



## Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 06:06 PM EST

PDB ID : 6VPX  
EMDB ID : EMD-21335  
Title : Nanodisc of full-length HIV-1 Envelope glycoprotein clone AMC011 in complex with one PGT151 Fab and three 10E8 Fabs  
Authors : Rantalainen, K.; Ward, A.B.W.  
Deposited on : 2020-02-04  
Resolution : 5.00 Å (reported)  
Based on initial models : 6OLP, 5T80

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>.

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

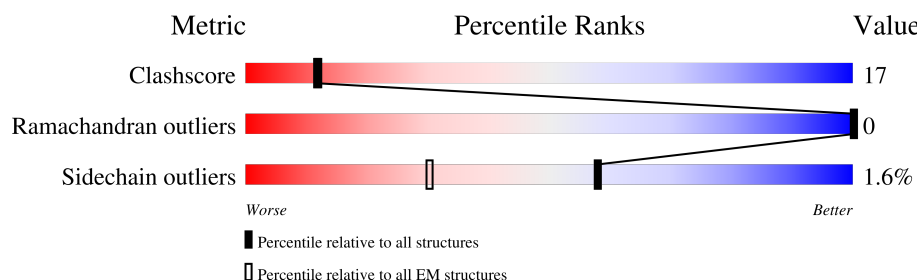
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 Å.

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





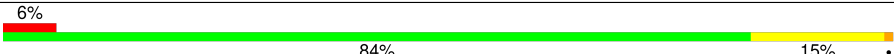
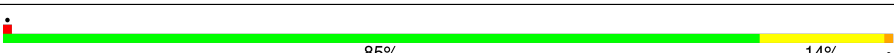
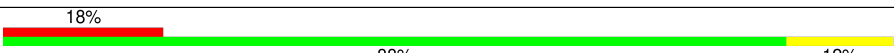
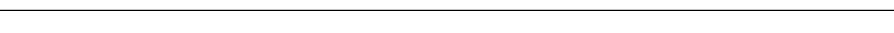





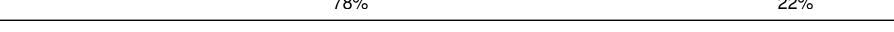


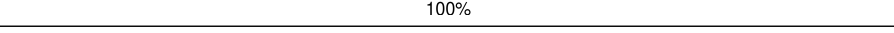
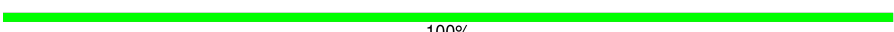
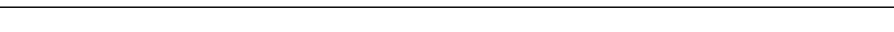


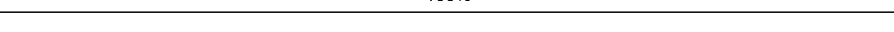
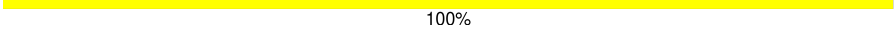

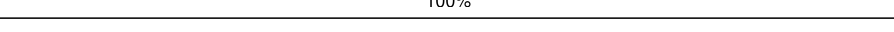
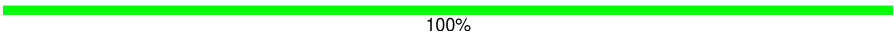

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	465	
1	C	465	
1	E	465	
2	B	153	
2	D	153	
2	F	153	
3	H	129	
3	K	129	

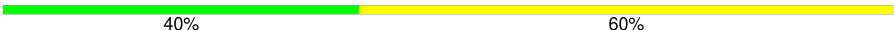

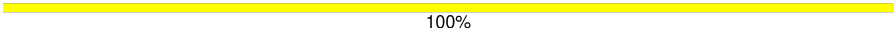




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	129	 76% 22%
4	L	108	 19% 85% 14%
4	N	108	 6% 84% 15%
4	O	108	 85% 14%
5	G	17	 18% 88% 12%
5	I	17	 88% 12%
5	J	17	 88% 12%
6	P	134	 75% 25%
7	Q	109	 78% 22%
8	R	2	 50% 50%
8	T	2	 100%
8	U	2	 100%
8	V	2	 50% 50%
8	X	2	 100%
8	Z	2	 100%
8	a	2	 100%
8	b	2	 100%
8	d	2	 100%
8	e	2	 100%
8	f	2	 100%
8	i	2	 100%
9	S	2	 100%
10	W	4	 75% 25%
11	Y	3	 67% 33%
11	c	3	 100%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
12	g	5	 40%60%
13	h	2	 50%50%
13	n	2	 100%
14	j	3	 33%67%33%
14	k	3	 33%67%
15	l	9	 11%89%
16	m	8	 50%50%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22655 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	1	0
			3390	2148	586	630	26		
1	E	419	Total	C	N	O	S	0	0
			3288	2085	571	606	26		
1	C	438	Total	C	N	O	S	0	0
			3454	2185	600	643	26		

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total	C	N	O	S	0	0
			1014	643	170	195	6		
2	B	143	Total	C	N	O	S	0	0
			1137	717	197	217	6		
2	F	120	Total	C	N	O	S	0	0
			954	601	165	182	6		

- Molecule 3 is a protein called Antibody 10E8 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	129	Total	C	N	O	S	1	0
			1025	657	171	191	6		
3	K	129	Total	C	N	O	S	1	0
			1025	657	171	191	6		
3	M	129	Total	C	N	O	S	1	0
			1016	649	171	190	6		

- Molecule 4 is a protein called Antibody 10E8 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	108	Total	C	N	O	S	3	0
			825	508	147	166	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	108	Total	C	N	O	S	3	0
			825	508	147	166	4		
4	O	108	Total	C	N	O	S	3	0
			825	508	147	166	4		

- Molecule 5 is a protein called MPER peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	17	Total	C	N	O		0	0
			153	106	24	23			
5	I	17	Total	C	N	O		0	0
			153	106	24	23			
5	J	17	Total	C	N	O		0	0
			153	106	24	23			

- Molecule 6 is a protein called Antibody PGT151 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	134	Total	C	N	O	S	0	0
			1062	676	184	196	6		

- Molecule 7 is a protein called Antibody PGT151 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	109	Total	C	N	O	S	0	0
			838	527	142	165	4		

- Molecule 8 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
8	R	2	Total	C	N	O		0	0
			28	16	2	10			
8	T	2	Total	C	N	O		0	0
			28	16	2	10			
8	U	2	Total	C	N	O		0	0
			28	16	2	10			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	b	2	Total	C	N	O	0	0
			28	16	2	10		
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



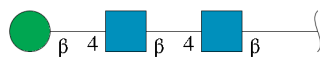
Mol	Chain	Residues	Atoms				AltConf	Trace
9	S	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



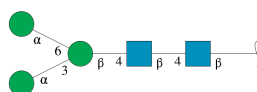
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 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
11	Y	3	Total	C	N	O	0	0
			39	22	2	15		
11	c	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 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
12	g	5	Total	C	N	O	0	0
			61	34	2	25		

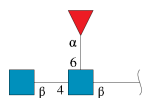
- Molecule 13 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	2	Total	C	N	O	0	0
			24	14	1	9		
13	n	2	Total	C	N	O	0	0
			24	14	1	9		

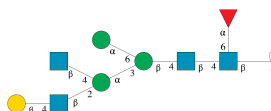
- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.





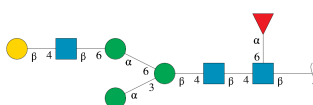
Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	3	Total	C	N	O	0	0
			38	22	2	14		
14	k	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 15 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
15	l	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 16 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-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
16	m	8	Total	C	N	O	0	0
			96	54	3	39		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

Continued on next page...

*Continued from previous page...*

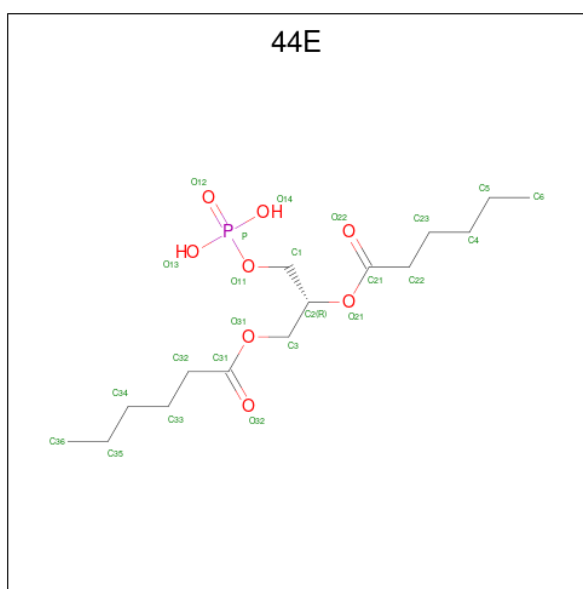
Mol	Chain	Residues	Atoms				AltConf
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14	8	1	5	
17	E	1	Total	C	N	O	0
			14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

*Continued on next page...*

Continued from previous page...

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

- Molecule 18 is (2R)-3-(phosphonoxy)propane-1,2-diyl dihexanoate (three-letter code: 44E) (formula: C<sub>15</sub>H<sub>29</sub>O<sub>8</sub>P).

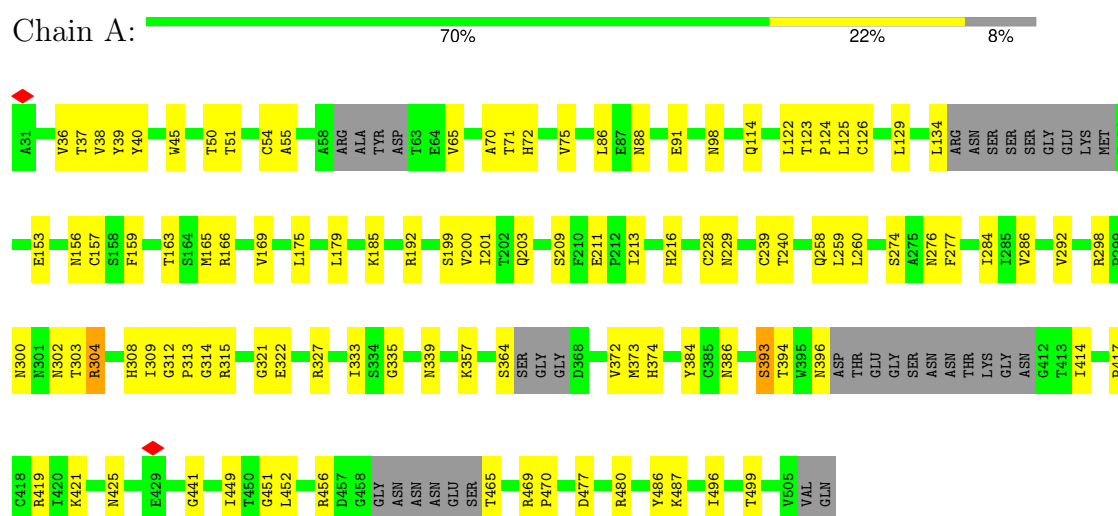


Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	O	P	0
			11	4	6	1	
18	N	1	Total	C	O	P	0
			11	4	6	1	
18	O	1	Total	C	O	P	0
			11	4	6	1	

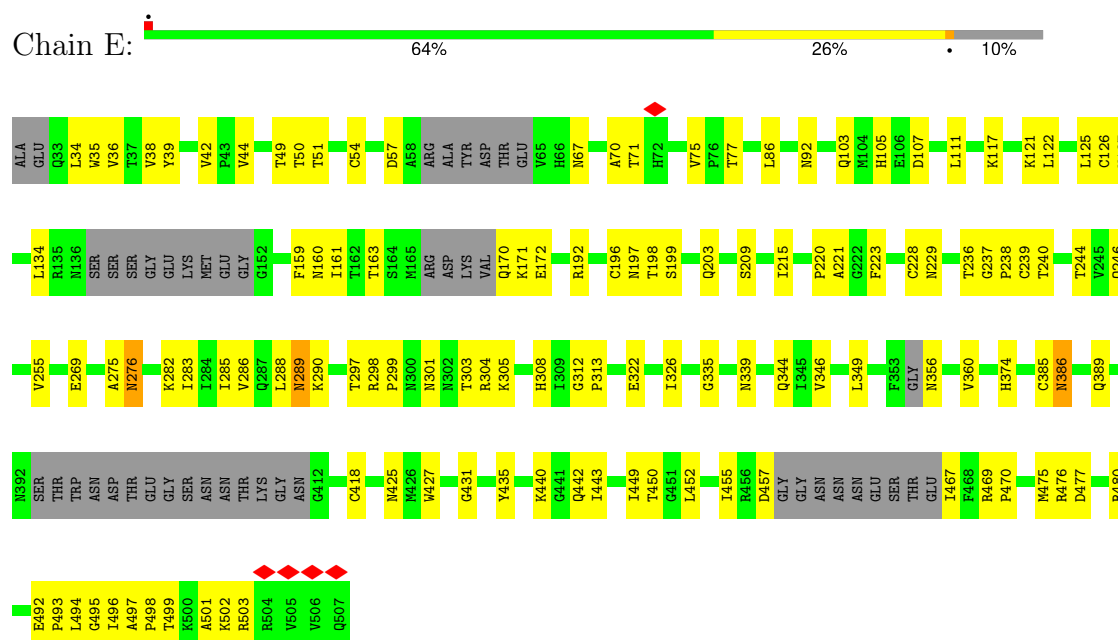
### 3 Residue-property plots

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

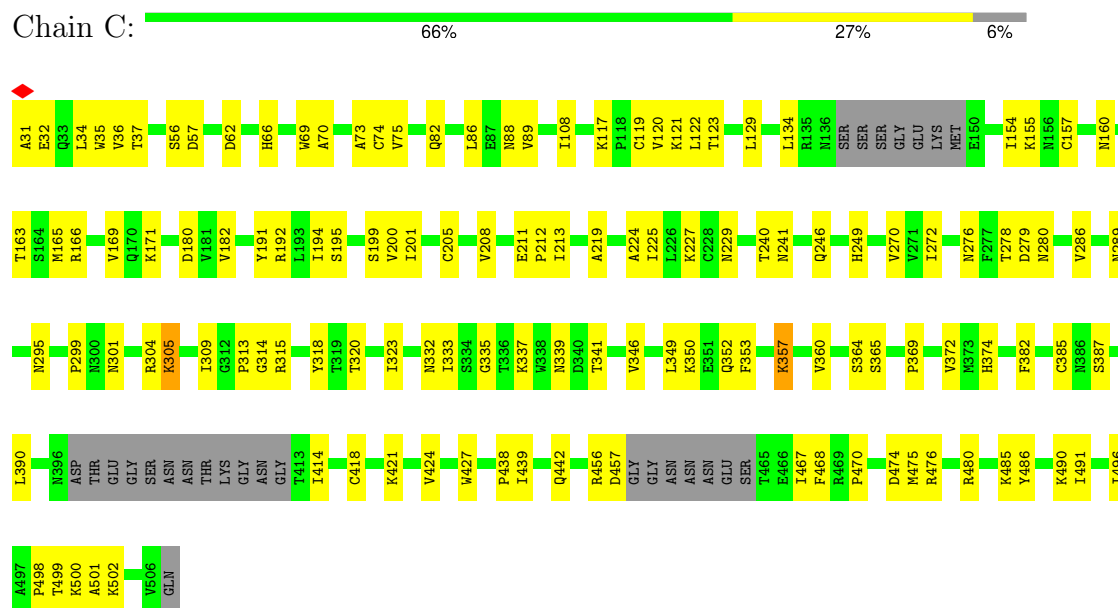
#### • Molecule 1: Envelope glycoprotein gp120



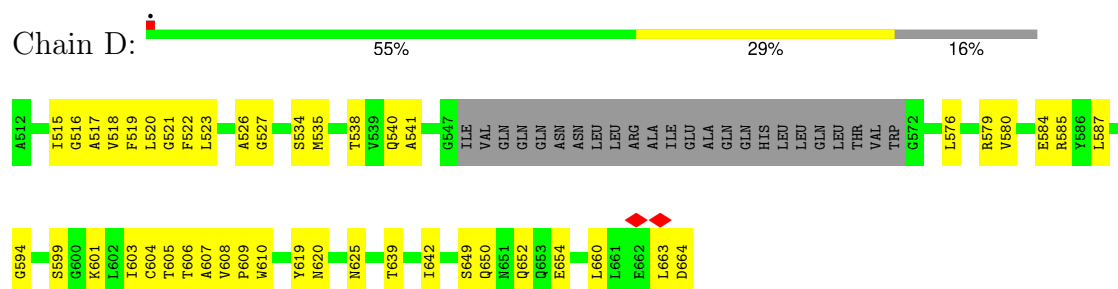
#### • Molecule 1: Envelope glycoprotein gp120



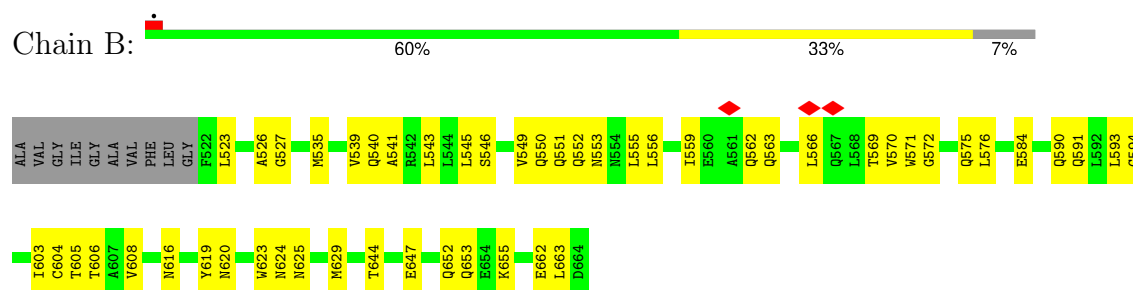
- Molecule 1: Envelope glycoprotein gp120



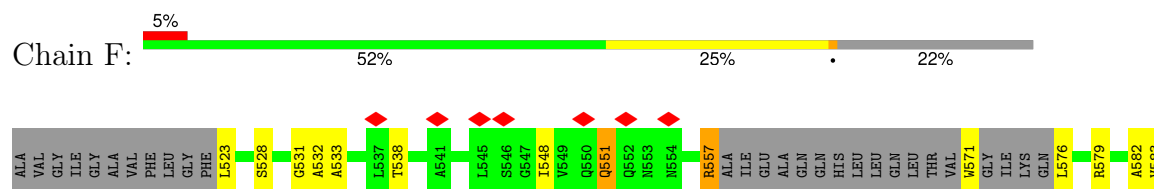
- Molecule 2: Envelope glycoprotein gp41

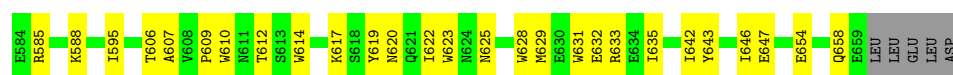


- Molecule 2: Envelope glycoprotein gp41

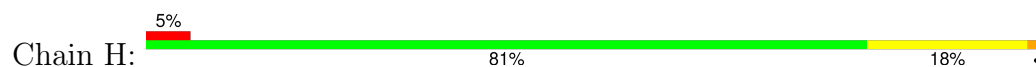


- Molecule 2: Envelope glycoprotein gp41

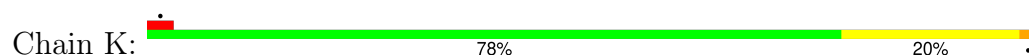




• Molecule 3: Antibody 10E8 Fab heavy chain



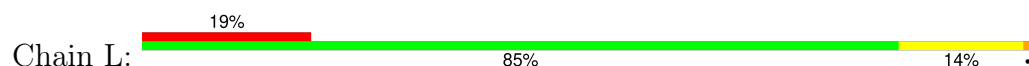
• Molecule 3: Antibody 10E8 Fab heavy chain



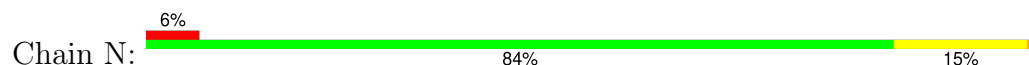
• Molecule 3: Antibody 10E8 Fab heavy chain



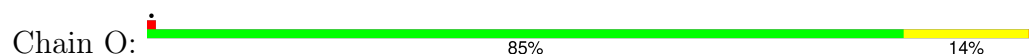
• Molecule 4: Antibody 10E8 Fab light chain



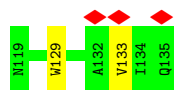
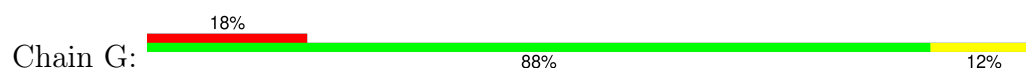
• Molecule 4: Antibody 10E8 Fab light chain



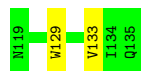
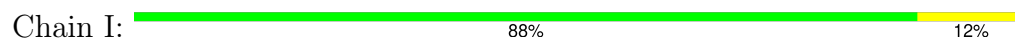
• Molecule 4: Antibody 10E8 Fab light chain



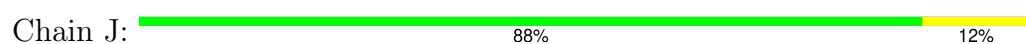
• Molecule 5: MPER peptide



- Molecule 5: MPER peptide



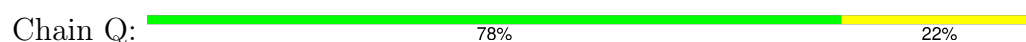
- Molecule 5: MPER peptide



- Molecule 6: Antibody PGT151 Fab heavy chain



- Molecule 7: Antibody PGT151 Fab light chain



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50%  50%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  75% 25%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  67% 33%



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1  
MAG2  
BMA3

- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  40% 60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 13: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  50% 50%

MAG1  
FUC2

- Molecule 13: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%

MAG1  
FUC2

- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  33% 67% 33%

MAG1  
MAG2  
FUC3

- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  33% 67%

MAG1  
MAG2  
FUC3

- Molecule 15: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  11% 89%

NAG1	NAG2	BRG3	MAN4	NAG5	GAL6	NAG7	MAN8	FUC9
------	------	------	------	------	------	------	------	------

- Molecule 16: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  50% 50%

NAG1	NAG2	BRG3	MAN4	NAG5	GAL6	NAG7	FUC8
------	------	------	------	------	------	------	------

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.169	Depositor
Minimum map value	-1.395	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.269	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, BMA, GAL, NAG, 44E

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	0.43	0/3460	0.61	0/4695
1	C	0.41	0/3527	0.60	0/4790
1	E	0.41	0/3353	0.58	0/4546
2	B	0.47	0/1156	0.62	0/1568
2	D	0.50	0/1031	0.58	0/1397
2	F	0.45	0/970	0.57	0/1313
3	H	0.41	0/1057	0.52	0/1435
3	K	0.41	0/1057	0.52	0/1435
3	M	0.41	0/1047	0.52	0/1421
4	L	0.44	0/845	0.58	0/1141
4	N	0.44	0/845	0.58	0/1141
4	O	0.45	0/845	0.58	0/1141
5	G	0.41	0/159	0.43	0/219
5	I	0.41	0/159	0.43	0/219
5	J	0.40	0/159	0.43	0/219
6	P	0.48	0/1091	0.56	0/1482
7	Q	0.45	0/856	0.64	1/1156 (0.1%)
All	All	0.43	0/21617	0.58	1/29318 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	96	LEU	CA-CB-CG	5.78	128.59	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	3390	0	3345	116	0
1	C	3454	0	3406	133	0
1	E	3288	0	3252	248	0
2	B	1137	0	1116	127	0
2	D	1014	0	993	132	0
2	F	954	0	920	217	0
3	H	1025	0	960	40	0
3	K	1025	0	958	47	0
3	M	1016	0	947	56	0
4	L	825	0	792	11	0
4	N	825	0	792	12	0
4	O	825	0	792	10	0
5	G	153	0	149	2	0
5	I	153	0	149	2	0
5	J	153	0	149	2	0
6	P	1062	0	1024	32	0
7	Q	838	0	817	14	0
8	R	28	0	25	0	0
8	T	28	0	25	0	0
8	U	28	0	25	0	0
8	V	28	0	25	0	0
8	X	28	0	25	0	0
8	Z	28	0	25	0	0
8	a	28	0	25	0	0
8	b	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	i	28	0	25	0	0
9	S	28	0	25	0	0
10	W	50	0	43	0	0
11	Y	39	0	34	0	0
11	c	39	0	34	0	0
12	g	61	0	52	0	0
13	h	24	0	22	0	0
13	n	24	0	22	0	0
14	j	38	0	34	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	k	38	0	34	0	0
15	l	110	0	94	0	0
16	m	96	0	82	0	0
17	A	126	0	117	0	0
17	C	182	0	169	0	0
17	D	14	0	13	1	0
17	E	224	0	208	5	0
17	F	56	0	52	4	0
18	L	11	0	5	0	0
18	N	11	0	5	0	0
18	O	11	0	5	0	0
All	All	22655	0	21911	752	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 17.

All (752) 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:E:36:VAL:HG22	2:F:610:TRP:CE3	1.15	1.64
1:E:497:ALA:HA	2:F:631:TRP:CZ2	1.26	1.62
2:D:619:TYR:CE2	3:H:75:ILE:HA	1.35	1.56
1:E:36:VAL:HG13	2:F:610:TRP:CZ3	1.40	1.54
1:E:36:VAL:HG22	2:F:610:TRP:CD2	1.42	1.52
1:E:36:VAL:CG2	2:F:610:TRP:CE3	1.92	1.52
2:B:545:LEU:CD1	2:F:595:ILE:HD11	1.37	1.50
1:E:36:VAL:HG21	2:F:614:TRP:CZ3	1.48	1.48
2:D:663:LEU:CD2	3:M:73:ASN:HB3	1.24	1.45
2:D:663:LEU:HD21	3:M:73:ASN:CB	1.07	1.45
2:B:540:GLN:NE2	2:F:647:GLU:HG3	1.32	1.43
2:B:556:LEU:CD2	2:F:585:ARG:HH21	1.32	1.43
2:B:556:LEU:HD21	2:F:585:ARG:NH2	1.10	1.40
1:E:221:ALA:HB3	2:F:582:ALA:CB	1.51	1.40
1:E:496:ILE:O	2:F:631:TRP:NE1	1.57	1.37
1:E:497:ALA:CA	2:F:631:TRP:CZ2	2.06	1.37
2:B:545:LEU:HD11	2:F:595:ILE:CD1	1.55	1.36
1:E:221:ALA:CB	2:F:582:ALA:HB1	1.57	1.35
2:B:540:GLN:NE2	2:F:647:GLU:CG	1.87	1.35
1:E:498:PRO:HD2	2:F:631:TRP:CH2	1.62	1.33
1:E:497:ALA:CA	2:F:631:TRP:HZ2	1.37	1.31
1:C:500:LYS:NZ	3:H:30:ASP:OD1	1.61	1.31

