



## Full wwPDB EM Validation Report ⓘ

Sep 16, 2023 – 12:28 PM EDT

PDB ID : 7TXD  
EMDB ID : EMD-26157  
Title : Cryo-EM structure of BG505 SOSIP HIV-1 Env trimer in complex with CD4 receptor (D1D2) and broadly neutralizing darpin bnD.9  
Authors : Cerutti, G.; Gorman, J.; Kwong, P.D.; Shapiro, L.  
Deposited on : 2022-02-08  
Resolution : 3.87 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

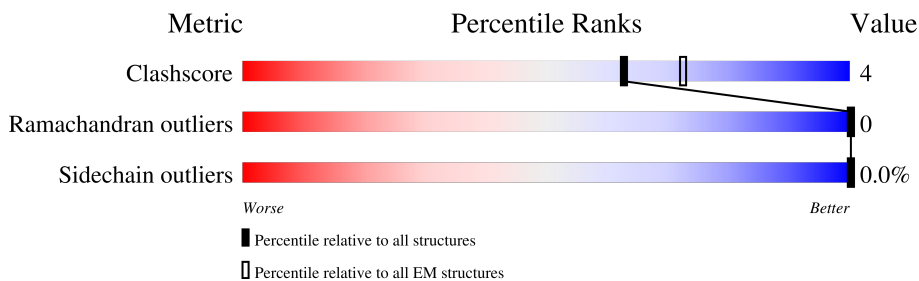
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.87 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.



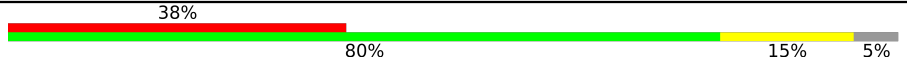

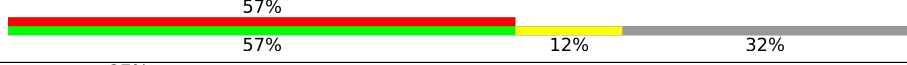

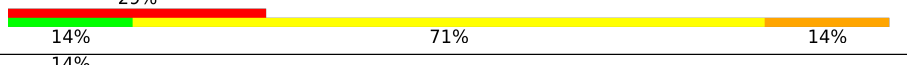
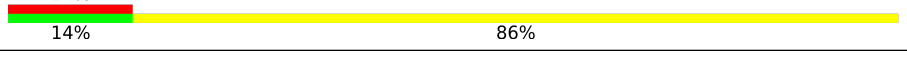
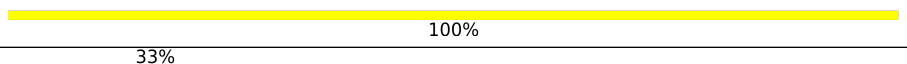

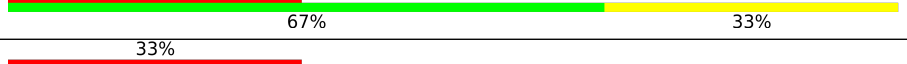
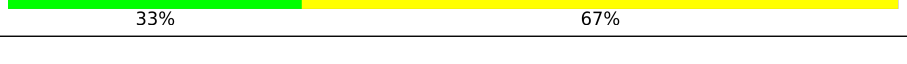

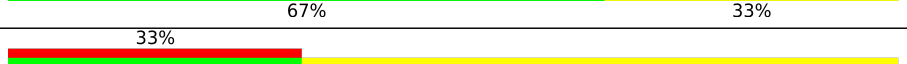
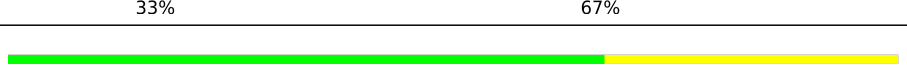

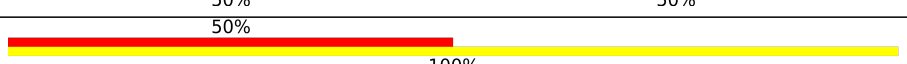
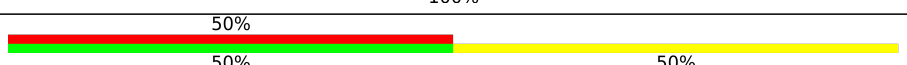
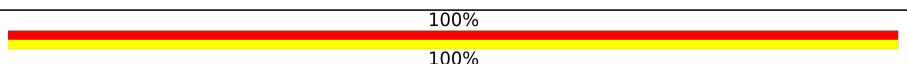

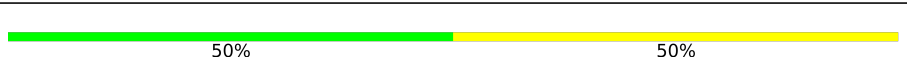

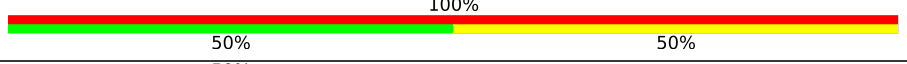
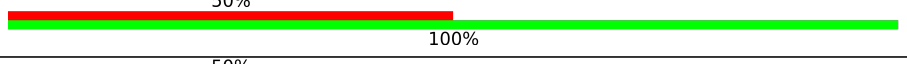
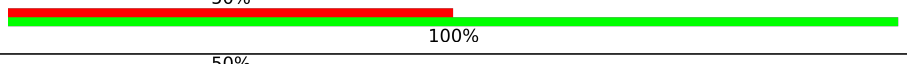
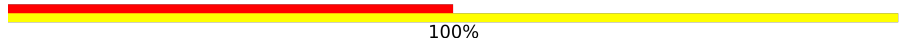

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	
1	C	481	
1	E	481	
2	B	153	
2	D	153	
2	F	153	
3	G	185	
3	H	185	

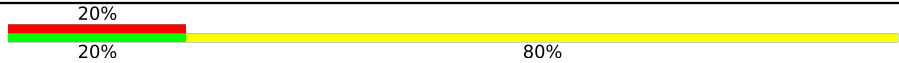
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Mol	Chain	Length	Quality of chain
3	I	185	
4	J	196	
4	K	196	
4	L	196	
5	M	7	
5	b	7	
6	N	3	
6	P	3	
6	T	3	
6	Y	3	
6	Z	3	
6	c	3	
6	e	3	
6	f	3	
7	O	2	
7	Q	2	
7	R	2	
7	S	2	
7	U	2	
7	W	2	
7	X	2	
7	a	2	
7	d	2	
7	g	2	
7	h	2	

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Mol	Chain	Length	Quality of chain
8	V	5	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '20%', a green segment in the middle labeled '20%', and a yellow segment on the right labeled '80%'. The total length of the bar represents 100%.</p>

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 20555 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
			Total	C	N	O	S		
1	A	397	3101	1951	547	579	24	0	0
1	C	397	3101	1951	547	579	24	0	0
1	E	397	3101	1951	547	579	24	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	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
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
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 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	127	Total	C	N	O	S	0	0
			1004	640	175	183	6		
2	D	113	Total	C	N	O	S	0	0
			900	568	159	167	6		
2	F	122	Total	C	N	O	S	0	0
			965	605	172	182	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
3	H	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		
3	I	176	Total	C	N	O	S	0	0
			1370	856	240	270	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	184	ASN	-	expression tag	UNP P01730
G	185	THR	-	expression tag	UNP P01730
H	184	ASN	-	expression tag	UNP P01730
H	185	THR	-	expression tag	UNP P01730
I	184	ASN	-	expression tag	UNP P01730
I	185	THR	-	expression tag	UNP P01730

- Molecule 4 is a protein called Broadly neutralizing darpin bnd.9.

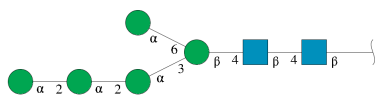
Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	134	Total	C	N	O	S	0	0
			1002	634	174	193	1		

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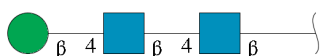
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	134	Total	C	N	O	S	0	0
			1002	634	174	193	1		
4	L	134	Total	C	N	O	S	0	0
			1002	634	174	193	1		

- Molecule 5 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
			Total	C	N	O		
5	M	7	Total	C	N	O	0	0
			83	46	2	35		
5	b	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 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
			Total	C	N	O		
6	N	3	Total	C	N	O	0	0
			39	22	2	15		
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	T	3	Total	C	N	O	0	0
			39	22	2	15		
6	Y	3	Total	C	N	O	0	0
			39	22	2	15		
6	Z	3	Total	C	N	O	0	0
			39	22	2	15		
6	c	3	Total	C	N	O	0	0
			39	22	2	15		
6	e	3	Total	C	N	O	0	0
			39	22	2	15		

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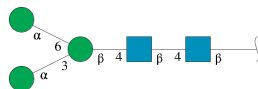
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	f	3	39	22	2	15	0	0

- 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
			Total	C	N	O		
7	O	2	28	16	2	10	0	0
7	Q	2	28	16	2	10	0	0
7	R	2	28	16	2	10	0	0
7	S	2	28	16	2	10	0	0
7	U	2	28	16	2	10	0	0
7	W	2	28	16	2	10	0	0
7	X	2	28	16	2	10	0	0
7	a	2	28	16	2	10	0	0
7	d	2	28	16	2	10	0	0
7	g	2	28	16	2	10	0	0
7	h	2	28	16	2	10	0	0

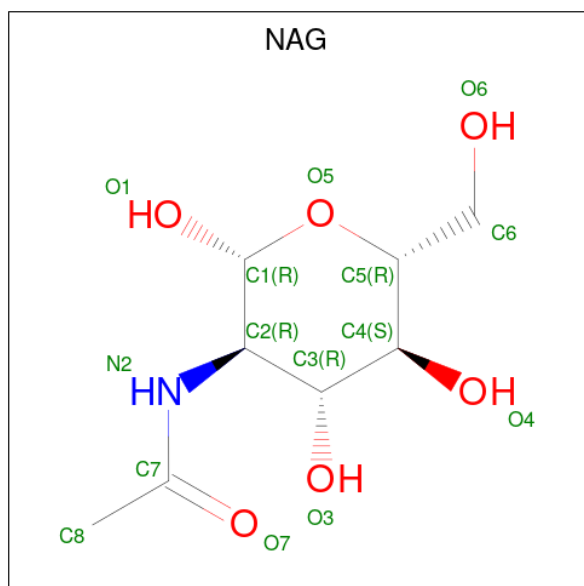
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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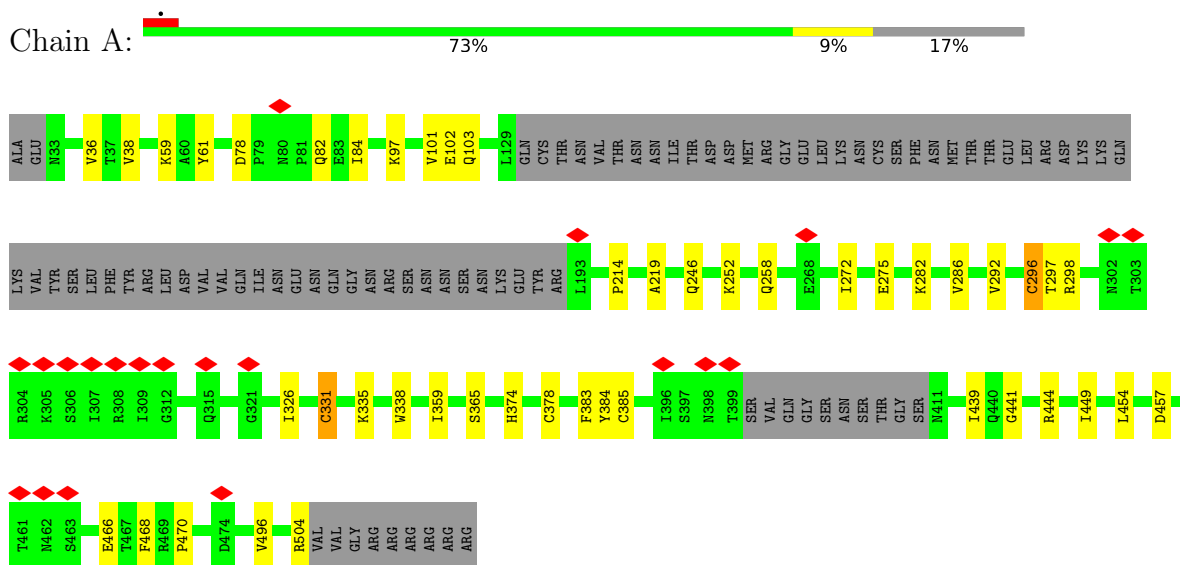
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	C	1	Total 14	C 8	N 1	O 5	0
9	C	1	Total 14	C 8	N 1	O 5	0
9	C	1	Total 14	C 8	N 1	O 5	0
9	C	1	Total 14	C 8	N 1	O 5	0
9	C	1	Total 14	C 8	N 1	O 5	0
9	C	1	Total 14	C 8	N 1	O 5	0
9	D	1	Total 14	C 8	N 1	O 5	0
9	D	1	Total 14	C 8	N 1	O 5	0
9	D	1	Total 14	C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

### 3 Residue-property plots

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

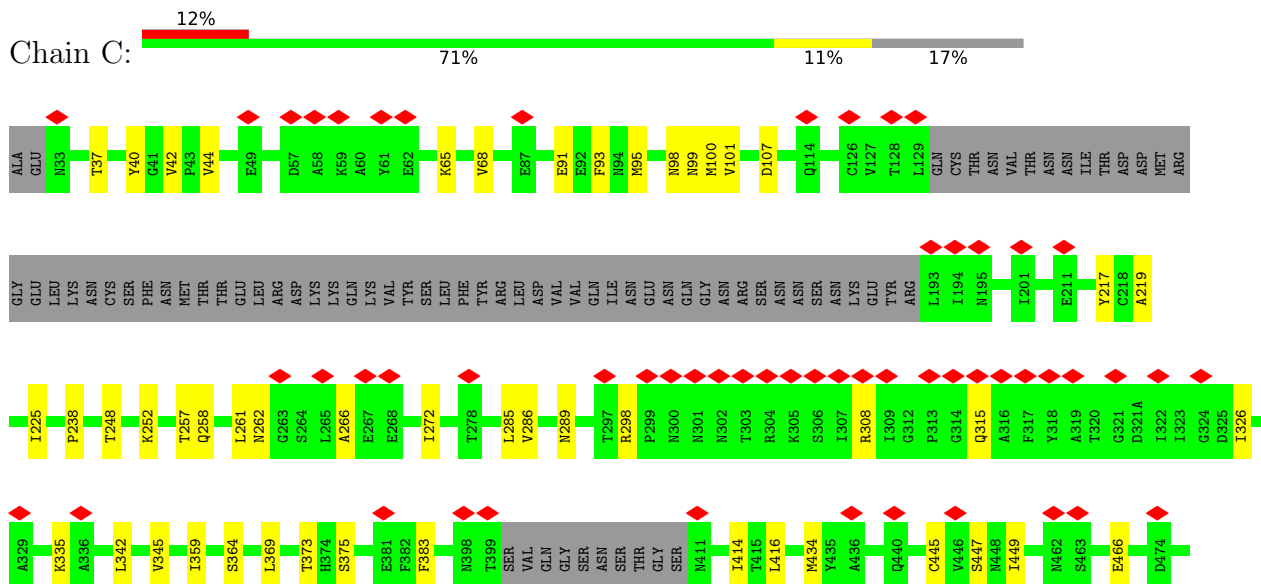
- Molecule 1: Envelope glycoprotein gp120

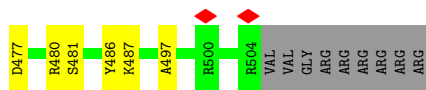
Chain A:



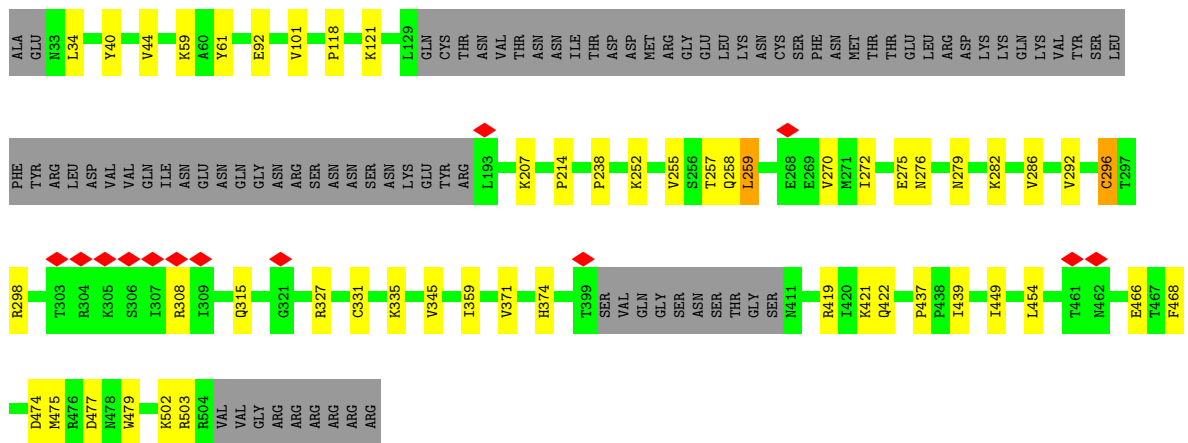
- Molecule 1: Envelope glycoprotein gp120

Chain C:

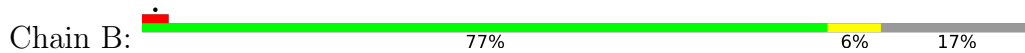




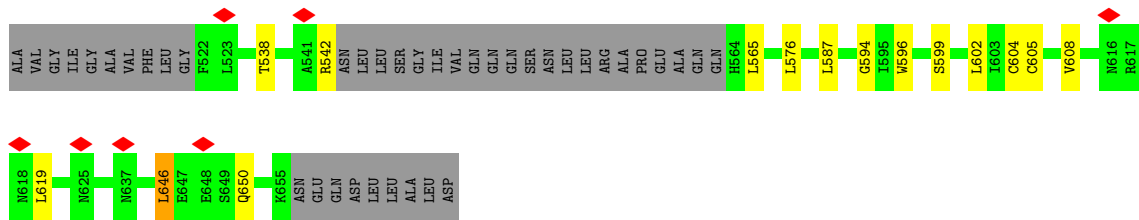
• Molecule 1: Envelope glycoprotein gp120



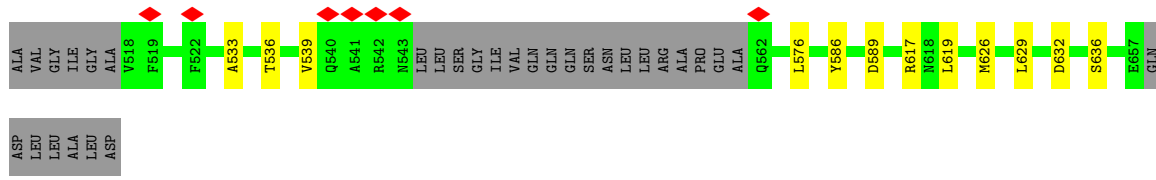
• Molecule 2: Envelope glycoprotein gp41



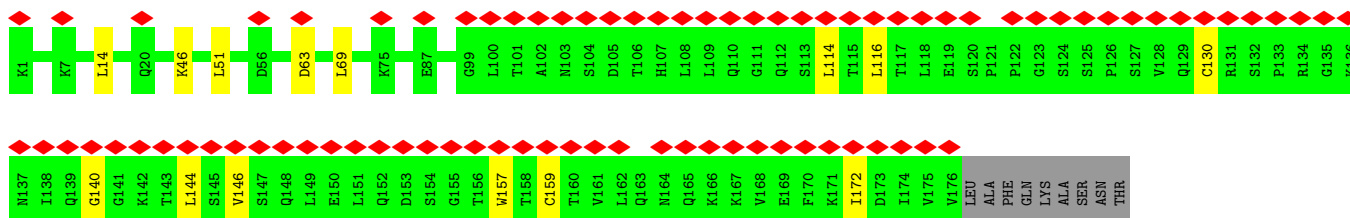
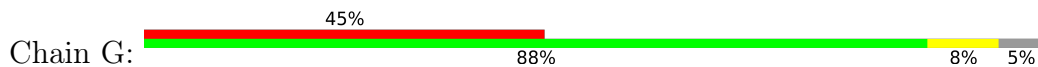
• Molecule 2: Envelope glycoprotein gp41



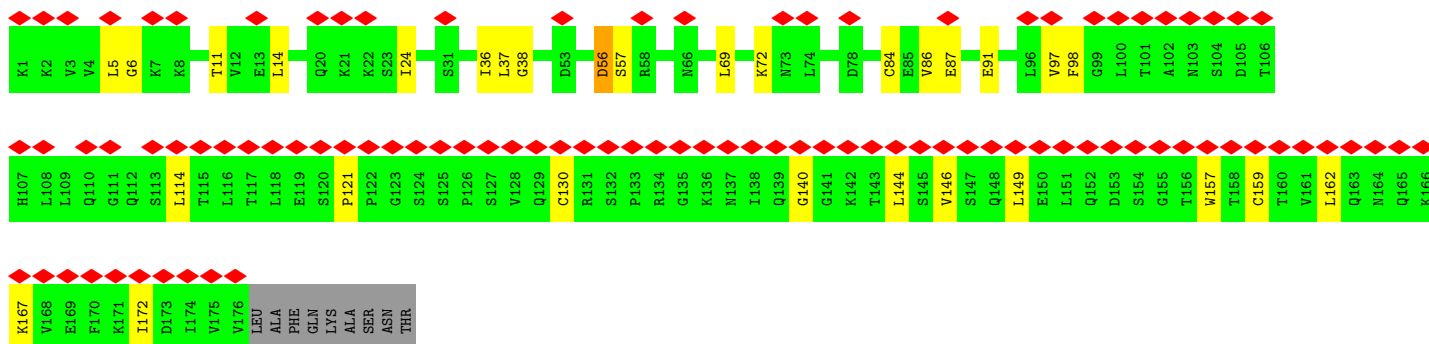
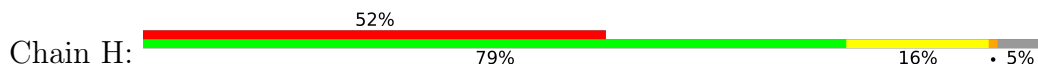
• Molecule 2: Envelope glycoprotein gp41



