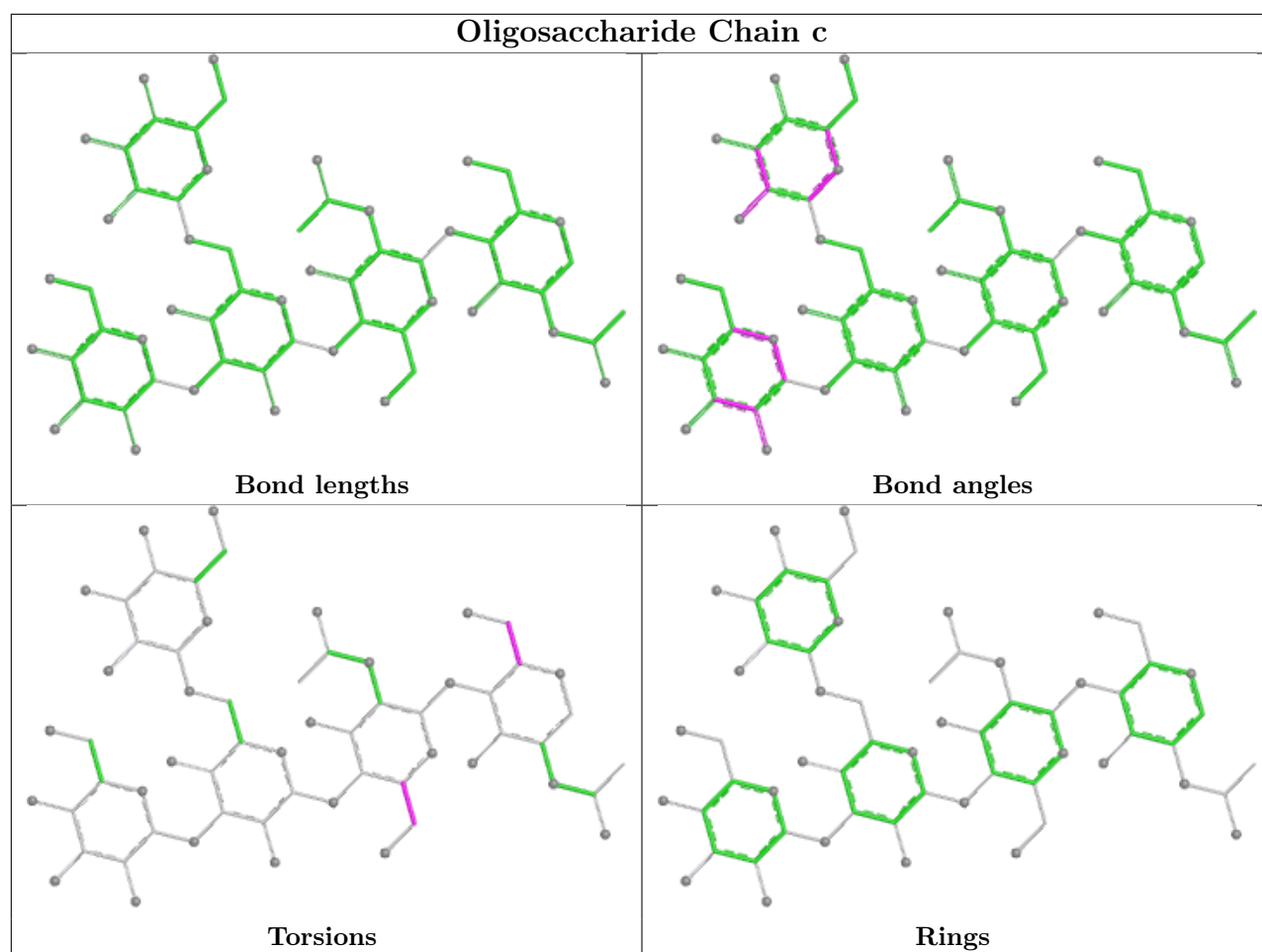


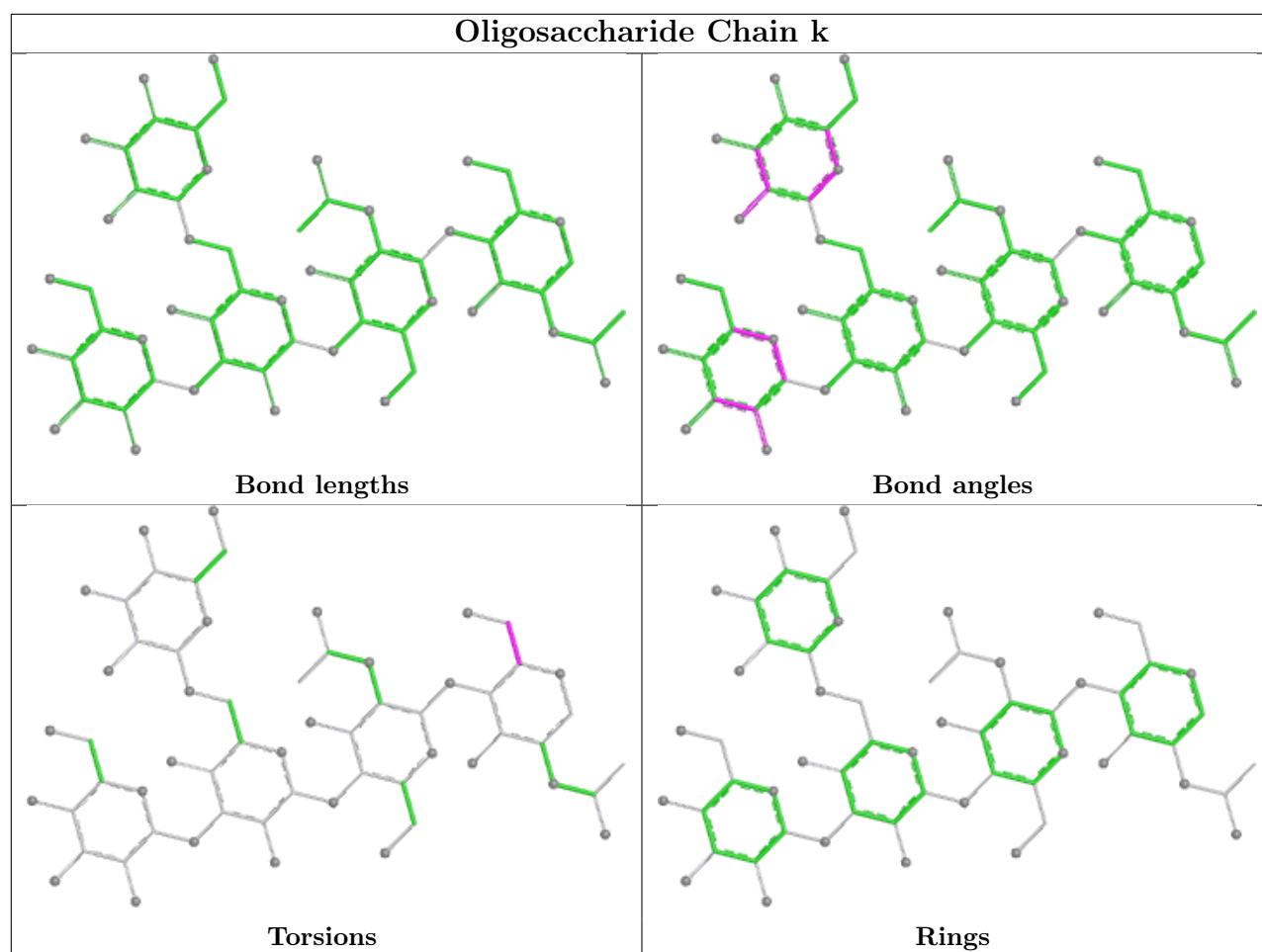


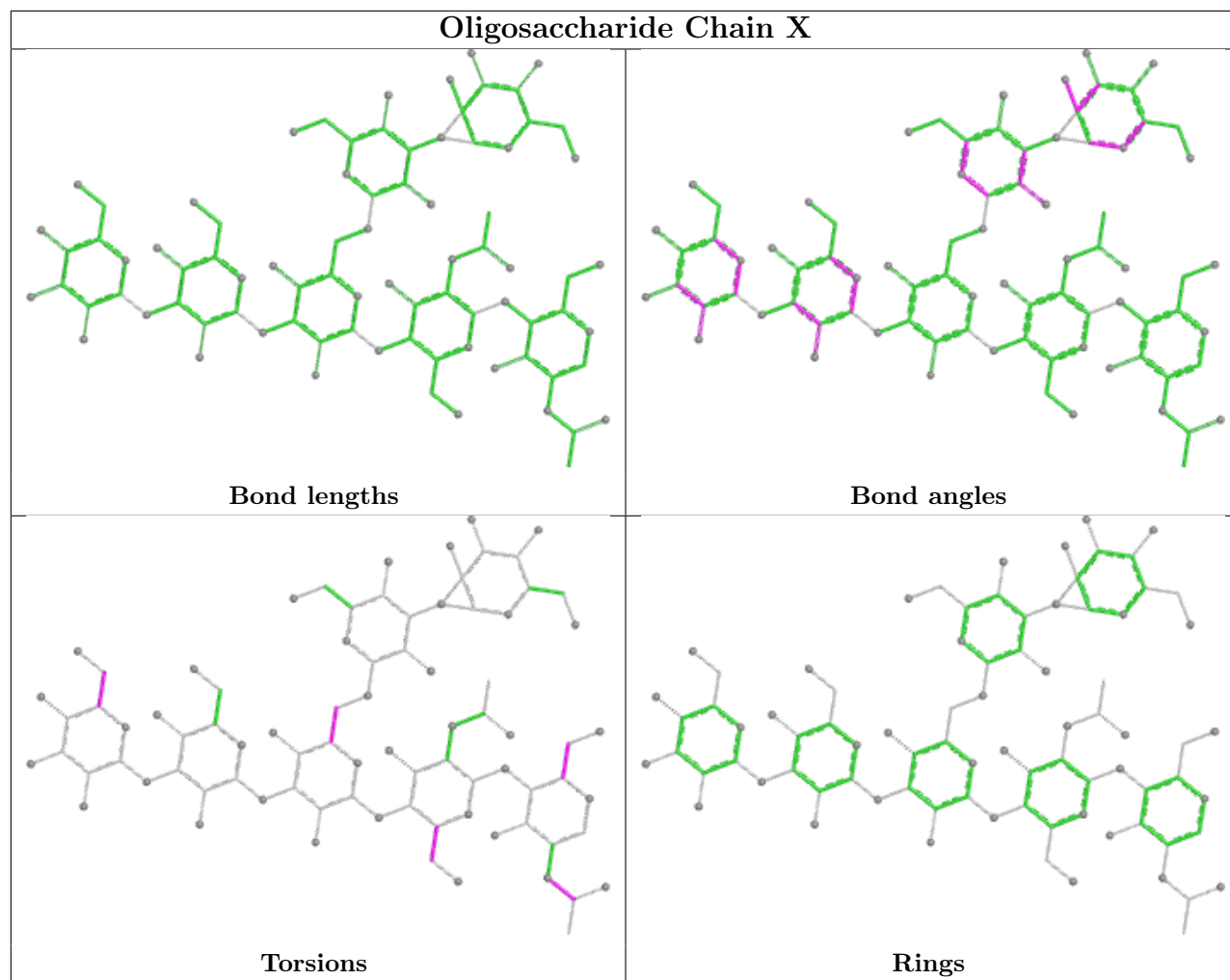


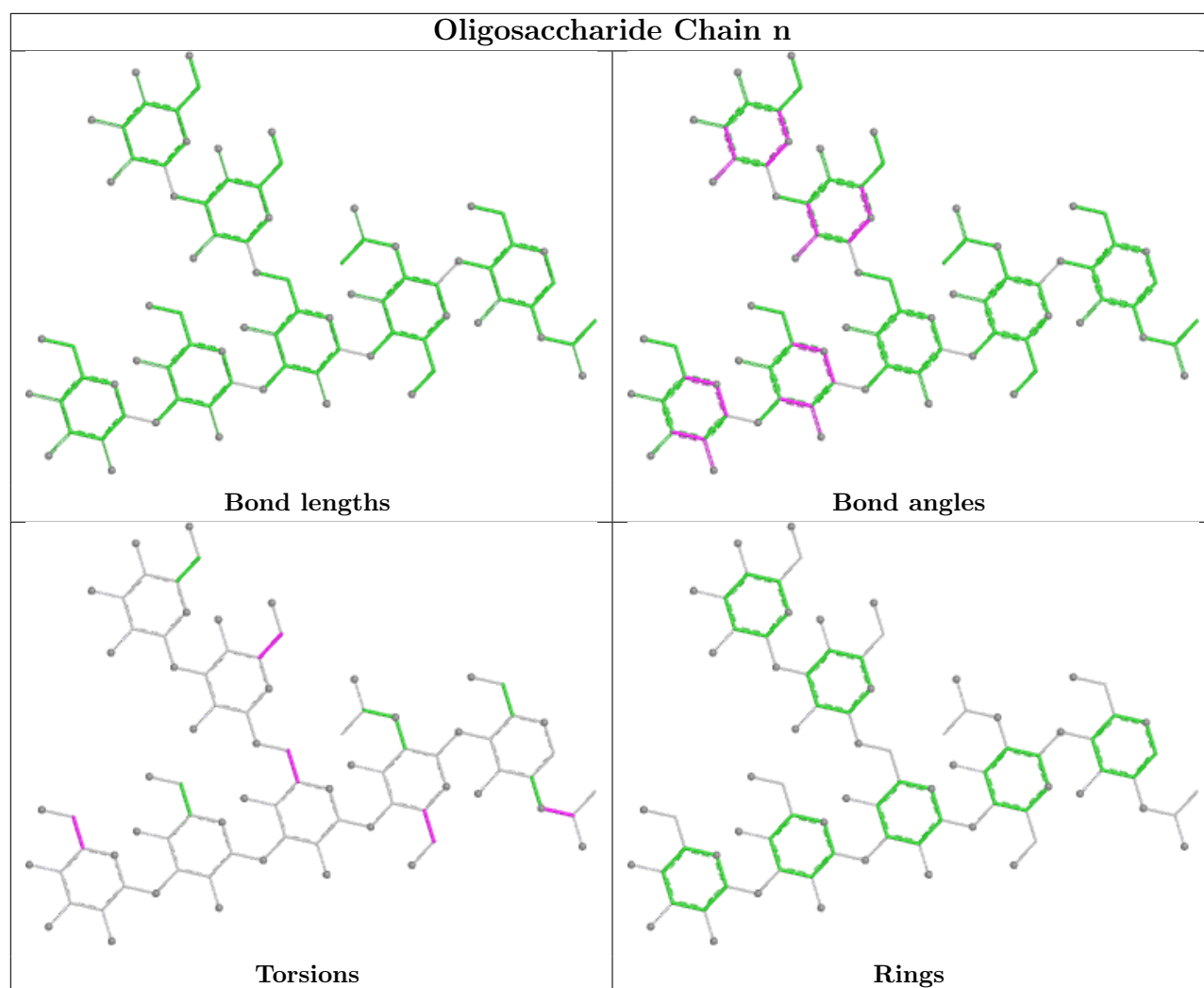


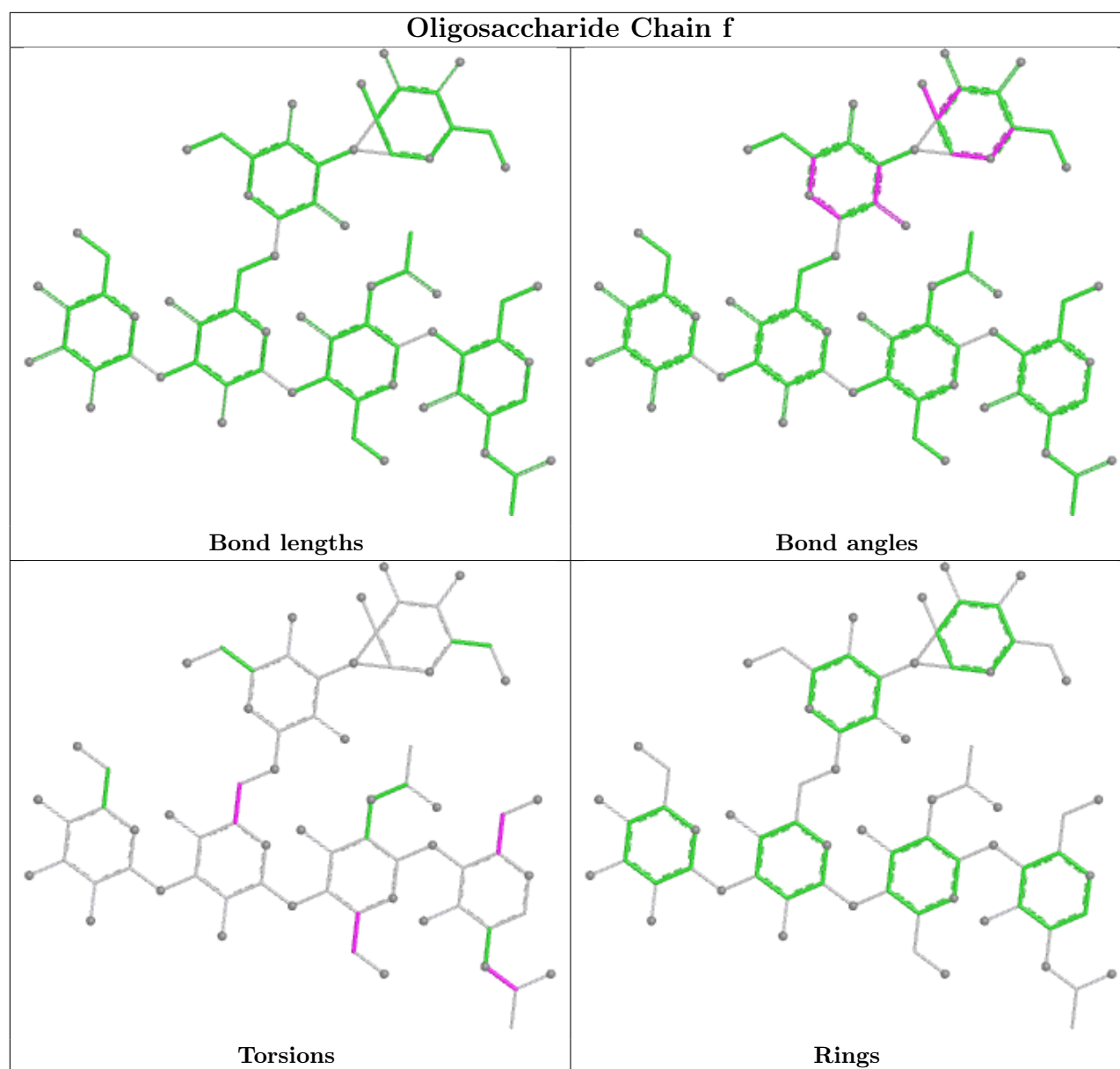












5.6 Ligand geometry [i](#)

16 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	B	601	1	14,14,15	0.32	0	17,19,21	0.53	0
11	NAG	A	603	1	14,14,15	0.25	0	17,19,21	0.50	0
11	NAG	B	603	1	14,14,15	0.25	0	17,19,21	0.51	0
11	NAG	C	601	1	14,14,15	0.36	0	17,19,21	0.51	0
11	NAG	C	602	1	14,14,15	0.27	0	17,19,21	0.52	0
11	NAG	C	604	1	14,14,15	0.22	0	17,19,21	0.45	0
11	NAG	C	603	1	14,14,15	0.25	0	17,19,21	0.50	0
11	NAG	D	701	2	14,14,15	0.42	0	17,19,21	1.26	1 (5%)
11	NAG	E	701	2	14,14,15	0.42	0	17,19,21	1.27	1 (5%)
11	NAG	F	701	2	14,14,15	0.42	0	17,19,21	1.27	1 (5%)
12	MAN	Q	201	-	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
11	NAG	A	604	1	14,14,15	0.23	0	17,19,21	0.45	0
11	NAG	A	601	1	14,14,15	0.30	0	17,19,21	0.53	0
11	NAG	B	602	1	14,14,15	0.26	0	17,19,21	0.52	0
11	NAG	A	602	1	14,14,15	0.27	0	17,19,21	0.51	0
11	NAG	B	604	1	14,14,15	0.23	0	17,19,21	0.45	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	B	601	1	-	2/6/23/26	0/1/1/1
