



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:54 PM UTC

PDB ID : 9EHL / pdb_00009ehl
EMDB ID : EMD-48059
Title : Structure of HIV-1 BG505 SOSIP.664 Env trimer in complex with IOMAm5
and 10-1074 Broadly Neutralizing Antibodies - Class I
Authors : Dam, K.A.; Yang, Z.; Bjorkman, P.J.
Deposited on : 2024-11-23
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

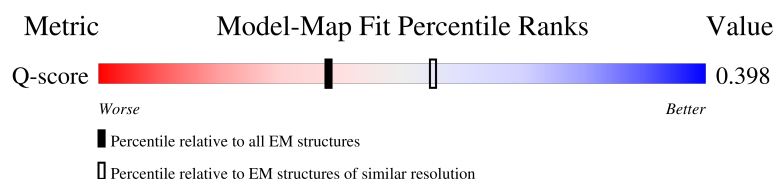
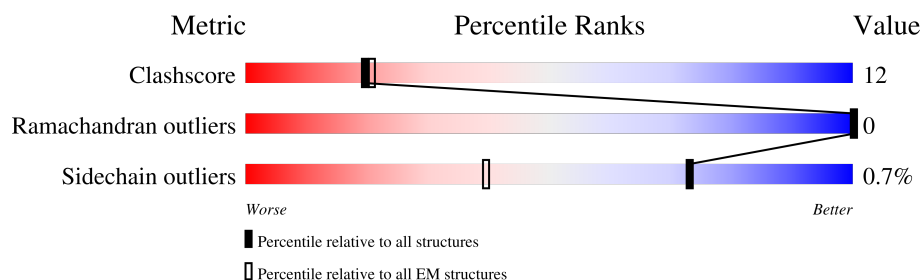
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



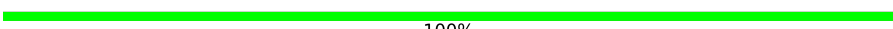
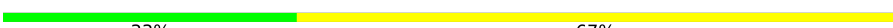
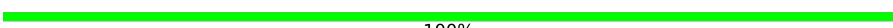
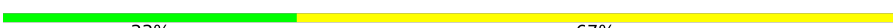
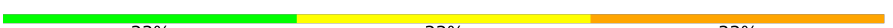
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	A	506	 63% 26% 11%
1	B	506	 62% 26% • 11%
1	C	506	 65% 23% 11%
2	D	153	 58% 25% 18%

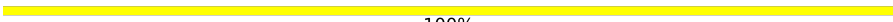
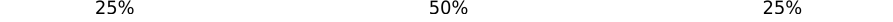
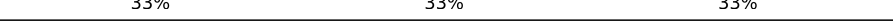
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	153	
2	F	153	
3	G	128	
3	H	128	
3	I	128	
4	J	111	
4	K	111	
4	L	111	
5	M	134	
5	N	134	
5	O	134	
6	P	110	
6	Q	110	
6	R	110	
7	S	3	
7	X	3	
7	b	3	
7	f	3	
7	i	3	
7	k	3	
7	n	3	
7	p	3	
7	r	3	
8	T	2	
8	W	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	Y	2	 100%
8	c	2	 50% 50%
8	e	2	 100%
8	g	2	 50% 50%
8	l	2	 50% 50%
8	o	2	 50% 50%
8	q	2	 50% 50%
9	U	4	 50% 50%
9	d	4	 50% 50%
9	h	4	 75% 25%
10	V	4	 75% 25%
10	m	4	 25% 50% 25%
11	Z	3	 33% 67%
12	a	6	 50% 33% 17%
12	j	6	 33% 33% 33%
13	s	6	 33% 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	NAG	C	604	X	-	-	-
7	NAG	n	1	X	-	-	-
7	NAG	p	2	X	-	-	-
8	NAG	T	1	X	-	-	-
8	NAG	T	2	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26143 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 HIV-1 BG505 SOSIP gp120,Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
1	B	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
1	C	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	engineered mutation	UNP Q2N0S5
A	501	CYS	ALA	engineered mutation	UNP Q2N0S5
A	509	ARG	-	insertion	UNP Q2N0S5
A	510	ARG	-	insertion	UNP Q2N0S5
A	511	ARG	-	insertion	UNP Q2N0S5
A	512	ARG	-	insertion	UNP Q2N0S5
A	513	ARG	-	insertion	UNP Q2N0S5
B	332	ASN	THR	engineered mutation	UNP Q2N0S5
B	501	CYS	ALA	engineered mutation	UNP Q2N0S5
B	509	ARG	-	insertion	UNP Q2N0S5
B	510	ARG	-	insertion	UNP Q2N0S5
B	511	ARG	-	insertion	UNP Q2N0S5
B	512	ARG	-	insertion	UNP Q2N0S5
B	513	ARG	-	insertion	UNP Q2N0S5
C	332	ASN	THR	engineered mutation	UNP Q2N0S5
C	501	CYS	ALA	engineered mutation	UNP Q2N0S5
C	509	ARG	-	insertion	UNP Q2N0S5
C	510	ARG	-	insertion	UNP Q2N0S5
C	511	ARG	-	insertion	UNP Q2N0S5
C	512	ARG	-	insertion	UNP Q2N0S5
C	513	ARG	-	insertion	UNP Q2N0S5

- Molecule 2 is a protein called HIV-1 BG505 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
2	E	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
2	F	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	559	PRO	ILE	engineered mutation	UNP Q2N0S5
D	605	CYS	THR	engineered mutation	UNP Q2N0S5
E	559	PRO	ILE	engineered mutation	UNP Q2N0S5
E	605	CYS	THR	engineered mutation	UNP Q2N0S5
F	559	PRO	ILE	engineered mutation	UNP Q2N0S5
F	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 3 is a protein called IOMamin5 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	127	Total	C	N	O	S	0	0
			998	632	176	182	8		
3	H	127	Total	C	N	O	S	0	0
			998	632	176	182	8		
3	I	127	Total	C	N	O	S	0	0
			998	632	176	182	8		

- Molecule 4 is a protein called IOMamin5 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	110	Total	C	N	O	S	0	0
			801	498	135	165	3		
4	K	110	Total	C	N	O	S	0	0
			801	498	135	165	3		
4	L	110	Total	C	N	O	S	0	0
			801	498	135	165	3		

- Molecule 5 is a protein called 10-1074 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	134	Total	C	N	O	S	0	0
			1047	660	176	207	4		

Continued on next page...

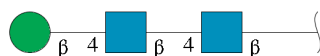
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	134	Total	C	N	O	S	0	0
			1047	660	176	207	4		
5	O	134	Total	C	N	O	S	0	0
			1047	660	176	207	4		

- Molecule 6 is a protein called 10-1074 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	109	Total	C	N	O	S	0	0
			840	525	155	157	3		
6	Q	109	Total	C	N	O	S	0	0
			840	525	155	157	3		
6	R	109	Total	C	N	O	S	0	0
			840	525	155	157	3		

- Molecule 7 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.



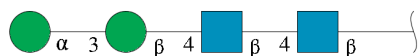
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	3	Total	C	N	O	0	0
			39	22	2	15		
7	X	3	Total	C	N	O	0	0
			39	22	2	15		
7	b	3	Total	C	N	O	0	0
			39	22	2	15		
7	f	3	Total	C	N	O	0	0
			39	22	2	15		
7	i	3	Total	C	N	O	0	0
			39	22	2	15		
7	k	3	Total	C	N	O	0	0
			39	22	2	15		
7	n	3	Total	C	N	O	0	0
			39	22	2	15		
7	p	3	Total	C	N	O	0	0
			39	22	2	15		
7	r	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	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	g	2	Total	C	N	O	0	0
			28	16	2	10		
8	l	2	Total	C	N	O	0	0
			28	16	2	10		
8	o	2	Total	C	N	O	0	0
			28	16	2	10		
8	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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
9	U	4	Total	C	N	O	0	0
			50	28	2	20		
9	d	4	Total	C	N	O	0	0
			50	28	2	20		
9	h	4	Total	C	N	O	0	0
			50	28	2	20		

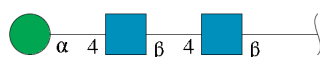
- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



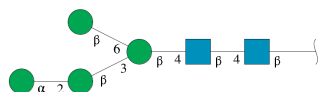
Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	4	Total	C	N	O	0	0
			50	28	2	20		
10	m	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



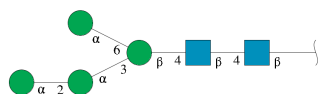
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-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.



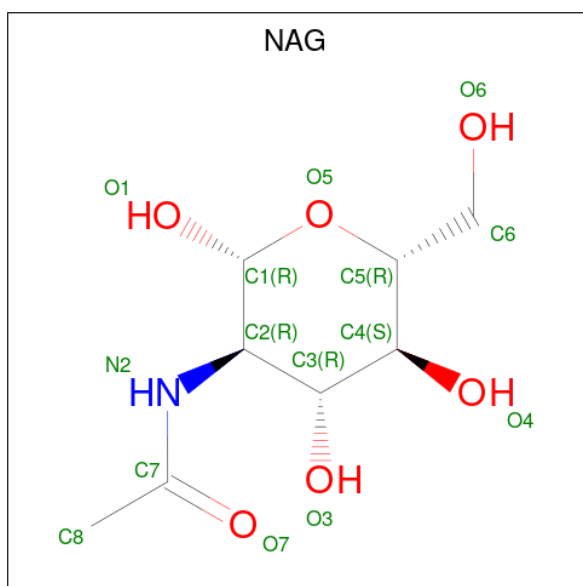
Mol	Chain	Residues	Atoms				AltConf	Trace
12	a	6	Total	C	N	O	0	0
			72	40	2	30		
12	j	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	s	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

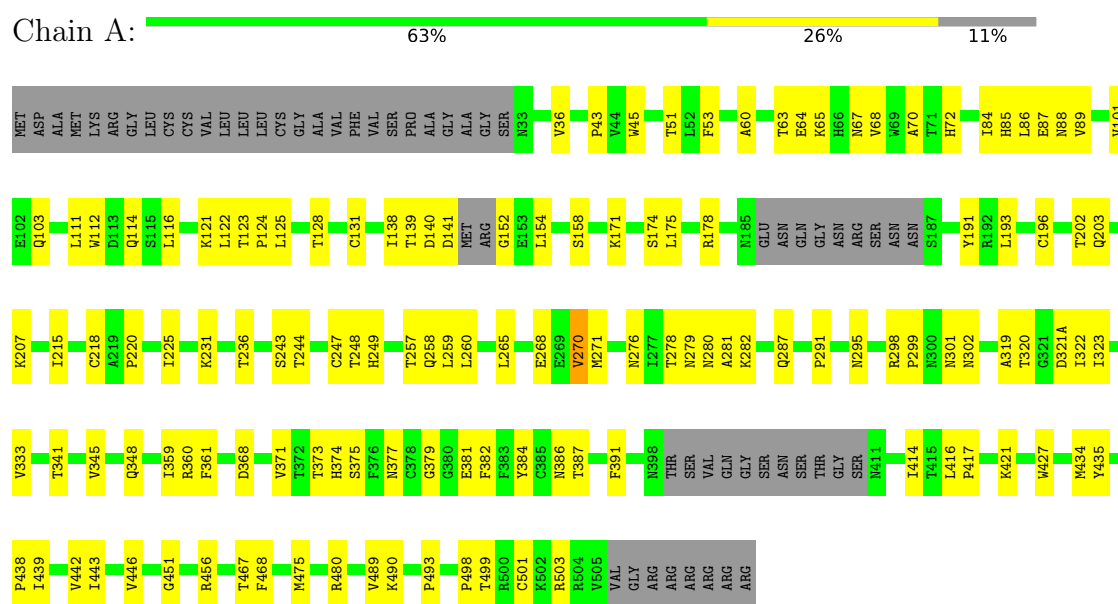
Continued from previous page...

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

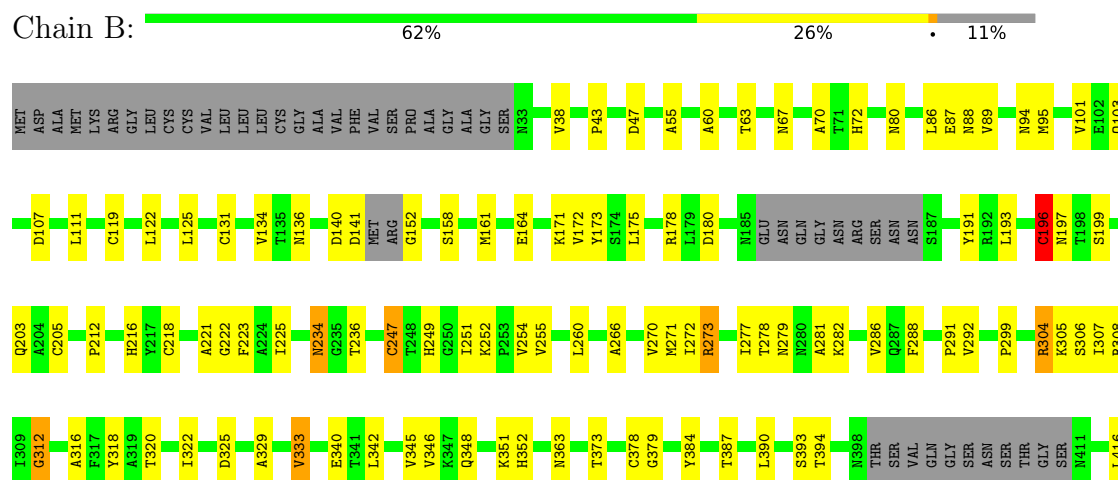
3 Residue-property plots

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

• Molecule 1: HIV-1 BG505 SOSIP gp120,Envelope glycoprotein gp120



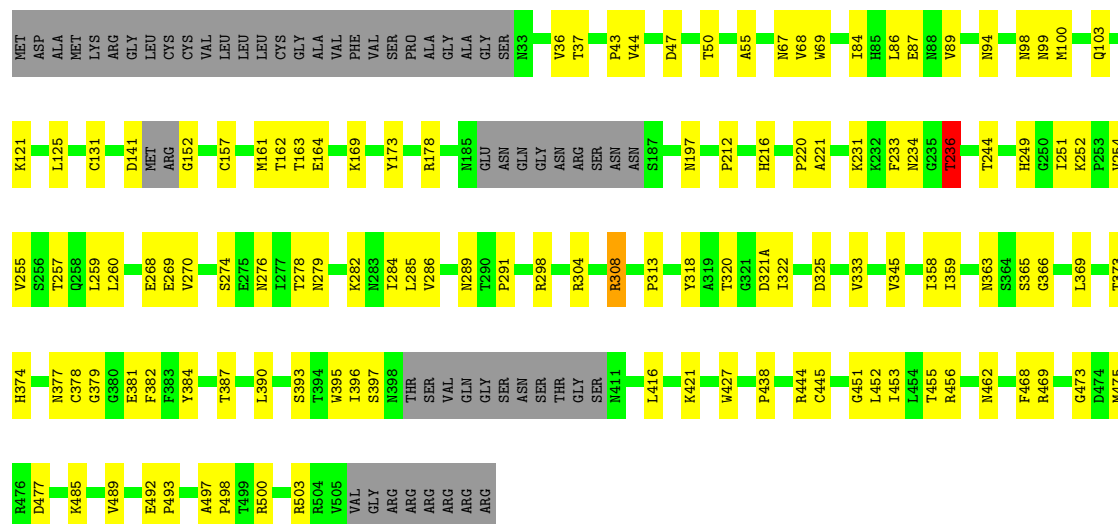
• Molecule 1: HIV-1 BG505 SOSIP gp120,Envelope glycoprotein gp120