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:619:TYR:CD2	3:H:75:ILE:HA	1.67	1.30
1:E:34:LEU:O	2:F:610:TRP:CB	1.81	1.29
2:D:663:LEU:HD22	3:M:30:ASP:CG	1.53	1.28
2:D:518:VAL:N	6:P:113:GLY:O	1.65	1.27
2:D:515:ILE:HG22	6:P:115:ASN:O	1.16	1.27
1:E:35:TRP:HA	2:F:610:TRP:N	1.50	1.26
2:D:664:ASP:OD2	3:M:52(B):PRO:HB3	1.33	1.25
1:A:308:HIS:NE2	1:E:197:ASN:O	1.68	1.25
1:A:499:THR:OG1	3:K:74:SER:HB2	1.36	1.25
2:D:663:LEU:HD23	3:M:30:ASP:OD2	1.36	1.25
1:E:111:LEU:HD21	2:F:571:TRP:CH2	1.73	1.24
2:D:652:GLN:OE1	2:F:538:THR:HG21	1.35	1.23
2:B:545:LEU:CG	2:F:595:ILE:HD11	1.69	1.22
2:B:535:MET:HB3	3:K:19:ARG:CZ	1.68	1.22
1:E:36:VAL:CA	2:F:610:TRP:HE3	1.55	1.20
1:A:166:ARG:CB	1:E:127:VAL:HG12	1.73	1.19
1:A:314:GLY:N	1:E:198:THR:C	1.96	1.19
2:D:619:TYR:CE2	3:H:74:SER:O	1.93	1.19
1:E:36:VAL:CB	2:F:610:TRP:CE3	2.26	1.18
2:D:619:TYR:CE2	3:H:75:ILE:CA	2.24	1.18
1:E:221:ALA:CB	2:F:582:ALA:CB	2.18	1.18
17:F:902:NAG:H83	3:M:5:VAL:HG11	1.24	1.18
1:E:36:VAL:CG1	2:F:610:TRP:CZ3	2.28	1.17
2:D:619:TYR:CZ	3:H:74:SER:O	1.95	1.17
1:E:34:LEU:C	2:F:610:TRP:HB3	1.64	1.16
2:D:619:TYR:OH	3:H:74:SER:O	1.62	1.16
2:D:518:VAL:HG21	6:P:115:ASN:OD1	1.44	1.15
2:D:663:LEU:CD2	3:M:30:ASP:OD2	1.95	1.14
1:E:111:LEU:HD21	2:F:571:TRP:HH2	1.00	1.14
1:A:314:GLY:CA	1:E:198:THR:C	2.15	1.13
2:D:619:TYR:HE2	3:H:75:ILE:CA	1.59	1.13
1:E:36:VAL:CG2	2:F:614:TRP:HZ3	1.60	1.12
1:E:503:ARG:HD2	2:F:607:ALA:CB	1.78	1.12
1:E:221:ALA:HB3	2:F:582:ALA:HB2	1.16	1.11
2:D:663:LEU:CD2	3:M:30:ASP:CG	2.19	1.11
1:E:38:VAL:HG21	2:F:646:ILE:HD13	1.32	1.10
1:E:36:VAL:HG23	2:F:610:TRP:HA	1.18	1.10
2:B:556:LEU:CD2	2:F:585:ARG:NH2	2.00	1.10
2:D:663:LEU:HD21	3:M:73:ASN:HB2	1.21	1.09
1:E:498:PRO:HB3	2:F:610:TRP:CD2	1.87	1.09
2:D:584:GLU:OE1	2:F:579:ARG:NH2	1.84	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:CD1	2:D:607:ALA:O	2.06	1.09
2:B:556:LEU:HD21	2:F:585:ARG:CZ	1.83	1.09
1:E:497:ALA:CB	2:F:631:TRP:CZ2	2.36	1.08
1:E:34:LEU:O	2:F:610:TRP:HB3	0.90	1.08
1:E:36:VAL:CB	2:F:610:TRP:HE3	1.63	1.08
1:C:34:LEU:O	2:D:609:PRO:HA	1.52	1.08
2:D:603:ILE:HG12	2:B:655:LYS:HB3	1.33	1.08
1:E:503:ARG:HE	2:F:606:THR:HA	1.12	1.07
1:E:498:PRO:CD	2:F:631:TRP:HH2	1.68	1.06
1:E:36:VAL:HA	2:F:610:TRP:HE3	1.20	1.04
17:F:902:NAG:C8	3:M:5:VAL:HG11	1.88	1.04
1:A:313:PRO:C	1:E:199:SER:HA	1.78	1.03
1:E:36:VAL:HA	2:F:610:TRP:CE3	1.93	1.03
2:D:663:LEU:CD2	3:M:73:ASN:CB	1.83	1.03
1:E:498:PRO:CD	2:F:631:TRP:CH2	2.41	1.03
2:D:587:LEU:CD1	2:F:583:VAL:HG13	1.87	1.03
1:E:38:VAL:CG2	2:F:646:ILE:HD13	1.89	1.02
1:A:313:PRO:CB	1:E:196:CYS:O	2.06	1.02
1:E:497:ALA:HB2	2:F:631:TRP:CE2	1.95	1.02
1:A:499:THR:OG1	3:K:74:SER:CB	2.08	1.01
2:B:540:GLN:NE2	2:F:647:GLU:HG2	1.73	1.01
1:A:308:HIS:CE1	1:E:197:ASN:HA	1.96	1.01
2:D:587:LEU:HD11	2:F:583:VAL:CG1	1.90	1.01
2:D:587:LEU:HD11	2:F:583:VAL:HG13	1.43	1.00
1:E:494:LEU:HD23	2:F:643:TYR:OH	1.61	0.99
2:D:534:SER:O	2:B:652:GLN:NE2	1.94	0.99
2:F:620:ASN:HD22	3:M:25:SER:HB2	1.26	0.99
1:E:36:VAL:CA	2:F:610:TRP:CE3	2.45	0.98
1:A:166:ARG:HB2	1:E:127:VAL:HG12	1.00	0.98
1:A:308:HIS:HE1	1:E:197:ASN:HA	1.23	0.98
1:E:496:ILE:C	2:F:631:TRP:HE1	1.67	0.97
1:A:313:PRO:C	1:E:199:SER:CA	2.32	0.97
2:D:664:ASP:OD1	3:M:52(B):PRO:CG	2.12	0.97
2:B:624:ASN:CA	3:K:77:PHE:HZ	1.76	0.97
2:B:540:GLN:HE22	2:F:647:GLU:CG	1.64	0.96
2:F:532:ALA:HB1	3:M:19:ARG:NH2	1.78	0.96
2:B:540:GLN:HE22	2:F:647:GLU:HG3	0.83	0.96
1:A:313:PRO:C	1:E:199:SER:N	2.19	0.96
1:E:503:ARG:NE	2:F:606:THR:HA	1.80	0.96
2:D:515:ILE:CG2	6:P:115:ASN:O	2.11	0.96
1:C:498:PRO:HG3	2:D:610:TRP:CD2	2.00	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:TRP:HA	2:F:610:TRP:H	1.05	0.95
2:D:663:LEU:HD22	3:M:73:ASN:HB3	1.47	0.95
1:A:166:ARG:HB2	1:E:127:VAL:CG1	1.96	0.94
1:E:503:ARG:CG	2:F:607:ALA:HB2	1.96	0.94
2:B:545:LEU:CD1	2:F:595:ILE:CD1	2.29	0.93
1:A:308:HIS:CE1	1:E:197:ASN:CA	2.51	0.93
1:E:496:ILE:HG13	2:F:635:ILE:HD12	1.50	0.92
1:C:35:TRP:CD1	2:D:607:ALA:C	2.43	0.92
1:C:35:TRP:HA	2:D:608:VAL:O	1.68	0.92
2:D:515:ILE:HG22	6:P:115:ASN:C	1.90	0.92
1:E:498:PRO:HD2	2:F:631:TRP:HH2	1.00	0.92
1:E:36:VAL:HG13	2:F:610:TRP:CE3	2.05	0.92
1:E:497:ALA:CB	2:F:631:TRP:CE2	2.53	0.92
1:E:502:LYS:HE3	2:F:609:PRO:HG3	1.52	0.92
1:E:503:ARG:CD	2:F:607:ALA:CB	2.48	0.92
1:A:165:MET:SD	1:E:192:ARG:HG3	2.10	0.91
1:A:313:PRO:C	1:E:198:THR:C	2.29	0.91
1:E:36:VAL:HG23	2:F:610:TRP:CA	2.01	0.91
1:A:313:PRO:HB3	1:E:196:CYS:O	1.67	0.91
1:E:36:VAL:CG2	2:F:614:TRP:CZ3	2.42	0.91
2:F:531:GLY:O	3:M:79:TYR:OH	1.89	0.91
2:D:619:TYR:CD2	3:H:75:ILE:HG22	2.06	0.90
1:E:35:TRP:CA	2:F:610:TRP:HB2	2.00	0.90
2:B:535:MET:CB	3:K:19:ARG:CZ	2.49	0.90
1:A:308:HIS:CE1	1:E:197:ASN:O	2.24	0.90
1:E:503:ARG:CD	2:F:607:ALA:HB2	2.01	0.89
1:E:498:PRO:HB3	2:F:610:TRP:CE2	2.07	0.89
1:E:36:VAL:HG21	2:F:614:TRP:CE3	2.08	0.89
1:E:38:VAL:CG2	2:F:646:ILE:CD1	2.49	0.89
2:D:663:LEU:CD2	3:M:73:ASN:HB2	1.81	0.88
1:E:111:LEU:CD2	2:F:571:TRP:CH2	2.56	0.88
1:E:494:LEU:CD2	2:F:643:TYR:OH	2.21	0.88
1:E:35:TRP:C	2:F:610:TRP:HB2	1.93	0.88
2:B:545:LEU:HD11	2:F:595:ILE:CG1	2.04	0.88
1:C:36:VAL:HG12	2:D:608:VAL:HB	1.54	0.88
2:D:619:TYR:CE2	3:H:75:ILE:CG2	2.55	0.88
1:E:221:ALA:HB1	2:F:582:ALA:HB1	1.55	0.88
1:E:111:LEU:CD2	2:F:571:TRP:HH2	1.86	0.88
2:B:545:LEU:HD11	2:F:595:ILE:HD11	0.88	0.88
1:C:35:TRP:HD1	2:D:607:ALA:O	1.53	0.87
1:A:166:ARG:HG3	1:E:127:VAL:CG1	2.04	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:619:TYR:CD2	3:H:75:ILE:CA	2.52	0.86
2:D:587:LEU:CD1	2:F:583:VAL:CG1	2.52	0.85
1:E:36:VAL:CG1	2:F:610:TRP:CE3	2.54	0.85
1:E:38:VAL:HG22	2:F:646:ILE:CD1	2.06	0.85
1:E:503:ARG:HE	2:F:606:THR:CA	1.87	0.85
1:A:308:HIS:CE1	1:E:197:ASN:C	2.50	0.85
2:D:664:ASP:OD1	3:M:52(B):PRO:HG2	1.76	0.85
1:E:36:VAL:CG2	2:F:610:TRP:CD2	2.36	0.85
1:A:166:ARG:CG	1:E:127:VAL:CG1	2.55	0.84
2:D:664:ASP:CG	3:M:52(B):PRO:HB3	1.97	0.84
1:E:35:TRP:CA	2:F:610:TRP:H	1.89	0.84
2:D:619:TYR:HE2	3:H:75:ILE:HA	1.02	0.84
2:D:517:ALA:HA	6:P:114:ARG:HB3	1.60	0.83
1:E:503:ARG:HD2	2:F:607:ALA:HB3	1.58	0.83
2:D:603:ILE:CG1	2:B:655:LYS:HB3	2.08	0.83
2:B:535:MET:CB	3:K:19:ARG:NE	2.41	0.83
1:E:49:THR:OG1	2:B:562:GLN:OE1	1.96	0.83
2:B:535:MET:SD	3:K:19:ARG:HD2	2.19	0.83
1:A:166:ARG:CG	1:E:127:VAL:HG12	2.07	0.82
1:A:39:TYR:HD1	2:B:603:ILE:HG12	1.44	0.82
2:B:535:MET:SD	3:K:19:ARG:CD	2.68	0.82
1:E:36:VAL:CG1	2:F:610:TRP:HZ3	1.80	0.82
2:F:532:ALA:CB	3:M:19:ARG:NH2	2.42	0.82
1:E:35:TRP:HA	2:F:610:TRP:CB	2.11	0.81
2:B:540:GLN:CD	2:F:647:GLU:HG3	2.01	0.80
1:E:497:ALA:HB2	2:F:631:TRP:NE1	1.96	0.80
1:E:313:PRO:HB2	1:C:123:THR:HG23	1.63	0.80
1:A:314:GLY:HA2	1:E:198:THR:C	2.00	0.80
3:H:82:MET:HB3	3:H:82(C):LEU:HD21	1.64	0.80
1:E:38:VAL:HG22	2:F:646:ILE:HD11	1.64	0.80
3:K:82:MET:HB3	3:K:82(C):LEU:HD21	1.64	0.79
2:B:620:ASN:HD21	3:K:25:SER:HB2	1.47	0.79
1:E:313:PRO:HB2	1:C:123:THR:CG2	2.12	0.79
2:B:545:LEU:CG	2:F:595:ILE:CD1	2.55	0.79
3:M:82:MET:HB3	3:M:82(C):LEU:HD21	1.64	0.79
1:A:39:TYR:CD1	2:B:603:ILE:HG12	2.17	0.78
1:A:200:VAL:HG22	1:C:313:PRO:HB2	1.65	0.78
1:C:496:ILE:HD11	2:D:642:ILE:HD13	1.64	0.78
1:A:499:THR:CB	3:K:74:SER:HB2	2.13	0.78
2:D:619:TYR:CE2	3:H:75:ILE:HG22	2.18	0.78
1:A:499:THR:OG1	3:K:74:SER:CA	2.32	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:GLN:CD	2:F:647:GLU:CG	2.51	0.77
1:E:503:ARG:HG2	2:F:607:ALA:HB2	1.64	0.77
1:C:35:TRP:HD1	2:D:607:ALA:C	1.82	0.77
1:E:86:LEU:HD22	2:F:523:LEU:O	1.84	0.76
1:E:313:PRO:CB	1:C:123:THR:CG2	2.62	0.76
2:F:532:ALA:CA	3:M:19:ARG:NH2	2.48	0.76
1:E:35:TRP:HA	2:F:610:TRP:CA	2.15	0.76
1:A:499:THR:OG1	3:K:74:SER:O	2.04	0.76
1:E:35:TRP:CA	2:F:610:TRP:CB	2.64	0.75
2:B:535:MET:HB3	3:K:19:ARG:NE	1.99	0.75
2:B:535:MET:HB3	3:K:19:ARG:NH2	2.00	0.75
1:E:498:PRO:HD2	2:F:631:TRP:CZ2	2.22	0.75
1:C:502:LYS:HE3	2:D:607:ALA:HB1	1.67	0.75
2:B:624:ASN:CA	3:K:77:PHE:CZ	2.66	0.75
1:E:503:ARG:NE	2:F:606:THR:CA	2.49	0.75
2:D:538:THR:HG21	2:B:647:GLU:HB3	1.66	0.75
1:C:82:GLN:NE2	6:P:116:TYR:OH	2.19	0.74
1:A:166:ARG:CB	1:E:127:VAL:CG1	2.61	0.74
2:D:520:LEU:O	6:P:113:GLY:N	2.20	0.74
2:D:663:LEU:HD22	3:M:30:ASP:CB	2.18	0.74
1:E:496:ILE:O	2:F:631:TRP:CE2	2.38	0.73
1:A:308:HIS:NE2	1:E:197:ASN:C	2.41	0.73
2:F:619:TYR:HE2	3:M:76:ASN:HB2	1.53	0.73
1:E:495:GLY:HA3	2:F:632:GLU:OE2	1.90	0.72
1:E:498:PRO:HD3	2:F:610:TRP:CH2	2.24	0.72
1:E:36:VAL:HG22	2:F:610:TRP:CG	2.20	0.72
1:E:34:LEU:C	2:F:610:TRP:CB	2.45	0.71
2:B:556:LEU:HD11	2:F:585:ARG:NE	2.05	0.71
2:D:587:LEU:HD11	2:F:583:VAL:HG11	1.72	0.71
1:E:288:LEU:HD11	1:E:452:LEU:CD1	2.20	0.71
1:E:313:PRO:CB	1:C:123:THR:HG23	2.20	0.71
2:F:620:ASN:ND2	3:M:25:SER:HB2	2.04	0.71
2:B:540:GLN:CD	2:F:647:GLU:OE2	2.30	0.70
2:B:545:LEU:CD2	2:F:595:ILE:HD11	2.20	0.70
2:F:532:ALA:HB1	3:M:19:ARG:HH22	1.54	0.70
2:D:515:ILE:HG21	6:P:115:ASN:HB2	1.73	0.69
2:D:619:TYR:HE2	3:H:74:SER:O	1.58	0.69
1:E:498:PRO:HB3	2:F:610:TRP:CG	2.26	0.69
1:C:31:ALA:HA	3:H:27:PHE:HA	1.73	0.69
1:A:39:TYR:CE1	2:B:603:ILE:HG23	2.28	0.69
2:B:545:LEU:HD21	2:F:595:ILE:CD1	2.22	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:515:ILE:CG2	6:P:115:ASN:C	2.60	0.68
2:D:620:ASN:ND2	3:H:75:ILE:O	2.27	0.68
1:C:37:THR:HG23	2:D:604:CYS:O	1.94	0.68
2:B:549:VAL:HG23	2:F:588:LYS:HG3	1.76	0.68
1:E:288:LEU:HD11	1:E:452:LEU:HD11	1.76	0.67
2:D:619:TYR:HE2	3:H:74:SER:C	1.96	0.67
2:D:603:ILE:HD11	2:B:655:LYS:O	1.94	0.67
2:B:556:LEU:CD1	2:F:585:ARG:NE	2.58	0.67
2:D:619:TYR:CE2	3:H:74:SER:C	2.68	0.67
2:D:619:TYR:CD2	3:H:75:ILE:CG2	2.78	0.67
2:B:545:LEU:HG	2:F:595:ILE:HD11	1.75	0.66
1:E:494:LEU:CD2	2:F:643:TYR:CZ	2.78	0.66
2:D:587:LEU:HD13	2:F:583:VAL:HG13	1.74	0.66
1:E:36:VAL:CG2	2:F:610:TRP:HA	2.11	0.65
2:F:620:ASN:ND2	3:M:24:ALA:O	2.27	0.65
2:F:532:ALA:C	3:M:19:ARG:HH22	2.00	0.65
1:E:42:VAL:HG21	2:F:628:TRP:CZ3	2.32	0.64
1:C:34:LEU:O	2:D:609:PRO:CA	2.38	0.64
1:A:166:ARG:HG3	1:E:127:VAL:HG13	1.79	0.64
2:F:531:GLY:C	3:M:79:TYR:OH	2.36	0.64
7:Q:61:ARG:HH22	7:Q:79:GLU:HB2	1.62	0.64
1:A:499:THR:HG1	3:K:74:SER:C	2.00	0.64
2:D:619:TYR:HE2	3:H:75:ILE:N	1.96	0.64
2:B:553:ASN:OD1	2:F:588:LYS:NZ	2.29	0.64
2:F:532:ALA:CA	3:M:19:ARG:HH22	2.10	0.64
1:A:499:THR:OG1	3:K:74:SER:C	2.37	0.63
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.81	0.63
1:E:44:VAL:HG21	2:F:632:GLU:HG3	1.80	0.63
1:E:497:ALA:CA	2:F:631:TRP:CE2	2.74	0.63
3:K:2:VAL:HA	3:K:26:GLY:HA3	1.81	0.63
1:E:75:VAL:HB	2:F:551:GLN:HG2	1.81	0.63
2:D:664:ASP:CG	3:M:52(B):PRO:CB	2.65	0.63
1:E:34:LEU:O	2:F:610:TRP:CA	2.47	0.63
1:E:498:PRO:CD	2:F:631:TRP:CZ2	2.77	0.63
1:E:496:ILE:HG21	2:F:642:ILE:HG21	1.81	0.62
1:E:497:ALA:HB1	2:F:631:TRP:CZ2	2.33	0.62
1:C:498:PRO:HB3	2:D:610:TRP:HB2	1.79	0.62
3:M:2:VAL:HA	3:M:26:GLY:HA3	1.80	0.62
1:C:502:LYS:HA	2:D:606:THR:O	1.99	0.62
2:B:619:TYR:CE2	3:K:75:ILE:C	2.72	0.62
1:A:36:VAL:HG23	2:B:608:VAL:O	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:CA	2:D:608:VAL:O	2.44	0.62
1:A:308:HIS:CD2	1:E:197:ASN:O	2.50	0.62
1:C:501:ALA:HB1	2:B:662:GLU:CG	2.30	0.62
1:E:496:ILE:O	2:F:635:ILE:HD13	2.00	0.62
1:A:37:THR:HG23	2:B:604:CYS:O	2.00	0.62
1:A:88:ASN:HB2	2:B:527:GLY:HA3	1.80	0.62
1:A:313:PRO:CA	1:E:196:CYS:O	2.48	0.61
1:E:161:ILE:HG22	1:E:170:GLN:HG3	1.81	0.61
1:C:498:PRO:HG3	2:D:610:TRP:CE2	2.36	0.61
1:A:277:PHE:O	1:A:456:ARG:NH1	2.34	0.61
2:B:535:MET:CG	3:K:19:ARG:NE	2.64	0.61
1:A:165:MET:HG2	1:E:126:CYS:SG	2.40	0.61
2:D:663:LEU:HD21	3:M:73:ASN:HB3	0.63	0.61
2:D:538:THR:HB	2:B:647:GLU:OE1	2.00	0.60
2:B:535:MET:CB	3:K:19:ARG:NH2	2.61	0.60
3:M:50:ARG:NH2	3:M:58:ASP:OD2	2.34	0.60
2:D:518:VAL:CG2	6:P:115:ASN:OD1	2.35	0.60
1:A:357:LYS:HB3	1:A:465:THR:HA	1.83	0.60
1:E:503:ARG:NE	2:F:606:THR:C	2.55	0.60
1:C:498:PRO:HD3	2:D:610:TRP:CZ3	2.36	0.60
2:B:556:LEU:CD2	2:F:585:ARG:CZ	2.65	0.60
2:B:619:TYR:CE2	3:K:75:ILE:O	2.55	0.60
1:C:500:LYS:HB2	2:B:663:LEU:HD12	1.84	0.60
1:E:35:TRP:NE1	2:F:609:PRO:CG	2.41	0.60
1:A:54:CYS:HB3	2:B:571:TRP:CZ3	2.37	0.60
1:A:313:PRO:HB2	1:E:199:SER:O	2.02	0.60
1:C:31:ALA:HB2	3:H:27:PHE:N	2.16	0.60
2:D:664:ASP:OD1	3:M:52(B):PRO:CB	2.50	0.60
1:E:498:PRO:HD3	2:F:610:TRP:CZ2	2.36	0.59
1:E:503:ARG:NE	2:F:607:ALA:N	2.39	0.59
3:K:50:ARG:NH2	3:K:58:ASP:OD2	2.34	0.59
1:A:126:CYS:O	1:C:165:MET:O	2.20	0.59
1:A:373:MET:HG2	1:A:384:TYR:HB3	1.85	0.59
1:E:494:LEU:HD23	2:F:643:TYR:CZ	2.36	0.59
2:F:617:LYS:HD3	2:F:622:ILE:HD11	1.84	0.59
1:A:335:GLY:O	1:A:339:ASN:ND2	2.35	0.59
1:E:49:THR:CB	2:B:562:GLN:OE1	2.50	0.59
2:B:620:ASN:ND2	3:K:25:SER:HB2	2.16	0.59
3:H:50:ARG:NH2	3:H:58:ASP:OD2	2.34	0.59
1:C:498:PRO:HG3	2:D:610:TRP:CE3	2.36	0.59
1:C:346:VAL:HA	1:C:349:LEU:HB2	1.84	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:29:PHE:O	6:P:72:ARG:NH2	2.34	0.59
2:D:663:LEU:HB3	3:M:30:ASP:HB3	1.84	0.59
1:E:344:GLN:NE2	17:E:609:NAG:O7	2.35	0.58
2:D:619:TYR:CE2	3:H:75:ILE:HG23	2.38	0.58
1:E:35:TRP:HA	2:F:610:TRP:HB2	1.76	0.58
1:C:502:LYS:H	2:B:662:GLU:CG	2.17	0.58
1:E:290:LYS:O	1:E:290:LYS:HG3	2.03	0.58
2:F:654:GLU:O	2:F:658:GLN:NE2	2.34	0.58
1:A:98:ASN:ND2	1:A:486:TYR:O	2.36	0.58
1:A:314:GLY:HA3	1:E:198:THR:C	2.18	0.58
1:C:31:ALA:HB2	3:H:26:GLY:C	2.24	0.58
2:D:664:ASP:OD2	3:M:52(B):PRO:CB	2.28	0.58
2:B:549:VAL:HG23	2:F:588:LYS:CD	2.34	0.58
2:B:545:LEU:CD2	2:F:595:ILE:CD1	2.80	0.58
2:F:532:ALA:HA	3:M:19:ARG:NH2	2.17	0.58
2:B:546:SER:O	2:B:550:GLN:NE2	2.37	0.58
2:B:549:VAL:HG23	2:F:588:LYS:CG	2.33	0.58
1:C:122:LEU:HB2	1:C:201:ILE:HG23	1.86	0.57
1:C:498:PRO:CG	2:D:610:TRP:CD2	2.83	0.57
2:B:619:TYR:HE2	3:K:75:ILE:O	1.87	0.57
1:E:35:TRP:CA	2:F:610:TRP:N	2.45	0.57
1:A:209:SER:OG	1:A:211:GLU:OE1	2.22	0.57
1:A:300:ASN:HD21	1:A:327:ARG:H	1.52	0.57
1:E:36:VAL:HG13	2:F:610:TRP:HZ3	0.84	0.57
1:E:494:LEU:HD21	2:F:643:TYR:CZ	2.40	0.57
1:C:305:LYS:HD3	1:C:318:TYR:HB3	1.87	0.57
1:E:496:ILE:H	2:F:635:ILE:CD1	2.18	0.57
2:D:594:GLY:HA2	2:D:599:SER:HB3	1.87	0.57
2:F:532:ALA:HA	3:M:19:ARG:HH21	1.70	0.57
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.38	0.56
2:B:546:SER:OG	2:B:550:GLN:NE2	2.38	0.56
1:A:393[B]:SER:OG	1:A:394:THR:N	2.39	0.56
1:E:71:THR:HG23	2:F:557:ARG:HA	1.87	0.56
1:A:239:CYS:SG	1:A:240:THR:N	2.79	0.56
1:E:35:TRP:NE1	2:F:609:PRO:HG3	2.21	0.56
1:E:122:LEU:HD13	1:E:125:LEU:HD12	1.87	0.56
1:C:501:ALA:HB3	2:D:605:THR:HG21	1.88	0.56
2:B:556:LEU:CD2	2:F:585:ARG:NE	2.69	0.56
2:F:532:ALA:CB	3:M:19:ARG:HH22	2.12	0.56
1:A:298:ARG:NH2	1:A:441:GLY:O	2.39	0.56
1:E:44:VAL:HG11	2:F:632:GLU:HG3	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ASN:CB	2:D:527:GLY:O	2.54	0.56
1:A:36:VAL:HB	2:B:606:THR:OG1	2.04	0.56
1:C:272:ILE:HG12	1:C:286:VAL:HA	1.88	0.56
1:E:35:TRP:HE1	2:F:609:PRO:CG	1.88	0.55
1:E:304:ARG:HG2	1:E:440:LYS:HD3	1.88	0.55
1:E:160:ASN:HA	1:E:171:LYS:H	1.71	0.55
1:E:288:LEU:N	1:E:450:THR:O	2.40	0.55
1:C:74:CYS:SG	1:C:75:VAL:N	2.80	0.55
1:C:350:LYS:NZ	1:C:357:LYS:O	2.29	0.55
7:Q:25:SER:OG	7:Q:27:GLU:O	2.24	0.55
1:E:111:LEU:CD2	2:F:571:TRP:CZ3	2.90	0.55
4:O:16:GLY:O	4:O:77:GLY:HA2	2.07	0.55
1:A:129:LEU:HD12	1:A:157:CYS:HB3	1.89	0.55
2:D:619:TYR:CE2	3:H:75:ILE:CB	2.90	0.55
1:A:165:MET:SD	1:E:192:ARG:CG	2.91	0.54
2:D:603:ILE:HG12	2:B:655:LYS:CB	2.23	0.54
1:A:314:GLY:HA3	1:E:199:SER:CA	2.37	0.54
1:C:476:ARG:O	1:C:480:ARG:N	2.38	0.54
1:C:501:ALA:HB1	2:B:662:GLU:HB3	1.88	0.54
4:N:16:GLY:O	4:N:77:GLY:HA2	2.07	0.54
1:E:386:ASN:HB3	1:E:389:GLN:HE22	1.71	0.54
1:E:503:ARG:NE	2:F:607:ALA:H	2.05	0.54
2:D:541:ALA:O	2:B:591:GLN:NE2	2.39	0.54
4:L:16:GLY:O	4:L:77:GLY:HA2	2.07	0.54
1:C:32:GLU:HG3	1:C:500:LYS:HG2	1.90	0.54
1:C:427:TRP:HZ2	1:C:475:MET:H	1.56	0.54
1:E:269:GLU:O	1:E:289:ASN:HB3	2.07	0.54
1:C:457:ASP:HB3	1:C:467:ILE:HB	1.89	0.54
2:D:639:THR:HA	2:D:642:ILE:HD12	1.88	0.54
2:F:532:ALA:O	3:M:19:ARG:NH2	2.40	0.54
1:E:246:GLN:OE1	2:F:548:ILE:HG21	2.09	0.53
1:C:56:SER:OG	1:C:57:ASP:N	2.41	0.53
2:B:551:GLN:O	2:B:555:LEU:N	2.37	0.53
3:K:68:THR:HB	3:K:81:GLU:HB3	1.90	0.53
1:E:276:ASN:H	1:E:282:LYS:HG3	1.72	0.53
2:D:580:VAL:HG11	2:F:576:LEU:HD12	1.90	0.53
2:B:535:MET:CG	3:K:19:ARG:HD2	2.37	0.53
3:M:68:THR:HB	3:M:81:GLU:HB3	1.91	0.53
1:A:122:LEU:HB3	1:A:125:LEU:HD12	1.91	0.53
1:A:199:SER:HA	1:C:314:GLY:HA3	1.90	0.53
1:E:36:VAL:CG2	2:F:610:TRP:CG	2.85	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:CG2	2:F:610:TRP:HE3	1.69	0.53
1:E:36:VAL:N	2:F:610:TRP:HB2	2.23	0.53
1:C:31:ALA:HA	3:H:27:PHE:CA	2.38	0.53
2:B:556:LEU:CD2	2:F:585:ARG:HE	2.21	0.53
7:Q:32:SER:HB3	7:Q:91:SER:HB2	1.90	0.53
1:E:496:ILE:HD11	2:F:635:ILE:HB	1.90	0.53
1:A:304:ARG:HA	1:A:321:GLY:H	1.74	0.53
1:E:308:HIS:NE2	1:E:312:GLY:O	2.42	0.53
1:C:456:ARG:HG2	1:C:468:PHE:HE1	1.74	0.53
2:B:545:LEU:HG	2:F:595:ILE:CD1	2.35	0.53
1:E:159:PHE:O	1:E:172:GLU:N	2.39	0.53
1:C:364:SER:HB2	1:C:470:PRO:HG2	1.91	0.52
1:A:88:ASN:HB2	2:B:527:GLY:CA	2.40	0.52
1:E:288:LEU:HD11	1:E:452:LEU:HD12	1.90	0.52
2:B:563:GLN:HB3	2:B:566:LEU:HG	1.91	0.52
3:H:68:THR:HB	3:H:81:GLU:HB3	1.91	0.52
1:C:224:ALA:HB2	2:D:522:PHE:HE2	1.74	0.52
1:A:393[A]:SER:OG	1:A:394:THR:N	2.39	0.52
1:E:290:LYS:O	1:E:290:LYS:CG	2.56	0.52
1:C:117:LYS:O	1:C:121:LYS:NZ	2.40	0.52
1:C:299:PRO:O	1:C:442:GLN:NE2	2.42	0.52
1:A:313:PRO:HB2	1:E:196:CYS:O	2.01	0.52
1:C:369:PRO:HA	1:C:372:VAL:HB	1.91	0.52
1:E:344:GLN:NE2	17:E:609:NAG:O3	2.43	0.52
1:C:498:PRO:CG	2:D:610:TRP:CE3	2.92	0.52
1:A:114:GLN:OE1	2:B:570:VAL:HG23	2.09	0.52
1:C:502:LYS:HG3	2:D:607:ALA:HA	1.92	0.52
2:B:549:VAL:HG23	2:F:588:LYS:HE2	1.92	0.52
2:D:603:ILE:CD1	2:B:655:LYS:HB3	2.39	0.51
1:E:221:ALA:HB2	2:F:582:ALA:HB1	1.77	0.51
1:C:498:PRO:CB	2:D:610:TRP:HB2	2.39	0.51
1:A:274:SER:HB2	1:A:284:ILE:HA	1.92	0.51
1:E:38:VAL:CG2	2:F:646:ILE:HD11	2.30	0.51
2:D:535:MET:CE	2:B:653:GLN:OE1	2.58	0.51
6:P:69:LEU:HB3	6:P:82:GLU:HB3	1.90	0.51
1:E:38:VAL:HA	1:E:496:ILE:HG22	1.93	0.51
2:D:664:ASP:OD1	3:M:52(B):PRO:HG3	2.05	0.51
4:N:81:GLU:CD	4:N:81:GLU:H	2.14	0.51
6:P:40:ALA:HB3	6:P:43:LYS:HB2	1.91	0.51
1:A:71:THR:OG1	2:B:571:TRP:NE1	2.43	0.51
1:C:387:SER:HB2	1:C:390:LEU:HD12	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:PRO:HB3	2:D:610:TRP:CE3	2.46	0.51
3:K:22:CYS:HB3	3:K:78:LEU:HB3	1.93	0.51
1:A:91:GLU:OE2	1:A:487:LYS:NZ	2.43	0.51
1:E:244:THR:OG1	2:F:523:LEU:HD12	2.11	0.51
3:H:22:CYS:HB3	3:H:78:LEU:HB3	1.93	0.51
1:C:34:LEU:HB2	2:D:610:TRP:HB3	1.92	0.51
2:B:535:MET:HG3	3:K:19:ARG:HD2	1.92	0.51
1:E:161:ILE:HB	1:E:170:GLN:HA	1.93	0.50
2:D:516:GLY:O	6:P:114:ARG:HB2	2.10	0.50
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.43	0.50
4:N:61:ARG:NH2	4:N:82:ASP:OD1	2.43	0.50
1:A:122:LEU:HD12	1:A:201:ILE:HG22	1.93	0.50
2:B:556:LEU:HD22	2:F:585:ARG:HE	1.76	0.50
2:F:629:MET:HB3	2:F:633:ARG:HH12	1.77	0.50
1:C:276:ASN:HD22	1:C:279:ASP:HB2	1.76	0.50
1:C:382:PHE:HD2	1:C:424:VAL:HG21	1.75	0.50
3:M:22:CYS:HB3	3:M:78:LEU:HB3	1.93	0.50
1:A:37:THR:OG1	2:B:605:THR:HG22	2.12	0.50
1:E:385:CYS:HA	1:E:418:CYS:HA	1.94	0.50
2:D:650:GLN:O	2:D:654:GLU:N	2.42	0.50
1:E:42:VAL:HG21	2:F:628:TRP:CE3	2.46	0.50
1:E:134:LEU:HD23	1:E:326:ILE:HD11	1.93	0.50
1:A:179:LEU:O	1:A:421:LYS:NZ	2.35	0.50
1:E:42:VAL:CG2	2:F:628:TRP:CZ3	2.95	0.50
1:C:36:VAL:CG1	2:D:608:VAL:HB	2.35	0.50
1:C:500:LYS:HD2	2:B:663:LEU:CD1	2.41	0.50
2:B:535:MET:CG	3:K:19:ARG:CD	2.89	0.50
2:B:540:GLN:OE1	2:F:647:GLU:OE2	2.30	0.50
1:A:65:VAL:HG22	1:A:72:HIS:HB3	1.93	0.50
1:A:314:GLY:HA3	1:E:199:SER:HA	1.93	0.50
1:E:39:TYR:OH	2:F:623:TRP:HH2	1.94	0.50
3:M:29:PHE:O	3:M:71:ARG:NH2	2.45	0.50
2:D:652:GLN:OE1	2:F:538:THR:CG2	2.31	0.49
3:K:29:PHE:O	3:K:71:ARG:NH2	2.45	0.49
1:E:236:THR:OG1	1:E:237:GLY:N	2.45	0.49
4:L:81:GLU:H	4:L:81:GLU:CD	2.14	0.49
1:A:129:LEU:HD13	1:A:159:PHE:HB3	1.94	0.49
1:E:50:THR:OG1	1:E:51:THR:N	2.44	0.49
1:E:289:ASN:O	1:E:290:LYS:HG2	2.12	0.49
1:E:457:ASP:O	1:E:469:ARG:NH2	2.44	0.49
1:E:502:LYS:HE3	2:F:609:PRO:CG	2.33	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:GLY:O	6:P:114:ARG:CB	2.61	0.49
3:H:29:PHE:O	3:H:71:ARG:NH2	2.45	0.49
2:D:663:LEU:HD22	3:M:30:ASP:OD1	2.07	0.49
1:E:228:CYS:SG	1:E:229:ASN:N	2.85	0.49
1:E:105:HIS:CD2	1:E:476:ARG:HE	2.30	0.49
4:O:81:GLU:CD	4:O:81:GLU:H	2.14	0.49
7:Q:61:ARG:NH1	7:Q:77:ARG:O	2.45	0.49
1:C:490:LYS:NZ	2:D:585:ARG:HE	2.10	0.49
3:M:55:TRP:CE3	3:M:71:ARG:HD3	2.48	0.49
7:Q:63:VAL:HG23	7:Q:74:ARG:HB3	1.94	0.49
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.94	0.49
1:E:246:GLN:OE1	2:F:548:ILE:CG2	2.61	0.49
1:C:501:ALA:CB	2:B:662:GLU:HB3	2.42	0.49
2:D:579:ARG:HH21	2:B:584:GLU:CD	2.16	0.49
7:Q:90:GLN:HE21	7:Q:97:THR:H	1.59	0.49
1:E:117:LYS:O	1:E:121:LYS:NZ	2.46	0.49
1:C:69:TRP:HZ3	1:C:108:ILE:HD12	1.77	0.49
1:C:421:LYS:HE3	1:C:424:VAL:HA	1.95	0.49
2:B:535:MET:SD	3:K:19:ARG:HD3	2.50	0.49
1:A:129:LEU:HD23	1:A:192:ARG:HA	1.94	0.49
1:C:501:ALA:HB1	2:B:662:GLU:HG2	1.94	0.49
1:E:498:PRO:CB	2:F:610:TRP:CD2	2.78	0.48
1:C:333:ILE:HG23	1:C:414:ILE:HB	1.95	0.48
1:E:67:ASN:HB3	1:E:70:ALA:HB2	1.95	0.48
3:H:55:TRP:CE3	3:H:71:ARG:HD3	2.48	0.48
7:Q:6:GLN:HE21	7:Q:101:GLY:H	1.60	0.48
1:E:36:VAL:HG23	2:F:610:TRP:CB	2.44	0.48
1:E:44:VAL:HG23	1:E:492:GLU:HB2	1.94	0.48
1:E:255:VAL:HG22	1:E:475:MET:HE2	1.95	0.48
1:E:498:PRO:HD3	2:F:631:TRP:CH2	2.42	0.48
1:E:42:VAL:CG2	2:F:628:TRP:CE3	2.96	0.48
1:E:298:ARG:N	1:E:443:ILE:O	2.46	0.48
2:B:539:VAL:O	2:B:541:ALA:N	2.46	0.48
6:P:51:ILE:HD11	6:P:70:VAL:HB	1.96	0.48
6:P:52:SER:HB3	6:P:57:HIS:HB3	1.96	0.48
1:A:258:GLN:NE2	1:A:372:VAL:O	2.41	0.48
1:C:134:LEU:N	1:C:154:ILE:O	2.46	0.48
4:N:103:LYS:HZ1	4:N:105:THR:HG23	1.79	0.48
1:E:92:ASN:HA	1:E:238:PRO:HA	1.96	0.48
1:E:246:GLN:HE22	2:F:548:ILE:HB	1.79	0.48
1:E:288:LEU:HD12	1:E:449:ILE:HG22	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:CG	1:E:127:VAL:HG13	2.37	0.47
1:C:70:ALA:HB1	1:C:73:ALA:H	1.79	0.47
1:A:70:ALA:HB2	1:A:213:ILE:HD13	1.96	0.47
1:E:303:THR:OG1	1:E:322:GLU:N	2.47	0.47
1:C:119:CYS:SG	1:C:205:CYS:N	2.87	0.47
1:C:301:ASN:HD22	1:C:323:ILE:HD12	1.79	0.47
2:D:521:GLY:HA2	6:P:112:SER:HA	1.97	0.47
3:K:55:TRP:CE3	3:K:71:ARG:HD3	2.48	0.47
1:E:221:ALA:HB2	2:F:582:ALA:CB	2.33	0.47
1:E:427:TRP:CD1	1:E:475:MET:HG2	2.50	0.47
1:A:386:ASN:HB3	1:A:417:PRO:HG2	1.95	0.47
1:C:491:ILE:O	2:D:585:ARG:NH2	2.48	0.47
1:A:286:VAL:HB	1:A:452:LEU:HB3	1.96	0.47
2:D:619:TYR:HD2	3:H:75:ILE:CA	2.18	0.47
2:B:623:TRP:CE3	3:K:75:ILE:HG12	2.50	0.47
1:A:45:TRP:CZ2	2:B:629:MET:SD	3.08	0.47
1:A:228:CYS:SG	1:A:229:ASN:N	2.87	0.47
1:E:286:VAL:CG1	1:E:452:LEU:HB2	2.44	0.47
1:C:502:LYS:H	2:B:662:GLU:HG3	1.79	0.47
2:B:569:THR:HG23	2:B:572:GLY:H	1.78	0.47
2:B:623:TRP:HB3	3:K:77:PHE:CE1	2.50	0.47
4:L:22:THR:HG22	4:L:72:SER:HB3	1.96	0.47
1:C:88:ASN:HB2	2:D:527:GLY:O	2.14	0.47
1:C:304:ARG:HG3	1:C:305:LYS:H	1.79	0.47
17:F:902:NAG:C8	3:M:5:VAL:CG1	2.78	0.47
4:N:22:THR:HG22	4:N:72:SER:HB3	1.96	0.47
2:F:528:SER:HB2	2:F:533:ALA:HB2	1.97	0.47
1:E:103:GLN:NE2	1:E:107:ASP:OD2	2.41	0.47
1:C:500:LYS:HD2	2:B:663:LEU:HD11	1.96	0.47
1:A:364:SER:HB2	1:A:470:PRO:HD2	1.97	0.46
1:E:220:PRO:HG2	1:E:223:PHE:HD2	1.80	0.46
2:B:540:GLN:CD	2:F:647:GLU:CD	2.73	0.46
1:E:57:ASP:HA	1:E:77:THR:HA	1.96	0.46
2:B:619:TYR:HE2	3:K:75:ILE:C	2.19	0.46
4:O:22:THR:HG22	4:O:72:SER:HB3	1.96	0.46
1:A:165:MET:SD	1:E:192:ARG:NH1	2.88	0.46
1:E:42:VAL:N	1:E:493:PRO:O	2.47	0.46
1:E:335:GLY:O	1:E:339:ASN:ND2	2.48	0.46
3:K:51:ILE:HD13	3:K:71:ARG:HD2	1.97	0.46
3:M:51:ILE:HD13	3:M:71:ARG:HD2	1.97	0.46
1:A:312:GLY:HA3	1:A:315:ARG:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:HA	1:A:469:ARG:HD2	1.98	0.46
1:E:54:CYS:HB2	1:E:215:ILE:HD11	1.97	0.46
1:E:313:PRO:HG2	1:C:123:THR:HG22	1.98	0.46
1:A:298:ARG:NH1	1:A:302:ASN:HD22	2.14	0.46
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.48	0.46
2:D:519:PHE:CE2	6:P:108:LEU:HD21	2.51	0.46
1:E:269:GLU:HA	17:E:609:NAG:H82	1.96	0.46
2:B:540:GLN:HB2	2:B:543:LEU:HD23	1.96	0.46
3:K:50:ARG:HD3	3:K:100(J):GLU:OE1	2.16	0.46
1:A:36:VAL:O	2:B:606:THR:OG1	2.26	0.46
1:C:360:VAL:HG21	1:C:467:ILE:HD13	1.97	0.46
7:Q:46:LEU:HD21	7:Q:49:PHE:HB3	1.96	0.46
1:A:75:VAL:HG23	2:B:575:GLN:NE2	2.31	0.46
3:M:50:ARG:HD3	3:M:100(J):GLU:OE1	2.16	0.46
1:C:36:VAL:N	2:D:608:VAL:O	2.47	0.46
2:D:603:ILE:HD11	2:B:655:LYS:C	2.36	0.46
1:C:70:ALA:HB2	1:C:213:ILE:HD11	1.98	0.46
3:H:72:LEU:HB3	3:H:75:ILE:HD11	1.98	0.46
6:P:134:SER:OG	6:P:135:SER:N	2.49	0.46
1:E:269:GLU:HG2	17:E:609:NAG:H82	1.98	0.45
1:E:313:PRO:HG2	1:C:123:THR:CG2	2.46	0.45
2:B:619:TYR:HE2	3:K:76:ASN:HB2	1.81	0.45
3:M:72:LEU:HB3	3:M:75:ILE:HD11	1.98	0.45
1:A:45:TRP:CE2	2:B:629:MET:SD	3.10	0.45
1:E:283:ILE:HG12	1:E:455:ILE:HD11	1.98	0.45
3:H:51:ILE:HD13	3:H:71:ARG:HD2	1.97	0.45
1:E:494:LEU:HD21	2:F:643:TYR:CE1	2.51	0.45
1:C:89:VAL:HG22	2:D:526:ALA:O	2.15	0.45
1:C:502:LYS:H	2:B:662:GLU:HG2	1.81	0.45
2:B:559:ILE:HA	2:B:562:GLN:HB2	1.99	0.45
2:B:545:LEU:HD11	2:F:595:ILE:HG13	1.94	0.45
1:E:44:VAL:HG12	2:F:629:MET:HA	1.97	0.45
1:E:503:ARG:CZ	2:F:606:THR:HA	2.45	0.45
1:C:163:THR:OG1	1:C:309:ILE:O	2.29	0.45
3:K:72:LEU:HB3	3:K:75:ILE:HD11	1.98	0.45
3:K:101:GLN:H	3:K:101:GLN:HG2	1.62	0.45
6:P:3:GLN:HB3	6:P:25:SER:HB2	1.98	0.45
6:P:22:CYS:HB3	6:P:79:LEU:HB3	1.98	0.45
7:Q:27(B):LEU:HD21	7:Q:90:GLN:HB2	1.99	0.45
1:C:364:SER:OG	1:C:365:SER:N	2.49	0.45
1:C:499:THR:OG1	1:C:500:LYS:N	2.48	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:ARG:NH2	4:O:82:ASP:OD1	2.43	0.45
1:C:501:ALA:HB1	2:B:662:GLU:CB	2.47	0.45
2:F:533:ALA:HB3	2:F:628:TRP:HE1	1.82	0.45
3:H:50:ARG:HD3	3:H:100(J):GLU:OE1	2.16	0.45
4:N:24:ARG:HG2	4:N:70:ARG:HB3	1.99	0.45
5:I:129:TRP:CE2	5:I:133:VAL:HG21	2.52	0.45
1:C:180:ASP:HA	1:C:194:ILE:HG12	1.99	0.45
2:B:545:LEU:HD21	2:F:595:ILE:HD13	1.97	0.45
2:B:556:LEU:CD1	2:F:585:ARG:HE	2.28	0.45
3:M:34:MET:HB3	3:M:78:LEU:HD22	1.99	0.45
5:J:129:TRP:CE2	5:J:133:VAL:HG21	2.52	0.45
1:A:313:PRO:HA	1:E:196:CYS:O	2.15	0.44
6:P:47:TRP:HH2	6:P:59:VAL:HG12	1.82	0.44
1:A:499:THR:CG2	3:K:74:SER:HB2	2.47	0.44
1:C:34:LEU:O	2:D:610:TRP:N	2.47	0.44
2:D:580:VAL:HG21	2:F:576:LEU:HD11	1.99	0.44
1:E:275:ALA:HB3	1:E:282:LYS:HG3	1.99	0.44
1:E:496:ILE:HG13	2:F:635:ILE:CD1	2.34	0.44
1:A:50:THR:OG1	1:A:51:THR:N	2.51	0.44
1:C:249:HIS:ND1	1:C:486:TYR:OH	2.42	0.44
1:C:490:LYS:HE3	2:D:585:ARG:CZ	2.48	0.44
2:D:601:LYS:HD3	2:B:655:LYS:HZ2	1.82	0.44
3:H:34:MET:HB3	3:H:78:LEU:HD22	1.99	0.44
1:E:36:VAL:HG21	2:F:614:TRP:HZ3	0.78	0.44
1:E:360:VAL:HG22	1:E:467:ILE:HB	1.99	0.44
5:G:129:TRP:CE2	5:G:133:VAL:HG21	2.52	0.44
1:E:34:LEU:HD12	2:F:612:THR:HG22	2.00	0.44
1:C:374:HIS:N	1:C:385:CYS:O	2.46	0.44
1:E:203:GLN:HA	1:E:435:TYR:HB3	2.00	0.44
1:C:89:VAL:HG23	2:D:527:GLY:HA3	2.00	0.44
4:N:89:SER:HB2	4:N:98:PHE:CE1	2.52	0.44
4:L:89:SER:HB2	4:L:98:PHE:CE1	2.52	0.44
3:K:34:MET:HB3	3:K:78:LEU:HD22	1.99	0.44
1:A:123:THR:HG22	1:C:166:ARG:HD2	2.00	0.44
1:C:160:ASN:HB3	1:C:169:VAL:HB	2.00	0.44
4:O:89:SER:HB2	4:O:98:PHE:CE1	2.53	0.44
1:E:374:HIS:HB3	1:E:385:CYS:HB2	2.00	0.43
1:C:35:TRP:NE1	2:D:607:ALA:O	2.46	0.43
2:B:552:GLN:HA	2:B:555:LEU:HB3	2.01	0.43
7:Q:36:TYR:HB3	7:Q:46:LEU:HD12	2.00	0.43
4:L:24:ARG:HG2	4:L:70:ARG:HB3	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASN:O	1:C:332:ASN:N	2.49	0.43
1:C:352:GLN:HG2	1:C:353:PHE:HD1	1.83	0.43
1:E:67:ASN:HA	1:E:209:SER:HB3	2.00	0.43
1:C:246:GLN:HG3	6:P:111:TRP:CE3	2.53	0.43
2:B:644:THR:OG1	6:P:110:ARG:NH1	2.51	0.43
4:N:24:ARG:HG2	4:N:70:ARG:CB	2.49	0.43
6:P:69:LEU:N	6:P:82:GLU:O	2.48	0.43
1:A:54:CYS:HB3	2:B:571:TRP:CH2	2.52	0.43
1:C:227:LYS:HG3	1:C:485:LYS:HB3	2.00	0.43
4:L:103:LYS:HZ1	4:L:105:THR:HG23	1.82	0.43
4:O:24:ARG:HG2	4:O:70:ARG:HB3	1.99	0.43
1:A:303:THR:OG1	1:A:322:GLU:O	2.26	0.43
1:E:499:THR:HG23	1:E:501:ALA:H	1.83	0.43
1:C:219:ALA:HB2	1:C:225:ILE:HG13	2.01	0.43
2:D:619:TYR:CD2	3:H:75:ILE:CB	3.02	0.43
4:L:103:LYS:NZ	4:L:105:THR:HG23	2.33	0.43
3:M:51:ILE:HG13	3:M:57:VAL:HG22	2.01	0.43
4:O:24:ARG:HG2	4:O:70:ARG:CB	2.49	0.43
1:C:199:SER:OG	1:C:200:VAL:N	2.51	0.43
2:B:619:TYR:OH	3:K:74:SER:O	2.33	0.43
3:K:51:ILE:HG13	3:K:57:VAL:HG22	2.01	0.43
1:A:259:LEU:HB2	1:A:374:HIS:HE1	1.84	0.43
1:E:313:PRO:CG	1:C:123:THR:CG2	2.97	0.43
1:C:88:ASN:HB3	2:D:527:GLY:O	2.17	0.43
1:C:229:ASN:ND2	1:C:241:ASN:O	2.39	0.43
3:H:51:ILE:HG13	3:H:57:VAL:HG22	2.01	0.43
1:E:346:VAL:HA	1:E:349:LEU:HB2	2.00	0.43
1:C:62:ASP:OD1	1:C:62:ASP:N	2.51	0.43
1:C:66:HIS:HB2	1:C:208:VAL:HA	2.00	0.43
1:C:337:LYS:O	1:C:341:THR:OG1	2.32	0.43
6:P:2:VAL:HG21	6:P:26:ASP:H	1.84	0.43
1:C:194:ILE:HD12	1:C:195:SER:HB3	2.01	0.43
1:C:246:GLN:HG3	6:P:111:TRP:CD2	2.54	0.43
1:C:439:ILE:H	1:C:439:ILE:HG13	1.58	0.43
2:D:523:LEU:HA	2:D:540:GLN:HE21	1.84	0.43
4:L:24:ARG:HG2	4:L:70:ARG:CB	2.49	0.43
4:N:103:LYS:NZ	4:N:105:THR:HG23	2.33	0.43
1:C:385:CYS:HA	1:C:418:CYS:HA	2.01	0.42
1:A:260:LEU:HB2	1:A:451:GLY:HA3	2.01	0.42
1:E:36:VAL:CG2	2:F:614:TRP:CE3	2.91	0.42
4:O:103:LYS:NZ	4:O:105:THR:HG23	2.33	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:TRP:N	2:F:610:TRP:CB	2.82	0.42
1:C:182:VAL:HG23	1:C:194:ILE:HG22	2.01	0.42
1:C:474:ASP:OD2	1:C:476:ARG:NE	2.45	0.42
2:D:649:SER:OG	2:D:650:GLN:N	2.52	0.42
1:E:286:VAL:HG13	1:E:286:VAL:O	2.20	0.42
1:C:304:ARG:HE	1:C:305:LYS:HD2	1.84	0.42
1:E:297:THR:HG23	1:E:299:PRO:HD3	2.01	0.42
1:A:124:PRO:HB2	1:A:309:ILE:HD11	2.01	0.42
1:A:153:GLU:OE1	1:A:419:ARG:NH2	2.52	0.42
1:E:496:ILE:HD12	2:F:635:ILE:HG21	2.02	0.42
1:C:70:ALA:O	1:C:74:CYS:N	2.53	0.42
2:F:617:LYS:HA	17:F:901:NAG:H82	2.00	0.42
3:K:40:PRO:HG2	3:K:43:LYS:HD2	2.02	0.42
1:E:44:VAL:HG11	2:F:632:GLU:CG	2.50	0.42
1:E:301:ASN:HB2	1:E:442:GLN:HE21	1.85	0.42
1:E:469:ARG:HA	1:E:470:PRO:HD3	1.89	0.42
1:C:320:THR:HG22	1:C:438:PRO:HD2	2.02	0.42
2:B:540:GLN:HE21	2:F:647:GLU:HG2	1.74	0.42
6:P:38:ARG:NH2	6:P:46:GLU:OE1	2.42	0.42
1:A:40:TYR:HB2	2:B:593:LEU:HD11	2.02	0.41
1:A:122:LEU:HD11	1:A:203:GLN:HB2	2.02	0.41
1:A:333:ILE:O	1:A:414:ILE:N	2.48	0.41
1:E:163:THR:HA	1:E:308:HIS:HD2	1.85	0.41
6:P:39:GLN:OE1	6:P:95:ARG:NH1	2.43	0.41
1:A:38:VAL:HG22	1:A:496:ILE:HG22	2.02	0.41
1:A:39:TYR:CE1	2:B:603:ILE:CG2	3.02	0.41
1:A:86:LEU:HD11	2:B:526:ALA:HB3	2.02	0.41
1:C:278:THR:O	1:C:456:ARG:NH1	2.53	0.41
1:C:280:ASN:OD1	1:C:456:ARG:NH1	2.53	0.41
2:D:660:LEU:HD21	3:M:72:LEU:HD13	2.02	0.41
1:C:155:LYS:HG3	1:C:191:TYR:HE2	1.86	0.41
1:C:211:GLU:HA	1:C:212:PRO:HD3	1.82	0.41
2:B:549:VAL:HG23	2:F:588:LYS:CE	2.49	0.41
2:F:619:TYR:CE2	3:M:76:ASN:HB2	2.43	0.41
3:H:40:PRO:HG2	3:H:43:LYS:HD2	2.02	0.41
5:G:129:TRP:CZ2	5:G:133:VAL:HG21	2.55	0.41
5:I:129:TRP:CZ2	5:I:133:VAL:HG21	2.55	0.41
3:M:40:PRO:HG2	3:M:43:LYS:HD2	2.02	0.41
5:J:129:TRP:CZ2	5:J:133:VAL:HG21	2.55	0.41
6:P:6:GLU:HB2	6:P:129:THR:HG23	2.03	0.41
1:A:292:VAL:O	1:A:449:ILE:N	2.47	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:GLN:O	2:B:594:GLY:N	2.53	0.41
2:F:528:SER:HB3	2:F:532:ALA:HB3	2.02	0.41
7:Q:13:VAL:N	7:Q:105:ASP:O	2.41	0.41
1:E:239:CYS:SG	1:E:240:THR:N	2.93	0.41
1:C:335:GLY:O	1:C:339:ASN:ND2	2.54	0.41
1:C:129:LEU:HD22	1:C:157:CYS:HB3	2.02	0.41
1:C:490:LYS:HZ1	2:D:585:ARG:HE	1.69	0.41
4:L:55:PRO:HG2	4:L:58:VAL:HG21	2.03	0.41
4:L:89:SER:HB2	4:L:98:PHE:CD1	2.56	0.41
4:O:89:SER:HB2	4:O:98:PHE:CD1	2.56	0.41
7:Q:27(B):LEU:HG	7:Q:92:LYS:HE2	2.03	0.41
2:D:625:ASN:OD1	17:D:901:NAG:N2	2.54	0.41
1:C:86:LEU:HD22	2:D:523:LEU:O	2.21	0.40
2:D:576:LEU:HD21	2:B:576:LEU:HD21	2.02	0.40
4:O:55:PRO:HG2	4:O:58:VAL:HG21	2.03	0.40
1:A:156:ASN:HA	1:A:175:LEU:HD23	2.01	0.40
1:E:285:ILE:HD13	1:E:285:ILE:HA	1.77	0.40
1:C:120:VAL:HG22	1:C:315:ARG:HD2	2.02	0.40
1:C:240:THR:OG1	1:C:241:ASN:N	2.54	0.40
4:N:89:SER:HB2	4:N:98:PHE:CD1	2.56	0.40
1:A:314:GLY:HA3	1:E:199:SER:HB3	2.03	0.40
1:C:36:VAL:O	2:D:606:THR:OG1	2.31	0.40
7:Q:49:PHE:CD2	7:Q:50:GLU:HG2	2.56	0.40
1:A:45:TRP:CZ3	2:B:523:LEU:HD22	2.57	0.40
1:A:134:LEU:HD21	1:A:156:ASN:HD22	1.86	0.40
1:A:163:THR:HG22	1:A:169:VAL:HG12	2.03	0.40
2:D:601:LYS:HG2	2:B:655:LYS:HZ1	1.87	0.40
4:N:44:PRO:O	4:N:45:ILE:HD13	2.22	0.40
1:E:199:SER:OG	1:E:431:GLY:O	2.31	0.40
17:E:621:NAG:H81	2:F:528:SER:OG	2.21	0.40
1:C:270:VAL:HG22	1:C:289:ASN:H	1.87	0.40
7:Q:58:VAL:HG13	7:Q:62:PHE:HD2	1.87	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	419/465 (90%)	370 (88%)	49 (12%)	0	100	100
1	C	430/465 (92%)	371 (86%)	59 (14%)	0	100	100
1	E	405/465 (87%)	357 (88%)	48 (12%)	0	100	100
2	B	141/153 (92%)	129 (92%)	12 (8%)	0	100	100
2	D	125/153 (82%)	113 (90%)	12 (10%)	0	100	100
2	F	115/153 (75%)	100 (87%)	15 (13%)	0	100	100
3	H	128/129 (99%)	125 (98%)	3 (2%)	0	100	100
3	K	128/129 (99%)	125 (98%)	3 (2%)	0	100	100
3	M	128/129 (99%)	125 (98%)	3 (2%)	0	100	100
4	L	109/108 (101%)	107 (98%)	2 (2%)	0	100	100
4	N	109/108 (101%)	107 (98%)	2 (2%)	0	100	100
4	O	109/108 (101%)	107 (98%)	2 (2%)	0	100	100
5	G	15/17 (88%)	15 (100%)	0	0	100	100
5	I	15/17 (88%)	15 (100%)	0	0	100	100
5	J	15/17 (88%)	15 (100%)	0	0	100	100
6	P	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
7	Q	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
All	All	2630/2859 (92%)	2395 (91%)	235 (9%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/413 (94%)	379 (98%)	7 (2%)	54	71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	392/413 (95%)	388 (99%)	4 (1%)	73	82
1	E	374/413 (91%)	368 (98%)	6 (2%)	58	74
2	B	122/130 (94%)	120 (98%)	2 (2%)	58	74
2	D	108/130 (83%)	108 (100%)	0	100	100
2	F	102/130 (78%)	99 (97%)	3 (3%)	37	57
3	H	106/105 (101%)	103 (97%)	3 (3%)	38	58
3	K	106/105 (101%)	103 (97%)	3 (3%)	38	58
3	M	104/105 (99%)	101 (97%)	3 (3%)	37	57
4	L	89/87 (102%)	87 (98%)	2 (2%)	47	65
4	N	89/87 (102%)	87 (98%)	2 (2%)	47	65
4	O	89/87 (102%)	87 (98%)	2 (2%)	47	65
5	G	16/16 (100%)	16 (100%)	0	100	100
5	I	16/16 (100%)	16 (100%)	0	100	100
5	J	16/16 (100%)	16 (100%)	0	100	100
6	P	115/115 (100%)	115 (100%)	0	100	100
7	Q	96/96 (100%)	96 (100%)	0	100	100
All	All	2326/2464 (94%)	2289 (98%)	37 (2%)	58	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	276	ASN
1	A	304	ARG
1	A	393[A]	SER
1	A	393[B]	SER
1	A	396	ASN
1	A	425	ASN
1	E	276	ASN
1	E	289	ASN
1	E	305	LYS
1	E	356	ASN
1	E	386	ASN
1	E	425	ASN
1	C	171	LYS
1	C	192	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	305	LYS
1	C	357	LYS
2	B	616	ASN
2	B	625	ASN
2	F	551	GLN
2	F	557	ARG
2	F	625	ASN
3	H	50	ARG
3	H	72	LEU
3	H	105	ARG
4	L	97	VAL
4	L	105	THR
3	K	50	ARG
3	K	72	LEU
3	K	105	ARG
4	N	97	VAL
4	N	105	THR
3	M	50	ARG
3	M	72	LEU
3	M	105	ARG
4	O	97	VAL
4	O	105	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	216	HIS
1	A	300	ASN
1	A	339	ASN
1	A	396	ASN
1	A	425	ASN
1	E	105	HIS
1	E	339	ASN
1	E	344	GLN
1	E	386	ASN
1	E	422	GLN
1	E	425	ASN
1	E	442	GLN
1	C	82	GLN
1	C	287	GLN
1	C	300	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	339	ASN
2	D	590	GLN
2	D	651	ASN
2	B	550	GLN
2	B	616	ASN
2	B	620	ASN
2	F	540	GLN
2	F	620	ASN
3	H	31	ASN
3	K	31	ASN
3	M	31	ASN
7	Q	6	GLN
7	Q	27(D)	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 ⓘ