11	NAG	A	603	1	-	0/6/23/26	0/1/1/1
11	NAG	B	603	1	-	0/6/23/26	0/1/1/1
11	NAG	C	601	1	-	3/6/23/26	0/1/1/1
11	NAG	C	602	1	-	3/6/23/26	0/1/1/1
11	NAG	C	604	1	-	2/6/23/26	0/1/1/1
11	NAG	C	603	1	-	0/6/23/26	0/1/1/1
11	NAG	D	701	2	-	0/6/23/26	0/1/1/1
11	NAG	E	701	2	-	0/6/23/26	0/1/1/1
11	NAG	F	701	2	-	0/6/23/26	0/1/1/1
12	MAN	Q	201	-	-	1/2/19/22	0/1/1/1
11	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	601	1	-	2/6/23/26	0/1/1/1
11	NAG	B	602	1	-	3/6/23/26	0/1/1/1
11	NAG	A	602	1	-	3/6/23/26	0/1/1/1
11	NAG	B	604	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	701	NAG	C1-O5-C5	4.81	118.64	112.19
11	E	701	NAG	C1-O5-C5	4.80	118.62	112.19
11	D	701	NAG	C1-O5-C5	4.80	118.62	112.19
12	Q	201	MAN	C1-O5-C5	2.40	115.40	112.19
12	Q	201	MAN	O2-C2-C3	-2.17	105.67	110.15

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	604	NAG	C4-C5-C6-O6
11	A	604	NAG	C4-C5-C6-O6
11	C	604	NAG	C4-C5-C6-O6
11	B	604	NAG	O5-C5-C6-O6
11	A	604	NAG	O5-C5-C6-O6
11	C	604	NAG	O5-C5-C6-O6
11	B	602	NAG	O5-C5-C6-O6
11	C	602	NAG	O5-C5-C6-O6
11	A	602	NAG	O5-C5-C6-O6
12	Q	201	MAN	O5-C5-C6-O6