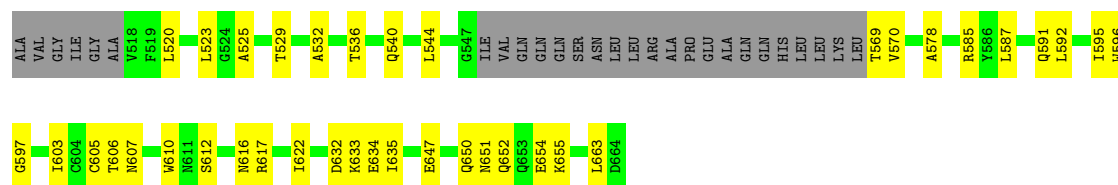
- Molecule 1: HIV-1 BG505 SOSIP gp120,Envelope glycoprotein gp120

Chain C: 65% 23% 11%



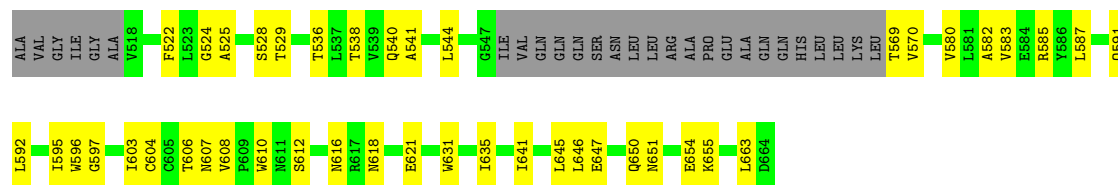
- Molecule 2: HIV-1 BG505 SOSIP gp41

Chain D: 58% 25% 18%



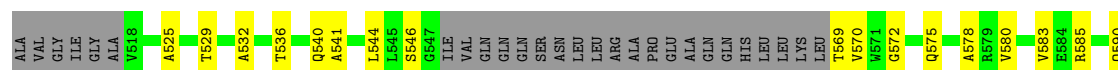
- Molecule 2: HIV-1 BG505 SOSIP gp41

Chain E: 54% 28% 18%



- Molecule 2: HIV-1 BG505 SOSIP gp41

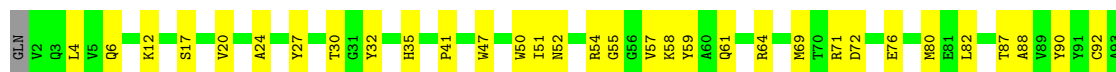
Chain F: 60% 22% 18%





• Molecule 3: IOMamin5 Fab Heavy Chain

Chain G: 63% 36%



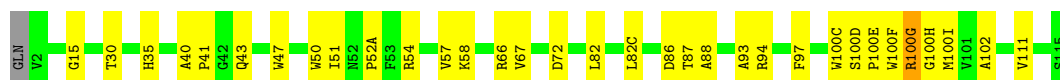
• Molecule 3: IOMamin5 Fab Heavy Chain

Chain H: 70% 30%



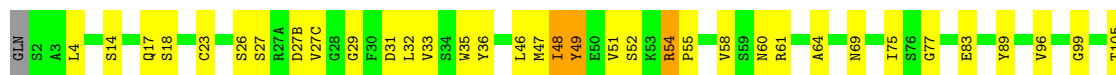
• Molecule 3: IOMamin5 Fab Heavy Chain

Chain I: 73% 25%



• Molecule 4: IOMamin5 Fab Light Chain

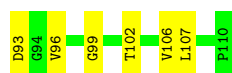
Chain J: 67% 30%



• Molecule 4: IOMamin5 Fab Light Chain

Chain K: 58% 39%





- Molecule 4: IOMamin5 Fab Light Chain

Chain L: 79% 20%



- Molecule 5: 10-1074 Fab Heavy Chain

Chain M: 74% 26%



- Molecule 5: 10-1074 Fab Heavy Chain

Chain N: 73% 27%



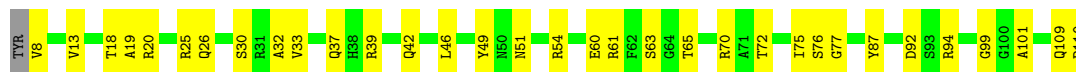
- Molecule 5: 10-1074 Fab Heavy Chain

Chain O: 73% 27%



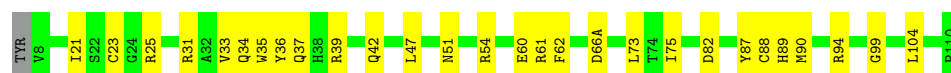
- Molecule 6: 10-1074 Fab Light Chain

Chain P: 69% 30%



- Molecule 6: 10-1074 Fab Light Chain

Chain Q:  74% 25%

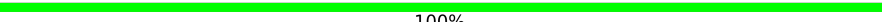


- Molecule 6: 10-1074 Fab Light Chain

Chain R:  69% 29%



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

Chain S:  100%



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

Chain X:  67% 33%

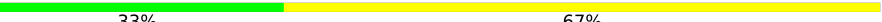


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  67% 33%

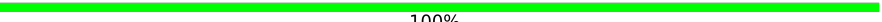


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  33% 67%



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

Chain i:  100%



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

Chain k:  33% 67%

 MAG1
MAG2
BMA3

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

Chain n:  33% 67%

 MAG1
MAG2
BMA3

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

Chain p:  33% 33% 33%

 MAG1
MAG2
BMA3

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

Chain r:  67% 33%

 MAG1
MAG2
BMA3

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

Chain T:  50% 50%

 MAG1
MAG2

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

Chain W:  100%

 MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

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

Chain e:  100%

MAG1
MAG2

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

Chain g:  50% 50%

MAG1
MAG2

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

Chain i:  50% 50%

MAG1
MAG2

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

Chain o:  50% 50%

MAG1
MAG2

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

Chain q:  50% 50%

MAG1
MAG2

- Molecule 9: 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 U:  50% 50%

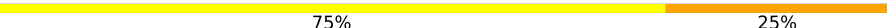


- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50% 50%



- Molecule 9: 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 h:  75% 25%

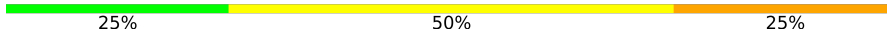


- Molecule 10: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  75% 25%



- Molecule 10: beta-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 m:  25% 50% 25%



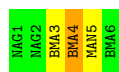
- Molecule 11: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  33% 67%

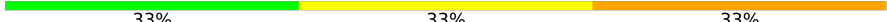


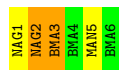
- Molecule 12: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 33% 17%



- Molecule 12: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[beta-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 j:  33% 33% 33%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.000283	Depositor
Map size (Å)	299.52002, 299.52002, 299.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3605	0.48	0/4895
1	B	0.49	0/3605	0.60	0/4895
1	C	0.49	0/3605	0.59	2/4895 (0.0%)
2	D	0.17	0/1019	0.35	0/1382
2	E	0.17	0/1019	0.38	0/1382
2	F	0.16	0/1019	0.35	0/1382
3	G	0.16	0/1026	0.35	0/1390
3	H	0.15	0/1026	0.36	0/1390
3	I	0.19	0/1026	0.50	2/1390 (0.1%)
4	J	0.36	0/818	0.46	0/1109
4	K	0.45	0/818	0.56	0/1109
4	L	0.44	0/818	0.50	0/1109
5	M	0.12	0/1072	0.32	0/1459
5	N	0.11	0/1072	0.29	0/1459
5	O	0.11	0/1072	0.31	0/1459
6	P	0.12	0/862	0.36	0/1172
6	Q	0.13	0/862	0.35	0/1172
6	R	0.36	0/862	0.49	1/1172 (0.1%)
All	All	0.34	0/25206	0.47	5/34221 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4
1	C	0	1
4	J	0	1
4	K	0	1
6	R	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	100(H)	GLY	N-CA-C	8.71	122.28	110.69
1	C	197	ASN	N-CA-C	-5.97	107.23	114.75
3	I	100(G)	ARG	N-CA-C	5.70	117.49	111.28
1	C	236	THR	CA-CB-OG1	-5.51	101.33	109.60
6	R	66(B)	ILE	N-CA-C	-5.07	107.77	112.43

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	CYS	Peptide
1	B	273	ARG	Sidechain
1	B	304	ARG	Sidechain
1	B	312	GLY	Peptide
1	C	308	ARG	Sidechain
4	J	54	ARG	Sidechain
4	K	61	ARG	Sidechain
6	R	70	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3532	0	3460	96	0
1	B	3532	0	3459	102	0
1	C	3532	0	3462	91	0
2	D	1001	0	976	32	0
2	E	1001	0	976	36	0
2	F	1001	0	976	27	0
3	G	998	0	955	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	998	0	955	30	0
3	I	998	0	954	48	0
4	J	801	0	768	28	0
4	K	801	0	768	36	0
4	L	801	0	768	19	0
5	M	1047	0	1010	28	0
5	N	1047	0	1010	23	0
5	O	1047	0	1010	27	0
6	P	840	0	803	23	0
6	Q	840	0	803	21	0
6	R	840	0	803	21	0
7	S	39	0	34	0	0
7	X	39	0	34	0	0
7	b	39	0	34	0	0
7	f	39	0	34	1	0
7	i	39	0	34	0	0
7	k	39	0	34	2	0
7	n	39	0	34	5	0
7	p	39	0	34	1	0
7	r	39	0	34	1	0
8	T	28	0	25	2	0
8	W	28	0	25	0	0
8	Y	28	0	25	0	0
8	c	28	0	25	1	0
8	e	28	0	25	1	0
8	g	28	0	25	1	0
8	l	28	0	25	0	0
8	o	28	0	25	0	0
8	q	28	0	25	0	0
9	U	50	0	43	0	0
9	d	50	0	43	3	0
9	h	50	0	43	4	0
10	V	50	0	43	1	0
10	m	50	0	43	3	0
11	Z	39	0	34	2	0
12	a	72	0	61	1	0
12	j	72	0	61	5	0
13	s	72	0	61	5	0
14	A	98	0	91	4	0
14	B	98	0	91	6	0
14	C	98	0	91	4	0
14	D	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	28	0	26	0	0
14	F	28	0	26	0	0
All	All	26143	0	25230	640	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 12.