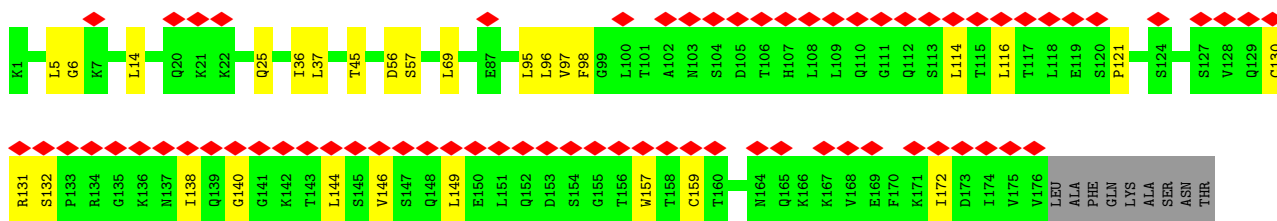
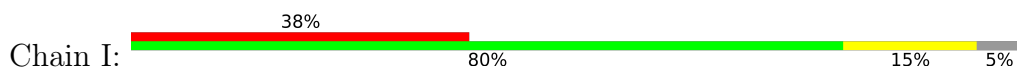
• Molecule 3: T-cell surface glycoprotein CD4



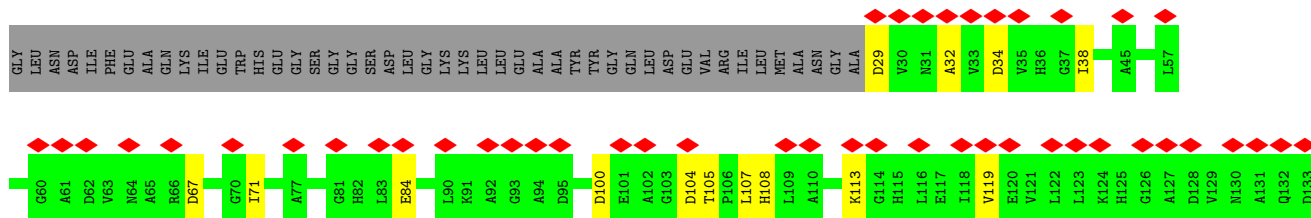
• Molecule 3: T-cell surface glycoprotein CD4



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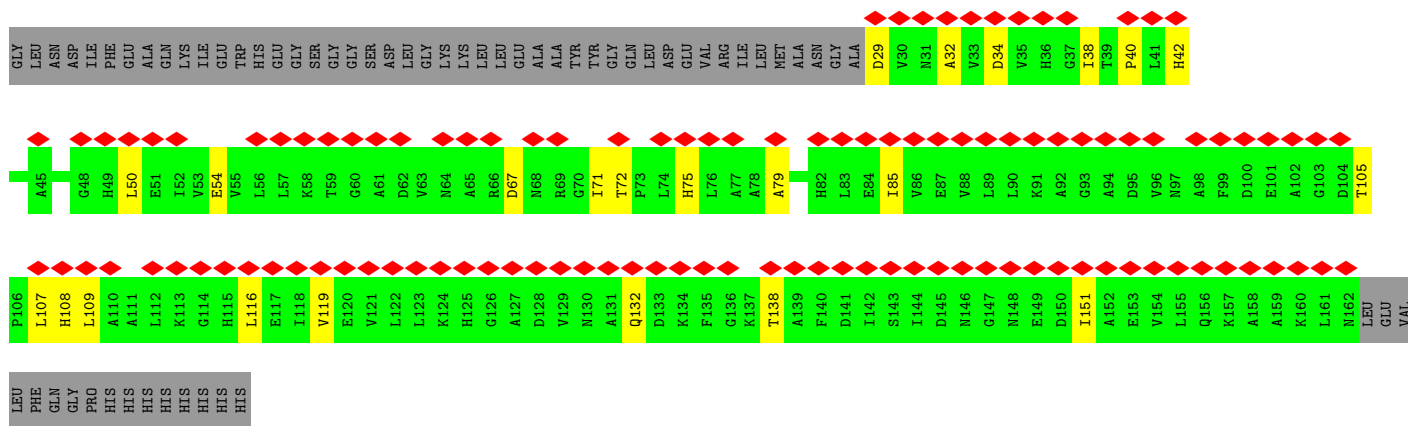


• Molecule 4: Broadly neutralizing darpin bnd.9

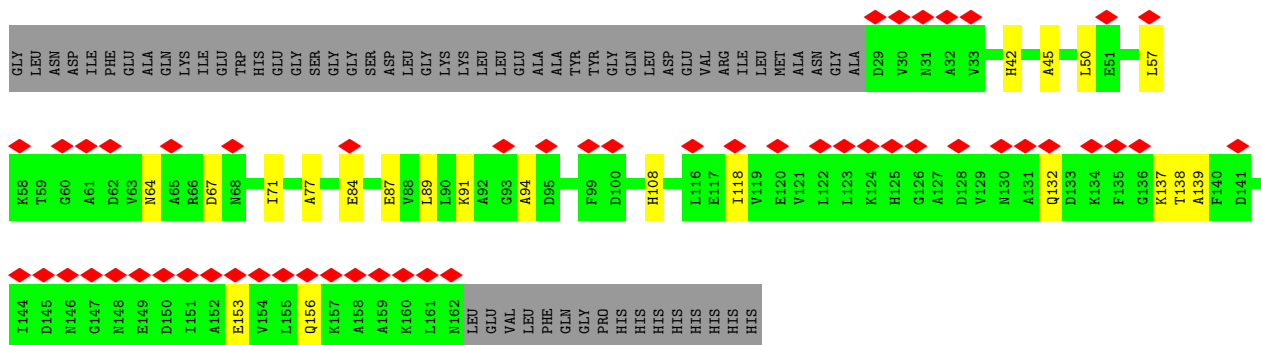




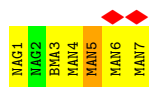
- Molecule 4: Broadly neutralizing darpin bnd.9



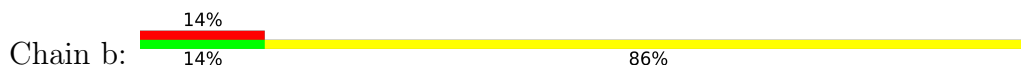
- Molecule 4: Broadly neutralizing darpin bnd.9



- Molecule 5: 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 5: 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 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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





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



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



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



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



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



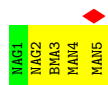
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115325	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.520	Depositor
Minimum map value	-0.672	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.27	Depositor
Map size ( $\text{\AA}$ )	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	2/3170 (0.1%)	0.64	3/4311 (0.1%)
1	C	0.30	0/3170	0.59	1/4311 (0.0%)
1	E	0.29	0/3170	0.59	3/4311 (0.1%)
2	B	0.30	0/1023	0.62	1/1387 (0.1%)
2	D	0.30	0/917	0.75	2/1243 (0.2%)
2	F	0.30	0/982	0.59	0/1331
3	G	0.28	0/1389	0.62	2/1873 (0.1%)
3	H	0.30	0/1389	0.66	1/1873 (0.1%)
3	I	0.27	0/1389	0.58	0/1873
4	J	0.33	0/1017	0.60	1/1382 (0.1%)
4	K	0.33	0/1017	0.58	0/1382
4	L	0.31	0/1017	0.59	0/1382
All	All	0.30	2/19650 (0.0%)	0.61	14/26659 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	CYS	CB-SG	7.46	1.95	1.82
1	A	296	CYS	CB-SG	-6.65	1.71	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	CYS	CA-CB-SG	12.91	137.25	114.00
3	G	63	ASP	CB-CG-OD2	8.55	126.00	118.30
1	E	296	CYS	CA-CB-SG	7.49	127.48	114.00
2	D	646	LEU	CA-CB-CG	6.95	131.28	115.30
1	A	78	ASP	CB-CG-OD2	6.87	124.48	118.30
3	H	56	ASP	CB-CG-OD2	6.73	124.36	118.30
1	E	477	ASP	CB-CG-OD1	6.57	124.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ASP	CB-CG-OD2	6.42	124.08	118.30
1	E	259	LEU	CA-CB-CG	6.21	129.59	115.30
2	D	619	LEU	CA-CB-CG	6.08	129.28	115.30
2	B	544	LEU	CA-CB-CG	5.53	128.01	115.30
3	G	51	LEU	CA-CB-CG	5.53	128.01	115.30
1	C	416	LEU	CA-CB-CG	5.39	127.70	115.30
4	J	155	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3101	0	3043	30	0
1	C	3101	0	3044	32	0
1	E	3101	0	3043	29	0
2	B	1004	0	995	7	0
2	D	900	0	878	10	0
2	F	965	0	929	9	0
3	G	1370	0	1398	8	0
3	H	1370	0	1398	17	0
3	I	1370	0	1398	18	0
4	J	1002	0	1002	9	0
4	K	1002	0	1002	13	0
4	L	1002	0	1002	12	0
5	M	83	0	70	1	0
5	b	83	0	70	0	0
6	N	39	0	34	0	0
6	P	39	0	34	0	0
6	T	39	0	34	0	0
6	Y	39	0	34	0	0
6	Z	39	0	34	1	0
6	c	39	0	34	0	0
6	e	39	0	34	0	0
6	f	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	28	0	25	0	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	1	0
7	a	28	0	25	0	0
7	d	28	0	25	0	0
7	g	28	0	25	0	0
7	h	28	0	25	0	0
8	V	61	0	52	1	0
9	A	84	0	78	1	0
9	B	42	0	39	0	0
9	C	98	0	91	0	0
9	D	42	0	39	0	0
9	E	112	0	104	1	0
9	F	42	0	39	0	0
All	All	20555	0	20261	179	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 4.

All (179) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:CYS:HB3	1:A:331:CYS:HA	1.74	0.69
1:C:257:THR:HG22	1:C:258:GLN:HG3	1.79	0.64
2:D:608:VAL:HG21	2:D:646:LEU:HD13	1.81	0.63
3:H:130:CYS:HA	3:H:159:CYS:HA	1.81	0.60
3:I:131:ARG:NH1	3:I:132:SER:O	2.34	0.60
3:H:140:GLY:HA3	3:H:144:LEU:HD21	1.83	0.60
1:E:257:THR:HG22	1:E:258:GLN:HG3	1.84	0.59
4:L:64:ASN:OD1	4:L:94:ALA:HA	2.02	0.59
4:K:29:ASP:HB3	4:K:32:ALA:HB2	1.84	0.59
1:E:359:ILE:HG22	1:E:466:GLU:HB2	1.84	0.58
1:C:477:ASP:OD1	1:C:480:ARG:NH2	2.37	0.58
3:H:98:PHE:HB3	3:H:121:PRO:HD3	1.86	0.57
1:E:101:VAL:HG23	1:E:479:TRP:HB2	1.86	0.57
1:E:371:VAL:HG11	3:I:45:THR:HG22	1.87	0.57
1:A:36:VAL:HG22	2:B:610:TRP:HE3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:84:CYS:HB2	3:H:91:GLU:HB3	1.89	0.55
1:E:296:CYS:HB3	1:E:331:CYS:HA	1.89	0.55
1:E:298:ARG:NH2	1:E:439:ILE:O	2.39	0.55
1:E:454:LEU:HD12	1:E:468:PHE:HB3	1.87	0.55
1:A:59:LYS:HG2	1:A:61:TYR:OH	2.07	0.54
1:A:359:ILE:HG22	1:A:466:GLU:HB2	1.89	0.54
1:E:292:VAL:HB	1:E:449:ILE:HB	1.88	0.54
3:I:130:CYS:HB2	3:I:138:ILE:HB	1.88	0.54
1:C:308:ARG:HB3	1:C:315:GLN:HG2	1.88	0.54
3:I:98:PHE:HB3	3:I:121:PRO:HD3	1.90	0.54
1:A:374:HIS:O	1:A:384:TYR:HA	2.08	0.54
4:J:67:ASP:OD1	4:J:71:ILE:N	2.39	0.54
1:A:258:GLN:HG2	1:A:470:PRO:HB2	1.90	0.54
1:E:275:GLU:OE1	1:E:282:LYS:NZ	2.41	0.54
3:I:130:CYS:HA	3:I:159:CYS:HA	1.90	0.54
1:A:298:ARG:NH2	1:A:439:ILE:O	2.41	0.53
1:C:434:MET:CE	4:K:40:PRO:HB3	2.39	0.53
1:E:270:VAL:HG11	1:E:345:VAL:HG12	1.90	0.53
3:G:140:GLY:HA3	3:G:144:LEU:HD21	1.91	0.53
1:E:255:VAL:HA	1:E:475:MET:HE1	1.90	0.53
1:A:298:ARG:NH1	1:A:326:ILE:O	2.42	0.52
1:E:207:LYS:NZ	1:E:437:PRO:O	2.42	0.52
1:E:327:ARG:NH2	1:E:422:GLN:OE1	2.40	0.52
2:B:617:ARG:NH2	2:B:626:MET:SD	2.82	0.52
1:A:374:HIS:HB3	1:A:385:CYS:HB2	1.91	0.52
1:C:445:CYS:HB3	8:V:2:NAG:H61	1.91	0.52
4:L:45:ALA:HB1	4:L:77:ALA:HB2	1.92	0.52
1:A:275:GLU:HB3	1:A:282:LYS:HG3	1.91	0.52
2:F:617:ARG:NH1	2:F:626:MET:SD	2.83	0.51
3:I:114:LEU:HB3	3:I:146:VAL:HB	1.92	0.51
1:C:91:GLU:O	1:C:238:PRO:HA	2.11	0.51
1:C:37:THR:HG22	2:D:605:CYS:HA	1.93	0.51
3:G:130:CYS:HA	3:G:159:CYS:HA	1.91	0.51
1:C:447:SER:HA	7:X:1:NAG:H82	1.91	0.51
4:J:34:ASP:OD1	4:J:38:ILE:N	2.44	0.51
4:L:108:HIS:HD2	4:L:139:ALA:HB2	1.76	0.50
3:I:114:LEU:HD12	3:I:149:LEU:HD22	1.92	0.50
4:K:38:ILE:HG23	4:K:42:HIS:HB2	1.94	0.50
1:A:219:ALA:O	1:A:246:GLN:NE2	2.44	0.50
1:A:441:GLY:HA3	5:M:5:MAN:H61	1.94	0.50
2:D:594:GLY:HA2	2:D:599:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:105:THR:OG1	4:K:108:HIS:ND1	2.42	0.49
4:K:132:GLN:HG2	4:K:138:THR:HG22	1.93	0.49
1:C:298:ARG:NH1	1:C:326:ILE:O	2.45	0.49
1:E:474:ASP:OD2	3:I:25:GLN:NE2	2.41	0.49
3:I:56:ASP:OD2	3:I:57:SER:N	2.46	0.49
4:K:67:ASP:OD1	4:K:71:ILE:N	2.44	0.49
3:I:5:LEU:HD12	3:I:98:PHE:HE1	1.77	0.49
1:C:272:ILE:HG22	1:C:286:VAL:HG22	1.94	0.49
2:D:596:TRP:HA	2:D:650:GLN:HG3	1.93	0.49
4:J:141:ASP:HA	4:J:144:ILE:HG12	1.95	0.49
1:E:34:LEU:HD21	2:F:619:LEU:HD22	1.95	0.49
3:I:116:LEU:HD12	3:I:144:LEU:HB2	1.95	0.49
4:J:105:THR:OG1	4:J:108:HIS:ND1	2.37	0.49
4:L:57:LEU:HD21	4:L:89:LEU:HD23	1.95	0.49
1:C:107:ASP:OD2	1:C:217:TYR:OH	2.31	0.48
3:H:114:LEU:HB3	3:H:146:VAL:HB	1.95	0.48
1:A:101:VAL:C	1:A:103:GLN:H	2.16	0.48
1:A:454:LEU:HD23	1:A:468:PHE:HB3	1.95	0.48
3:H:36:ILE:HG22	3:H:37:LEU:HD12	1.94	0.48
3:I:140:GLY:HA3	3:I:144:LEU:HD21	1.96	0.48
2:D:538:THR:O	2:D:542:ARG:NH1	2.47	0.48
1:E:308:ARG:O	1:E:315:GLN:NE2	2.46	0.48
1:E:44:VAL:HG22	2:F:629:LEU:HA	1.96	0.48
1:A:496:VAL:HG11	2:B:642:ILE:HG21	1.95	0.47
4:L:87:GLU:O	4:L:91:LYS:HG2	2.12	0.47
3:H:162:LEU:HD12	3:H:167:LYS:HD3	1.96	0.47
3:I:6:GLY:HA3	3:I:97:VAL:HG22	1.95	0.47
2:F:533:ALA:HA	2:F:536:THR:HG22	1.96	0.47
4:K:34:ASP:OD1	4:K:38:ILE:N	2.47	0.47
1:E:272:ILE:HG22	1:E:286:VAL:HG22	1.97	0.47
1:A:38:VAL:HG12	1:A:496:VAL:HG22	1.96	0.47
4:J:100:ASP:OD1	4:J:104:ASP:N	2.44	0.47
4:J:29:ASP:HB3	4:J:32:ALA:HB2	1.95	0.47
3:G:114:LEU:HB3	3:G:146:VAL:HB	1.97	0.46
4:K:107:LEU:HD11	4:K:119:VAL:HG13	1.97	0.46
2:D:604:CYS:SG	2:D:605:CYS:N	2.89	0.46
1:A:297:THR:HG22	1:A:444:ARG:HG3	1.98	0.46
2:B:577:GLN:HG2	2:D:576:LEU:HD21	1.97	0.46
3:H:157:TRP:HB2	3:H:172:ILE:HD12	1.96	0.46
1:C:40:TYR:HB3	2:D:602:LEU:HD13	1.98	0.46
1:C:252:LYS:HD2	1:C:262:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:14:LEU:HD12	3:I:69:LEU:HD23	1.98	0.46
4:L:132:GLN:HG2	4:L:138:THR:HG22	1.97	0.46
1:A:214:PRO:HD3	1:A:252:LYS:HE2	1.98	0.46
3:G:14:LEU:HB2	3:G:69:LEU:HB3	1.98	0.46
1:E:259:LEU:HD22	1:E:374:HIS:HD2	1.81	0.46
3:G:116:LEU:HD12	3:G:144:LEU:HB2	1.98	0.46
1:E:258:GLN:NE2	1:E:371:VAL:O	2.49	0.45
1:E:419:ARG:HG2	1:E:421:LYS:HG2	1.98	0.45
3:H:11:THR:HG22	3:H:72:LYS:HG2	1.98	0.45
1:A:292:VAL:HB	1:A:449:ILE:HB	1.98	0.45
3:H:5:LEU:HD12	3:H:98:PHE:HE1	1.81	0.45
1:C:37:THR:OG1	1:C:497:ALA:O	2.32	0.45
1:C:266:ALA:HB3	1:C:289:ASN:HA	1.98	0.45
1:C:93:PHE:HE1	1:C:487:LYS:HB2	1.82	0.45
1:C:364:SER:HB2	6:Z:1:NAG:H82	1.99	0.45
3:H:24:ILE:HD11	3:H:86:VAL:HG12	1.97	0.45
3:H:56:ASP:OD2	3:H:57:SER:N	2.50	0.45
3:I:36:ILE:HG22	3:I:37:LEU:HD12	1.99	0.45
1:C:342:LEU:HA	1:C:345:VAL:HG12	1.99	0.45
4:L:118:ILE:HD12	4:L:118:ILE:HA	1.82	0.45
1:C:95:MET:HA	1:C:98:ASN:HB2	2.00	0.44
4:L:67:ASP:OD1	4:L:71:ILE:N	2.40	0.44
4:L:153:GLU:HA	4:L:156:GLN:HG3	1.99	0.44
1:E:214:PRO:HD3	1:E:252:LYS:HE2	2.00	0.44
3:H:114:LEU:HD12	3:H:149:LEU:HD22	1.99	0.44
3:I:5:LEU:HD13	3:I:96:LEU:HB2	1.99	0.44
1:E:92:GLU:HA	1:E:238:PRO:HB3	1.99	0.44
2:F:536:THR:HA	2:F:539:VAL:HG22	1.98	0.44
4:K:50:LEU:HG	4:K:54:GLU:OE2	2.18	0.44
1:C:65:LYS:HA	1:C:68:VAL:HG12	1.99	0.44
3:H:6:GLY:HA3	3:H:97:VAL:HG22	2.00	0.44
4:K:72:THR:HG23	4:K:75:HIS:H	1.83	0.44
1:A:292:VAL:HG11	1:A:338:TRP:HD1	1.82	0.44
1:C:219:ALA:HB2	1:C:225:ILE:HG13	1.99	0.44
1:E:276:ASN:HB3	1:E:279:ASN:HB2	2.00	0.44
4:J:113:LYS:HA	4:J:113:LYS:HD3	1.75	0.44
2:B:576:LEU:HD21	2:F:576:LEU:HB3	1.99	0.44
1:C:42:VAL:HG12	1:C:44:VAL:HG23	2.00	0.43
3:G:146:VAL:HG21	3:G:157:TRP:HZ3	1.83	0.43
1:A:365:SER:OG	3:G:46:LYS:O	2.30	0.43
1:C:369:LEU:O	1:C:373:THR:OG1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:TYR:HE2	2:F:589:ASP:HB3	1.82	0.43
1:A:272:ILE:HG22	1:A:286:VAL:HG22	2.00	0.43
1:C:335:LYS:HE2	1:C:414:ILE:HB	2.00	0.43
4:K:79:ALA:HB2	4:K:109:LEU:HB3	1.99	0.43
4:L:42:HIS:NE2	4:L:71:ILE:O	2.49	0.43
1:C:285:LEU:HD23	1:C:481:SER:HB2	2.01	0.43
2:B:570:VAL:HG21	2:D:565:LEU:HD13	2.00	0.43
1:A:378:CYS:HB2	1:A:383:PHE:HE1	1.84	0.42
1:E:502:LYS:NZ	1:E:503:ARG:O	2.45	0.42
1:A:335:LYS:HD3	9:A:603:NAG:H81	2.00	0.42
1:E:118:PRO:HG2	1:E:121:LYS:HD3	2.00	0.42
3:I:157:TRP:HB2	3:I:172:ILE:HD12	1.99	0.42
1:A:101:VAL:O	1:A:103:GLN:N	2.52	0.42
4:K:116:LEU:HD13	4:K:151:ILE:HG12	2.02	0.42
3:H:87:GLU:OE2	3:H:87:GLU:N	2.53	0.42
4:J:84:GLU:H	4:J:84:GLU:HG3	1.65	0.42
1:A:101:VAL:C	1:A:103:GLN:N	2.73	0.42
2:D:587:LEU:HD12	2:F:586:TYR:HE2	1.85	0.42
1:C:449:ILE:HD13	1:C:449:ILE:HA	1.93	0.42
3:H:14:LEU:O	3:H:69:LEU:N	2.53	0.42
2:F:632:ASP:O	2:F:636:SER:OG	2.37	0.41
1:A:97:LYS:HA	1:A:97:LYS:HD3	1.88	0.41
3:I:14:LEU:HD11	3:I:95:LEU:HD12	2.02	0.41
1:C:99:ASN:O	1:C:100:MET:C	2.59	0.41
1:C:248:THR:HA	1:C:486:TYR:HE1	1.86	0.41
1:C:99:ASN:O	1:C:101:VAL:N	2.54	0.41
1:C:261:LEU:HA	1:C:449:ILE:HD13	2.03	0.41
1:C:375:SER:HA	1:C:383:PHE:O	2.20	0.41
4:L:50:LEU:HD13	4:L:84:GLU:HB3	2.02	0.41
1:C:359:ILE:HG22	1:C:466:GLU:HB2	2.03	0.41
3:G:157:TRP:HB2	3:G:172:ILE:HD12	2.03	0.41
3:H:37:LEU:HB3	3:H:38:GLY:H	1.77	0.41
2:B:638:TYR:O	2:B:642:ILE:HG12	2.21	0.40
1:E:59:LYS:HB3	1:E:61:TYR:CE1	2.56	0.40
4:J:107:LEU:HD11	4:J:119:VAL:HG13	2.02	0.40
1:A:102:GLU:H	1:A:102:GLU:HG2	1.76	0.40
1:E:335:LYS:NZ	9:E:608:NAG:O7	2.51	0.40
1:A:59:LYS:HB3	1:A:61:TYR:CE1	2.57	0.40
4:K:50:LEU:HD13	4:K:85:ILE:HG12	2.04	0.40
1:A:82:GLN:HE21	1:A:84:ILE:HD11	1.87	0.40
4:L:137:LYS:HB2	4:L:137:LYS:HE2	1.79	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	391/481 (81%)	375 (96%)	16 (4%)	0	100	100
1	C	391/481 (81%)	378 (97%)	13 (3%)	0	100	100
1	E	391/481 (81%)	376 (96%)	15 (4%)	0	100	100
2	B	123/153 (80%)	120 (98%)	3 (2%)	0	100	100
2	D	109/153 (71%)	106 (97%)	3 (3%)	0	100	100
2	F	118/153 (77%)	118 (100%)	0	0	100	100
3	G	174/185 (94%)	163 (94%)	11 (6%)	0	100	100
3	H	174/185 (94%)	157 (90%)	17 (10%)	0	100	100
3	I	174/185 (94%)	157 (90%)	17 (10%)	0	100	100
4	J	132/196 (67%)	126 (96%)	6 (4%)	0	100	100
4	K	132/196 (67%)	128 (97%)	4 (3%)	0	100	100
4	L	132/196 (67%)	127 (96%)	5 (4%)	0	100	100
All	All	2441/3045 (80%)	2331 (96%)	110 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/428 (82%)	349 (100%)	1 (0%)	92	95
1	C	350/428 (82%)	350 (100%)	0	100	100
1	E	350/428 (82%)	350 (100%)	0	100	100
2	B	107/129 (83%)	107 (100%)	0	100	100
2	D	96/129 (74%)	96 (100%)	0	100	100
2	F	102/129 (79%)	102 (100%)	0	100	100
3	G	160/167 (96%)	160 (100%)	0	100	100
3	H	160/167 (96%)	160 (100%)	0	100	100
3	I	160/167 (96%)	160 (100%)	0	100	100
4	J	103/152 (68%)	103 (100%)	0	100	100
4	K	103/152 (68%)	103 (100%)	0	100	100
4	L	103/152 (68%)	103 (100%)	0	100	100
All	All	2144/2628 (82%)	2143 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	504	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