11	C	601	NAG	O5-C5-C6-O6
11	A	602	NAG	C1-C2-N2-C7
11	B	602	NAG	C1-C2-N2-C7
11	C	602	NAG	C1-C2-N2-C7
11	A	601	NAG	C3-C2-N2-C7
11	A	602	NAG	C3-C2-N2-C7
11	B	601	NAG	C3-C2-N2-C7
11	B	602	NAG	C3-C2-N2-C7
11	C	601	NAG	C3-C2-N2-C7
11	C	602	NAG	C3-C2-N2-C7
11	A	601	NAG	C1-C2-N2-C7
11	B	601	NAG	C1-C2-N2-C7
11	C	601	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	603	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	603	NAG	1	0
11	C	601	NAG	1	0
11	C	603	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	3
1	C	3
2	E	1
2	F	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	397:SER	C	411:ASN	N	27.34
1	B	397:SER	C	411:ASN	N	27.34
1	C	397:SER	C	411:ASN	N	27.23
1	E	546:SER	C	565:LEU	N	26.04
1	F	546:SER	C	565:LEU	N	26.04
1	D	546:SER	C	565:LEU	N	26.01
1	B	61:TYR	C	64:LYS	N	5.83
1	C	61:TYR	C	64:LYS	N	5.83
1	A	61:TYR	C	64:LYS	N	5.81
1	A	142:ARG	C	152:GLY	N	5.00
1	B	142:ARG	C	152:GLY	N	5.00
1	C	142:ARG	C	152:GLY	N	4.99

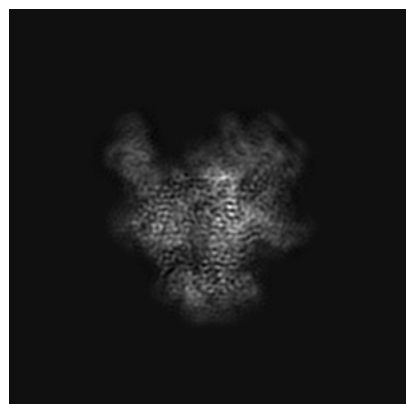
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26490. These allow visual inspection of the internal detail of the map and identification of artifacts.