All (640) 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)
3:I:100(E):PRO:HG2	4:L:32:LEU:HD21	1.18	1.14
1:C:278:THR:HG22	7:n:1:NAG:HN2	1.12	1.09
3:I:100(C):TRP:HD1	3:I:100(F):TRP:N	1.49	1.08
3:I:100(C):TRP:CD1	3:I:100(F):TRP:H	1.71	1.07
3:I:100(E):PRO:CG	4:L:32:LEU:HD21	1.76	1.05
3:I:100(C):TRP:CD1	3:I:100(F):TRP:HA	1.99	0.98
3:I:100(E):PRO:HG2	4:L:32:LEU:CD2	2.00	0.92
3:I:100(C):TRP:CD1	3:I:100(F):TRP:CA	2.58	0.85
5:M:17:THR:HA	5:M:82:LEU:O	1.75	0.85
3:I:100(C):TRP:CD1	3:I:100(F):TRP:N	2.35	0.84
3:G:87:THR:HG23	3:G:110:THR:HA	1.61	0.81
5:O:36:TRP:HE1	5:O:78:LEU:HD22	1.46	0.81
1:C:212:PRO:HB2	1:C:252:LYS:HB3	1.62	0.81
1:C:278:THR:CG2	7:n:1:NAG:HN2	1.92	0.80
3:I:100(C):TRP:NE1	3:I:100(F):TRP:HA	1.97	0.80
3:I:100(C):TRP:HD1	3:I:100(F):TRP:H	0.84	0.80
1:A:218:CYS:HA	1:A:247:CYS:HB3	1.65	0.78
1:B:87:GLU:H	14:B:602:NAG:H82	1.48	0.77
5:M:18:LEU:HB3	5:M:82:LEU:HD13	1.67	0.76
1:A:225:ILE:HD12	1:A:247:CYS:HA	1.71	0.73
6:P:26:GLN:HE22	6:P:70:ARG:HG2	1.53	0.73
1:A:499:THR:HG23	1:A:501:CYS:H	1.55	0.72
3:I:100(D):SER:N	3:I:100(E):PRO:CD	2.51	0.72
1:C:231:LYS:HB3	1:C:268:GLU:HG2	1.71	0.72
1:B:286:VAL:HB	1:B:452:LEU:HB2	1.72	0.72
4:J:47:MET:HA	4:J:58:VAL:HG21	1.72	0.72
4:J:46:LEU:HD21	4:J:49:TYR:HB3	1.71	0.72
1:C:291:PRO:HG3	14:C:607:NAG:H82	1.73	0.71
6:R:12:SER:HB3	6:R:107:LEU:HD22	1.73	0.70
1:A:384:TYR:HE1	1:A:421:LYS:HB3	1.55	0.70
1:C:87:GLU:HB2	14:C:602:NAG:HN2	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:NE2	1:A:371:VAL:O	2.24	0.70
4:J:89:TYR:HE1	4:J:96:VAL:HG13	1.56	0.70
2:D:595:ILE:O	2:D:651:ASN:ND2	2.24	0.69
5:N:3:GLN:HE22	5:N:5:GLN:HB2	1.58	0.69
5:M:100:ARG:NH1	6:P:30:SER:OG	2.25	0.69
2:F:525:ALA:HB3	2:F:536:THR:HG21	1.75	0.69
4:J:29:GLY:HA2	11:Z:3:MAN:H2	1.75	0.68
1:B:266:ALA:HB1	1:B:271:MET:HG2	1.76	0.68
1:C:152:GLY:HA3	1:C:178:ARG:HH21	1.58	0.68
6:Q:37:GLN:HB2	6:Q:47:LEU:HD11	1.76	0.67
1:A:291:PRO:HG3	14:A:607:NAG:H82	1.77	0.67
1:B:272:ILE:HG22	1:B:286:VAL:HG22	1.77	0.67
1:C:278:THR:HG22	7:n:1:NAG:N2	1.98	0.67
5:N:39:GLN:HB2	5:N:45:LEU:HD23	1.77	0.67
2:E:595:ILE:HD12	2:F:602:LEU:HD11	1.77	0.66
2:E:591:GLN:NE2	2:F:541:ALA:O	2.28	0.66
3:H:94:ARG:HB2	3:H:102:ALA:HB3	1.77	0.66
1:C:43:PRO:HG3	2:F:540:GLN:HE22	1.61	0.66
3:I:100(I):MET:O	4:L:46:LEU:HD22	1.97	0.65
4:K:35:TRP:HB2	4:K:48:ILE:HB	1.78	0.65
1:C:94:ASN:HA	1:C:236:THR:HG22	1.78	0.65
5:M:2:VAL:HA	5:M:25:SER:O	1.97	0.65
5:M:54:ARG:NH1	5:M:56:SER:O	2.29	0.64
6:Q:21:ILE:HB	6:Q:73:LEU:HB3	1.79	0.64
1:C:308:ARG:HH22	9:h:1:NAG:H81	1.60	0.64
4:L:27(B):ASP:HB3	4:L:92:ALA:HB2	1.79	0.64
1:B:340:GLU:HG2	14:B:601:NAG:H62	1.78	0.64
5:N:37:ILE:HB	5:N:91:TYR:HB2	1.78	0.64
1:B:70:ALA:HA	1:B:111:LEU:HD21	1.80	0.64
3:G:41:PRO:HD3	3:G:88:ALA:HA	1.80	0.64
1:C:387:THR:HG22	1:C:416:LEU:HD13	1.79	0.63
5:N:27:ASP:OD2	5:N:31:ASN:ND2	2.31	0.63
1:C:322:ILE:O	6:R:94:ARG:NH1	2.30	0.63
6:P:54:ARG:NH1	6:P:60:GLU:OE1	2.31	0.63
1:C:456:ARG:NH1	4:L:93:ASP:OD1	2.31	0.63
4:L:23:CYS:HB3	4:L:71:ALA:HB3	1.79	0.63
1:B:140:ASP:OD2	1:B:152:GLY:N	2.32	0.63
1:B:453:ILE:HG21	1:B:472:GLY:HA3	1.81	0.63
3:I:100(E):PRO:CG	4:L:32:LEU:CD2	2.58	0.63
1:C:270:VAL:HG21	1:C:345:VAL:HA	1.80	0.63
1:A:298:ARG:NH1	1:A:381:GLU:OE1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:HG11	1:B:307:ILE:HG21	1.80	0.63
1:B:304:ARG:HD2	1:B:438:PRO:HG2	1.78	0.63
1:C:445:CYS:HA	10:m:2:NAG:H2	1.81	0.62
1:A:320:THR:HG22	1:A:438:PRO:HB3	1.80	0.62
4:K:46:LEU:HD21	4:K:49:TYR:HB3	1.79	0.62
2:F:590:GLN:HE22	2:F:601:LYS:HE3	1.65	0.62
1:B:333:VAL:HG11	1:B:390:LEU:HD21	1.81	0.62
6:Q:51:ASN:HB2	12:j:5:MAN:H62	1.80	0.62
6:P:8:VAL:HG12	6:P:101:ALA:HB3	1.81	0.62
1:C:384:TYR:HE2	1:C:421:LYS:HD3	1.65	0.62
3:G:35:HIS:HD2	3:G:50:TRP:HB3	1.64	0.62
2:F:660:LEU:HA	2:F:663:LEU:HG	1.82	0.61
4:J:18:SER:HA	4:J:75:ILE:O	2.00	0.61
3:H:41:PRO:HD3	3:H:88:ALA:HA	1.82	0.61
1:C:492:GLU:OE2	2:F:585:ARG:NH2	2.34	0.61
3:I:35:HIS:HD2	3:I:50:TRP:HB3	1.65	0.61
1:A:360:ARG:HB3	1:A:467:THR:HG22	1.83	0.61
3:H:4:LEU:HD11	3:H:94:ARG:HG3	1.81	0.61
5:M:94:THR:OG1	5:M:101:ASP:OD1	2.18	0.61
1:A:70:ALA:HA	1:A:111:LEU:HD21	1.82	0.61
2:D:591:GLN:NE2	2:E:541:ALA:O	2.34	0.61
1:C:269:GLU:HA	1:C:289:ASN:HD22	1.65	0.61
1:A:387:THR:HG22	1:A:416:LEU:HD13	1.81	0.61
2:E:525:ALA:HB3	2:E:536:THR:HG21	1.82	0.61
1:B:387:THR:HA	1:B:416:LEU:HD22	1.81	0.60
2:D:634:GLU:HG3	2:D:635:ILE:HG12	1.82	0.60
3:I:40:ALA:HB3	3:I:43:GLN:HB3	1.83	0.60
6:R:9:ARG:HH11	6:R:11:LEU:HD11	1.65	0.60
6:R:39:ARG:HB2	6:R:42:GLN:HB3	1.82	0.60
1:B:279:ASN:HB3	1:B:282:LYS:HG2	1.84	0.60
3:H:19:THR:HG23	9:h:4:MAN:H61	1.83	0.60
1:B:225:ILE:HG12	1:B:488:VAL:HG12	1.82	0.60
3:G:24:ALA:HB1	3:G:27:TYR:HE1	1.67	0.60
3:G:100(C):TRP:CH2	3:G:100(F):TRP:HA	2.37	0.60
1:A:152:GLY:HA3	1:A:178:ARG:HE	1.67	0.60
1:B:55:ALA:HB3	1:B:216:HIS:HB2	1.84	0.60
2:D:612:SER:O	2:D:616:ASN:ND2	2.33	0.60
5:O:12:VAL:HG21	5:O:18:LEU:HD21	1.84	0.60
1:B:125:LEU:HA	1:B:161:MET:HE1	1.84	0.59
1:C:444:ARG:H	10:m:3:BMA:H62	1.67	0.59
1:C:503:ARG:HH21	2:F:606:THR:HG22	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:100(C):TRP:H	3:H:100(G):ARG:HH22	1.51	0.59
4:J:46:LEU:HG	4:J:55:PRO:HG3	1.84	0.59
3:G:4:LEU:HD11	3:G:94:ARG:HG3	1.85	0.59
1:A:270:VAL:HG13	1:A:348:GLN:HG3	1.84	0.59
3:G:59:TYR:O	3:G:64:ARG:NH2	2.36	0.59
3:H:95:GLU:HA	3:H:100(I):MET:HA	1.84	0.58
1:B:443:ILE:HA	9:d:3:BMA:H62	1.84	0.58
1:C:455:THR:OG1	3:I:58:LYS:NZ	2.36	0.58
1:A:158:SER:HB3	1:A:171:LYS:HE2	1.85	0.58
5:N:36:TRP:HE1	5:N:78:LEU:HG	1.69	0.58
2:E:607:ASN:HB2	2:E:650:GLN:HE22	1.68	0.58
1:B:122:LEU:HD13	1:B:125:LEU:HD22	1.85	0.58
1:A:379:GLY:HA2	10:V:2:NAG:H61	1.85	0.58
6:P:37:GLN:HE22	6:P:39:ARG:HG2	1.69	0.58
3:I:35:HIS:ND1	3:I:100(I):MET:HE2	2.17	0.58
5:O:33:TYR:HB2	5:O:95:ALA:HB3	1.85	0.58
1:B:43:PRO:HG3	2:E:540:GLN:HE22	1.68	0.57
4:J:61:ARG:NH2	4:J:77:GLY:O	2.36	0.57
2:D:647:GLU:OE1	2:E:538:THR:OG1	2.19	0.57
3:I:66:ARG:NH2	3:I:86:ASP:OD2	2.37	0.57
4:J:89:TYR:CE1	4:J:96:VAL:HG13	2.39	0.57
1:C:233:PHE:HE2	1:C:485:LYS:HA	1.70	0.57
6:R:54:ARG:NH1	6:R:60:GLU:OE1	2.38	0.57
2:F:596:TRP:HD1	2:F:647:GLU:HB3	1.68	0.57
5:O:100(E):VAL:HG22	13:s:2:NAG:H81	1.86	0.57
1:A:51:THR:HA	1:A:103:GLN:HE22	1.70	0.57
1:A:278:THR:O	1:A:456:ARG:NH2	2.38	0.57
3:G:51:ILE:HG23	3:G:57:VAL:HG12	1.87	0.57
4:K:27(B):ASP:HB3	4:K:92:ALA:HB2	1.86	0.57
5:O:38:ARG:NE	5:O:46:GLU:OE2	2.37	0.57
1:B:291:PRO:HG3	14:B:606:NAG:H82	1.87	0.57
1:C:358:ILE:HG12	1:C:396:ILE:HG22	1.87	0.57
1:C:396:ILE:HG13	1:C:397:SER:H	1.70	0.57
4:J:52:SER:HA	4:J:64:ALA:HB3	1.87	0.57
1:B:218:CYS:HA	1:B:247:CYS:HB3	1.87	0.57
2:D:529:THR:HG23	2:D:532:ALA:H	1.70	0.57
6:P:18:THR:HA	6:P:75:ILE:O	2.04	0.57
6:P:39:ARG:HB2	6:P:42:GLN:HB3	1.86	0.57
2:E:587:LEU:HD12	2:F:583:VAL:HG23	1.87	0.56
3:G:61:GLN:OE1	3:G:64:ARG:NH1	2.38	0.56
3:H:87:THR:HG22	3:H:111:VAL:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:650:GLN:NE2	2:D:654:GLU:OE1	2.38	0.56
4:J:27:SER:OG	4:J:69:ASN:ND2	2.38	0.56
6:R:25:ARG:HE	6:R:90:MET:HB3	1.70	0.56
2:E:596:TRP:CD1	2:E:647:GLU:HB3	2.41	0.56
5:M:47:TRP:O	5:M:60:ASN:ND2	2.38	0.56
6:R:19:ALA:HB3	6:R:75:ILE:HB	1.86	0.56
3:I:35:HIS:CD2	3:I:50:TRP:HB3	2.40	0.56
3:I:100(C):TRP:CB	3:I:100(G):ARG:HH21	2.18	0.56
3:I:100(C):TRP:HE1	3:I:100(F):TRP:CG	2.24	0.56
1:A:101:VAL:HG11	1:A:480:ARG:HG2	1.88	0.56
1:B:378:CYS:SG	1:B:379:GLY:N	2.79	0.56
6:Q:39:ARG:HB2	6:Q:42:GLN:HB3	1.87	0.56
1:B:225:ILE:HD12	1:B:247:CYS:HA	1.87	0.56
5:O:90:TYR:HE2	5:O:109:VAL:HG22	1.70	0.56
1:C:475:MET:HE2	3:I:54:ARG:HH12	1.71	0.56
2:D:569:THR:OG1	2:D:570:VAL:N	2.38	0.56
1:B:196:CYS:O	1:C:313:PRO:HB3	2.06	0.55
1:C:427:TRP:H	3:I:54:ARG:HH21	1.54	0.55
6:P:109:GLN:HE21	6:P:110:PRO:HD2	1.71	0.55
6:R:21:ILE:HB	6:R:73:LEU:HB3	1.87	0.55
1:A:231:LYS:HD2	1:A:268:GLU:HG3	1.89	0.55
5:N:94:THR:OG1	5:N:101:ASP:OD1	2.24	0.55
1:A:322:ILE:O	6:P:94:ARG:NH1	2.38	0.55
1:C:178:ARG:HH12	14:C:603:NAG:H62	1.70	0.55
1:B:197:ASN:O	1:B:199:SER:N	2.36	0.55
1:B:387:THR:HG22	1:B:416:LEU:HD13	1.87	0.55
1:C:98:ASN:HD21	1:C:100:MET:HB2	1.71	0.55
1:B:47:ASP:HA	1:B:489:VAL:HG12	1.88	0.55
2:D:525:ALA:HB3	2:D:536:THR:HG21	1.87	0.55
3:H:38:ARG:HH21	3:H:46:GLU:HG2	1.72	0.55
1:B:445:CYS:HA	9:d:2:NAG:HN2	1.72	0.55
2:D:603:ILE:HD13	2:F:655:LYS:HB3	1.88	0.55
3:G:100(B):ASP:OD2	3:G:100(G):ARG:NH2	2.36	0.55
5:O:18:LEU:HD23	5:O:82(C):VAL:HG21	1.89	0.54
1:C:173:TYR:OH	1:C:321(A):ASP:OD1	2.23	0.54
5:M:33:TYR:CD1	5:M:52:SER:HA	2.43	0.54
1:C:221:ALA:HB2	2:F:546:SER:HB3	1.89	0.54
5:N:100(A):ILE:HB	12:j:3:BMA:H5	1.89	0.54
3:G:100(D):SER:OG	3:G:100(E):PRO:HD3	2.08	0.54
4:L:61:ARG:HA	4:L:76:SER:OG	2.08	0.54
1:B:38:VAL:HB	2:E:604:CYS:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:SER:OG	1:C:395:TRP:NE1	2.39	0.54
5:M:40:SER:HB3	5:M:43:LYS:HB2	1.89	0.54
1:C:44:VAL:HG12	1:C:492:GLU:HB2	1.90	0.53
3:G:17:SER:HA	3:G:82:LEU:O	2.08	0.53
5:O:54:ARG:NH1	5:O:56:SER:O	2.41	0.53
4:L:34:SER:HB2	4:L:89:TYR:HD2	1.73	0.53
5:O:86:ASP:O	5:O:90:TYR:OH	2.24	0.53
5:O:87:THR:HG23	5:O:110:THR:HA	1.89	0.53
6:R:61:ARG:NH1	6:R:77:GLY:O	2.41	0.53
6:R:54:ARG:HH21	6:R:63:SER:HA	1.73	0.53
1:A:387:THR:HA	1:A:416:LEU:HD22	1.91	0.53
1:C:274:SER:C	1:C:276:ASN:N	2.66	0.53
1:C:276:ASN:HB3	1:C:282:LYS:HG3	1.90	0.53
6:R:66(A):ASP:H	13:s:5:MAN:H2	1.73	0.53
1:B:306:SER:HA	1:B:318:TYR:HA	1.91	0.53
1:C:500:ARG:HB2	2:E:663:LEU:HD12	1.91	0.53
1:C:87:GLU:HB2	14:C:602:NAG:N2	2.22	0.53
4:K:22:SER:HA	4:K:72:SER:HA	1.90	0.53
1:B:348:GLN:HA	1:B:351:LYS:HZ3	1.74	0.53
2:E:597:GLY:N	2:E:651:ASN:HD21	2.07	0.53
3:G:100(E):PRO:HG2	4:J:32:LEU:HD21	1.90	0.53
5:N:33:TYR:HB2	5:N:95:ALA:HB3	1.90	0.53
5:N:54:ARG:CZ	5:N:56:SER:HB2	2.39	0.53
1:B:86:LEU:HB2	1:B:89:VAL:HG11	1.89	0.52
5:N:100(D):VAL:HA	12:j:2:NAG:H2	1.91	0.52
1:B:119:CYS:SG	1:B:205:CYS:N	2.74	0.52
1:B:260:LEU:HD12	1:B:451:GLY:HA3	1.92	0.52
4:J:27(B):ASP:OD1	4:J:27(B):ASP:N	2.42	0.52
1:A:203:GLN:HA	1:A:435:TYR:HB3	1.91	0.52
2:F:569:THR:OG1	2:F:570:VAL:N	2.42	0.52
6:Q:33:VAL:HG12	6:Q:51:ASN:OD1	2.10	0.52
1:A:43:PRO:HG3	2:D:540:GLN:HE22	1.74	0.52
1:A:64:GLU:O	1:A:68:VAL:HG23	2.10	0.52
1:A:493:PRO:HG3	2:D:544:LEU:HD21	1.91	0.52
2:F:645:LEU:O	2:F:649:SER:OG	2.28	0.52
4:J:31:ASP:O	4:J:51:VAL:HB	2.10	0.52
4:K:9:SER:HA	4:K:102:THR:HG23	1.91	0.52
1:A:280:ASN:HB2	1:A:456:ARG:O	2.10	0.52
1:C:212:PRO:HG2	1:C:254:VAL:HG12	1.91	0.52
4:K:85:ASP:OD1	4:K:86:TYR:N	2.41	0.52
5:O:38:ARG:HB3	5:O:90:TYR:HD1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:CYS:SG	1:C:379:GLY:N	2.83	0.52
2:F:572:GLY:O	2:F:575:GLN:NE2	2.42	0.52
5:M:100:ARG:NE	12:a:4:BMA:H5	2.25	0.52
4:K:47:MET:O	4:K:55:PRO:HD2	2.10	0.52
6:Q:31:ARG:O	6:Q:51:ASN:ND2	2.43	0.52
1:A:257:THR:OG1	1:A:375:SER:OG	2.24	0.51
1:A:140:ASP:OD2	1:A:152:GLY:N	2.42	0.51
1:C:47:ASP:HA	1:C:489:VAL:HG12	1.92	0.51
3:I:51:ILE:HG23	3:I:57:VAL:HG12	1.92	0.51
1:A:45:TRP:HB2	1:A:489:VAL:HB	1.92	0.51
4:J:4:LEU:HB2	4:J:99:GLY:HA2	1.91	0.51
1:B:260:LEU:HB2	1:B:451:GLY:HA3	1.93	0.51
2:E:596:TRP:HD1	2:E:647:GLU:HB3	1.75	0.51
1:B:171:LYS:HE3	8:c:1:NAG:H82	1.92	0.51
1:C:86:LEU:HD21	1:C:244:THR:HG22	1.92	0.51
4:K:47:MET:HB3	4:K:58:VAL:CG2	2.41	0.51
6:P:18:THR:O	6:P:20:ARG:NH2	2.43	0.51
3:H:35:HIS:CD2	3:H:50:TRP:HB3	2.45	0.51
1:B:325:ASP:OD1	1:B:325:ASP:N	2.40	0.51
1:B:384:TYR:HE2	1:B:421:LYS:HD3	1.76	0.51
1:C:286:VAL:HB	1:C:452:LEU:HB2	1.93	0.51
1:C:462:ASN:HA	4:L:27(A):ARG:HH22	1.75	0.51
3:H:98:ASP:OD1	3:H:99:SER:N	2.44	0.51
1:B:196:CYS:O	1:B:196:CYS:SG	2.68	0.51
2:D:587:LEU:HD12	2:E:583:VAL:HG23	1.92	0.51
4:J:26:SER:OG	4:J:27:SER:N	2.43	0.51
1:C:325:ASP:OD1	1:C:325:ASP:N	2.43	0.51
6:P:65:THR:OG1	6:P:72:THR:O	2.29	0.51
1:B:55:ALA:O	1:B:216:HIS:ND1	2.42	0.50
1:C:274:SER:C	1:C:276:ASN:H	2.19	0.50
1:B:270:VAL:HG11	1:B:345:VAL:HG22	1.94	0.50
1:A:498:PRO:HB3	2:D:610:TRP:CD2	2.47	0.50
5:M:75:LYS:HE3	5:M:77:GLN:HB2	1.93	0.50
5:N:100:ARG:NH2	6:Q:66(A):ASP:OD2	2.44	0.50
5:O:100(A):ILE:O	13:s:3:BMA:H5	2.11	0.50
6:P:46:LEU:HD21	6:P:49:TYR:HB3	1.94	0.50
1:A:65:LYS:NZ	1:A:207:LYS:O	2.39	0.50
1:A:279:ASN:HD22	1:A:282:LYS:HE2	1.76	0.50
1:C:173:TYR:CE2	7:k:1:NAG:H3	2.46	0.50
2:E:592:LEU:HA	2:E:595:ILE:HG22	1.92	0.50
4:K:4:LEU:HB2	4:K:99:GLY:HA2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:47:TRP:NE1	5:M:49:GLY:O	2.45	0.50
4:L:34:SER:HB2	4:L:89:TYR:HB3	1.94	0.50
1:B:278:THR:HB	4:K:30:PHE:HZ	1.75	0.50
5:M:38:ARG:HH21	5:M:80:LEU:HD21	1.75	0.50
6:Q:37:GLN:HE22	6:Q:39:ARG:HG2	1.76	0.50
1:A:236:THR:HB	14:A:604:NAG:H5	1.94	0.50
4:K:89:TYR:CE1	4:K:96:VAL:HG13	2.47	0.50
1:B:134:VAL:O	1:B:136:ASN:ND2	2.45	0.49
5:N:59:TYR:CE1	5:N:69:ILE:HG22	2.47	0.49
4:J:35:TRP:HB2	4:J:48:ILE:HB	1.94	0.49
5:O:52:SER:HB2	5:O:54:ARG:NH1	2.27	0.49
1:C:333:VAL:HG21	1:C:390:LEU:HD11	1.93	0.49
3:I:87:THR:OG1	3:I:111:VAL:O	2.30	0.49
1:C:279:ASN:CG	3:I:100(F):TRP:HE1	2.21	0.49
3:I:100(D):SER:N	3:I:100(E):PRO:HD3	2.27	0.49
1:B:462:ASN:H	4:K:27(A):ARG:HH22	1.60	0.49
5:N:18:LEU:HD13	5:N:82(C):VAL:HG21	1.95	0.49
1:B:496:VAL:O	2:E:631:TRP:NE1	2.35	0.49
3:H:47:TRP:CD2	4:K:96:VAL:HB	2.48	0.49
2:E:608:VAL:HG21	2:E:646:LEU:HA	1.94	0.48
3:I:41:PRO:HD3	3:I:88:ALA:HA	1.95	0.48
3:I:100(D):SER:HB3	3:I:100(E):PRO:HD3	1.94	0.48
4:K:6:GLN:NE2	4:K:88:CYS:H	2.11	0.48
5:N:51:ILE:HD11	5:N:69:ILE:HG23	1.95	0.48
6:Q:66(A):ASP:CB	12:j:5:MAN:H5	2.43	0.48
1:A:141:ASP:OD1	1:A:141:ASP:N	2.46	0.48
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.94	0.48
3:H:40:ALA:HB3	3:H:43:GLN:HB2	1.95	0.48
3:H:100(B):ASP:OD1	3:H:100(G):ARG:NH2	2.35	0.48
3:I:97:PHE:CD1	3:I:100(G):ARG:HD2	2.48	0.48
3:I:100(C):TRP:HE1	3:I:100(F):TRP:CD1	2.31	0.48
6:P:33:VAL:N	6:P:51:ASN:OD1	2.45	0.48
7:p:1:NAG:H61	7:p:2:NAG:C7	2.42	0.48
1:B:500:ARG:HB2	2:D:663:LEU:HG	1.95	0.48
3:I:87:THR:HG23	3:I:111:VAL:H	1.78	0.48
6:P:54:ARG:HH21	6:P:63:SER:HA	1.78	0.48
1:A:279:ASN:HB3	1:A:282:LYS:HG2	1.94	0.48
3:I:100(D):SER:N	3:I:100(E):PRO:HD2	2.26	0.48
5:M:35:THR:OG1	5:M:47:TRP:NE1	2.38	0.48
5:O:90:TYR:CE2	5:O:109:VAL:HG22	2.48	0.48
6:Q:61:ARG:NH1	6:Q:82:ASP:OD2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD11	1:A:291:PRO:HD3	1.96	0.48
1:A:439:ILE:HB	1:A:443:ILE:HD11	1.94	0.48
3:H:61:GLN:OE1	3:H:64:ARG:NH1	2.47	0.48
5:M:5:GLN:NE2	5:M:6:GLU:O	2.46	0.48
1:A:341:THR:O	1:A:345:VAL:HG23	2.13	0.48
1:B:212:PRO:HG2	1:B:254:VAL:HG12	1.94	0.48
1:B:475:MET:HE2	3:H:54:ARG:HH12	1.78	0.48
2:E:525:ALA:HB1	2:E:528:SER:HB3	1.96	0.48
3:I:67:VAL:HG12	3:I:82:LEU:HD13	1.94	0.48
3:I:100(C):TRP:NE1	3:I:100(F):TRP:CD1	2.81	0.48
3:I:100(C):TRP:HB2	3:I:100(G):ARG:HH21	1.79	0.48
4:K:23:CYS:HB3	4:K:71:ALA:HB3	1.95	0.48
5:M:35:THR:OG1	5:M:49:GLY:O	2.23	0.48
5:M:90:TYR:O	5:M:106:GLY:HA2	2.14	0.48
1:B:444:ARG:HH21	9:d:2:NAG:H82	1.79	0.48
1:B:469:ARG:HH21	3:H:64:ARG:HD3	1.79	0.48
4:K:80:ALA:HB2	4:K:107:LEU:HD21	1.94	0.48
1:B:178:ARG:NH2	14:B:603:NAG:H4	2.28	0.48
6:Q:66(A):ASP:HB3	12:j:5:MAN:H5	1.96	0.48
1:B:101:VAL:HG11	1:B:480:ARG:HG2	1.96	0.48
1:B:322:ILE:O	6:Q:94:ARG:NH1	2.47	0.48
1:C:220:PRO:HB3	2:F:578:ALA:HB1	1.96	0.48
1:C:298:ARG:NH1	1:C:381:GLU:OE1	2.47	0.48
1:B:67:ASN:OD1	1:B:72:HIS:HB2	2.14	0.47
1:B:131:CYS:SG	1:B:191:TYR:HB2	2.55	0.47
1:B:279:ASN:ND2	3:H:100(F):TRP:HZ3	2.12	0.47
1:B:460:SER:HB2	4:K:93:ASP:HB3	1.96	0.47
4:K:37:GLN:HB2	4:K:47:MET:SD	2.55	0.47
4:L:21:ILE:HD12	4:L:73:LEU:HD23	1.96	0.47
5:N:5:GLN:NE2	5:N:6:GLU:O	2.48	0.47
5:N:38:ARG:HD3	5:N:48:ILE:HD12	1.95	0.47
1:B:212:PRO:HB2	1:B:252:LYS:HB3	1.96	0.47
3:I:100(C):TRP:HB3	3:I:100(G):ARG:NH2	2.30	0.47
1:A:171:LYS:HD3	8:T:1:NAG:H5	1.96	0.47
1:A:84:ILE:HB	1:A:244:THR:HG23	1.97	0.47
1:B:363:ASN:O	1:B:469:ARG:NH1	2.48	0.47
4:K:47:MET:O	4:K:54:ARG:HB2	2.15	0.47
1:B:249:HIS:O	1:B:251:ILE:HG13	2.15	0.47
2:E:569:THR:OG1	2:E:570:VAL:N	2.42	0.47
6:Q:21:ILE:HD11	6:Q:104:LEU:HD22	1.96	0.47
6:Q:36:TYR:HB2	6:Q:87:TYR:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:THR:OG1	1:C:497:ALA:O	2.31	0.47
1:C:249:HIS:O	1:C:251:ILE:HG13	2.13	0.47
1:C:260:LEU:HD21	1:C:453:ILE:HD11	1.97	0.47
6:R:14:ALA:HB3	6:R:17:GLU:HG3	1.97	0.47
1:B:281:ALA:H	3:H:100(F):TRP:HH2	1.63	0.46
1:C:257:THR:O	1:C:453:ILE:HD12	2.15	0.46
4:K:67:SER:OG	4:K:70:THR:OG1	2.32	0.46
6:R:92:ASP:OD1	6:R:95:SER:OG	2.28	0.46
1:A:503:ARG:NH2	2:D:597:GLY:HA3	2.30	0.46
1:C:163:THR:OG1	1:C:164:GLU:N	2.47	0.46
5:M:29:MET:HA	5:M:34:TRP:HZ2	1.80	0.46
1:B:456:ARG:O	3:H:58:LYS:NZ	2.41	0.46
1:C:473:GLY:O	3:I:54:ARG:NH1	2.47	0.46
5:O:94:THR:OG1	5:O:101:ASP:OD1	2.33	0.46
1:A:60:ALA:O	1:A:63:THR:OG1	2.30	0.46
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.80	0.46
1:B:342:LEU:O	1:B:346:VAL:HG23	2.15	0.46
3:G:100(E):PRO:HG3	11:Z:1:NAG:H83	1.96	0.46
1:B:278:THR:HB	4:K:30:PHE:CZ	2.50	0.46
1:B:439:ILE:HB	1:B:443:ILE:HD11	1.98	0.46
2:D:596:TRP:C	2:D:651:ASN:HD21	2.24	0.46
3:I:72:ASP:CG	7:r:2:NAG:H2	2.40	0.46
5:N:54:ARG:NH1	5:N:56:SER:O	2.46	0.46
1:A:299:PRO:HA	1:A:442:VAL:HG13	1.97	0.46
1:B:491:ILE:HG13	2:E:522:PHE:HZ	1.81	0.46
1:B:498:PRO:HB3	2:E:610:TRP:CD2	2.51	0.46
1:C:162:THR:HG22	1:C:169:LYS:HE2	1.97	0.46
3:G:52:ASN:O	3:G:55:GLY:HA2	2.16	0.46
3:H:100(B):ASP:OD1	3:H:100(C):TRP:N	2.45	0.46
1:C:279:ASN:HD22	1:C:282:LYS:HE2	1.80	0.46
1:B:94:ASN:HA	1:B:236:THR:HA	1.98	0.46
3:I:47:TRP:CD2	4:L:96:VAL:HB	2.51	0.46
1:B:292:VAL:HB	1:B:449:ILE:HB	1.97	0.46
2:D:655:LYS:HB3	2:E:603:ILE:HG13	1.97	0.46
4:K:31:ASP:OD1	4:K:31:ASP:N	2.41	0.46
5:N:65:SER:O	5:N:65:SER:OG	2.32	0.46
1:B:158:SER:HA	1:B:173:TYR:HA	1.96	0.46
1:B:221:ALA:HB3	2:E:582:ALA:HB1	1.97	0.46
1:A:193:LEU:HB2	1:A:196:CYS:SG	2.56	0.45
1:A:270:VAL:HA	1:A:287:GLN:O	2.16	0.45
3:H:101:VAL:HG12	4:K:46:LEU:HD22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:30:THR:HA	3:I:52(A):PRO:HB2	1.98	0.45
1:B:218:CYS:HA	1:B:247:CYS:CB	2.46	0.45
1:A:373:THR:OG1	1:A:384:TYR:HB3	2.16	0.45
1:C:36:VAL:HG12	2:F:610:TRP:HE3	1.80	0.45
1:C:384:TYR:CE2	1:C:421:LYS:HD3	2.50	0.45
3:I:35:HIS:CG	3:I:100(I):MET:HE2	2.51	0.45
5:O:100:ARG:NH2	13:s:5:MAN:H3	2.31	0.45
6:R:21:ILE:O	6:R:72:THR:HA	2.17	0.45
5:O:33:TYR:HD1	5:O:52:SER:HA	1.82	0.45
6:Q:34:GLN:HB2	6:Q:89:HIS:HB3	1.99	0.45
1:A:259:LEU:HD12	1:A:374:HIS:CD2	2.51	0.45
2:D:652:GLN:HE21	2:E:538:THR:HG22	1.82	0.45
4:J:27(C):VAL:HG13	4:J:33:VAL:HG21	1.98	0.45
4:J:48:ILE:HG21	4:J:64:ALA:HB2	1.98	0.45
2:E:528:SER:OG	2:E:529:THR:N	2.50	0.45
2:E:618:ASN:ND2	2:E:621:GLU:OE2	2.49	0.45
2:E:641:ILE:O	2:E:645:LEU:HD12	2.17	0.45
4:K:47:MET:HE3	4:K:47:MET:HB2	1.83	0.45
3:G:98:ASP:OD1	3:G:99:SER:N	2.49	0.45
3:I:100(C):TRP:CB	3:I:100(G):ARG:NH2	2.80	0.45
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.87	0.45
1:A:70:ALA:HB1	1:A:215:ILE:HD11	1.98	0.44
1:A:427:TRP:H	3:G:54:ARG:HH21	1.63	0.44
1:A:321(A):ASP:OD1	1:A:321(A):ASP:N	2.50	0.44
1:B:476:ARG:HA	1:B:479:TRP:CD1	2.52	0.44
2:E:655:LYS:NZ	2:F:601:LYS:H	2.14	0.44
3:G:20:VAL:HG12	3:G:80:MET:HB3	1.99	0.44
3:H:51:ILE:HG23	3:H:57:VAL:HG12	1.99	0.44
5:M:52:SER:HB2	5:M:54:ARG:HD3	1.98	0.44
1:A:220:PRO:HB3	2:D:578:ALA:HB1	1.99	0.44
3:H:79:TYR:CE1	9:h:3:BMA:H3	2.53	0.44
4:J:48:ILE:HD13	4:J:54:ARG:HG2	1.98	0.44
6:R:31:ARG:NH2	6:R:66(A):ASP:HA	2.33	0.44
1:B:305:LYS:HE3	1:B:307:ILE:HD11	1.99	0.44
1:C:84:ILE:HB	1:C:244:THR:HG23	2.00	0.44
1:C:173:TYR:CG	7:k:1:NAG:H5	2.52	0.44
4:K:34:SER:N	4:K:89:TYR:O	2.51	0.44
5:N:23:SER:HA	5:N:77:GLN:HG2	1.99	0.44
1:A:174:SER:OG	1:A:319:ALA:HB1	2.18	0.44
1:A:298:ARG:NH1	1:A:302:ASN:HD22	2.16	0.44
3:I:100(C):TRP:O	3:I:100(C):TRP:CG	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:GLU:CB	4:K:53:LYS:HB3	2.48	0.44
4:K:106:VAL:O	4:K:107:LEU:HG	2.17	0.44
6:R:89:HIS:CE1	6:R:91:TRP:HE1	2.35	0.44
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.79	0.44
1:B:384:TYR:CE2	1:B:421:LYS:HD3	2.53	0.44
2:D:606:THR:OG1	2:D:607:ASN:N	2.50	0.44
2:F:617:ARG:HB2	2:F:622:ILE:HD11	1.99	0.44
2:D:617:ARG:HB2	2:D:622:ILE:HD11	1.99	0.44
1:A:301:ASN:HB3	1:A:323:ILE:O	2.17	0.44
1:C:304:ARG:HD3	1:C:318:TYR:CD2	2.53	0.44
6:P:32:ALA:HA	6:P:51:ASN:HD21	1.83	0.44
1:A:175:LEU:O	1:A:320:THR:OG1	2.30	0.43
1:B:80:ASN:OD1	1:B:80:ASN:N	2.51	0.43
1:B:492:GLU:OE2	2:E:585:ARG:NH2	2.51	0.43
2:D:632:ASP:OD1	2:D:633:LYS:N	2.51	0.43
6:P:37:GLN:NE2	6:P:39:ARG:HG2	2.33	0.43
1:A:295:ASN:OD1	1:A:446:VAL:HG13	2.17	0.43
1:A:503:ARG:NE	2:D:605:CYS:O	2.42	0.43
1:B:95:MET:SD	1:B:273:ARG:HD3	2.59	0.43
1:B:175:LEU:O	1:B:320:THR:OG1	2.30	0.43
3:H:20:VAL:HG12	3:H:80:MET:HE3	2.00	0.43
3:I:35:HIS:N	3:I:93:ALA:O	2.41	0.43
1:A:67:ASN:OD1	1:A:72:HIS:HB2	2.18	0.43
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.52	0.43
4:K:27:SER:HA	4:K:69:ASN:OD1	2.18	0.43
6:R:26:GLN:OE1	6:R:70:ARG:NH2	2.51	0.43
1:A:202:THR:O	1:A:435:TYR:N	2.52	0.43
1:C:498:PRO:HB3	2:F:610:TRP:CD2	2.53	0.43
2:E:580:VAL:HG21	2:F:580:VAL:HG22	2.01	0.43
4:K:6:GLN:HE21	4:K:99:GLY:HA3	1.84	0.43
1:A:87:GLU:H	14:A:602:NAG:C8	2.31	0.43
1:C:279:ASN:HB3	1:C:282:LYS:HG2	2.01	0.43
1:C:493:PRO:HG3	2:F:544:LEU:HD21	2.00	0.43
2:D:523:LEU:HA	2:D:540:GLN:HE21	1.83	0.43
6:Q:54:ARG:NH1	6:Q:60:GLU:OE1	2.52	0.43
1:B:234:ASN:HA	1:B:273:ARG:HG2	2.01	0.43
3:G:100(I):MET:O	3:G:103:TRP:NE1	2.52	0.43
4:L:63:SER:O	4:L:73:LEU:HD12	2.19	0.43
1:B:306:SER:H	1:B:318:TYR:HA	1.83	0.43
3:G:47:TRP:CD2	4:J:96:VAL:HB	2.54	0.43
6:Q:25:ARG:HH22	6:Q:99:GLY:HA3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASN:O	1:C:68:VAL:C	2.62	0.43
2:E:612:SER:O	2:E:616:ASN:HB2	2.19	0.43
3:I:94:ARG:HB2	3:I:102:ALA:HB3	2.00	0.43
4:K:6:GLN:HE22	4:K:88:CYS:H	1.66	0.43
6:Q:23:CYS:HB3	6:Q:88:CYS:HB2	1.92	0.43
1:A:85:HIS:HA	1:A:243:SER:HB2	2.01	0.43
1:B:164:GLU:HA	1:B:312:GLY:O	2.19	0.43
4:J:4:LEU:HD13	4:J:23:CYS:SG	2.59	0.43
5:M:34:TRP:CZ3	5:M:94:THR:HG22	2.54	0.43
5:N:87:THR:HG23	5:N:110:THR:HA	2.00	0.43
5:O:17:THR:HA	5:O:82:LEU:O	2.19	0.43
5:O:92:CYS:O	5:O:104:GLY:N	2.52	0.43
6:Q:35:TRP:CD2	6:Q:73:LEU:HD22	2.53	0.43
6:R:70:ARG:O	6:R:72:THR:HG23	2.19	0.43
1:A:248:THR:OG1	1:A:249:HIS:N	2.52	0.42
1:B:180:ASP:OD2	1:B:422:GLN:HB2	2.19	0.42
14:B:602:NAG:H81	2:E:524:GLY:O	2.18	0.42
1:C:274:SER:HB2	1:C:284:ILE:HG13	2.00	0.42
1:C:377:ASN:HB2	1:C:382:PHE:CD2	2.54	0.42
3:H:35:HIS:ND1	3:H:100(I):MET:SD	2.92	0.42
5:N:54:ARG:H	5:N:54:ARG:HD3	1.84	0.42
1:A:53:PHE:N	1:A:218:CYS:O	2.51	0.42
1:A:298:ARG:HB3	1:A:443:ILE:HB	2.00	0.42
1:B:320:THR:HG22	1:B:438:PRO:HB3	2.01	0.42
1:B:393:SER:OG	1:B:394:THR:N	2.52	0.42
1:C:131:CYS:HA	1:C:157:CYS:HA	2.01	0.42
3:H:27:TYR:CE1	3:H:94:ARG:HD2	2.53	0.42
3:H:79:TYR:CD2	9:h:3:BMA:H5	2.53	0.42
5:O:72:ASP:OD2	5:O:74:SER:OG	2.27	0.42
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.84	0.42
3:H:6:GLN:NE2	3:H:92:CYS:SG	2.77	0.42
4:K:65:SER:OG	4:K:66:LYS:N	2.52	0.42
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.87	0.42
1:B:103:GLN:O	1:B:107:ASP:HB2	2.19	0.42
1:B:427:TRP:H	3:H:54:ARG:HH21	1.66	0.42
1:C:121:LYS:HE3	1:C:121:LYS:HB2	1.87	0.42
3:G:6:GLN:NE2	3:G:92:CYS:SG	2.76	0.42
4:J:54:ARG:CZ	4:J:60:ASN:HA	2.50	0.42
1:A:490:LYS:HD2	2:D:585:ARG:NH2	2.34	0.42
1:B:503:ARG:HH12	2:E:654:GLU:CD	2.27	0.42
1:C:260:LEU:HB2	1:C:451:GLY:HA3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:HD21	1:C:477:ASP:HB3	2.02	0.42
2:D:587:LEU:HD23	2:D:587:LEU:HA	1.86	0.42
2:F:661:LEU:HD23	2:F:661:LEU:O	2.20	0.42
3:G:100(I):MET:HB2	4:J:36:TYR:CE1	2.54	0.42
4:J:33:VAL:HA	4:J:89:TYR:O	2.20	0.42
4:K:27(B):ASP:O	4:K:90:SER:OG	2.33	0.42
1:B:222:GLY:HA2	2:E:544:LEU:HD12	2.01	0.42
1:C:304:ARG:HD3	1:C:318:TYR:HD2	1.84	0.42
5:O:47:TRP:CZ2	5:O:100(P):MET:HE3	2.55	0.42
5:O:100:ARG:NH2	6:R:66(A):ASP:OD2	2.52	0.42
6:P:13:VAL:HG11	6:P:19:ALA:HB2	2.01	0.42
1:A:260:LEU:HD12	1:A:451:GLY:HA3	2.01	0.42
1:A:302:ASN:OD1	1:A:322:ILE:HG12	2.18	0.42
1:A:333:VAL:O	1:A:414:ILE:HG22	2.18	0.42
1:C:36:VAL:HG12	2:F:610:TRP:CE3	2.54	0.42
1:C:125:LEU:HA	1:C:161:MET:HE1	2.02	0.42
3:G:12:LYS:O	3:G:111:VAL:HA	2.19	0.42
1:B:373:THR:OG1	1:B:384:TYR:HB3	2.19	0.42
5:M:45:LEU:HG	6:P:87:TYR:CZ	2.54	0.42
1:A:116:LEU:HD11	1:A:434:MET:HG3	2.02	0.42
1:B:288:PHE:CZ	1:B:452:LEU:HG	2.55	0.42
4:J:109:GLN:H	4:J:109:GLN:CD	2.27	0.42
5:M:29:MET:HE2	5:M:29:MET:HB3	1.96	0.42
5:M:86:ASP:O	5:M:90:TYR:OH	2.34	0.42
1:A:475:MET:HE2	3:G:54:ARG:HH12	1.85	0.42
2:E:631:TRP:O	2:E:635:ILE:HG12	2.20	0.42
3:G:90:TYR:O	3:G:106:GLY:HA2	2.19	0.42
3:I:15:GLY:N	3:I:82(C):LEU:O	2.45	0.42
3:I:100(F):TRP:N	3:I:100(F):TRP:CD1	2.88	0.42
5:M:35:THR:HG1	5:M:47:TRP:HE1	1.65	0.42
5:O:34:TRP:CZ3	5:O:94:THR:HG22	2.53	0.42
1:A:114:GLN:CD	2:D:570:VAL:HG11	2.45	0.41
1:A:490:LYS:HD2	2:D:585:ARG:HH22	1.85	0.41
1:B:223:PHE:CE2	1:B:490:LYS:HB3	2.55	0.41
1:B:277:ILE:HG12	1:B:352:HIS:HB3	2.02	0.41
1:B:299:PRO:HD3	1:B:329:ALA:HA	2.01	0.41
3:G:51:ILE:HD11	3:G:69:MET:HB3	2.02	0.41
5:M:45:LEU:HG	6:P:87:TYR:CE1	2.55	0.41
6:P:18:THR:HG23	6:P:76:SER:HA	2.02	0.41
6:P:25:ARG:HH12	6:P:99:GLY:HA2	1.85	0.41
8:e:1:NAG:H61	8:e:2:NAG:O5	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:O	1:A:243:SER:HB2	2.20	0.41
1:A:138:ILE:HG22	1:A:139:THR:H	1.85	0.41
4:J:83:GLU:HG3	4:J:105:THR:HA	2.02	0.41
4:K:50:GLU:HB3	4:K:53:LYS:HB3	2.01	0.41
6:Q:33:VAL:HG23	6:Q:90:MET:HA	2.03	0.41
1:A:280:ASN:OD1	1:A:281:ALA:N	2.54	0.41
1:B:308:ARG:HA	1:B:316:ALA:HA	2.03	0.41
4:K:47:MET:HB3	4:K:58:VAL:HG23	2.03	0.41
4:L:36:TYR:O	4:L:86:TYR:HA	2.20	0.41
6:P:61:ARG:NH1	6:P:77:GLY:O	2.53	0.41
1:C:141:ASP:OD1	1:C:141:ASP:N	2.52	0.41
2:F:657:GLU:HA	2:F:660:LEU:HG	2.03	0.41
3:G:27:TYR:HE2	3:G:32:TYR:HB2	1.86	0.41
3:G:30:THR:HG22	3:G:30:THR:O	2.20	0.41
3:G:50:TRP:CE2	3:G:58:LYS:HB3	2.56	0.41
1:A:123:THR:HG23	1:A:124:PRO:HD3	2.02	0.41
1:A:259:LEU:HD12	1:A:374:HIS:CG	2.56	0.41
2:D:520:LEU:HD23	2:D:520:LEU:HA	1.88	0.41
4:L:28:GLY:O	7:n:3:BMA:H5	2.20	0.41
5:N:14:PRO:HD3	5:N:112:SER:O	2.21	0.41
5:O:47:TRP:HE3	6:R:96:TRP:CE3	2.38	0.41
6:P:92:ASP:OD1	6:P:92:ASP:N	2.53	0.41
2:F:529:THR:HG23	2:F:532:ALA:H	1.83	0.41
4:J:14:SER:HB3	4:J:17:GLN:CD	2.45	0.41
5:M:6:GLU:HB2	5:M:107:THR:HG23	2.02	0.41
1:A:368:ASP:OD2	3:G:71:ARG:NH1	2.54	0.41
1:A:131:CYS:SG	1:A:191:TYR:HB2	2.61	0.41
1:B:178:ARG:HH22	14:B:603:NAG:H4	1.85	0.41
1:C:276:ASN:CB	1:C:282:LYS:HG3	2.50	0.41
1:C:278:THR:CG2	7:n:1:NAG:N2	2.73	0.41
1:C:369:LEU:O	1:C:373:THR:OG1	2.30	0.41
2:D:592:LEU:HD23	2:D:592:LEU:HA	1.94	0.41
3:G:100(F):TRP:HB3	4:J:89:TYR:OH	2.21	0.41
4:K:79:GLN:O	4:K:106:VAL:HG21	2.21	0.41
4:L:47:MET:HB2	4:L:47:MET:HE2	1.82	0.41
5:M:27:ASP:OD2	5:M:31:ASN:ND2	2.48	0.41
6:R:33:VAL:HG12	6:R:51:ASN:OD1	2.21	0.41
1:A:122:LEU:HD22	1:A:125:LEU:HD23	2.02	0.41
1:A:377:ASN:HB2	1:A:382:PHE:CD2	2.55	0.41
1:C:86:LEU:HB2	1:C:89:VAL:HG11	2.02	0.41
1:C:365:SER:OG	1:C:366:GLY:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:631:TRP:O	2:F:635:ILE:HG12	2.20	0.41
6:Q:62:PHE:HD1	6:Q:75:ILE:HG12	1.86	0.41
1:A:36:VAL:HG12	2:D:610:TRP:HE3	1.86	0.40
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.87	0.40
1:A:375:SER:HB3	1:A:384:TYR:CD2	2.55	0.40
1:B:193:LEU:HB2	1:B:196:CYS:HB3	2.02	0.40
1:C:50:THR:C	1:C:103:GLN:HE22	2.29	0.40
1:C:359:ILE:HD12	1:C:468:PHE:HE2	1.86	0.40
1:C:363:ASN:O	1:C:469:ARG:NH1	2.54	0.40
5:M:4:LEU:HD13	5:M:92:CYS:SG	2.61	0.40
1:A:87:GLU:H	14:A:602:NAG:H82	1.87	0.40
1:A:112:TRP:CG	1:A:427:TRP:HZ3	2.40	0.40
1:B:60:ALA:O	1:B:63:THR:OG1	2.28	0.40
1:C:98:ASN:OD1	1:C:99:ASN:N	2.55	0.40
1:C:259:LEU:HD12	1:C:374:HIS:CD2	2.57	0.40
3:H:17:SER:HA	3:H:82(A):SER:HA	2.02	0.40
5:O:37:ILE:HG21	5:O:45:LEU:HD23	2.03	0.40
1:A:121:LYS:HE3	1:A:121:LYS:HB2	1.95	0.40
1:A:386:ASN:OD1	1:A:417:PRO:HD2	2.20	0.40
1:B:141:ASP:OD1	1:B:141:ASP:N	2.55	0.40
1:C:320:THR:HG22	1:C:438:PRO:HB3	2.04	0.40
1:C:444:ARG:O	10:m:2:NAG:H4	2.21	0.40
3:G:72:ASP:O	3:G:76:GLU:N	2.54	0.40
5:N:89:VAL:HG12	5:N:108:THR:HG22	2.03	0.40
7:f:1:NAG:H62	8:g:2:NAG:HN2	1.87	0.40
1:A:128:THR:O	8:T:1:NAG:H81	2.22	0.40
1:A:279:ASN:ND2	3:G:100(D):SER:O	2.54	0.40
2:E:606:THR:HG23	2:E:608:VAL:H	1.87	0.40
1:A:86:LEU:HB2	1:A:89:VAL:HG11	2.04	0.40
1:A:361:PHE:HB3	1:A:391:PHE:HB3	2.02	0.40
1:B:203:GLN:HA	1:B:435:TYR:HB3	2.04	0.40
4:K:59:SER:OG	4:K:61:ARG:NE	2.54	0.40
4:L:90:SER:OG	4:L:91:TYR:N	2.55	0.40
5:O:3:GLN:O	5:O:24:VAL:HA	2.21	0.40
5:O:100(C):GLY:O	13:s:2:NAG:H4	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	441/506 (87%)	409 (93%)	32 (7%)	0	100	100
1	B	441/506 (87%)	409 (93%)	32 (7%)	0	100	100
1	C	441/506 (87%)	410 (93%)	31 (7%)	0	100	100
2	D	122/153 (80%)	106 (87%)	16 (13%)	0	100	100
2	E	122/153 (80%)	113 (93%)	9 (7%)	0	100	100
2	F	122/153 (80%)	113 (93%)	9 (7%)	0	100	100
3	G	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
3	H	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
3	I	125/128 (98%)	121 (97%)	4 (3%)	0	100	100
4	J	108/111 (97%)	99 (92%)	9 (8%)	0	100	100
4	K	108/111 (97%)	99 (92%)	9 (8%)	0	100	100
4	L	108/111 (97%)	100 (93%)	8 (7%)	0	100	100
5	M	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
5	N	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
5	O	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
6	P	107/110 (97%)	98 (92%)	9 (8%)	0	100	100
6	Q	107/110 (97%)	101 (94%)	6 (6%)	0	100	100
6	R	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
All	All	3105/3426 (91%)	2894 (93%)	211 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/446 (90%)	397 (99%)	4 (1%)	68	75
1	B	401/446 (90%)	395 (98%)	6 (2%)	57	70
1	C	401/446 (90%)	397 (99%)	4 (1%)	68	75
2	D	108/129 (84%)	108 (100%)	0	100	100
2	E	108/129 (84%)	108 (100%)	0	100	100
2	F	108/129 (84%)	108 (100%)	0	100	100
3	G	104/105 (99%)	104 (100%)	0	100	100
3	H	104/105 (99%)	104 (100%)	0	100	100
3	I	104/105 (99%)	104 (100%)	0	100	100
4	J	87/88 (99%)	85 (98%)	2 (2%)	44	63
4	K	87/88 (99%)	84 (97%)	3 (3%)	32	55
4	L	87/88 (99%)	87 (100%)	0	100	100
5	M	117/117 (100%)	117 (100%)	0	100	100
5	N	117/117 (100%)	117 (100%)	0	100	100
5	O	117/117 (100%)	117 (100%)	0	100	100
6	P	87/88 (99%)	87 (100%)	0	100	100
6	Q	87/88 (99%)	87 (100%)	0	100	100
6	R	87/88 (99%)	87 (100%)	0	100	100
All	All	2712/2919 (93%)	2693 (99%)	19 (1%)	73	78

