



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:14 PM UTC

PDB ID : 7YBL / pdb_00007ybl
EMDB ID : EMD-33725
Title : SARS-CoV-2 B.1.620 variant spike (close state)
Authors : Wang, X.; Fu, W.
Deposited on : 2022-06-29
Resolution : 3.60 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:

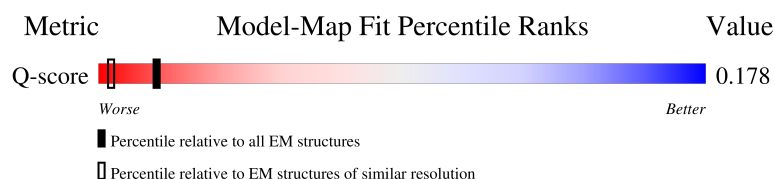
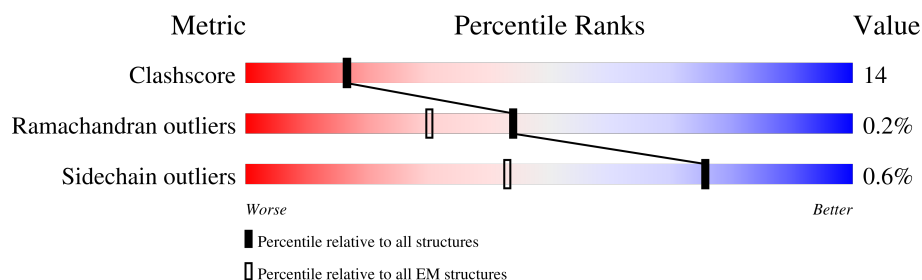
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1270	26% 61% 23% 15%
1	B	1270	26% 62% 22% 15%
1	C	1270	26% 62% 22% 15%
2	D	2	100% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	100%
2	I	2	50%
2	O	2	100%
2	Q	2	100%
2	T	2	50%
2	Z	2	100%
2	b	2	100%
2	e	2	50%
3	E	3	100%
3	G	3	100%
3	H	3	67%
3	J	3	33%
3	K	3	67%
3	M	3	67%
3	N	3	33%
3	P	3	100%
3	R	3	100%
3	S	3	67%
3	U	3	67%
3	V	3	67%
3	X	3	67%
3	Y	3	33%
3	a	3	100%
3	c	3	100%
3	d	3	67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	f	3	33% 67% 33%
3	g	3	67% 67% 33%
3	i	3	33% 67% 33%
3	j	3	33% 67% 33%
4	L	3	67% 100%
4	W	3	67% 67% 33%
4	h	3	67% 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26819 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1078	Total	C	N	O	S	0	0
			8442	5390	1411	1604	37		
1	B	1078	Total	C	N	O	S	0	0
			8442	5390	1411	1604	37		
1	C	1078	Total	C	N	O	S	0	0
			8442	5390	1411	1604	37		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	SER	PRO	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	126	ALA	VAL	conflict	UNP P0DTC2
A	142B	ASP	-	insertion	UNP P0DTC2
A	142C	GLU	-	insertion	UNP P0DTC2
A	142D	LEU	TYR	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	242	TYR	HIS	conflict	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1027	ILE	THR	conflict	UNP P0DTC2
A	1118	HIS	ASP	conflict	UNP P0DTC2
B	26	SER	PRO	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	126	ALA	VAL	conflict	UNP P0DTC2
B	142B	ASP	-	insertion	UNP P0DTC2
B	142C	GLU	-	insertion	UNP P0DTC2
B	142D	LEU	TYR	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	242	TYR	HIS	conflict	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1027	ILE	THR	conflict	UNP P0DTC2
B	1118	HIS	ASP	conflict	UNP P0DTC2
C	26	SER	PRO	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	126	ALA	VAL	conflict	UNP P0DTC2
C	142B	ASP	-	insertion	UNP P0DTC2
C	142C	GLU	-	insertion	UNP P0DTC2
C	142D	LEU	TYR	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	242	TYR	HIS	conflict	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

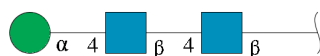
Chain	Residue	Modelled	Actual	Comment	Reference
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1027	ILE	THR	conflict	UNP P0DTC2
C	1118	HIS	ASP	conflict	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		

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



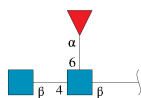
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

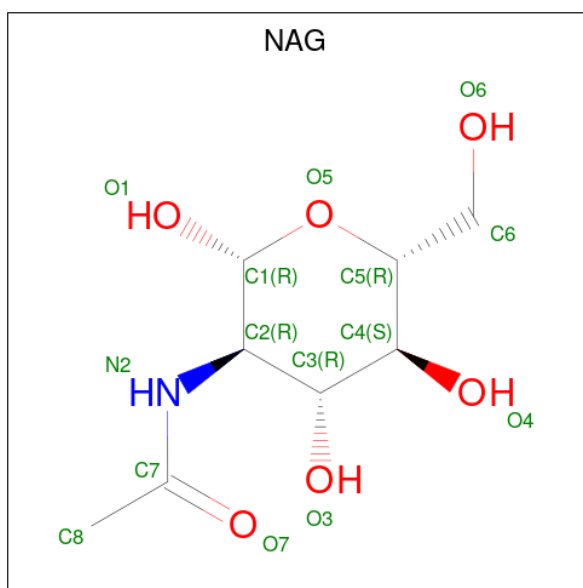
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Y	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	g	3	Total	C	N	O	0	0
			39	22	2	15		
3	i	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	3	Total	C	N	O	0	0
			38	22	2	14		
4	W	3	Total	C	N	O	0	0
			38	22	2	14		
4	h	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

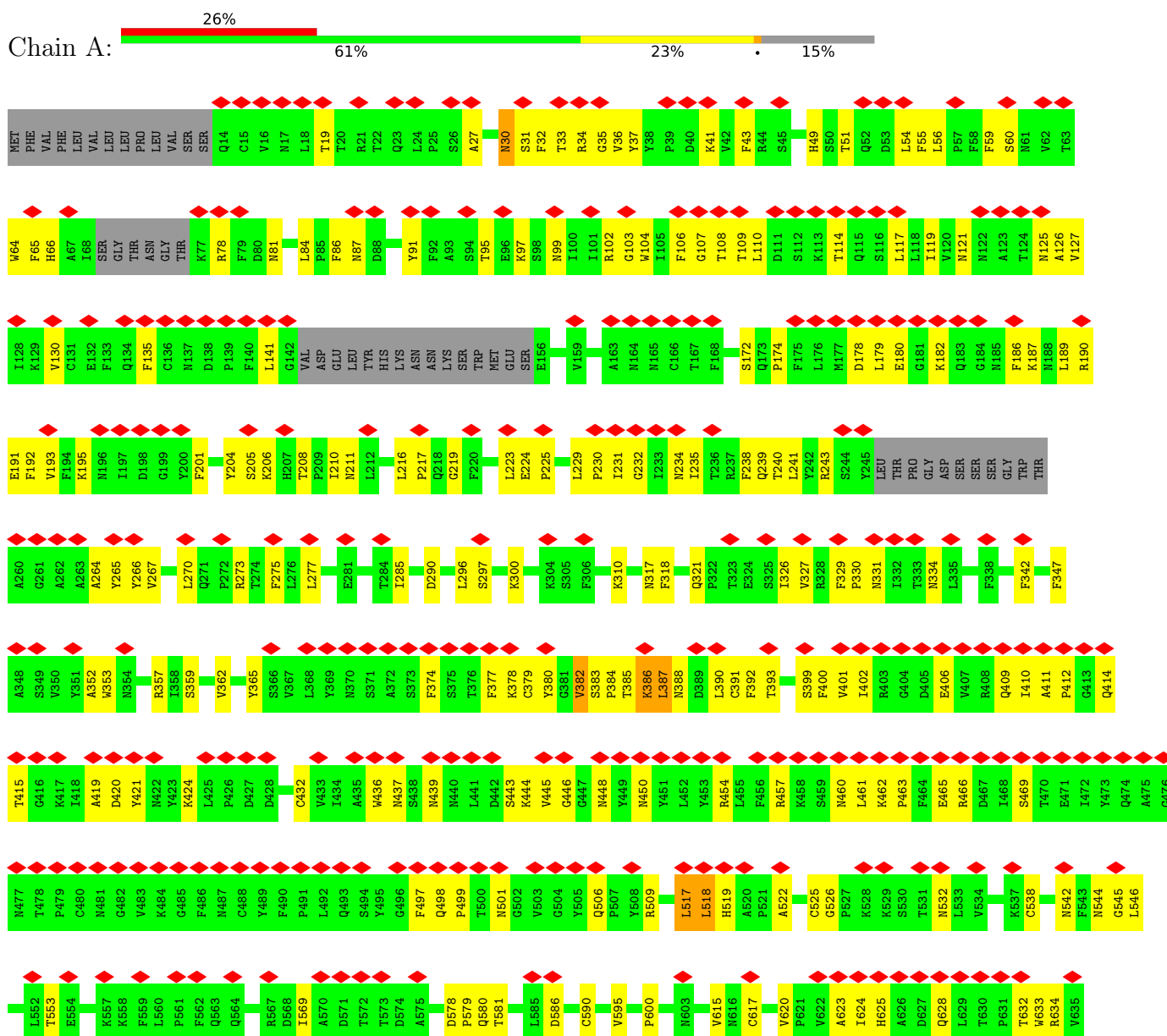
Continued from previous page...

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

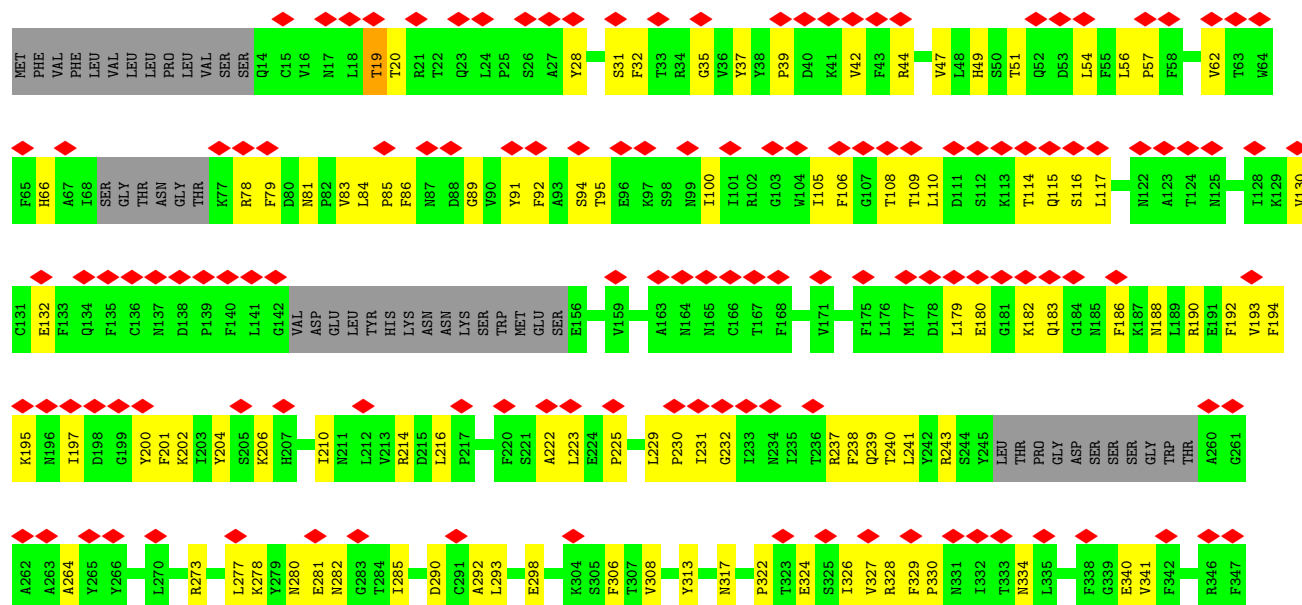
3 Residue-property plots

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: Spike glycoprotein











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



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



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



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



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



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

Chain b: 

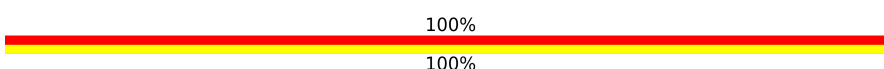


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

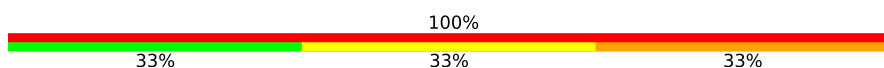


- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 



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

Chain G: 



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

Chain H: 



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

Chain J: 



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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	315257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	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: FUC, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/8640	0.55	5/11758 (0.0%)
1	B	0.28	1/8640 (0.0%)	0.59	12/11758 (0.1%)
1	C	0.27	0/8640	0.62	17/11758 (0.1%)
All	All	0.29	1/25920 (0.0%)	0.59	34/35274 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	977	LEU	C-N	9.92	1.47	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	993	ILE	O-C-N	-19.47	99.87	122.06
1	B	993	ILE	O-C-N	-18.42	104.00	121.87
1	B	993	ILE	CA-C-N	12.69	136.94	120.44
1	B	993	ILE	C-N-CA	12.69	136.94	120.44
1	C	977	LEU	O-C-N	-12.27	107.87	122.22
1	B	977	LEU	O-C-N	-11.66	109.76	122.12
1	C	993	ILE	CA-C-N	11.03	139.45	120.58
1	C	993	ILE	C-N-CA	11.03	139.45	120.58
1	C	977	LEU	CA-C-N	10.75	135.55	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	977	LEU	C-N-CA	10.75	135.55	120.29
1	C	986	PRO	CA-N-CD	-9.15	99.19	112.00
1	B	986	PRO	CA-N-CD	-9.15	99.19	112.00
1	B	987	PRO	CA-N-CD	-9.02	99.37	112.00
1	C	987	PRO	CA-N-CD	-9.01	99.39	112.00
1	A	817	PRO	CA-N-CD	-8.99	99.41	112.00
1	C	817	PRO	CA-N-CD	-8.98	99.43	112.00
1	C	899	PRO	CA-N-CD	-8.96	99.45	112.00
1	B	899	PRO	CA-N-CD	-8.96	99.45	112.00
1	A	899	PRO	CA-N-CD	-8.93	99.50	112.00
1	B	817	PRO	CA-N-CD	-8.88	99.58	112.00
1	B	977	LEU	CA-C-N	8.87	132.88	120.29
1	B	977	LEU	C-N-CA	8.87	132.88	120.29
1	A	892	PRO	CA-N-CD	-8.66	99.87	112.00
1	C	892	PRO	CA-N-CD	-8.65	99.88	112.00
1	B	892	PRO	CA-N-CD	-8.64	99.90	112.00
1	C	85	PRO	CA-C-N	6.82	132.69	122.87
1	C	85	PRO	C-N-CA	6.82	132.69	122.87
1	C	942	PRO	N-CA-CB	6.60	110.12	102.33
1	B	942	PRO	N-CA-CB	6.56	110.14	103.25
1	A	942	PRO	N-CA-CB	6.53	110.10	103.25
1	A	19	THR	CB-CA-C	-6.38	109.20	116.54
1	C	19	THR	CB-CA-C	-6.11	109.52	116.54
1	C	85	PRO	N-CA-C	5.97	119.87	111.33
1	C	322	PRO	CA-N-CD	-5.62	104.13	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	993	ILE	Mainchain

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	8442	0	8226	251	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8442	0	8227	263	0
1	C	8442	0	8226	255	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	I	28	0	25	0	0
2	O	28	0	25	0	0
2	Q	28	0	25	0	0
2	T	28	0	25	1	0
2	Z	28	0	25	0	0
2	b	28	0	25	0	0
2	e	28	0	25	1	0
3	E	39	0	34	2	0
3	G	39	0	34	1	0
3	H	39	0	34	0	0
3	J	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	2	0
3	N	39	0	34	0	0
3	P	39	0	34	1	0
3	R	39	0	34	2	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	0	0
3	Y	39	0	34	1	0
3	a	39	0	34	1	0
3	c	39	0	34	0	0
3	d	39	0	34	1	0
3	f	39	0	34	0	0
3	g	39	0	34	0	0
3	i	39	0	34	0	0
3	j	39	0	34	2	0
4	L	38	0	34	0	0
4	W	38	0	34	0	0
4	h	38	0	34	0	0
5	A	98	0	91	2	0
5	B	98	0	91	2	0
5	C	112	0	104	1	0
All	All	26819	0	26006	740	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 14.