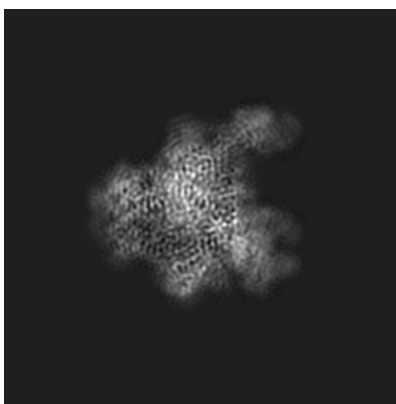
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

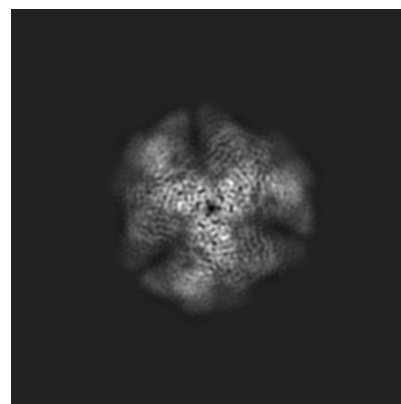
6.1.1 Primary map



X

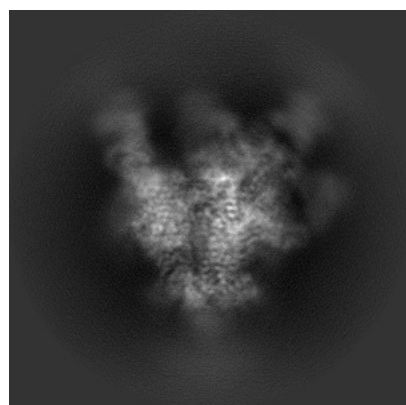


Y

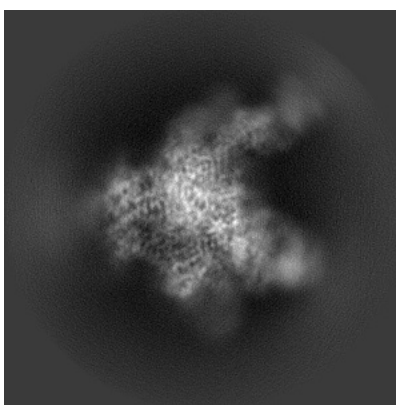


Z

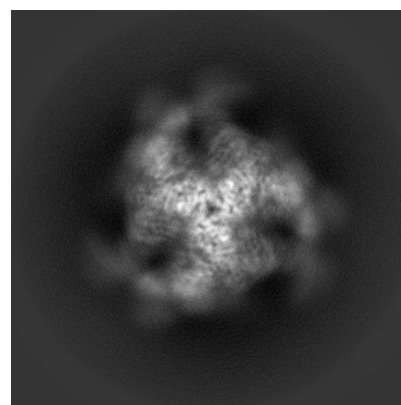
6.1.2 Raw map



X



Y

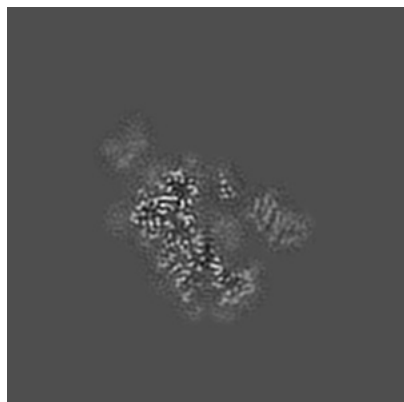


Z

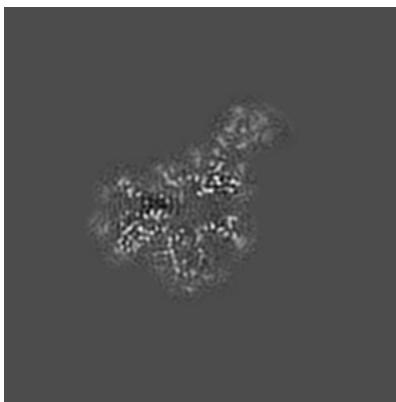
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

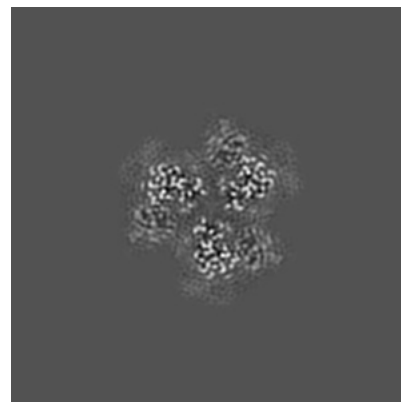
6.2.1 Primary map



X Index: 168

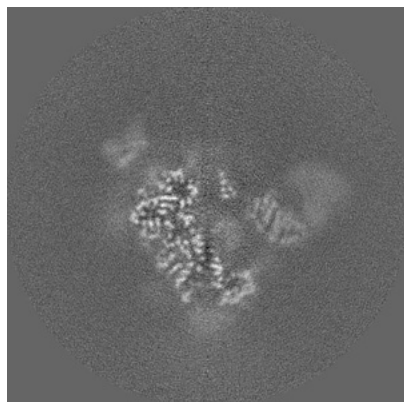


Y Index: 168

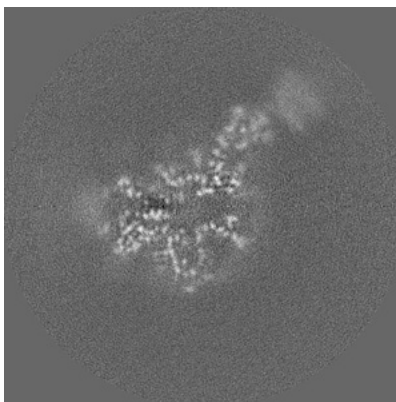


Z Index: 168

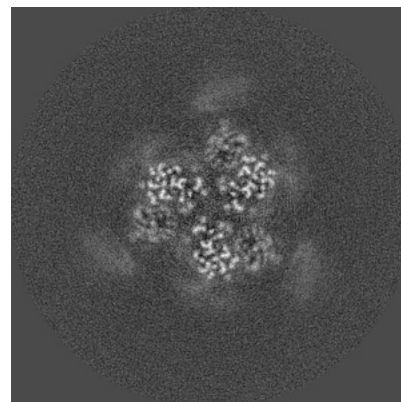
6.2.2 Raw map



X Index: 168



Y Index: 168

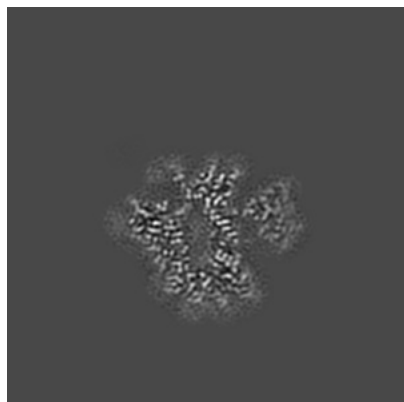


Z Index: 168

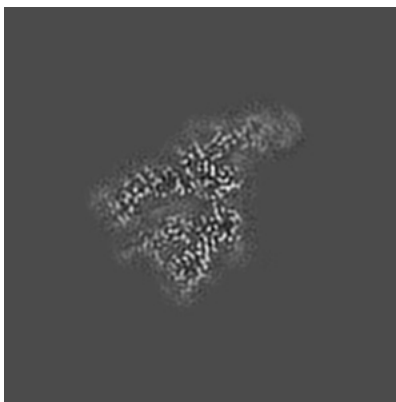
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