65 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
5	NAG	M	1	5,1	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
5	NAG	M	2	5	14,14,15	0.30	0	17,19,21	0.52	0
5	BMA	M	3	5	11,11,12	0.67	0	15,15,17	1.06	1 (6%)
5	MAN	M	4	5	11,11,12	0.87	1 (9%)	15,15,17	1.29	2 (13%)
5	MAN	M	5	5	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
5	MAN	M	6	5	11,11,12	0.87	0	15,15,17	0.96	2 (13%)
5	MAN	M	7	5	11,11,12	0.83	0	15,15,17	1.15	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.34	0	17,19,21	0.60	1 (5%)
6	NAG	N	2	6	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
6	BMA	N	3	6	11,11,12	0.75	0	15,15,17	0.86	1 (6%)
7	NAG	O	1	7,1	14,14,15	0.78	1 (7%)	17,19,21	0.65	1 (5%)
7	NAG	O	2	7	14,14,15	0.41	0	17,19,21	0.45	0
6	NAG	P	1	6,1	14,14,15	0.23	0	17,19,21	0.58	0
6	NAG	P	2	6	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
6	BMA	P	3	6	11,11,12	0.83	0	15,15,17	0.78	0
7	NAG	Q	1	7,1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
7	NAG	Q	2	7	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
7	NAG	R	1	7,1	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
7	NAG	R	2	7	14,14,15	0.59	0	17,19,21	0.57	0
7	NAG	S	1	7,1	14,14,15	0.44	0	17,19,21	1.01	1 (5%)
7	NAG	S	2	7	14,14,15	0.51	0	17,19,21	1.04	2 (11%)
6	NAG	T	1	6,1	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
6	NAG	T	2	6	14,14,15	0.31	0	17,19,21	0.56	0
6	BMA	T	3	6	11,11,12	0.78	0	15,15,17	0.86	0
7	NAG	U	1	2,7	14,14,15	0.27	0	17,19,21	0.53	0
7	NAG	U	2	7	14,14,15	0.52	0	17,19,21	1.04	2 (11%)
8	NAG	V	1	8,1	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	V	2	8	14,14,15	0.23	0	17,19,21	0.61	0
8	BMA	V	3	8	11,11,12	1.53	3 (27%)	15,15,17	1.00	0
8	MAN	V	4	8	11,11,12	0.85	0	15,15,17	1.12	2 (13%)
8	MAN	V	5	8	11,11,12	0.78	0	15,15,17	1.13	2 (13%)
7	NAG	W	1	7,1	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
7	NAG	W	2	7	14,14,15	0.36	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	X	1	7,1	14,14,15	0.65	0	17,19,21	0.65	1 (5%)
7	NAG	X	2	7	14,14,15	0.39	0	17,19,21	0.45	0
6	NAG	Y	1	6,1	14,14,15	0.34	0	17,19,21	0.55	0
6	NAG	Y	2	6	14,14,15	0.76	1 (7%)	17,19,21	2.24	3 (17%)
6	BMA	Y	3	6	11,11,12	0.76	0	15,15,17	0.93	1 (6%)
6	NAG	Z	1	6,1	14,14,15	0.29	0	17,19,21	0.53	0
6	NAG	Z	2	6	14,14,15	0.30	0	17,19,21	0.56	0
6	BMA	Z	3	6	11,11,12	0.79	0	15,15,17	0.86	0
7	NAG	a	1	7,1	14,14,15	0.30	0	17,19,21	0.61	0
7	NAG	a	2	7	14,14,15	0.62	0	17,19,21	1.05	2 (11%)
5	NAG	b	1	5,1	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	b	2	5	14,14,15	0.72	0	17,19,21	2.28	3 (17%)
5	BMA	b	3	5	11,11,12	0.80	0	15,15,17	1.25	2 (13%)
5	MAN	b	4	5	11,11,12	0.83	1 (9%)	15,15,17	1.23	2 (13%)
5	MAN	b	5	5	11,11,12	0.90	0	15,15,17	1.48	3 (20%)
5	MAN	b	6	5	11,11,12	0.88	0	15,15,17	0.98	2 (13%)
5	MAN	b	7	5	11,11,12	0.79	0	15,15,17	1.14	2 (13%)
6	NAG	c	1	6,1	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
6	NAG	c	2	6	14,14,15	0.32	0	17,19,21	0.47	0
6	BMA	c	3	6	11,11,12	0.81	0	15,15,17	0.79	0
7	NAG	d	1	7,1	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	d	2	7	14,14,15	0.38	0	17,19,21	0.47	0
6	NAG	e	1	6,1	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
6	NAG	e	2	6	14,14,15	0.37	0	17,19,21	0.60	1 (5%)
6	BMA	e	3	6	11,11,12	0.77	0	15,15,17	0.83	0
6	NAG	f	1	6,1	14,14,15	0.28	0	17,19,21	0.54	0
6	NAG	f	2	6	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
6	BMA	f	3	6	11,11,12	0.83	0	15,15,17	0.79	0
7	NAG	g	1	7,1	14,14,15	0.37	0	17,19,21	0.59	0
7	NAG	g	2	7	14,14,15	0.49	0	17,19,21	0.54	0
7	NAG	h	1	2,7	14,14,15	0.29	0	17,19,21	1.27	2 (11%)
7	NAG	h	2	7	14,14,15	0.38	0	17,19,21	1.07	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	3	BMA	C2-C3	2.93	1.56	1.52
8	V	3	BMA	O3-C3	2.51	1.48	1.43
8	V	3	BMA	C4-C3	2.37	1.58	1.52
5	M	4	MAN	C1-C2	2.34	1.57	1.52
7	O	1	NAG	O5-C1	2.19	1.47	1.43
6	Y	2	NAG	C1-C2	2.12	1.55	1.52
5	b	4	MAN	C1-C2	2.06	1.56	1.52

All (58) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	2	NAG	C2-N2-C7	7.87	134.11	122.90
6	Y	2	NAG	C2-N2-C7	7.86	134.10	122.90
5	b	5	MAN	O2-C2-C3	-3.79	102.54	110.14
6	Y	2	NAG	C1-C2-N2	3.70	116.81	110.49
5	M	4	MAN	C1-O5-C5	3.69	117.19	112.19
5	b	2	NAG	C1-C2-N2	3.58	116.61	110.49
5	M	5	MAN	O2-C2-C3	-3.56	103.00	110.14
5	b	3	BMA	C1-O5-C5	3.30	116.67	112.19
5	b	7	MAN	C1-O5-C5	3.17	116.49	112.19
7	h	2	NAG	C1-O5-C5	3.16	116.47	112.19
8	V	5	MAN	C1-O5-C5	3.10	116.39	112.19
5	b	5	MAN	C1-O5-C5	3.08	116.37	112.19
6	N	2	NAG	C2-N2-C7	3.08	127.29	122.90
6	T	1	NAG	C2-N2-C7	3.07	127.28	122.90
5	M	7	MAN	C1-O5-C5	3.07	116.35	112.19
7	Q	2	NAG	C2-N2-C7	3.06	127.26	122.90
6	e	1	NAG	C2-N2-C7	3.05	127.25	122.90
5	b	4	MAN	C1-O5-C5	3.05	116.32	112.19
7	S	1	NAG	C2-N2-C7	3.04	127.23	122.90
7	R	1	NAG	C2-N2-C7	3.04	127.23	122.90
7	a	2	NAG	C2-N2-C7	3.03	127.21	122.90
7	U	2	NAG	C2-N2-C7	3.01	127.18	122.90
7	S	2	NAG	C2-N2-C7	2.98	127.14	122.90
8	V	4	MAN	C1-O5-C5	2.83	116.02	112.19
5	b	4	MAN	O2-C2-C3	-2.77	104.60	110.14
5	M	3	BMA	C1-O5-C5	2.49	115.56	112.19
7	h	1	NAG	C4-C3-C2	-2.49	107.37	111.02
6	P	2	NAG	C1-O5-C5	2.46	115.53	112.19
5	M	4	MAN	O2-C2-C3	-2.44	105.25	110.14
5	M	5	MAN	C1-O5-C5	2.38	115.42	112.19
5	b	6	MAN	C1-O5-C5	2.28	115.28	112.19
7	h	2	NAG	C1-C2-N2	2.28	114.38	110.49
6	Y	3	BMA	C1-O5-C5	2.26	115.26	112.19
7	h	1	NAG	O4-C4-C3	2.25	115.56	110.35
5	b	6	MAN	O2-C2-C3	-2.23	105.67	110.14
8	V	5	MAN	O2-C2-C3	-2.21	105.70	110.14
7	U	2	NAG	C1-O5-C5	2.21	115.19	112.19
8	V	4	MAN	O2-C2-C3	-2.19	105.75	110.14
5	M	6	MAN	O2-C2-C3	-2.19	105.75	110.14
7	S	2	NAG	C1-O5-C5	2.19	115.15	112.19
5	M	7	MAN	O2-C2-C3	-2.18	105.76	110.14
5	M	6	MAN	C1-O5-C5	2.18	115.15	112.19
6	c	1	NAG	C1-O5-C5	2.17	115.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	2	NAG	C1-O5-C5	2.17	115.13	112.19
7	a	2	NAG	C1-O5-C5	2.16	115.12	112.19
5	b	7	MAN	O2-C2-C3	-2.13	105.88	110.14
7	X	1	NAG	C1-O5-C5	2.12	115.07	112.19
5	b	2	NAG	C8-C7-N2	2.11	119.68	116.10
7	Q	1	NAG	C1-O5-C5	2.10	115.04	112.19
6	Y	2	NAG	C8-C7-N2	2.09	119.63	116.10
7	W	1	NAG	C1-O5-C5	2.08	115.01	112.19
6	e	2	NAG	C1-O5-C5	2.05	114.97	112.19
6	N	3	BMA	C1-O5-C5	2.04	114.95	112.19
7	O	1	NAG	C1-O5-C5	2.02	114.93	112.19
5	M	1	NAG	C1-O5-C5	2.02	114.93	112.19
5	b	5	MAN	C1-C2-C3	-2.02	107.19	109.67
5	b	3	BMA	C1-C2-C3	2.01	112.14	109.67
6	N	1	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	h	1	NAG	O7-C7-N2-C2
6	f	1	NAG	O5-C5-C6-O6
7	h	1	NAG	C8-C7-N2-C2
6	e	1	NAG	O5-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
7	d	1	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
5	b	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	b	2	NAG	O7-C7-N2-C2
6	Y	2	NAG	C8-C7-N2-C2
6	Y	2	NAG	O7-C7-N2-C2
7	R	2	NAG	C8-C7-N2-C2
7	R	2	NAG	O7-C7-N2-C2
8	V	2	NAG	C8-C7-N2-C2
8	V	2	NAG	O7-C7-N2-C2
7	d	1	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
7	h	1	NAG	C1-C2-N2-C7
5	b	2	NAG	C4-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
8	V	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
6	f	3	BMA	O5-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
7	a	1	NAG	O5-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
8	V	3	BMA	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6

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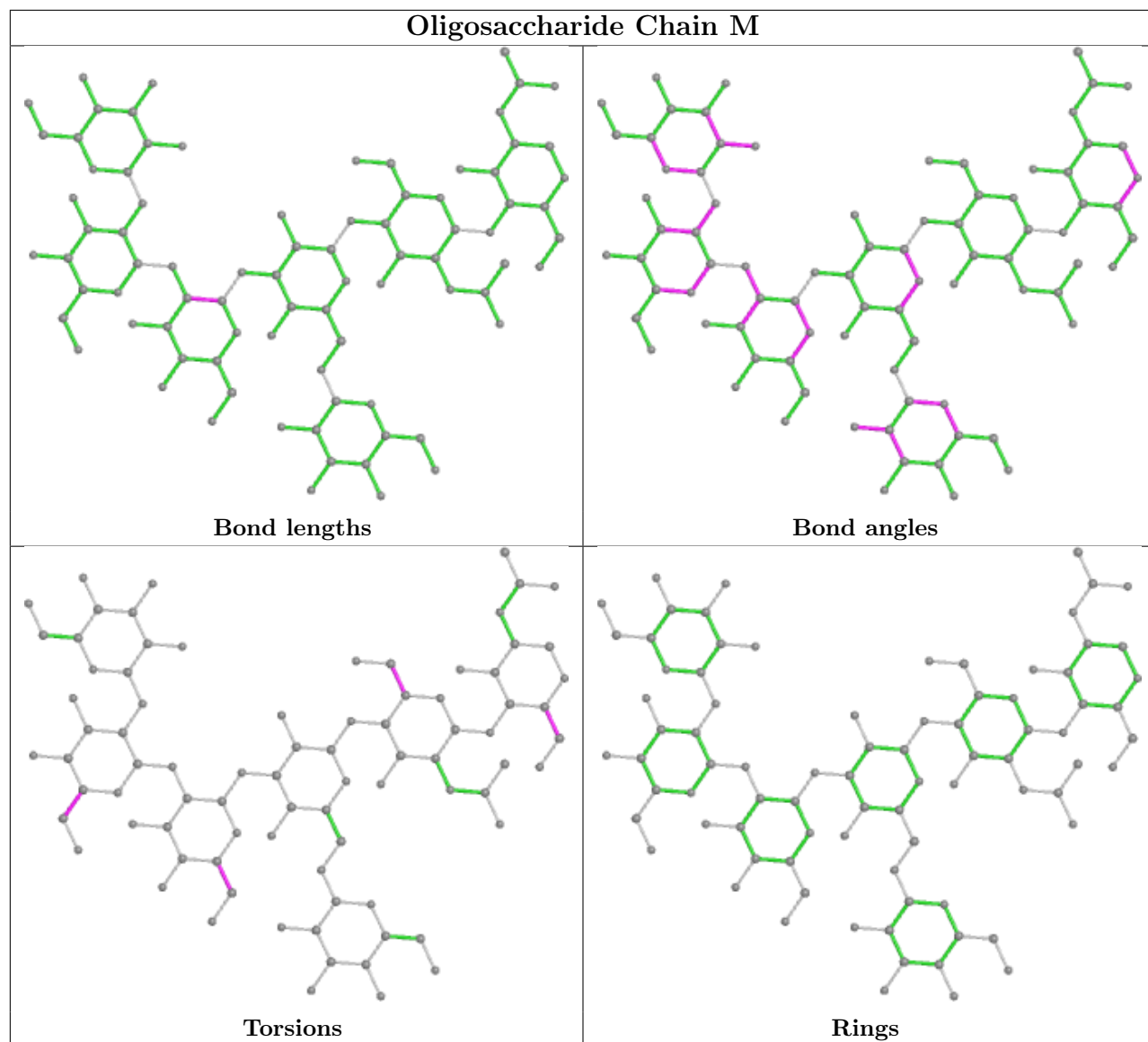
Mol	Chain	Res	Type	Atoms
5	b	2	NAG	C3-C2-N2-C7
8	V	3	BMA	O5-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
5	M	5	MAN	C4-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	X	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C3-C2-N2-C7
6	T	1	NAG	C3-C2-N2-C7
6	Y	2	NAG	C3-C2-N2-C7
6	e	1	NAG	C3-C2-N2-C7
7	Q	2	NAG	C3-C2-N2-C7
7	R	1	NAG	C3-C2-N2-C7
7	S	1	NAG	C3-C2-N2-C7
7	S	2	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
6	T	2	NAG	O5-C5-C6-O6

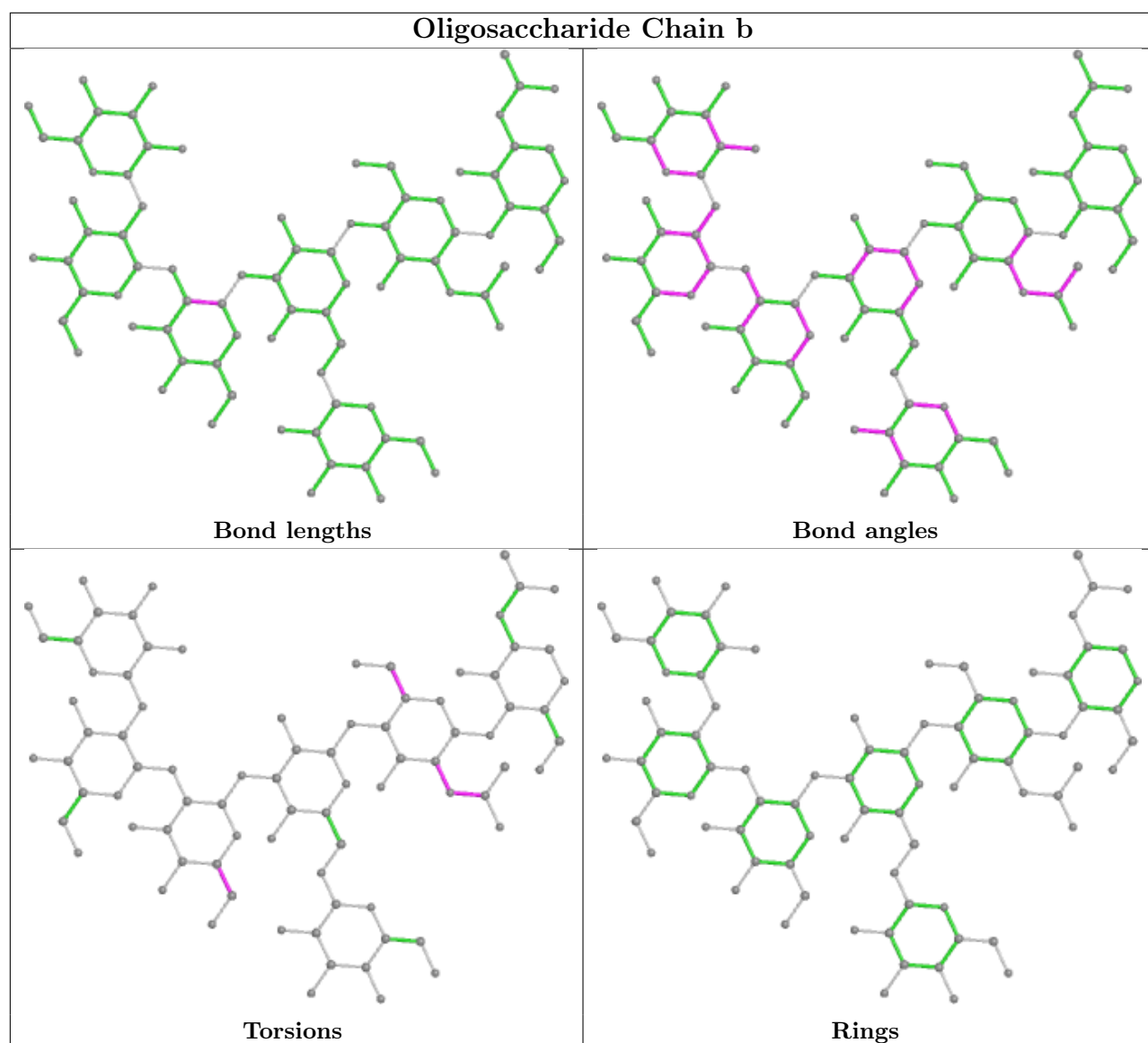
There are no ring outliers.