All (740) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:SER:OG	1:B:817:PRO:HD3	1.24	1.35
1:B:985:ASP:OD1	1:B:987:PRO:CD	1.82	1.26
1:C:816:SER:OG	1:C:817:PRO:HD3	1.15	1.25
1:B:985:ASP:CG	1:B:987:PRO:HD3	1.64	1.22
1:B:985:ASP:CG	1:B:987:PRO:CD	2.13	1.19
1:A:816:SER:OG	1:A:817:PRO:HD3	1.41	1.17
1:C:986:PRO:HD2	1:C:987:PRO:CD	1.78	1.13
1:B:985:ASP:HB2	1:B:986:PRO:HD3	1.26	1.12
1:A:817:PRO:HD2	1:A:818:ILE:H	1.12	1.10
1:C:987:PRO:HD2	1:C:988:GLU:H	1.12	1.10
1:C:816:SER:OG	1:C:817:PRO:CD	2.00	1.09
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.18	1.09
1:B:816:SER:OG	1:B:817:PRO:CD	2.02	1.08
1:B:817:PRO:HD2	1:B:818:ILE:H	1.12	1.08
1:B:985:ASP:OD1	1:B:987:PRO:HD2	1.54	1.07
1:C:817:PRO:HD2	1:C:818:ILE:H	1.11	1.06
1:A:899:PRO:HD2	1:A:900:MET:H	1.17	1.06
1:B:985:ASP:OD2	1:B:987:PRO:CG	2.04	1.06
1:C:365:TYR:HB3	1:C:387:LEU:CD1	1.86	1.05
1:B:985:ASP:CG	1:B:987:PRO:CG	2.30	1.05
1:C:365:TYR:CB	1:C:387:LEU:HD13	1.86	1.05
1:C:899:PRO:HD2	1:C:900:MET:H	1.19	1.03
1:C:985:ASP:C	1:C:987:PRO:HD3	1.83	1.03
1:C:365:TYR:HB3	1:C:387:LEU:HD13	1.44	1.00
1:C:365:TYR:CB	1:C:387:LEU:CD1	2.40	0.98
1:A:1118:HIS:CD2	1:A:1140:PRO:HG3	2.01	0.95
1:C:986:PRO:CD	1:C:987:PRO:HD3	1.97	0.94
1:C:816:SER:HG	1:C:817:PRO:HD3	1.23	0.92
1:B:985:ASP:OD2	1:B:987:PRO:HG3	1.67	0.92
1:C:365:TYR:CG	1:C:387:LEU:HD13	2.06	0.91
1:B:985:ASP:HB2	1:B:986:PRO:CD	2.02	0.88
1:C:986:PRO:HD2	1:C:987:PRO:HD3	1.49	0.88
1:B:985:ASP:C	1:B:987:PRO:HD3	1.97	0.88
1:B:817:PRO:HD2	1:B:818:ILE:N	1.88	0.88
1:B:987:PRO:HD2	1:B:988:GLU:H	1.38	0.88
1:C:986:PRO:HD2	1:C:987:PRO:N	1.87	0.87
1:B:1116:THR:HB	1:B:1140:PRO:HD3	1.56	0.86
1:A:817:PRO:HD2	1:A:818:ILE:N	1.89	0.86
1:B:899:PRO:HD2	1:B:900:MET:H	1.39	0.85
1:A:393:THR:HA	1:A:522:ALA:HA	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:CYS:SG	1:A:644:GLN:NE2	2.50	0.85
1:B:191:GLU:HB3	1:B:223:LEU:HD21	1.59	0.84
1:C:987:PRO:HD2	1:C:988:GLU:N	1.87	0.84
1:A:899:PRO:HD2	1:A:900:MET:N	1.91	0.84
1:B:986:PRO:HD2	1:B:987:PRO:CD	2.07	0.84
1:C:817:PRO:HD2	1:C:818:ILE:N	1.89	0.84
1:C:986:PRO:CD	1:C:987:PRO:CD	2.55	0.84
1:C:365:TYR:HB2	1:C:387:LEU:CB	2.08	0.83
1:C:899:PRO:HD2	1:C:900:MET:N	1.92	0.83
1:B:806:LEU:HD12	1:B:807:PRO:HD2	1.61	0.82
1:C:365:TYR:HB3	1:C:387:LEU:HD12	1.61	0.82
1:B:898:PHE:N	1:B:899:PRO:HD3	1.95	0.82
1:A:816:SER:OG	1:A:817:PRO:CD	2.27	0.82
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.13	0.81
1:B:444:LYS:HD3	1:B:446:GLY:H	1.44	0.81
1:A:898:PHE:N	1:A:899:PRO:HD3	1.96	0.80
1:B:391:CYS:HA	1:B:525:CYS:CB	2.07	0.80
1:B:985:ASP:CB	1:B:987:PRO:HD3	2.13	0.79
1:C:898:PHE:N	1:C:899:PRO:HD3	1.97	0.79
1:B:421:TYR:HA	1:B:457:ARG:HH21	1.47	0.79
1:B:817:PRO:CD	1:B:818:ILE:H	1.95	0.78
1:C:365:TYR:HB2	1:C:387:LEU:HB2	1.64	0.78
1:B:986:PRO:CD	1:B:987:PRO:HD3	2.13	0.77
1:A:897:PRO:C	1:A:899:PRO:HD3	2.09	0.77
1:B:985:ASP:OD2	1:B:987:PRO:HG2	1.84	0.77
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.18	0.76
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.19	0.76
1:B:637:SER:HA	1:B:651:ILE:HD11	1.67	0.76
1:C:985:ASP:C	1:C:987:PRO:CD	2.58	0.76
1:C:188:ASN:HB3	1:C:190:ARG:HH12	1.51	0.75
1:C:924:ALA:O	1:C:928:ASN:ND2	2.19	0.75
1:C:987:PRO:CD	1:C:988:GLU:H	1.95	0.75
1:A:37:TYR:H	1:A:55:PHE:HE1	1.35	0.74
1:A:125:ASN:ND2	1:A:172:SER:O	2.20	0.74
1:C:897:PRO:C	1:C:899:PRO:HD3	2.12	0.74
1:C:985:ASP:HB2	1:C:986:PRO:HD3	1.70	0.74
1:A:191:GLU:HB2	1:A:223:LEU:HD21	1.68	0.74
1:A:817:PRO:CD	1:A:818:ILE:H	1.97	0.73
1:C:817:PRO:CD	1:C:818:ILE:H	1.96	0.73
1:C:1116:THR:HB	1:C:1140:PRO:HD3	1.71	0.73
1:A:444:LYS:HD2	1:A:446:GLY:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:ASP:CB	1:B:986:PRO:HD3	2.14	0.72
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.23	0.72
1:A:897:PRO:C	1:A:899:PRO:CD	2.63	0.72
1:A:992:GLN:HG3	1:A:995:ARG:HH21	1.53	0.72
1:B:644:GLN:NE2	1:B:649:CYS:SG	2.62	0.72
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.70	0.72
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.72	0.71
1:B:433:VAL:HG23	1:B:512:VAL:HG22	1.73	0.71
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.24	0.70
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.72	0.70
1:C:1081:ILE:HD11	1:C:1135:ASN:HB3	1.74	0.70
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.23	0.70
1:B:1139:ASP:HB3	1:B:1142:GLN:HB2	1.74	0.70
1:B:816:SER:HG	1:B:817:PRO:HD3	1.56	0.70
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.25	0.69
1:B:985:ASP:OD1	1:B:987:PRO:HD3	1.68	0.69
1:B:924:ALA:O	1:B:928:ASN:ND2	2.25	0.69
1:B:439:ASN:HD22	1:B:506:GLN:HG2	1.58	0.69
1:B:899:PRO:HD2	1:B:900:MET:N	2.04	0.69
1:B:81:ASN:O	1:B:239:GLN:NE2	2.25	0.69
1:B:811:LYS:HD3	1:B:813:SER:H	1.57	0.69
1:B:986:PRO:CD	1:B:987:PRO:CD	2.71	0.69
1:C:897:PRO:C	1:C:899:PRO:CD	2.66	0.69
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.26	0.68
1:B:179:LEU:HD23	1:B:209:PRO:HD3	1.74	0.68
1:C:985:ASP:O	1:C:987:PRO:CD	2.42	0.68
1:A:27:ALA:HB3	1:A:64:TRP:HE3	1.57	0.68
1:B:987:PRO:HD2	1:B:988:GLU:N	2.01	0.68
1:B:1134:ASN:HB2	3:Y:1:NAG:HN2	1.57	0.68
1:C:81:ASN:HB3	1:C:239:GLN:HE21	1.58	0.68
1:A:517:LEU:C	1:A:519:HIS:H	2.02	0.68
1:B:461:LEU:HD12	1:B:465:GLU:HB3	1.75	0.68
1:A:983:ARG:HB3	1:A:984:LEU:HD22	1.76	0.68
1:C:986:PRO:CD	1:C:987:PRO:N	2.56	0.68
1:B:108:THR:HG23	1:B:109:THR:HG23	1.76	0.68
1:B:986:PRO:HD2	1:B:987:PRO:N	2.07	0.68
1:B:31:SER:OG	1:B:60:SER:OG	2.12	0.67
1:C:899:PRO:CD	1:C:900:MET:H	2.01	0.67
1:A:141:LEU:HB2	1:A:243:ARG:HA	1.75	0.67
1:A:34:ARG:HG3	1:A:216:LEU:HD11	1.77	0.67
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASP:HB3	1:A:986:PRO:HD2	1.76	0.67
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.28	0.67
1:B:978:ASN:HB3	1:C:547:THR:OG1	1.94	0.67
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.28	0.66
1:C:117:LEU:HD12	1:C:130:VAL:HG22	1.76	0.66
1:B:898:PHE:N	1:B:899:PRO:CD	2.58	0.66
1:A:517:LEU:HG	1:A:518:LEU:HD22	1.77	0.66
1:B:892:PRO:HD3	1:C:1069:PRO:HG2	1.77	0.66
1:C:328:ARG:NH1	1:C:531:THR:O	2.27	0.66
1:C:1134:ASN:HB2	3;j:1:NAG:HN2	1.60	0.66
1:A:899:PRO:CD	1:A:900:MET:H	2.00	0.66
1:B:985:ASP:C	1:B:987:PRO:CD	2.69	0.66
1:B:985:ASP:OD1	1:B:987:PRO:CG	2.38	0.66
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.60	0.66
1:A:99:ASN:O	1:A:102:ARG:NH1	2.27	0.66
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.78	0.66
1:B:985:ASP:CB	1:B:986:PRO:CD	2.71	0.66
1:A:817:PRO:CD	1:A:818:ILE:N	2.58	0.65
1:B:409:GLN:HB3	1:B:419:ALA:HB2	1.78	0.65
1:C:623:ALA:HB1	1:C:629:LEU:HD21	1.78	0.65
1:A:81:ASN:O	1:A:239:GLN:NE2	2.16	0.65
1:B:617:CYS:SG	1:B:644:GLN:NE2	2.67	0.65
1:A:99:ASN:ND2	1:A:178:ASP:OD1	2.30	0.65
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.77	0.65
1:C:78:ARG:HE	1:C:79:PHE:H	1.42	0.65
1:A:818:ILE:O	1:A:822:LEU:HD12	1.97	0.65
1:C:987:PRO:CD	1:C:988:GLU:N	2.56	0.65
1:A:899:PRO:CD	1:A:900:MET:N	2.59	0.65
1:B:897:PRO:C	1:B:899:PRO:HD3	2.21	0.65
1:B:379:CYS:HB3	1:B:382:VAL:HG13	1.79	0.65
1:C:334:ASN:ND2	1:C:360:ASN:O	2.25	0.65
1:A:1129:VAL:HG12	1:C:917:TYR:HB3	1.79	0.64
1:C:1093:GLY:H	1:C:1107:ARG:NH1	1.95	0.64
1:A:898:PHE:N	1:A:899:PRO:CD	2.59	0.64
1:C:95:THR:OG1	1:C:264:ALA:O	2.15	0.64
1:C:898:PHE:N	1:C:899:PRO:CD	2.61	0.64
1:C:899:PRO:CD	1:C:900:MET:N	2.60	0.64
1:B:384:PRO:HA	1:B:387:LEU:HG	1.80	0.64
1:B:817:PRO:CD	1:B:818:ILE:N	2.56	0.64
1:B:897:PRO:C	1:B:899:PRO:CD	2.71	0.64
1:C:817:PRO:CD	1:C:818:ILE:N	2.57	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:PRO:HD2	1:B:987:PRO:HD3	1.79	0.63
1:A:127:VAL:HG21	3:E:1:NAG:H62	1.81	0.63
1:B:892:PRO:HD2	1:B:892:PRO:O	1.99	0.63
1:C:866:THR:H	1:C:869:MET:HE2	1.63	0.63
1:A:201:PHE:HB3	1:A:229:LEU:HB3	1.81	0.63
1:B:986:PRO:N	1:B:987:PRO:HD3	2.12	0.63
1:A:383:SER:HB2	1:A:386:LYS:HG2	1.81	0.62
1:A:393:THR:CA	1:A:522:ALA:HA	2.27	0.62
1:A:406:GLU:OE2	1:A:409:GLN:NE2	2.32	0.62
1:A:977:LEU:O	1:A:981:LEU:HG	1.99	0.62
1:B:420:ASP:O	1:B:457:ARG:NH2	2.32	0.62
1:C:37:TYR:HA	1:C:223:LEU:H	1.64	0.62
1:A:866:THR:H	1:A:869:MET:HE2	1.64	0.62
1:C:365:TYR:HB2	1:C:387:LEU:CD1	2.28	0.62
1:B:866:THR:H	1:B:869:MET:HE2	1.64	0.62
1:A:892:PRO:HD2	1:A:892:PRO:O	1.99	0.62
1:C:379:CYS:HA	1:C:432:CYS:CB	2.29	0.62
1:B:31:SER:HG	1:B:60:SER:HG	1.48	0.62
1:B:357:ARG:NH2	1:B:359:SER:OG	2.33	0.62
1:B:66:HIS:CE1	1:B:262:ALA:HB1	2.35	0.61
1:C:115:GLN:HA	1:C:132:GLU:HA	1.81	0.61
1:A:342:PHE:HB2	5:A:1403:NAG:H82	1.82	0.61
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.81	0.61
1:C:892:PRO:HD2	1:C:892:PRO:O	2.00	0.61
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.83	0.61
1:C:365:TYR:CB	1:C:387:LEU:HD12	2.22	0.60
1:C:424:LYS:NZ	1:C:461:LEU:O	2.28	0.60
1:B:899:PRO:CD	1:B:900:MET:H	2.14	0.60
1:C:81:ASN:HB3	1:C:239:GLN:NE2	2.16	0.60
1:C:986:PRO:HD2	1:C:987:PRO:CG	2.29	0.60
1:B:985:ASP:CG	1:B:987:PRO:HG2	2.23	0.60
1:B:277:LEU:HD11	1:B:285:ILE:HD13	1.82	0.60
1:B:415:THR:OG1	1:B:420:ASP:OD2	2.20	0.60
1:C:637:SER:HA	1:C:651:ILE:HD11	1.84	0.60
1:A:992:GLN:HA	1:A:995:ARG:NE	2.17	0.59
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.84	0.59
1:C:81:ASN:HD21	1:C:240:THR:HG22	1.67	0.59
1:A:454:ARG:NH2	1:A:469:SER:O	2.30	0.59
1:C:986:PRO:N	1:C:987:PRO:HD3	2.18	0.59
1:B:37:TYR:CD2	1:B:193:VAL:HG21	2.38	0.59
1:B:987:PRO:CD	1:B:988:GLU:H	2.11	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:OG1	1:A:264:ALA:O	2.20	0.58
1:A:977:LEU:O	1:A:980:ILE:HG22	2.02	0.58
1:C:357:ARG:NH2	1:C:359:SER:OG	2.37	0.58
1:A:296:LEU:HD21	1:A:300:LYS:HE3	1.84	0.58
1:B:78:ARG:HE	1:B:79:PHE:H	1.49	0.58
1:C:66:HIS:CD2	1:C:214:ARG:HH22	2.21	0.58
1:A:1118:HIS:HD2	1:A:1140:PRO:HG3	1.65	0.58
1:A:461:LEU:HD12	1:A:465:GLU:HB2	1.86	0.58
1:B:212:LEU:HD13	1:B:217:PRO:HA	1.84	0.58
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.86	0.58
1:B:987:PRO:CD	1:B:988:GLU:N	2.66	0.58
1:B:1081:ILE:HG23	1:B:1088:HIS:HB2	1.85	0.58
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.39	0.58
1:A:108:THR:HG23	1:A:109:THR:HG23	1.86	0.57
1:B:331:ASN:OD1	5:B:1402:NAG:N2	2.37	0.57
1:B:346:ARG:NH1	1:B:442:ASP:OD1	2.36	0.57
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.85	0.57
1:A:620:VAL:HA	1:A:623:ALA:HB3	1.85	0.57
1:B:105:ILE:HD12	1:B:242:TYR:CE2	2.39	0.57
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.40	0.57
1:B:94:SER:HB3	1:B:101:ILE:HG13	1.86	0.57
1:C:81:ASN:HD21	1:C:240:THR:H	1.53	0.57
1:C:722:VAL:HG22	1:C:930:ALA:HB1	1.86	0.57
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.87	0.57
1:A:731:MET:HB2	1:A:955:ASN:HD21	1.70	0.57
1:B:457:ARG:NH1	1:B:459:SER:O	2.38	0.56
1:C:390:LEU:HD23	1:C:391:CYS:H	1.70	0.56
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.87	0.56
1:C:108:THR:HG23	1:C:109:THR:HG23	1.87	0.56
1:B:53:ASP:OD1	1:B:54:LEU:N	2.35	0.56
1:C:384:PRO:HA	1:C:387:LEU:CD1	2.36	0.56
1:B:206:LYS:HB2	1:B:223:LEU:HD23	1.87	0.56
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.70	0.56
1:B:328:ARG:NH1	1:B:531:THR:O	2.36	0.56
1:B:899:PRO:CD	1:B:900:MET:N	2.69	0.56
1:A:265:TYR:HE2	1:A:267:VAL:HG23	1.71	0.56
1:B:234:ASN:N	1:C:465:GLU:OE2	2.39	0.56
1:A:206:LYS:HB3	1:A:223:LEU:HD23	1.87	0.55
1:B:457:ARG:HH22	1:B:461:LEU:H	1.54	0.55
1:A:382:VAL:HG23	1:A:387:LEU:HD21	1.88	0.55
1:B:431:GLY:HA2	1:B:515:PHE:CE1	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1050:MET:HE2	1:B:1052:PHE:CZ	2.41	0.55
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.89	0.55
1:A:801:ASN:HB3	1:A:928:ASN:OD1	2.07	0.55
1:A:989:ALA:O	1:A:993:ILE:HG13	2.06	0.55
1:A:110:LEU:HG	1:A:135:PHE:HD2	1.72	0.55
1:A:1139:ASP:HB3	1:A:1142:GLN:HG2	1.88	0.55
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.42	0.55
1:C:634:ARG:CZ	1:C:637:SER:HB2	2.37	0.55
1:A:661:GLU:N	1:A:661:GLU:OE1	2.40	0.55
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.89	0.55
1:C:206:LYS:HD2	1:C:222:ALA:O	2.06	0.55
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.40	0.55
1:A:30:ASN:O	1:A:30:ASN:ND2	2.37	0.55
1:A:384:PRO:HA	1:A:387:LEU:HG	1.89	0.55
1:C:91:TYR:HD1	1:C:193:VAL:HG22	1.72	0.55
1:A:357:ARG:NH2	1:A:359:SER:OG	2.40	0.54
1:A:984:LEU:HB3	1:A:988:GLU:HG2	1.89	0.54
1:B:365:TYR:CG	1:B:387:LEU:HD13	2.42	0.54
1:C:193:VAL:HB	1:C:204:TYR:HD2	1.72	0.54
1:B:91:TYR:OH	1:B:191:GLU:OE2	2.17	0.54
1:B:453:TYR:OH	1:B:455:LEU:HD13	2.07	0.54
1:A:55:PHE:HB2	1:A:275:PHE:CE1	2.43	0.54
1:B:897:PRO:HB2	1:B:900:MET:HG3	1.90	0.54
1:A:35:GLY:HA2	1:A:91:TYR:CE1	2.41	0.54
1:A:409:GLN:HB3	1:A:419:ALA:HB2	1.90	0.54
1:C:1081:ILE:HG23	1:C:1088:HIS:HB2	1.90	0.54
1:B:391:CYS:C	1:B:392:PHE:HD1	2.15	0.54
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.73	0.54
1:A:37:TYR:HD2	1:A:193:VAL:HG21	1.72	0.54
1:A:201:PHE:O	1:A:229:LEU:N	2.31	0.54
1:A:31:SER:O	1:A:59:PHE:N	2.41	0.53
1:A:64:TRP:CZ2	1:A:66:HIS:HB2	2.42	0.53
1:C:81:ASN:ND2	1:C:240:THR:O	2.37	0.53
1:A:644:GLN:NE2	1:A:649:CYS:SG	2.81	0.53
1:B:326:ILE:HD13	1:B:533:LEU:HA	1.88	0.53
1:C:278:LYS:HB2	1:C:306:PHE:HE2	1.73	0.53
1:C:327:VAL:H	1:C:531:THR:HG22	1.73	0.53
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.90	0.53
1:C:979:ASP:OD1	1:C:983:ARG:NH2	2.41	0.53
1:B:869:MET:HG2	1:C:699:LEU:HD21	1.90	0.53
1:A:81:ASN:ND2	1:A:240:THR:O	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:N	1:A:210:ILE:O	2.42	0.53
1:B:206:LYS:NZ	1:B:222:ALA:H	2.07	0.53
1:C:801:ASN:HB3	1:C:928:ASN:OD1	2.09	0.53
1:C:994:ASP:OD1	1:C:995:ARG:N	2.41	0.53
1:B:989:ALA:O	1:B:993:ILE:HG12	2.09	0.53
1:C:229:LEU:HD12	1:C:230:PRO:HD2	1.91	0.53
1:A:1118:HIS:NE2	1:A:1140:PRO:HG3	2.23	0.52
1:C:81:ASN:ND2	1:C:240:THR:H	2.07	0.52
1:C:278:LYS:HB2	1:C:306:PHE:CE2	2.45	0.52
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.43	0.52
1:A:424:LYS:NZ	1:A:461:LEU:O	2.34	0.52
1:B:346:ARG:HH21	1:B:450:ASN:HD21	1.57	0.52
1:C:897:PRO:HB2	1:C:900:MET:HE3	1.91	0.52
1:A:517:LEU:C	1:A:519:HIS:N	2.65	0.52
1:C:452:LEU:HG	1:C:494:SER:HA	1.91	0.52
1:A:41:LYS:HA	1:B:562:PHE:CE2	2.44	0.52
1:A:469:SER:HB2	1:C:114:THR:HG22	1.91	0.52
1:A:705:VAL:HG11	1:C:883:THR:HG21	1.92	0.52
1:C:179:LEU:HG	1:C:180:GLU:H	1.75	0.52
1:A:892:PRO:HD3	1:B:1069:PRO:HG2	1.92	0.52
1:B:33:THR:HA	1:B:58:PHE:CD1	2.45	0.52
1:B:393:THR:HA	1:B:522:ALA:HA	1.92	0.52
1:B:634:ARG:NH1	1:B:637:SER:HB2	2.25	0.52
1:C:1091:ARG:HG2	1:C:1091:ARG:HH11	1.74	0.52
1:B:596:SER:HB3	1:B:613:GLN:HE22	1.75	0.52
1:A:637:SER:HA	1:A:651:ILE:HD11	1.91	0.51
1:C:444:LYS:HD3	1:C:446:GLY:H	1.76	0.51
1:C:461:LEU:HD12	1:C:465:GLU:HB3	1.92	0.51
1:C:804:GLN:O	1:C:817:PRO:CD	2.59	0.51
1:C:54:LEU:HD12	1:C:197:ILE:HD11	1.91	0.51
1:C:84:LEU:HB2	1:C:238:PHE:CE1	2.46	0.51
1:A:36:VAL:HG11	1:A:277:LEU:HD21	1.91	0.51
1:C:729:VAL:HG11	1:C:781:VAL:HG11	1.93	0.51
1:A:379:CYS:HA	1:A:432:CYS:HA	1.92	0.51
1:B:290:ASP:O	1:B:297:SER:HB3	2.10	0.51
1:B:365:TYR:CD1	1:B:387:LEU:HB3	2.45	0.51
1:B:816:SER:HG	1:B:817:PRO:CD	2.18	0.51
1:C:759:PHE:O	1:C:763:LEU:HG	2.11	0.51
1:C:1139:ASP:HB3	1:C:1142:GLN:HB2	1.92	0.51
1:A:383:SER:HB2	1:A:386:LYS:CG	2.40	0.51
1:B:27:ALA:HB3	1:B:64:TRP:CE3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:VAL:HG11	1:A:781:VAL:HG11	1.92	0.51
1:A:187:LYS:HB2	1:A:210:ILE:HG13	1.93	0.51
1:A:986:PRO:N	1:A:987:PRO:HD2	2.25	0.50
1:C:106:PHE:O	1:C:116:SER:HB3	2.11	0.50
1:C:341:VAL:HG11	1:C:397:ALA:HB1	1.91	0.50
1:A:290:ASP:O	1:A:297:SER:HB3	2.12	0.50
1:A:578:ASP:HB3	1:A:581:THR:O	2.11	0.50
1:B:213:VAL:HG22	1:B:214:ARG:HG2	1.93	0.50
1:C:201:PHE:HB3	1:C:229:LEU:HB3	1.93	0.50
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.92	0.50
1:B:1031:GLU:OE1	1:C:1039:ARG:NE	2.37	0.50
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.93	0.50
1:A:186:PHE:CD1	1:A:211:ASN:HB3	2.45	0.50
1:A:1104:VAL:HG13	1:A:1115:ILE:HG12	1.93	0.50
1:C:736:VAL:HG22	1:C:858:LEU:HG	1.94	0.50
1:B:222:ALA:HB2	1:B:285:ILE:HD12	1.93	0.50
1:A:978:ASN:H	1:A:978:ASN:HD22	1.58	0.50
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.20	0.50
1:B:326:ILE:HD11	1:B:534:VAL:HG12	1.93	0.50
1:B:334:ASN:ND2	1:B:360:ASN:O	2.33	0.50
1:B:366:SER:HB3	1:B:388:ASN:HD21	1.77	0.49
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.47	0.49
1:B:384:PRO:HA	1:B:387:LEU:CG	2.41	0.49
1:B:909:ILE:HG12	1:B:1047:TYR:HB3	1.94	0.49
1:A:1116:THR:OG1	1:A:1140:PRO:HD3	2.11	0.49
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.76	0.49
1:C:624:ILE:HD12	1:C:634:ARG:HE	1.78	0.49
1:A:462:LYS:HB2	1:A:465:GLU:HG3	1.94	0.49
1:C:37:TYR:CD2	1:C:193:VAL:HG21	2.47	0.49
1:B:346:ARG:HH22	1:B:448:ASN:HD21	1.61	0.49
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.95	0.49
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.95	0.49
1:B:1138:TYR:OH	1:B:1143:PRO:HG3	2.12	0.49
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.44	0.49
1:A:444:LYS:HD2	1:A:446:GLY:N	2.26	0.49
1:B:985:ASP:CA	1:B:987:PRO:HD3	2.42	0.49
1:C:92:PHE:HE1	1:C:94:SER:HB3	1.77	0.49
1:C:293:LEU:O	1:C:633:TRP:HB3	2.13	0.49
1:A:331:ASN:OD1	1:A:331:ASN:N	2.46	0.49
1:A:752:LEU:HD11	1:A:990:GLU:HB3	1.94	0.49
1:B:35:GLY:HA2	1:B:91:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:HE2	1:B:557:LYS:HD2	1.78	0.49
1:B:66:HIS:HE1	1:B:262:ALA:HB1	1.76	0.49
1:B:457:ARG:HH22	1:B:460:ASN:HA	1.78	0.49
1:B:986:PRO:HD2	1:B:987:PRO:CG	2.42	0.49
1:C:393:THR:HA	1:C:522:ALA:HA	1.95	0.49
1:A:34:ARG:HG2	1:A:216:LEU:HD21	1.94	0.49
1:B:32:PHE:HA	1:B:59:PHE:HD1	1.78	0.49
1:C:390:LEU:HD13	1:C:392:PHE:HE1	1.78	0.49
1:C:905:ARG:NH1	1:C:1050:MET:HB3	2.28	0.49
1:A:37:TYR:CD2	1:A:193:VAL:HG21	2.48	0.49
1:A:804:GLN:O	1:A:817:PRO:CD	2.61	0.49
1:A:983:ARG:HA	1:A:983:ARG:NE	2.28	0.49
1:B:28:TYR:CE2	5:B:1401:NAG:H5	2.48	0.49
1:A:49:HIS:HE1	1:A:51:THR:HB	1.78	0.48
1:B:94:SER:HB2	1:B:190:ARG:HB2	1.93	0.48
1:B:117:LEU:HD12	1:B:130:VAL:HB	1.95	0.48
1:A:386:LYS:HG3	1:C:983:ARG:O	2.13	0.48
1:B:179:LEU:HG	1:B:180:GLU:H	1.77	0.48
1:B:401:VAL:HG21	1:B:451:TYR:CE2	2.48	0.48
1:C:35:GLY:HA2	1:C:91:TYR:CE1	2.48	0.48
1:C:985:ASP:HB2	1:C:986:PRO:CD	2.41	0.48
1:A:378:LYS:HE3	1:A:380:TYR:OH	2.13	0.48
1:B:384:PRO:HA	1:B:387:LEU:CD1	2.43	0.48
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.62	0.48
1:C:44:ARG:HB2	1:C:49:HIS:HE1	1.78	0.48
1:C:538:CYS:HB3	1:C:590:CYS:HB3	1.66	0.48
1:C:431:GLY:HA2	1:C:515:PHE:CE1	2.49	0.48
1:C:804:GLN:O	1:C:817:PRO:CG	2.61	0.48
1:A:390:LEU:HD23	1:A:392:PHE:CZ	2.48	0.48
1:B:187:LYS:N	1:B:210:ILE:O	2.47	0.48
1:C:200:TYR:HB2	1:C:202:LYS:HZ3	1.78	0.48
1:C:919:ASN:O	1:C:923:ILE:HG12	2.14	0.48
1:A:86:PHE:CE2	1:A:238:PHE:HB3	2.48	0.48
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.78	0.48
1:A:205:SER:O	1:A:224:GLU:N	2.42	0.48
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.95	0.48
1:B:187:LYS:O	1:B:210:ILE:N	2.33	0.48
1:C:388:ASN:HA	1:C:527:PRO:HD2	1.95	0.48
1:A:33:THR:OG1	1:A:219:GLY:O	2.27	0.48
1:A:229:LEU:HD12	1:A:230:PRO:HD2	1.96	0.48
1:A:318:PHE:CZ	1:A:615:VAL:HG21	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:ASN:HB3	1:B:928:ASN:OD1	2.13	0.48
1:C:83:VAL:HG12	1:C:237:ARG:HB2	1.96	0.48
1:C:105:ILE:HD11	1:C:241:LEU:HD21	1.96	0.48
1:C:909:ILE:HG12	1:C:1047:TYR:HB3	1.95	0.48
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.95	0.48
1:A:990:GLU:HA	1:A:993:ILE:HD12	1.96	0.48
1:A:30:ASN:C	1:A:30:ASN:HD22	2.14	0.47
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.31	0.47
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.96	0.47
1:B:142:GLY:H	1:B:156:GLU:HB2	1.79	0.47
1:C:927:PHE:CZ	1:C:931:ILE:HD11	2.49	0.47
2:T:1:NAG:H61	2:T:2:NAG:HN2	1.78	0.47
1:C:617:CYS:O	1:C:620:VAL:HG12	2.14	0.47
1:A:84:LEU:HB2	1:A:238:PHE:CE1	2.48	0.47
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.30	0.47
1:C:231:ILE:HG13	1:C:232:GLY:N	2.29	0.47
1:C:329:PHE:CE2	1:C:528:LYS:HB3	2.49	0.47
1:C:366:SER:H	1:C:388:ASN:HD21	1.63	0.47
1:C:708:SER:HG	1:C:711:SER:HG	1.61	0.47
1:B:462:LYS:HG2	3:G:1:NAG:H82	1.95	0.47
1:C:105:ILE:N	1:C:239:GLN:O	2.36	0.47
1:C:722:VAL:HG23	1:C:934:ILE:HG13	1.97	0.47
1:C:985:ASP:O	1:C:987:PRO:HD2	2.13	0.47
1:A:99:ASN:OD1	1:A:190:ARG:NH2	2.47	0.47
1:B:127:VAL:HA	1:B:171:VAL:HG12	1.95	0.47
1:A:380:TYR:CZ	1:A:412:PRO:HD2	2.48	0.47
1:B:179:LEU:HB2	1:B:207:HIS:CE1	2.50	0.47
1:B:788:ILE:HD11	1:C:699:LEU:HB3	1.97	0.47
1:C:889:GLY:HA3	1:C:1034:LEU:HD23	1.97	0.47
1:A:104:TRP:HZ2	1:A:192:PHE:CE2	2.32	0.47
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.78	0.47
1:A:546:LEU:C	1:A:546:LEU:HD23	2.40	0.47
1:B:201:PHE:O	1:B:229:LEU:N	2.35	0.47
1:B:345:THR:HG22	1:B:346:ARG:HG2	1.96	0.47
1:C:83:VAL:HA	1:C:238:PHE:O	2.15	0.47
1:C:462:LYS:HG3	3:R:1:NAG:H82	1.95	0.47
1:A:402:ILE:HD13	1:A:410:ILE:HD11	1.96	0.47
1:A:927:PHE:CZ	1:A:931:ILE:HD11	2.49	0.47
1:C:349:SER:OG	1:C:452:LEU:O	2.33	0.47
1:C:642:VAL:HG22	1:C:651:ILE:HG13	1.97	0.47
1:A:930:ALA:O	1:A:934:ILE:HG12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ARG:O	1:A:984:LEU:HB2	2.15	0.47
1:B:33:THR:OG1	1:B:219:GLY:O	2.22	0.47
1:A:102:ARG:NH1	1:A:243:ARG:HH21	2.12	0.47
1:A:206:LYS:CB	1:A:223:LEU:HD23	2.44	0.47
1:A:989:ALA:HA	1:A:992:GLN:OE1	2.14	0.47
1:B:174:PRO:HB2	1:B:176:LEU:HD22	1.97	0.47
1:A:388:ASN:O	1:A:526:GLY:HA3	2.15	0.46
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.74	0.46
1:B:380:TYR:CD1	1:B:380:TYR:N	2.83	0.46
1:B:380:TYR:HD1	1:B:431:GLY:O	1.99	0.46
1:B:401:VAL:HG21	1:B:451:TYR:CZ	2.50	0.46
1:B:986:PRO:CD	1:B:987:PRO:N	2.72	0.46
1:A:114:THR:HG22	1:B:469:SER:HB2	1.97	0.46
1:A:392:PHE:HA	1:A:517:LEU:HD22	1.97	0.46
1:B:94:SER:CB	1:B:101:ILE:HG13	2.45	0.46
1:B:105:ILE:HD12	1:B:242:TYR:CZ	2.50	0.46
1:A:334:ASN:O	1:A:362:VAL:N	2.49	0.46
1:A:983:ARG:NH1	1:B:390:LEU:HD13	2.30	0.46
1:A:1107:ARG:HD3	1:C:904:TYR:CE1	2.50	0.46
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.97	0.46
1:A:393:THR:HB	1:A:517:LEU:HB3	1.96	0.46
1:A:892:PRO:O	1:A:892:PRO:CD	2.64	0.46
1:B:873:TYR:CZ	1:C:699:LEU:HD12	2.51	0.46
1:A:125:ASN:HA	1:A:174:PRO:HB3	1.97	0.46
1:C:392:PHE:N	1:C:524:VAL:O	2.49	0.46
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.95	0.46
1:A:27:ALA:HB3	1:A:64:TRP:CE3	2.45	0.46
1:A:871:ALA:HA	1:A:874:THR:HG22	1.98	0.46
1:B:308:VAL:O	1:B:602:THR:OG1	2.22	0.46
1:B:1116:THR:HG22	1:B:1138:TYR:HD2	1.81	0.46
1:C:281:GLU:HG3	3:d:1:NAG:H82	1.98	0.46
1:C:365:TYR:CD1	1:C:387:LEU:HD13	2.47	0.46
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.98	0.46
1:C:86:PHE:HD1	1:C:89:GLY:HA2	1.80	0.46
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.96	0.46
1:C:81:ASN:ND2	1:C:239:GLN:HG2	2.31	0.46
1:C:100:ILE:HA	1:C:243:ARG:HG2	1.97	0.46
1:A:216:LEU:HD13	1:A:266:TYR:HE2	1.81	0.46
1:A:595:VAL:HG11	1:A:633:TRP:HH2	1.81	0.46
1:A:1156:PHE:O	1:A:1160:THR:HG23	2.16	0.46
1:A:352:ALA:HA	1:A:466:ARG:HD2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:HG3	1:A:463:PRO:HA	1.98	0.45
1:C:308:VAL:HG13	1:C:313:TYR:HE2	1.81	0.45
1:C:858:LEU:HD21	1:C:962:LEU:HD23	1.98	0.45
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.81	0.45
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.81	0.45
1:B:555:SER:HB3	1:B:586:ASP:N	2.31	0.45
1:C:384:PRO:HA	1:C:387:LEU:HG	1.98	0.45
1:C:557:LYS:NZ	1:C:575:ALA:HB2	2.31	0.45
1:A:1039:ARG:NE	1:C:1031:GLU:OE2	2.39	0.45
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.51	0.45
1:C:551:VAL:HG12	1:C:588:THR:O	2.17	0.45
1:A:1103:PHE:CZ	3:M:1:NAG:H62	2.52	0.45
1:B:114:THR:HG22	1:C:469:SER:HB2	1.98	0.45
1:B:293:LEU:O	1:B:633:TRP:HB3	2.17	0.45
1:B:538:CYS:HB3	1:B:590:CYS:HB3	1.79	0.45
1:B:892:PRO:O	1:B:892:PRO:CD	2.64	0.45
1:C:402:ILE:HD13	1:C:410:ILE:HD11	1.98	0.45
1:C:816:SER:CB	1:C:817:PRO:CD	2.93	0.45
1:C:1029:MET:HE1	1:C:1053:PRO:HB3	1.99	0.45
1:A:37:TYR:CB	1:A:223:LEU:HB2	2.47	0.45
1:A:91:TYR:HD1	1:A:193:VAL:HG22	1.81	0.45
1:A:231:ILE:HG13	1:A:232:GLY:N	2.32	0.45
1:A:902:MET:HB3	1:A:916:LEU:HD21	1.99	0.45
1:C:298:GLU:HG3	1:C:633:TRP:HE1	1.80	0.45
1:C:388:ASN:CA	1:C:527:PRO:HD2	2.47	0.45
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.98	0.45
1:C:892:PRO:O	1:C:892:PRO:CD	2.65	0.45
3:E:1:NAG:H61	3:E:2:NAG:N2	2.32	0.45
1:A:388:ASN:C	1:A:390:LEU:H	2.25	0.45
1:A:909:ILE:O	1:A:909:ILE:HG13	2.16	0.45
1:A:542:ASN:HA	1:A:546:LEU:O	2.16	0.45
1:C:324:GLU:O	1:C:539:VAL:HG13	2.17	0.45
1:C:665:PRO:HA	1:C:671:CYS:SG	2.57	0.45
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.52	0.45
1:A:883:THR:HG21	1:B:705:VAL:HG11	1.98	0.45
1:B:102:ARG:HD3	1:B:121:ASN:O	2.17	0.45
1:B:1156:PHE:O	1:B:1160:THR:HG23	2.17	0.45
1:A:439:ASN:O	1:A:443:SER:CB	2.65	0.45
1:B:122:ASN:O	1:B:124:THR:N	2.49	0.44
1:C:365:TYR:HB2	1:C:387:LEU:HB3	1.92	0.44
1:C:877:LEU:O	1:C:881:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:PRO:HG2	1:A:988:GLU:OE1	2.18	0.44
1:A:1103:PHE:HZ	3:M:1:NAG:H62	1.83	0.44
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.53	0.44
1:C:105:ILE:O	1:C:238:PHE:HB2	2.17	0.44
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.00	0.44
1:B:34:ARG:HG3	1:B:216:LEU:HD21	2.00	0.44
1:B:142:GLY:N	1:B:156:GLU:HB2	2.33	0.44
1:B:819:GLU:O	1:B:823:PHE:HD1	1.99	0.44
1:C:28:TYR:CD1	5:C:1401:NAG:H3	2.52	0.44
1:C:31:SER:HB3	1:C:62:VAL:HB	1.99	0.44
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.99	0.44
1:B:239:GLN:HB3	1:B:242:TYR:OH	2.18	0.44
1:B:390:LEU:HG	1:B:391:CYS:N	2.32	0.44
1:B:897:PRO:HB2	1:B:899:PRO:HD2	1.98	0.44
1:C:543:PHE:HD2	1:C:579:PRO:HD2	1.83	0.44
1:C:330:PRO:HG3	1:C:579:PRO:HB2	1.99	0.44
1:C:1117:THR:H	1:C:1140:PRO:HD3	1.82	0.44
1:B:384:PRO:HA	1:B:387:LEU:HD12	2.00	0.44
1:B:557:LYS:O	1:B:584:ILE:HG21	2.18	0.44
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.83	0.44
1:C:634:ARG:NH1	1:C:637:SER:HB2	2.33	0.44
1:A:538:CYS:HB3	1:A:590:CYS:HB3	1.79	0.44
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.53	0.44
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.82	0.44
1:A:448:ASN:HB3	1:A:497:PHE:HB2	2.00	0.44
1:A:877:LEU:O	1:A:881:THR:HG23	2.18	0.44
1:A:382:VAL:CG2	1:A:387:LEU:HD21	2.47	0.43
1:B:57:PRO:O	1:B:60:SER:HB3	2.18	0.43
1:B:378:LYS:NZ	1:B:411:ALA:HB2	2.32	0.43
1:A:909:ILE:HG12	1:A:1047:TYR:HB3	2.01	0.43
1:B:329:PHE:CE2	1:B:528:LYS:HB3	2.53	0.43
2:e:1:NAG:H61	2:e:2:NAG:N2	2.32	0.43
1:A:748:GLU:OE2	1:A:981:LEU:HD13	2.19	0.43
1:B:444:LYS:HD3	1:B:446:GLY:N	2.23	0.43
1:B:578:ASP:HB3	1:B:581:THR:O	2.17	0.43
1:C:490:PHE:HE2	1:C:492:LEU:HB2	1.82	0.43
1:A:195:LYS:HE2	1:A:204:TYR:OH	2.18	0.43
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.79	0.43
1:A:1031:GLU:OE1	1:B:1039:ARG:NE	2.30	0.43
1:B:64:TRP:CZ2	1:B:66:HIS:HB2	2.52	0.43
1:B:127:VAL:HB	3:P:1:NAG:H62	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.83	0.43
1:C:19:THR:OG1	1:C:20:THR:N	2.51	0.43
1:A:37:TYR:HB3	1:A:223:LEU:HB2	2.00	0.43
1:A:65:PHE:O	1:A:264:ALA:HB1	2.18	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.80	0.43
1:B:1050:MET:HE2	1:B:1052:PHE:HZ	1.83	0.43
1:C:410:ILE:HG21	1:C:433:VAL:HG21	2.00	0.43
1:A:189:LEU:HB3	1:A:208:THR:HG23	2.01	0.43
1:B:41:LYS:HA	1:C:562:PHE:CE2	2.54	0.43
1:B:552:LEU:HD23	1:B:552:LEU:H	1.84	0.43
1:B:1086:LYS:HB3	1:B:1122:VAL:HG13	2.00	0.43
1:C:47:VAL:HG23	1:C:49:HIS:NE2	2.34	0.43
1:C:182:LYS:O	1:C:183:GLN:HG3	2.18	0.43
1:C:277:LEU:HD11	1:C:285:ILE:HD13	2.01	0.43
1:C:355:ARG:HD3	1:C:396:TYR:HD2	1.83	0.43
1:C:662:CYS:HB2	1:C:671:CYS:HB2	1.25	0.43
1:C:1080:ALA:HB3	1:C:1129:VAL:HG11	1.99	0.43
1:A:327:VAL:HA	1:A:542:ASN:HB3	2.00	0.43
1:A:580:GLN:O	5:A:1402:NAG:H82	2.19	0.43
1:A:1141:LEU:HG	1:A:1145:LEU:HD13	2.00	0.43
1:A:985:ASP:C	1:A:987:PRO:HD2	2.44	0.43
1:B:107:GLY:N	1:B:235:ILE:HG23	2.34	0.43
1:B:902:MET:HB3	1:B:916:LEU:HD21	2.00	0.43
1:C:280:ASN:HD21	1:C:282:ASN:HB2	1.84	0.43
1:A:37:TYR:CE2	1:A:193:VAL:HG11	2.54	0.43
1:A:107:GLY:H	1:A:235:ILE:HG23	1.84	0.43
1:A:742:ILE:HD13	1:A:753:LEU:HD13	2.01	0.43
1:A:873:TYR:CE1	1:B:699:LEU:HD12	2.54	0.43
1:B:327:VAL:HA	1:B:542:ASN:HB3	2.01	0.43
1:B:994:ASP:O	1:B:998:THR:HG23	2.18	0.43
1:C:32:PHE:HD2	1:C:216:LEU:HD22	1.83	0.43
1:C:214:ARG:HE	1:C:214:ARG:HB3	1.65	0.43
1:B:457:ARG:HH22	1:B:461:LEU:N	2.16	0.43
1:B:625:HIS:HB2	1:B:634:ARG:HD2	2.01	0.43
1:B:948:LEU:O	1:B:951:VAL:HG12	2.19	0.43
1:C:564:GLN:HG3	1:C:565:PHE:CE1	2.54	0.43
3:j:1:NAG:H61	3:j:2:NAG:H82	2.01	0.43
1:B:871:ALA:HA	1:B:874:THR:HG22	2.00	0.42
1:C:985:ASP:CB	1:C:987:PRO:HD3	2.49	0.42
1:A:439:ASN:O	1:A:443:SER:HB2	2.19	0.42
1:A:659:SER:HB2	1:A:698:SER:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:GLN:OE1	1:B:703:ASN:ND2	2.50	0.42
1:B:86:PHE:HA	1:B:90:VAL:HG23	2.00	0.42
1:B:336:CYS:HA	1:B:337:PRO:HD3	1.88	0.42
1:B:639:GLY:C	1:B:641:ASN:H	2.27	0.42
1:A:110:LEU:O	1:A:110:LEU:HD23	2.20	0.42
1:A:1139:ASP:HB3	1:A:1142:GLN:CG	2.48	0.42
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.54	0.42
1:C:578:ASP:HB3	1:C:581:THR:O	2.19	0.42
1:A:377:PHE:HE2	1:A:384:PRO:HG3	1.83	0.42
1:B:515:PHE:HE2	1:B:517:LEU:HD11	1.84	0.42
1:C:367:VAL:HG23	1:C:368:LEU:HD12	2.00	0.42
1:C:458:LYS:HB3	3:R:2:NAG:H61	2.01	0.42
1:C:767:LEU:HA	1:C:767:LEU:HD23	1.82	0.42
1:C:1117:THR:H	1:C:1140:PRO:CD	2.33	0.42
1:A:210:ILE:HG21	1:A:217:PRO:HG3	2.01	0.42
1:A:273:ARG:HH22	1:A:632:THR:HG21	1.85	0.42
1:B:776:LYS:HA	1:B:776:LYS:HD2	1.89	0.42
1:A:37:TYR:HB3	1:A:223:LEU:HD12	2.00	0.42
1:A:87:ASN:OD1	1:A:87:ASN:N	2.53	0.42
1:A:390:LEU:HG	1:A:391:CYS:N	2.35	0.42
1:B:883:THR:HG21	1:C:705:VAL:HG11	2.02	0.42
1:B:1083:HIS:HB2	1:B:1137:VAL:HG23	2.02	0.42
1:C:192:PHE:HB3	1:C:194:PHE:CZ	2.55	0.42
1:C:278:LYS:HD2	1:C:306:PHE:CE2	2.54	0.42
1:C:340:GLU:N	1:C:340:GLU:OE1	2.53	0.42
1:A:109:THR:OG1	1:A:114:THR:OG1	2.20	0.42
1:A:1107:ARG:NH1	1:C:904:TYR:HE1	2.17	0.42
1:B:37:TYR:CB	1:B:223:LEU:HB2	2.50	0.42
1:B:714:ILE:HA	1:B:715:PRO:HD3	1.93	0.42
1:C:866:THR:O	1:C:870:ILE:HG13	2.20	0.42
1:A:179:LEU:HG	1:A:180:GLU:H	1.84	0.42
1:A:326:ILE:HD12	1:A:532:ASN:O	2.20	0.42
1:A:330:PRO:HD3	1:A:544:ASN:ND2	2.35	0.42
1:A:816:SER:CB	1:A:817:PRO:CD	2.98	0.42
1:B:318:PHE:HE1	1:B:629:LEU:HD22	1.85	0.42
1:A:518:LEU:HG	1:C:983:ARG:HH21	1.85	0.42
1:A:625:HIS:HB2	1:A:634:ARG:HD2	2.02	0.42
1:B:159:VAL:HG13	1:B:160:TYR:CD2	2.55	0.42
1:A:329:PHE:HE1	1:A:545:GLY:H	1.67	0.42
1:C:452:LEU:HD23	1:C:492:LEU:HB3	2.00	0.42
1:C:1081:ILE:CD1	1:C:1135:ASN:HB3	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLN:HB2	1:A:628:GLN:O	2.20	0.41
1:B:818:ILE:O	1:B:822:LEU:HD23	2.19	0.41
1:C:84:LEU:HA	1:C:84:LEU:HD23	1.76	0.41
1:A:1107:ARG:HH11	1:C:904:TYR:HE1	1.68	0.41
1:B:84:LEU:HD22	1:B:267:VAL:HG11	2.03	0.41
1:B:402:ILE:HD13	1:B:410:ILE:HD11	2.02	0.41
1:C:984:LEU:HD13	1:C:988:GLU:OE2	2.19	0.41
1:A:41:LYS:HA	1:B:562:PHE:HE2	1.84	0.41
1:B:124:THR:O	1:B:174:PRO:HD3	2.20	0.41
1:B:212:LEU:HD22	1:B:215:ASP:O	2.21	0.41
1:B:457:ARG:NH2	1:B:460:ASN:HA	2.35	0.41
1:B:617:CYS:HB3	1:B:649:CYS:HB3	1.90	0.41
1:B:666:ILE:HD11	1:B:672:ALA:HB2	2.02	0.41
1:C:290:ASP:CG	1:C:293:LEU:HB2	2.44	0.41
1:C:804:GLN:O	1:C:817:PRO:HG2	2.20	0.41
1:A:182:LYS:HD3	1:A:182:LYS:HA	1.87	0.41
1:A:353:TRP:HB3	1:A:400:PHE:HB3	2.01	0.41
1:A:448:ASN:OD1	1:A:450:ASN:ND2	2.53	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.21	0.41
1:B:102:ARG:HD2	1:B:243:ARG:NH1	2.36	0.41
1:C:117:LEU:HD12	1:C:130:VAL:CG2	2.45	0.41
1:C:222:ALA:CB	1:C:285:ILE:HD12	2.50	0.41
1:A:54:LEU:HB3	1:A:270:LEU:HG	2.03	0.41
1:C:195:LYS:HE2	1:C:204:TYR:OH	2.21	0.41
1:C:921:LYS:HD2	1:C:922:LEU:N	2.36	0.41
1:A:97:LYS:HE3	1:A:187:LYS:HG2	2.03	0.41
1:A:119:ILE:O	1:A:241:LEU:HD11	2.20	0.41
1:B:56:LEU:HD22	1:B:91:TYR:CD2	2.54	0.41
1:B:206:LYS:HD2	1:B:222:ALA:O	2.21	0.41
1:C:190:ARG:HB3	1:C:192:PHE:CE2	2.56	0.41
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.56	0.41
1:A:517:LEU:O	1:A:519:HIS:N	2.54	0.41
1:A:665:PRO:HA	1:A:671:CYS:SG	2.60	0.41
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.39	0.41
1:C:822:LEU:HD21	1:C:1061:VAL:HG21	2.02	0.41
1:C:1105:THR:HG22	1:C:1111:GLU:C	2.46	0.41
1:A:31:SER:OG	1:A:60:SER:OG	2.29	0.41
1:A:365:TYR:CD1	1:A:387:LEU:HB3	2.56	0.41
1:C:110:LEU:O	1:C:110:LEU:HD23	2.20	0.41
1:C:329:PHE:HE2	1:C:528:LYS:HB3	1.85	0.41
1:C:659:SER:OG	1:C:698:SER:HB3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:HA	1:A:126:ALA:HA	2.03	0.41
1:A:234:ASN:N	1:B:465:GLU:OE2	2.53	0.41
1:A:624:ILE:HA	1:A:634:ARG:CZ	2.51	0.41
1:A:624:ILE:HD12	1:A:634:ARG:NE	2.36	0.41
1:B:117:LEU:HA	1:B:130:VAL:HA	2.02	0.41
1:B:821:LEU:HD21	1:B:939:SER:HB2	2.03	0.41
1:B:1141:LEU:HG	1:B:1145:LEU:HD13	2.03	0.41
1:C:42:VAL:HG12	1:C:44:ARG:HG3	2.02	0.41
1:C:186:PHE:HB3	1:C:210:ILE:O	2.20	0.41
1:C:431:GLY:HA2	1:C:515:PHE:CZ	2.56	0.41
1:C:564:GLN:HG3	1:C:565:PHE:CD1	2.56	0.41
3:a:1:NAG:H61	3:a:2:NAG:N2	2.36	0.41
1:A:30:ASN:ND2	1:A:30:ASN:C	2.78	0.41
1:A:384:PRO:O	1:A:387:LEU:HB2	2.21	0.41
1:A:420:ASP:HB3	1:A:460:ASN:ND2	2.36	0.41
1:A:445:VAL:HG12	1:A:499:PRO:HG3	2.03	0.41
1:A:1029:MET:SD	1:A:1033:VAL:HG21	2.61	0.41
1:B:130:VAL:HG12	1:B:168:PHE:HB3	2.03	0.41
1:B:391:CYS:C	1:B:392:PHE:CD1	2.99	0.41
1:B:877:LEU:O	1:B:881:THR:HG23	2.21	0.41
1:B:909:ILE:HG13	1:B:909:ILE:O	2.20	0.41
1:C:553:THR:HB	1:C:586:ASP:OD1	2.20	0.41
1:A:788:ILE:HD11	1:B:699:LEU:HB3	2.03	0.40
1:B:546:LEU:HD21	1:B:573:THR:HG21	2.03	0.40
1:C:193:VAL:HB	1:C:204:TYR:CD2	2.53	0.40
1:C:365:TYR:CG	1:C:387:LEU:HB3	2.55	0.40
1:A:32:PHE:H	1:A:216:LEU:HD23	1.87	0.40
1:A:117:LEU:HD12	1:A:130:VAL:HG22	2.03	0.40
1:A:1082:CYS:HA	1:A:1086:LYS:O	2.21	0.40
1:B:94:SER:HB3	1:B:96:GLU:OE1	2.22	0.40
1:B:1097:SER:HB2	1:B:1102:TRP:CE3	2.56	0.40
1:C:392:PHE:HD2	1:C:395:VAL:HG22	1.84	0.40
1:C:985:ASP:CG	1:C:987:PRO:HD3	2.46	0.40
1:A:103:GLY:C	1:A:104:TRP:CG	3.00	0.40
1:A:277:LEU:HD22	1:A:285:ILE:HD13	2.03	0.40
1:A:569:ILE:HD11	1:C:47:VAL:HG11	2.03	0.40
1:C:379:CYS:HB3	1:C:382:VAL:HG12	2.03	0.40
1:A:415:THR:HG1	1:A:420:ASP:CG	2.28	0.40
1:A:498:GLN:O	1:A:501:ASN:ND2	2.54	0.40
1:A:553:THR:HB	1:A:586:ASP:OD1	2.21	0.40
1:B:633:TRP:CD1	1:B:633:TRP:H	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:ILE:HG13	1:C:909:ILE:O	2.22	0.40
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.62	0.40
1:C:56:LEU:HD22	1:C:91:TYR:CD2	2.57	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	1066/1270 (84%)	996 (93%)	68 (6%)	2 (0%)	43	72
1	B	1066/1270 (84%)	999 (94%)	63 (6%)	4 (0%)	30	61
1	C	1066/1270 (84%)	1010 (95%)	56 (5%)	0	100	100
All	All	3198/3810 (84%)	3005 (94%)	187 (6%)	6 (0%)	44	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	987	PRO
1	B	241	LEU
1	B	942	PRO
1	A	518	LEU
1	A	78	ARG
1	B	78	ARG