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	270	VAL
1	A	271	MET
1	A	276	ASN
1	B	88	ASN
1	B	196	CYS
1	B	234	ASN
1	B	247	CYS
1	B	255	VAL
1	B	333	VAL
1	C	69	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	234	ASN
1	C	236	THR
1	C	255	VAL
4	J	48	ILE
4	J	49	TYR
4	K	50	GLU
4	K	51	VAL
4	K	58	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	428	GLN
1	B	136	ASN
1	B	203	GLN
1	B	258	GLN
1	B	293	GLN
1	B	300	ASN
1	B	398	ASN
1	B	422	GLN
1	B	428	GLN
1	B	432	GLN
1	B	478	ASN
1	C	99	ASN
1	C	374	HIS
1	C	432	GLN
2	D	591	GLN
2	D	607	ASN
2	D	651	ASN
2	E	540	GLN
2	E	590	GLN
2	E	618	ASN
2	F	590	GLN
2	F	652	GLN
2	F	653	GLN
2	F	658	GLN
3	G	39	GLN
3	I	52	ASN
4	J	17	GLN
4	J	38	GLN
4	J	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	6	GLN
4	K	17	GLN
4	L	39	HIS
4	L	69	ASN
5	M	5	GLN
5	M	30	ASN
5	M	82(A)	ASN
5	N	3	GLN
5	N	5	GLN
5	O	1	GLN
5	O	5	GLN
5	O	30	ASN
6	P	26	GLN
6	P	37	GLN
6	P	52	GLN
6	P	109	GLN
6	Q	37	GLN
6	R	37	GLN
6	R	89	HIS
6	R	109	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