68 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	$\# Z  > 2$
8	NAG	R	1	8,1	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
8	NAG	R	2	8	14,14,15	0.34	0	17,19,21	0.44	0
9	NAG	S	1	9,1	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
9	NAG	S	2	9	14,14,15	0.54	0	17,19,21	1.07	1 (5%)
8	NAG	T	1	8,1	14,14,15	0.26	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	T	2	8	14,14,15	0.33	0	17,19,21	0.45	0
8	NAG	U	1	8,1	14,14,15	0.42	0	17,19,21	0.64	0
8	NAG	U	2	8	14,14,15	0.46	0	17,19,21	0.46	0
8	NAG	V	1	8,1	14,14,15	0.26	0	17,19,21	1.07	1 (5%)
8	NAG	V	2	8	14,14,15	0.42	0	17,19,21	0.60	0
10	NAG	W	1	10,1	14,14,15	0.37	0	17,19,21	0.48	0
10	NAG	W	2	10	14,14,15	0.24	0	17,19,21	0.58	0
10	BMA	W	3	10	11,11,12	0.78	0	15,15,17	0.94	0
10	MAN	W	4	10	11,11,12	0.85	1 (9%)	15,15,17	1.48	2 (13%)
8	NAG	X	1	8,1	14,14,15	0.44	0	17,19,21	0.63	0
8	NAG	X	2	8	14,14,15	0.25	0	17,19,21	0.59	0
11	NAG	Y	1	11,1	14,14,15	0.31	0	17,19,21	0.56	0
11	NAG	Y	2	11	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
11	BMA	Y	3	11	11,11,12	0.68	0	15,15,17	0.77	0
8	NAG	Z	1	8,1	14,14,15	0.49	0	17,19,21	1.08	1 (5%)
8	NAG	Z	2	8	14,14,15	0.21	0	17,19,21	0.76	1 (5%)
8	NAG	a	1	8,1	14,14,15	0.62	0	17,19,21	0.98	1 (5%)
8	NAG	a	2	8	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
8	NAG	b	1	8,1	14,14,15	0.48	0	17,19,21	0.64	0
8	NAG	b	2	8	14,14,15	0.39	0	17,19,21	0.47	0
11	NAG	c	1	11,1	14,14,15	0.37	0	17,19,21	0.59	0
11	NAG	c	2	11	14,14,15	0.37	0	17,19,21	0.78	0
11	BMA	c	3	11	11,11,12	0.67	0	15,15,17	0.92	0
8	NAG	d	1	8,1	14,14,15	0.20	0	17,19,21	0.60	0
8	NAG	d	2	8	14,14,15	0.23	0	17,19,21	0.59	0
8	NAG	e	1	8,1	14,14,15	0.34	0	17,19,21	0.64	0
8	NAG	e	2	8	14,14,15	0.24	0	17,19,21	0.59	0
8	NAG	f	1	8,1	14,14,15	0.58	0	17,19,21	1.13	2 (11%)
8	NAG	f	2	8	14,14,15	0.44	0	17,19,21	0.63	1 (5%)
12	NAG	g	1	12,1	14,14,15	0.49	0	17,19,21	0.65	0
12	NAG	g	2	12	14,14,15	0.20	0	17,19,21	0.65	0
12	BMA	g	3	12	11,11,12	0.67	0	15,15,17	1.11	1 (6%)
12	MAN	g	4	12	11,11,12	1.09	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	g	5	12	11,11,12	0.83	1 (9%)	15,15,17	1.30	2 (13%)
13	NAG	h	1	13,1	14,14,15	0.46	0	17,19,21	0.60	0
13	FUC	h	2	13	10,10,11	0.87	1 (10%)	14,14,16	1.17	1 (7%)
8	NAG	i	1	8,1	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
8	NAG	i	2	8	14,14,15	0.49	0	17,19,21	1.00	1 (5%)
14	NAG	j	1	2,14	14,14,15	0.40	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	NAG	j	2	14	14,14,15	0.62	1 (7%)	17,19,21	0.72	0
14	FUC	j	3	14	10,10,11	0.75	0	14,14,16	1.02	0
14	NAG	k	1	2,14	14,14,15	0.74	1 (7%)	17,19,21	1.23	1 (5%)
14	NAG	k	2	14	14,14,15	0.20	0	17,19,21	0.45	0
14	FUC	k	3	14	10,10,11	1.00	1 (10%)	14,14,16	0.89	1 (7%)
15	NAG	l	1	2,15	14,14,15	0.64	1 (7%)	17,19,21	0.84	0
15	NAG	l	2	15	14,14,15	0.47	0	17,19,21	1.10	1 (5%)
15	BMA	l	3	15	11,11,12	1.04	0	15,15,17	1.57	3 (20%)
15	MAN	l	4	15	11,11,12	0.96	1 (9%)	15,15,17	1.74	2 (13%)
15	NAG	l	5	15	14,14,15	0.21	0	17,19,21	0.77	1 (5%)
15	GAL	l	6	15	11,11,12	0.65	0	15,15,17	1.02	0
15	NAG	l	7	15	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
15	MAN	l	8	15	11,11,12	0.93	0	15,15,17	0.98	1 (6%)
15	FUC	l	9	15	10,10,11	0.97	1 (10%)	14,14,16	0.86	0
16	NAG	m	1	2,16	14,14,15	0.54	0	17,19,21	0.51	0
16	NAG	m	2	16	14,14,15	0.33	0	17,19,21	0.68	0
16	BMA	m	3	16	11,11,12	0.88	0	15,15,17	0.86	0
16	MAN	m	4	16	11,11,12	0.86	0	15,15,17	1.37	2 (13%)
16	NAG	m	5	16	14,14,15	0.23	0	17,19,21	0.73	1 (5%)
16	GAL	m	6	16	11,11,12	0.84	0	15,15,17	1.12	1 (6%)
16	MAN	m	7	16	11,11,12	1.01	1 (9%)	15,15,17	1.38	2 (13%)
16	FUC	m	8	16	10,10,11	0.65	0	14,14,16	0.70	0
13	NAG	n	1	2,13	14,14,15	0.81	1 (7%)	17,19,21	2.42	4 (23%)
13	FUC	n	2	13	10,10,11	1.38	2 (20%)	14,14,16	1.56	3 (21%)