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	944/1111 (85%)	935 (99%)	9 (1%)	68	75
1	B	944/1111 (85%)	941 (100%)	3 (0%)	86	83
1	C	944/1111 (85%)	939 (100%)	5 (0%)	81	80
All	All	2832/3333 (85%)	2815 (99%)	17 (1%)	76	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	382	VAL
1	A	385	THR
1	A	386	LYS
1	A	387	LEU
1	A	517	LEU
1	A	983	ARG
1	A	984	LEU
1	A	1018	ILE
1	B	380	TYR
1	B	778	THR
1	B	1018	ILE
1	C	380	TYR
1	C	385	THR
1	C	389	ASP
1	C	390	LEU
1	C	1014	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	49	HIS
1	A	115	GLN
1	A	188	ASN
1	A	450	ASN
1	A	460	ASN
1	A	501	ASN
1	A	544	ASN
1	A	755	GLN
1	A	774	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	804	GLN
1	A	872	GLN
1	A	953	ASN
1	A	955	ASN
1	A	978	ASN
1	A	1002	GLN
1	A	1064	HIS
1	B	49	HIS
1	B	218	GLN
1	B	239	GLN
1	B	388	ASN
1	B	409	GLN
1	B	439	ASN
1	B	655	HIS
1	B	755	GLN
1	B	777	ASN
1	B	953	ASN
1	B	1064	HIS
1	C	81	ASN
1	C	658	ASN
1	C	804	GLN
1	C	935	GLN
1	C	1005	GLN

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 ⓘ

90 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.51	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.50	0
3	NAG	E	1	1,3	14,14,15	0.17	0	17,19,21	0.60	0
3	NAG	E	2	3	14,14,15	0.31	0	17,19,21	0.44	0
3	MAN	E	3	3	11,11,12	0.70	0	15,15,17	1.12	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	G	1	1,3	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.40	0
3	MAN	G	3	3	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.46	0	17,19,21	0.46	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.49	0
3	MAN	H	3	3	11,11,12	0.73	0	15,15,17	1.25	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	J	1	1,3	14,14,15	0.18	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	MAN	J	3	3	11,11,12	0.75	0	15,15,17	1.26	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	MAN	K	3	3	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.19	0	17,19,21	0.59	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.49	0
4	FUC	L	3	4	10,10,11	0.78	0	14,14,16	0.81	0
3	NAG	M	1	1,3	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	M	2	3	14,14,15	0.22	0	17,19,21	0.37	0
3	MAN	M	3	3	11,11,12	0.73	0	15,15,17	1.24	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.33	0	17,19,21	0.39	0
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.40	0
3	MAN	N	3	3	11,11,12	0.72	0	15,15,17	1.36	2 (13%)
2	NAG	O	1	1,2	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	O	2	2	14,14,15	0.29	0	17,19,21	0.40	0
3	NAG	P	1	1,3	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.48	0
3	MAN	P	3	3	11,11,12	0.67	0	15,15,17	1.09	2 (13%)
2	NAG	Q	1	1,2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	Q	2	2	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	R	1	1,3	14,14,15	0.36	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	R	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	MAN	R	3	3	11,11,12	0.79	0	15,15,17	1.16	2 (13%)
3	NAG	S	1	3	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	S	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	MAN	S	3	3	11,11,12	0.74	0	15,15,17	1.21	2 (13%)
2	NAG	T	1	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	T	2	2	14,14,15	0.31	0	17,19,21	0.45	0
3	NAG	U	1	1,3	14,14,15	0.40	0	17,19,21	0.84	1 (5%)
3	NAG	U	2	3	14,14,15	0.23	0	17,19,21	0.53	0
3	MAN	U	3	3	11,11,12	0.80	0	15,15,17	1.20	2 (13%)
3	NAG	V	1	1,3	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	V	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	MAN	V	3	3	11,11,12	0.66	0	15,15,17	1.31	2 (13%)
4	NAG	W	1	1,4	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	NAG	W	2	4	14,14,15	0.25	0	17,19,21	0.51	0
4	FUC	W	3	4	10,10,11	0.80	0	14,14,16	0.90	0
3	NAG	X	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	X	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	MAN	X	3	3	11,11,12	0.76	0	15,15,17	1.27	2 (13%)
3	NAG	Y	1	1,3	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
3	NAG	Y	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	MAN	Y	3	3	11,11,12	0.72	0	15,15,17	1.20	2 (13%)
2	NAG	Z	1	1,2	14,14,15	0.34	0	17,19,21	0.55	0
2	NAG	Z	2	2	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	a	1	1,3	14,14,15	0.17	0	17,19,21	0.55	0
3	NAG	a	2	3	14,14,15	0.26	0	17,19,21	0.52	0
3	MAN	a	3	3	11,11,12	0.66	0	15,15,17	1.10	2 (13%)
2	NAG	b	1	1,2	14,14,15	0.29	0	17,19,21	0.38	0
2	NAG	b	2	2	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	c	1	1,3	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	MAN	c	3	3	11,11,12	0.82	0	15,15,17	1.14	2 (13%)
3	NAG	d	1	1,3	14,14,15	0.39	0	17,19,21	0.43	0
3	NAG	d	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	MAN	d	3	3	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
2	NAG	e	1	1,2	14,14,15	0.27	0	17,19,21	0.62	1 (5%)
2	NAG	e	2	2	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	f	1	1,3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	f	2	3	14,14,15	0.19	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	f	3	3	11,11,12	0.74	0	15,15,17	1.24	1 (6%)
3	NAG	g	1	1,3	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	g	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	MAN	g	3	3	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	NAG	h	1	1,4	14,14,15	0.20	0	17,19,21	0.75	1 (5%)
4	NAG	h	2	4	14,14,15	0.25	0	17,19,21	0.48	0
4	FUC	h	3	4	10,10,11	0.76	0	14,14,16	0.92	0
3	NAG	i	1	1,3	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	i	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	MAN	i	3	3	11,11,12	0.76	0	15,15,17	1.28	2 (13%)
3	NAG	j	1	1,3	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
3	NAG	j	2	3	14,14,15	0.25	0	17,19,21	0.39	0
3	MAN	j	3	3	11,11,12	0.70	0	15,15,17	1.14	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	1/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	MAN	G	3	3	-	0/2/19/22	1/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	MAN	H	3	3	-	0/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	MAN	J	3	3	-	2/2/19/22	1/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	MAN	K	3	3	-	1/2/19/22	1/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	MAN	M	3	3	-	1/2/19/22	1/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	MAN	N	3	3	-	2/2/19/22	1/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	MAN	P	3	3	-	2/2/19/22	1/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	MAN	R	3	3	-	0/2/19/22	1/1/1/1
3	NAG	S	1	3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	MAN	S	3	3	-	0/2/19/22	1/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	MAN	U	3	3	-	2/2/19/22	1/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	MAN	V	3	3	-	1/2/19/22	1/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	FUC	W	3	4	-	-	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	MAN	X	3	3	-	1/2/19/22	1/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	MAN	C1-O5-C5	4.37	118.04	112.19
3	V	3	MAN	C1-O5-C5	4.09	117.66	112.19
3	g	3	MAN	C1-O5-C5	4.04	117.60	112.19
3	J	3	MAN	C1-O5-C5	4.00	117.54	112.19
3	i	3	MAN	C1-O5-C5	3.97	117.51	112.19
3	X	3	MAN	C1-O5-C5	3.95	117.48	112.19
3	f	3	MAN	C1-O5-C5	3.95	117.47	112.19
3	K	3	MAN	C1-O5-C5	3.91	117.43	112.19
3	H	3	MAN	C1-O5-C5	3.84	117.33	112.19
3	M	3	MAN	C1-O5-C5	3.82	117.30	112.19
3	S	3	MAN	C1-O5-C5	3.72	117.17	112.19
3	U	3	MAN	C1-O5-C5	3.69	117.13	112.19
3	Y	3	MAN	C1-O5-C5	3.64	117.07	112.19
3	R	3	MAN	C1-O5-C5	3.46	116.83	112.19
3	j	3	MAN	C1-O5-C5	3.42	116.77	112.19
3	a	3	MAN	C1-O5-C5	3.37	116.70	112.19
3	c	3	MAN	C1-O5-C5	3.37	116.70	112.19
3	G	3	MAN	C1-O5-C5	3.34	116.66	112.19
3	E	3	MAN	C1-O5-C5	3.33	116.64	112.19
3	d	3	MAN	C1-O5-C5	3.31	116.62	112.19
3	P	3	MAN	C1-O5-C5	3.26	116.55	112.19
3	U	1	NAG	C1-O5-C5	3.02	116.23	112.19
3	c	1	NAG	C1-O5-C5	2.84	116.00	112.19
4	h	1	NAG	C1-O5-C5	2.69	115.79	112.19
4	W	1	NAG	C1-O5-C5	2.66	115.75	112.19
3	Y	1	NAG	C1-O5-C5	2.35	115.34	112.19
3	V	3	MAN	O2-C2-C3	-2.31	105.37	110.15
3	g	3	MAN	O2-C2-C3	-2.28	105.43	110.15
3	G	1	NAG	C1-O5-C5	2.25	115.20	112.19
3	K	3	MAN	O2-C2-C3	-2.23	105.54	110.15
3	R	3	MAN	O2-C2-C3	-2.21	105.57	110.15
3	c	3	MAN	O2-C2-C3	-2.19	105.61	110.15
3	j	3	MAN	O2-C2-C3	-2.19	105.61	110.15
3	G	3	MAN	O2-C2-C3	-2.18	105.64	110.15
3	X	3	MAN	O2-C2-C3	-2.18	105.64	110.15
3	i	3	MAN	O2-C2-C3	-2.17	105.65	110.15
3	Y	3	MAN	O2-C2-C3	-2.17	105.66	110.15
3	M	3	MAN	O2-C2-C3	-2.16	105.67	110.15
3	U	3	MAN	O2-C2-C3	-2.15	105.70	110.15
3	E	3	MAN	O2-C2-C3	-2.14	105.71	110.15
3	j	1	NAG	C1-O5-C5	2.14	115.05	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	MAN	O2-C2-C3	-2.14	105.73	110.15
3	H	3	MAN	O2-C2-C3	-2.13	105.73	110.15
3	S	3	MAN	O2-C2-C3	-2.13	105.73	110.15
3	P	3	MAN	O2-C2-C3	-2.11	105.79	110.15
3	a	3	MAN	O2-C2-C3	-2.08	105.84	110.15
3	d	3	MAN	O2-C2-C3	-2.05	105.91	110.15
2	e	1	NAG	C1-O5-C5	2.04	114.92	112.19
3	J	3	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	Y	3	MAN	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	j	3	MAN	C4-C5-C6-O6
3	P	3	MAN	O5-C5-C6-O6
3	Y	3	MAN	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	U	3	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	h	2	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	j	3	MAN	O5-C5-C6-O6
3	U	3	MAN	C4-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	N	3	MAN	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
3	P	3	MAN	C4-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
3	i	3	MAN	O5-C5-C6-O6
3	X	3	MAN	O5-C5-C6-O6
3	a	3	MAN	O5-C5-C6-O6
3	V	3	MAN	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
3	M	3	MAN	O5-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
3	J	3	MAN	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
3	K	3	MAN	O5-C5-C6-O6
3	N	3	MAN	O5-C5-C6-O6
3	g	3	MAN	O5-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	f	3	MAN	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	J	3	MAN	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

All (21) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	3	MAN	C1-C2-C3-C4-C5-O5
3	a	3	MAN	C1-C2-C3-C4-C5-O5
3	c	3	MAN	C1-C2-C3-C4-C5-O5
3	G	3	MAN	C1-C2-C3-C4-C5-O5
3	E	3	MAN	C1-C2-C3-C4-C5-O5
3	R	3	MAN	C1-C2-C3-C4-C5-O5
3	N	3	MAN	C1-C2-C3-C4-C5-O5
3	X	3	MAN	C1-C2-C3-C4-C5-O5

Continued on next page...

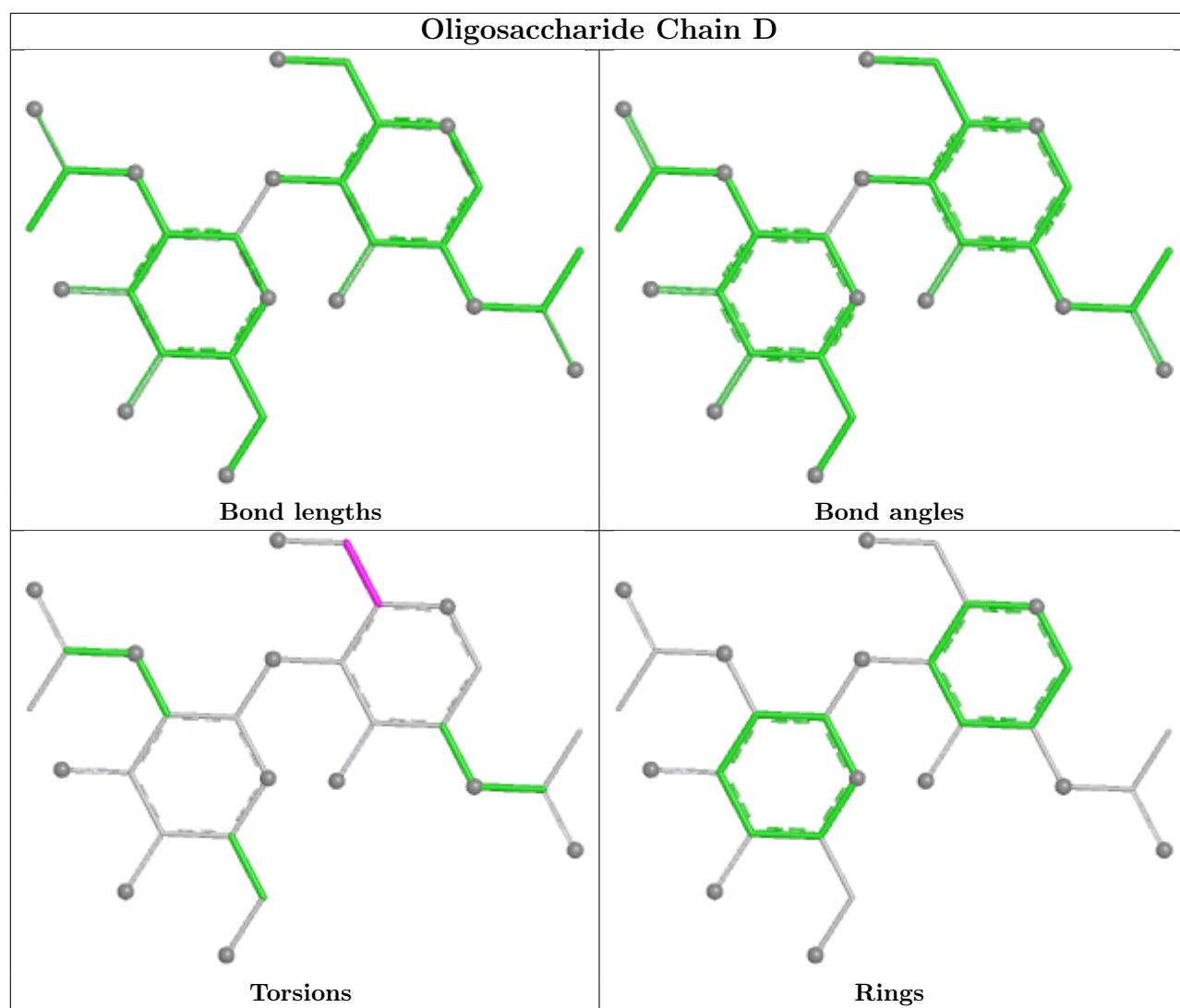
Continued from previous page...