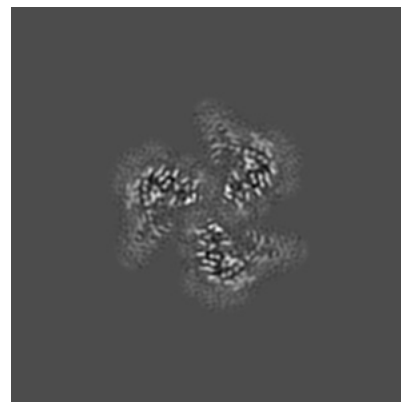
6.3.1 Primary map



X Index: 181

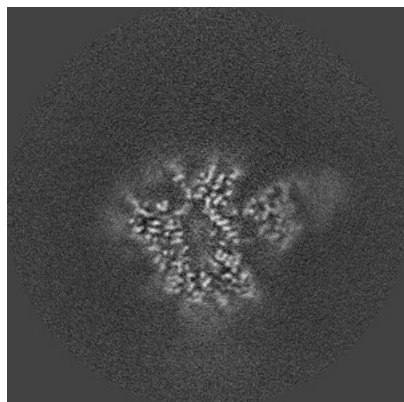


Y Index: 185

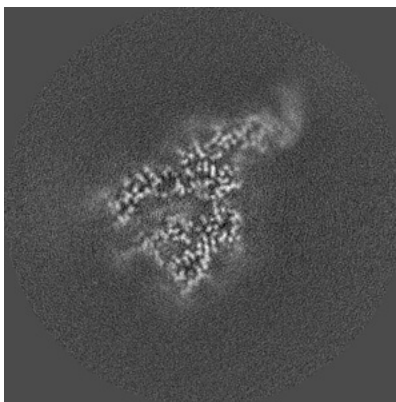


Z Index: 155

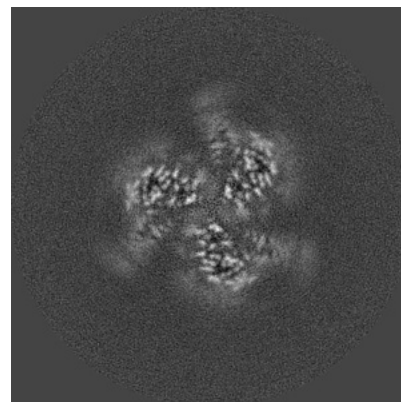
6.3.2 Raw map



X Index: 181



Y Index: 185

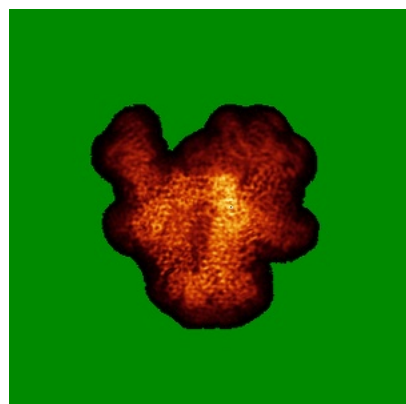


Z Index: 155

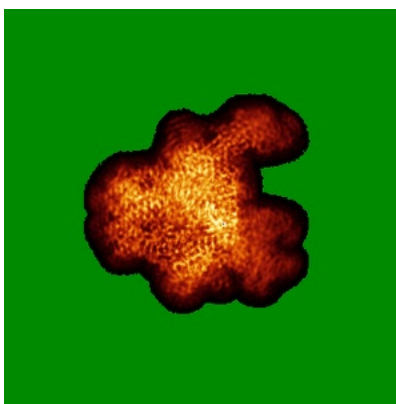
The images above show the largest variance slices of the map in three orthogonal directions.

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

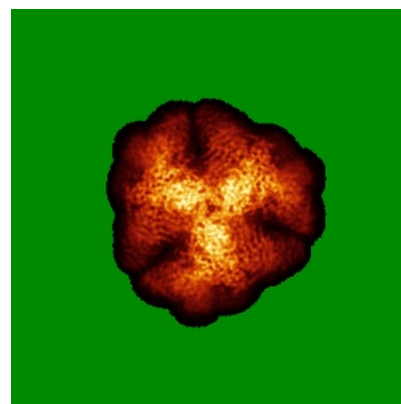
6.4.1 Primary map



X

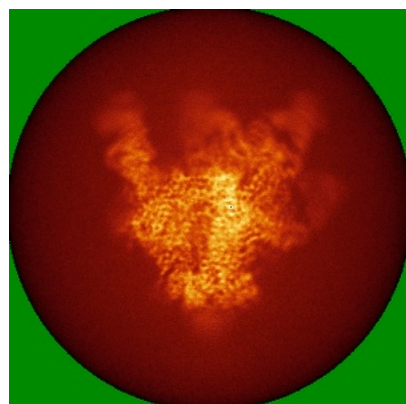


Y

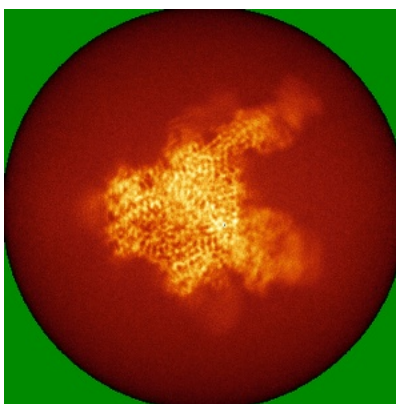


Z

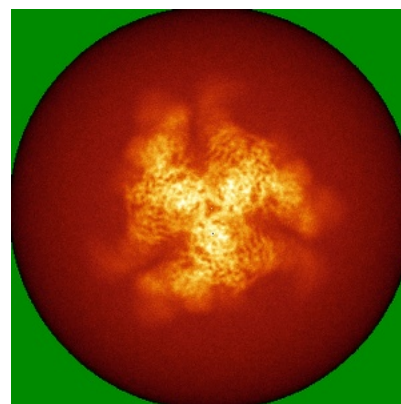
6.4.2 Raw map



X



Y

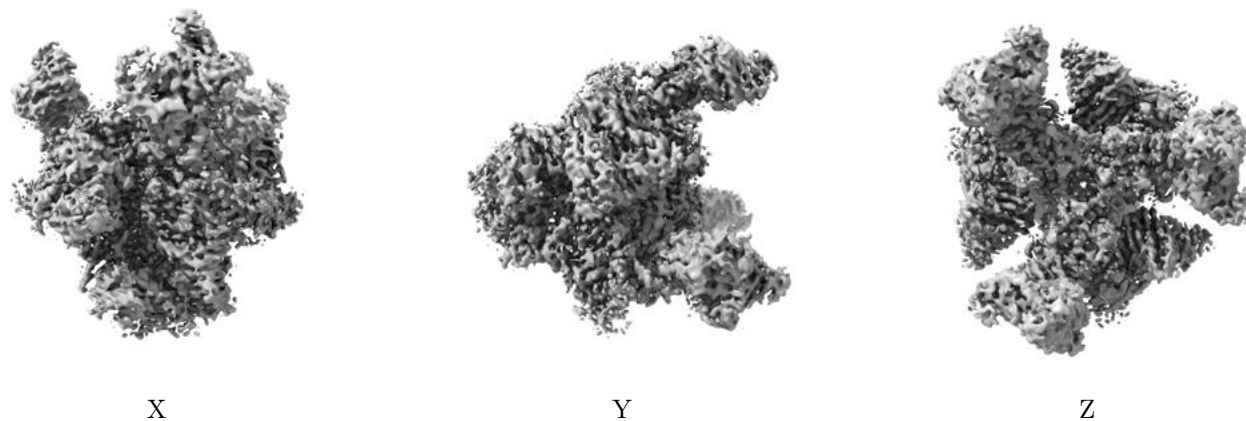


Z

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 0.0081. 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.