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
8	NAG	R	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
9	NAG	S	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	S	2	9	-	3/6/23/26	0/1/1/1
8	NAG	T	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	2/6/23/26	0/1/1/1

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	U	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	U	2	8	-	2/6/23/26	0/1/1/1
8	NAG	V	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
10	NAG	W	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	1/2/19/22	0/1/1/1
10	MAN	W	4	10	-	2/2/19/22	0/1/1/1
8	NAG	X	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
11	NAG	Y	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	1/2/19/22	0/1/1/1
8	NAG	Z	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
11	NAG	c	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	c	2	11	-	2/6/23/26	0/1/1/1
11	BMA	c	3	11	-	1/2/19/22	0/1/1/1
8	NAG	d	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	NAG	e	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	e	2	8	-	4/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
12	NAG	g	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	g	2	12	-	3/6/23/26	0/1/1/1
12	BMA	g	3	12	-	2/2/19/22	0/1/1/1
12	MAN	g	4	12	-	2/2/19/22	0/1/1/1
12	MAN	g	5	12	-	1/2/19/22	0/1/1/1
13	NAG	h	1	13,1	-	4/6/23/26	0/1/1/1
13	FUC	h	2	13	-	-	0/1/1/1
8	NAG	i	1	8,1	-	4/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	i	2	8	-	4/6/23/26	0/1/1/1
14	NAG	j	1	2,14	-	1/6/23/26	0/1/1/1
14	NAG	j	2	14	-	2/6/23/26	0/1/1/1
14	FUC	j	3	14	-	-	0/1/1/1
14	NAG	k	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	k	2	14	-	4/6/23/26	0/1/1/1
14	FUC	k	3	14	-	-	0/1/1/1
15	NAG	l	1	2,15	-	0/6/23/26	0/1/1/1
15	NAG	l	2	15	-	2/6/23/26	0/1/1/1
15	BMA	l	3	15	-	2/2/19/22	0/1/1/1
15	MAN	l	4	15	-	0/2/19/22	0/1/1/1
15	NAG	l	5	15	-	0/6/23/26	0/1/1/1
15	GAL	l	6	15	-	2/2/19/22	0/1/1/1
15	NAG	l	7	15	-	4/6/23/26	0/1/1/1
15	MAN	l	8	15	-	2/2/19/22	0/1/1/1
15	FUC	l	9	15	-	-	0/1/1/1
16	NAG	m	1	2,16	-	0/6/23/26	0/1/1/1
16	NAG	m	2	16	-	2/6/23/26	0/1/1/1
16	BMA	m	3	16	-	0/2/19/22	0/1/1/1
16	MAN	m	4	16	-	0/2/19/22	0/1/1/1
16	NAG	m	5	16	-	1/6/23/26	0/1/1/1
16	GAL	m	6	16	-	0/2/19/22	0/1/1/1
16	MAN	m	7	16	-	2/2/19/22	0/1/1/1
16	FUC	m	8	16	-	-	0/1/1/1
13	NAG	n	1	2,13	-	6/6/23/26	0/1/1/1
13	FUC	n	2	13	-	-	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	g	4	MAN	C1-C2	3.34	1.60	1.52
16	m	7	MAN	C1-C2	2.72	1.58	1.52
14	k	3	FUC	C1-C2	2.62	1.58	1.52
13	n	2	FUC	C2-C3	2.61	1.56	1.52
14	k	1	NAG	O5-C1	-2.48	1.39	1.43
12	g	5	MAN	C1-C2	2.36	1.57	1.52
13	n	1	NAG	C1-C2	2.30	1.55	1.52
15	l	1	NAG	O5-C1	-2.25	1.39	1.43
15	l	9	FUC	O5-C1	-2.22	1.40	1.43
14	j	2	NAG	O5-C1	-2.15	1.40	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	n	2	FUC	C4-C3	2.10	1.57	1.52
13	h	2	FUC	O5-C5	2.10	1.47	1.43
10	W	4	MAN	C1-C2	2.09	1.57	1.52
15	l	4	MAN	C2-C3	-2.01	1.49	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	n	1	NAG	C2-N2-C7	8.45	134.23	122.90
15	l	4	MAN	C1-O5-C5	4.85	118.68	112.19
10	W	4	MAN	C1-O5-C5	4.49	118.20	112.19
12	g	4	MAN	C1-O5-C5	3.83	117.32	112.19
14	k	1	NAG	C1-O5-C5	3.79	117.27	112.19
12	g	5	MAN	C1-O5-C5	3.77	117.24	112.19
15	l	4	MAN	O2-C2-C3	-3.61	102.67	110.15
16	m	7	MAN	C1-O5-C5	3.56	116.96	112.19
13	n	1	NAG	C1-C2-N2	3.49	115.93	110.43
8	Z	1	NAG	C2-N2-C7	3.46	127.54	122.90
8	R	1	NAG	C2-N2-C7	3.43	127.50	122.90
8	V	1	NAG	C2-N2-C7	3.33	127.36	122.90
8	i	2	NAG	C2-N2-C7	3.31	127.33	122.90
16	m	4	MAN	C1-O5-C5	3.30	116.60	112.19
15	l	2	NAG	C2-N2-C7	3.27	127.28	122.90
9	S	2	NAG	C2-N2-C7	3.25	127.25	122.90
15	l	7	NAG	C2-N2-C7	3.24	127.25	122.90
13	h	2	FUC	C1-O5-C5	3.21	120.53	112.97
8	a	1	NAG	C2-N2-C7	3.17	127.15	122.90
15	l	3	BMA	C1-C2-C3	3.16	114.25	109.64
8	a	2	NAG	C2-N2-C7	3.11	127.07	122.90
15	l	3	BMA	C1-O5-C5	3.10	116.34	112.19
8	i	1	NAG	C2-N2-C7	3.09	127.04	122.90
8	f	1	NAG	C2-N2-C7	3.05	126.98	122.90
13	n	2	FUC	C1-O5-C5	3.02	120.09	112.97
13	n	2	FUC	O5-C5-C4	2.98	114.92	109.55
16	m	4	MAN	O2-C2-C3	-2.98	103.98	110.15
12	g	3	BMA	C1-O5-C5	2.73	115.85	112.19
11	Y	2	NAG	C1-O5-C5	2.72	115.83	112.19
8	f	1	NAG	C1-O5-C5	2.60	115.67	112.19
12	g	5	MAN	O2-C2-C3	-2.54	104.88	110.15
16	m	5	NAG	C1-O5-C5	2.49	115.52	112.19
8	Z	2	NAG	C1-O5-C5	2.47	115.50	112.19
13	n	1	NAG	C1-O5-C5	-2.43	108.93	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	4	MAN	O2-C2-C3	-2.43	105.13	110.15
15	l	5	NAG	C1-O5-C5	2.42	115.44	112.19
13	n	2	FUC	C2-C3-C4	2.41	115.10	110.86
12	g	4	MAN	C1-C2-C3	2.40	113.14	109.64
9	S	1	NAG	C1-O5-C5	2.33	115.31	112.19
16	m	7	MAN	O2-C2-C3	-2.31	105.37	110.15
13	n	1	NAG	C8-C7-N2	2.25	119.84	116.12
10	W	4	MAN	O2-C2-C3	-2.24	105.51	110.15
15	l	8	MAN	C1-O5-C5	2.19	115.12	112.19
15	l	3	BMA	O2-C2-C3	-2.17	105.67	110.15
14	k	3	FUC	O2-C2-C1	2.16	114.16	109.22
8	f	2	NAG	C1-O5-C5	2.14	115.05	112.19
16	m	6	GAL	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	f	2	NAG	C4-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
12	g	1	NAG	O5-C5-C6-O6
15	l	8	MAN	O5-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	i	2	NAG	C4-C5-C6-O6
8	X	2	NAG	O5-C5-C6-O6
10	W	4	MAN	O5-C5-C6-O6
12	g	4	MAN	O5-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
14	j	2	NAG	O5-C5-C6-O6
16	m	7	MAN	O5-C5-C6-O6
12	g	1	NAG	C4-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
8	e	2	NAG	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
16	m	2	NAG	C4-C5-C6-O6
8	i	2	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	b	2	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
16	m	2	NAG	O5-C5-C6-O6
15	l	8	MAN	C4-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
14	j	2	NAG	C4-C5-C6-O6
16	m	7	MAN	C4-C5-C6-O6
11	Y	1	NAG	O5-C5-C6-O6
8	i	1	NAG	C4-C5-C6-O6
14	k	2	NAG	O5-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	X	2	NAG	C4-C5-C6-O6
11	Y	1	NAG	C4-C5-C6-O6
12	g	4	MAN	C4-C5-C6-O6
8	Z	2	NAG	C8-C7-N2-C2
8	Z	2	NAG	O7-C7-N2-C2
8	e	1	NAG	C8-C7-N2-C2
8	e	1	NAG	O7-C7-N2-C2
8	e	2	NAG	C8-C7-N2-C2
8	e	2	NAG	O7-C7-N2-C2
12	g	2	NAG	C8-C7-N2-C2
12	g	2	NAG	O7-C7-N2-C2
13	h	1	NAG	C8-C7-N2-C2
13	h	1	NAG	O7-C7-N2-C2
13	n	1	NAG	C8-C7-N2-C2
13	n	1	NAG	O7-C7-N2-C2
14	k	2	NAG	C8-C7-N2-C2
14	k	2	NAG	O7-C7-N2-C2
8	e	1	NAG	O5-C5-C6-O6
8	V	1	NAG	O5-C5-C6-O6
13	n	1	NAG	C4-C5-C6-O6
12	g	5	MAN	O5-C5-C6-O6
10	W	4	MAN	C4-C5-C6-O6
10	W	2	NAG	C4-C5-C6-O6
11	c	2	NAG	O5-C5-C6-O6
15	l	3	BMA	O5-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
10	W	2	NAG	O5-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	U	1	NAG	O5-C5-C6-O6
13	n	1	NAG	O5-C5-C6-O6
12	g	3	BMA	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
8	V	2	NAG	O5-C5-C6-O6
10	W	3	BMA	O5-C5-C6-O6
15	l	7	NAG	C4-C5-C6-O6
9	S	2	NAG	O5-C5-C6-O6
8	e	1	NAG	C4-C5-C6-O6
13	h	1	NAG	C4-C5-C6-O6
11	Y	3	BMA	O5-C5-C6-O6
16	m	5	NAG	O5-C5-C6-O6
11	c	3	BMA	O5-C5-C6-O6
15	l	3	BMA	C4-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
14	k	2	NAG	C4-C5-C6-O6
14	j	1	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
8	R	1	NAG	C1-C2-N2-C7
8	a	1	NAG	C1-C2-N2-C7
8	f	1	NAG	C1-C2-N2-C7
8	i	2	NAG	C1-C2-N2-C7
15	l	2	NAG	C1-C2-N2-C7
9	S	1	NAG	C4-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
15	l	7	NAG	O5-C5-C6-O6
15	l	6	GAL	C4-C5-C6-O6
8	R	1	NAG	C3-C2-N2-C7
9	S	2	NAG	C3-C2-N2-C7
13	h	1	NAG	O5-C5-C6-O6
12	g	3	BMA	O5-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
11	c	2	NAG	C4-C5-C6-O6
8	V	1	NAG	C1-C2-N2-C7
8	Z	1	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
8	i	1	NAG	C1-C2-N2-C7
9	S	2	NAG	C1-C2-N2-C7
13	n	1	NAG	C1-C2-N2-C7
15	l	7	NAG	C1-C2-N2-C7
15	l	6	GAL	O5-C5-C6-O6
8	X	1	NAG	C4-C5-C6-O6

*Continued on next page...*

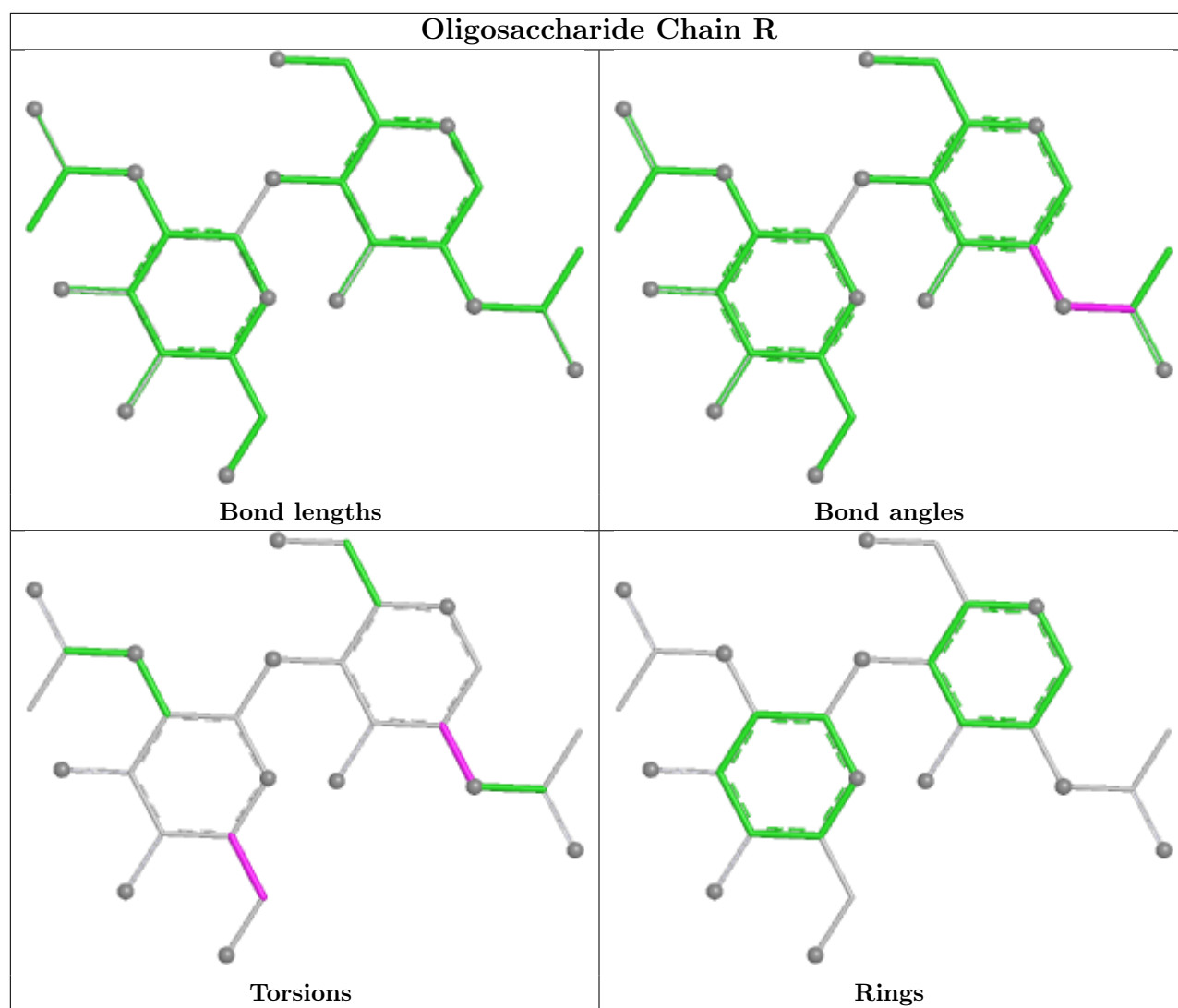
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	V	1	NAG	C3-C2-N2-C7
8	Z	1	NAG	C3-C2-N2-C7
8	a	1	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
8	i	1	NAG	C3-C2-N2-C7
8	i	2	NAG	C3-C2-N2-C7
13	n	1	NAG	C3-C2-N2-C7
15	l	2	NAG	C3-C2-N2-C7
15	l	7	NAG	C3-C2-N2-C7
12	g	2	NAG	C4-C5-C6-O6

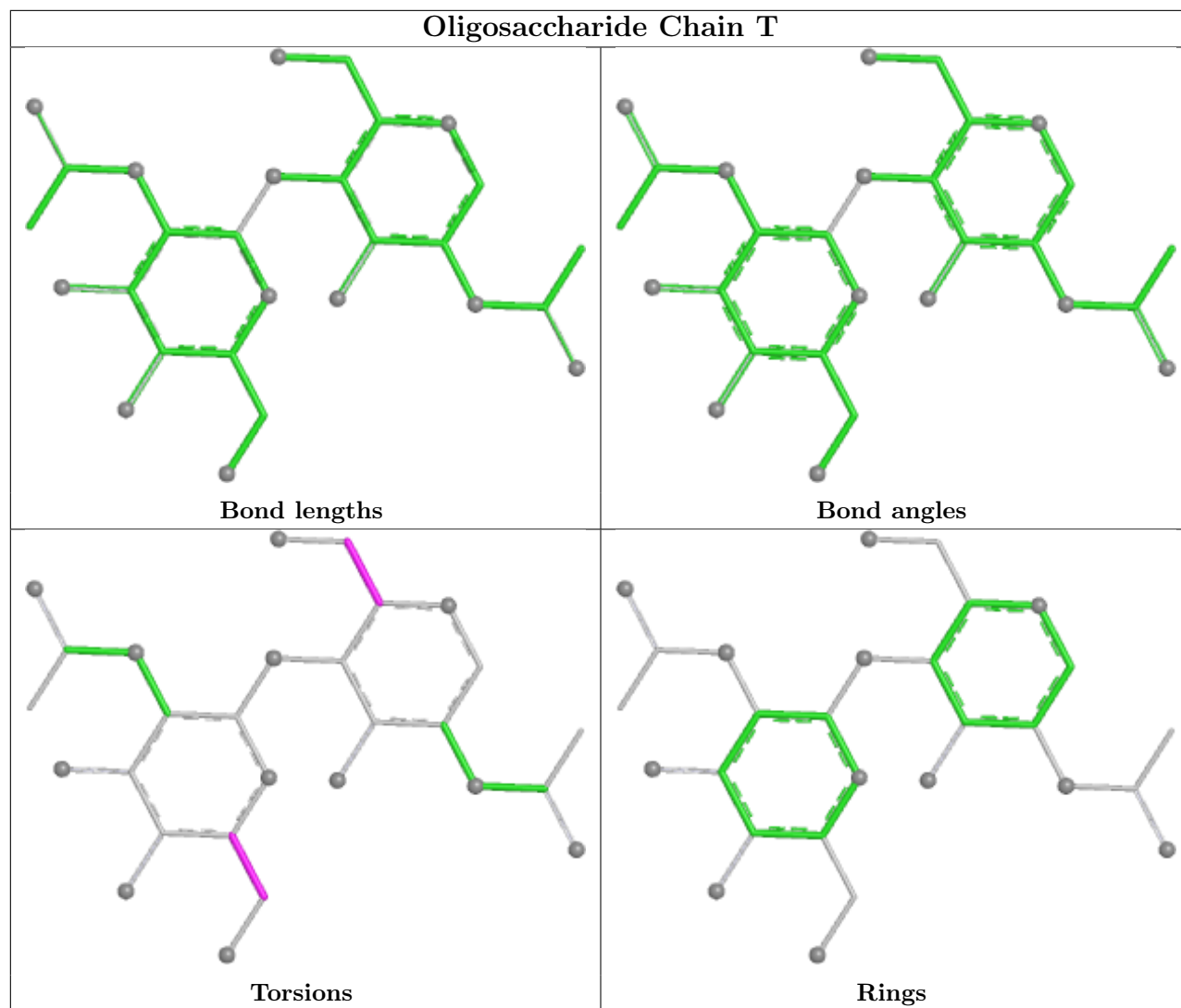
There are no ring outliers.

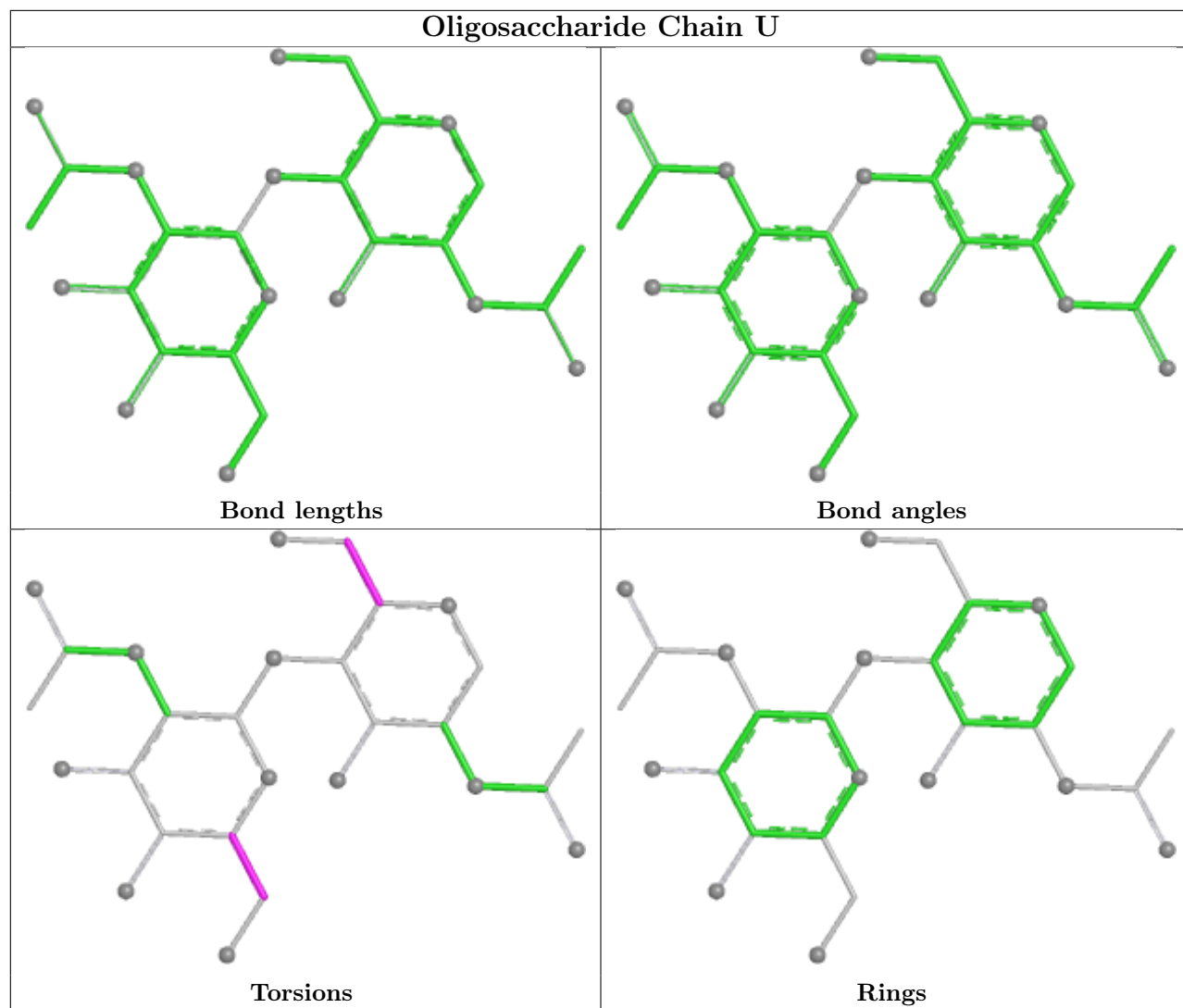
No monomer is involved in short contacts.

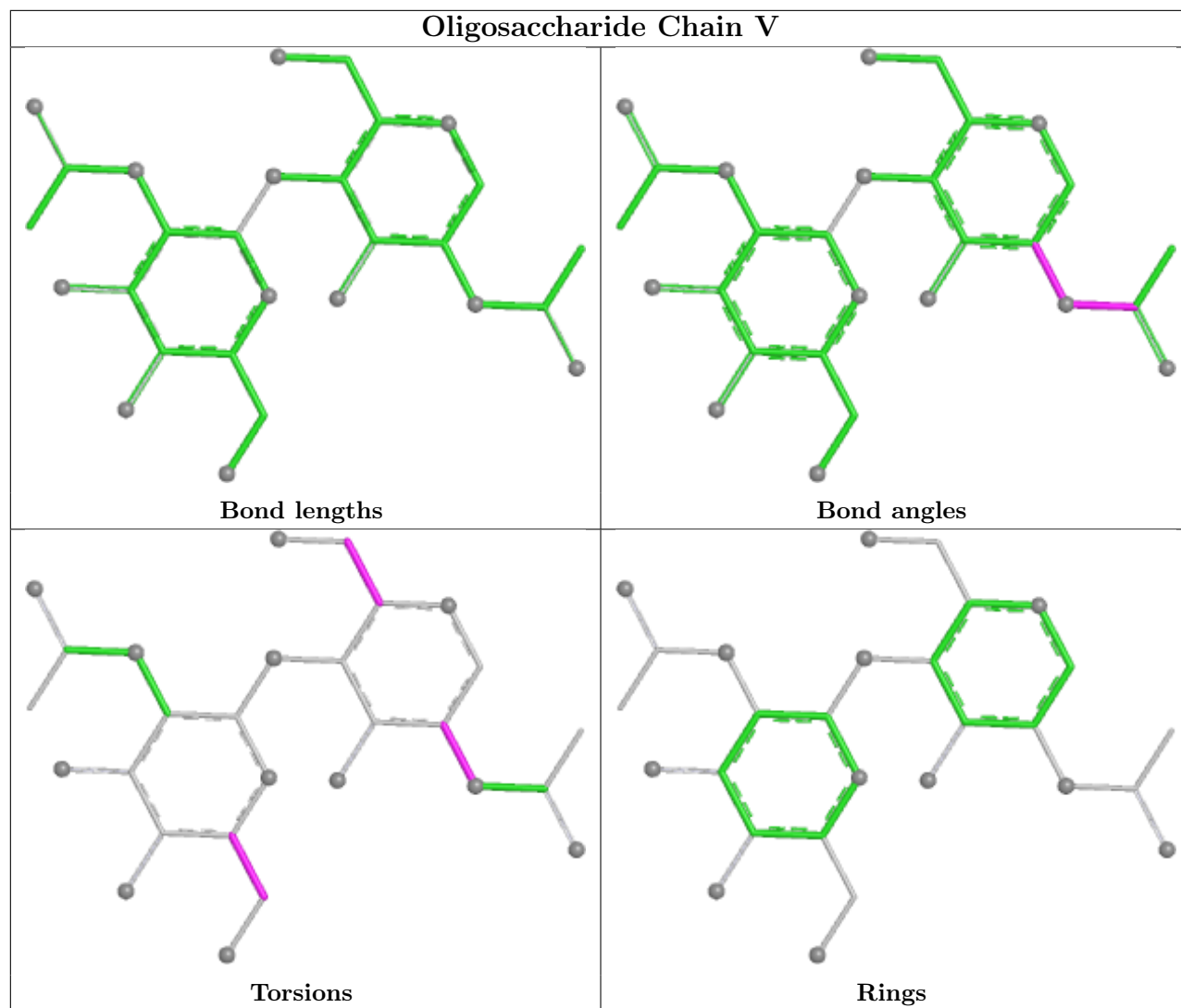
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