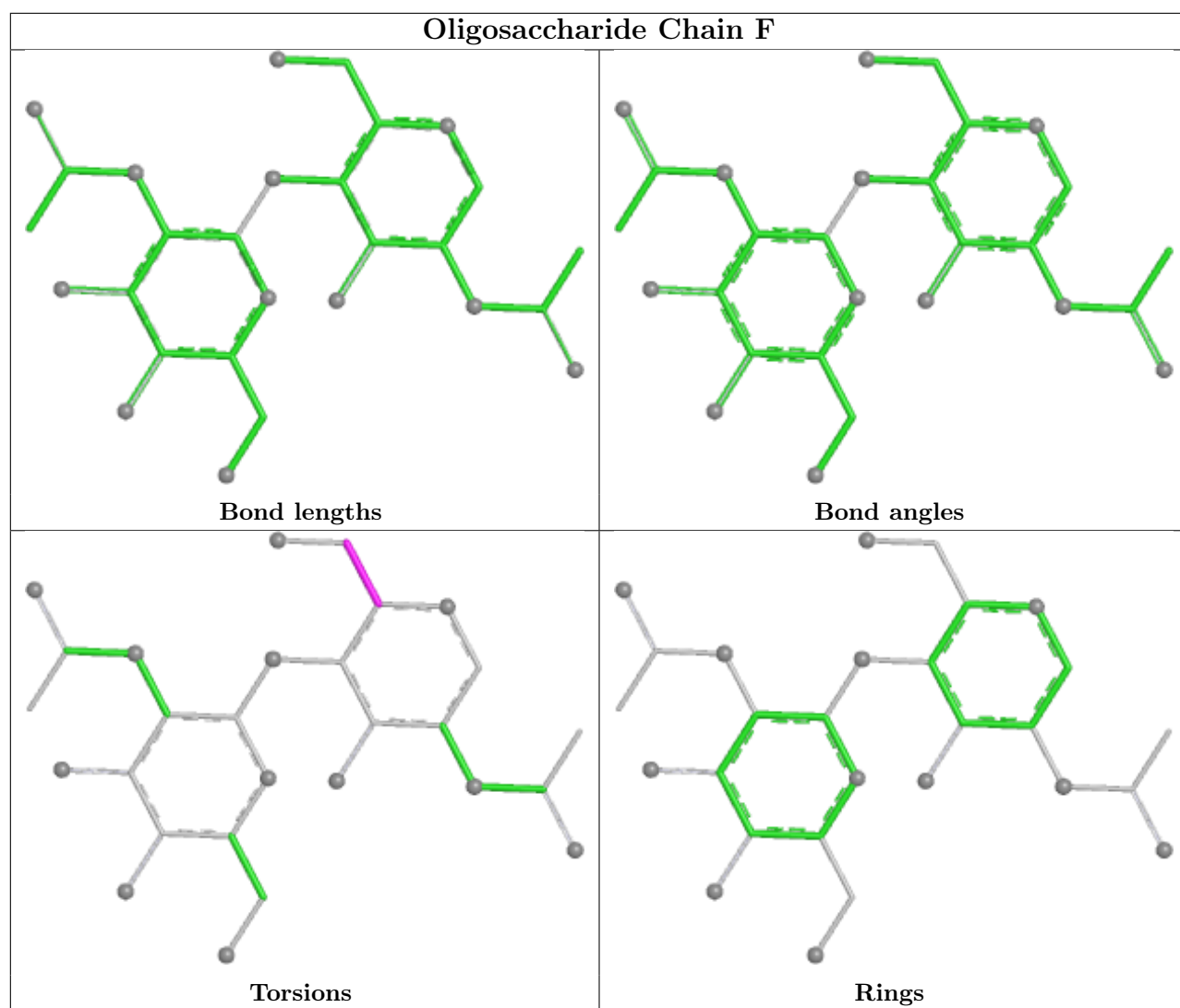
Mol	Chain	Res	Type	Atoms
3	i	3	MAN	C1-C2-C3-C4-C5-O5
3	M	3	MAN	C1-C2-C3-C4-C5-O5
3	d	3	MAN	C1-C2-C3-C4-C5-O5
3	K	3	MAN	C1-C2-C3-C4-C5-O5
3	S	3	MAN	C1-C2-C3-C4-C5-O5
3	j	3	MAN	C1-C2-C3-C4-C5-O5
3	Y	3	MAN	C1-C2-C3-C4-C5-O5
3	V	3	MAN	C1-C2-C3-C4-C5-O5
3	H	3	MAN	C1-C2-C3-C4-C5-O5
3	U	3	MAN	C1-C2-C3-C4-C5-O5
3	J	3	MAN	C1-C2-C3-C4-C5-O5
3	f	3	MAN	C1-C2-C3-C4-C5-O5
3	g	3	MAN	C1-C2-C3-C4-C5-O5

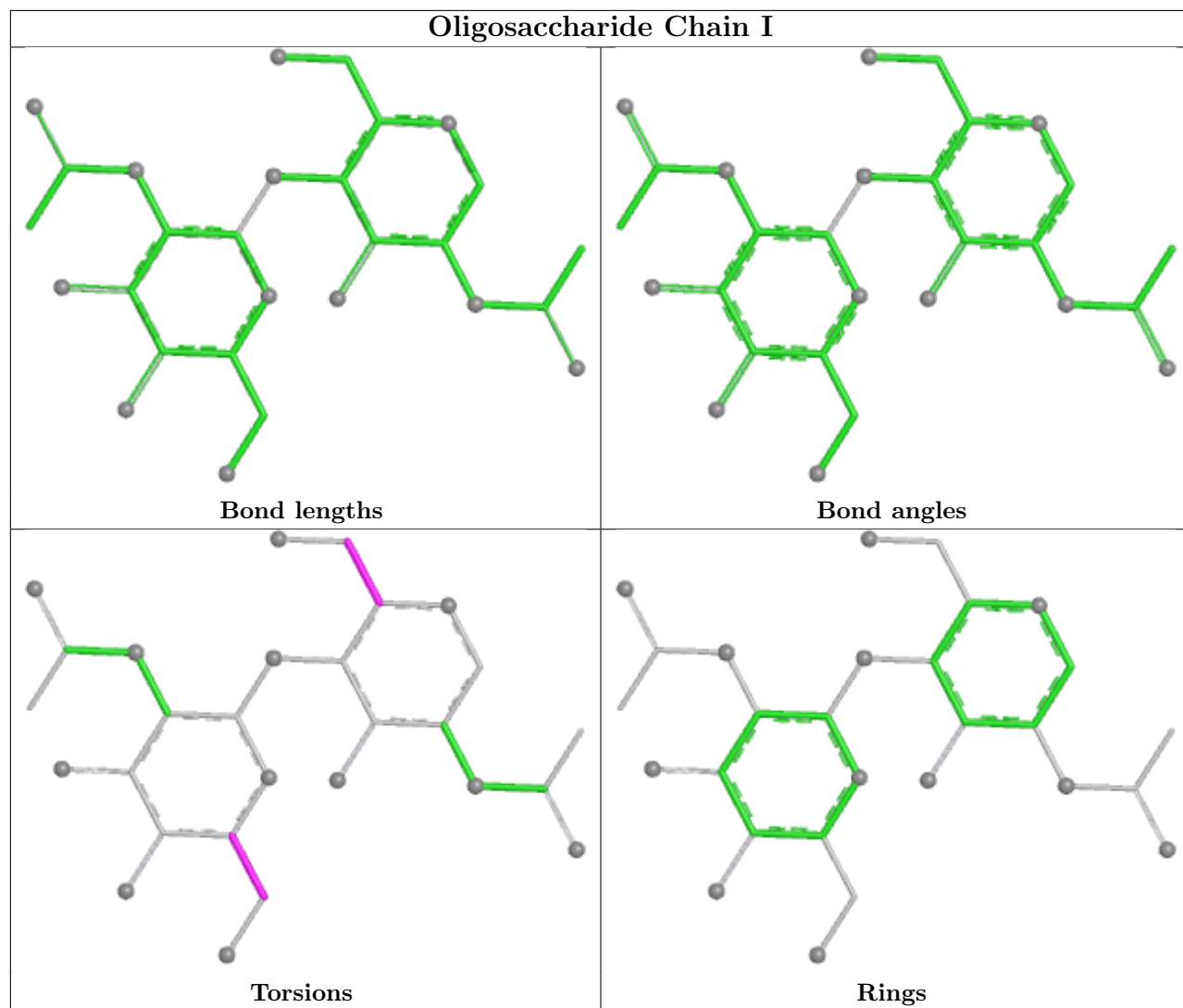
17 monomers are involved in 15 short contacts:

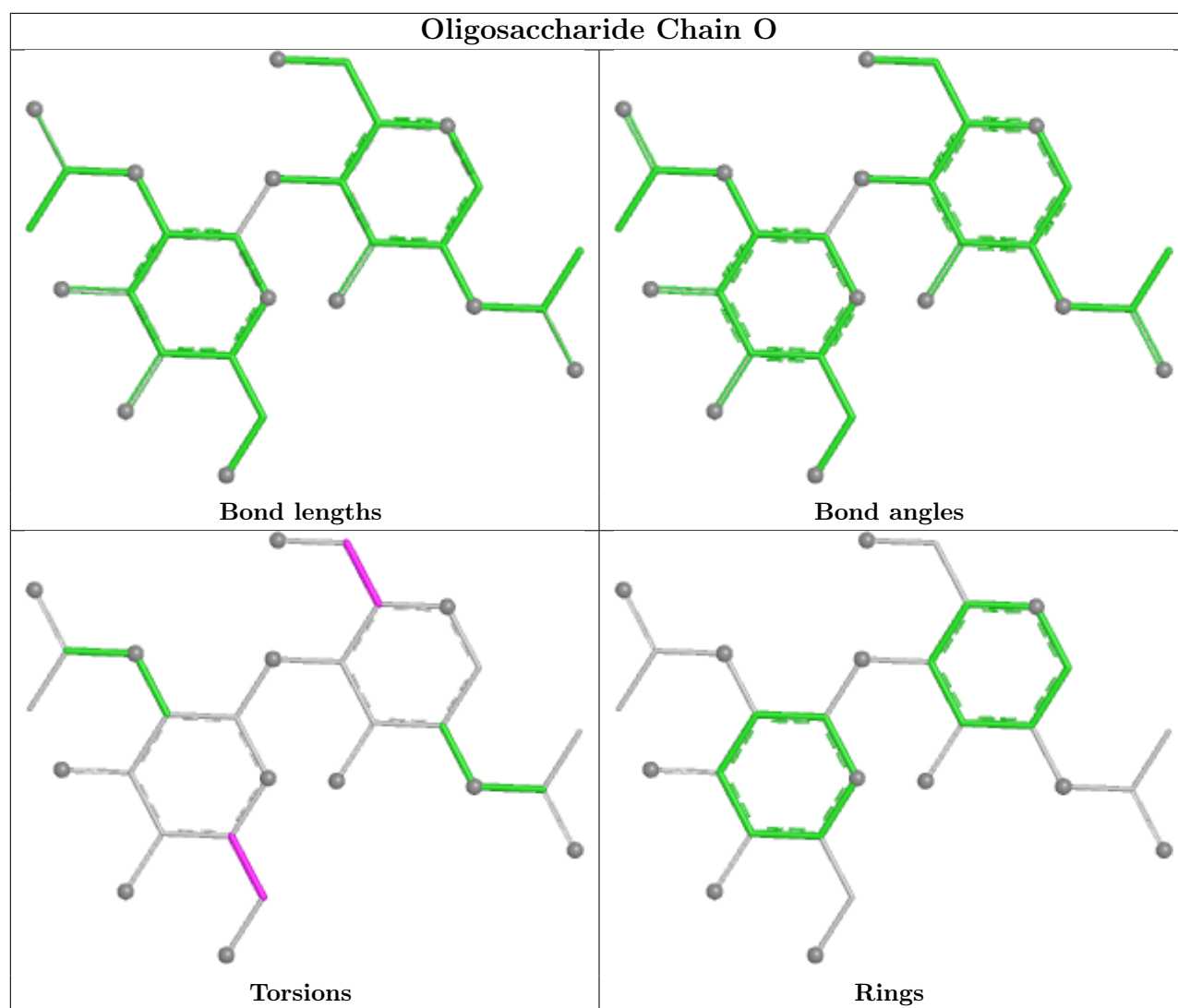
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	1	NAG	1	0
3	d	1	NAG	1	0
3	P	1	NAG	1	0
3	a	2	NAG	1	0
3	E	1	NAG	2	0
2	e	1	NAG	1	0
3	E	2	NAG	1	0
2	T	1	NAG	1	0
3	j	1	NAG	2	0
2	e	2	NAG	1	0
3	a	1	NAG	1	0
3	j	2	NAG	1	0
3	M	1	NAG	2	0
3	G	1	NAG	1	0
3	R	1	NAG	1	0
2	T	2	NAG	1	0
3	R	2	NAG	1	0

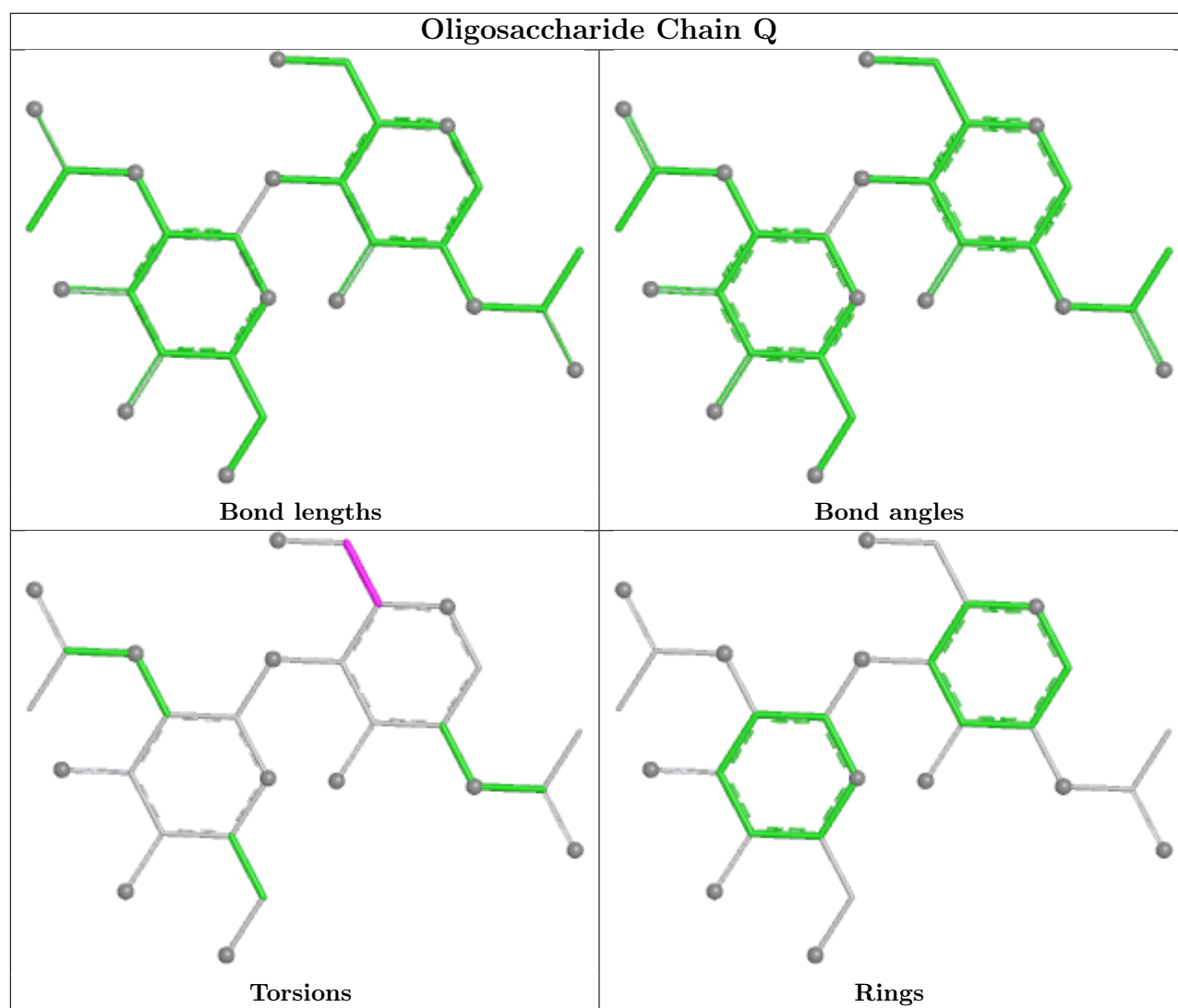
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