86 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	S	1	7,1	14,14,15	0.37	0	17,19,21	0.46	0
7	NAG	S	2	7	14,14,15	0.38	0	17,19,21	0.70	0
7	BMA	S	3	7	11,11,12	0.26	0	15,15,17	0.53	0
8	NAG	T	1	1,8	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
8	NAG	T	2	8	14,14,15	0.38	0	17,19,21	0.65	0
9	NAG	U	1	9,1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
9	NAG	U	2	9	14,14,15	0.37	0	17,19,21	0.87	1 (5%)
9	BMA	U	3	9	11,11,12	0.23	0	15,15,17	0.61	0
9	MAN	U	4	9	11,11,12	0.28	0	15,15,17	0.50	0
10	NAG	V	1	10,1	14,14,15	0.39	0	17,19,21	0.42	0
10	NAG	V	2	10	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
10	BMA	V	3	10	11,11,12	0.35	0	15,15,17	0.58	0
10	BMA	V	4	10	11,11,12	0.26	0	15,15,17	0.54	0
8	NAG	W	1	1,8	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
8	NAG	W	2	8	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
7	NAG	X	1	7,1	14,14,15	0.39	0	17,19,21	0.97	0
7	NAG	X	2	7	14,14,15	0.36	0	17,19,21	0.91	1 (5%)
7	BMA	X	3	7	11,11,12	0.26	0	15,15,17	0.53	0
8	NAG	Y	1	1,8	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
8	NAG	Y	2	8	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
11	NAG	Z	1	11,1	14,14,15	0.40	0	17,19,21	1.08	1 (5%)
11	NAG	Z	2	11	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
11	MAN	Z	3	11	11,11,12	0.32	0	15,15,17	1.02	1 (6%)
12	NAG	a	1	12,1	14,14,15	0.39	0	17,19,21	0.70	0
12	NAG	a	2	12	14,14,15	0.39	0	17,19,21	0.75	0
12	BMA	a	3	12	11,11,12	0.19	0	15,15,17	0.86	1 (6%)
12	BMA	a	4	12	11,11,12	0.28	0	15,15,17	1.06	1 (6%)
12	MAN	a	5	12	11,11,12	0.32	0	15,15,17	1.04	1 (6%)
12	BMA	a	6	12	11,11,12	0.27	0	15,15,17	0.52	0
7	NAG	b	1	7,1	14,14,15	0.37	0	17,19,21	0.62	0
7	NAG	b	2	7	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
7	BMA	b	3	7	11,11,12	0.27	0	15,15,17	0.53	0
8	NAG	c	1	1,8	14,14,15	0.40	0	17,19,21	0.58	0
8	NAG	c	2	8	14,14,15	0.37	0	17,19,21	0.50	0
9	NAG	d	1	9,1	14,14,15	0.40	0	17,19,21	0.72	0
9	NAG	d	2	9	14,14,15	0.39	0	17,19,21	0.95	1 (5%)
9	BMA	d	3	9	11,11,12	0.29	0	15,15,17	0.80	1 (6%)
9	MAN	d	4	9	11,11,12	0.30	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	e	1	1,8	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
8	NAG	e	2	8	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
7	NAG	f	1	7,1	14,14,15	0.40	0	17,19,21	0.49	0
7	NAG	f	2	7	14,14,15	0.38	0	17,19,21	0.90	2 (11%)
7	BMA	f	3	7	11,11,12	0.26	0	15,15,17	0.57	0
8	NAG	g	1	1,8	14,14,15	0.40	0	17,19,21	0.80	0
8	NAG	g	2	8	14,14,15	0.36	0	17,19,21	1.08	1 (5%)
9	NAG	h	1	9,1	14,14,15	0.39	0	17,19,21	0.68	0
9	NAG	h	2	9	14,14,15	0.39	0	17,19,21	1.00	2 (11%)
9	BMA	h	3	9	11,11,12	0.25	0	15,15,17	0.55	0
9	MAN	h	4	9	11,11,12	0.44	0	15,15,17	0.95	1 (6%)
7	NAG	i	1	7,1	14,14,15	0.35	0	17,19,21	0.56	0
7	NAG	i	2	7	14,14,15	0.37	0	17,19,21	0.66	0
7	BMA	i	3	7	11,11,12	0.27	0	15,15,17	0.57	0
12	NAG	j	1	12,1	14,14,15	0.39	0	17,19,21	2.18	2 (11%)
12	NAG	j	2	12	14,14,15	0.41	0	17,19,21	1.91	2 (11%)
12	BMA	j	3	12	11,11,12	0.26	0	15,15,17	0.69	1 (6%)
12	BMA	j	4	12	11,11,12	0.31	0	15,15,17	0.51	0
12	MAN	j	5	12	11,11,12	0.25	0	15,15,17	0.49	0
12	BMA	j	6	12	11,11,12	0.28	0	15,15,17	0.47	0
7	NAG	k	1	7,1	14,14,15	0.38	0	17,19,21	0.71	0
7	NAG	k	2	7	14,14,15	0.38	0	17,19,21	1.07	1 (5%)
7	BMA	k	3	7	11,11,12	0.28	0	15,15,17	0.54	0
8	NAG	l	1	1,8	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
8	NAG	l	2	8	14,14,15	0.37	0	17,19,21	0.52	0
10	NAG	m	1	10,1	14,14,15	0.37	0	17,19,21	0.89	2 (11%)
10	NAG	m	2	10	14,14,15	0.38	0	17,19,21	1.08	1 (5%)
10	BMA	m	3	10	11,11,12	0.34	0	15,15,17	0.48	0
10	BMA	m	4	10	11,11,12	0.30	0	15,15,17	0.44	0
7	NAG	n	1	7,1,3	14,14,15	0.62	0	17,19,21	4.36	6 (35%)
7	NAG	n	2	7	14,14,15	0.36	0	17,19,21	0.70	0
7	BMA	n	3	7	11,11,12	0.20	0	15,15,17	0.75	1 (6%)
8	NAG	o	1	1,8	14,14,15	0.38	0	17,19,21	0.81	0
8	NAG	o	2	8	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
7	NAG	p	1	7,1	14,14,15	0.40	0	17,19,21	0.80	0
7	NAG	p	2	7	14,14,15	0.41	0	17,19,21	1.41	2 (11%)
7	BMA	p	3	7	11,11,12	0.26	0	15,15,17	0.56	0
8	NAG	q	1	1,8	14,14,15	0.40	0	17,19,21	0.63	0
8	NAG	q	2	8	14,14,15	0.36	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	r	1	7,1	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	r	2	7	14,14,15	0.40	0	17,19,21	1.54	4 (23%)
7	BMA	r	3	7	11,11,12	0.33	0	15,15,17	0.39	0
13	NAG	s	1	13,1	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
13	NAG	s	2	13	14,14,15	0.37	0	17,19,21	0.58	0
13	BMA	s	3	13	11,11,12	0.29	0	15,15,17	0.70	0
13	MAN	s	4	13	11,11,12	0.32	0	15,15,17	0.51	0
13	MAN	s	5	13	11,11,12	0.39	0	15,15,17	0.57	0
13	MAN	s	6	13	11,11,12	0.32	0	15,15,17	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	S	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	3/6/23/26	0/1/1/1
7	BMA	S	3	7	-	1/2/19/22	0/1/1/1
8	NAG	T	1	1,8	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	T	2	8	1/1/5/7	2/6/23/26	0/1/1/1
9	NAG	U	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	5/6/23/26	0/1/1/1
9	BMA	U	3	9	-	1/2/19/22	0/1/1/1
9	MAN	U	4	9	-	2/2/19/22	0/1/1/1
10	NAG	V	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	V	2	10	-	4/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
10	BMA	V	4	10	-	0/2/19/22	0/1/1/1
8	NAG	W	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	1/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
11	NAG	Z	1	11,1	-	5/6/23/26	0/1/1/1
11	NAG	Z	2	11	-	1/6/23/26	0/1/1/1
11	MAN	Z	3	11	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	a	1	12,1	-	2/6/23/26	0/1/1/1
12	NAG	a	2	12	-	0/6/23/26	0/1/1/1
12	BMA	a	3	12	-	2/2/19/22	0/1/1/1
12	BMA	a	4	12	-	0/2/19/22	0/1/1/1
12	MAN	a	5	12	-	1/2/19/22	0/1/1/1
12	BMA	a	6	12	-	0/2/19/22	0/1/1/1
7	NAG	b	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	BMA	b	3	7	-	1/2/19/22	0/1/1/1
8	NAG	c	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
9	NAG	d	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
9	BMA	d	3	9	-	0/2/19/22	0/1/1/1
9	MAN	d	4	9	-	0/2/19/22	0/1/1/1
8	NAG	e	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
7	NAG	f	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	f	2	7	-	3/6/23/26	0/1/1/1
7	BMA	f	3	7	-	0/2/19/22	0/1/1/1
8	NAG	g	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
9	NAG	h	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	h	2	9	-	3/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
9	MAN	h	4	9	-	1/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	1/6/23/26	0/1/1/1
7	BMA	i	3	7	-	0/2/19/22	0/1/1/1
12	NAG	j	1	12,1	-	1/6/23/26	0/1/1/1
12	NAG	j	2	12	-	3/6/23/26	0/1/1/1
12	BMA	j	3	12	-	0/2/19/22	0/1/1/1
12	BMA	j	4	12	-	1/2/19/22	0/1/1/1
12	MAN	j	5	12	-	0/2/19/22	0/1/1/1
12	BMA	j	6	12	-	0/2/19/22	0/1/1/1
7	NAG	k	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	k	2	7	-	2/6/23/26	0/1/1/1
7	BMA	k	3	7	-	1/2/19/22	0/1/1/1
8	NAG	l	1	1,8	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	l	2	8	-	0/6/23/26	0/1/1/1
10	NAG	m	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	m	2	10	-	2/6/23/26	0/1/1/1
10	BMA	m	3	10	-	0/2/19/22	0/1/1/1
10	BMA	m	4	10	-	0/2/19/22	0/1/1/1
7	NAG	n	1	7,1,3	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	n	2	7	-	3/6/23/26	0/1/1/1
7	BMA	n	3	7	-	1/2/19/22	0/1/1/1
8	NAG	o	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
7	NAG	p	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	p	2	7	1/1/5/7	1/6/23/26	0/1/1/1
7	BMA	p	3	7	-	0/2/19/22	0/1/1/1
8	NAG	q	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
7	NAG	r	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	r	2	7	-	3/6/23/26	0/1/1/1
7	BMA	r	3	7	-	0/2/19/22	0/1/1/1
13	NAG	s	1	13,1	-	2/6/23/26	0/1/1/1
13	NAG	s	2	13	-	2/6/23/26	0/1/1/1
13	BMA	s	3	13	-	0/2/19/22	0/1/1/1
13	MAN	s	4	13	-	0/2/19/22	0/1/1/1
13	MAN	s	5	13	-	1/2/19/22	0/1/1/1
13	MAN	s	6	13	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	n	1	NAG	O5-C1-C2	-14.12	89.44	111.29
12	j	1	NAG	C2-N2-C7	8.32	134.05	122.90
7	n	1	NAG	C4-C3-C2	-6.37	101.69	111.02
7	n	1	NAG	C1-C2-N2	6.26	120.29	110.43
12	j	2	NAG	C1-C2-N2	5.46	119.04	110.43
7	n	1	NAG	C3-C4-C5	-5.23	100.75	110.23
12	j	2	NAG	C2-N2-C7	4.70	129.20	122.90
7	p	2	NAG	C2-N2-C7	4.53	128.97	122.90
7	k	2	NAG	C2-N2-C7	3.99	128.25	122.90
10	m	2	NAG	C2-N2-C7	3.72	127.88	122.90
8	g	2	NAG	C2-N2-C7	3.67	127.82	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	2	NAG	C2-N2-C7	3.40	127.46	122.90
7	b	2	NAG	C2-N2-C7	3.38	127.43	122.90
11	Z	2	NAG	C2-N2-C7	3.38	127.42	122.90
7	r	2	NAG	C1-O5-C5	3.34	116.66	112.19
8	q	2	NAG	C2-N2-C7	3.28	127.30	122.90
7	X	2	NAG	C2-N2-C7	3.24	127.24	122.90
9	d	2	NAG	C2-N2-C7	3.23	127.23	122.90
7	r	2	NAG	O4-C4-C3	-3.23	102.75	110.38
8	T	1	NAG	C2-N2-C7	3.09	127.05	122.90
12	a	5	MAN	C1-O5-C5	3.01	116.23	112.19
11	Z	3	MAN	C1-O5-C5	2.99	116.19	112.19
9	h	2	NAG	C1-C2-N2	2.70	114.68	110.43
12	a	4	BMA	O2-C2-C3	2.69	115.72	110.15
8	e	2	NAG	C1-C2-N2	2.67	114.64	110.43
12	j	1	NAG	C1-C2-N2	-2.66	106.25	110.43
11	Z	1	NAG	C2-N2-C7	2.66	126.46	122.90
9	h	4	MAN	C1-O5-C5	2.64	115.73	112.19
7	n	3	BMA	C1-O5-C5	2.52	115.57	112.19
7	r	2	NAG	C1-C2-N2	2.50	114.37	110.43
13	s	1	NAG	C2-N2-C7	2.43	126.16	122.90
7	p	2	NAG	C1-C2-N2	2.43	114.26	110.43
7	f	2	NAG	C1-C2-N2	2.39	114.20	110.43
9	d	3	BMA	C1-O5-C5	2.36	115.35	112.19
9	U	2	NAG	C1-C2-N2	2.29	114.04	110.43
10	m	1	NAG	C1-C2-N2	2.27	114.01	110.43
12	a	3	BMA	C1-O5-C5	2.20	115.13	112.19
8	Y	1	NAG	C1-C2-N2	2.16	113.84	110.43
10	V	2	NAG	C2-N2-C7	2.14	125.77	122.90
10	m	1	NAG	C2-N2-C7	-2.13	120.05	122.90
9	h	2	NAG	C2-N2-C7	2.12	125.74	122.90
9	U	1	NAG	C1-C2-N2	2.12	113.77	110.43
12	j	3	BMA	C1-O5-C5	2.11	115.01	112.19
7	n	1	NAG	C1-O5-C5	2.10	114.99	112.19
7	n	1	NAG	O5-C5-C4	-2.09	105.75	110.83
8	e	1	NAG	O4-C4-C3	-2.08	105.47	110.38
7	f	2	NAG	C2-N2-C7	2.07	125.67	122.90
8	W	2	NAG	C2-N2-C7	2.06	125.67	122.90
8	W	1	NAG	C1-O5-C5	2.06	114.95	112.19
7	r	2	NAG	C2-N2-C7	2.06	125.66	122.90
8	o	2	NAG	C2-N2-C7	2.02	125.61	122.90
8	l	1	NAG	C2-N2-C7	2.01	125.59	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	n	1	NAG	C1
7	p	2	NAG	C1
8	T	1	NAG	C1
8	T	2	NAG	C1