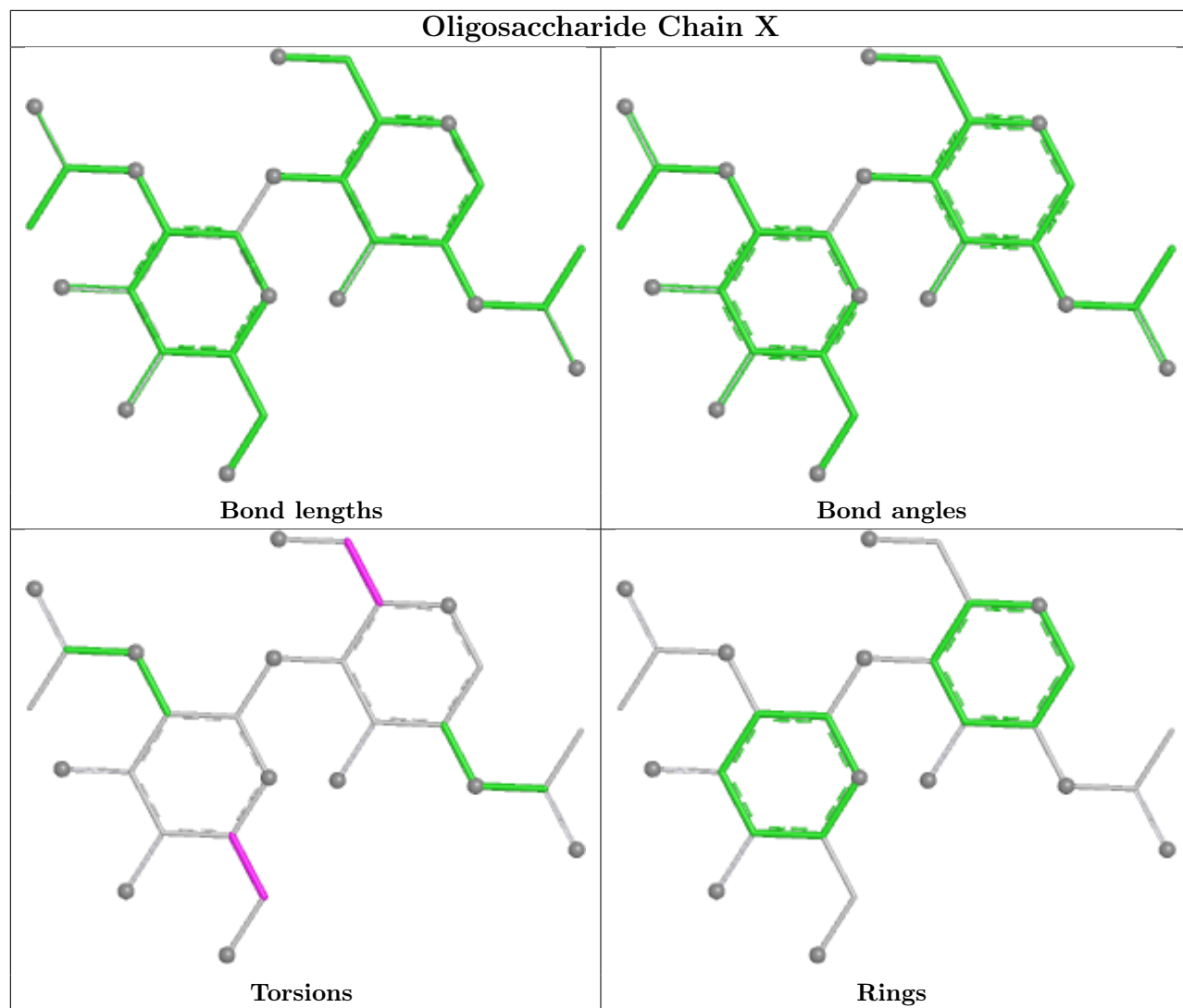


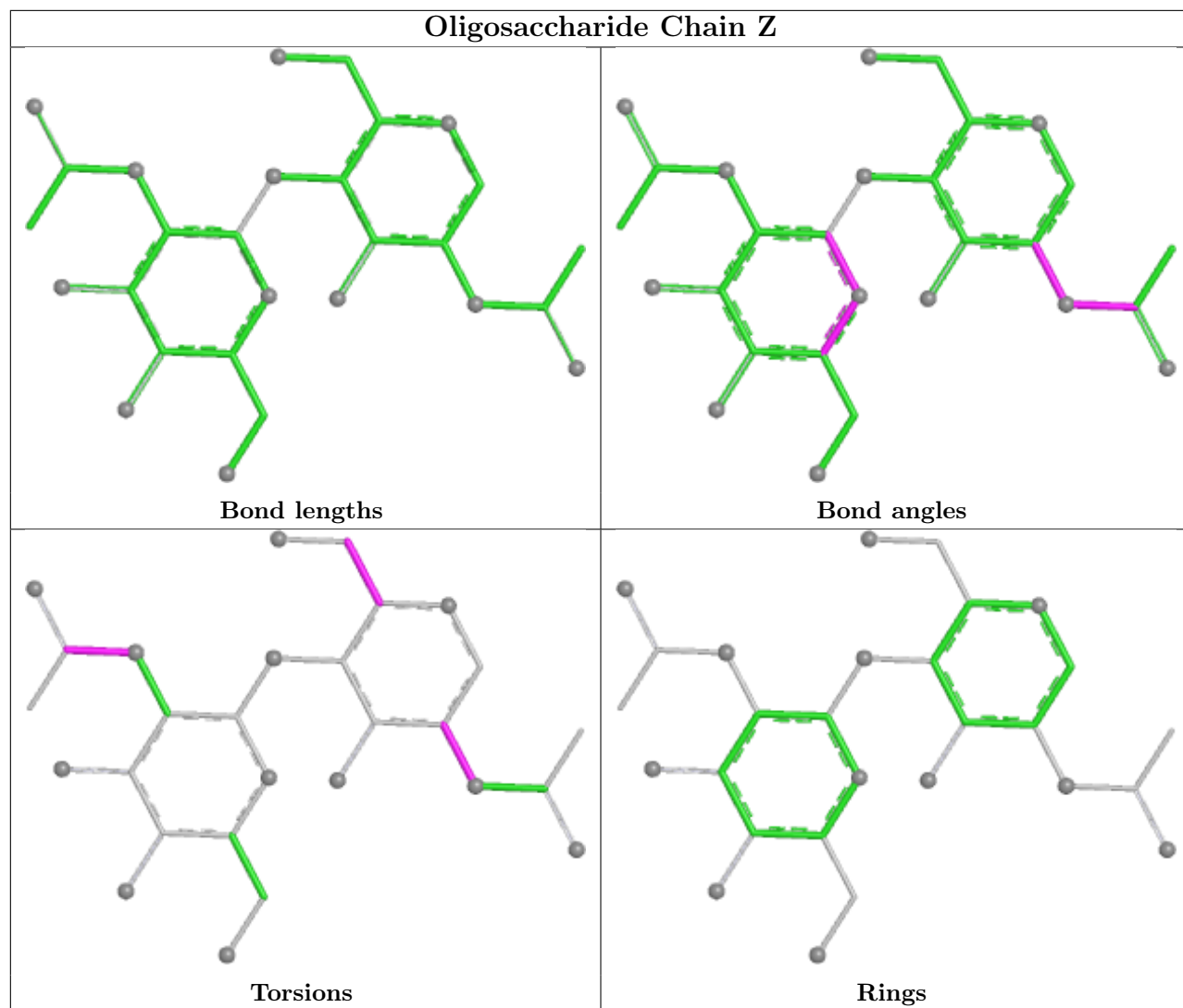


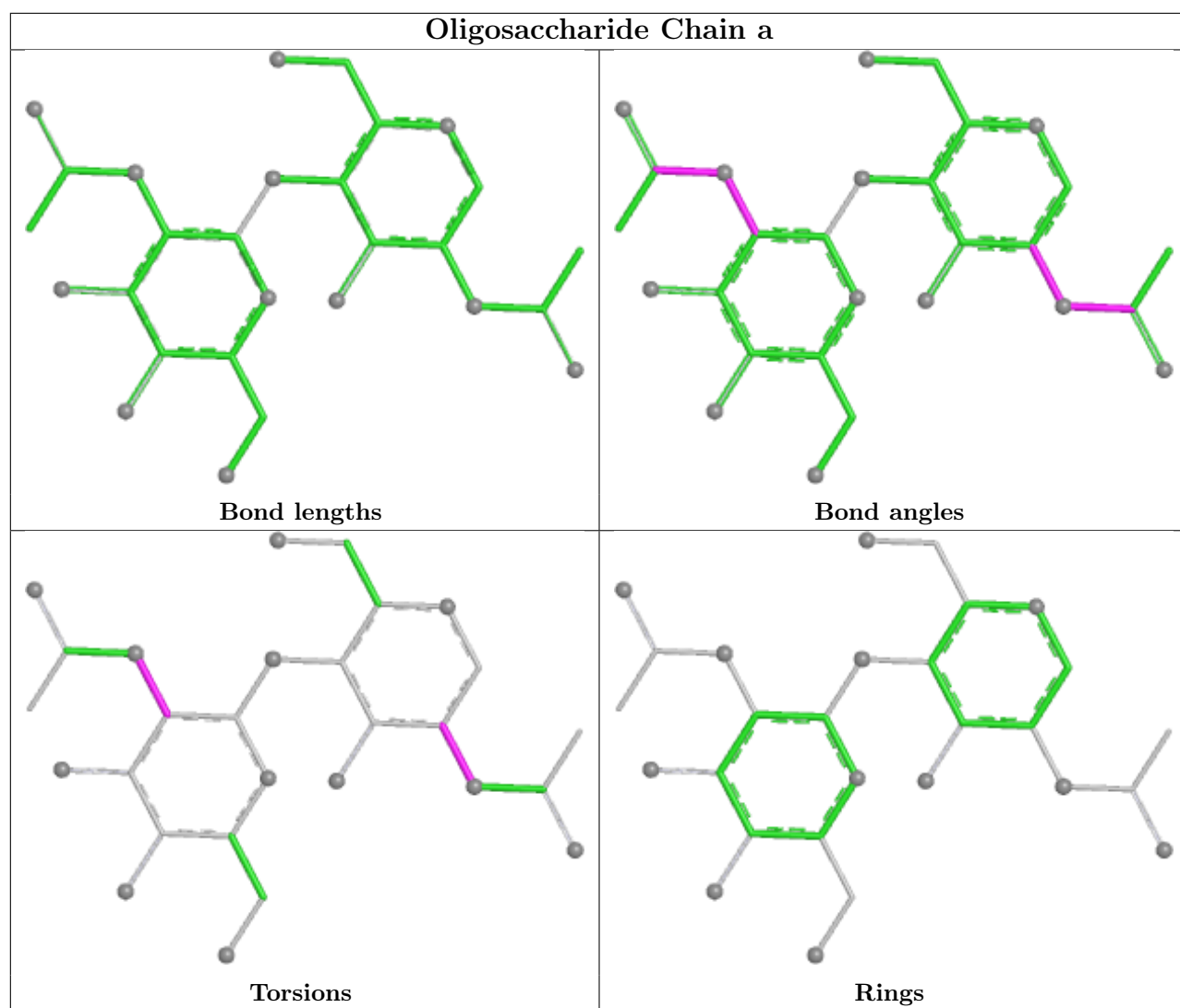


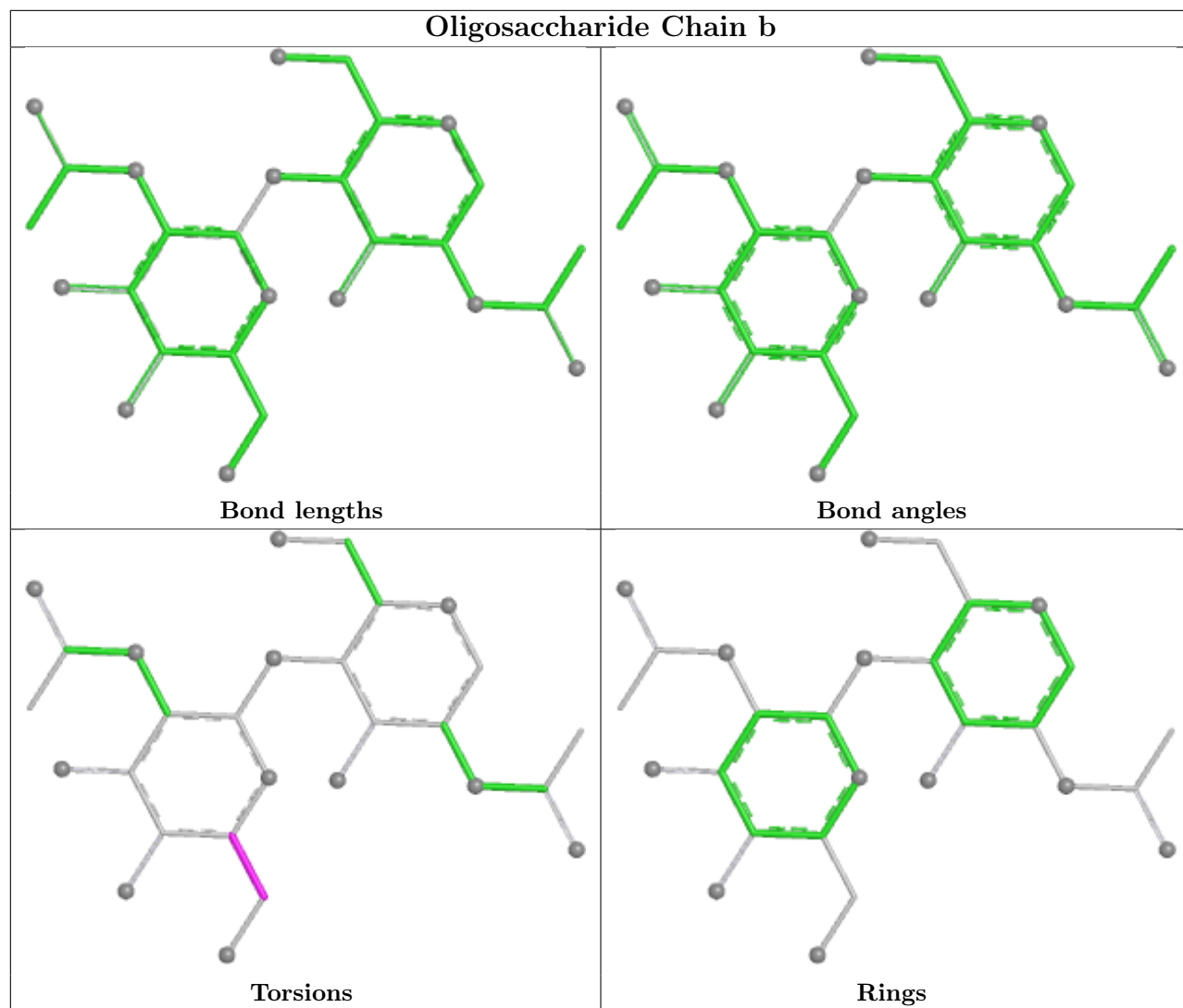


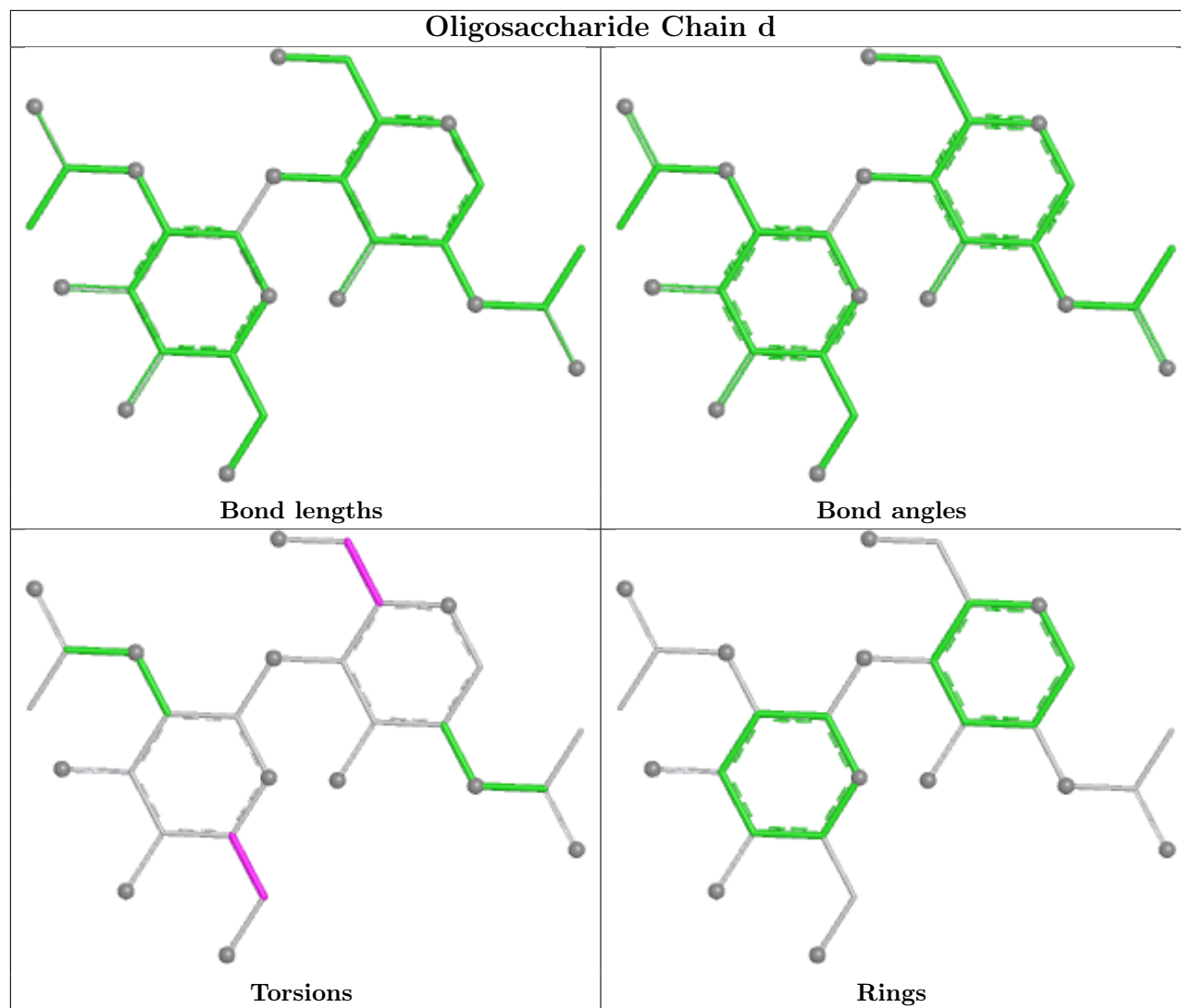




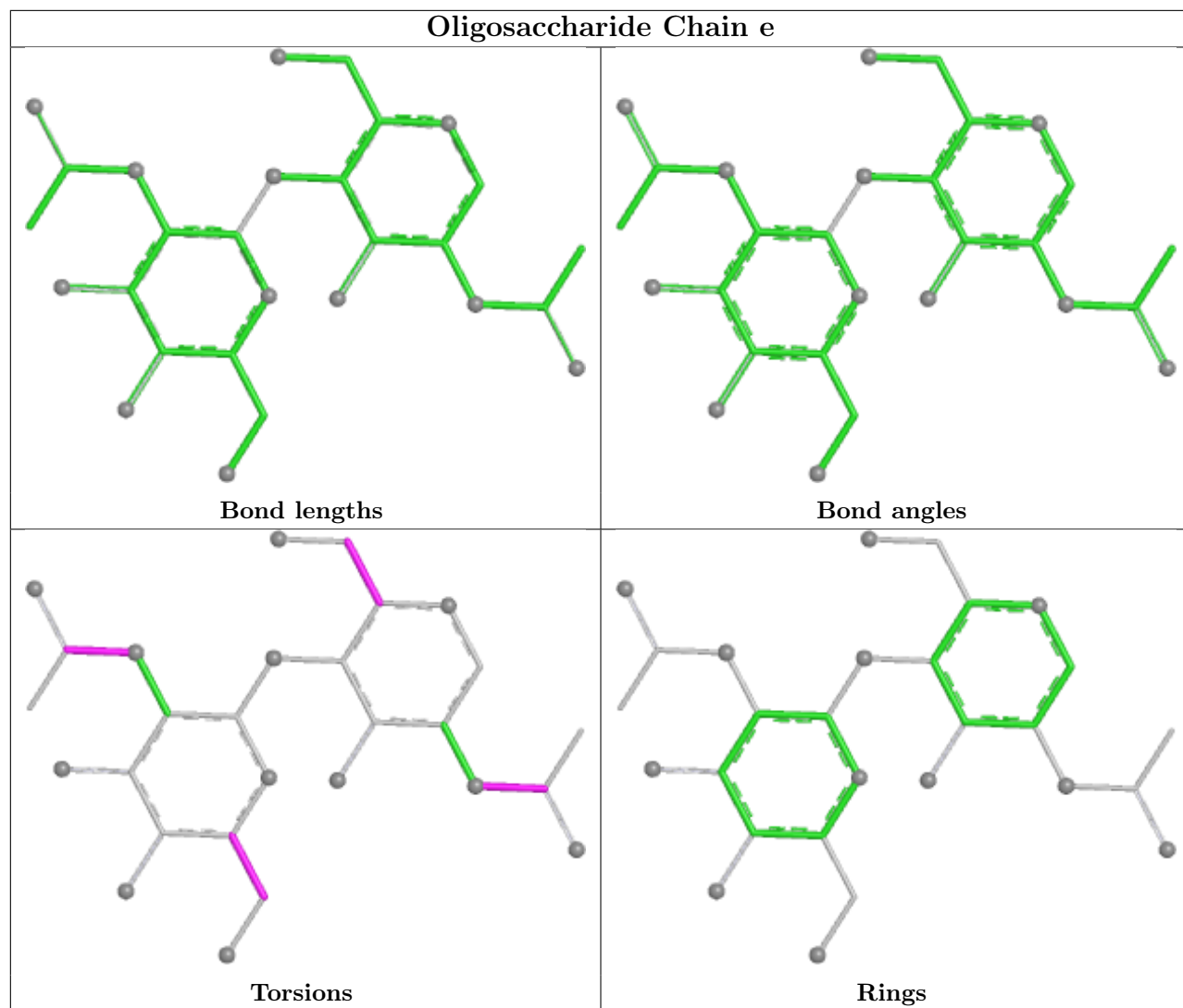


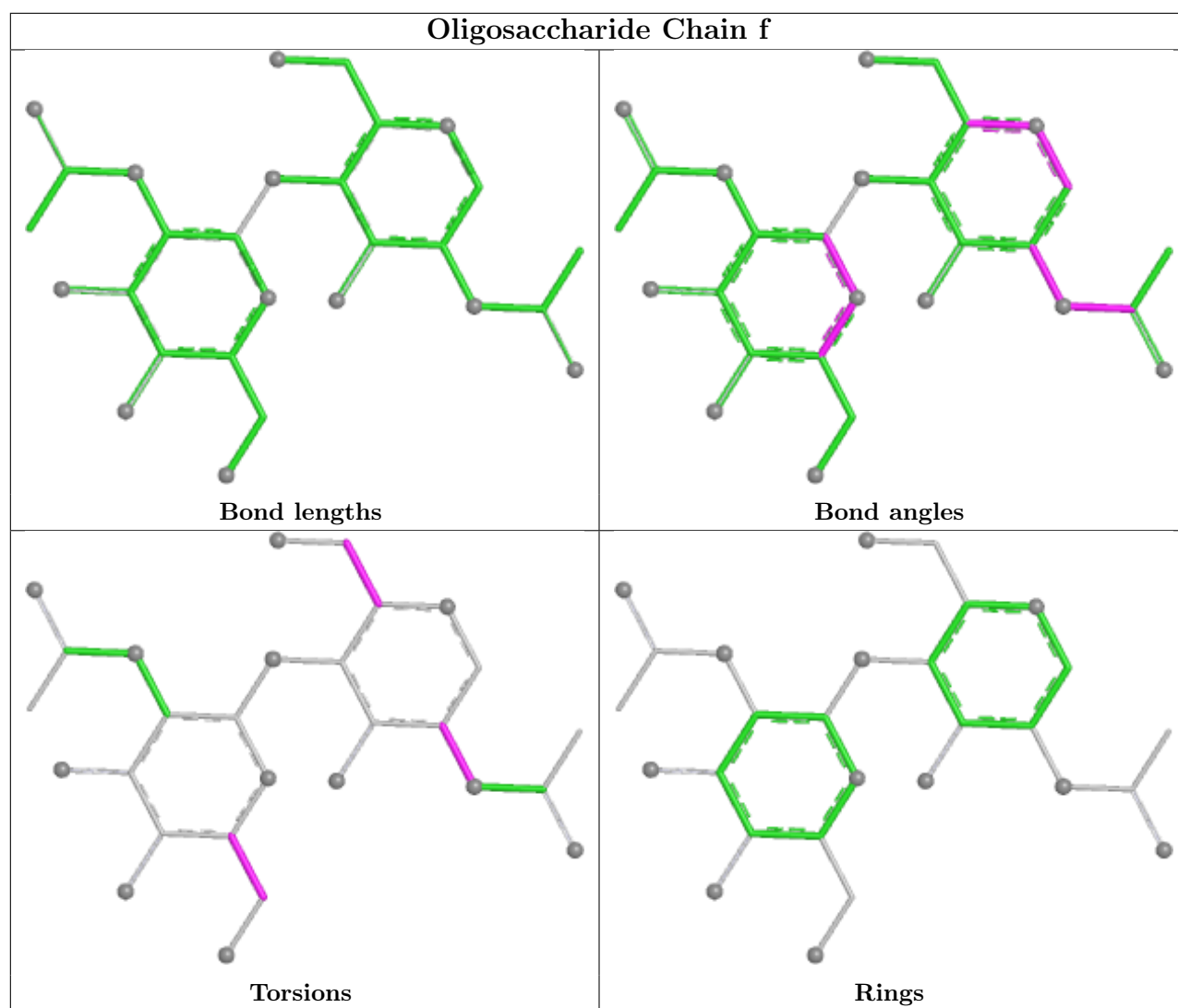


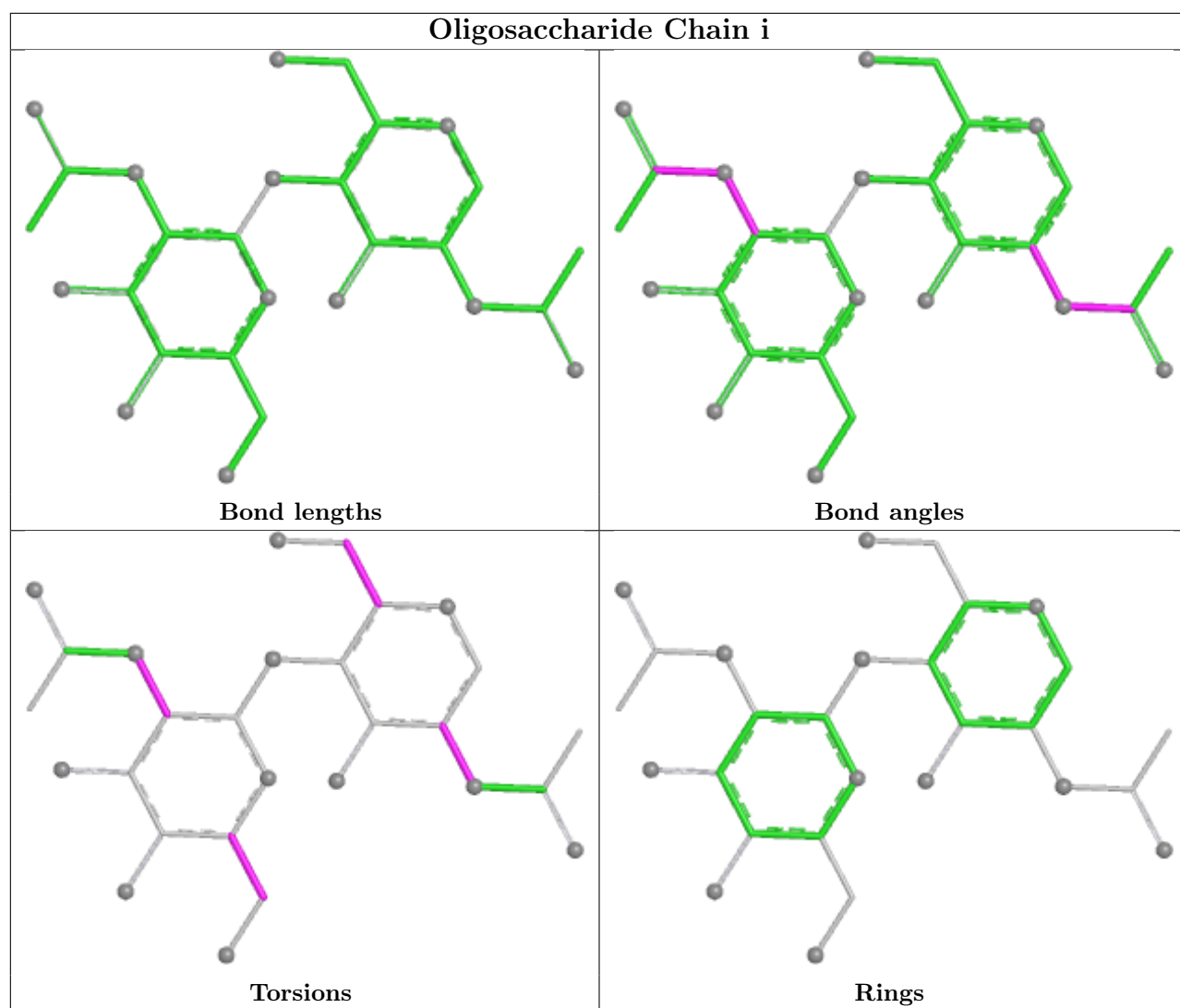


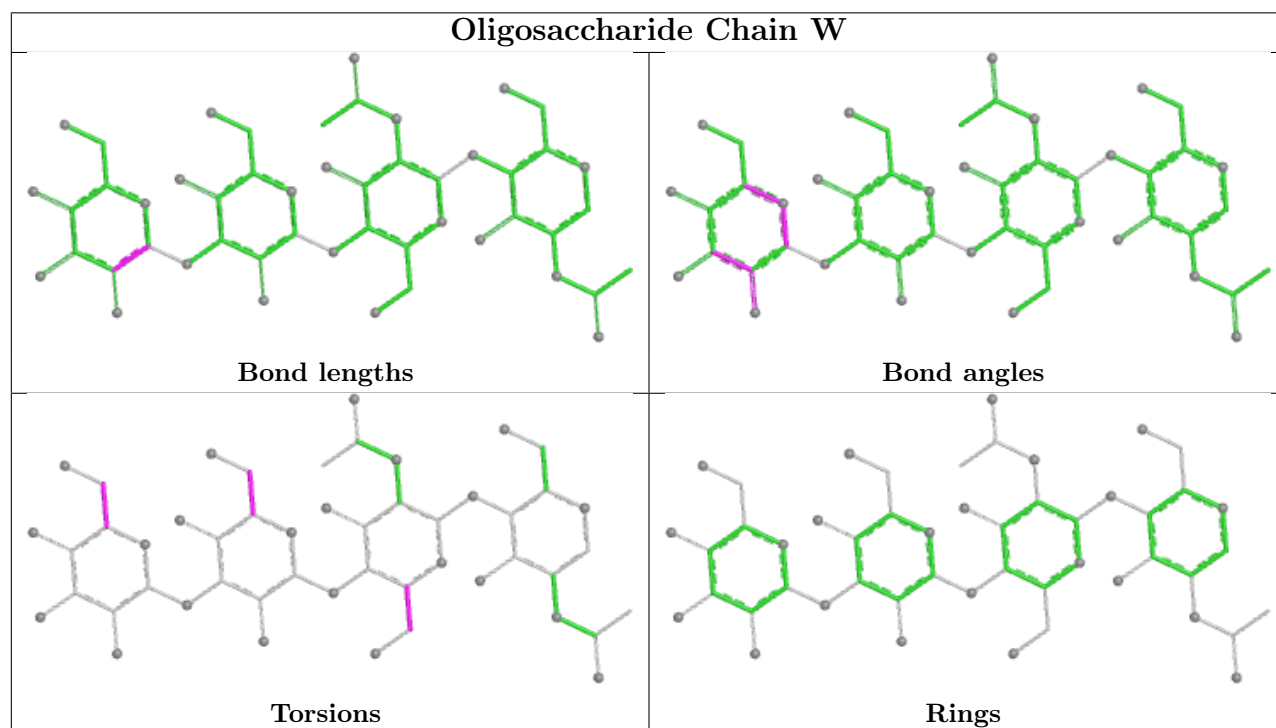
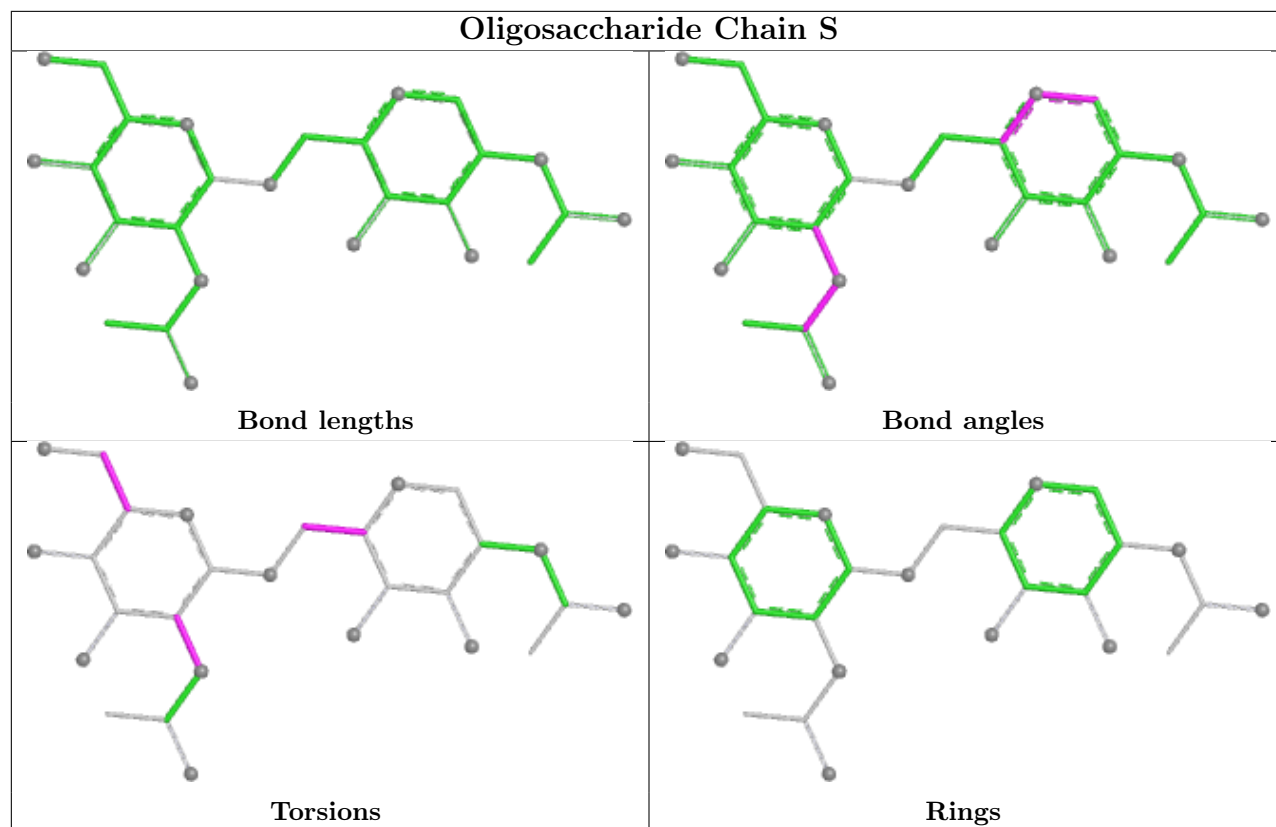