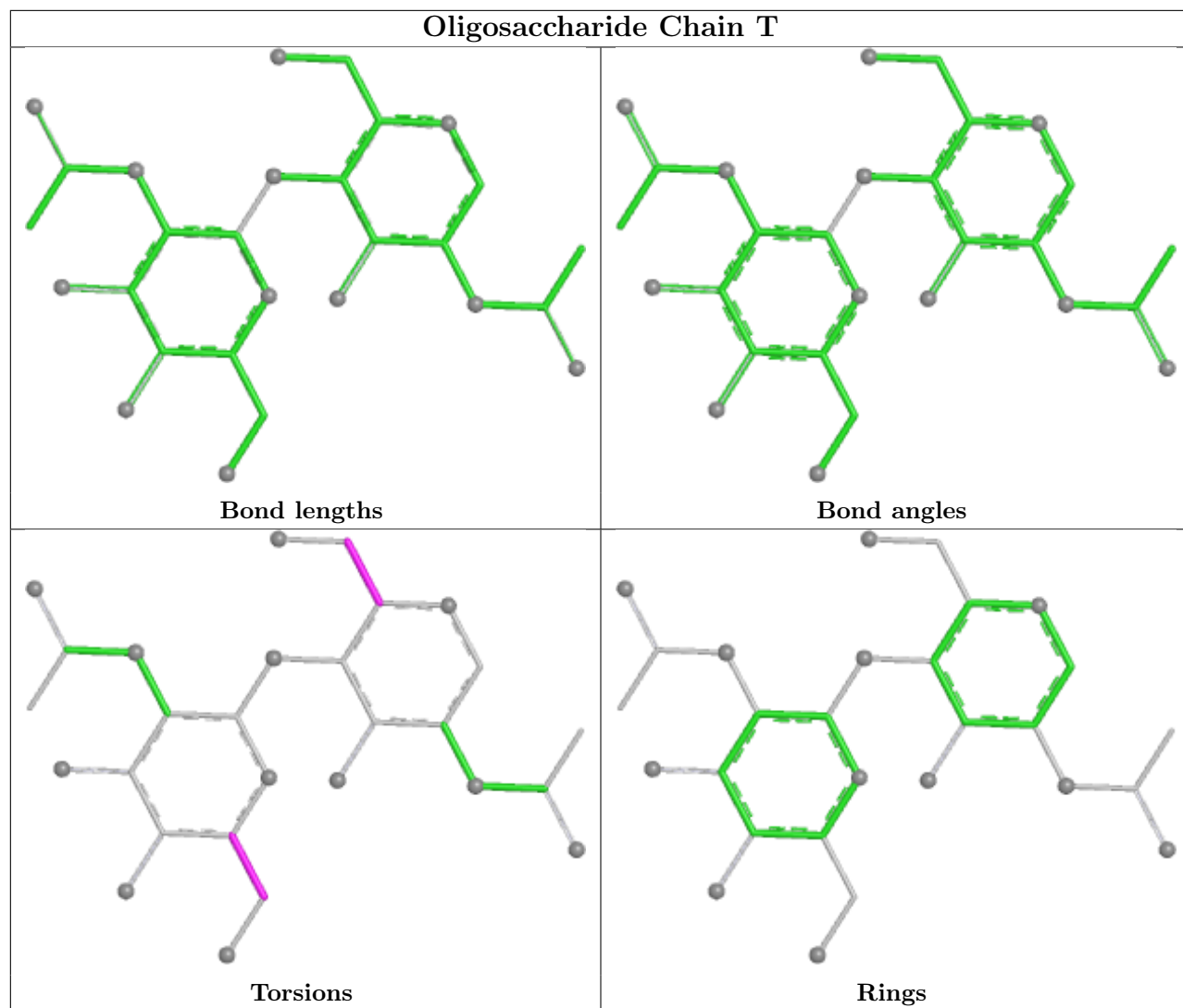


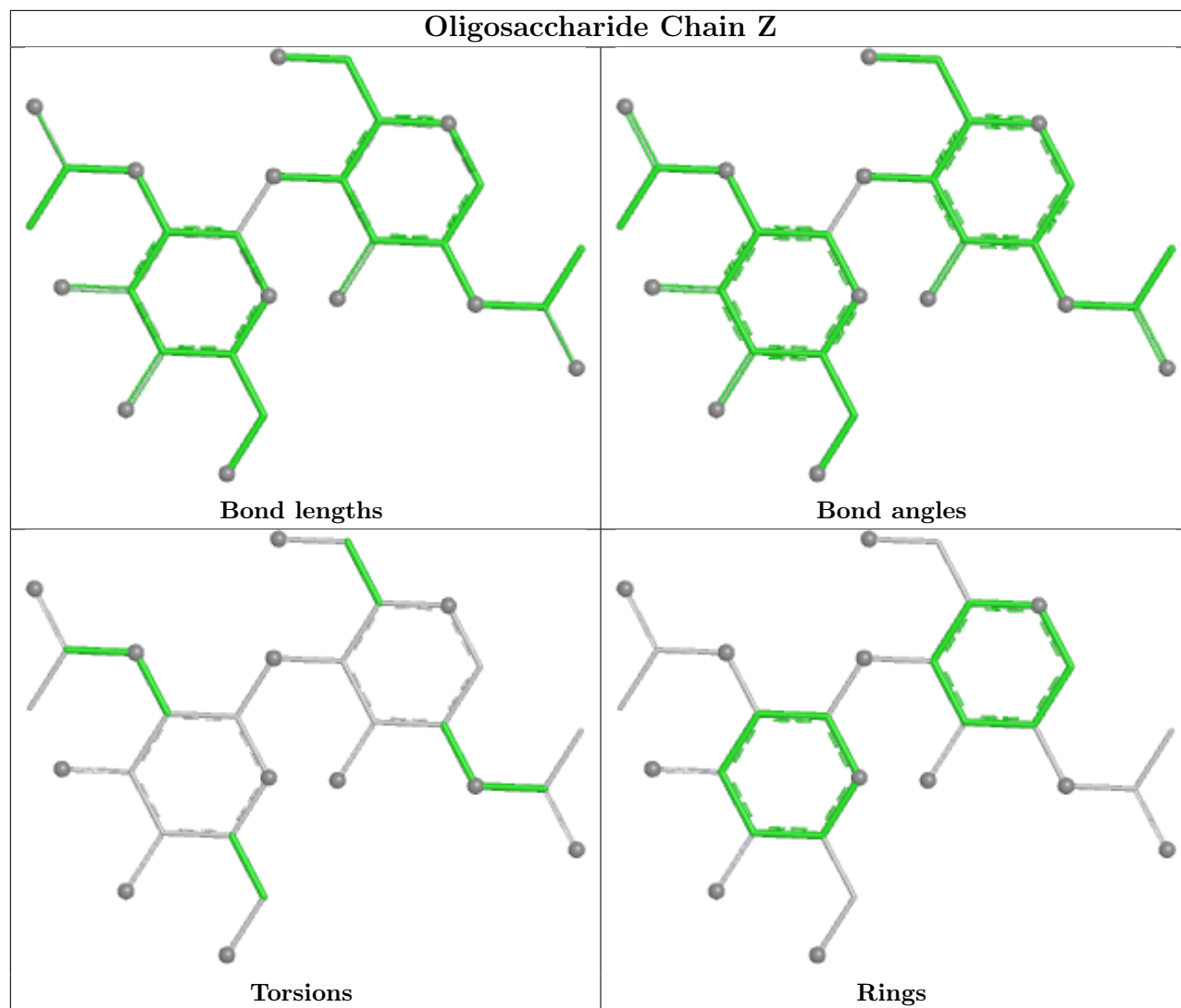


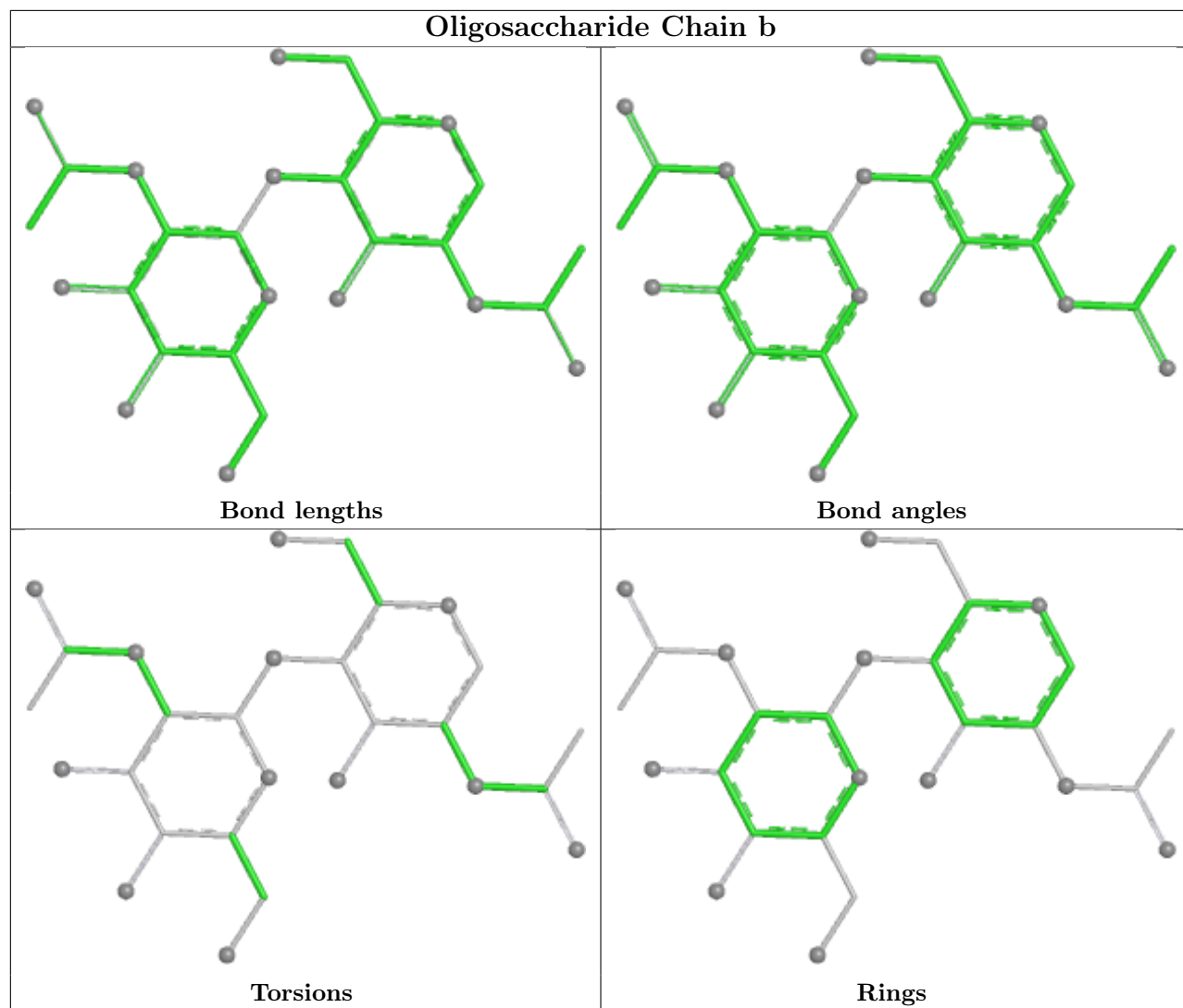


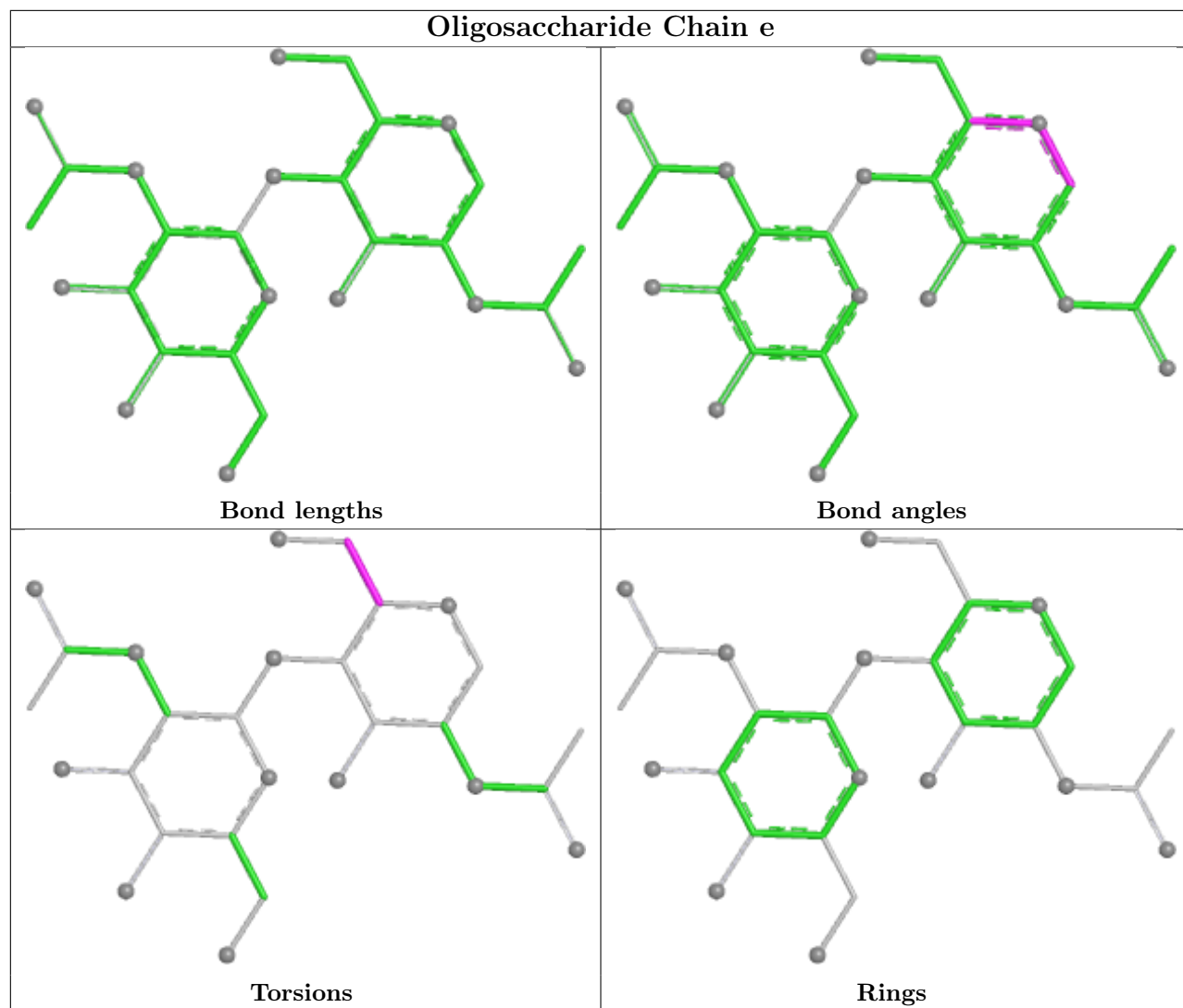


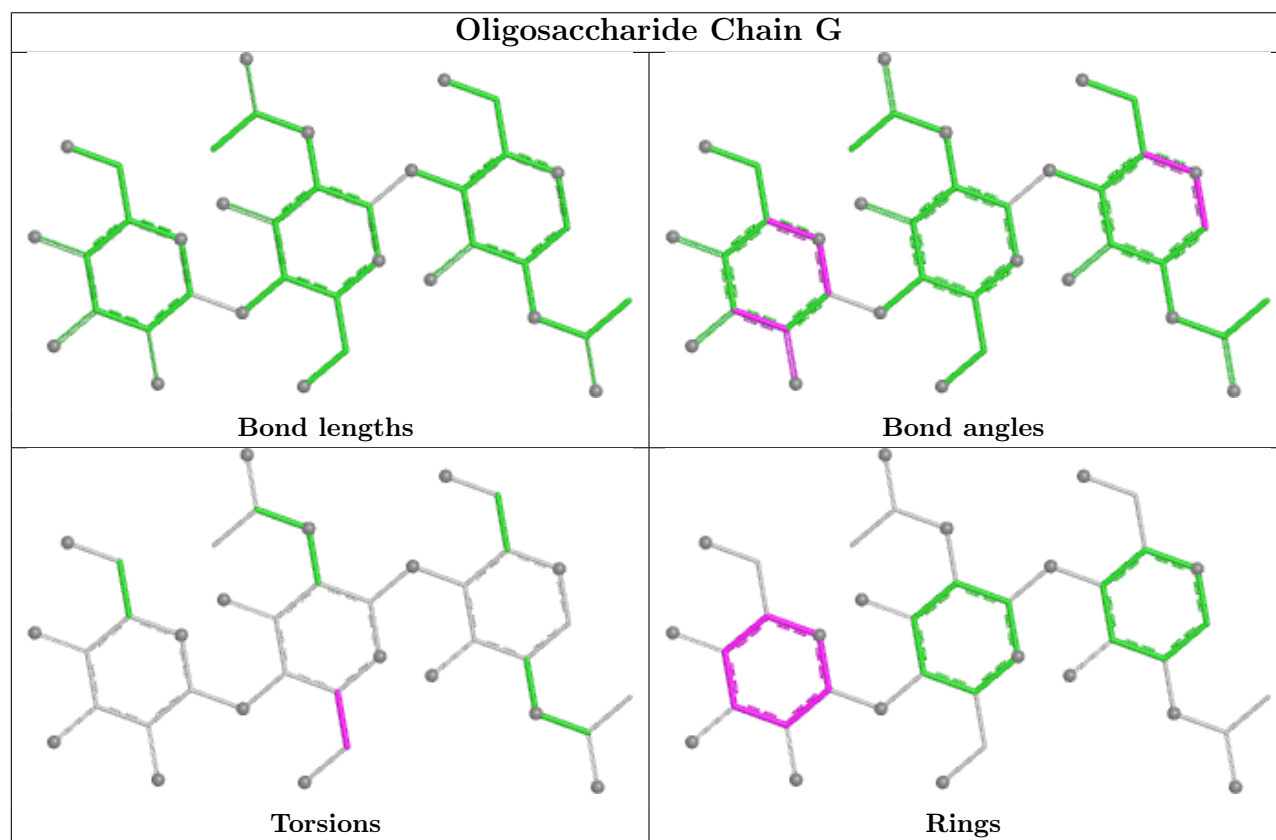
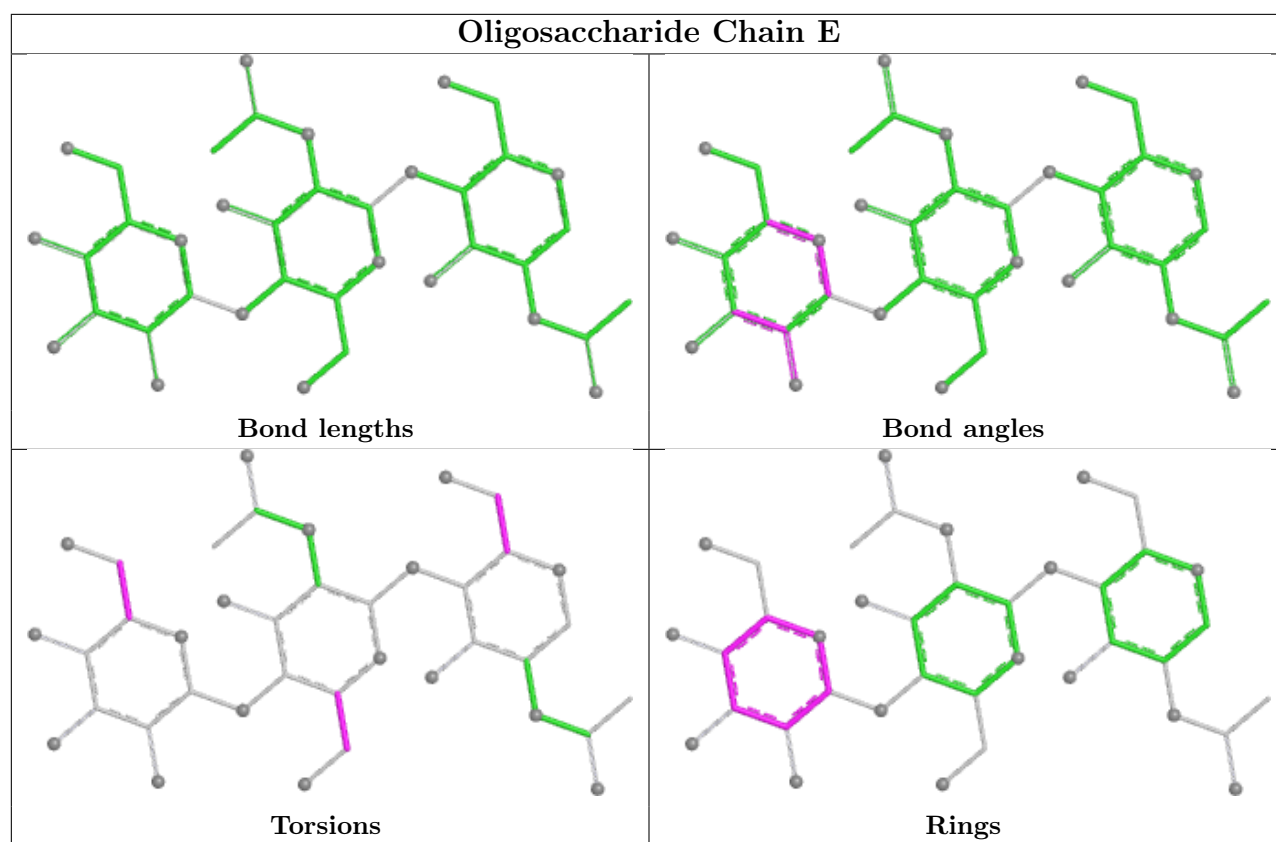


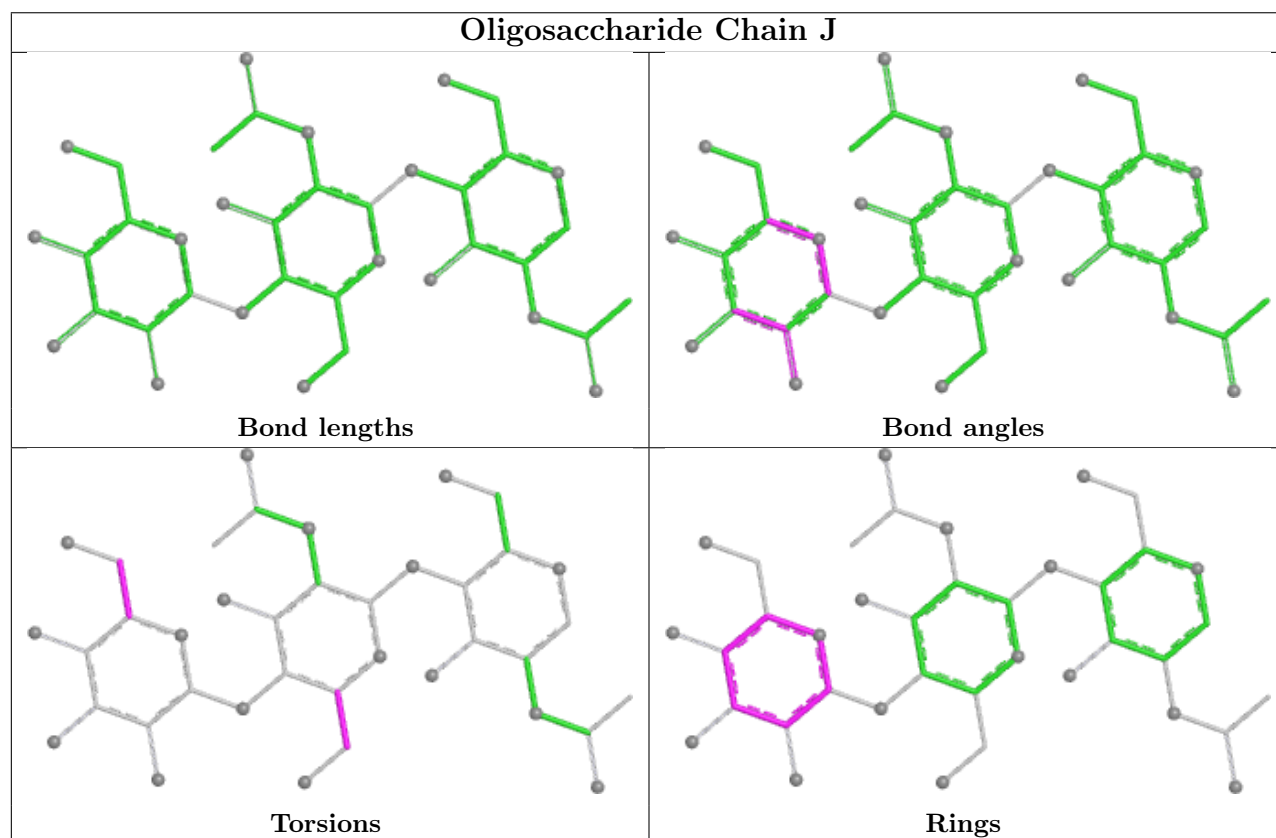
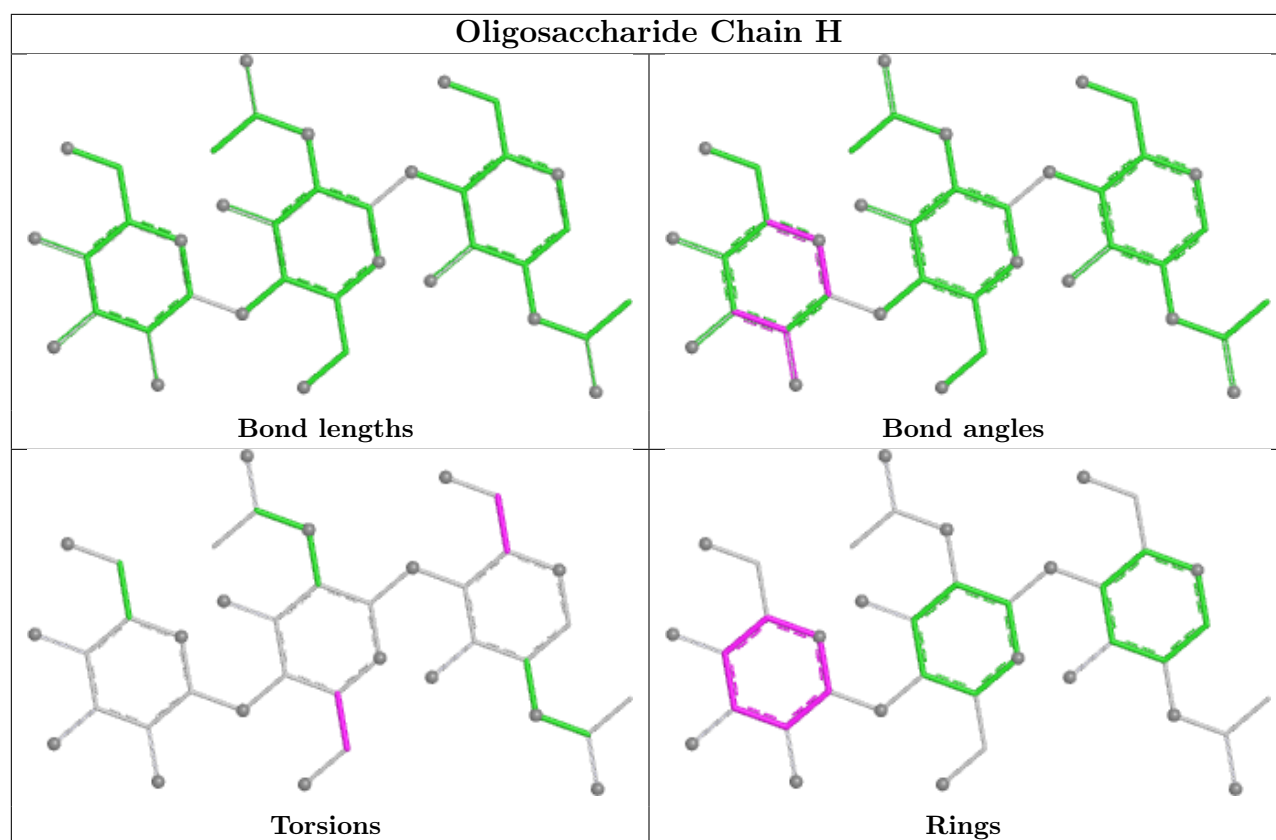


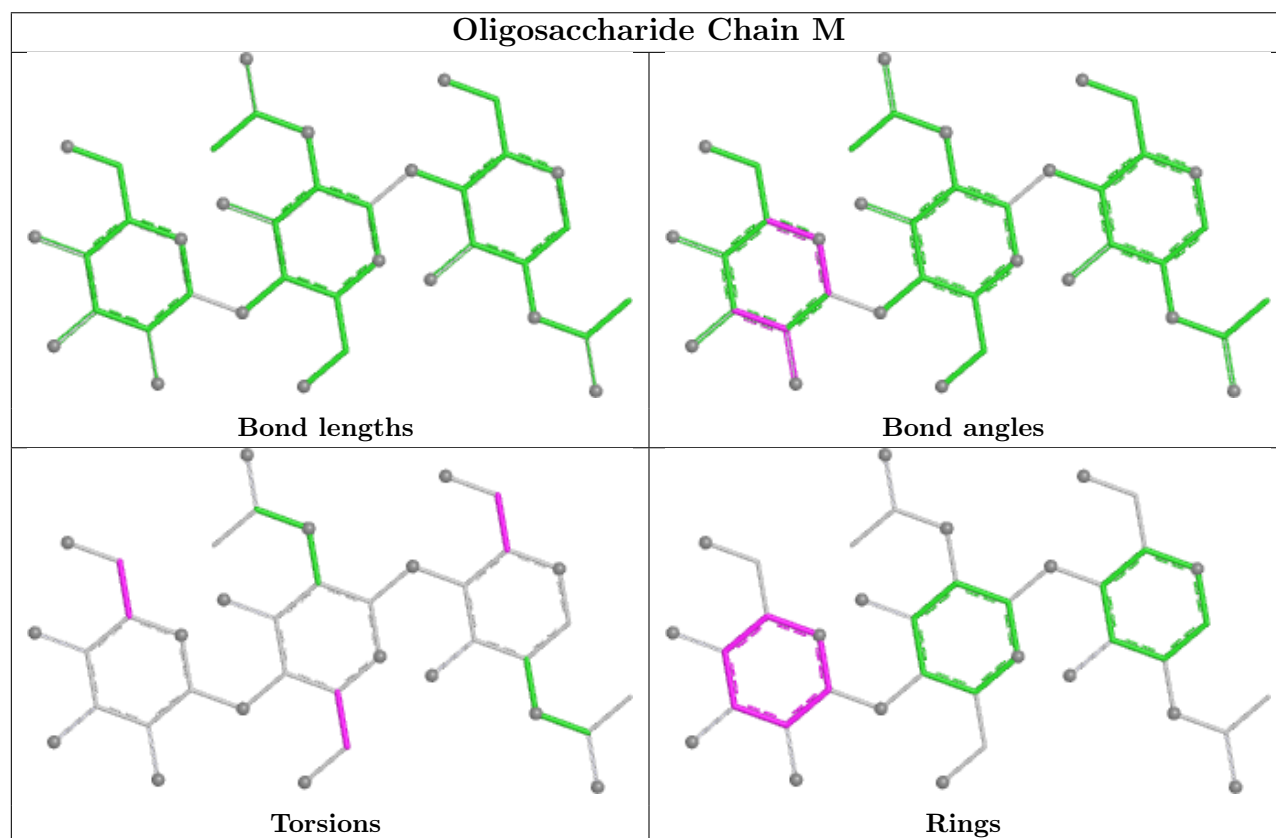
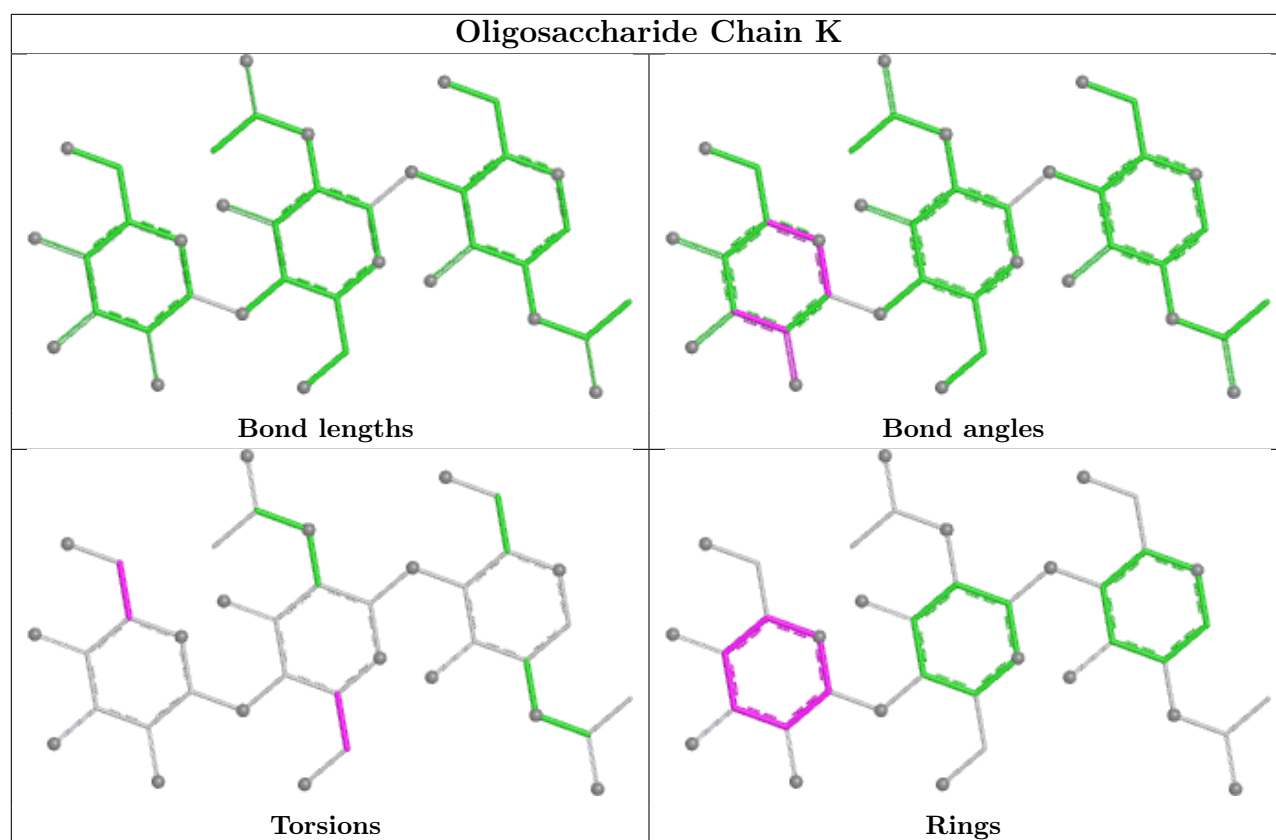


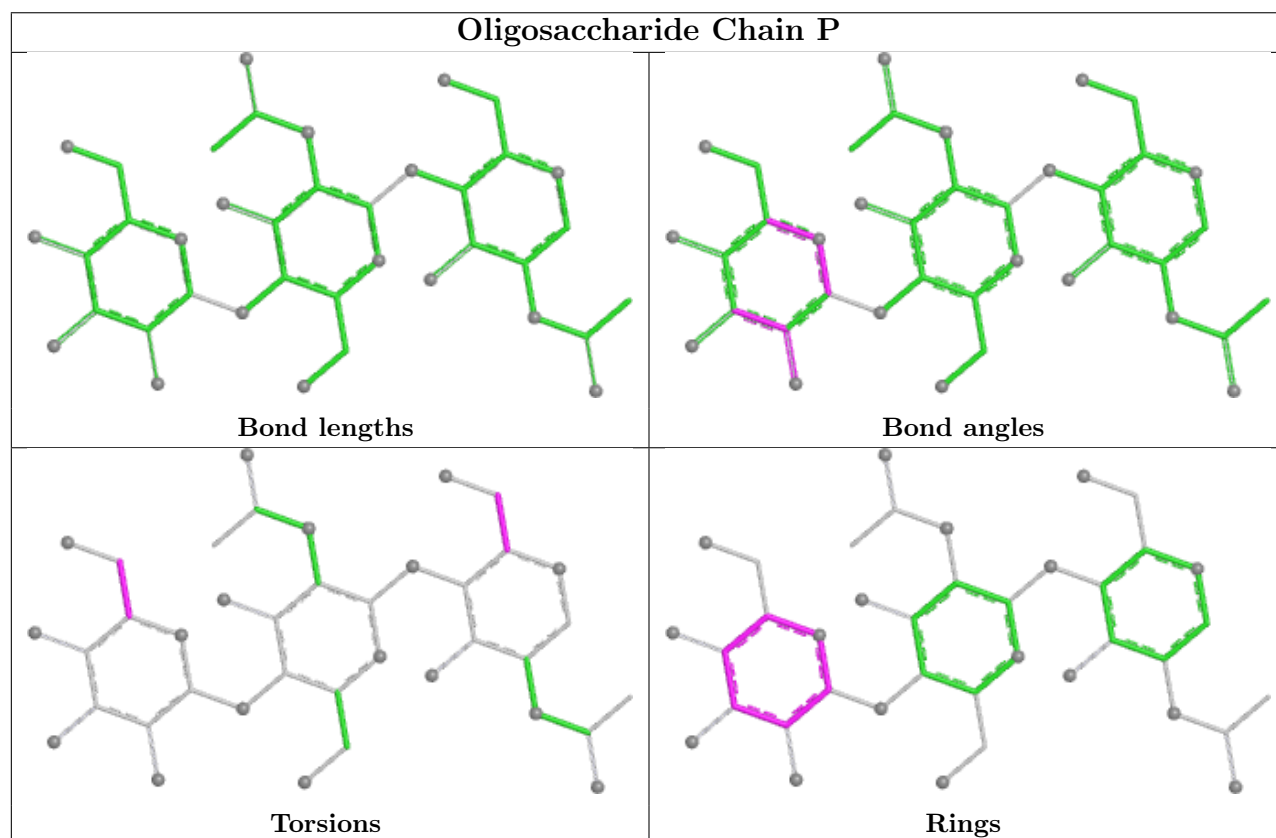
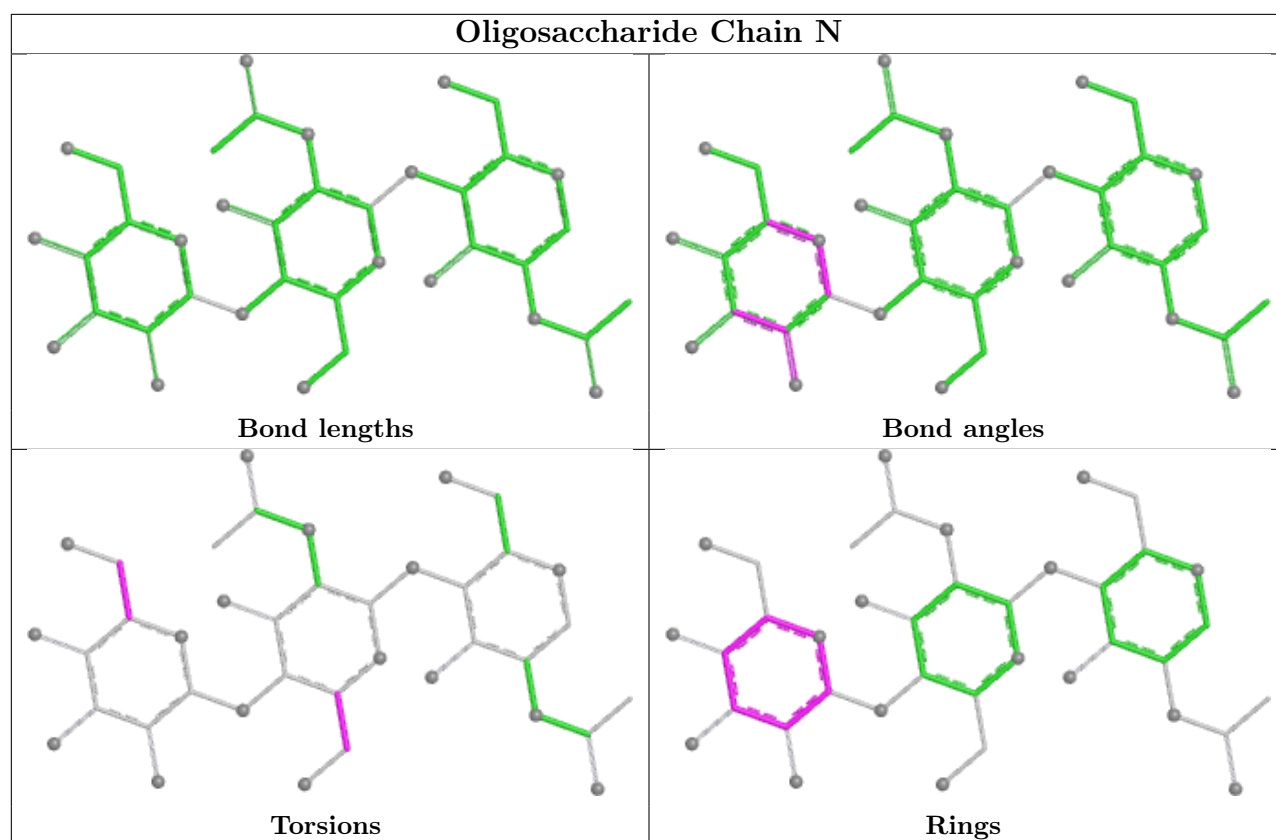