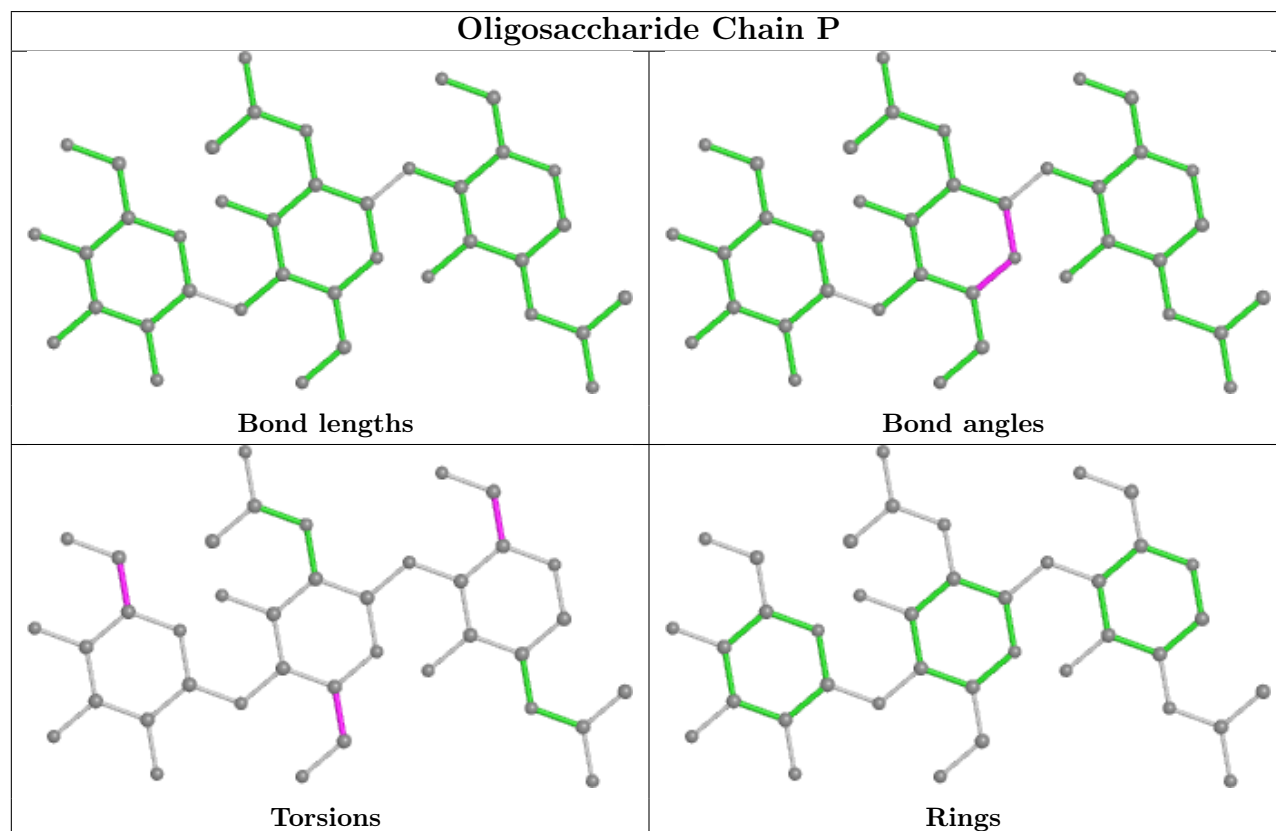
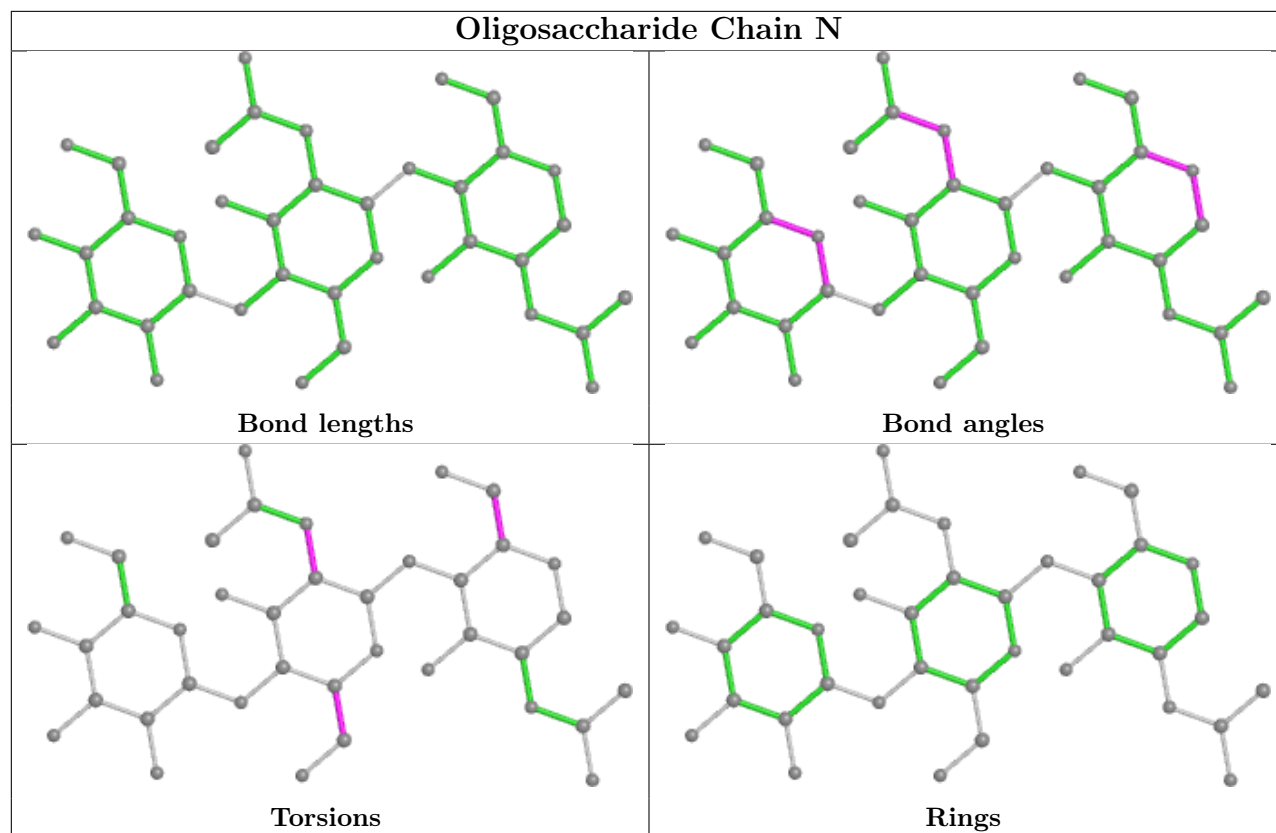
4 monomers are involved in 4 short contacts:

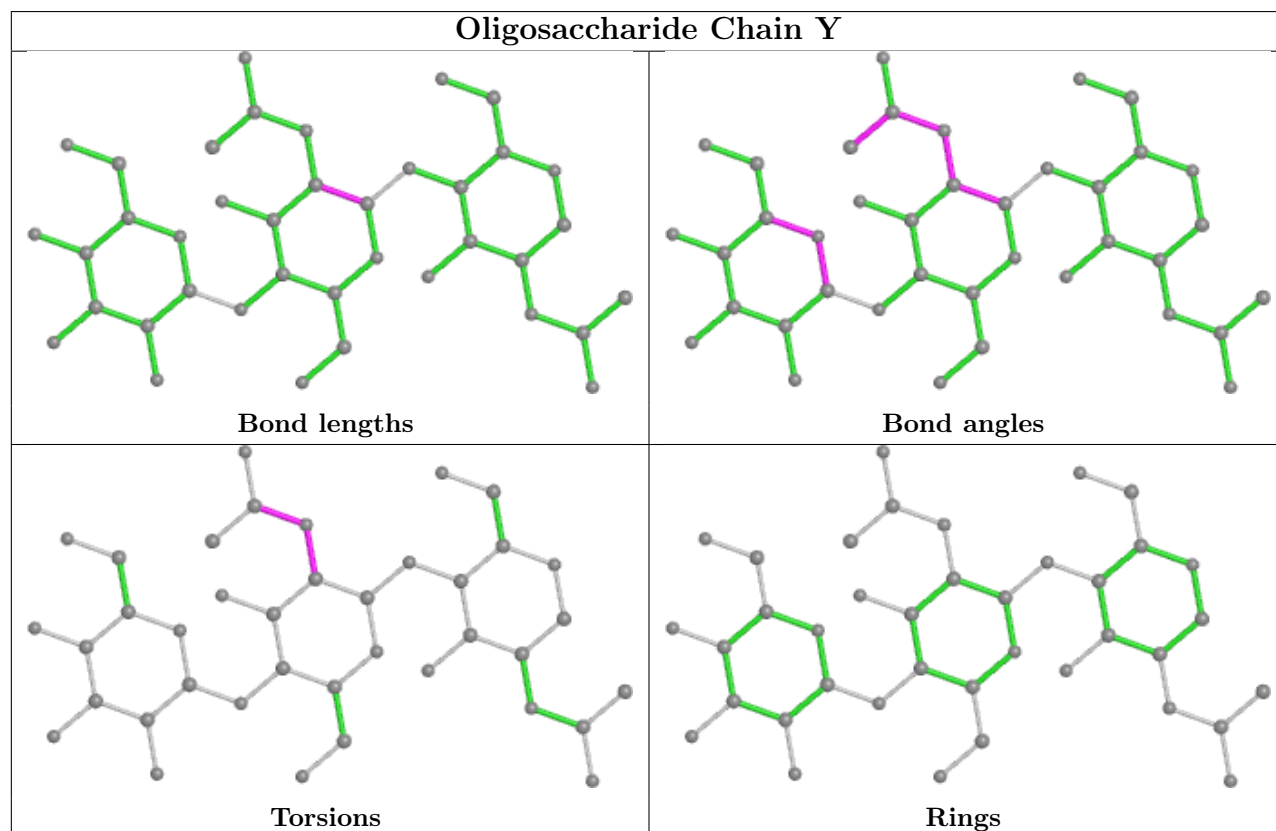
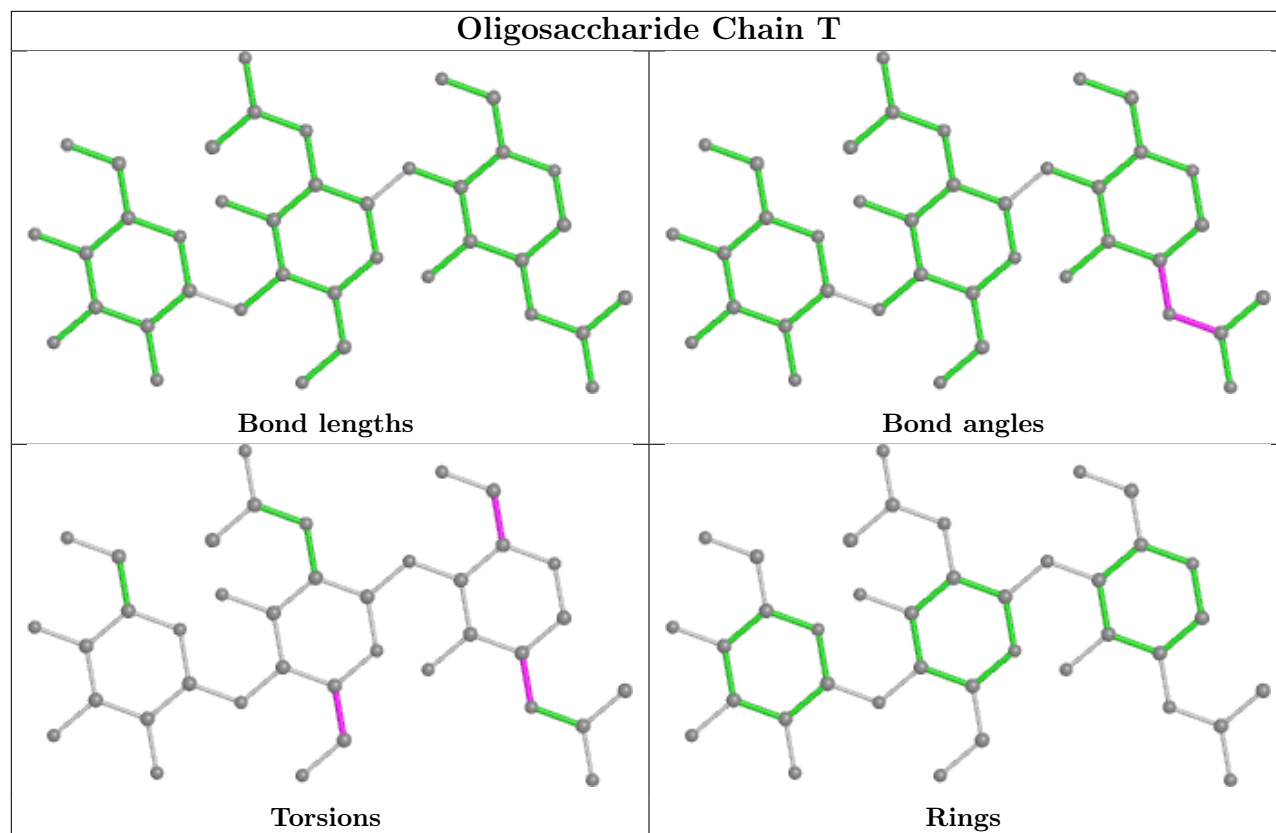
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	V	2	NAG	1	0
5	M	5	MAN	1	0
6	Z	1	NAG	1	0
7	X	1	NAG	1	0

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

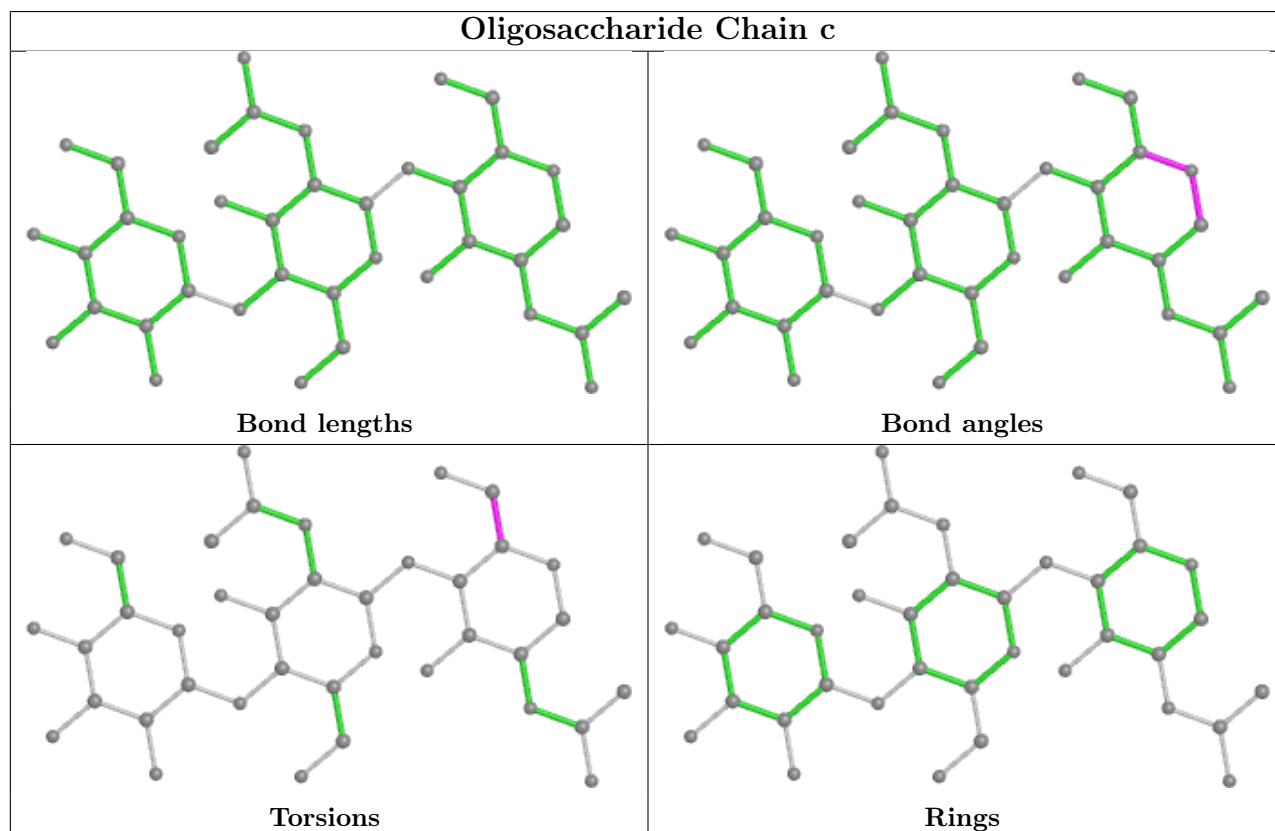
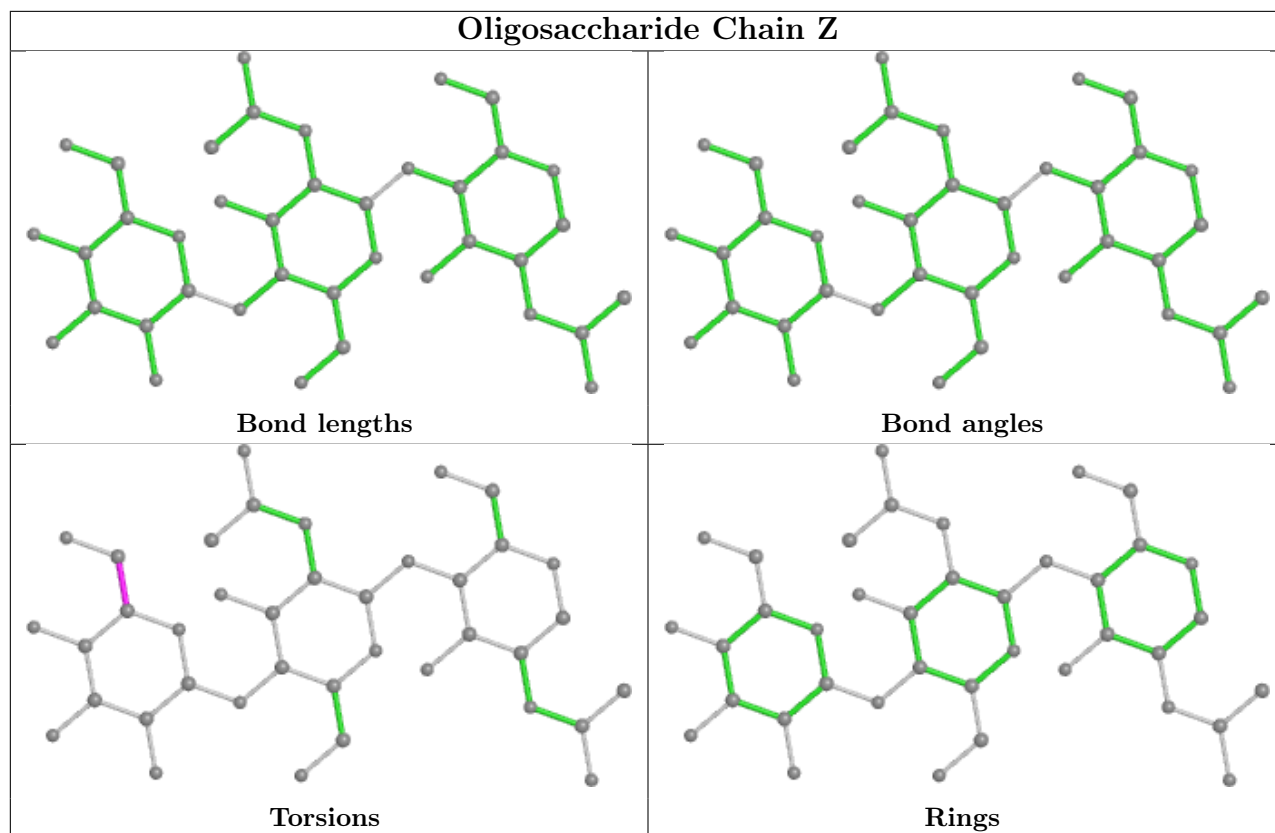