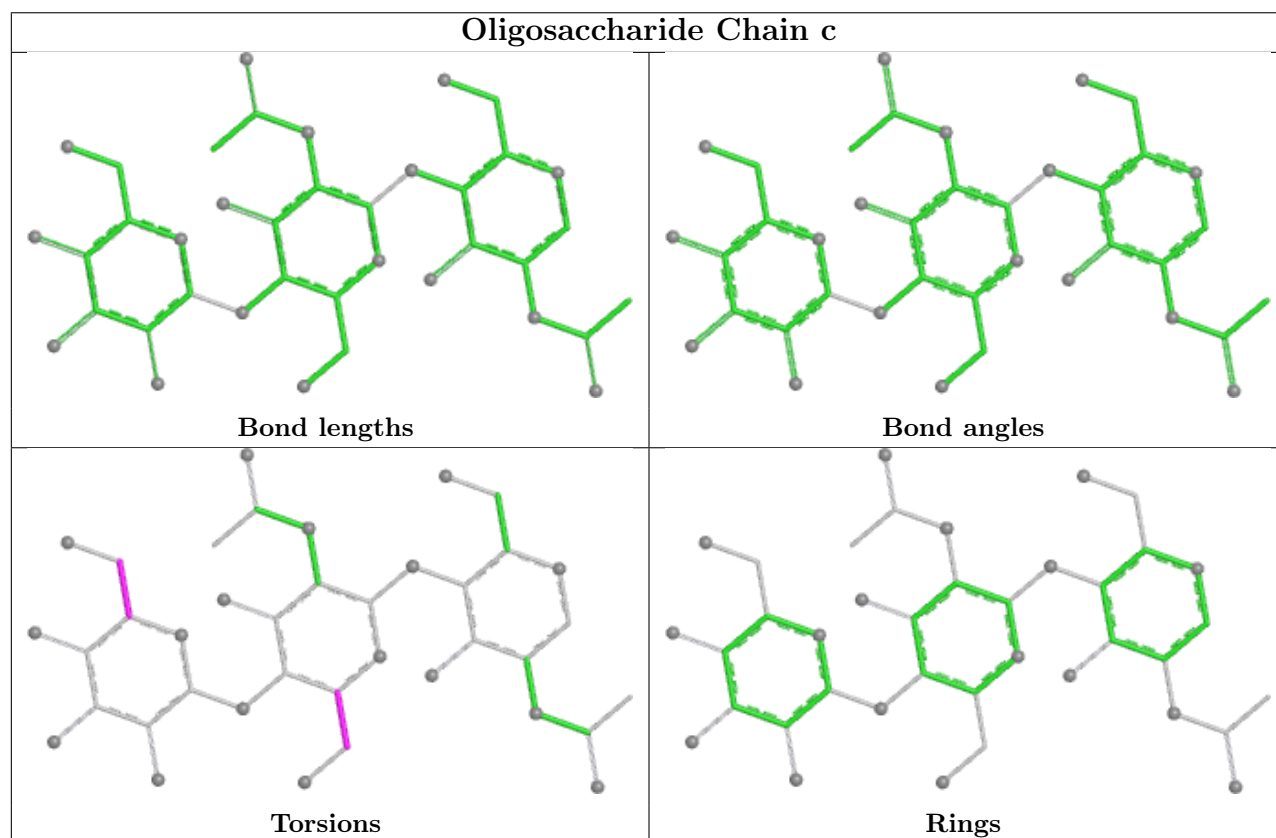
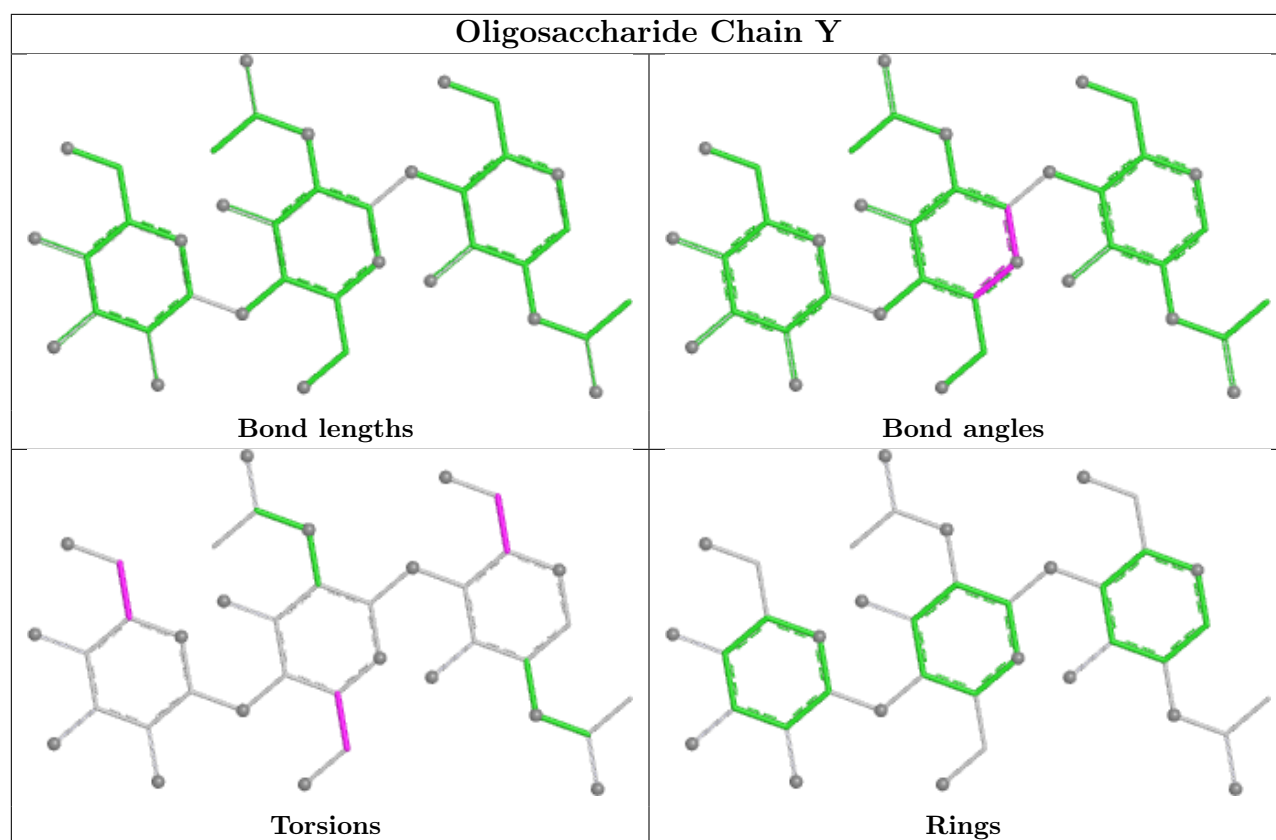


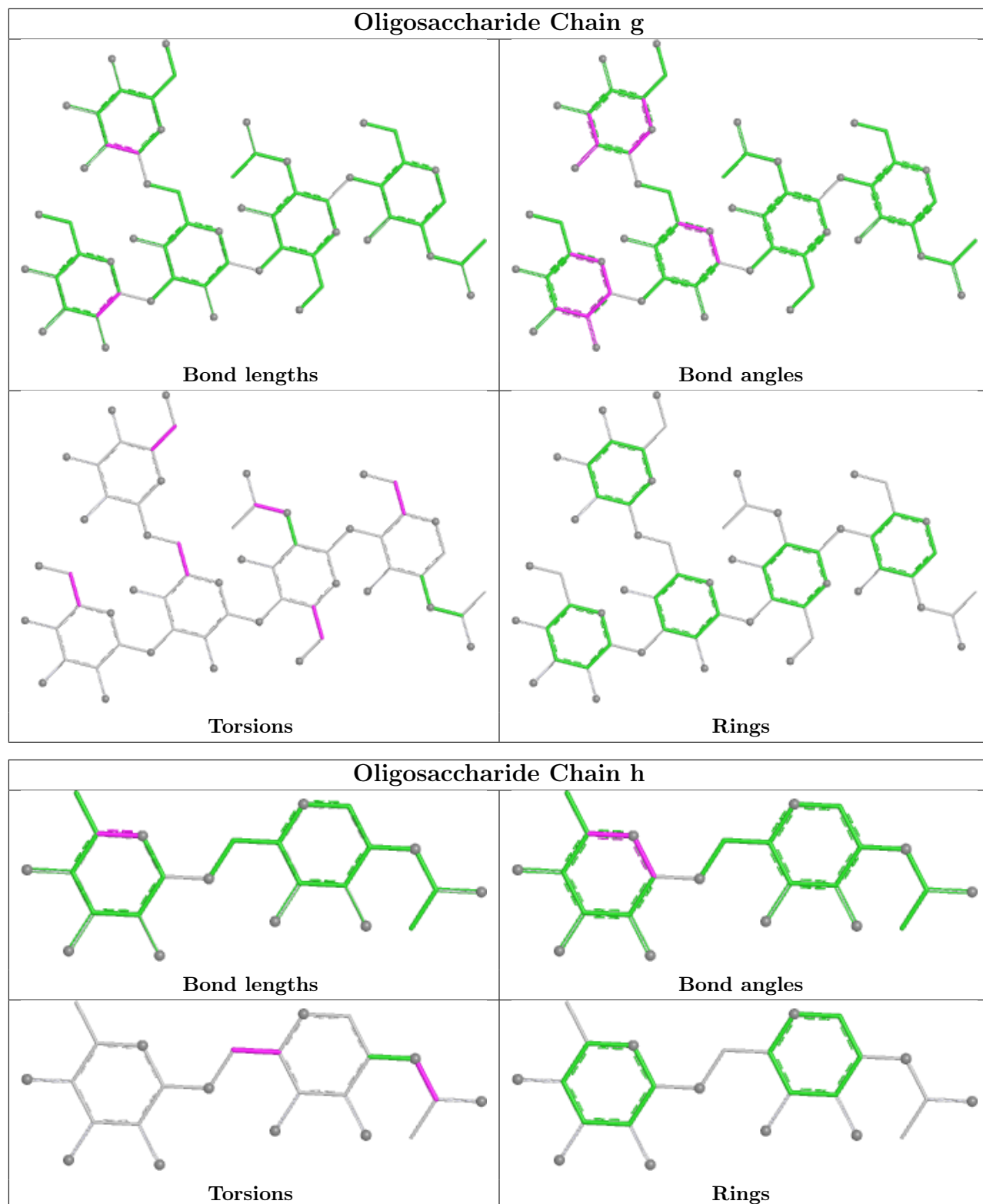


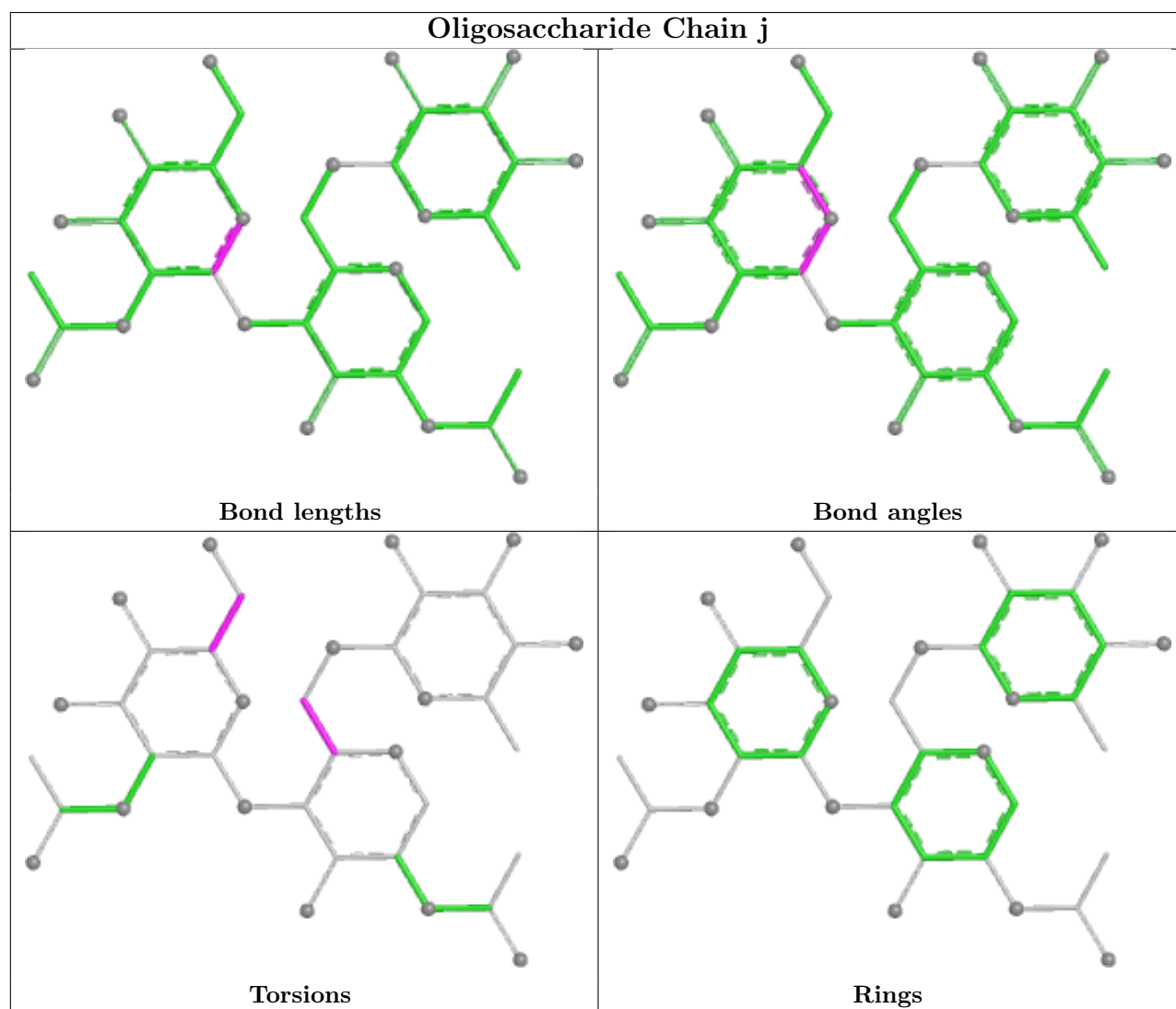
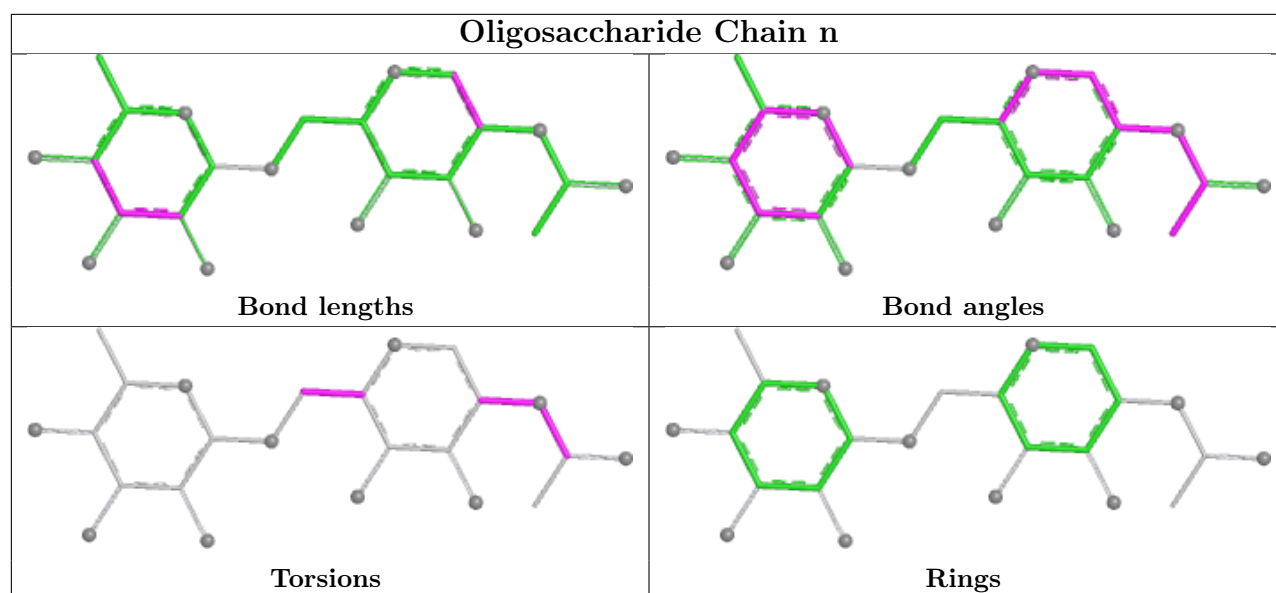