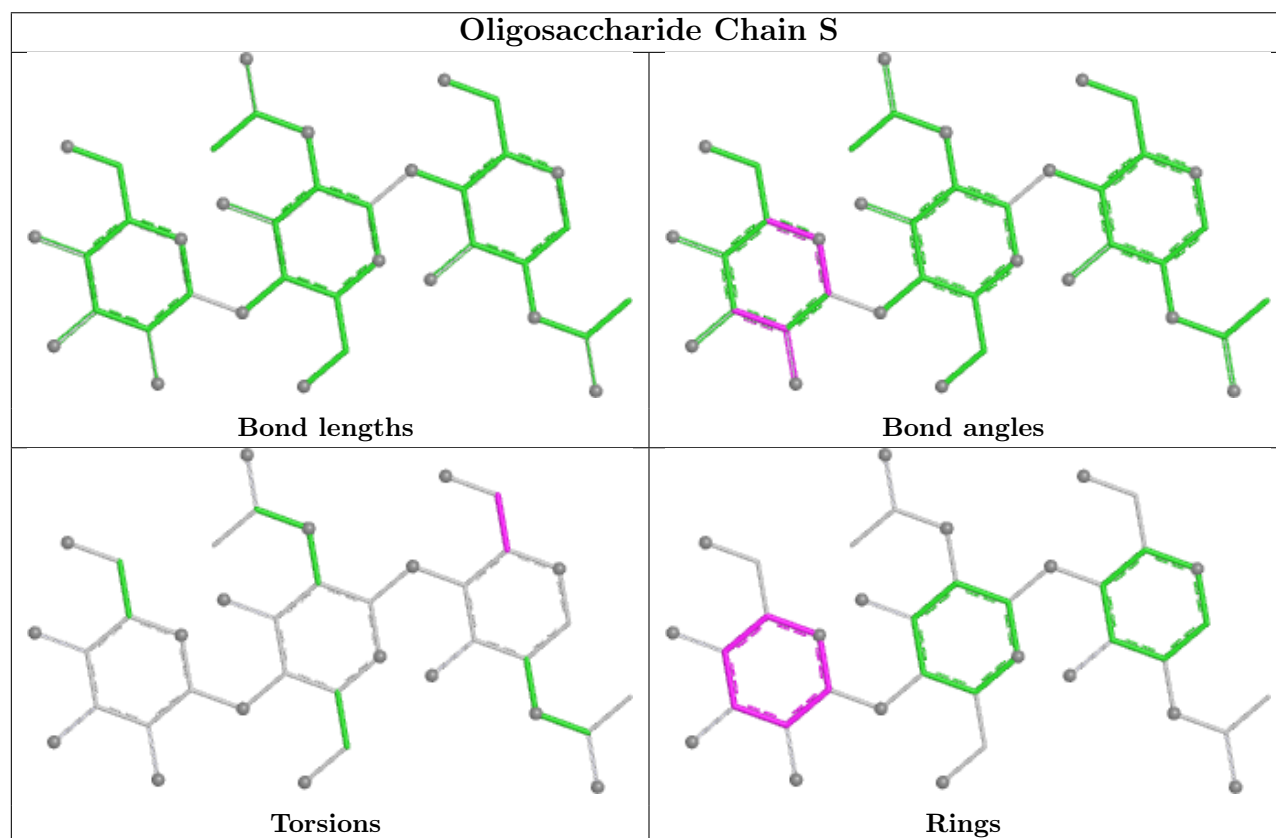
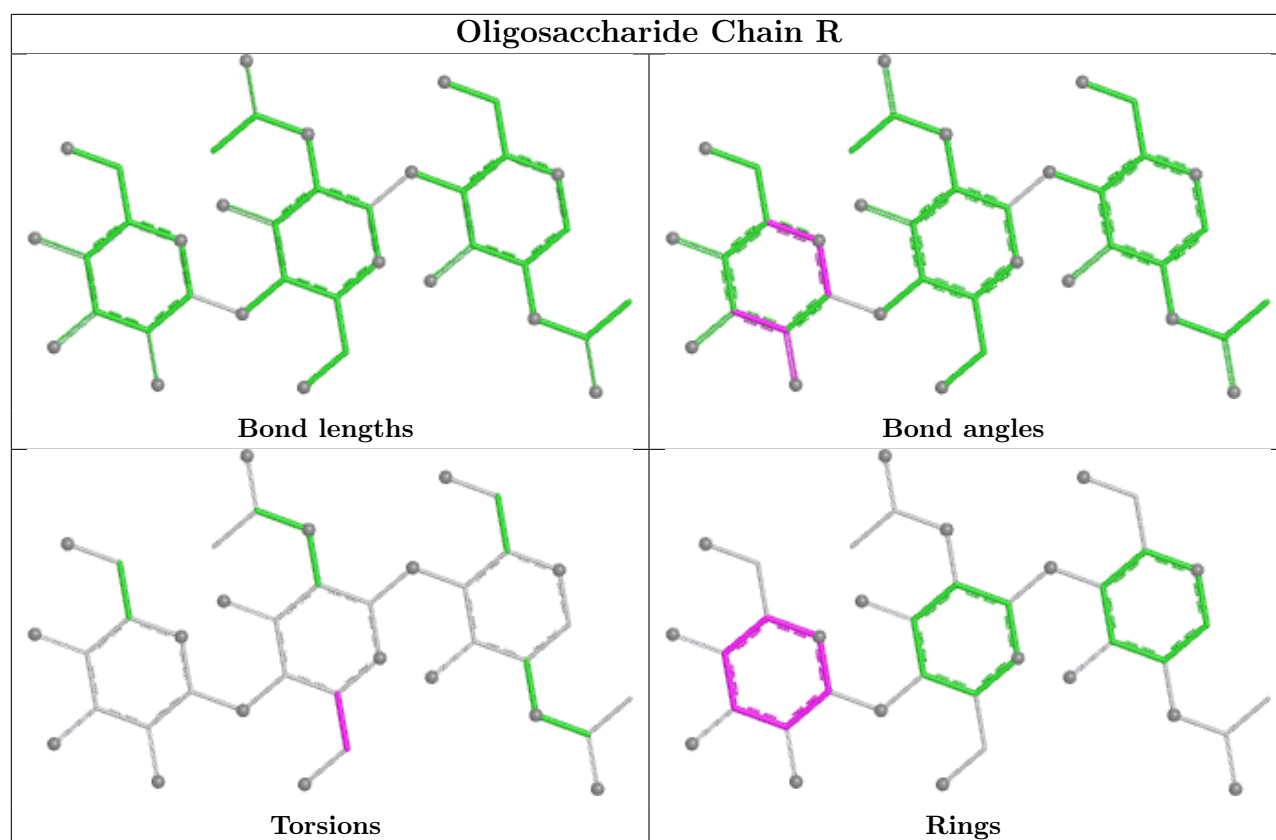


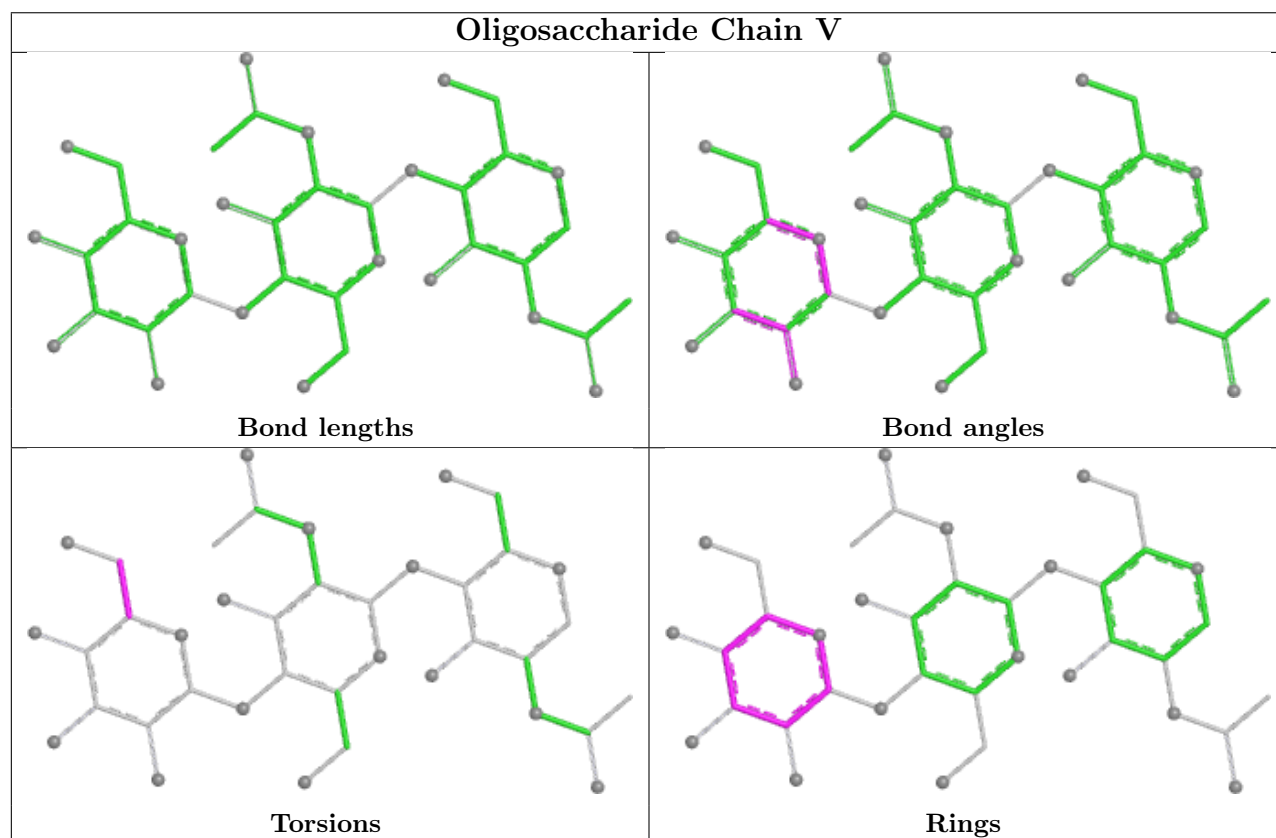
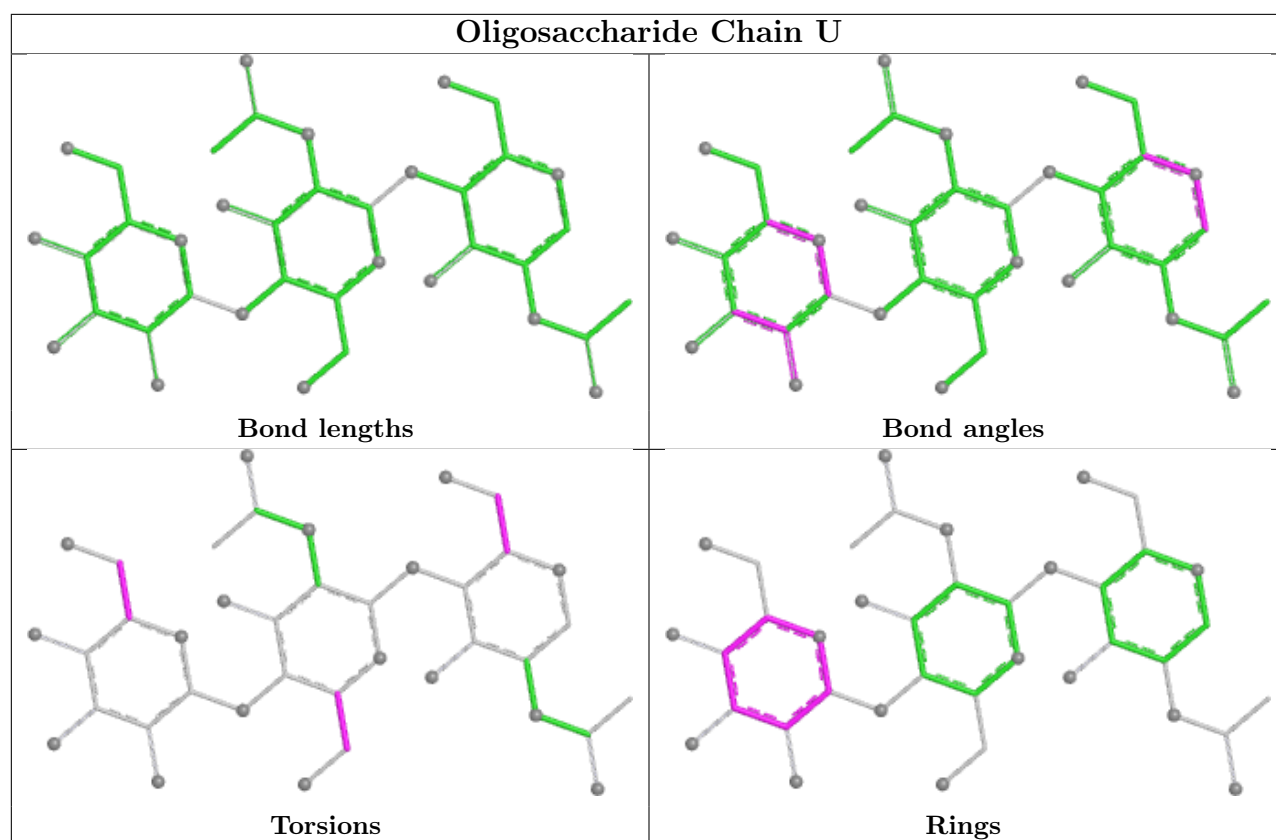


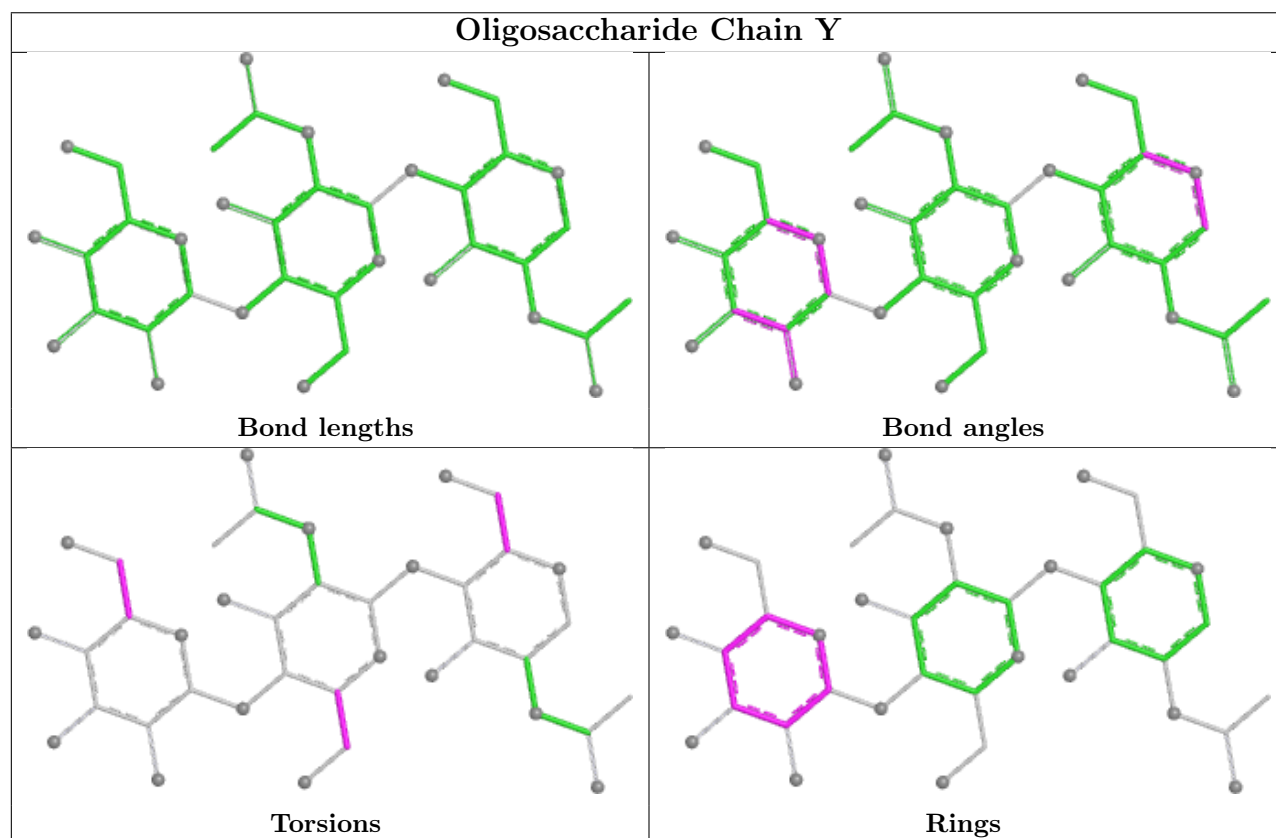
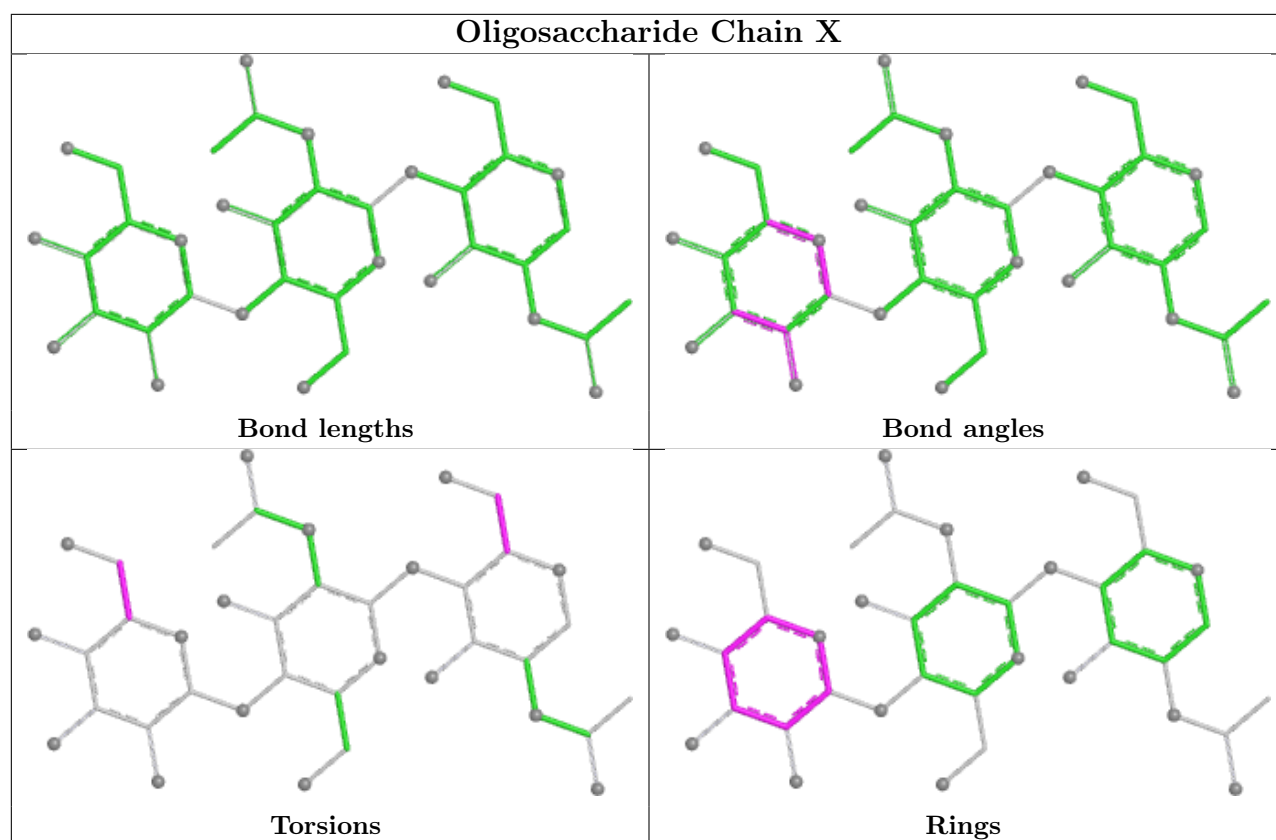


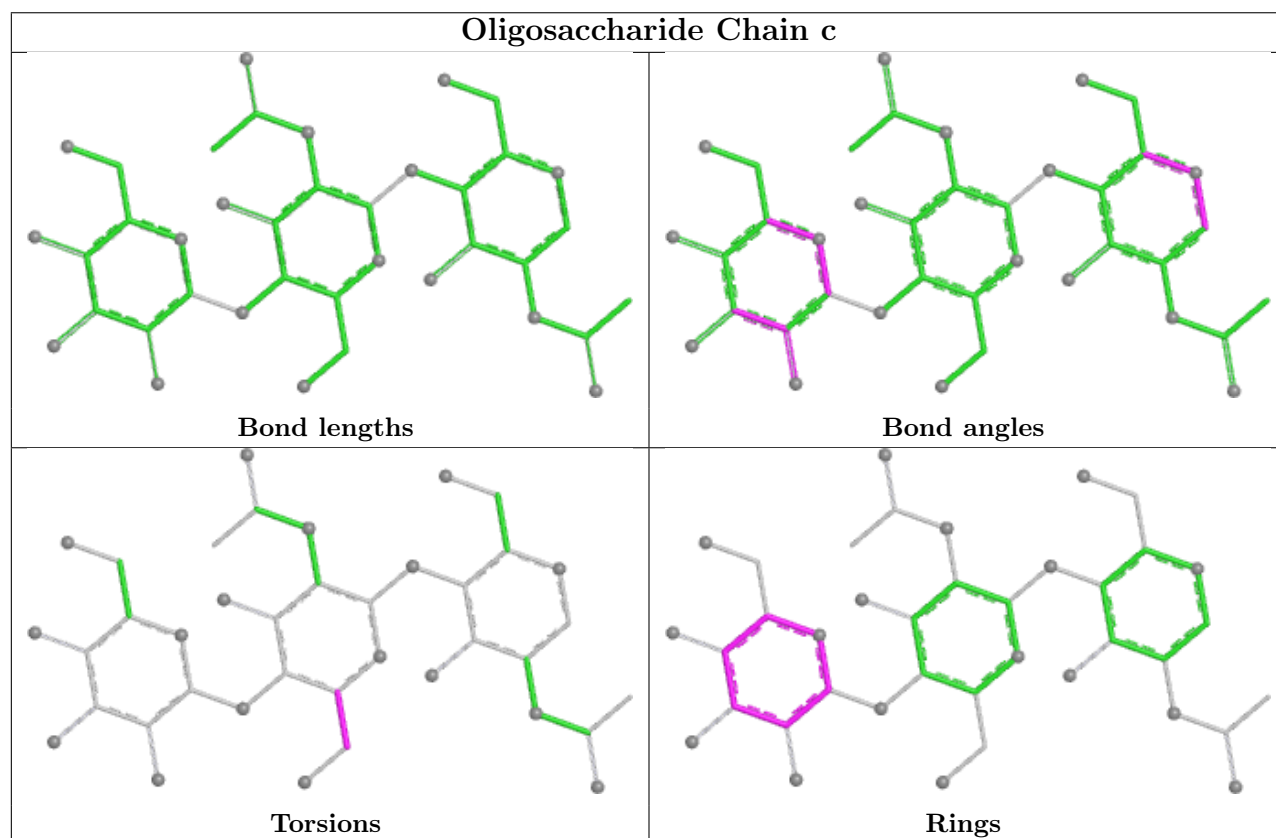
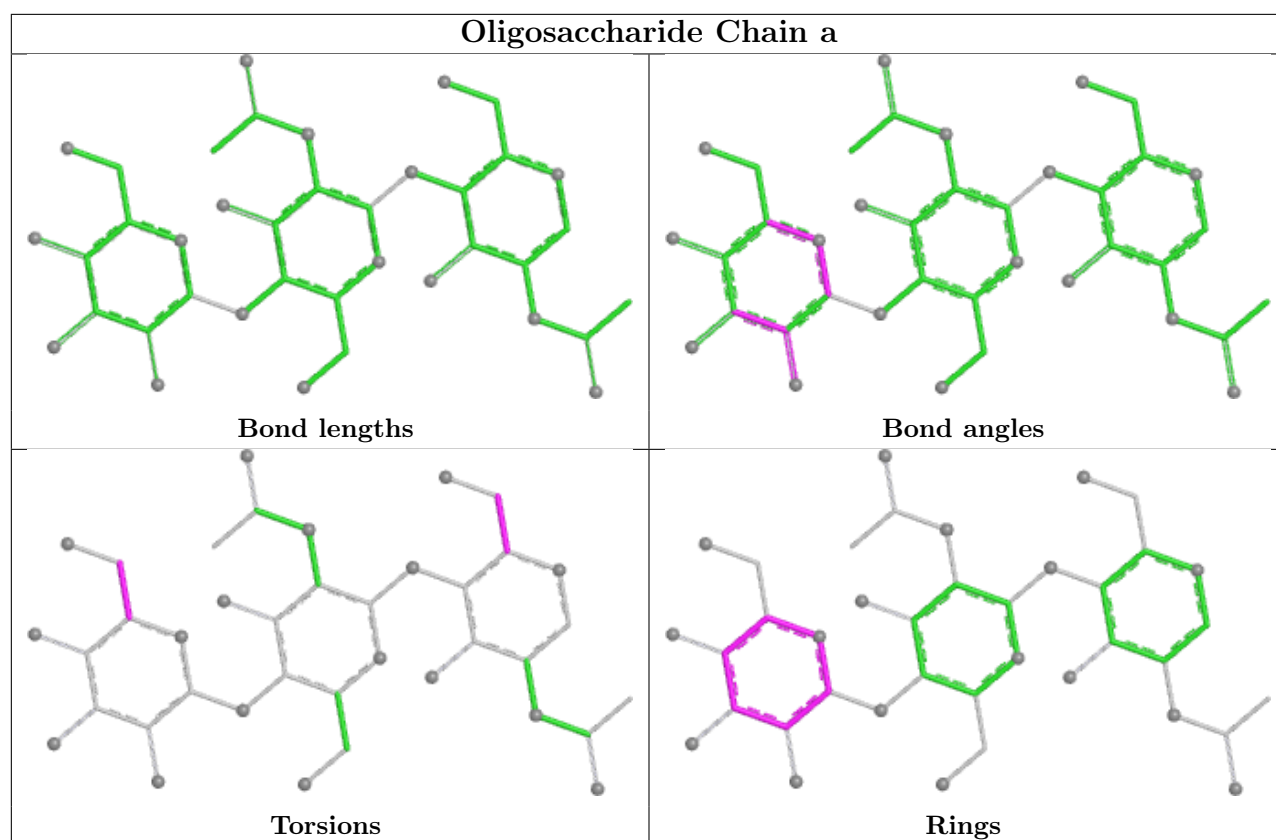


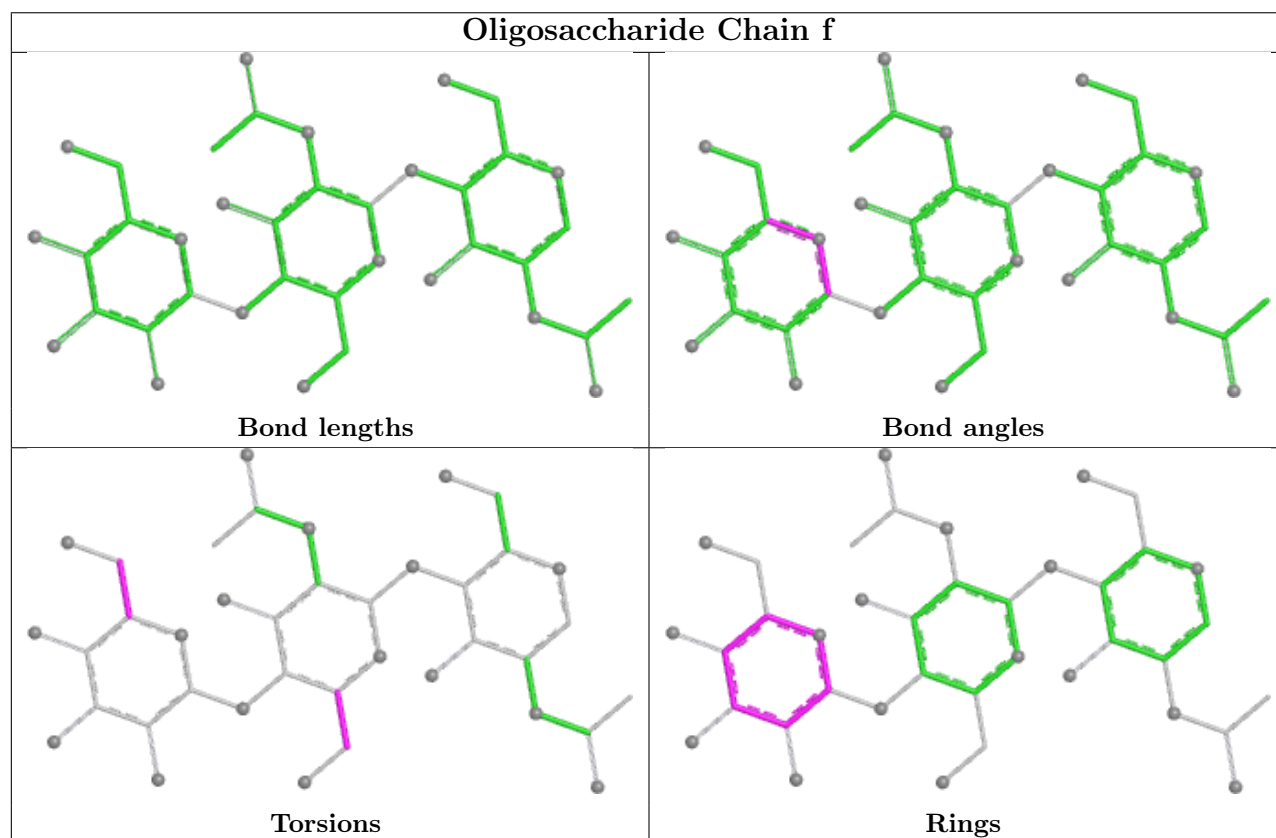
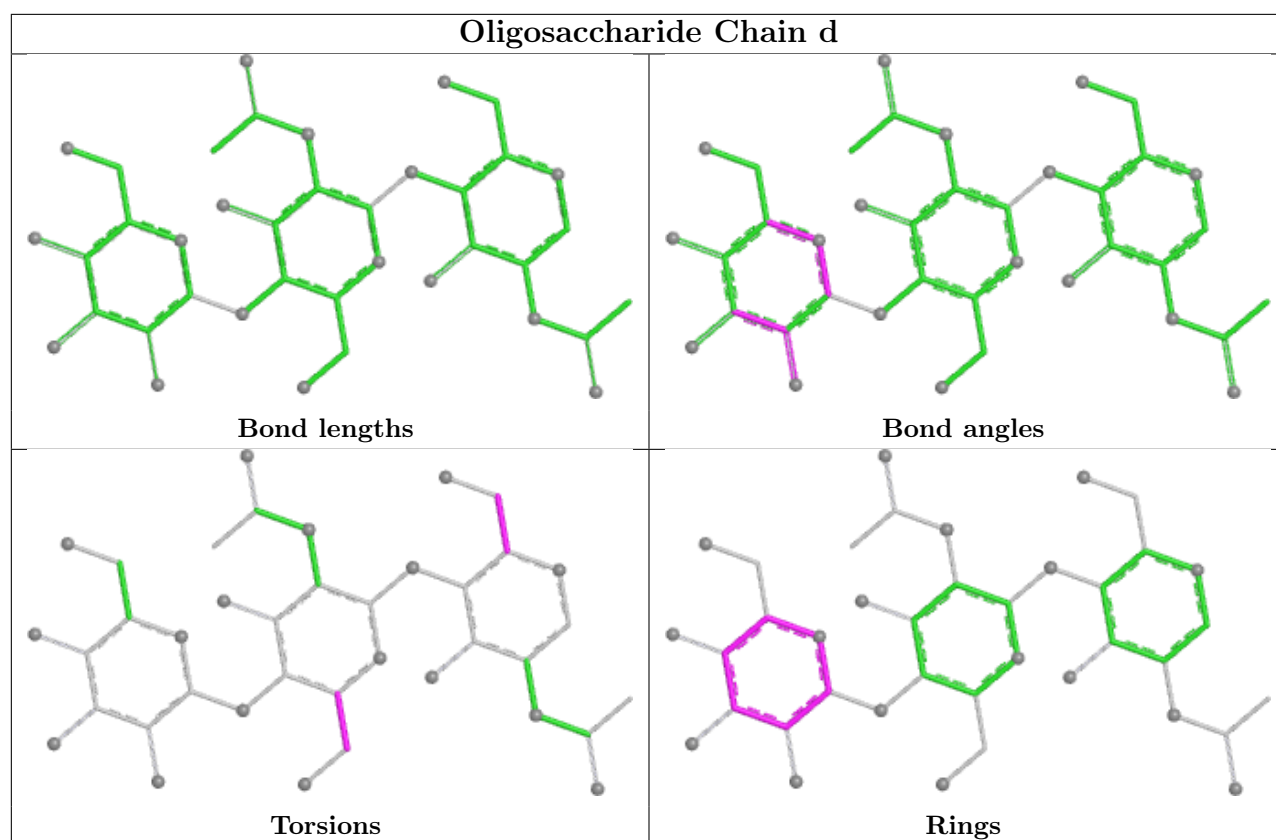