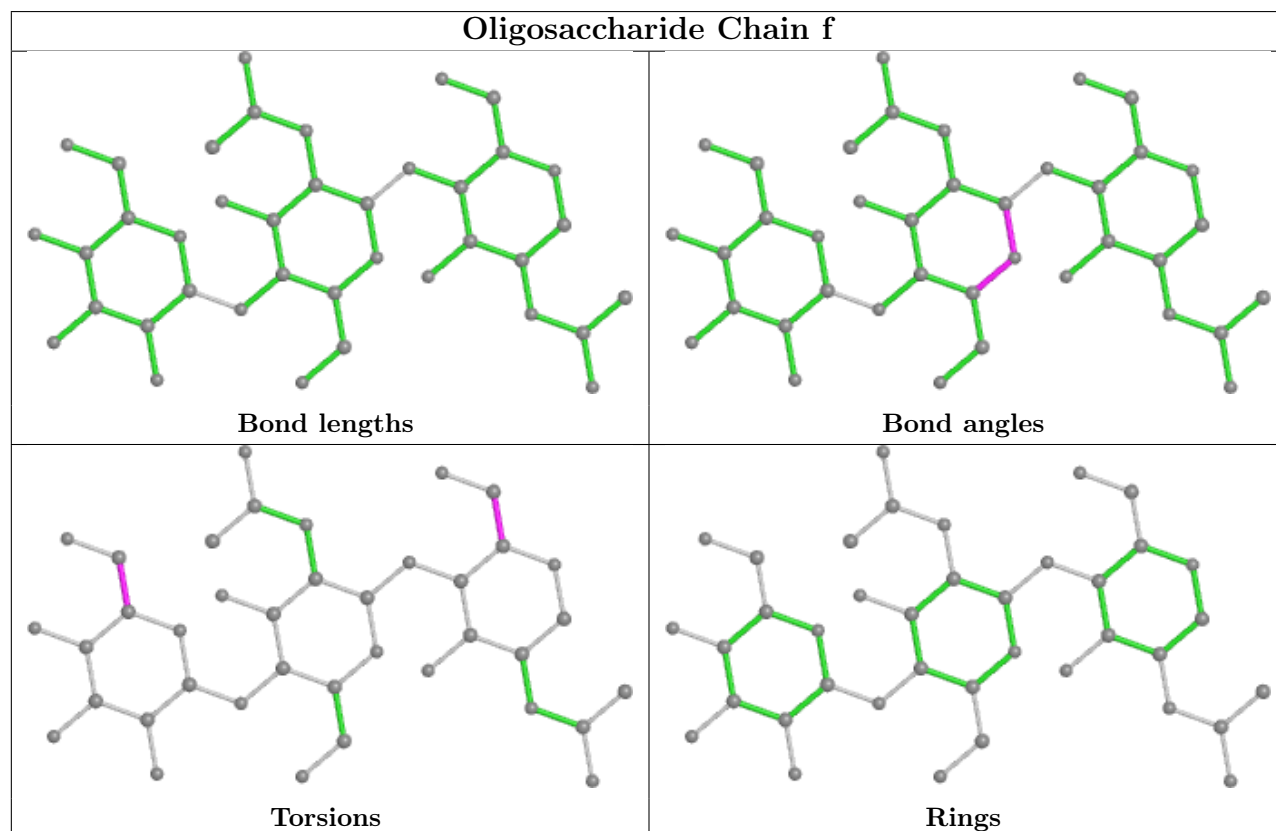
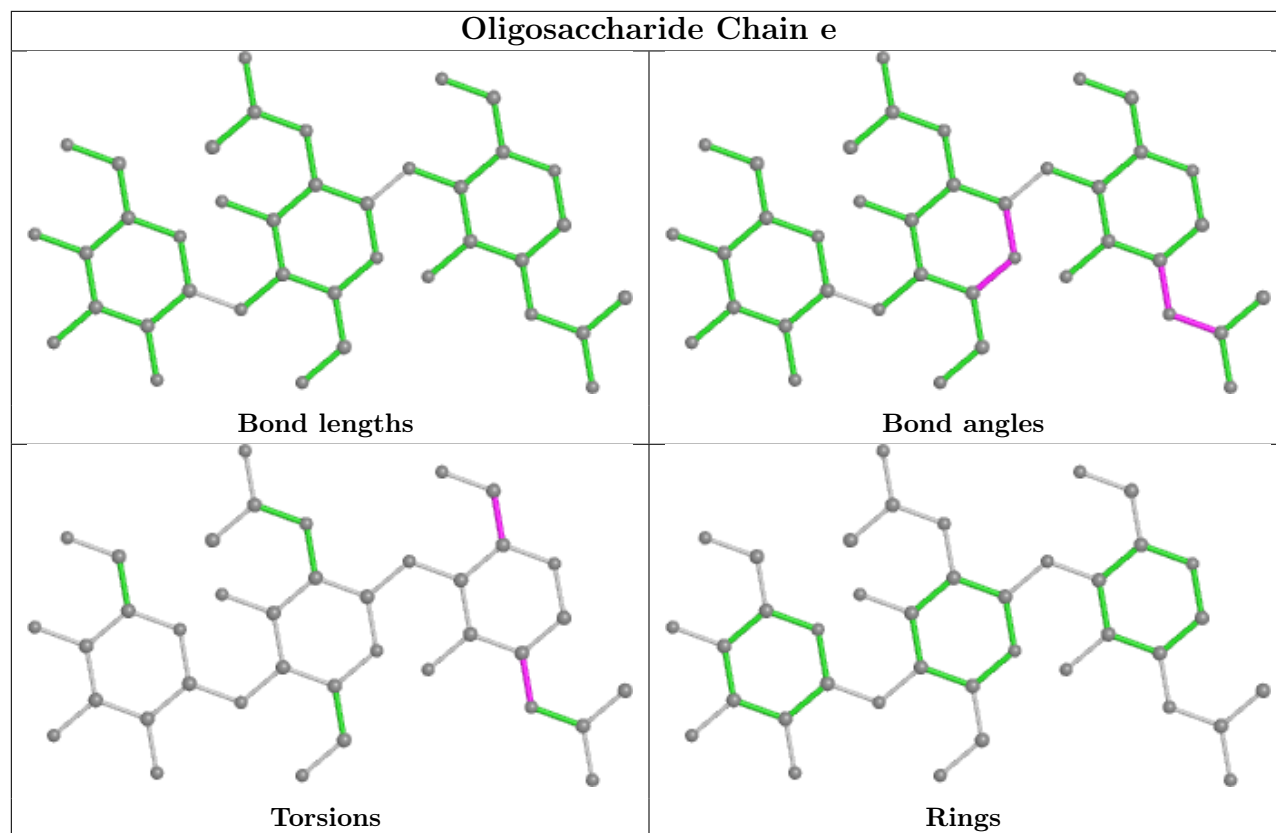