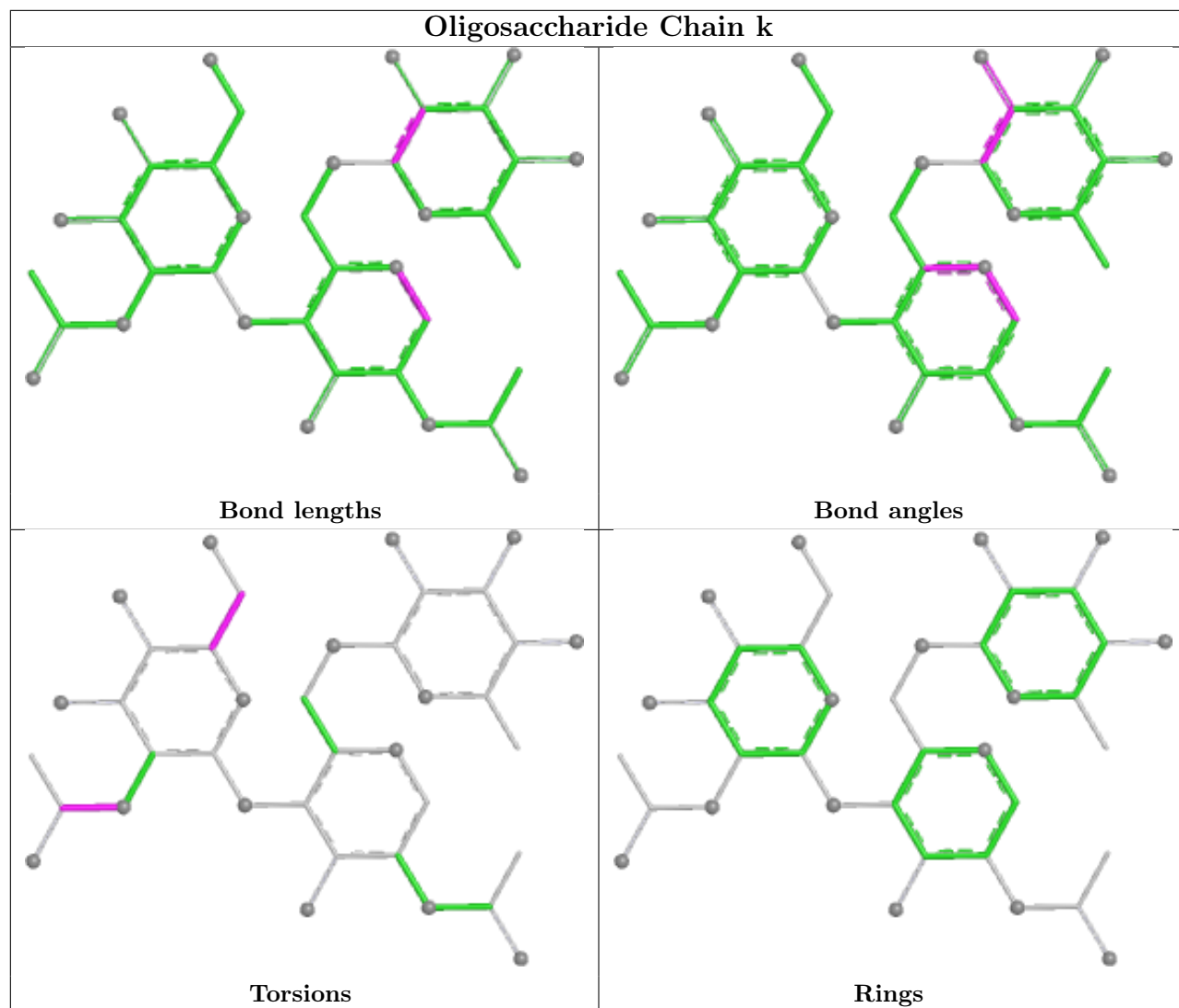




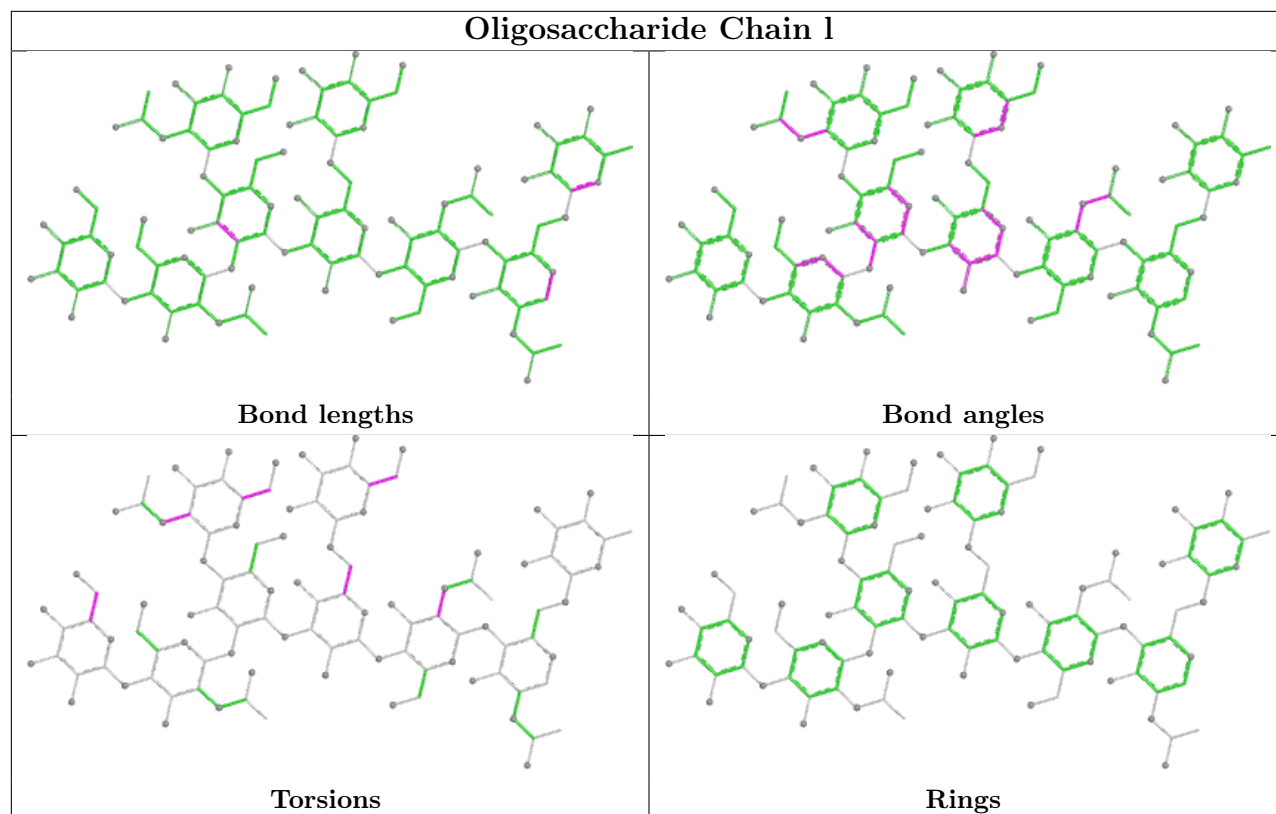


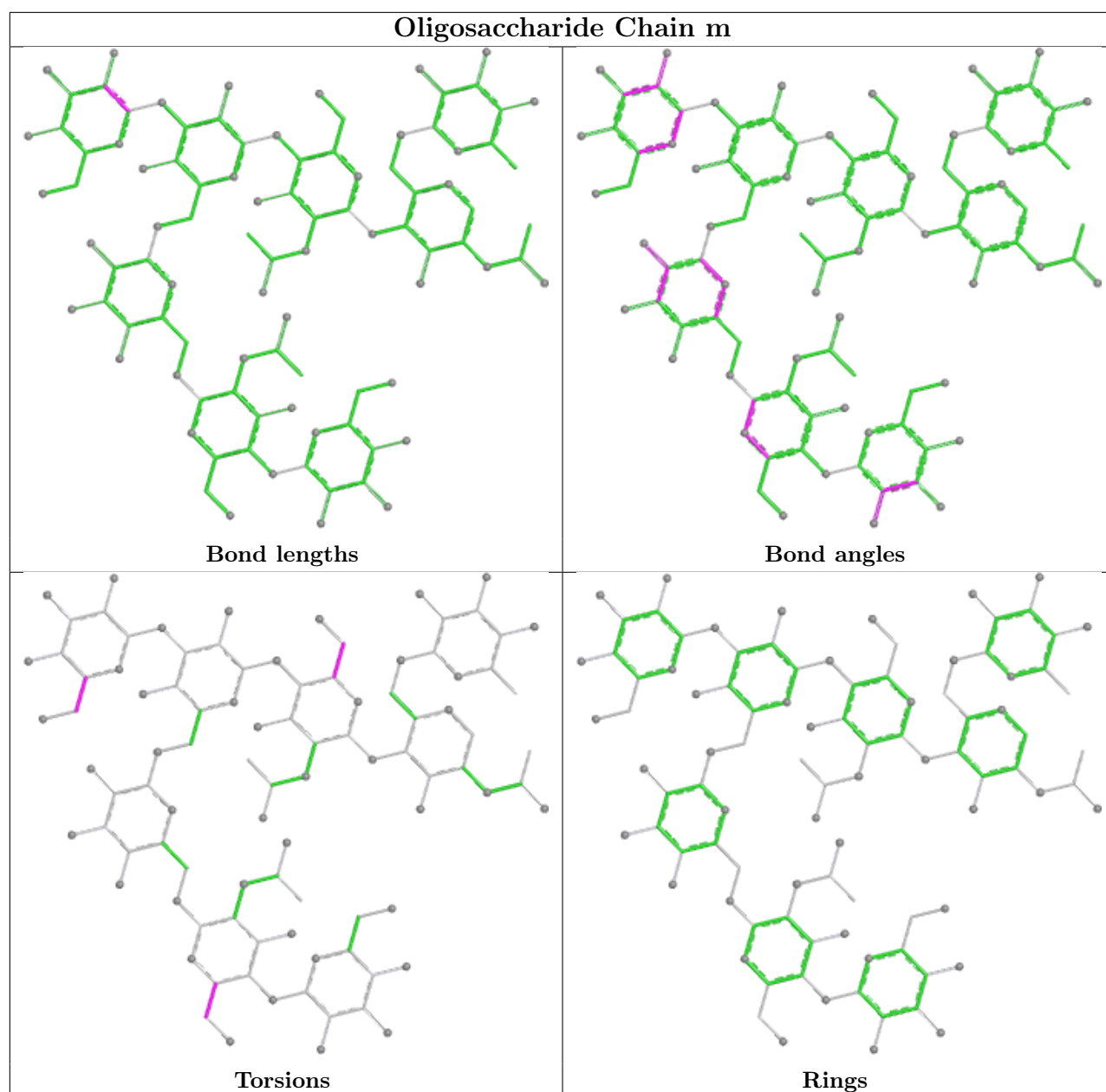












## 5.6 Ligand geometry [i](#)

46 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
17	NAG	E	620	1	14,14,15	0.50	0	17,19,21	0.71	1 (5%)
17	NAG	C	621	1	14,14,15	0.34	0	17,19,21	0.57	0
17	NAG	C	622	1	14,14,15	0.28	0	17,19,21	0.47	0
17	NAG	E	606	1	14,14,15	0.29	0	17,19,21	0.47	0
17	NAG	F	904	2	14,14,15	0.65	1 (7%)	17,19,21	0.50	0
17	NAG	C	606	1	14,14,15	0.19	0	17,19,21	0.40	0
17	NAG	E	613	1	14,14,15	0.26	0	17,19,21	0.45	0
17	NAG	A	631	1	14,14,15	0.55	0	17,19,21	0.62	1 (5%)
17	NAG	E	610	1	14,14,15	0.82	1 (7%)	17,19,21	2.38	3 (17%)
17	NAG	E	608	1	14,14,15	0.31	0	17,19,21	0.41	0
18	44E	O	301	-	10,10,23	2.08	1 (10%)	11,13,28	1.52	1 (9%)
17	NAG	A	605	1	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
17	NAG	A	619	1	14,14,15	0.44	0	17,19,21	0.54	0
17	NAG	A	632	1	14,14,15	0.69	1 (7%)	17,19,21	1.01	1 (5%)
17	NAG	E	621	1	14,14,15	0.84	1 (7%)	17,19,21	1.06	1 (5%)
17	NAG	C	614	1	14,14,15	0.63	0	17,19,21	0.68	1 (5%)
17	NAG	E	617	1	14,14,15	0.82	1 (7%)	17,19,21	2.32	3 (17%)
17	NAG	C	624	1	14,14,15	0.74	1 (7%)	17,19,21	0.93	1 (5%)
17	NAG	F	902	2	14,14,15	0.35	0	17,19,21	0.41	0
17	NAG	E	611	1	14,14,15	0.26	0	17,19,21	0.53	0
17	NAG	E	619	1	14,14,15	0.31	0	17,19,21	0.41	0
17	NAG	C	615	1	14,14,15	1.23	1 (7%)	17,19,21	1.62	1 (5%)
17	NAG	C	603	1	14,14,15	0.44	0	17,19,21	0.60	1 (5%)
17	NAG	A	618	1	14,14,15	0.19	0	17,19,21	0.51	0
17	NAG	E	609	1	14,14,15	1.00	1 (7%)	17,19,21	0.63	0
17	NAG	C	617	1	14,14,15	0.31	0	17,19,21	0.61	0
18	44E	N	301	-	10,10,23	2.09	1 (10%)	11,13,28	1.49	1 (9%)
17	NAG	F	901	2	14,14,15	0.20	0	17,19,21	0.69	1 (5%)
17	NAG	A	628	1	14,14,15	0.22	0	17,19,21	0.59	0
17	NAG	C	616	1	14,14,15	0.47	0	17,19,21	0.35	0
17	NAG	A	625	1	14,14,15	0.67	1 (7%)	17,19,21	0.91	0
17	NAG	C	620	1	14,14,15	0.25	0	17,19,21	0.67	0
17	NAG	E	607	1	14,14,15	0.26	0	17,19,21	0.63	0
17	NAG	F	903	2	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
17	NAG	E	615	1	14,14,15	0.29	0	17,19,21	0.43	0
17	NAG	C	623	1	14,14,15	0.31	0	17,19,21	0.44	0
17	NAG	E	614	1	14,14,15	0.54	0	17,19,21	1.08	2 (11%)
17	NAG	A	603	1	14,14,15	0.30	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	NAG	C	628	1	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
17	NAG	D	901	2	14,14,15	0.50	0	17,19,21	0.48	0
17	NAG	C	627	1	14,14,15	0.32	0	17,19,21	0.55	0
17	NAG	E	618	1	14,14,15	0.51	0	17,19,21	0.65	1 (5%)
17	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.61	1 (5%)
18	44E	L	301	-	10,10,23	2.10	1 (10%)	11,13,28	1.48	1 (9%)
17	NAG	E	612	1	14,14,15	0.38	0	17,19,21	0.51	0
17	NAG	E	616	1	14,14,15	0.60	1 (7%)	17,19,21	1.68	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	E	620	1	-	2/6/23/26	0/1/1/1
17	NAG	C	621	1	-	2/6/23/26	0/1/1/1
17	NAG	C	622	1	-	3/6/23/26	0/1/1/1
17	NAG	E	606	1	-	2/6/23/26	0/1/1/1
17	NAG	F	904	2	-	0/6/23/26	0/1/1/1
17	NAG	C	606	1	-	2/6/23/26	0/1/1/1
17	NAG	E	613	1	-	2/6/23/26	0/1/1/1
17	NAG	A	631	1	-	2/6/23/26	0/1/1/1
17	NAG	E	610	1	-	6/6/23/26	0/1/1/1
17	NAG	E	608	1	-	2/6/23/26	0/1/1/1
18	44E	O	301	-	-	6/9/9/25	-
17	NAG	A	605	1	-	0/6/23/26	0/1/1/1
17	NAG	A	619	1	-	4/6/23/26	0/1/1/1
17	NAG	A	632	1	-	4/6/23/26	0/1/1/1
17	NAG	E	621	1	-	2/6/23/26	0/1/1/1
17	NAG	C	614	1	-	2/6/23/26	0/1/1/1
17	NAG	E	617	1	-	6/6/23/26	0/1/1/1
17	NAG	C	624	1	-	3/6/23/26	0/1/1/1
17	NAG	F	902	2	-	2/6/23/26	0/1/1/1
17	NAG	E	611	1	-	2/6/23/26	0/1/1/1
17	NAG	E	619	1	-	2/6/23/26	0/1/1/1
17	NAG	C	615	1	-	4/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	C	603	1	-	1/6/23/26	0/1/1/1
17	NAG	A	618	1	-	2/6/23/26	0/1/1/1
17	NAG	E	609	1	-	2/6/23/26	0/1/1/1
17	NAG	C	617	1	-	4/6/23/26	0/1/1/1
18	44E	N	301	-	-	6/9/9/25	-
17	NAG	F	901	2	-	2/6/23/26	0/1/1/1
17	NAG	A	628	1	-	2/6/23/26	0/1/1/1
17	NAG	C	616	1	-	2/6/23/26	0/1/1/1
17	NAG	A	625	1	-	2/6/23/26	0/1/1/1
17	NAG	C	620	1	-	4/6/23/26	0/1/1/1
17	NAG	E	607	1	-	4/6/23/26	0/1/1/1
17	NAG	F	903	2	-	0/6/23/26	0/1/1/1
17	NAG	E	615	1	-	1/6/23/26	0/1/1/1
17	NAG	C	623	1	-	1/6/23/26	0/1/1/1
17	NAG	E	614	1	-	3/6/23/26	0/1/1/1
17	NAG	A	603	1	-	2/6/23/26	0/1/1/1
17	NAG	C	628	1	-	0/6/23/26	0/1/1/1
17	NAG	D	901	2	-	2/6/23/26	0/1/1/1
17	NAG	C	627	1	-	2/6/23/26	0/1/1/1
17	NAG	E	618	1	-	1/6/23/26	0/1/1/1
17	NAG	A	604	1	-	2/6/23/26	0/1/1/1
18	44E	L	301	-	-	6/9/9/25	-
17	NAG	E	612	1	-	1/6/23/26	0/1/1/1
17	NAG	E	616	1	-	4/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	301	44E	O21-C2	-5.89	1.38	1.46
18	N	301	44E	O21-C2	-5.87	1.38	1.46
18	O	301	44E	O21-C2	-5.84	1.38	1.46
17	C	615	NAG	O5-C1	4.43	1.51	1.43
17	E	609	NAG	C1-C2	3.41	1.57	1.52
17	E	621	NAG	O5-C1	2.65	1.48	1.43
17	C	624	NAG	C1-C2	2.49	1.55	1.52
17	E	617	NAG	C1-C2	2.39	1.55	1.52
17	A	632	NAG	C1-C2	2.34	1.55	1.52
17	E	610	NAG	C1-C2	2.27	1.55	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	625	NAG	O5-C1	-2.27	1.39	1.43
17	F	904	NAG	C1-C2	2.11	1.55	1.52
17	E	616	NAG	O5-C1	2.04	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	617	NAG	C2-N2-C7	8.33	134.06	122.90
17	E	610	NAG	C2-N2-C7	8.19	133.88	122.90
17	C	615	NAG	C1-O5-C5	6.43	120.81	112.19
17	E	616	NAG	C1-O5-C5	6.26	120.58	112.19
17	E	610	NAG	C1-C2-N2	4.15	116.98	110.43
18	O	301	44E	O21-C21-O22	-4.05	120.50	125.70
18	N	301	44E	O21-C21-O22	-4.04	120.52	125.70
18	L	301	44E	O21-C21-O22	-3.99	120.58	125.70
17	E	617	NAG	C1-C2-N2	3.52	115.98	110.43
17	E	621	NAG	C1-O5-C5	3.27	116.56	112.19
17	E	614	NAG	C2-N2-C7	3.14	127.11	122.90
17	A	632	NAG	C2-N2-C7	3.05	126.98	122.90
17	F	903	NAG	C1-O5-C5	3.04	116.26	112.19
17	C	624	NAG	C2-N2-C7	3.02	126.95	122.90
17	A	605	NAG	C1-O5-C5	2.94	116.12	112.19
17	E	620	NAG	C1-O5-C5	2.51	115.54	112.19
17	C	614	NAG	C1-O5-C5	2.36	115.34	112.19
17	E	617	NAG	C8-C7-N2	2.27	119.89	116.12
17	C	628	NAG	C1-O5-C5	2.21	115.15	112.19
17	E	618	NAG	C1-O5-C5	2.20	115.13	112.19
17	E	614	NAG	C1-O5-C5	2.15	115.07	112.19
17	F	901	NAG	C1-O5-C5	2.14	115.05	112.19
17	E	610	NAG	C8-C7-N2	2.13	119.64	116.12
17	C	603	NAG	C1-O5-C5	2.07	114.97	112.19
17	A	631	NAG	C1-O5-C5	2.03	114.91	112.19
17	A	604	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	301	44E	C1-O11-P-O13
18	L	301	44E	C1-O11-P-O14
18	L	301	44E	C1-O11-P-O12
18	L	301	44E	O11-C1-C2-O21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	L	301	44E	O22-C21-O21-C2
18	N	301	44E	C1-O11-P-O13
18	N	301	44E	C1-O11-P-O14
18	N	301	44E	C1-O11-P-O12
18	N	301	44E	O11-C1-C2-O21
18	N	301	44E	O22-C21-O21-C2
18	O	301	44E	C1-O11-P-O13
18	O	301	44E	C1-O11-P-O14
18	O	301	44E	C1-O11-P-O12
18	O	301	44E	O11-C1-C2-O21
18	O	301	44E	O22-C21-O21-C2
17	E	613	NAG	C4-C5-C6-O6
17	E	606	NAG	C4-C5-C6-O6
17	E	607	NAG	O5-C5-C6-O6
17	D	901	NAG	O5-C5-C6-O6
17	A	631	NAG	C4-C5-C6-O6
17	C	622	NAG	O5-C5-C6-O6
17	A	618	NAG	O5-C5-C6-O6
17	E	613	NAG	O5-C5-C6-O6
17	C	616	NAG	O5-C5-C6-O6
17	C	617	NAG	O5-C5-C6-O6
17	C	627	NAG	O5-C5-C6-O6
17	A	603	NAG	C4-C5-C6-O6
17	E	620	NAG	C4-C5-C6-O6
17	A	604	NAG	O5-C5-C6-O6
17	E	608	NAG	C4-C5-C6-O6
17	E	617	NAG	C4-C5-C6-O6
17	D	901	NAG	C4-C5-C6-O6
17	E	619	NAG	O5-C5-C6-O6
17	C	614	NAG	O5-C5-C6-O6
17	C	621	NAG	O5-C5-C6-O6
17	F	902	NAG	O5-C5-C6-O6
17	E	621	NAG	O5-C5-C6-O6
17	A	618	NAG	C4-C5-C6-O6
17	E	616	NAG	O5-C5-C6-O6
17	E	617	NAG	O5-C5-C6-O6
17	C	606	NAG	O5-C5-C6-O6
17	E	607	NAG	C4-C5-C6-O6
17	C	621	NAG	C4-C5-C6-O6
17	A	631	NAG	O5-C5-C6-O6
17	E	608	NAG	O5-C5-C6-O6
17	E	609	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	E	620	NAG	O5-C5-C6-O6
17	E	606	NAG	O5-C5-C6-O6
17	A	628	NAG	C4-C5-C6-O6
17	C	620	NAG	C4-C5-C6-O6
17	C	622	NAG	C4-C5-C6-O6
17	A	632	NAG	O5-C5-C6-O6
17	E	621	NAG	C4-C5-C6-O6
17	C	627	NAG	C4-C5-C6-O6
17	C	617	NAG	C4-C5-C6-O6
17	A	603	NAG	O5-C5-C6-O6
17	E	609	NAG	C4-C5-C6-O6
17	A	619	NAG	C8-C7-N2-C2
17	A	619	NAG	O7-C7-N2-C2
17	E	607	NAG	C8-C7-N2-C2
17	E	607	NAG	O7-C7-N2-C2
17	E	610	NAG	C8-C7-N2-C2
17	E	610	NAG	O7-C7-N2-C2
17	E	611	NAG	C8-C7-N2-C2
17	E	611	NAG	O7-C7-N2-C2
17	E	616	NAG	C8-C7-N2-C2
17	E	616	NAG	O7-C7-N2-C2
17	E	617	NAG	C8-C7-N2-C2
17	E	617	NAG	O7-C7-N2-C2
17	C	615	NAG	C8-C7-N2-C2
17	C	615	NAG	O7-C7-N2-C2
17	C	617	NAG	C8-C7-N2-C2
17	C	617	NAG	O7-C7-N2-C2
17	C	620	NAG	C8-C7-N2-C2
17	C	620	NAG	O7-C7-N2-C2
17	A	604	NAG	C4-C5-C6-O6
17	A	619	NAG	O5-C5-C6-O6
17	C	616	NAG	C4-C5-C6-O6
17	E	612	NAG	O5-C5-C6-O6
17	E	619	NAG	C4-C5-C6-O6
17	E	610	NAG	C4-C5-C6-O6
17	E	616	NAG	C4-C5-C6-O6
17	A	628	NAG	O5-C5-C6-O6
17	C	620	NAG	O5-C5-C6-O6
17	F	902	NAG	C4-C5-C6-O6
17	C	614	NAG	C4-C5-C6-O6
17	C	603	NAG	O5-C5-C6-O6
17	E	610	NAG	O5-C5-C6-O6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	C	606	NAG	C4-C5-C6-O6
17	C	624	NAG	O5-C5-C6-O6
17	E	614	NAG	O5-C5-C6-O6
17	E	618	NAG	O5-C5-C6-O6
17	A	625	NAG	C4-C5-C6-O6
18	L	301	44E	O11-C1-C2-C3
18	N	301	44E	O11-C1-C2-C3
18	O	301	44E	O11-C1-C2-C3
17	C	623	NAG	O5-C5-C6-O6
17	F	901	NAG	C4-C5-C6-O6
17	A	625	NAG	O5-C5-C6-O6
17	C	615	NAG	O5-C5-C6-O6
17	E	614	NAG	C3-C2-N2-C7
17	C	615	NAG	C4-C5-C6-O6
17	F	901	NAG	O5-C5-C6-O6
17	E	615	NAG	O5-C5-C6-O6
17	A	632	NAG	C4-C5-C6-O6
17	A	632	NAG	C1-C2-N2-C7
17	E	610	NAG	C1-C2-N2-C7
17	E	614	NAG	C1-C2-N2-C7
17	E	617	NAG	C1-C2-N2-C7
17	C	622	NAG	C1-C2-N2-C7
17	C	624	NAG	C1-C2-N2-C7
17	A	632	NAG	C3-C2-N2-C7
17	E	610	NAG	C3-C2-N2-C7
17	E	617	NAG	C3-C2-N2-C7
17	C	624	NAG	C3-C2-N2-C7
17	A	619	NAG	C4-C5-C6-O6

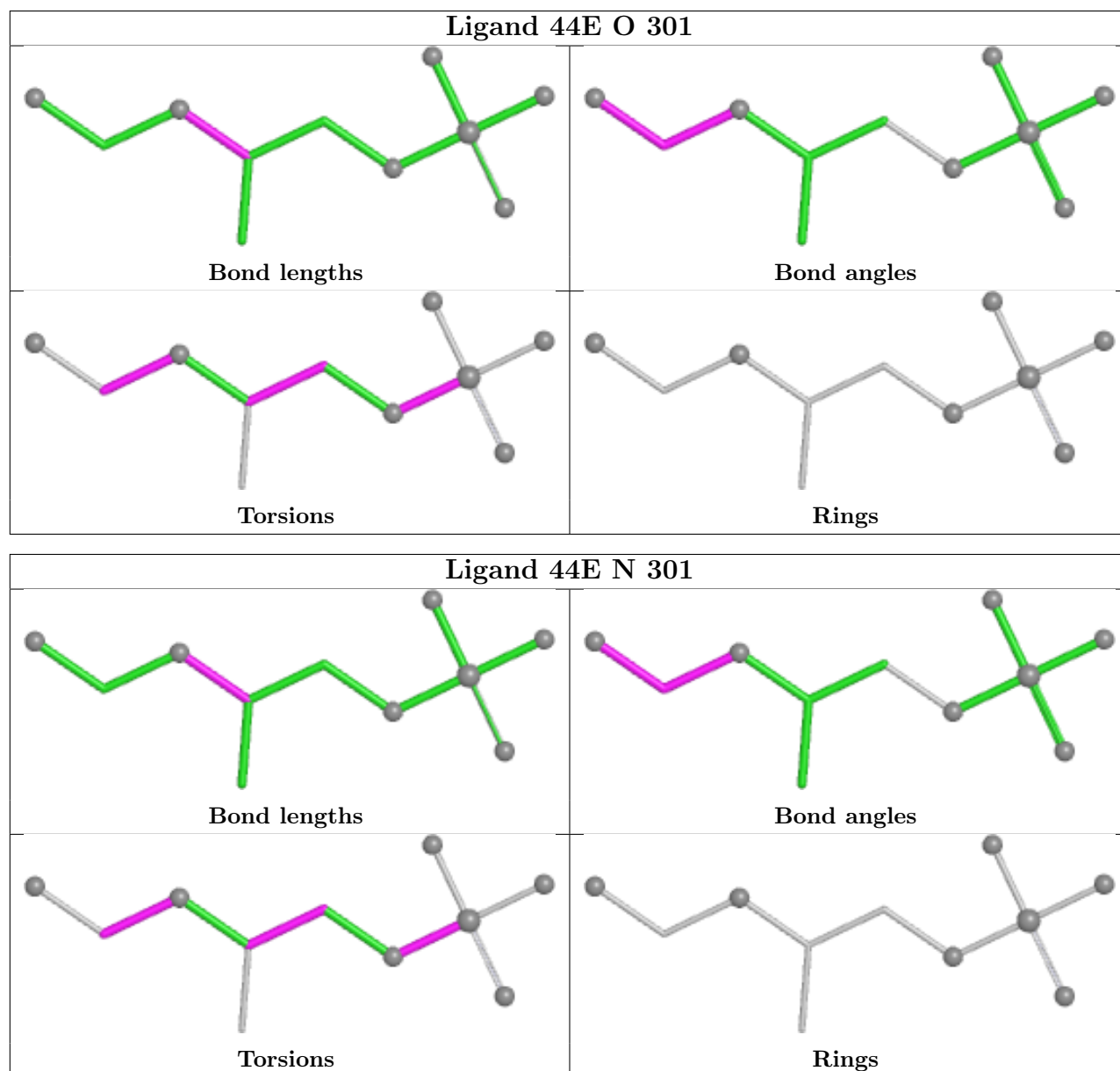
There are no ring outliers.

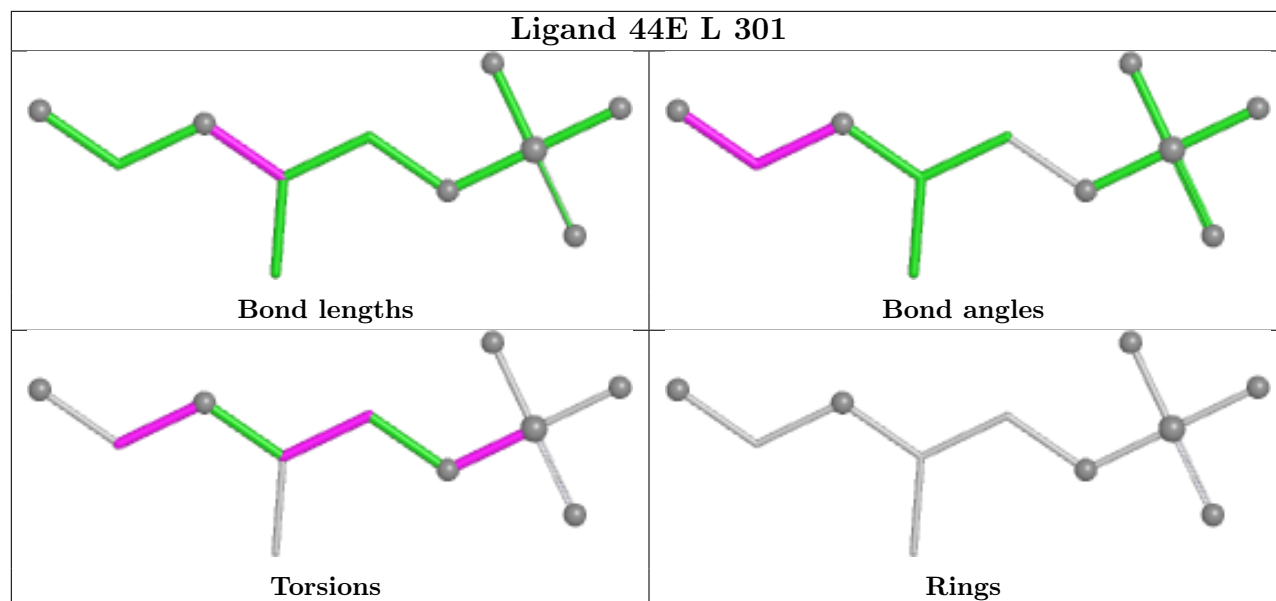
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	E	621	NAG	1	0
17	F	902	NAG	3	0
17	E	609	NAG	4	0
17	F	901	NAG	1	0
17	D	901	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

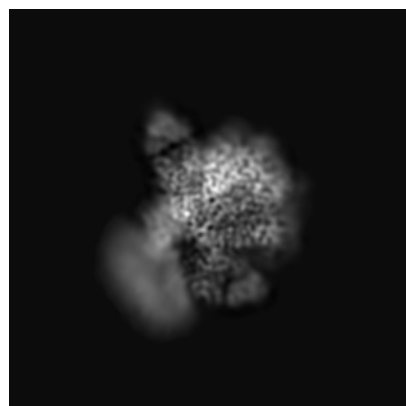
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21335. These allow visual inspection of the internal detail of the map and identification of artifacts.

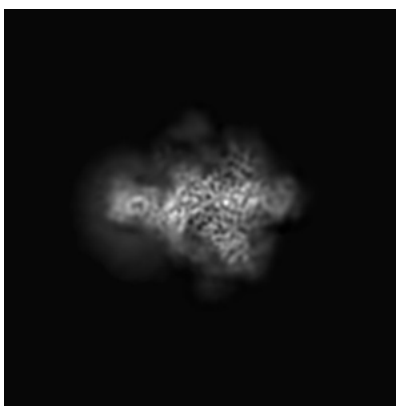
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

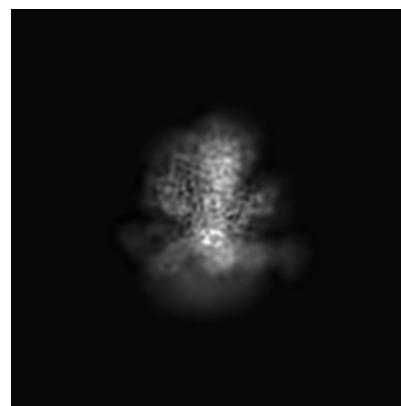
#### 6.1.1 Primary map



X

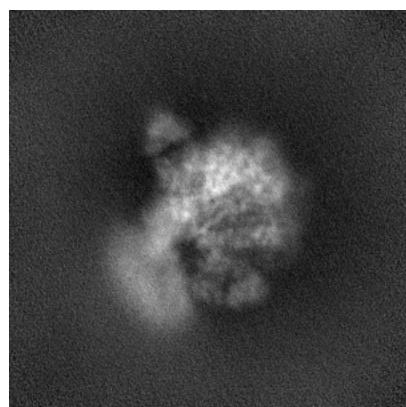


Y

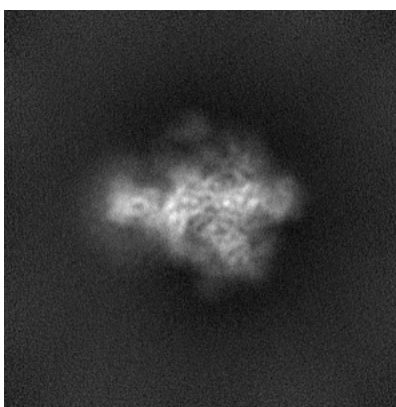


Z

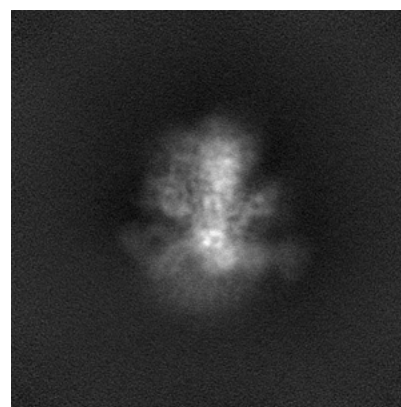
#### 6.1.2 Raw map



X



Y

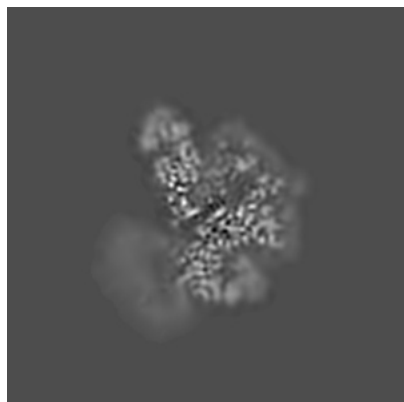


Z

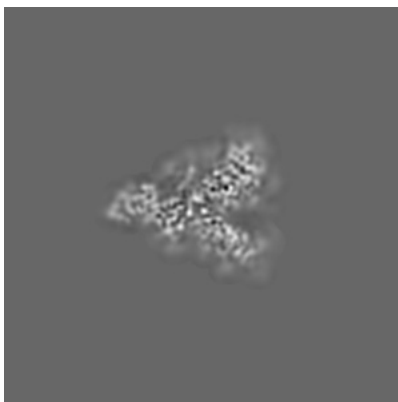
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

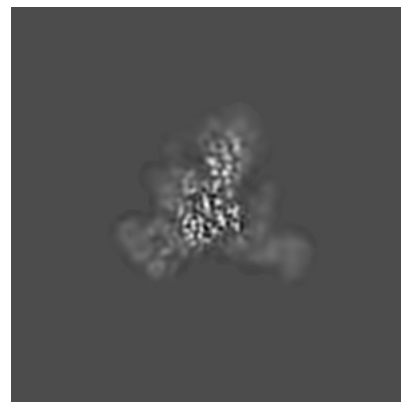
### 6.2.1 Primary map



X Index: 160

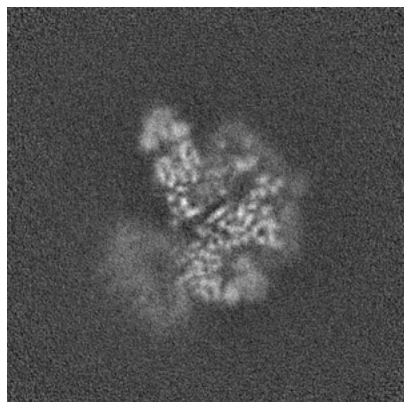


Y Index: 160

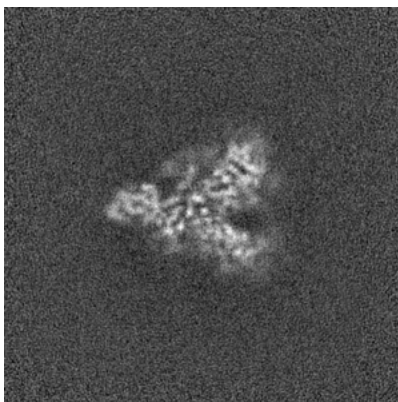


Z Index: 160

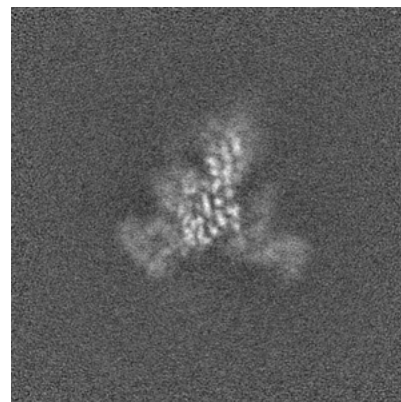
### 6.2.2 Raw map



X Index: 160



Y Index: 160

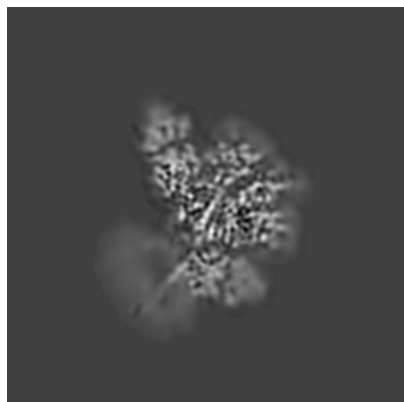


Z Index: 160

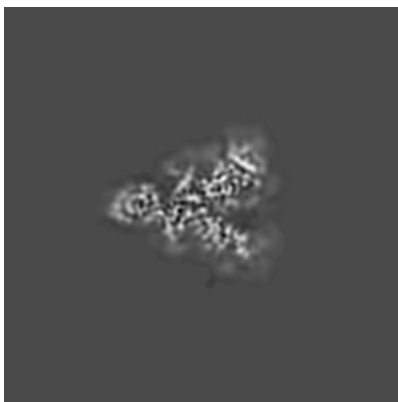
The images above show central slices of the map in three orthogonal directions.