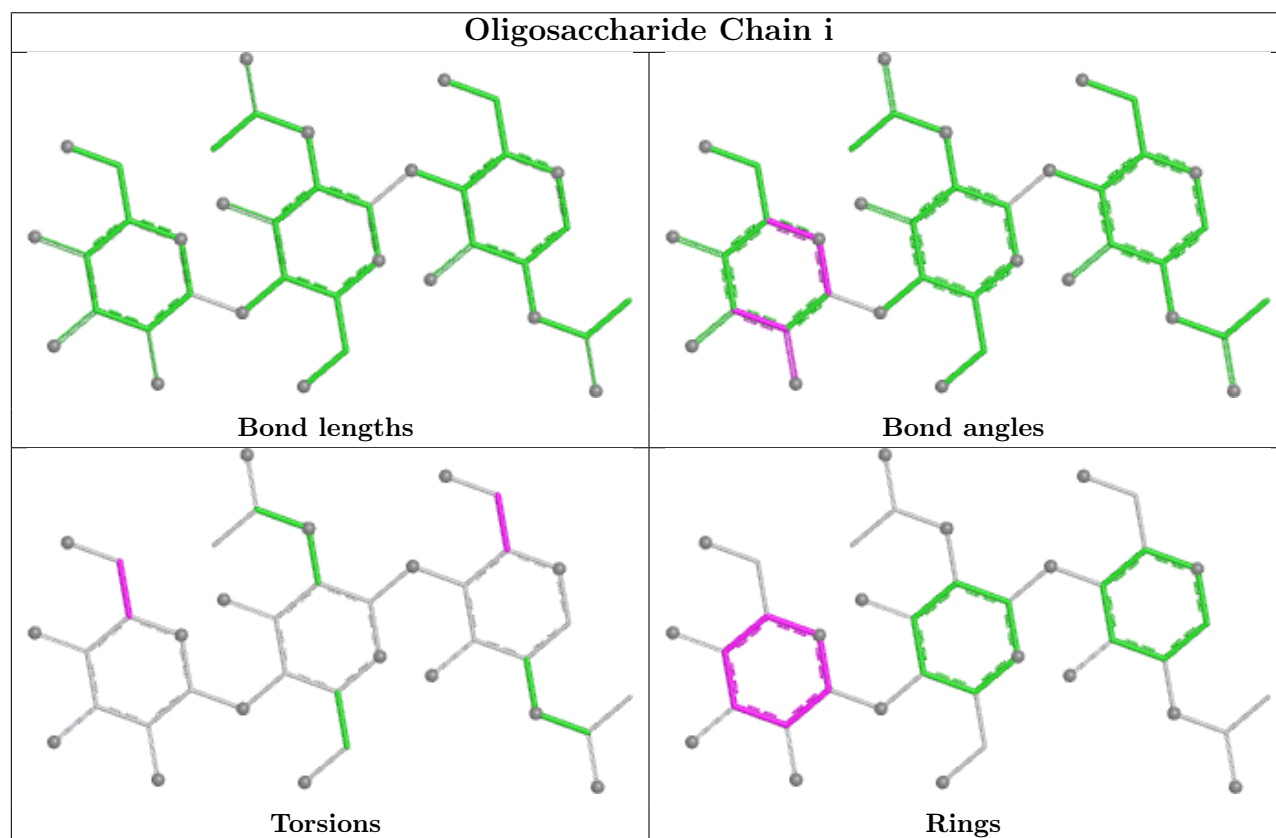
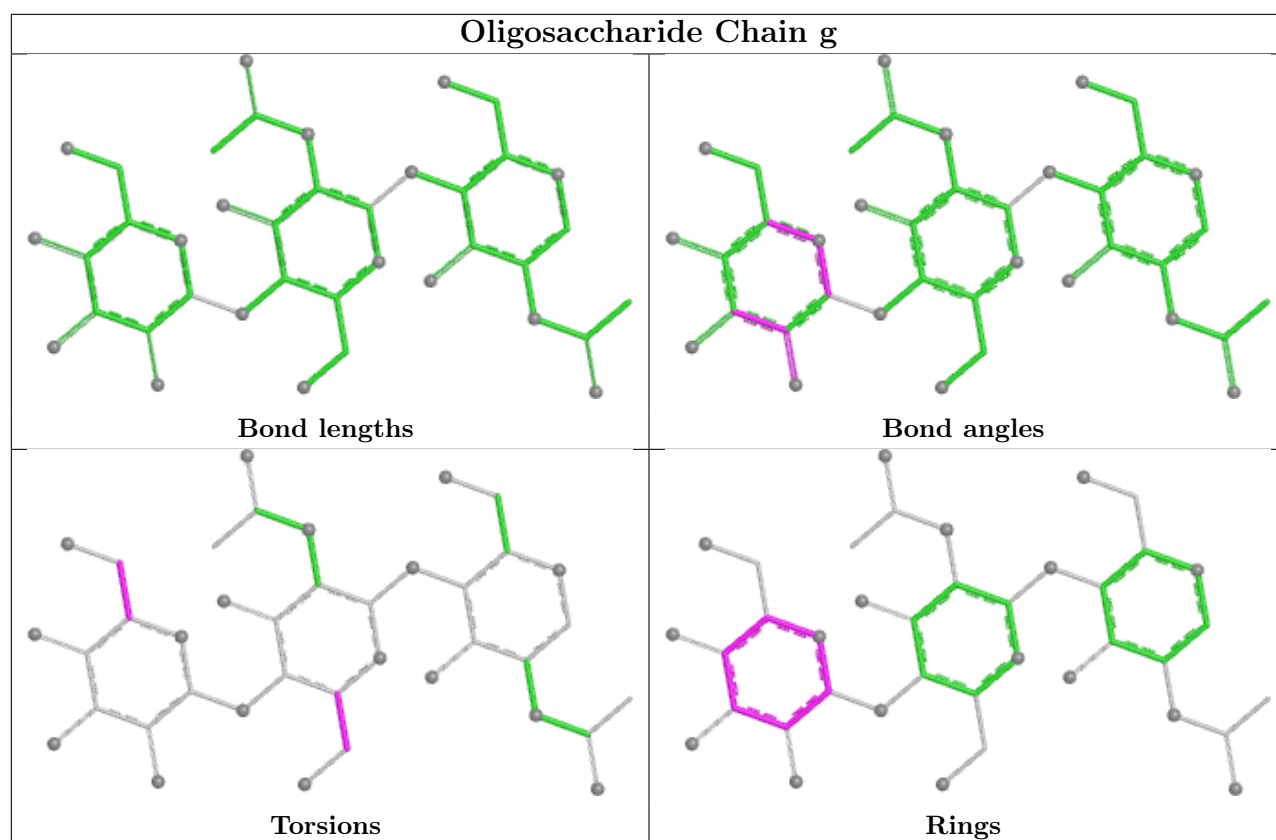


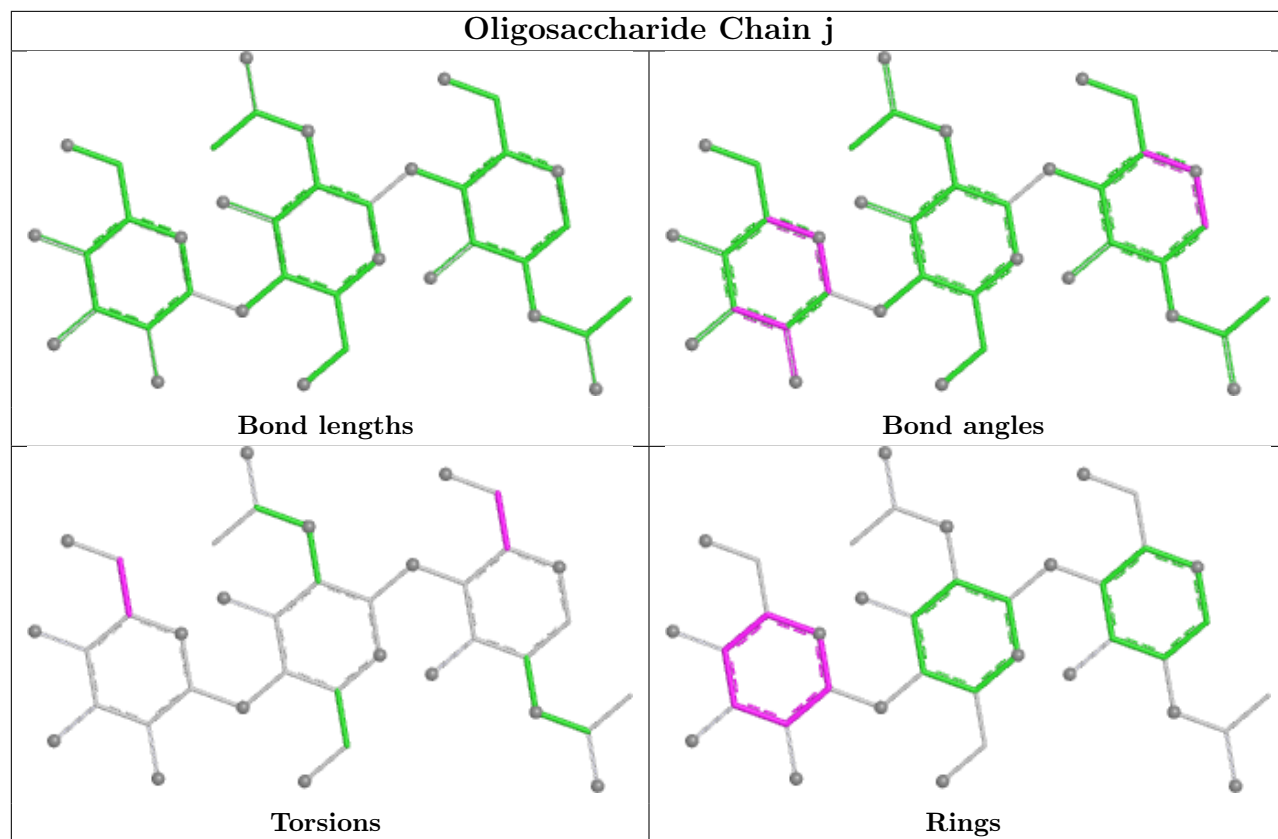


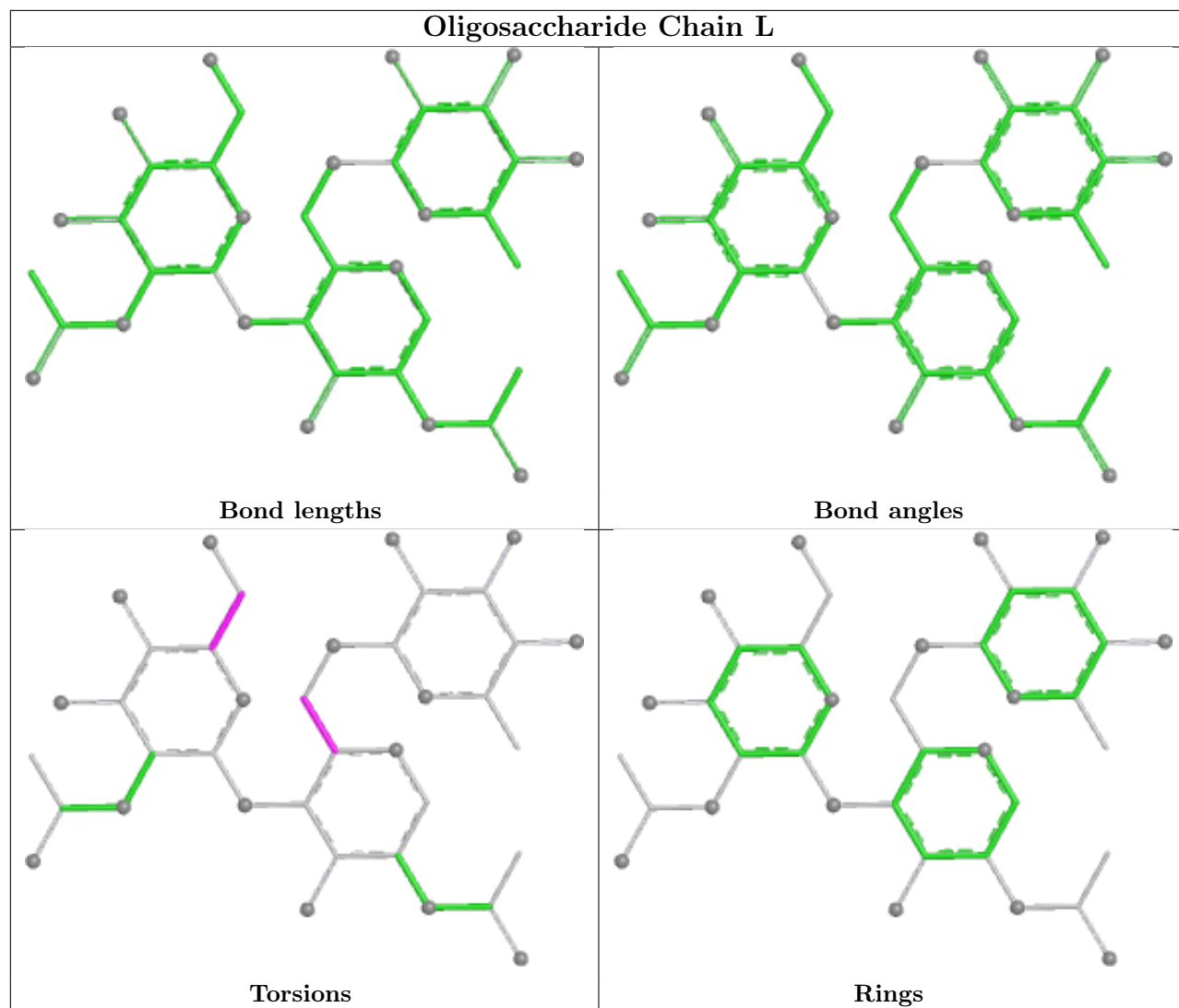


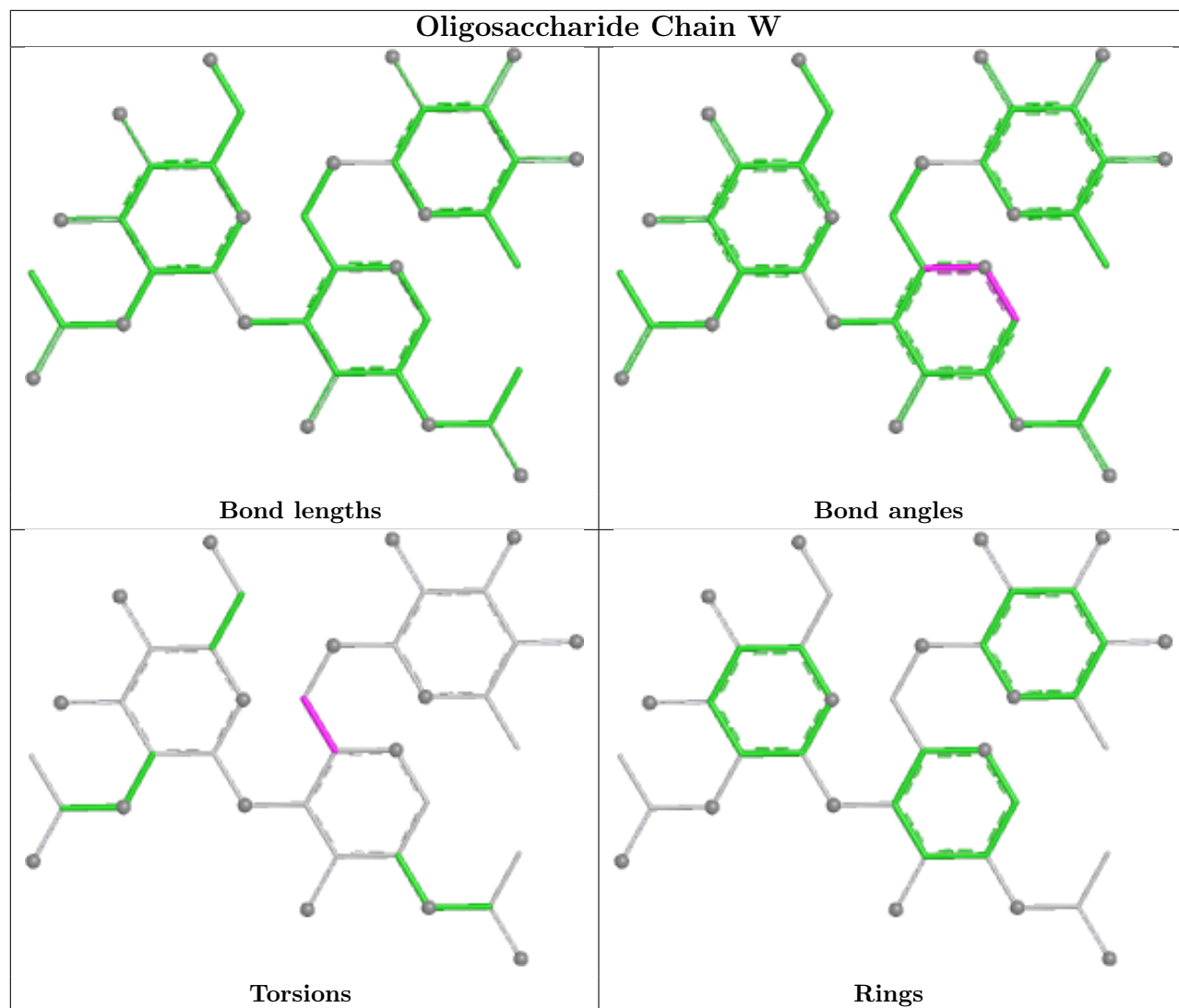


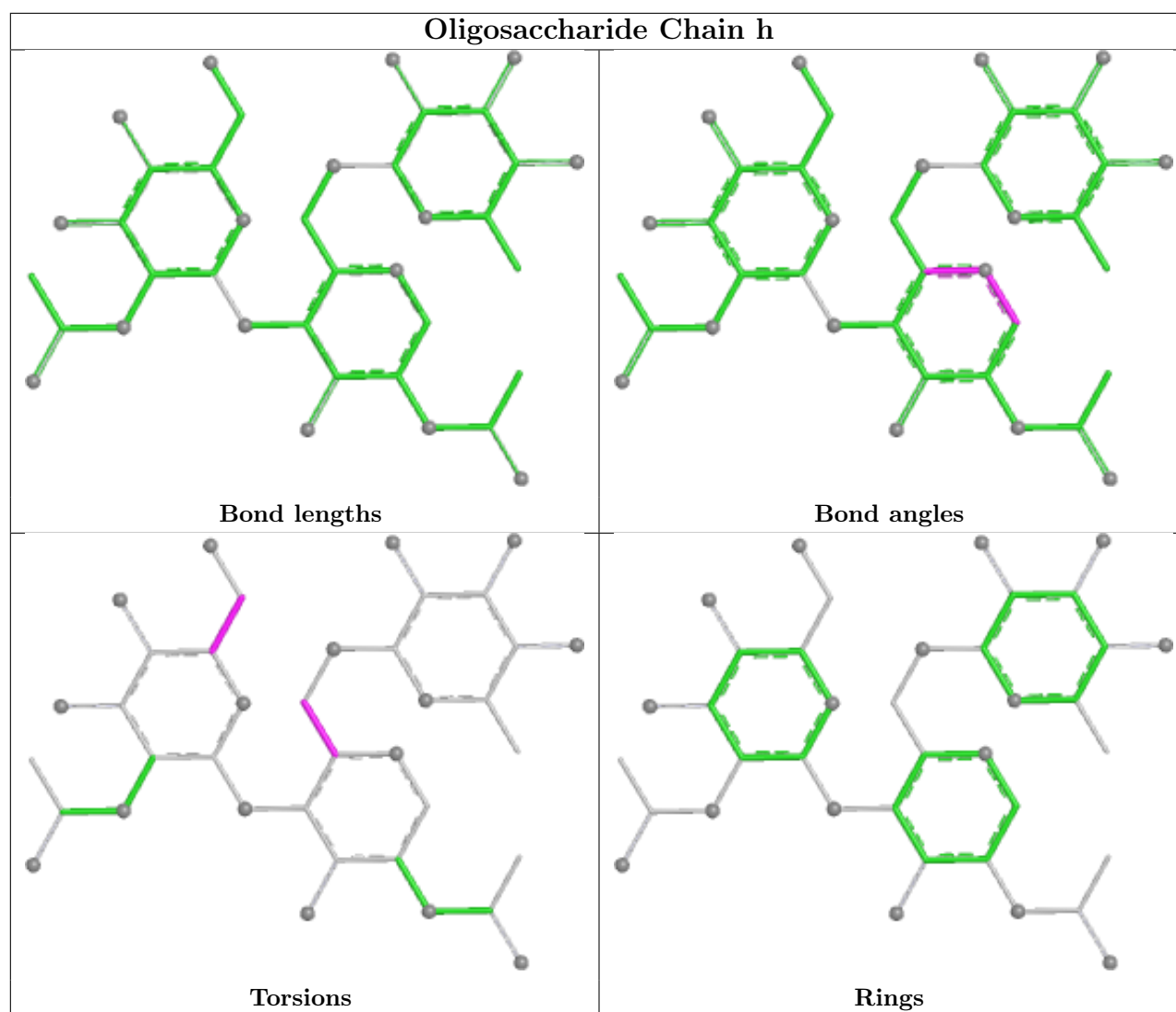












5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
5	NAG	C	1404	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	1404	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	B	1402	1	14,14,15	0.44	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1407	1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	A	1401	1	14,14,15	0.25	0	17,19,21	0.41	0
5	NAG	B	1401	1	14,14,15	0.22	0	17,19,21	0.51	0
5	NAG	C	1401	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	B	1407	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	B	1405	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	C	1406	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	A	1402	1	14,14,15	0.32	0	17,19,21	0.38	0
5	NAG	C	1402	-	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	B	1403	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	C	1405	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	C	1403	1	14,14,15	0.36	0	17,19,21	0.41	0
5	NAG	A	1405	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	A	1403	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	B	1404	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	1406	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1407	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	C	1408	1	14,14,15	0.24	0	17,19,21	0.48	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
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1402	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1407	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1405	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	NAG	1	0
5	B	1401	NAG	1	0
5	C	1401	NAG	1	0
5	A	1402	NAG	1	0
5	A	1403	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.

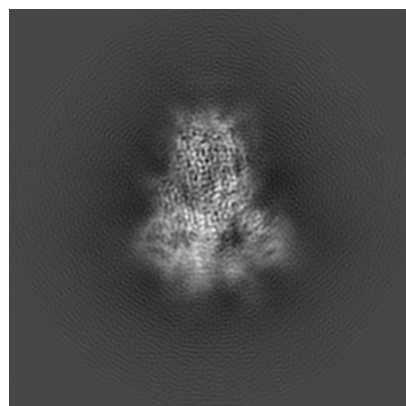
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33725. These allow visual inspection of the internal detail of the map and identification of artifacts.

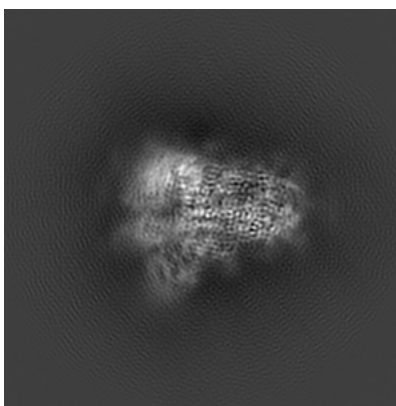
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

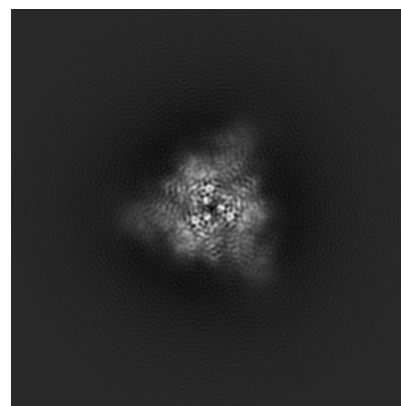
6.1.1 Primary map



X

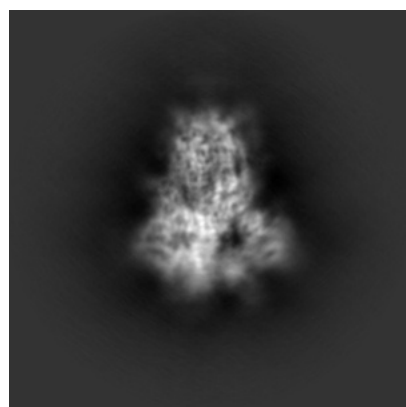


Y

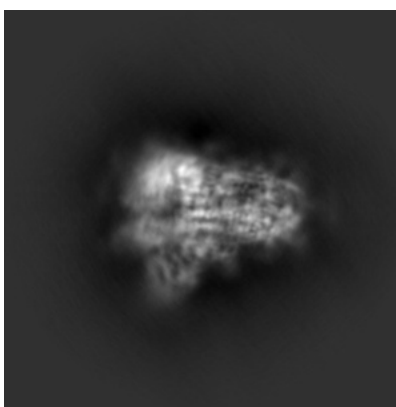


Z

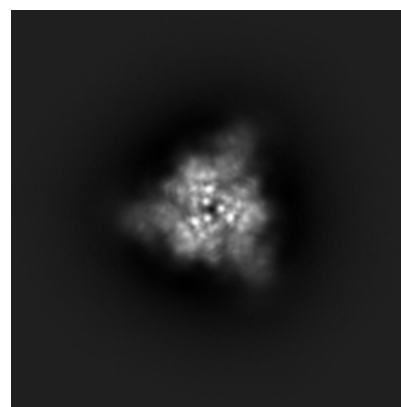
6.1.2 Raw map



X



Y

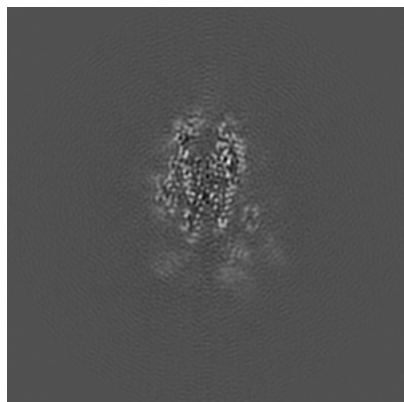


Z

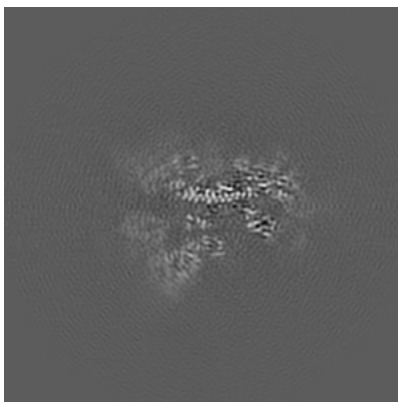
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

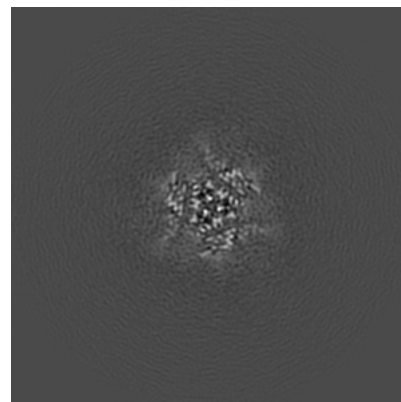
6.2.1 Primary map



X Index: 160

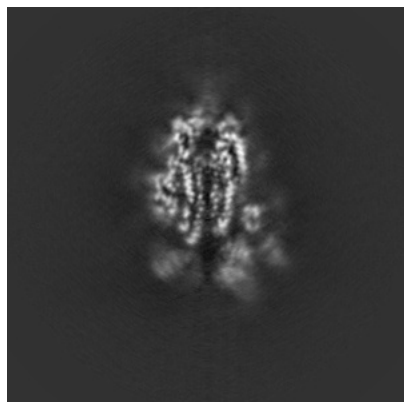


Y Index: 160

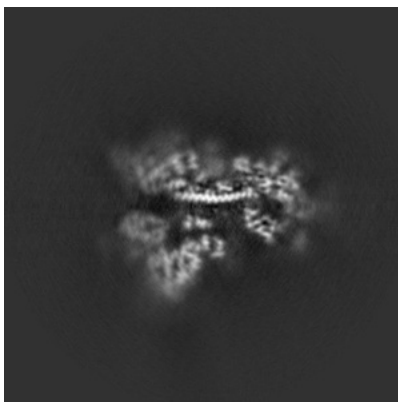


Z Index: 160

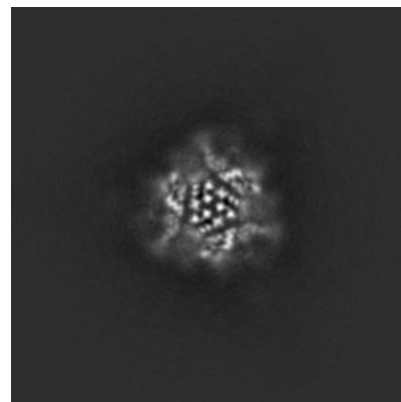
6.2.2 Raw map



X Index: 160



Y Index: 160

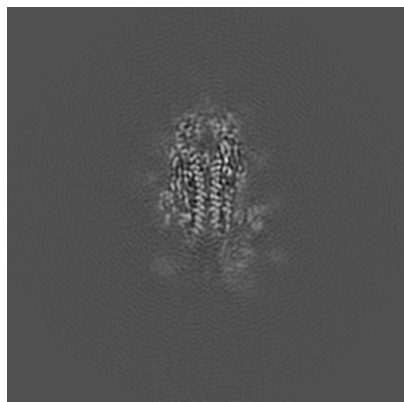


Z Index: 160

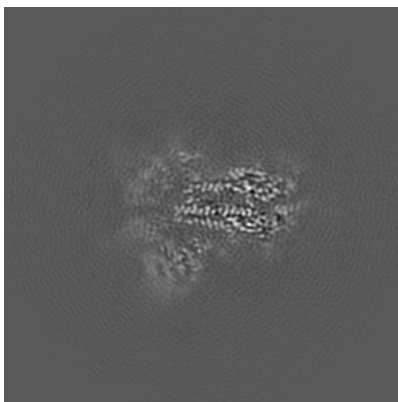
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