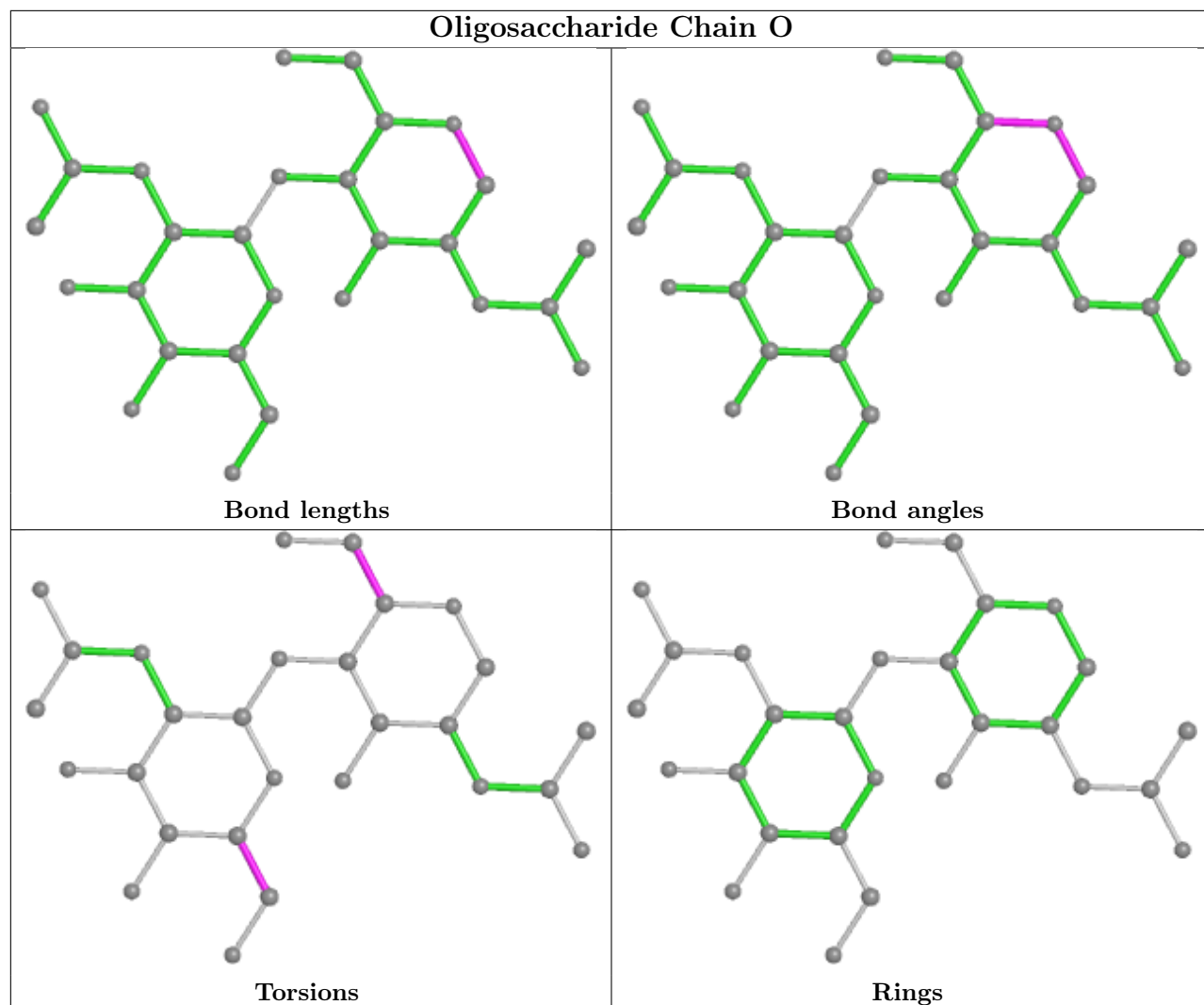


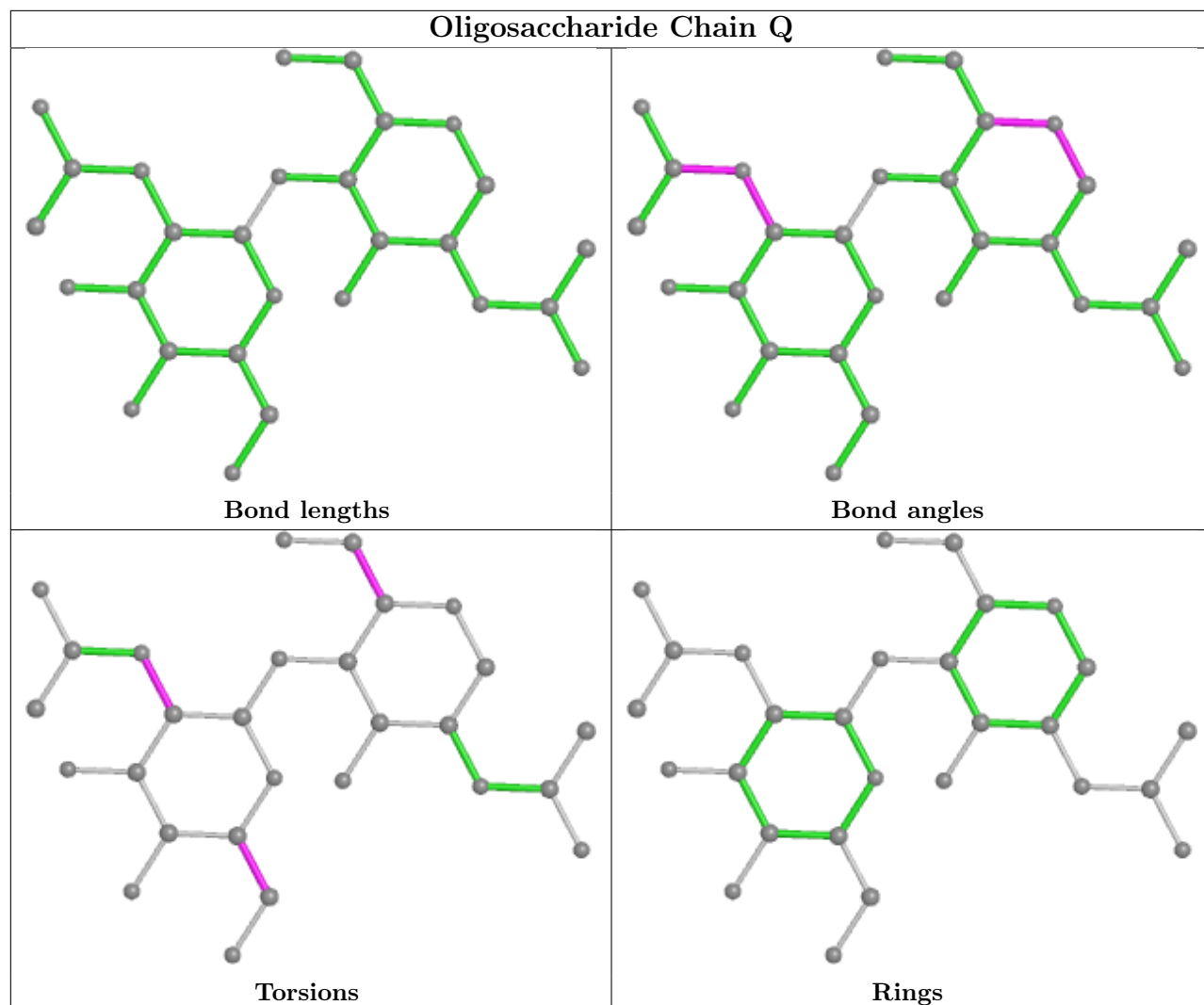


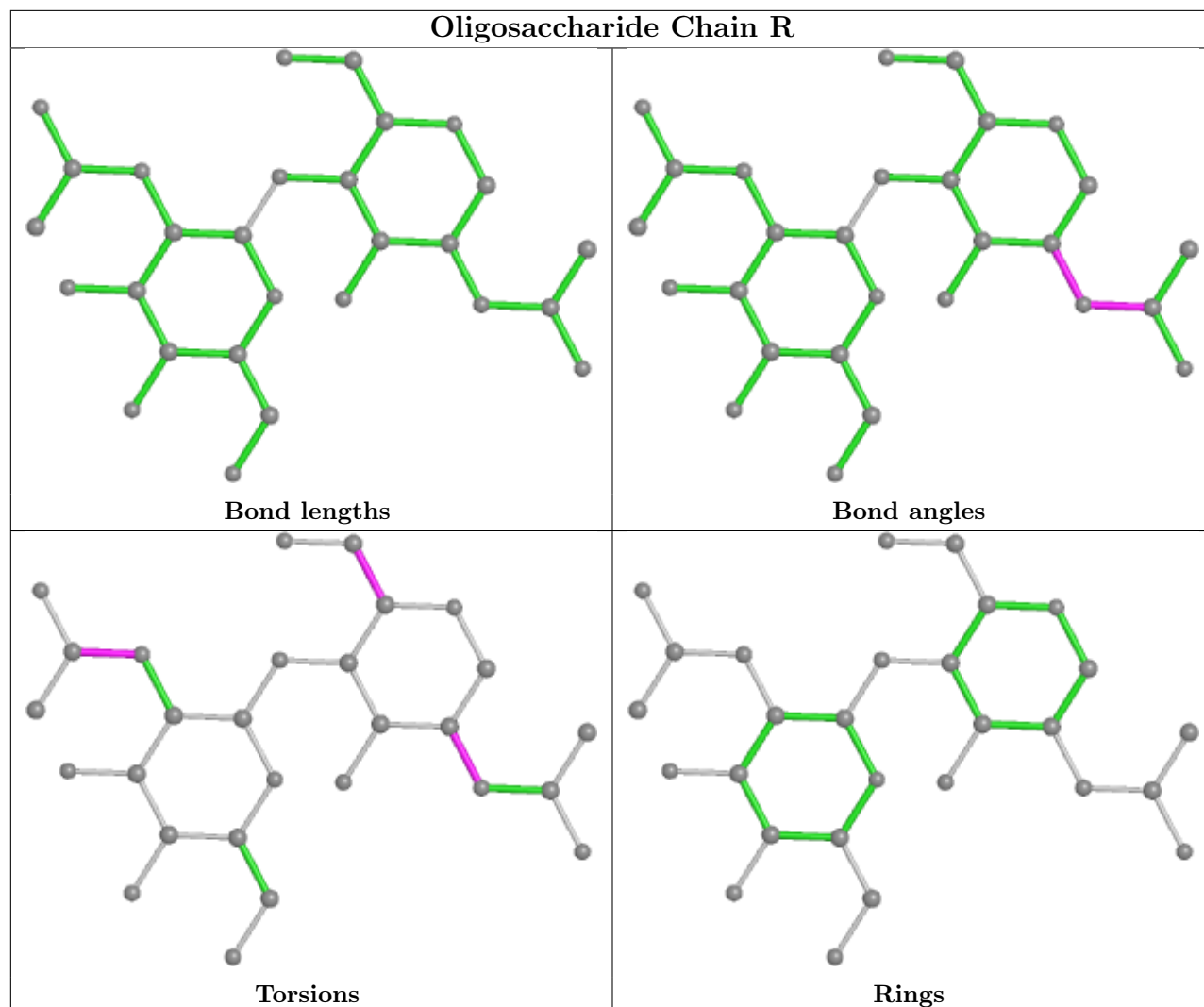


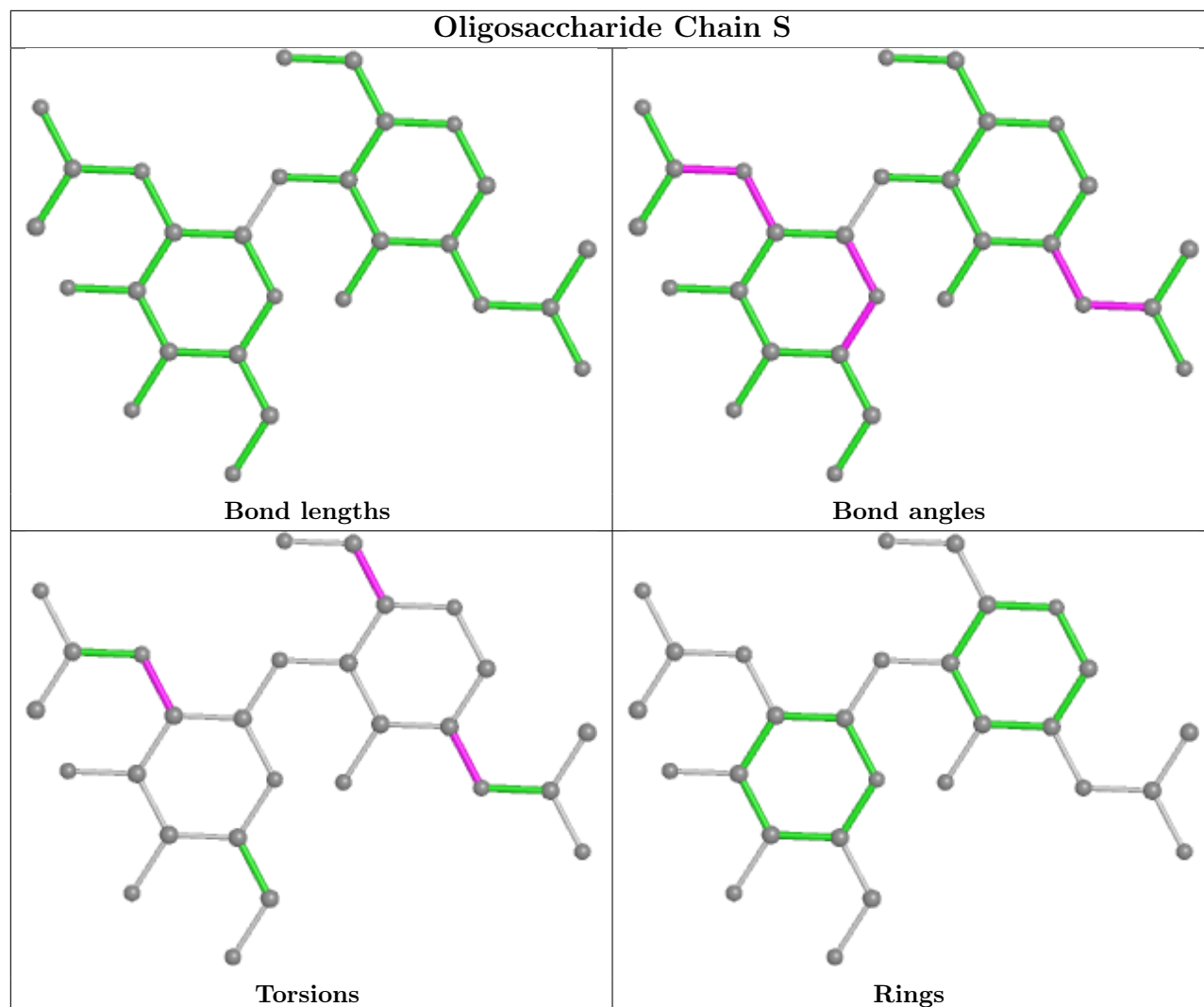


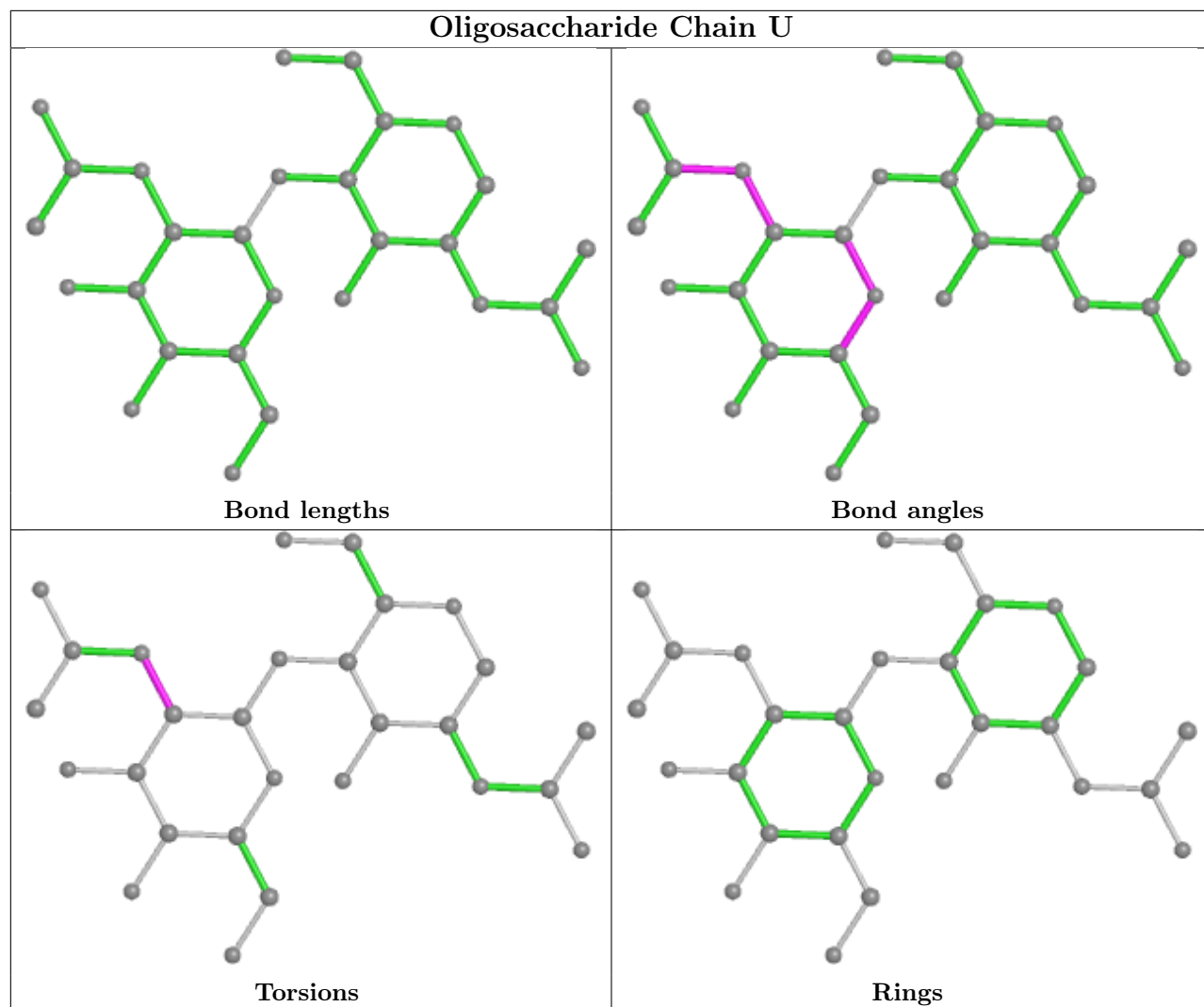


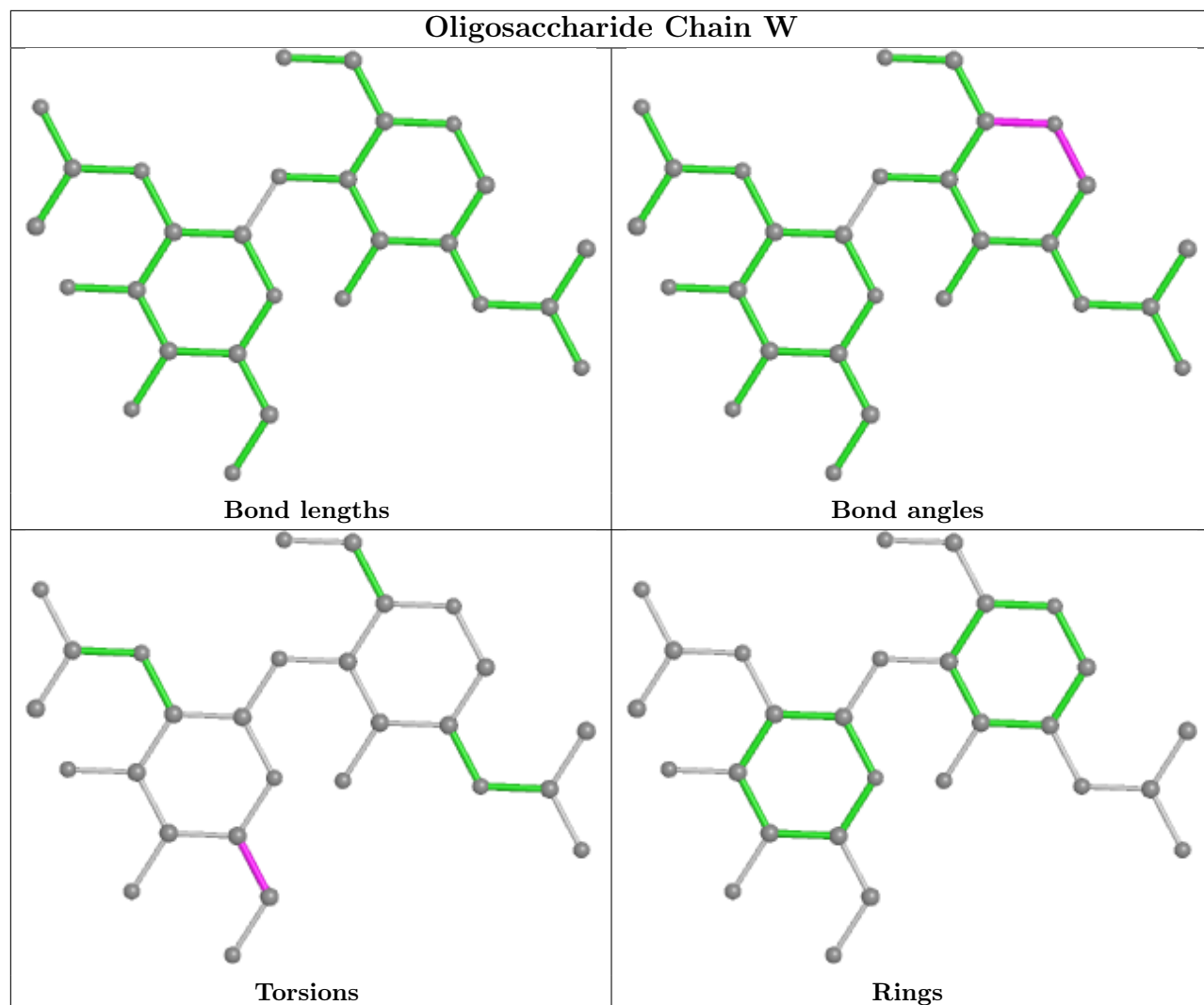




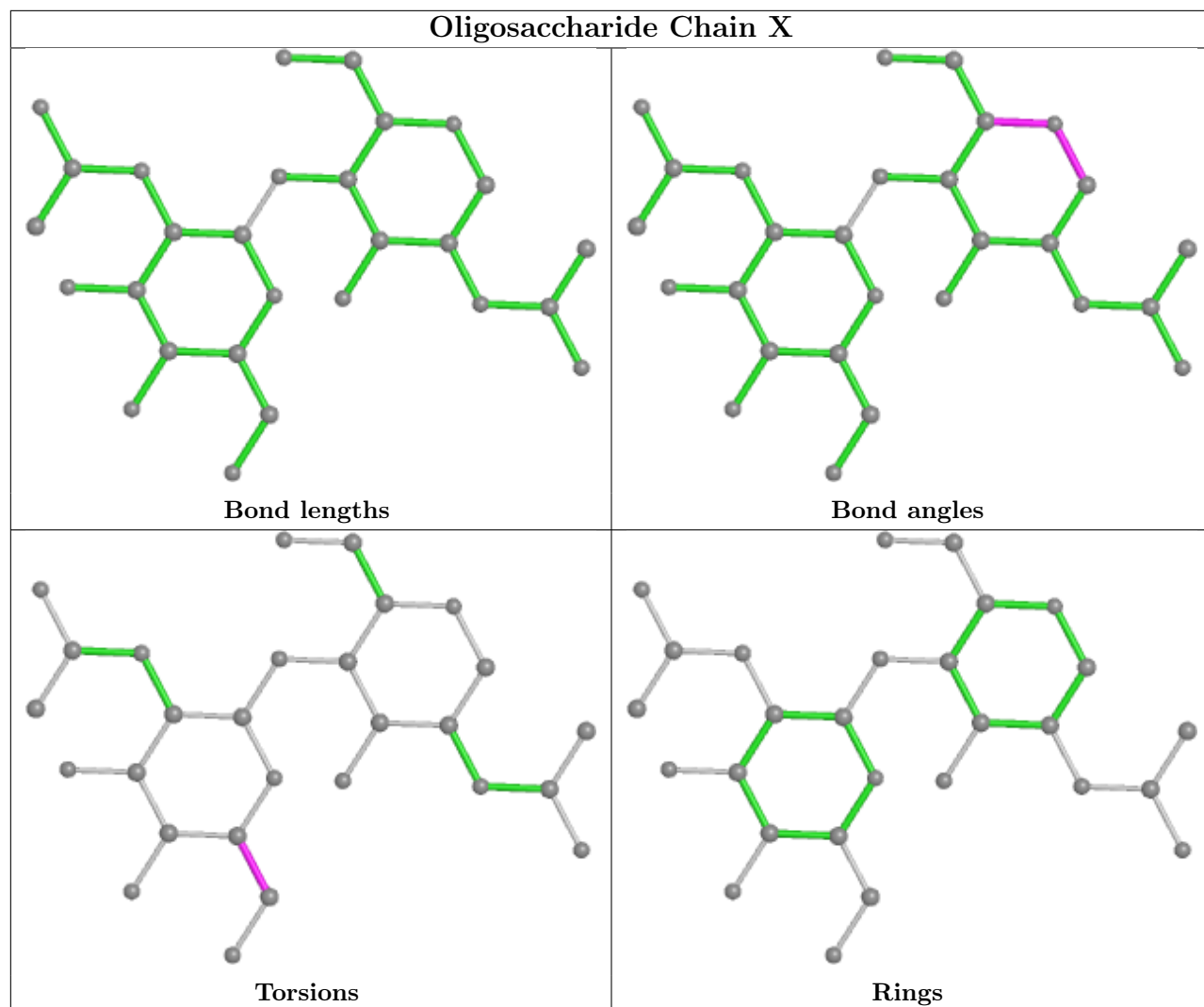


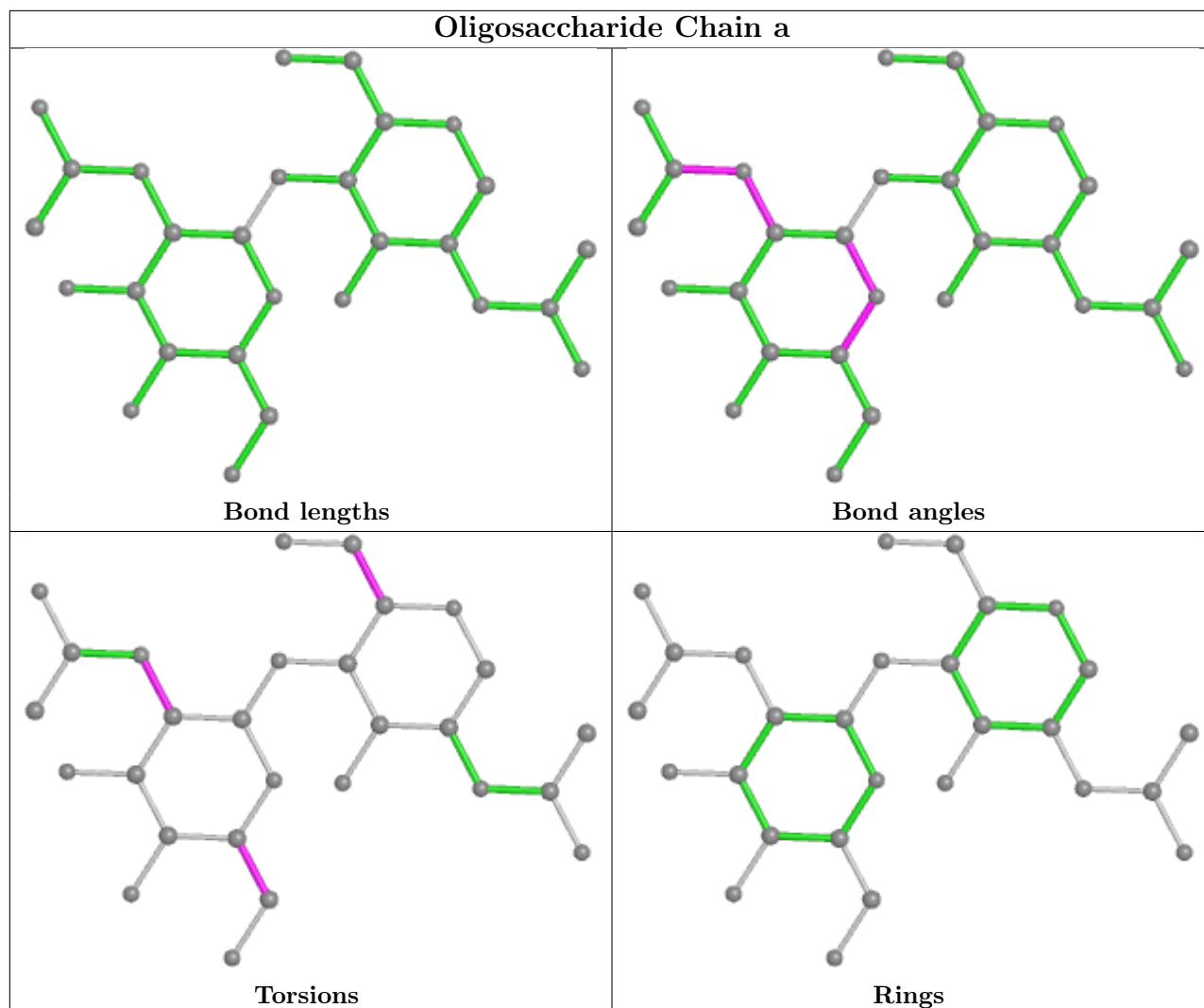


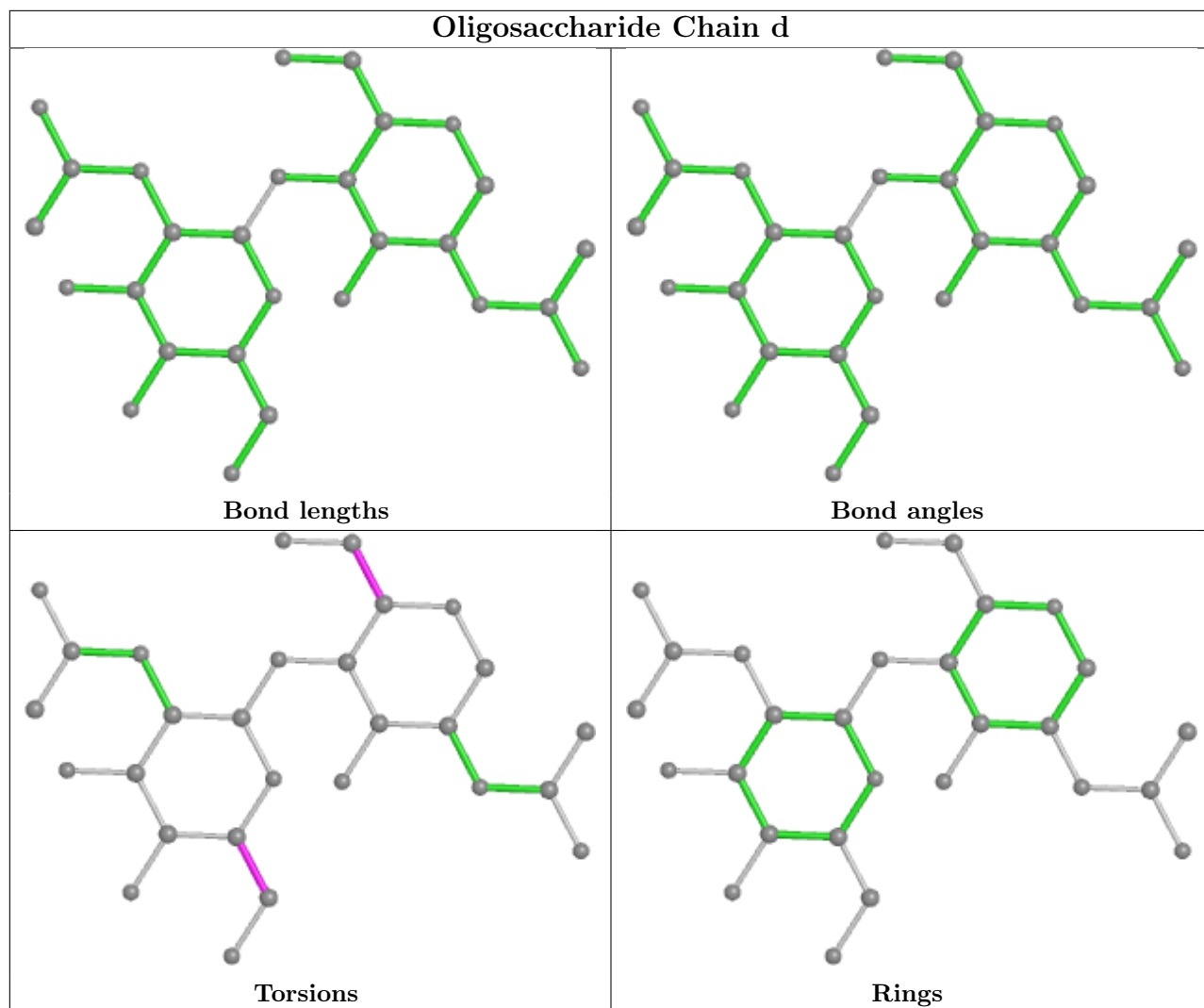


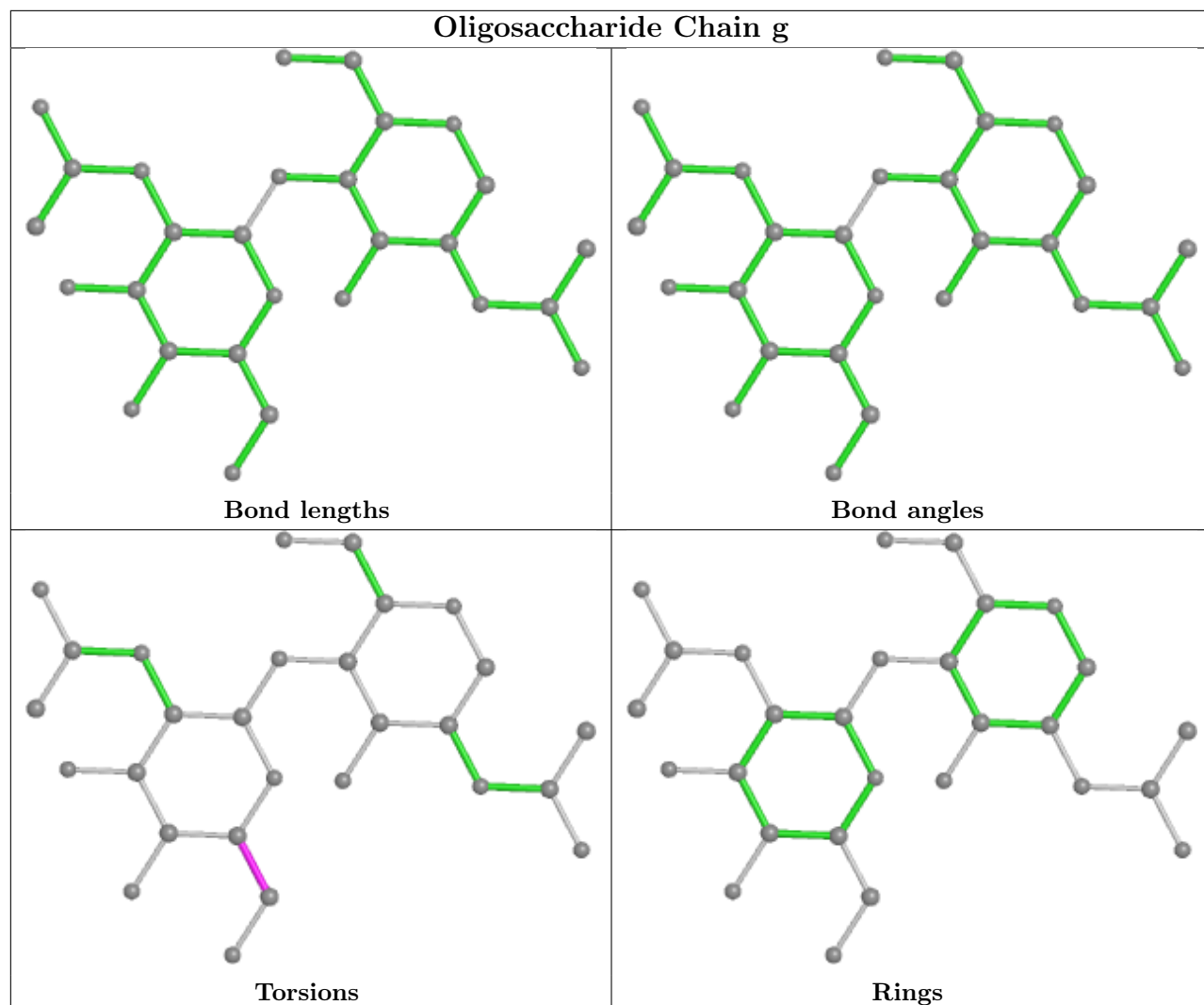


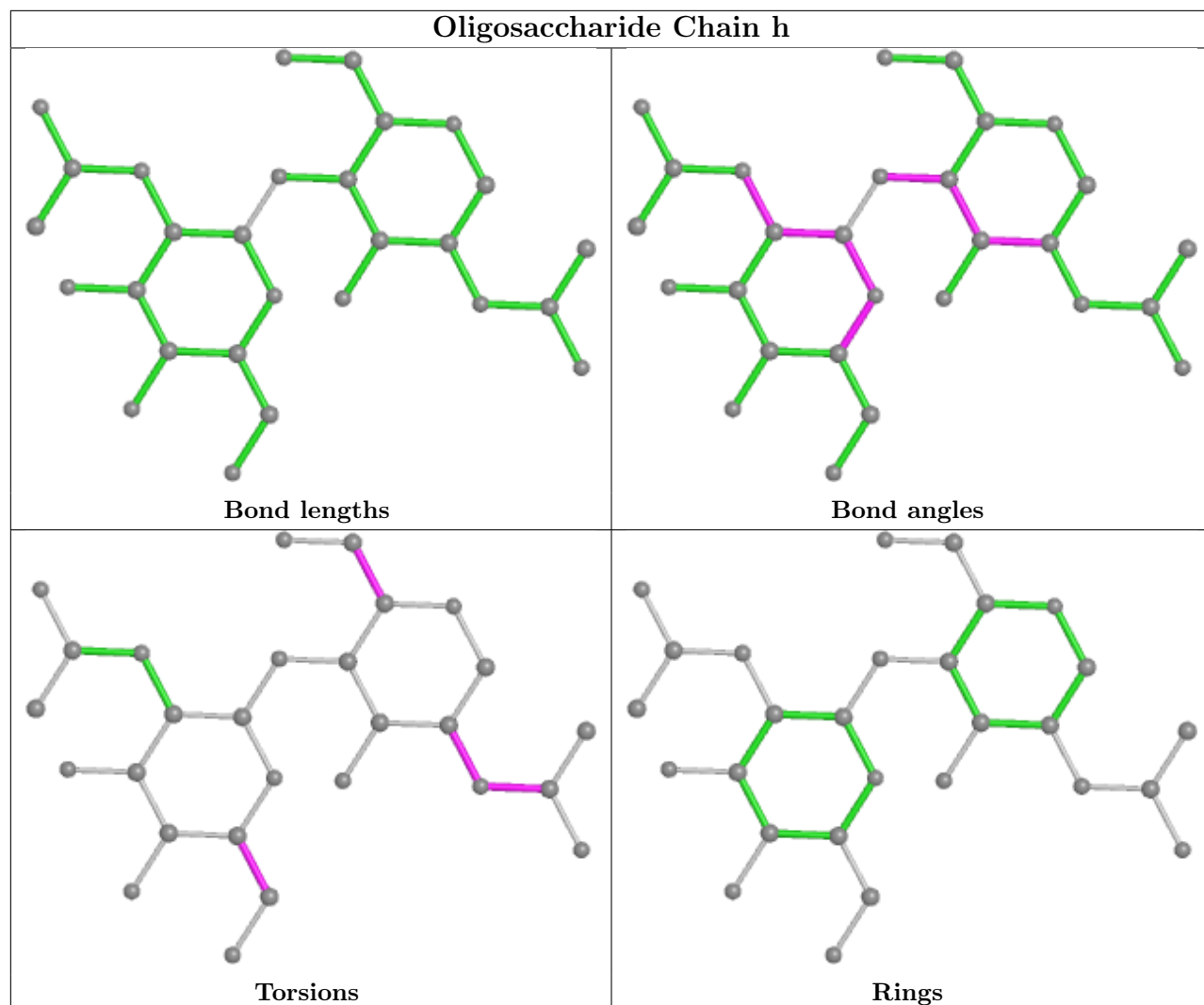


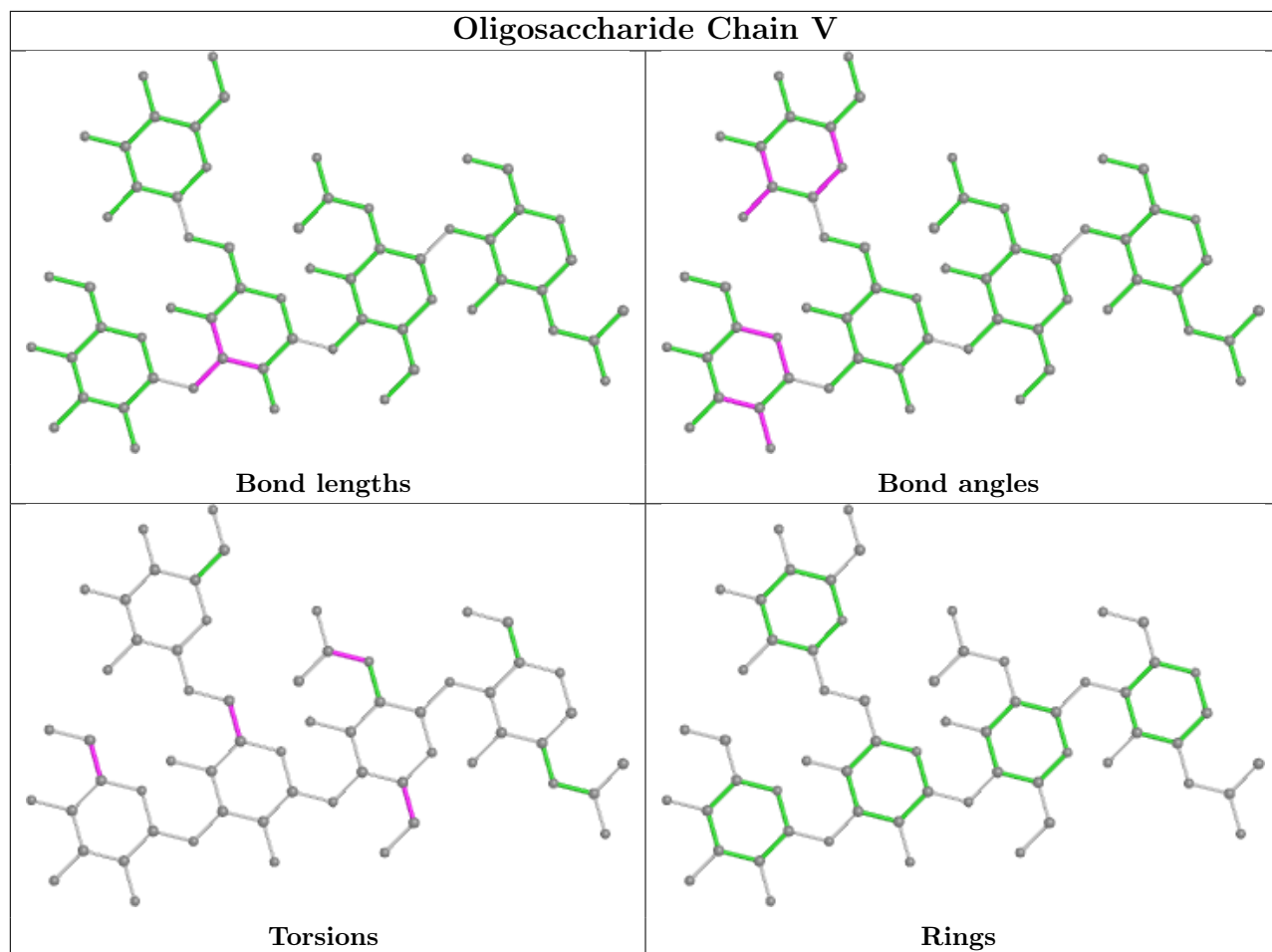












## 5.6 Ligand geometry [i](#)

30 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	$\# Z  > 2$
9	NAG	C	601	1	14,14,15	0.48	0	17,19,21	0.95	1 (5%)
9	NAG	D	703	2	14,14,15	0.40	0	17,19,21	0.54	0
9	NAG	C	602	1	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	A	605	1	14,14,15	0.44	0	17,19,21	0.55	0
9	NAG	A	602	1	14,14,15	0.30	0	17,19,21	0.51	0
9	NAG	F	701	2	14,14,15	0.56	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	D	701	2	14,14,15	0.39	0	17,19,21	0.62	0
9	NAG	F	703	2	14,14,15	0.27	0	17,19,21	0.59	0
9	NAG	B	703	2	14,14,15	0.36	0	17,19,21	0.51	0
9	NAG	D	702	2	14,14,15	0.57	0	17,19,21	0.97	1 (5%)
9	NAG	E	605	1	14,14,15	0.37	0	17,19,21	0.49	0
9	NAG	A	606	1	14,14,15	0.36	0	17,19,21	0.50	0
9	NAG	B	701	2	14,14,15	0.37	0	17,19,21	0.51	0
9	NAG	E	606	1	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
9	NAG	E	607	1	14,14,15	0.37	0	17,19,21	0.57	0
9	NAG	A	603	1	14,14,15	0.37	0	17,19,21	0.53	0
9	NAG	A	601	1	14,14,15	0.38	0	17,19,21	0.51	0
9	NAG	E	603	1	14,14,15	0.28	0	17,19,21	0.59	1 (5%)
9	NAG	C	605	1	14,14,15	0.42	0	17,19,21	0.36	0
9	NAG	E	608	1	14,14,15	0.35	0	17,19,21	0.43	0
9	NAG	E	601	1	14,14,15	0.36	0	17,19,21	0.49	0
9	NAG	F	702	2	14,14,15	0.97	1 (7%)	17,19,21	0.59	0
9	NAG	B	702	2	14,14,15	0.38	0	17,19,21	0.59	1 (5%)
9	NAG	E	602	1	14,14,15	0.31	0	17,19,21	0.56	0
9	NAG	E	604	1	14,14,15	0.35	0	17,19,21	0.50	0
9	NAG	A	604	1	14,14,15	0.33	0	17,19,21	0.48	0
9	NAG	C	607	1	14,14,15	0.37	0	17,19,21	0.51	0
9	NAG	C	603	1	14,14,15	0.45	0	17,19,21	0.54	0
9	NAG	C	604	1	14,14,15	0.44	0	17,19,21	0.48	0
9	NAG	C	606	1	14,14,15	0.64	1 (7%)	17,19,21	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	601	1	-	2/6/23/26	0/1/1/1
9	NAG	D	703	2	-	0/6/23/26	0/1/1/1
9	NAG	C	602	1	-	2/6/23/26	0/1/1/1
9	NAG	A	605	1	-	3/6/23/26	0/1/1/1
9	NAG	A	602	1	-	2/6/23/26	0/1/1/1
9	NAG	F	701	2	-	1/6/23/26	0/1/1/1
9	NAG	D	701	2	-	4/6/23/26	0/1/1/1
9	NAG	F	703	2	-	2/6/23/26	0/1/1/1
9	NAG	B	703	2	-	2/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	702	NAG	O5-C1	3.40	1.49	1.43
9	C	606	NAG	C1-C2	2.01	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	606	NAG	C2-N2-C7	3.08	127.28	122.90
9	F	701	NAG	C2-N2-C7	3.08	127.28	122.90
9	C	601	NAG	C2-N2-C7	3.05	127.25	122.90
9	C	606	NAG	C2-N2-C7	3.03	127.22	122.90