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	2	NAG	C1-C2-N2-C7
7	S	2	NAG	O7-C7-N2-C2
7	f	2	NAG	O7-C7-N2-C2
7	r	2	NAG	C1-C2-N2-C7
7	r	2	NAG	C8-C7-N2-C2
7	r	2	NAG	O7-C7-N2-C2
8	T	1	NAG	C3-C2-N2-C7
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
8	T	2	NAG	C8-C7-N2-C2
8	T	2	NAG	O7-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
9	U	1	NAG	C8-C7-N2-C2
9	U	1	NAG	O7-C7-N2-C2
9	U	2	NAG	C1-C2-N2-C7
9	U	2	NAG	C8-C7-N2-C2
9	U	2	NAG	O7-C7-N2-C2
9	h	1	NAG	C8-C7-N2-C2
9	h	2	NAG	C1-C2-N2-C7
9	h	2	NAG	C8-C7-N2-C2
9	h	2	NAG	O7-C7-N2-C2
10	V	2	NAG	C8-C7-N2-C2
10	V	2	NAG	O7-C7-N2-C2
12	a	1	NAG	C8-C7-N2-C2
12	a	1	NAG	O7-C7-N2-C2
12	j	1	NAG	C3-C2-N2-C7
12	j	2	NAG	C1-C2-N2-C7
13	s	1	NAG	C8-C7-N2-C2
13	s	1	NAG	O7-C7-N2-C2
7	S	2	NAG	C8-C7-N2-C2
7	f	2	NAG	C8-C7-N2-C2
8	c	1	NAG	C8-C7-N2-C2
8	c	1	NAG	O7-C7-N2-C2
9	h	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	U	4	MAN	C4-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6
11	Z	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
12	j	2	NAG	C8-C7-N2-C2
9	U	4	MAN	O5-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
7	n	2	NAG	C8-C7-N2-C2
12	j	2	NAG	O7-C7-N2-C2
7	n	1	NAG	C8-C7-N2-C2
7	n	1	NAG	O7-C7-N2-C2
7	n	2	NAG	O7-C7-N2-C2
8	g	1	NAG	C8-C7-N2-C2
8	g	1	NAG	O7-C7-N2-C2
8	q	1	NAG	C8-C7-N2-C2
8	q	1	NAG	O7-C7-N2-C2
13	s	2	NAG	C8-C7-N2-C2
13	s	2	NAG	O7-C7-N2-C2
9	U	2	NAG	C4-C5-C6-O6
7	S	1	NAG	C8-C7-N2-C2
8	l	1	NAG	C8-C7-N2-C2
7	f	1	NAG	O5-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
9	d	1	NAG	O5-C5-C6-O6
7	S	1	NAG	O7-C7-N2-C2
8	l	1	NAG	O7-C7-N2-C2
10	V	2	NAG	C4-C5-C6-O6
11	Z	1	NAG	C4-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
7	k	3	BMA	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
11	Z	3	MAN	O5-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
8	g	2	NAG	O5-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
12	a	5	MAN	O5-C5-C6-O6
12	j	4	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	s	5	MAN	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
9	h	4	MAN	O5-C5-C6-O6
7	f	2	NAG	C3-C2-N2-C7
7	p	2	NAG	C3-C2-N2-C7
8	q	2	NAG	C3-C2-N2-C7
12	a	3	BMA	C4-C5-C6-O6
11	Z	1	NAG	C8-C7-N2-C2
7	X	2	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7
7	k	2	NAG	C3-C2-N2-C7
8	Y	2	NAG	C3-C2-N2-C7
8	g	2	NAG	C3-C2-N2-C7
9	d	2	NAG	C3-C2-N2-C7
10	m	2	NAG	C3-C2-N2-C7
11	Z	1	NAG	C3-C2-N2-C7
11	Z	2	NAG	C3-C2-N2-C7
11	Z	1	NAG	O7-C7-N2-C2
8	W	1	NAG	C8-C7-N2-C2
7	k	2	NAG	C1-C2-N2-C7
9	d	2	NAG	C1-C2-N2-C7
10	m	2	NAG	C1-C2-N2-C7
7	n	3	BMA	O5-C5-C6-O6
12	a	3	BMA	O5-C5-C6-O6
7	i	2	NAG	C3-C2-N2-C7
8	W	2	NAG	C3-C2-N2-C7
8	W	1	NAG	O7-C7-N2-C2