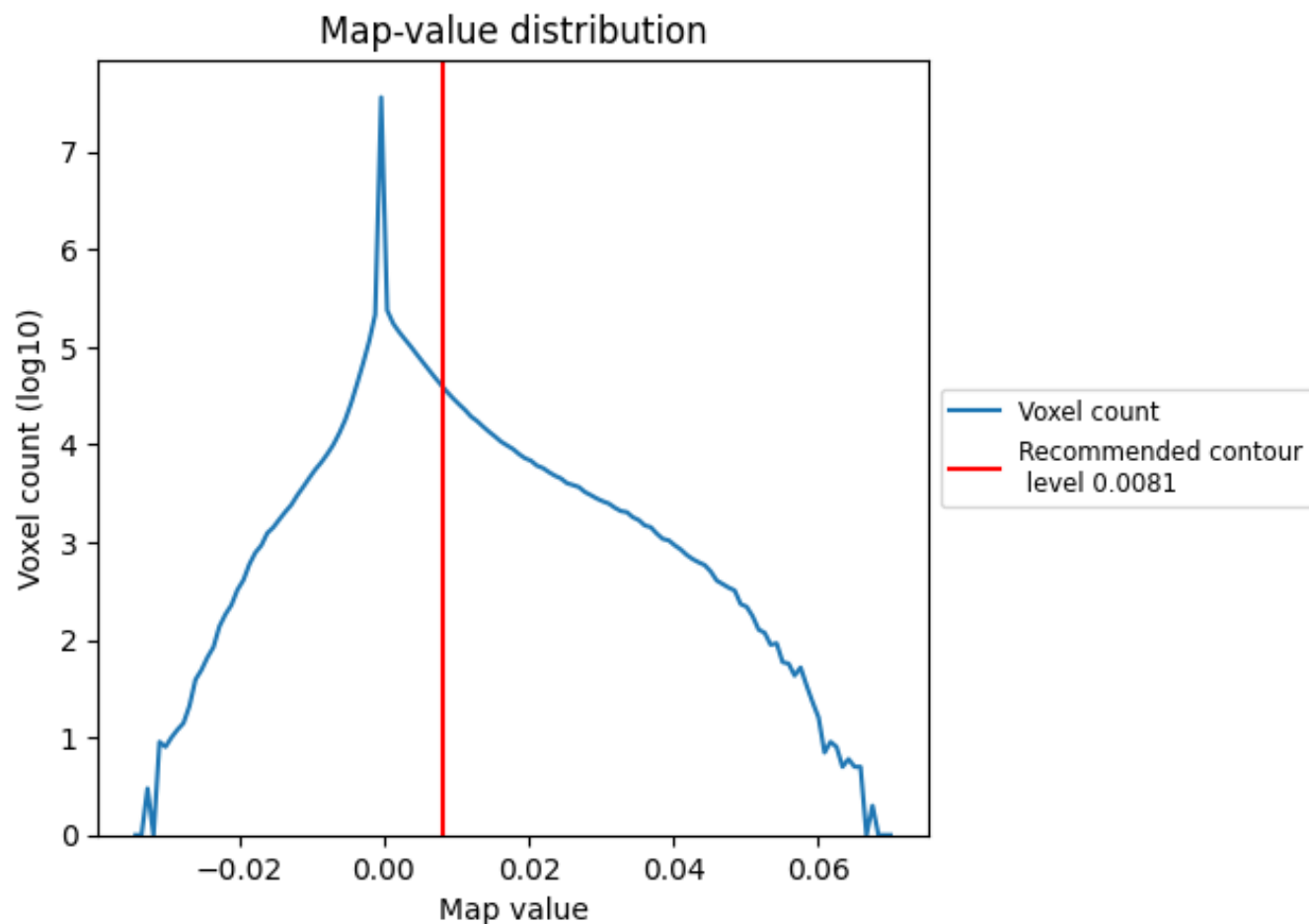
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

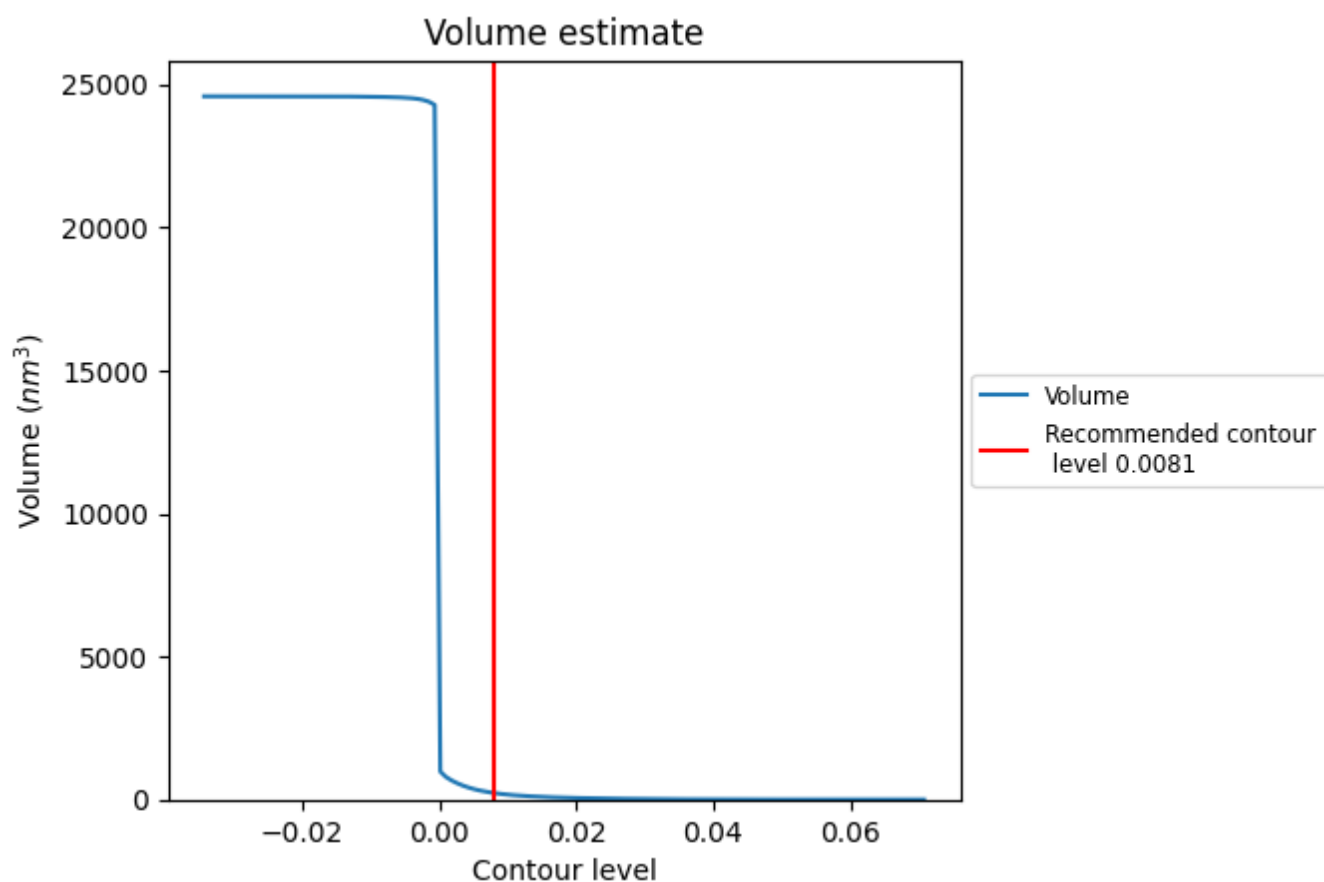
This section contains the results of statistical analysis of the map.

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.

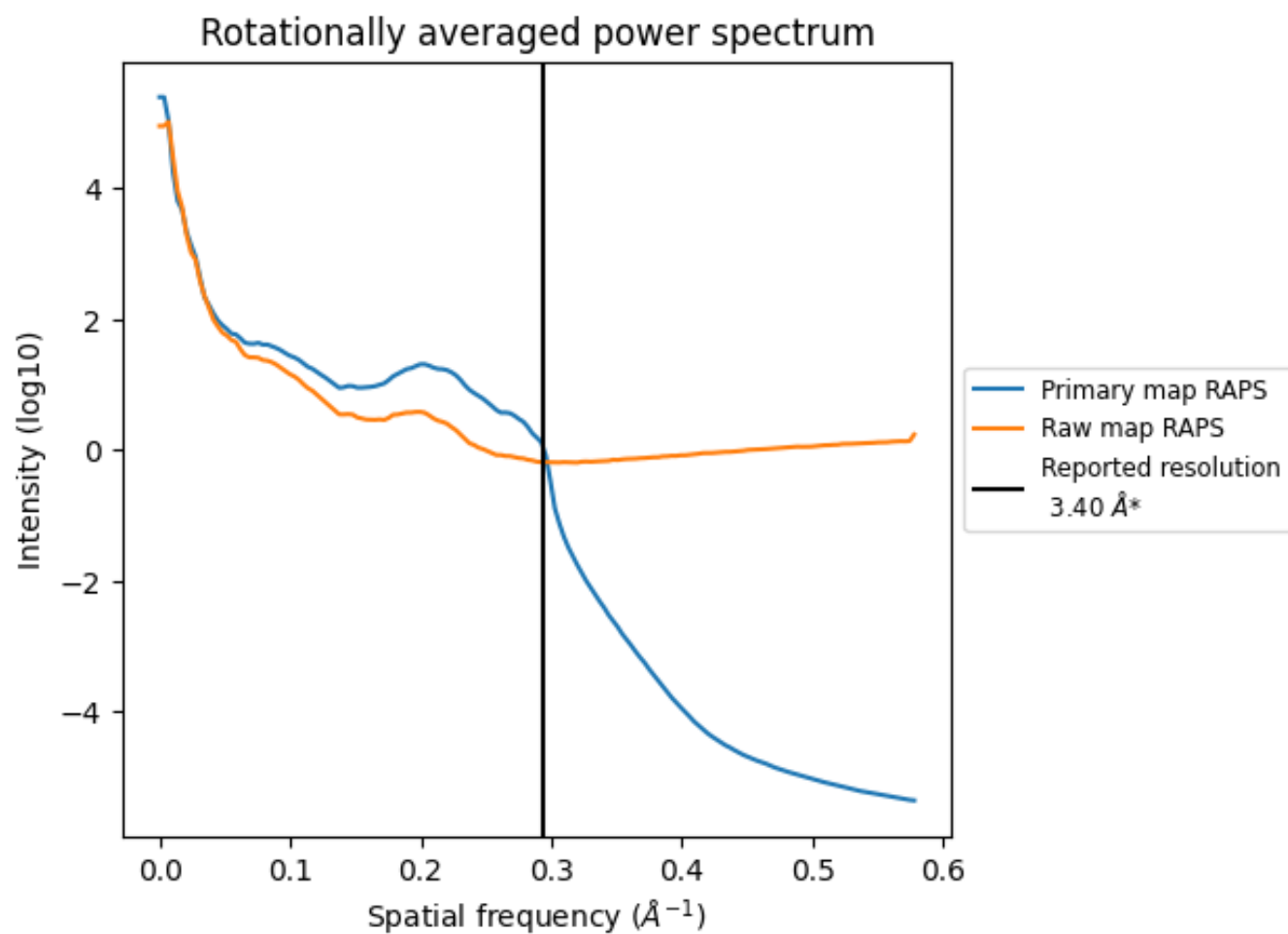
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 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 ⓘ