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

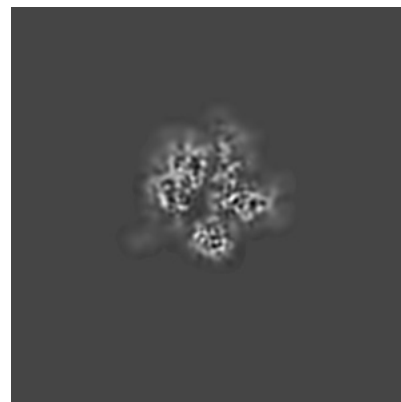
### 6.3.1 Primary map



X Index: 166

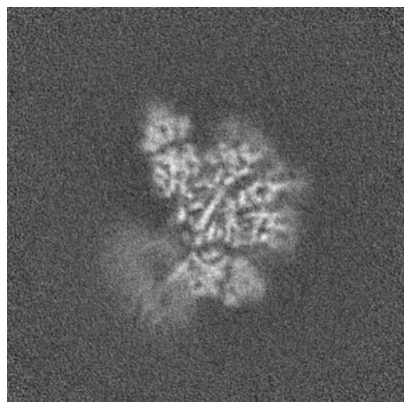


Y Index: 158

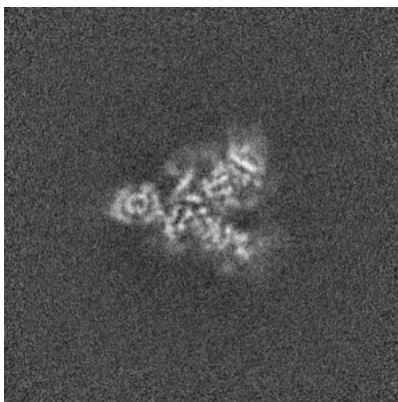


Z Index: 185

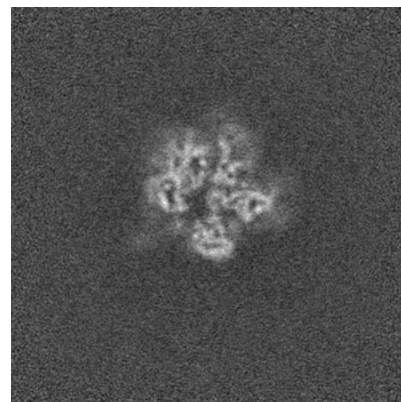
### 6.3.2 Raw map



X Index: 166



Y Index: 158



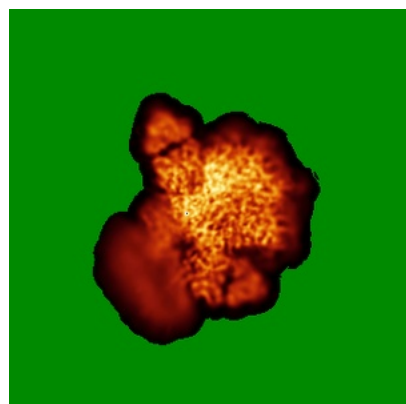
Z Index: 186

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

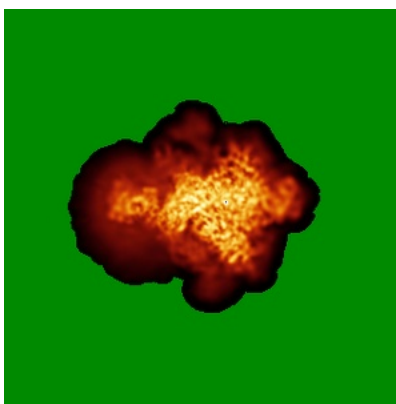


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

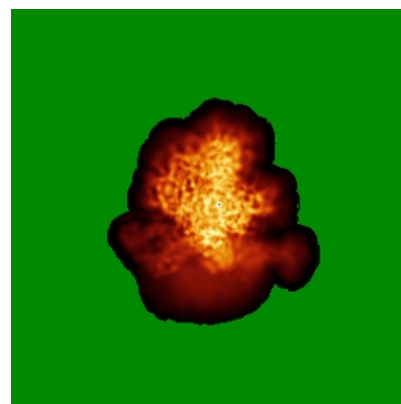
### 6.4.1 Primary map



X

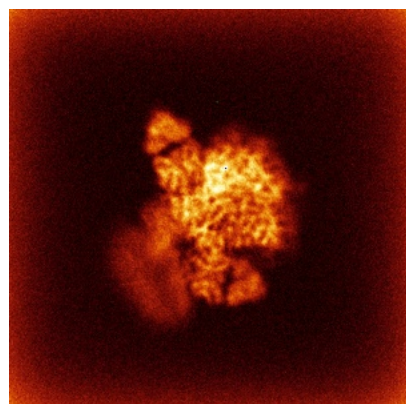


Y

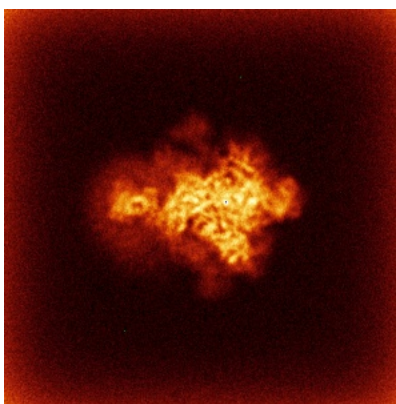


Z

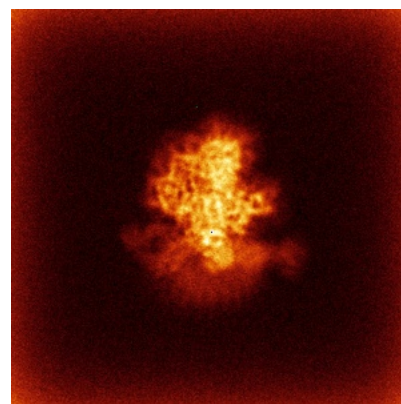
### 6.4.2 Raw map



X



Y

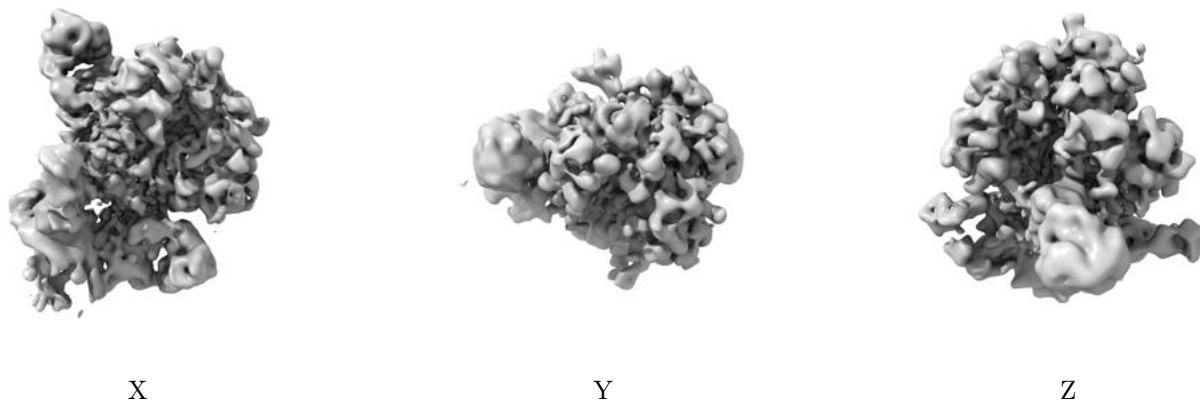


Z

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

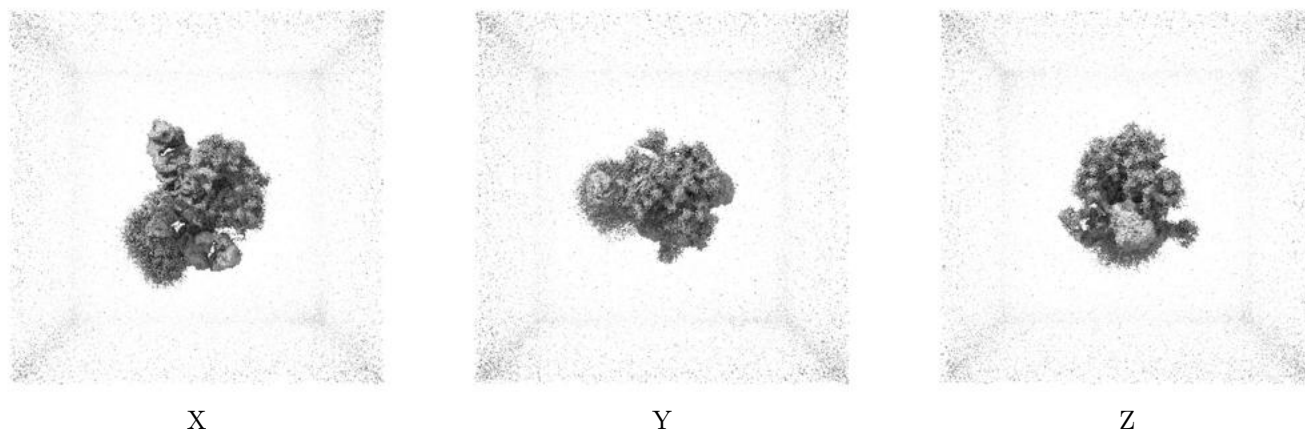
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.269. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



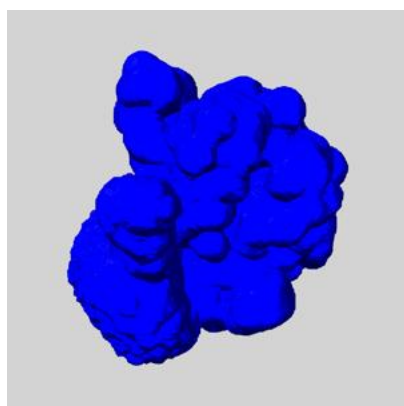
## 6.6 Mask visualisation [i](#)

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

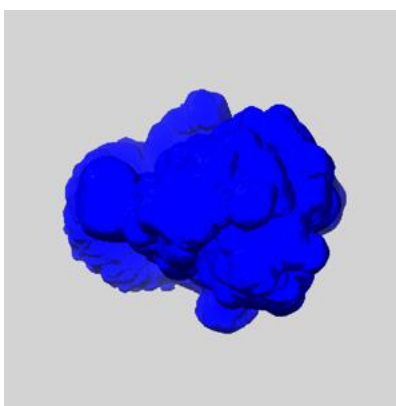
A mask typically either:

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

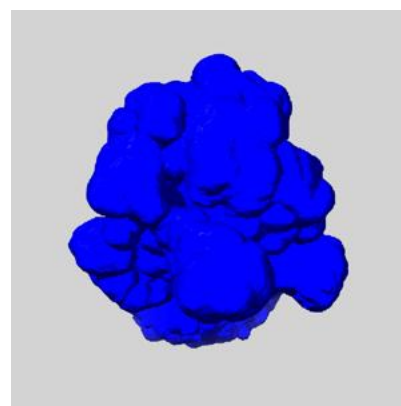
### 6.6.1 emd\_21335\_msk\_1.map [i](#)



X



Y

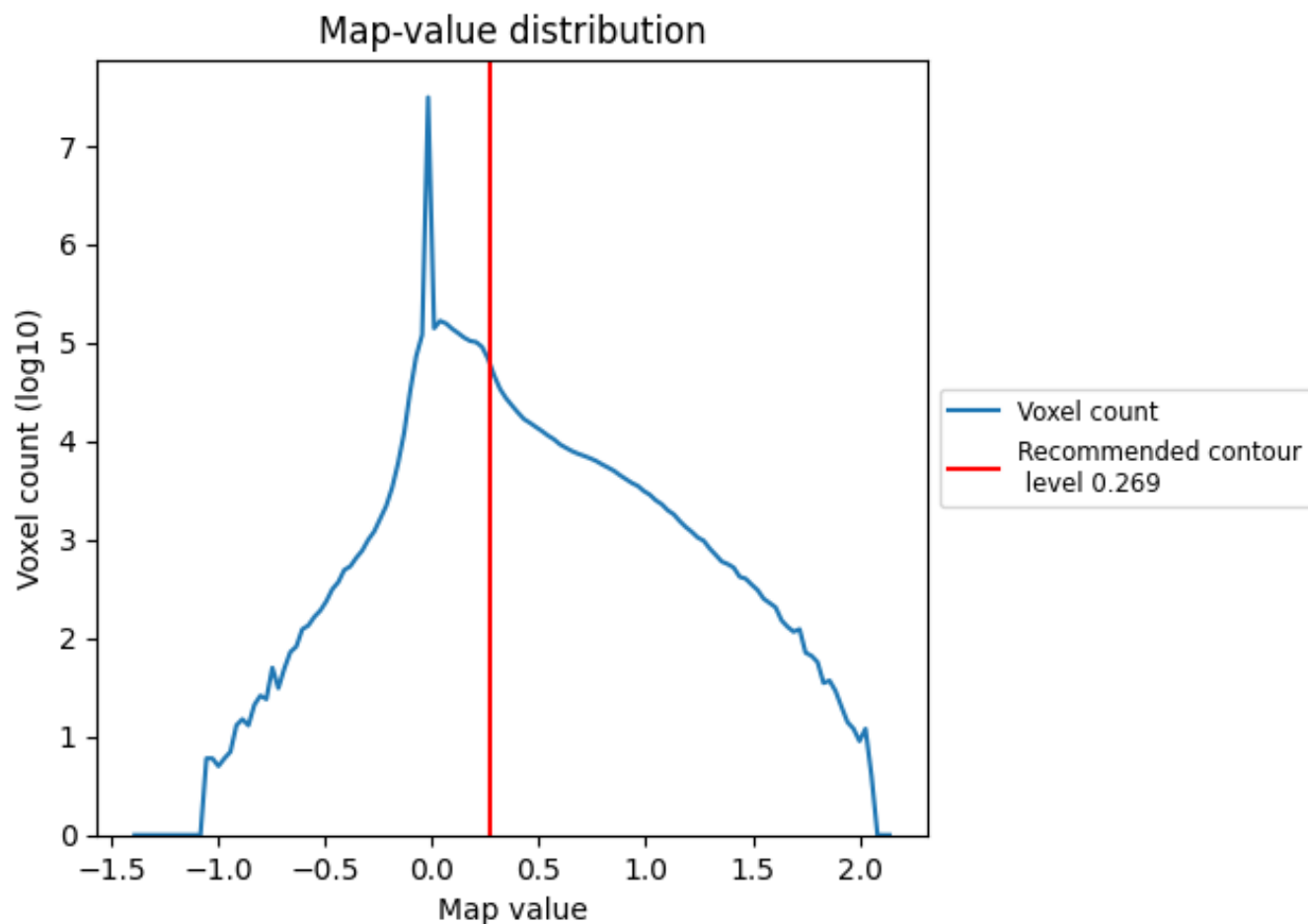


Z

## 7 Map analysis [i](#)

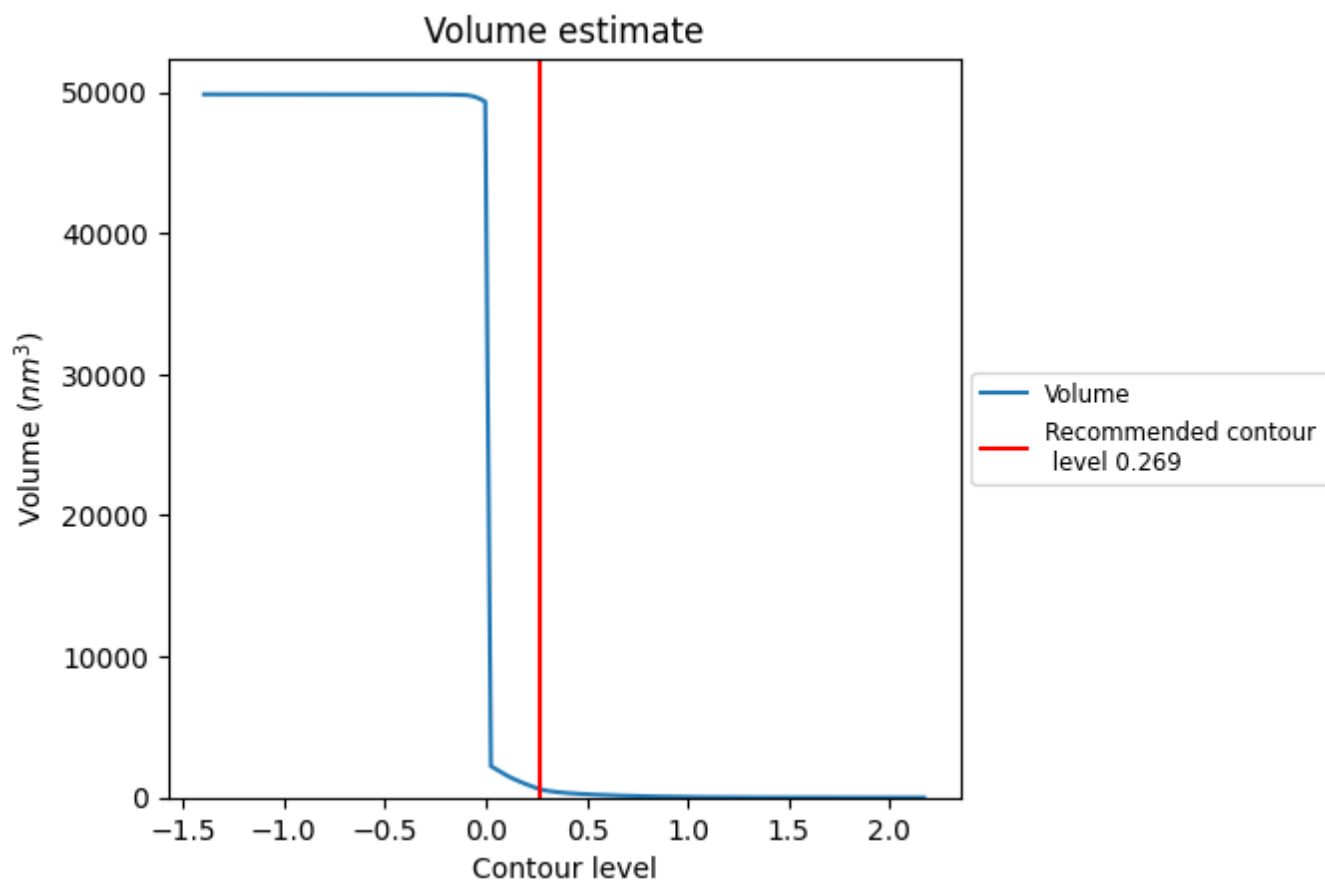
This section contains the results of statistical analysis of the map.

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



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

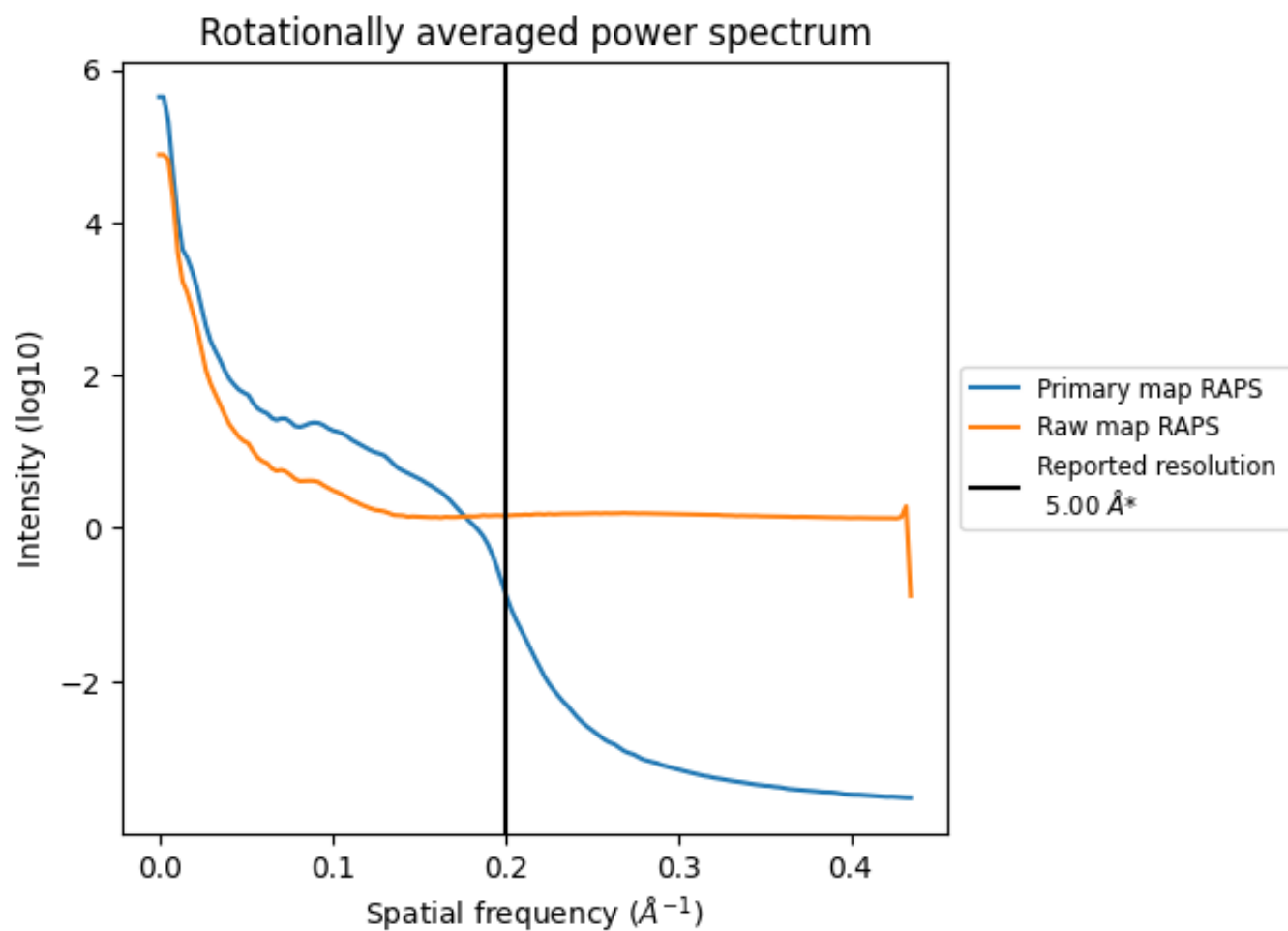
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 595  $\text{nm}^3$ ; this corresponds to an approximate mass of 538 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 ⓘ

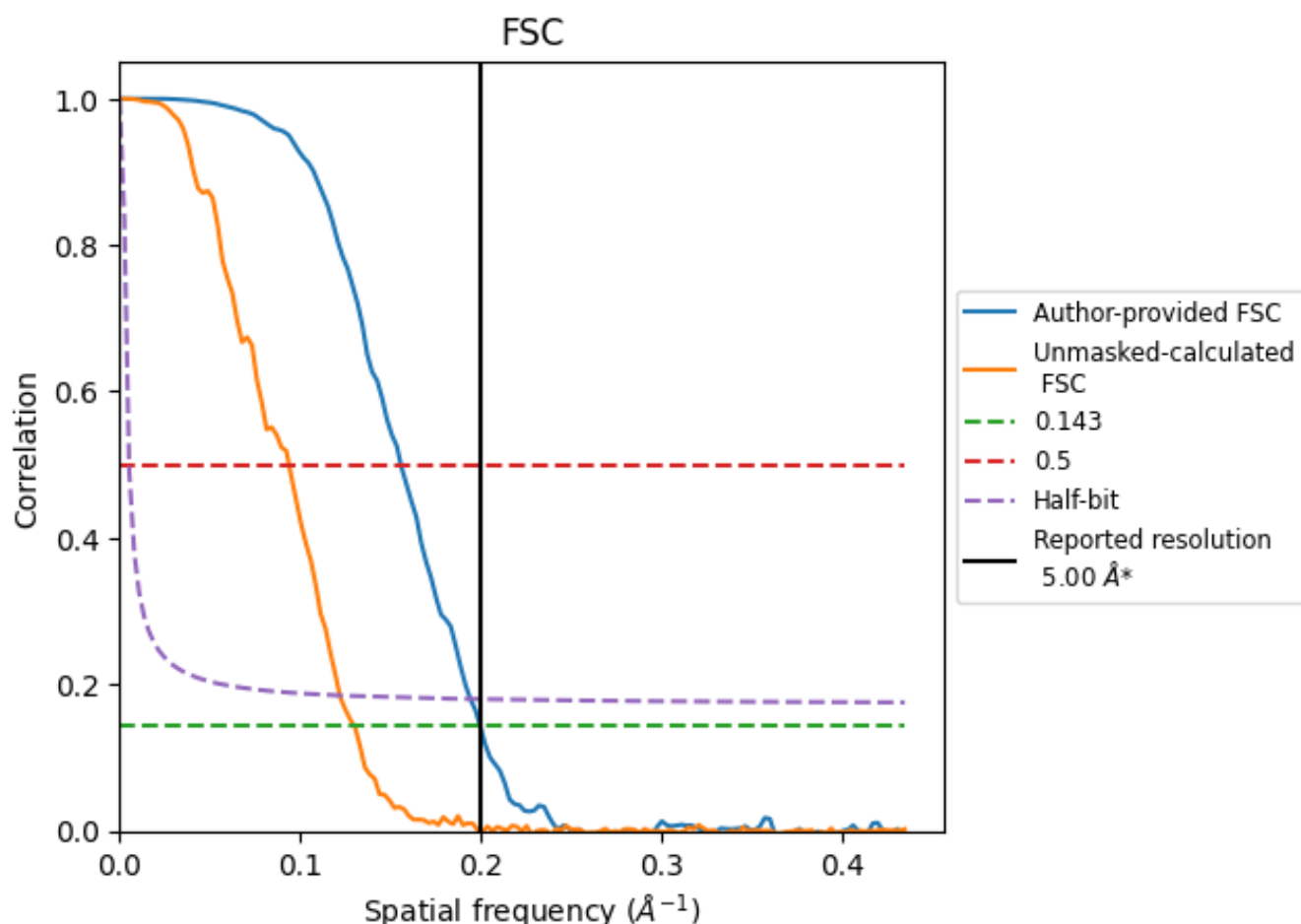


\*Reported resolution corresponds to spatial frequency of 0.200 Å<sup>-1</sup>

## 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 0.200 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

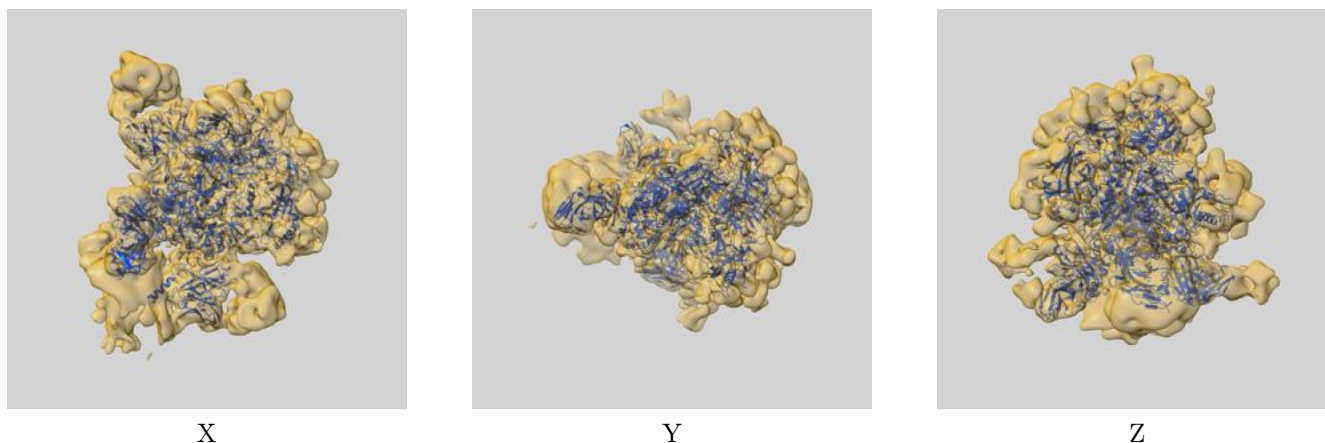
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	5.01	6.41	5.15
Unmasked-calculated*	7.69	10.65	8.20

\*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 7.69 differs from the reported value 5.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-21335 and PDB model 6VPX. Per-residue inclusion information can be found in section 3 on page 13.

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



The images above show the 3D surface view of the map at the recommended contour level 0.269 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.

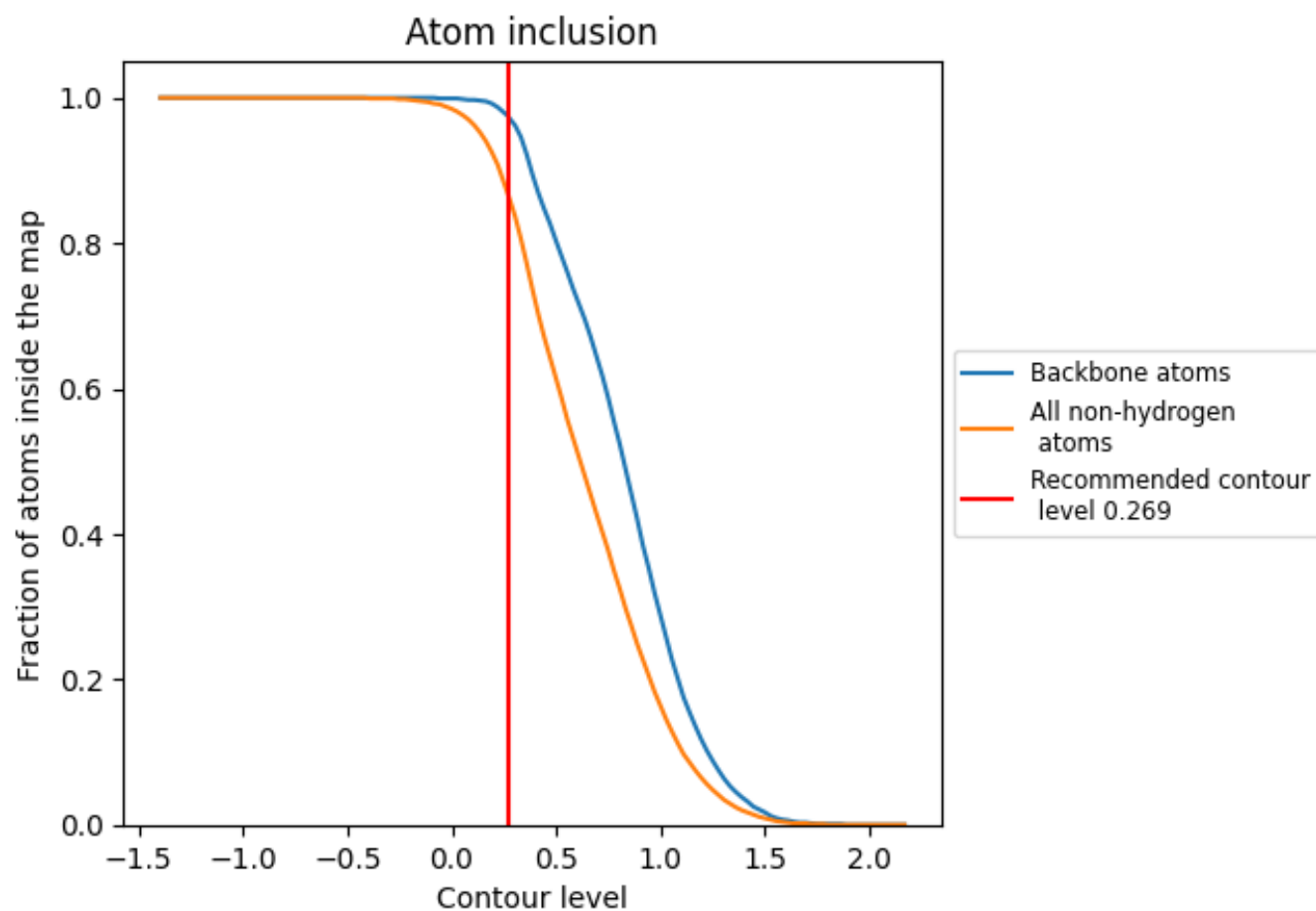
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.269).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.269) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.2000
A	 0.9030	 0.2370
B	 0.8280	 0.2080
C	 0.8940	 0.2250
D	 0.8250	 0.2090
E	 0.8770	 0.2020
F	 0.7990	 0.1590
G	 0.8270	 0.1490
H	 0.8560	 0.1220
I	 0.8070	 0.1630
J	 0.8400	 0.1490
K	 0.7620	 0.1320
L	 0.7610	 0.1090
M	 0.9010	 0.1950
N	 0.7240	 0.1460
O	 0.9150	 0.1710
P	 0.9440	 0.2340
Q	 0.9320	 0.1980
R	 1.0000	 0.3200
S	 0.8930	 0.3930
T	 0.9290	 0.2550
U	 0.9290	 0.3300
V	 0.9290	 0.2670
W	 0.9800	 0.4060
X	 1.0000	 0.2890
Y	 0.9230	 0.2810
Z	 0.9640	 0.2630
a	 0.9290	 0.2110
b	 0.8570	 0.2230
c	 0.9740	 0.3160
d	 0.8930	 0.2540
e	 1.0000	 0.3290
f	 0.7500	 0.2210
g	 0.9670	 0.4010
h	 0.9580	 0.1890



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.9640	 0.2870
j	 0.6320	 0.1860
k	 0.7370	 0.2310
l	 0.9460	 0.3150
m	 0.9480	 0.3770
n	 0.8750	 0.1690