9	D	702	NAG	C2-N2-C7	3.02	127.20	122.90
9	B	702	NAG	C1-O5-C5	2.07	115.00	112.19
9	E	603	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.



All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	702	NAG	C4-C5-C6-O6
9	A	603	NAG	O5-C5-C6-O6
9	F	702	NAG	O5-C5-C6-O6
9	E	602	NAG	O5-C5-C6-O6
9	A	603	NAG	C4-C5-C6-O6
9	C	604	NAG	O5-C5-C6-O6
9	D	701	NAG	C4-C5-C6-O6
9	D	701	NAG	O5-C5-C6-O6
9	E	602	NAG	C4-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6
9	A	602	NAG	C8-C7-N2-C2
9	A	602	NAG	O7-C7-N2-C2
9	A	605	NAG	C8-C7-N2-C2
9	A	605	NAG	O7-C7-N2-C2
9	C	602	NAG	C8-C7-N2-C2
9	C	602	NAG	O7-C7-N2-C2
9	C	603	NAG	C8-C7-N2-C2
9	C	603	NAG	O7-C7-N2-C2
9	D	701	NAG	C8-C7-N2-C2
9	D	701	NAG	O7-C7-N2-C2
9	E	602	NAG	C8-C7-N2-C2
9	E	602	NAG	O7-C7-N2-C2
9	C	606	NAG	O5-C5-C6-O6
9	F	703	NAG	C8-C7-N2-C2
9	C	604	NAG	C4-C5-C6-O6
9	A	605	NAG	O5-C5-C6-O6
9	F	703	NAG	O7-C7-N2-C2
9	B	701	NAG	O5-C5-C6-O6
9	E	604	NAG	O5-C5-C6-O6
9	A	604	NAG	O5-C5-C6-O6
9	C	603	NAG	O5-C5-C6-O6
9	E	601	NAG	O5-C5-C6-O6
9	B	702	NAG	C4-C5-C6-O6
9	E	603	NAG	C4-C5-C6-O6
9	B	702	NAG	O5-C5-C6-O6
9	E	603	NAG	O5-C5-C6-O6
9	E	606	NAG	C4-C5-C6-O6
9	E	606	NAG	O5-C5-C6-O6
9	A	601	NAG	C4-C5-C6-O6
9	C	606	NAG	C4-C5-C6-O6
9	B	703	NAG	C4-C5-C6-O6
9	C	607	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	601	NAG	C4-C5-C6-O6
9	C	601	NAG	C3-C2-N2-C7
9	C	606	NAG	C3-C2-N2-C7
9	D	702	NAG	C3-C2-N2-C7
9	E	606	NAG	C3-C2-N2-C7
9	F	701	NAG	C3-C2-N2-C7
9	C	607	NAG	O5-C5-C6-O6
9	B	703	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	603	NAG	1	0
9	E	608	NAG	1	0

## 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.

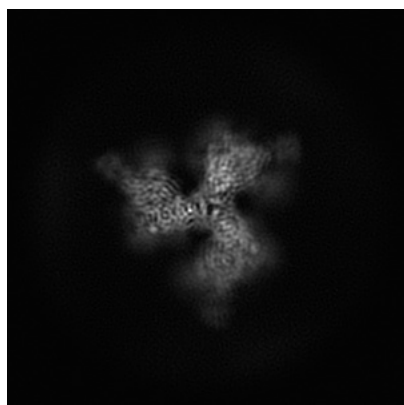
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26157. These allow visual inspection of the internal detail of the map and identification of artifacts.

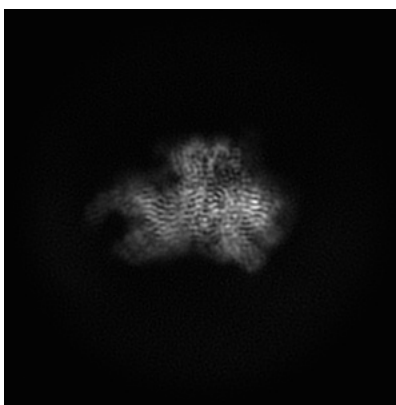
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

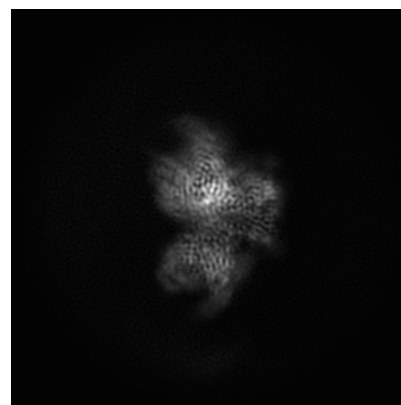
#### 6.1.1 Primary map



X



Y

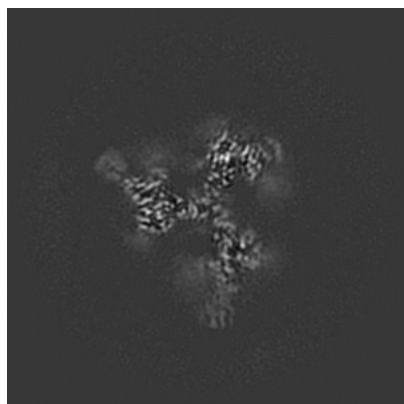


Z

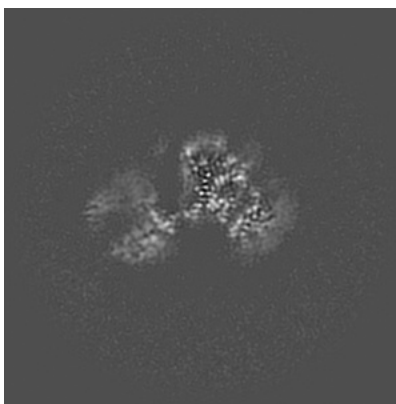
The images above show the map projected in three orthogonal directions.

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

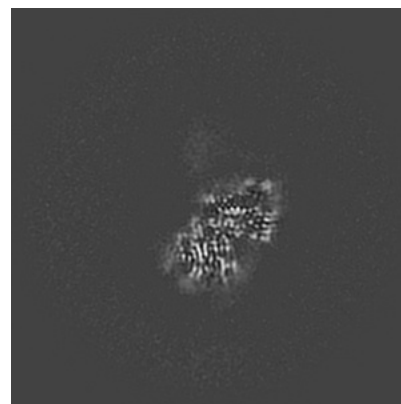
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

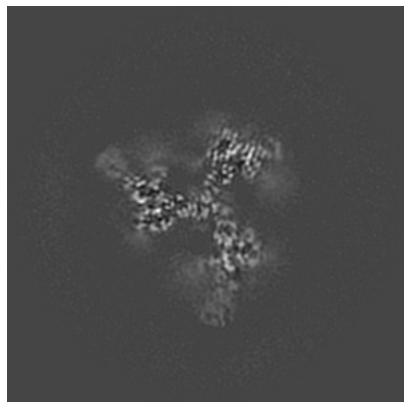


Z Index: 160

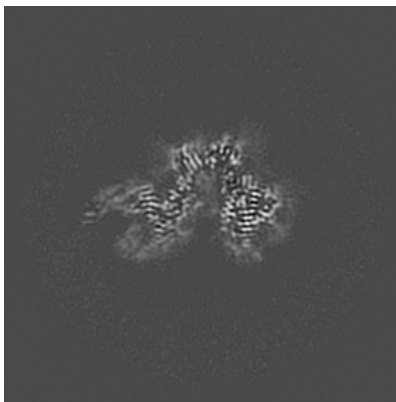
The images above show central slices of the map in three orthogonal directions.

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

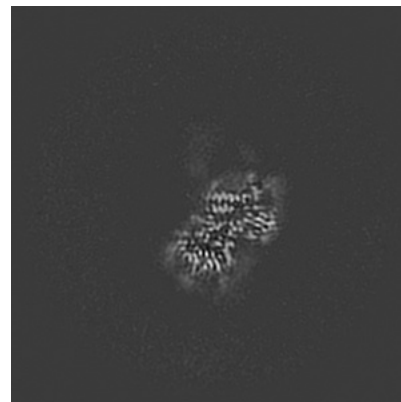
### 6.3.1 Primary map



X Index: 161



Y Index: 174

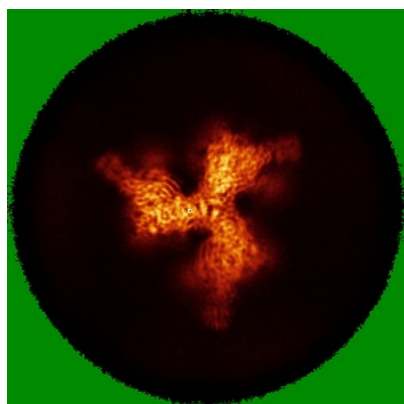


Z Index: 157

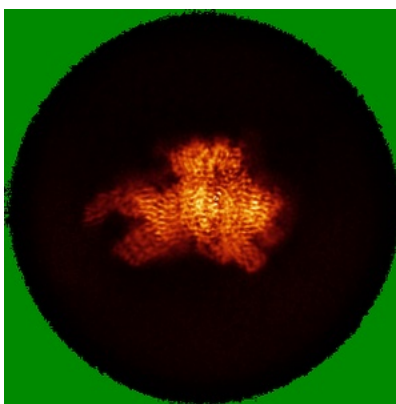
The images above show the largest variance slices of the map in three orthogonal directions.