There are no ring outliers.

29 monomers are involved in 38 short contacts:

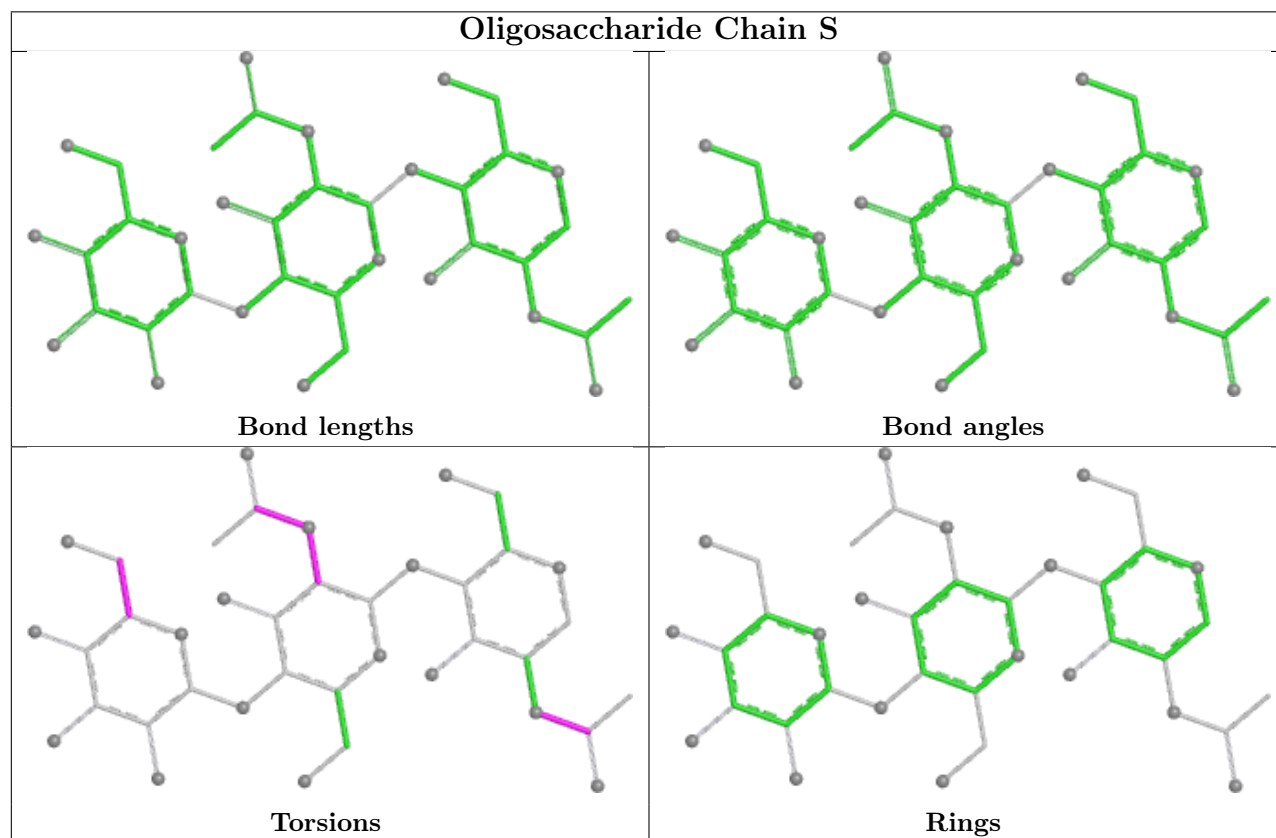
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	s	2	NAG	2	0
10	V	2	NAG	1	0
11	Z	3	MAN	1	0
8	c	1	NAG	1	0
8	g	2	NAG	1	0
7	k	1	NAG	2	0
7	f	1	NAG	1	0
10	m	2	NAG	2	0
12	j	3	BMA	1	0
9	d	3	BMA	1	0