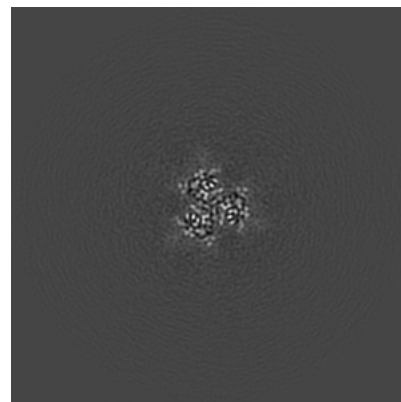
6.3.1 Primary map



X Index: 156

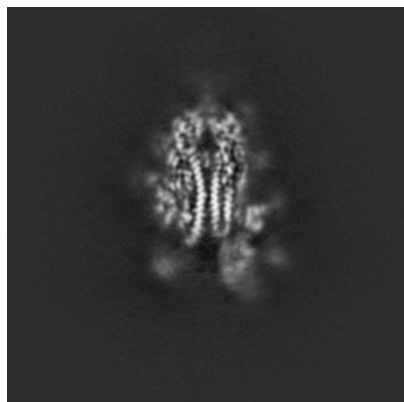


Y Index: 152

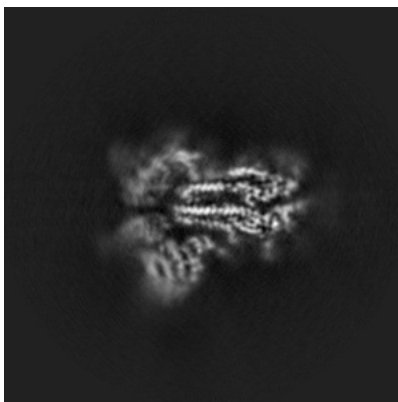


Z Index: 196

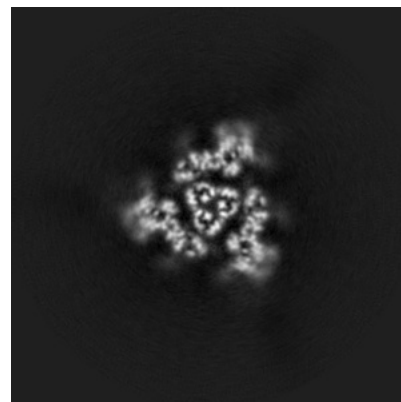
6.3.2 Raw map



X Index: 157



Y Index: 153

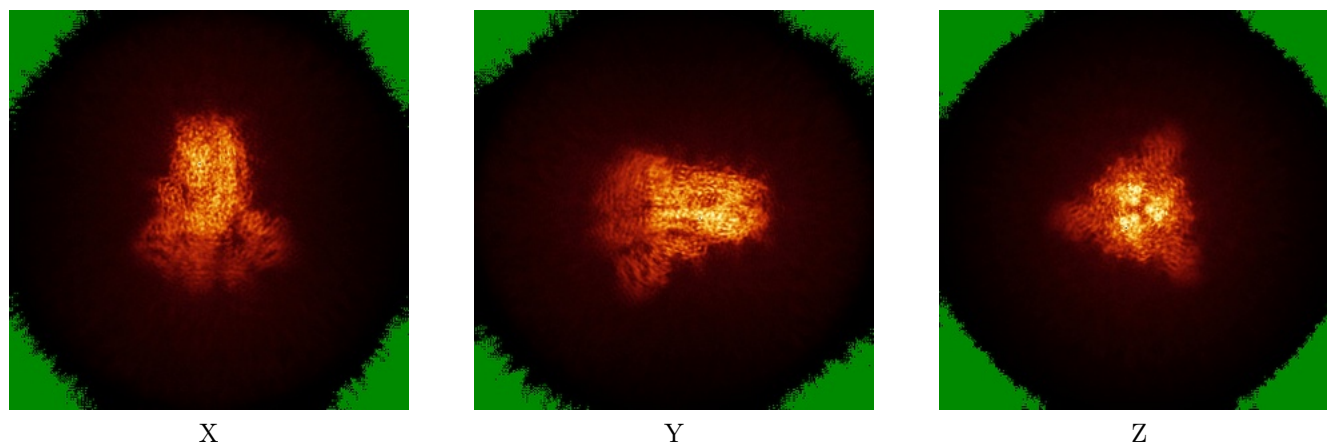


Z Index: 144

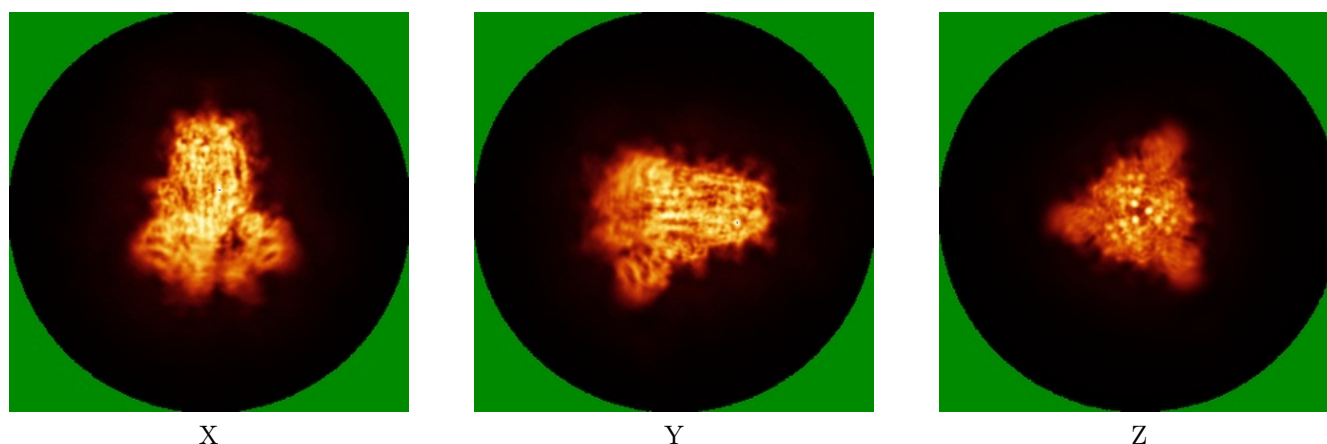
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

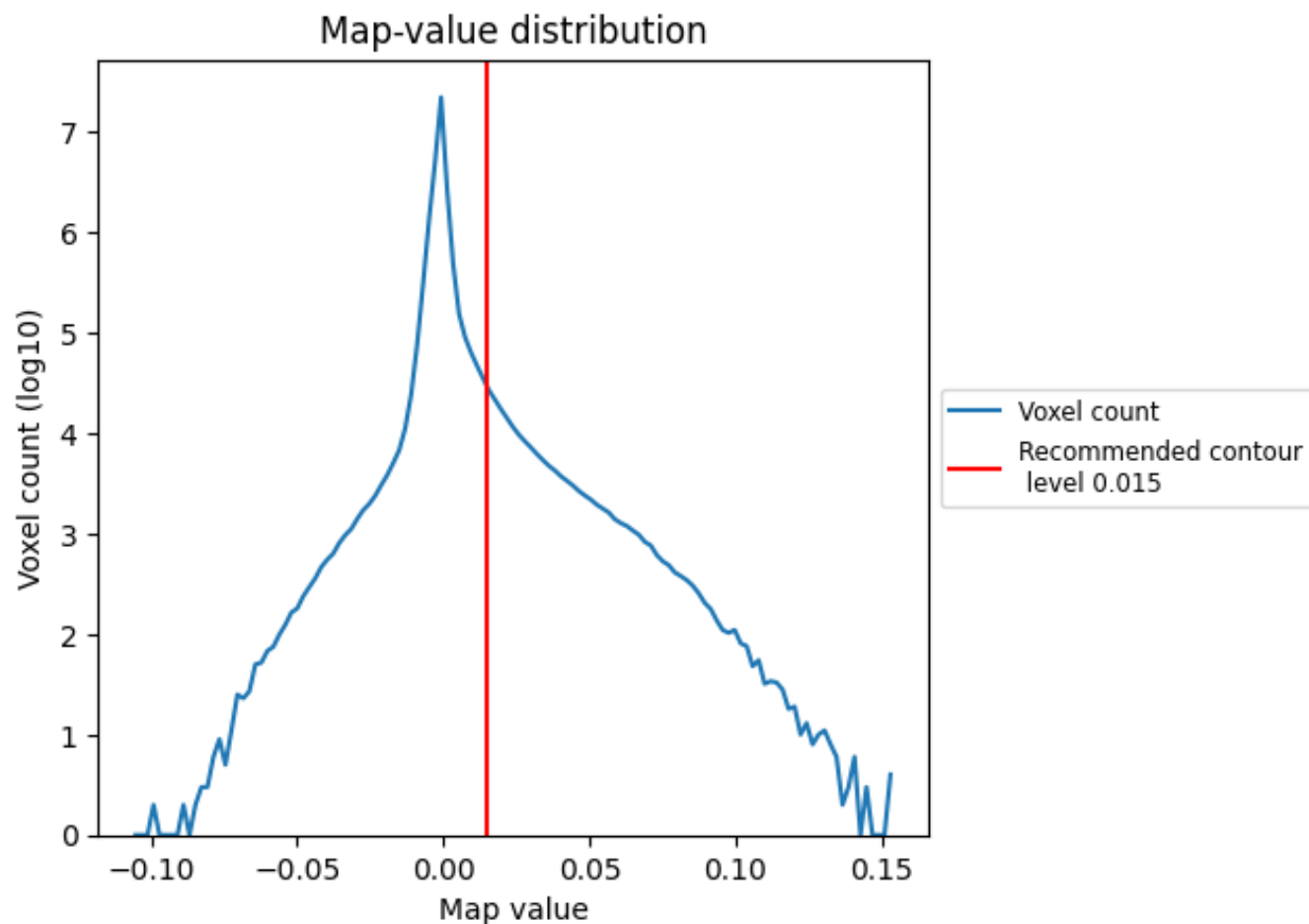
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

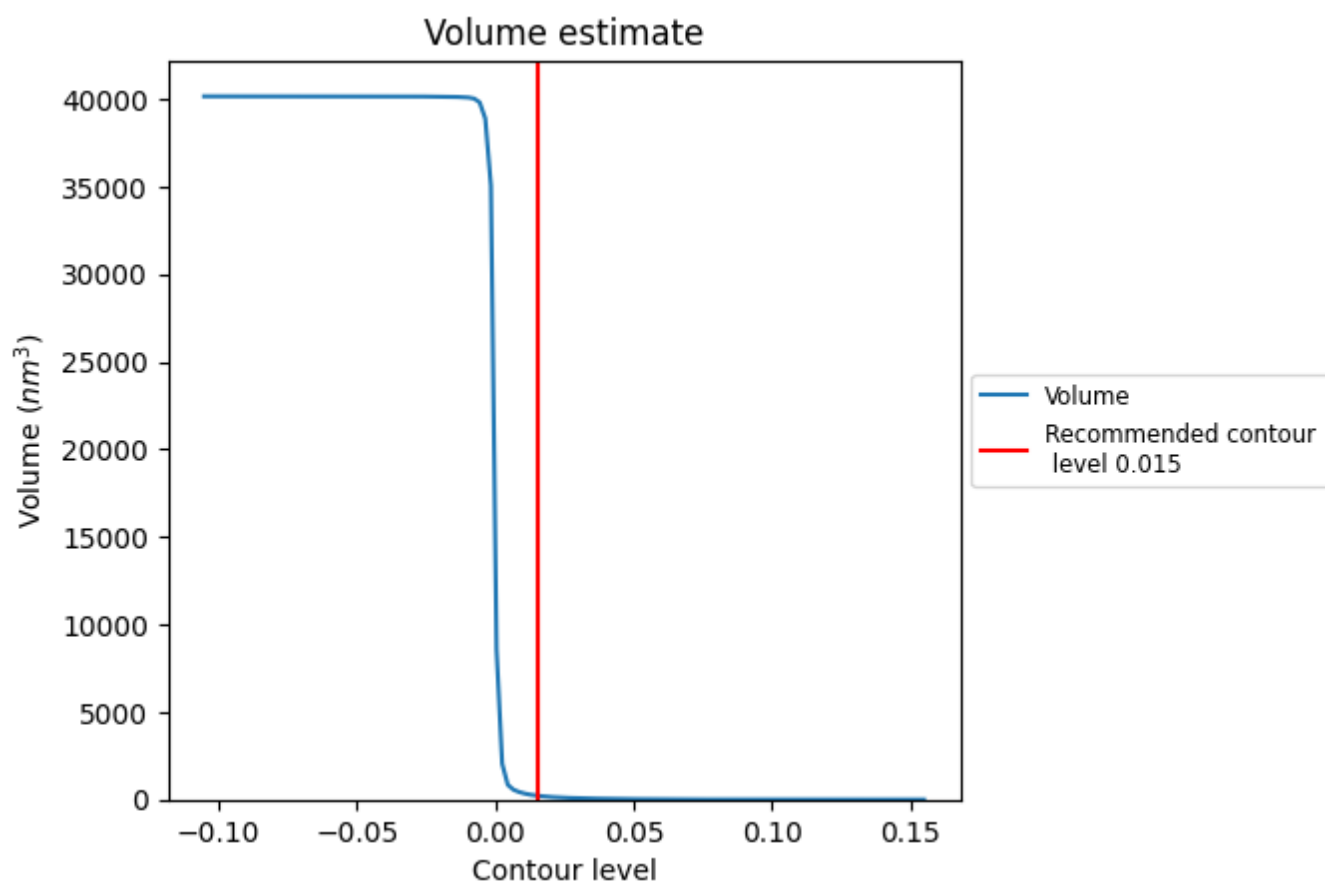
This section contains the results of statistical analysis of the map.

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.

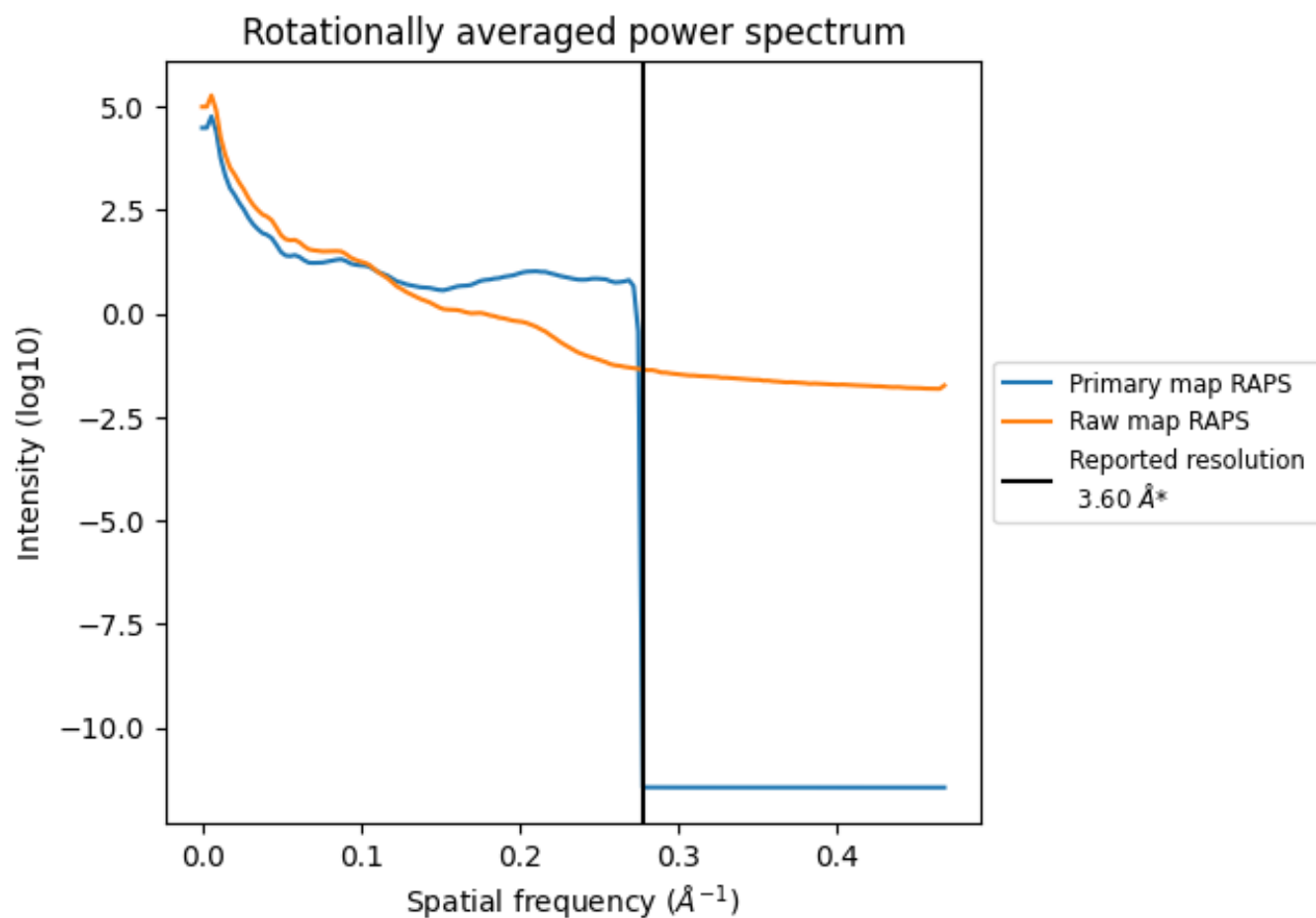
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm^3 ; this corresponds to an approximate mass of 201 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 ⓘ

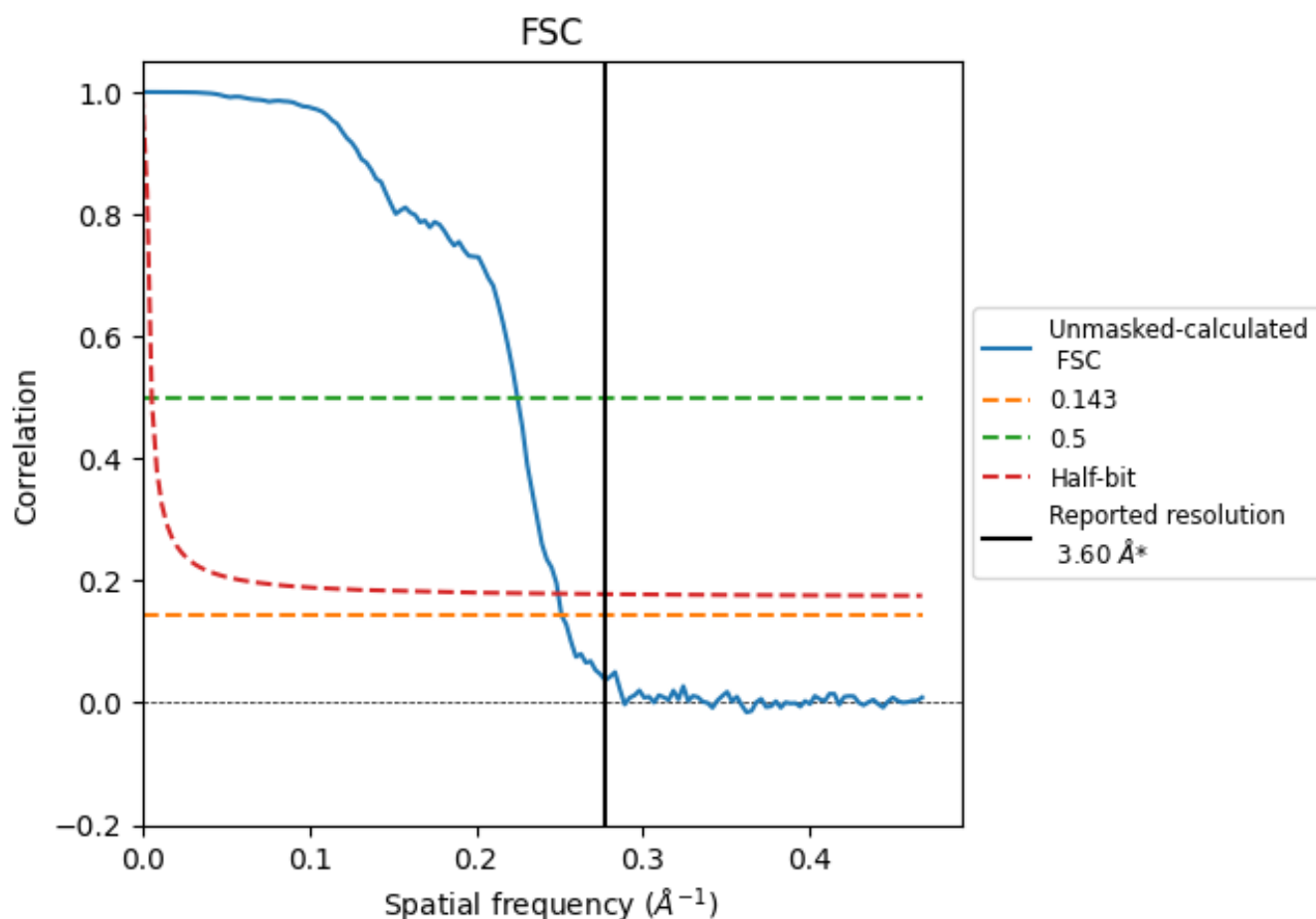


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

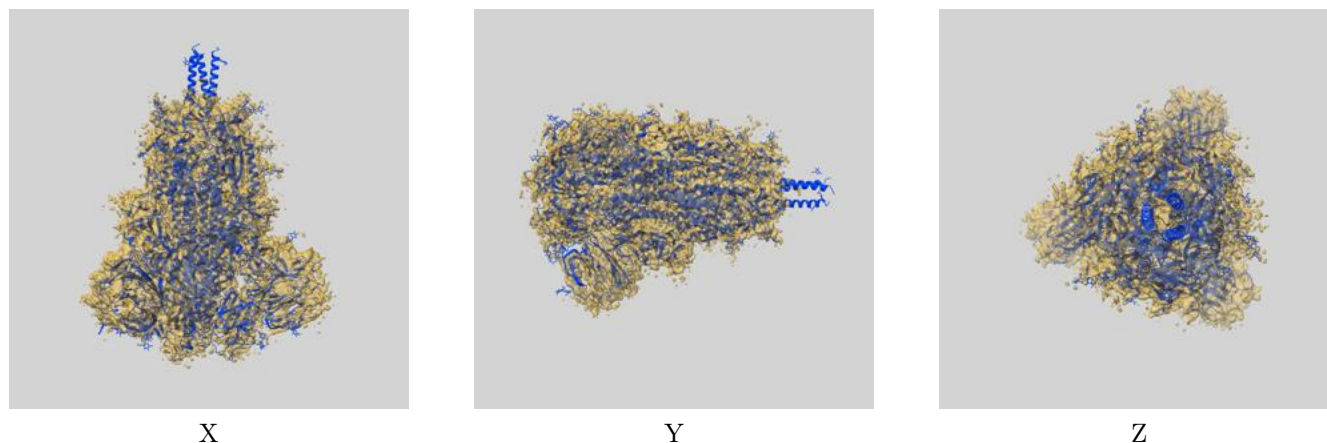
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	4.45	4.01

*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 3.98 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

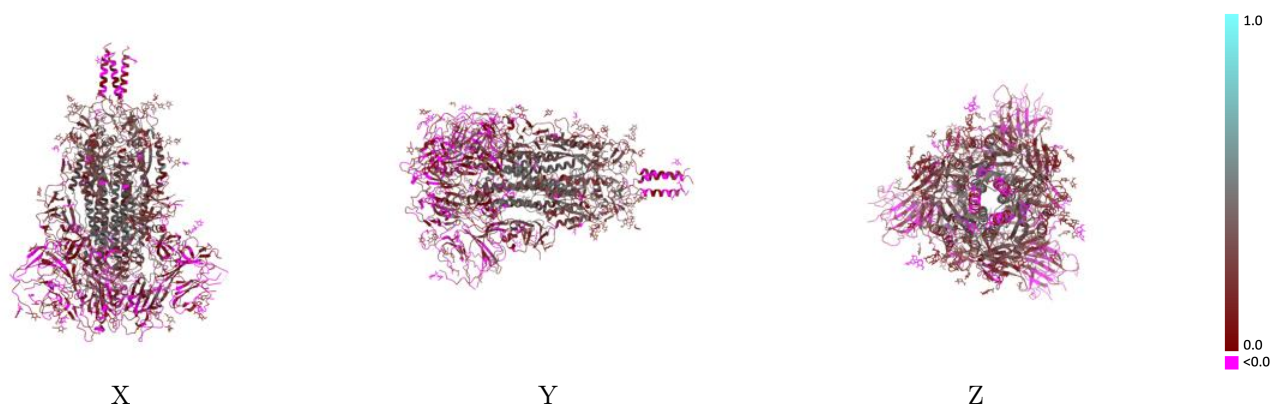
This section contains information regarding the fit between EMDB map EMD-33725 and PDB model 7YBL. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

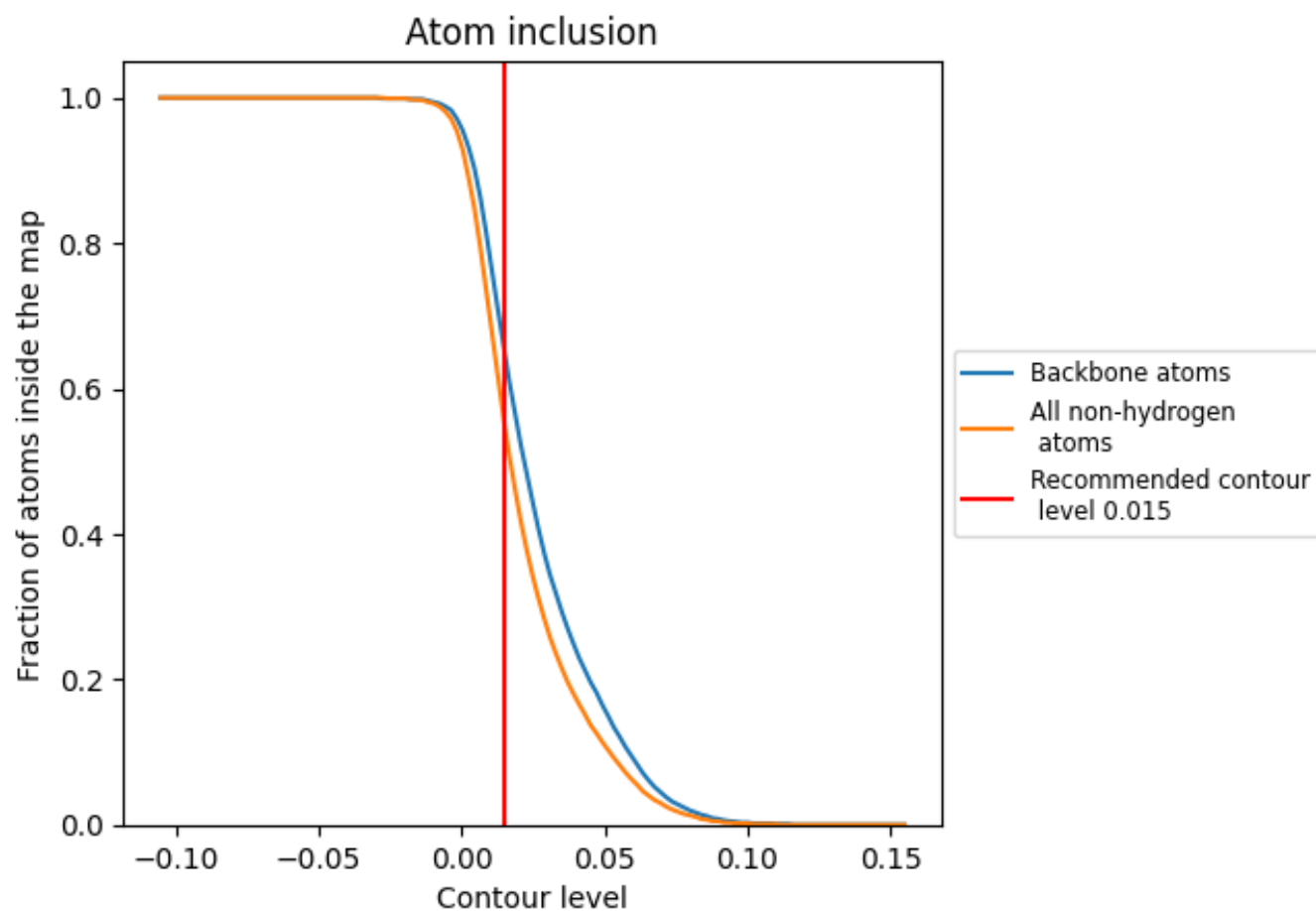


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 55% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5510	 0.1780
A	 0.5620	 0.1820
B	 0.5690	 0.1830
C	 0.5660	 0.1830
D	 0.0000	 -0.0600
E	 0.0000	 0.0130
F	 0.0360	 0.1780
G	 0.0000	 -0.0290
H	 0.2050	 0.0440
I	 0.2860	 0.0710
J	 0.4360	 0.1730
K	 0.3850	 0.0370
L	 0.2370	 0.0490
M	 0.3850	 0.2130
N	 0.4360	 0.2340
O	 0.0000	 -0.0770
P	 0.0260	 0.0490
Q	 0.0360	 0.1640
R	 0.0000	 -0.0200
S	 0.1790	 0.0310
T	 0.2860	 0.0450
U	 0.4100	 0.1120
V	 0.3850	 0.0670
W	 0.2630	 0.1230
X	 0.3850	 0.2170
Y	 0.4360	 0.2610
Z	 0.0000	 -0.0790
a	 0.0000	 0.0130
b	 0.0360	 0.1790
c	 0.0000	 -0.0100
d	 0.2310	 0.0730
e	 0.2860	 0.1170
f	 0.4620	 0.1490
g	 0.4360	 0.0380
h	 0.2630	 0.0750



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.4100	 0.2140
j	 0.5130	 0.2370