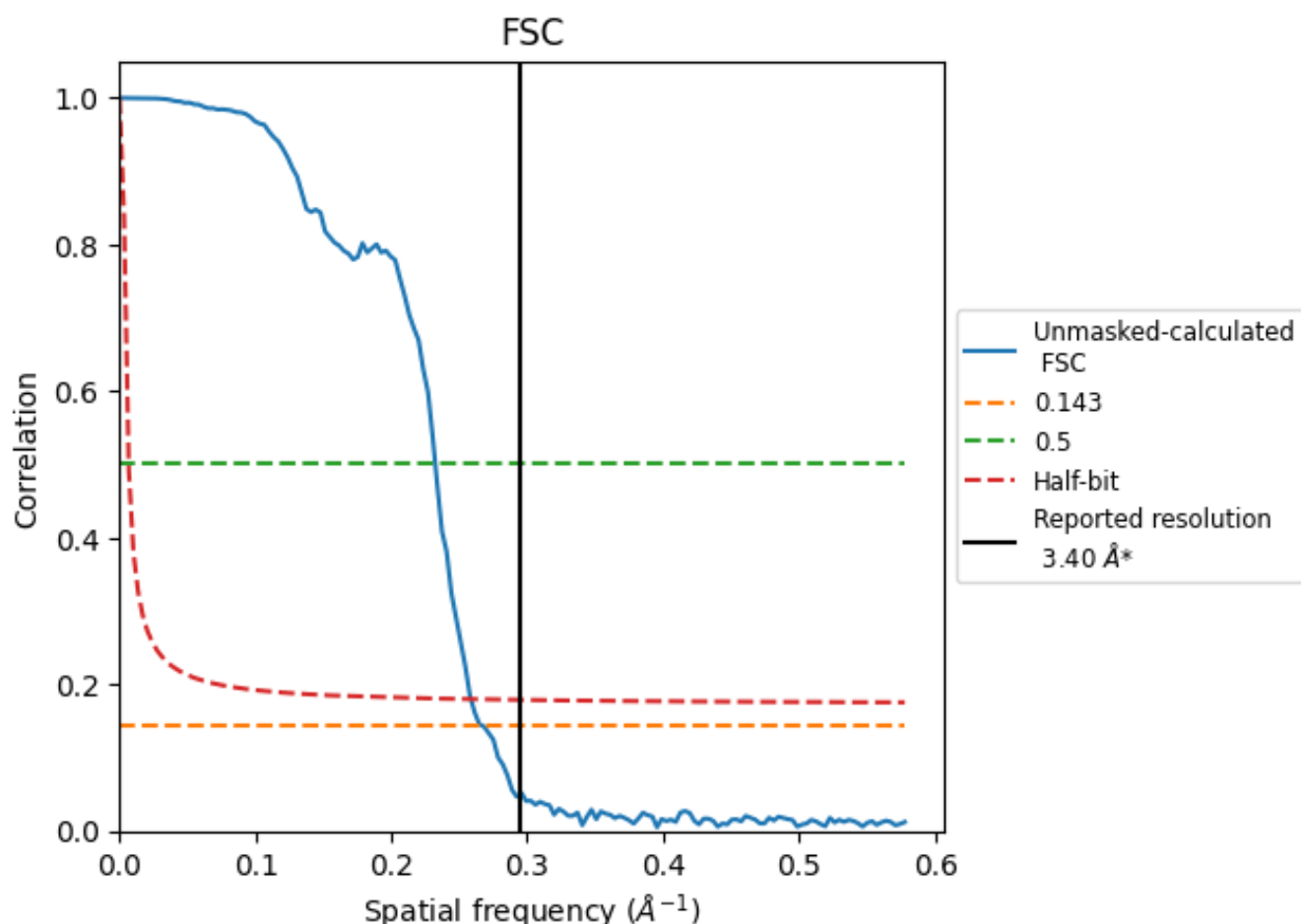


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

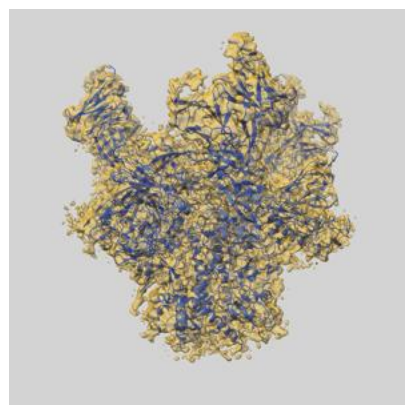
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.30	3.87

*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 3.74 differs from the reported value 3.4 by more than 10 %

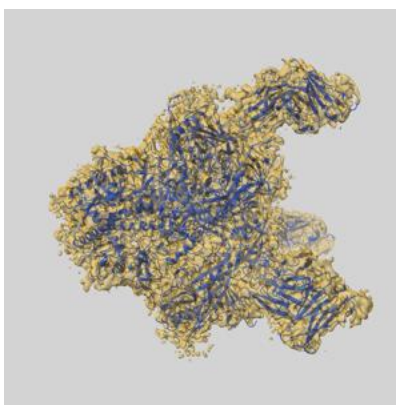
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26490 and PDB model 7UGN. Per-residue inclusion information can be found in section [3](#) on page [15](#).