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

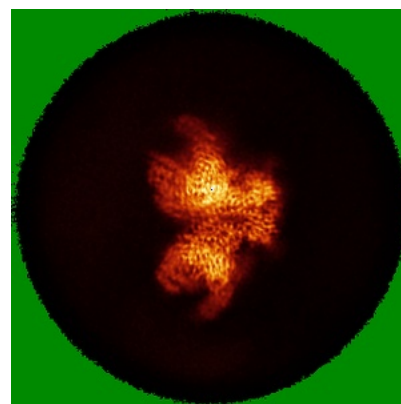
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

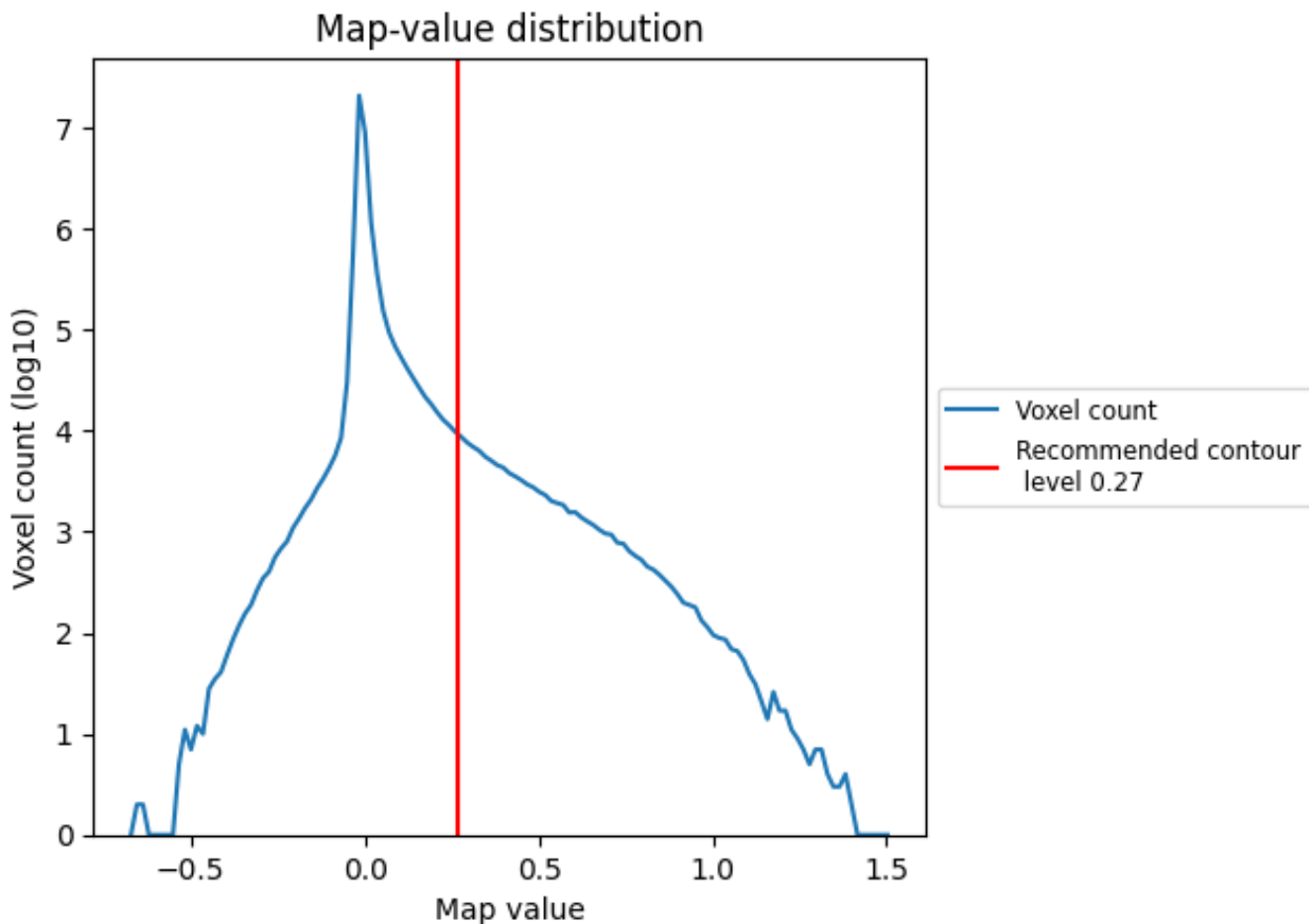
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

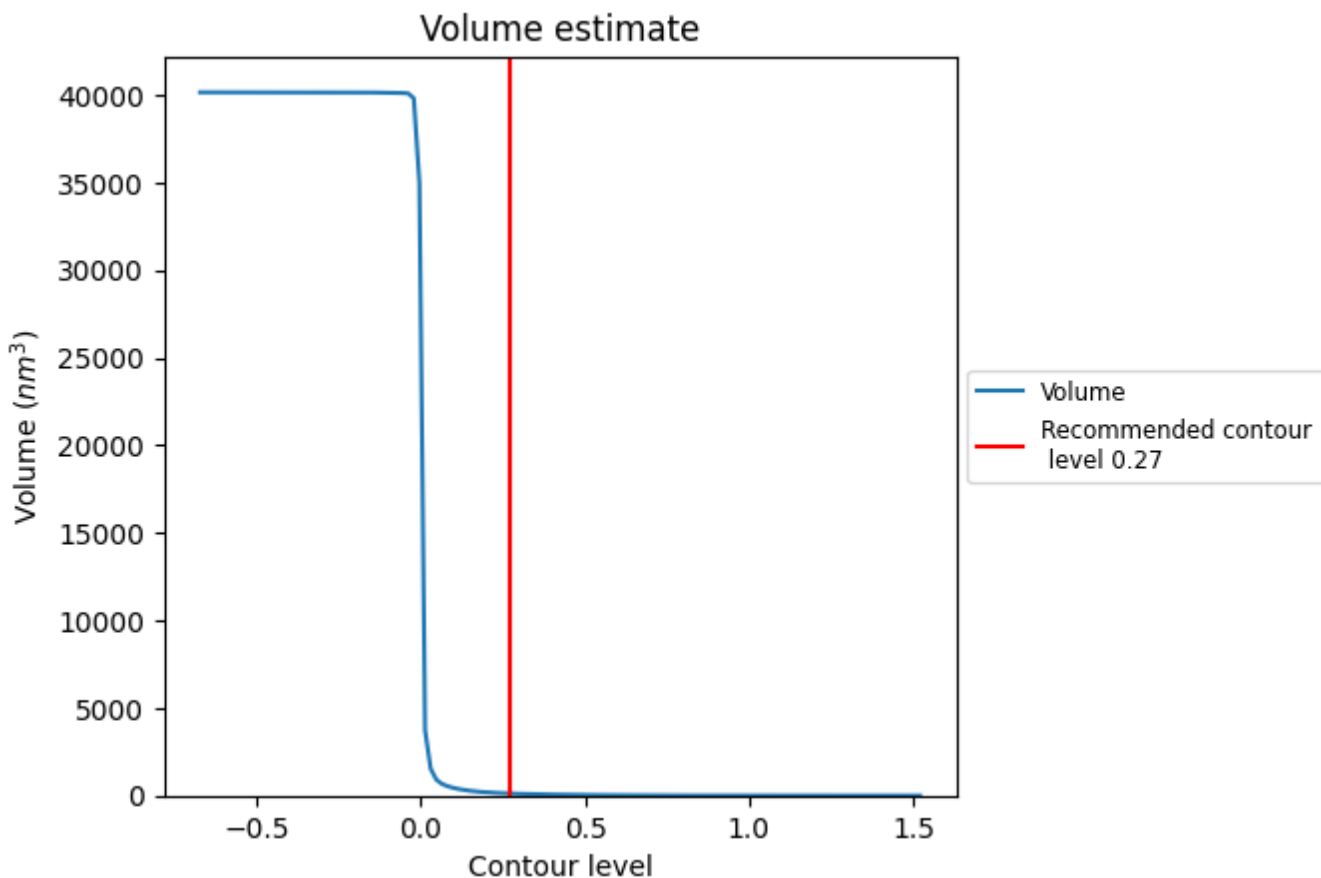
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

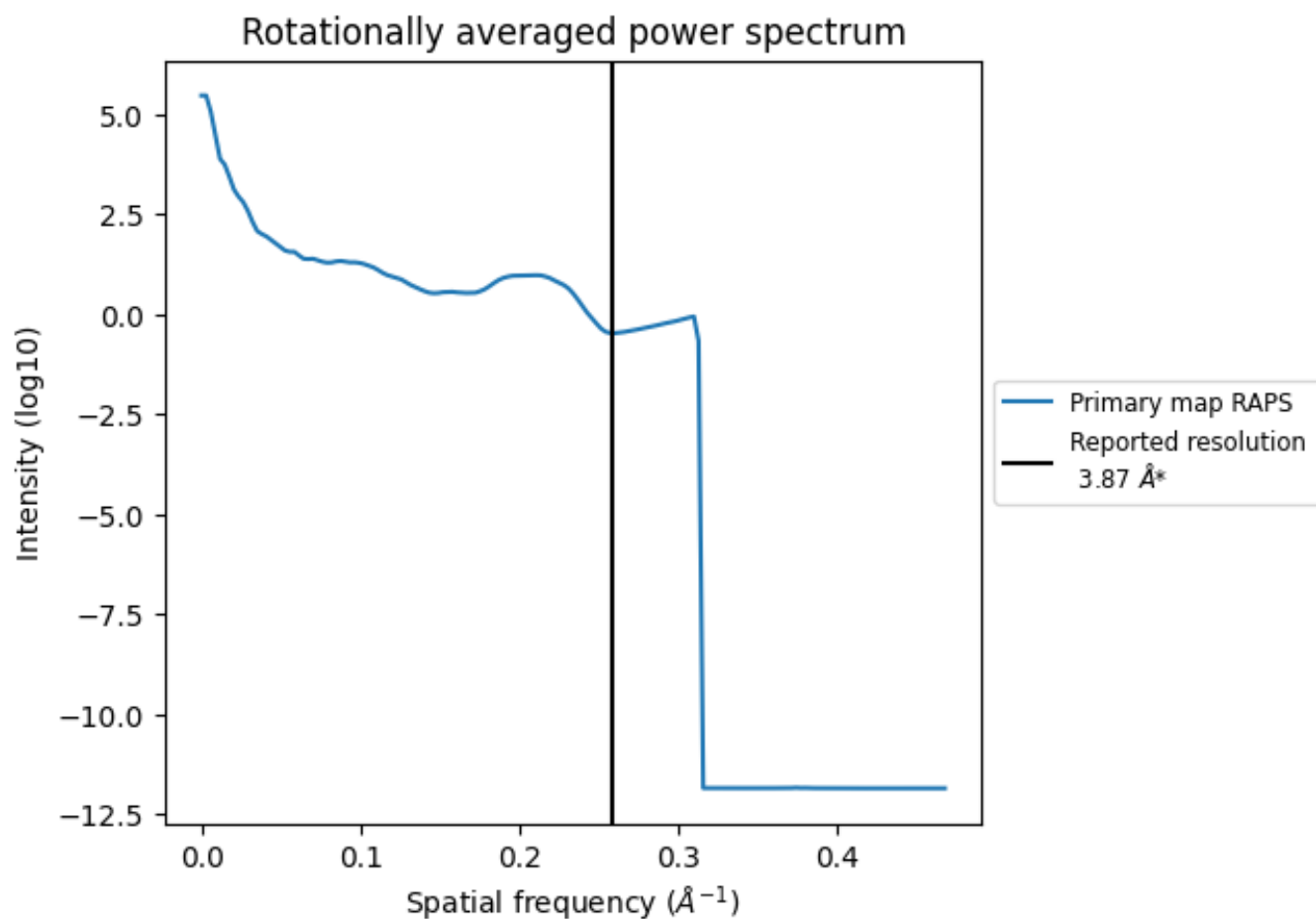
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 119 nm<sup>3</sup>; this corresponds to an approximate mass of 107 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.258 \text{\AA}^{-1}$



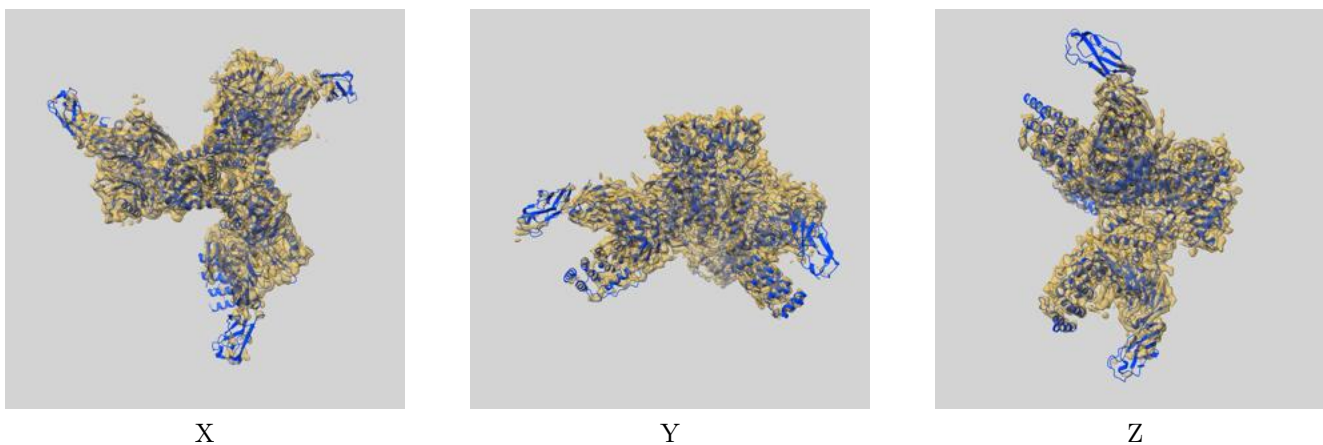
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

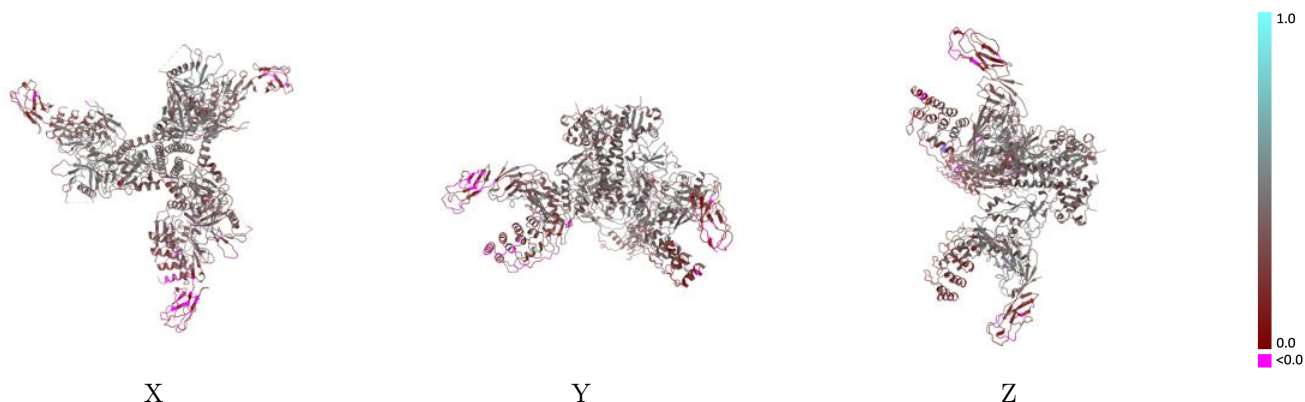
This section contains information regarding the fit between EMDB map EMD-26157 and PDB model 7TXD. Per-residue inclusion information can be found in section 3 on page 11.

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



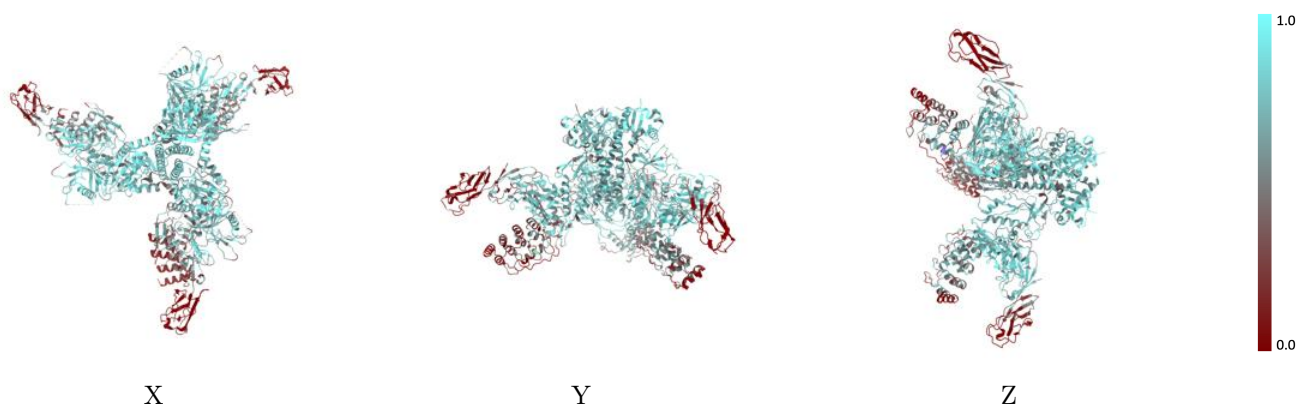
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



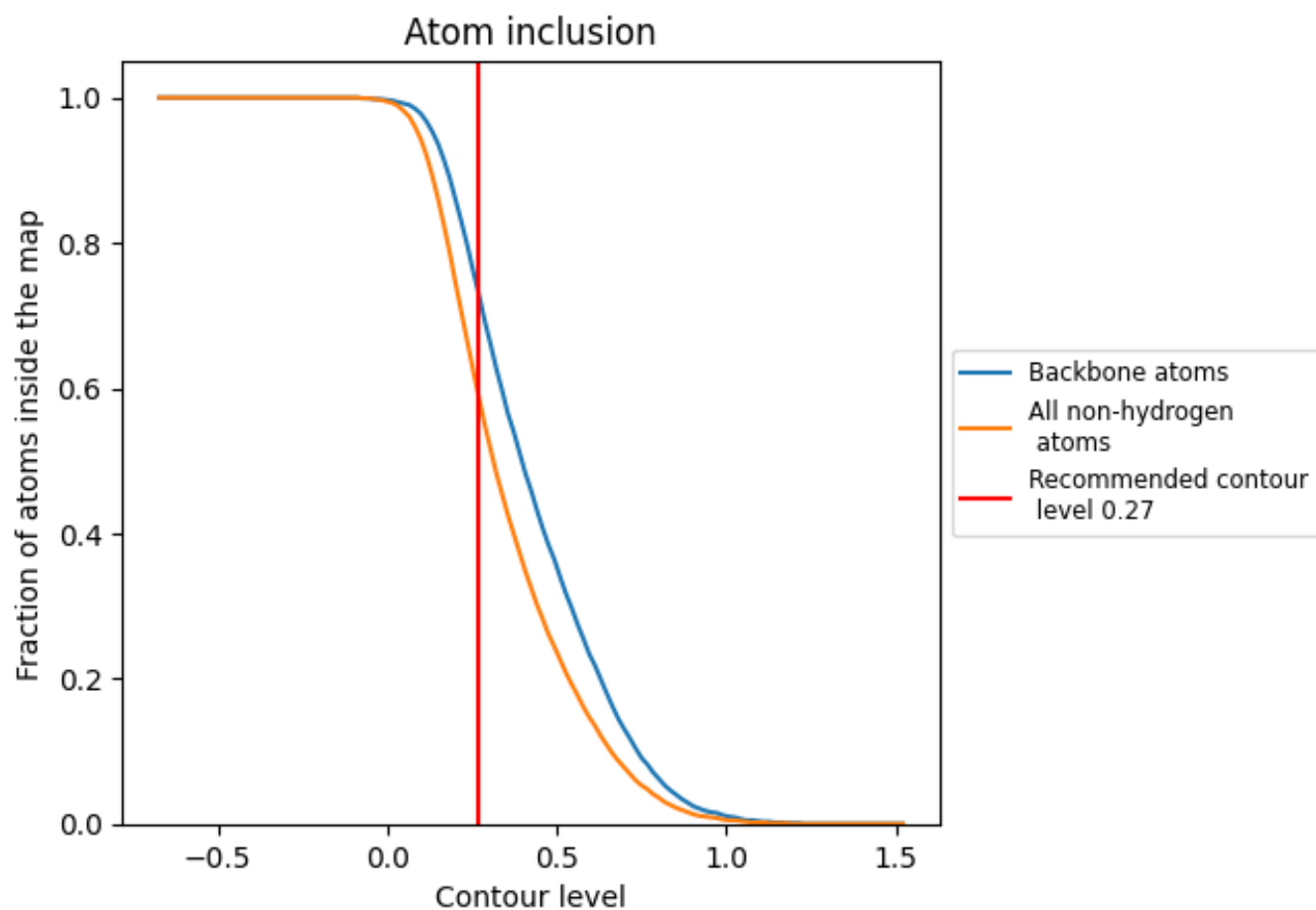
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.3520
A	 0.7310	 0.4150
B	 0.7230	 0.4000
C	 0.6280	 0.3570
D	 0.6750	 0.3700
E	 0.7550	 0.4180
F	 0.7170	 0.3870
G	 0.4150	 0.2940
H	 0.3500	 0.2350
I	 0.4760	 0.3310
J	 0.4070	 0.2800
K	 0.1810	 0.1980
L	 0.4660	 0.2720
M	 0.5900	 0.4440
N	 0.6920	 0.4350
O	 0.4640	 0.4230
P	 0.6150	 0.4590
Q	 0.2860	 0.3540
R	 0.3210	 0.3180
S	 0.1070	 0.3710
T	 0.4620	 0.4150
U	 0.3570	 0.3460
V	 0.6720	 0.3750
W	 0.5710	 0.3850
X	 0.3570	 0.2860
Y	 0.4620	 0.3390
Z	 0.6920	 0.3670
a	 0.2500	 0.2770
b	 0.6630	 0.4420
c	 0.6670	 0.4180
d	 0.4640	 0.4150
e	 0.5130	 0.3850
f	 0.7440	 0.4580
g	 0.4290	 0.3990
h	 0.3930	 0.3250