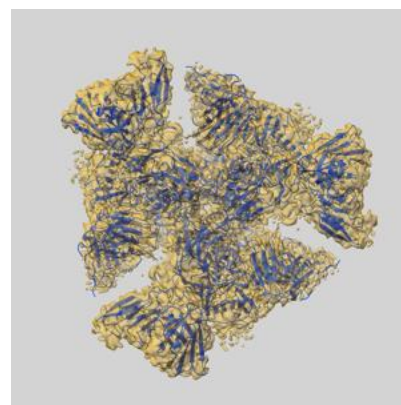
9.1 Map-model overlay [i](#)



X



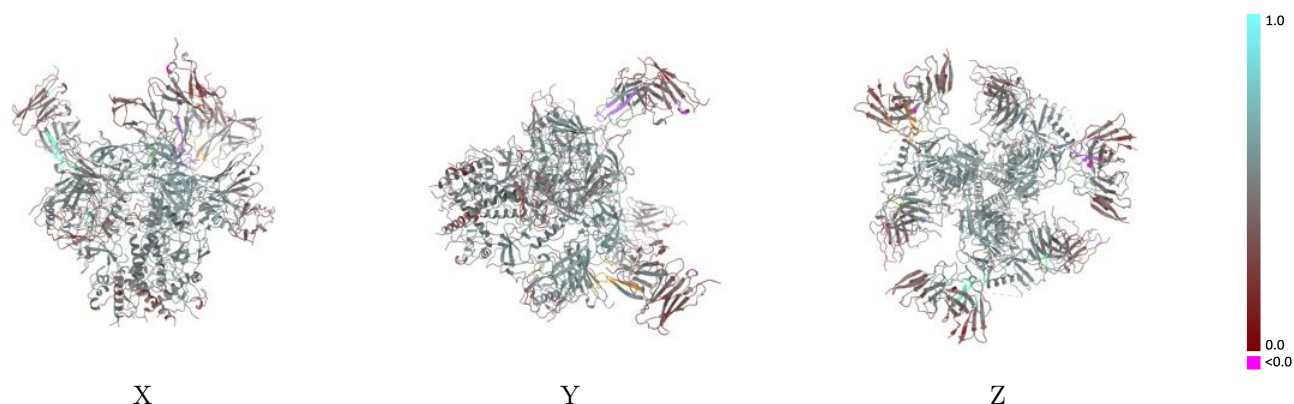
Y



Z

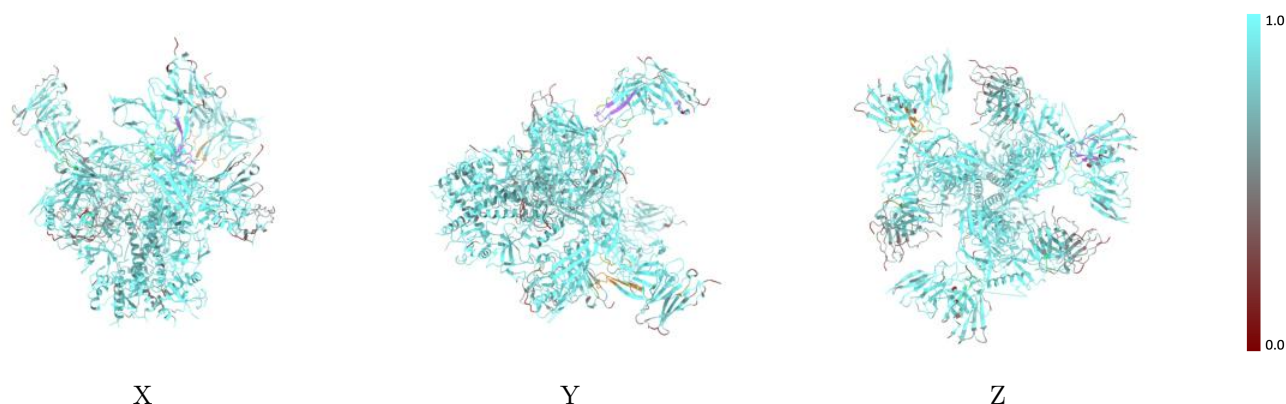
The images above show the 3D surface view of the map at the recommended contour level 0.0081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



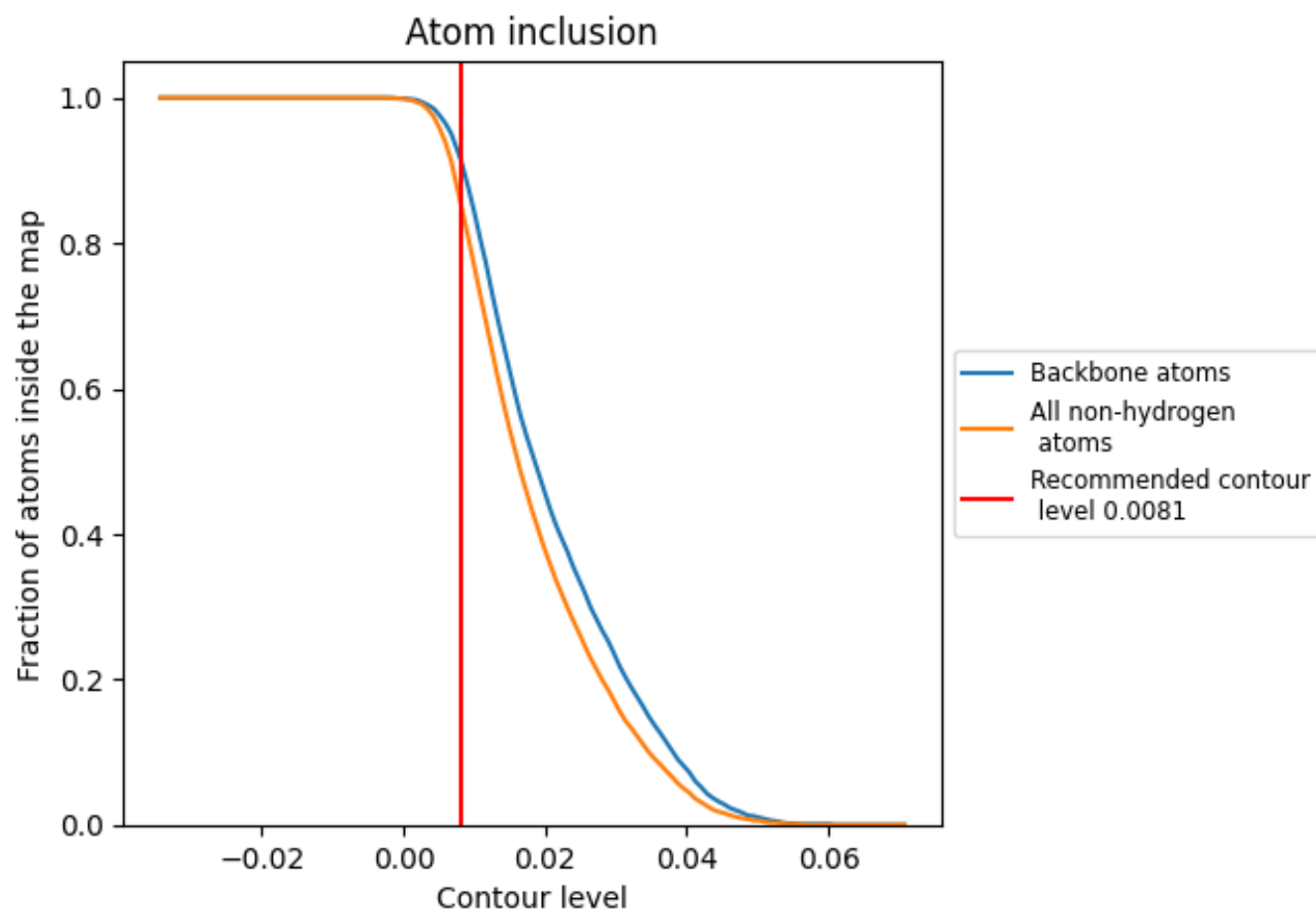
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0081).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.4770
A	 0.9300	 0.5310
B	 0.9320	 0.5320
C	 0.9280	 0.5290
D	 0.8800	 0.4740
E	 0.8770	 0.4730
F	 0.8760	 0.4760
G	 0.7770	 0.4780
H	 0.7770	 0.4820
I	 0.7720	 0.4710
J	 0.5940	 0.3650
K	 0.6110	 0.3840
L	 0.6020	 0.3780
M	 0.8150	 0.3950
N	 0.8180	 0.4100
O	 0.8170	 0.4080
P	 0.8980	 0.4400
Q	 0.9030	 0.4480
R	 0.8930	 0.4500
S	 0.8930	 0.5290
T	 0.5360	 0.3530
U	 0.9020	 0.5150
V	 0.9290	 0.5400
W	 0.7860	 0.4280
X	 0.8920	 0.4430
Y	 0.7500	 0.4980
Z	 0.5360	 0.2370
a	 0.8930	 0.5280
b	 0.5360	 0.3420
c	 0.9020	 0.5050
d	 0.9290	 0.5420
e	 0.7860	 0.4550
f	 0.9030	 0.4560
g	 0.7500	 0.4940
h	 0.5360	 0.2260



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Chain	Atom inclusion	Q-score
i	 0.8930	 0.4910
j	 0.5360	 0.3090
k	 0.8850	 0.4730
l	 0.9290	 0.5310
m	 0.7860	 0.4410
n	 0.8680	 0.4130
o	 0.7500	 0.4850
p	 0.6790	 0.3680