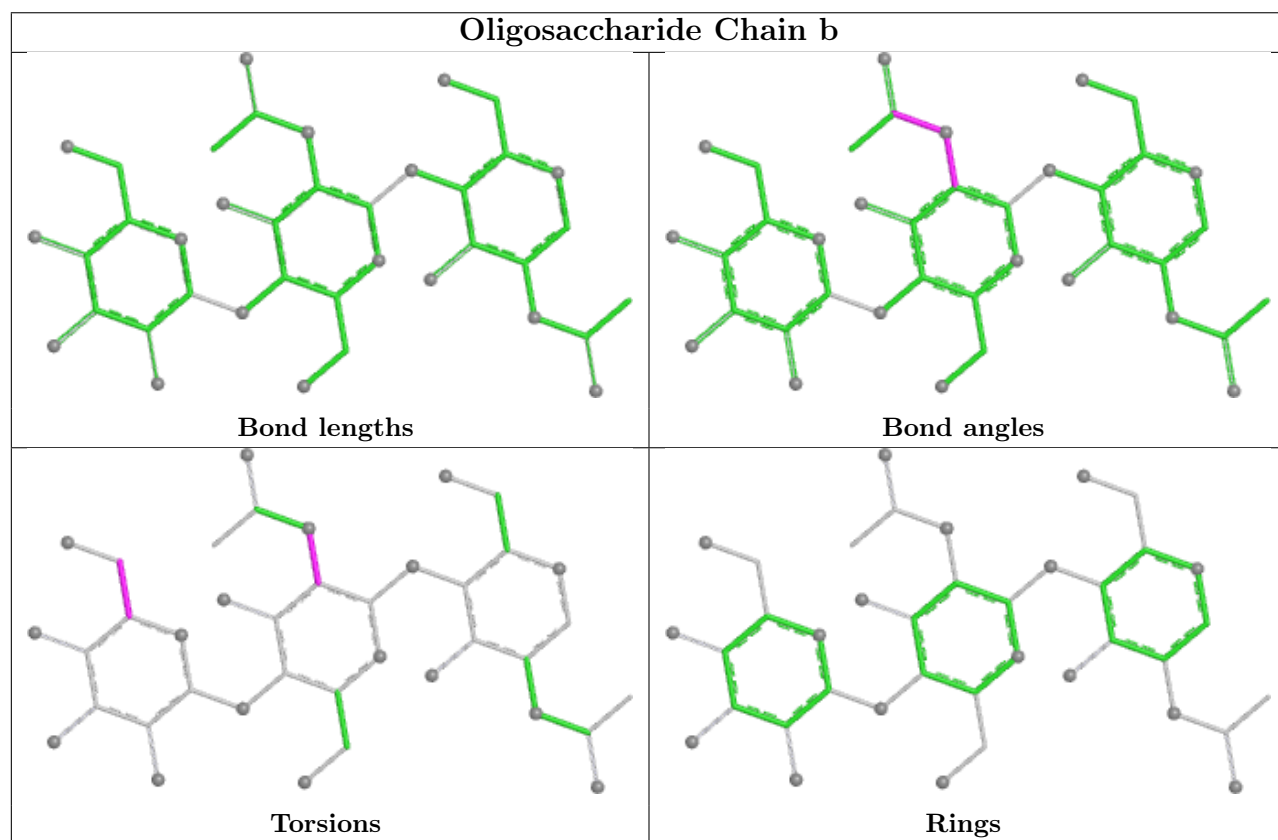
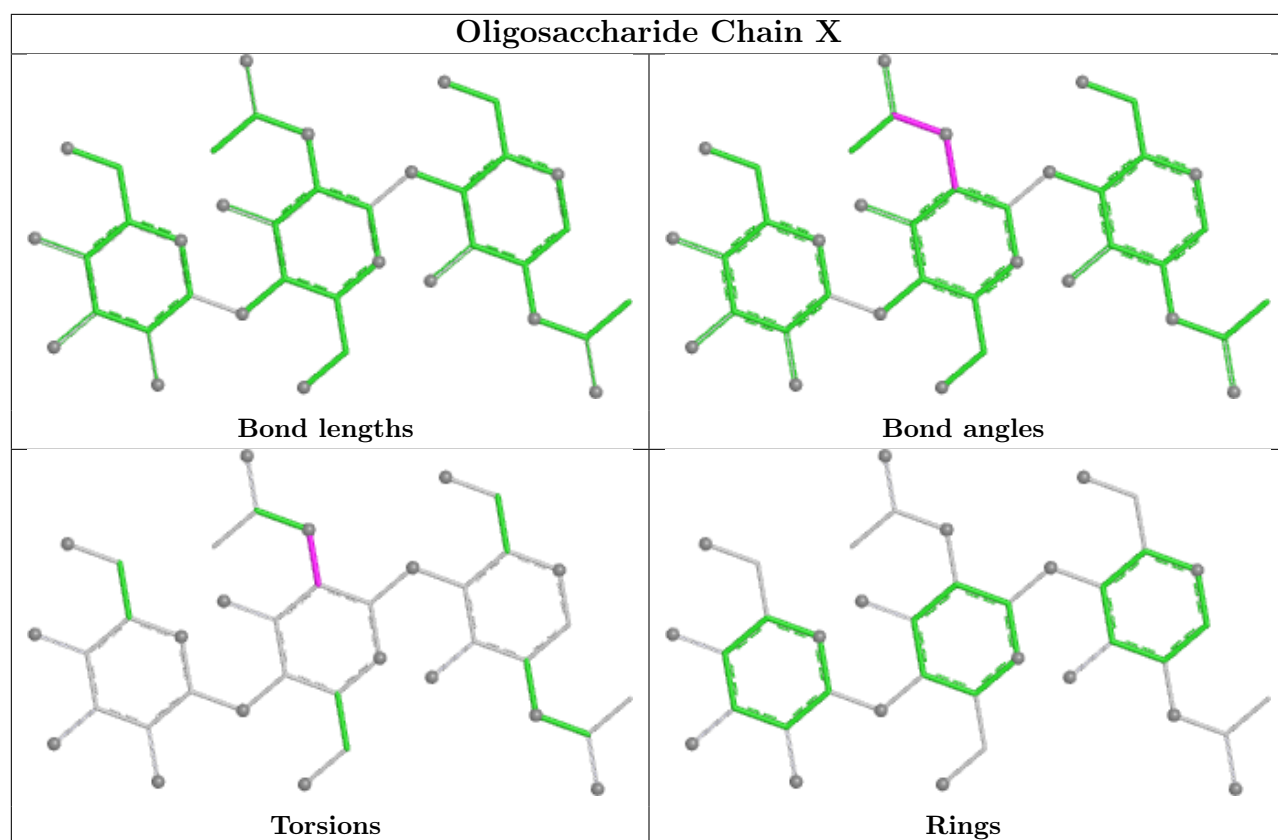
Continued on next page...

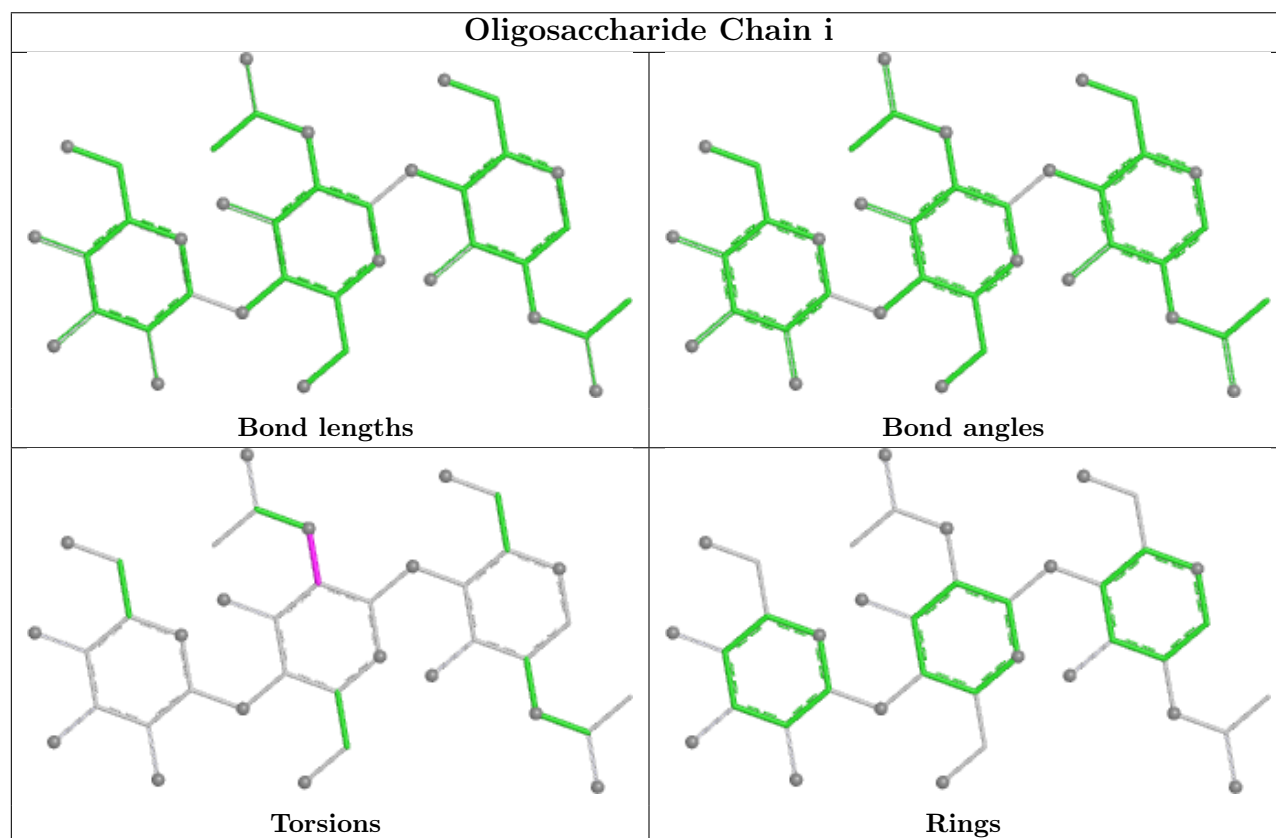
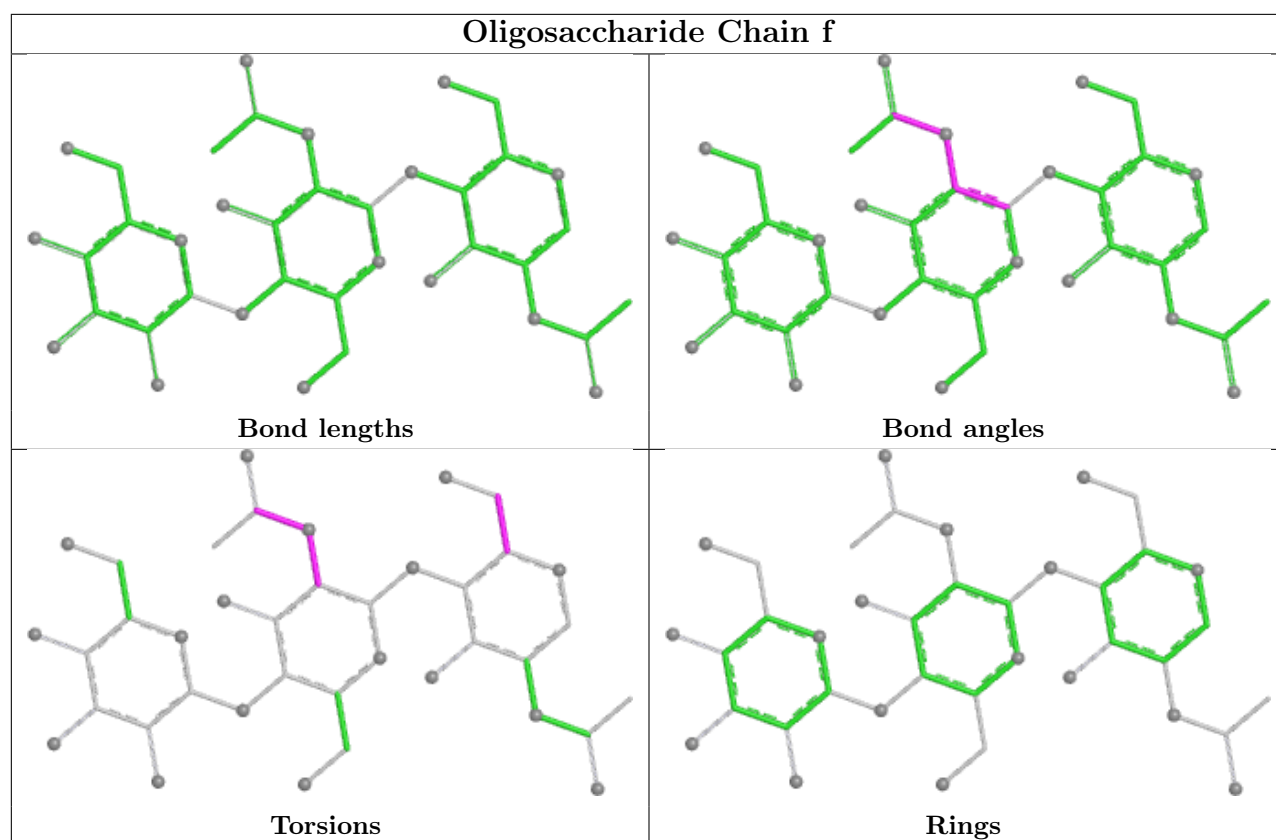
Continued from previous page...

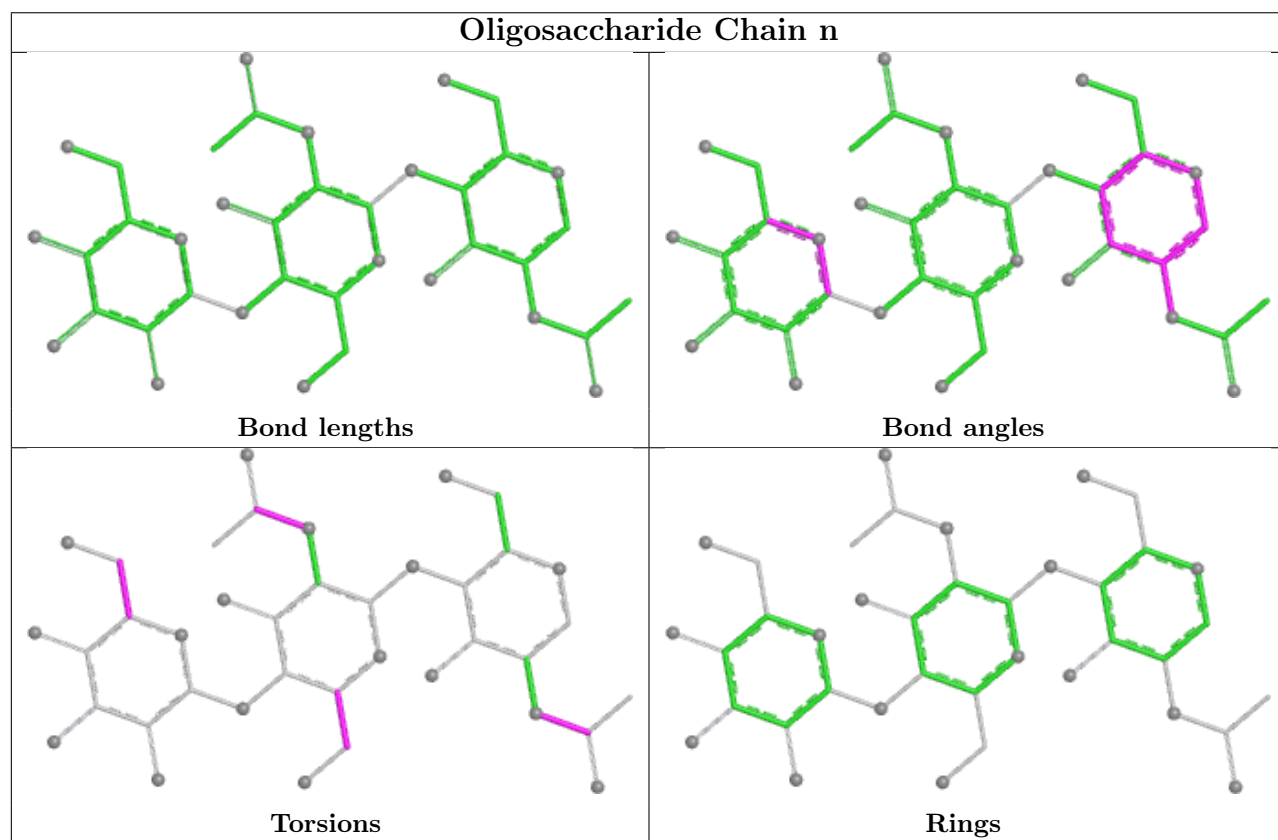
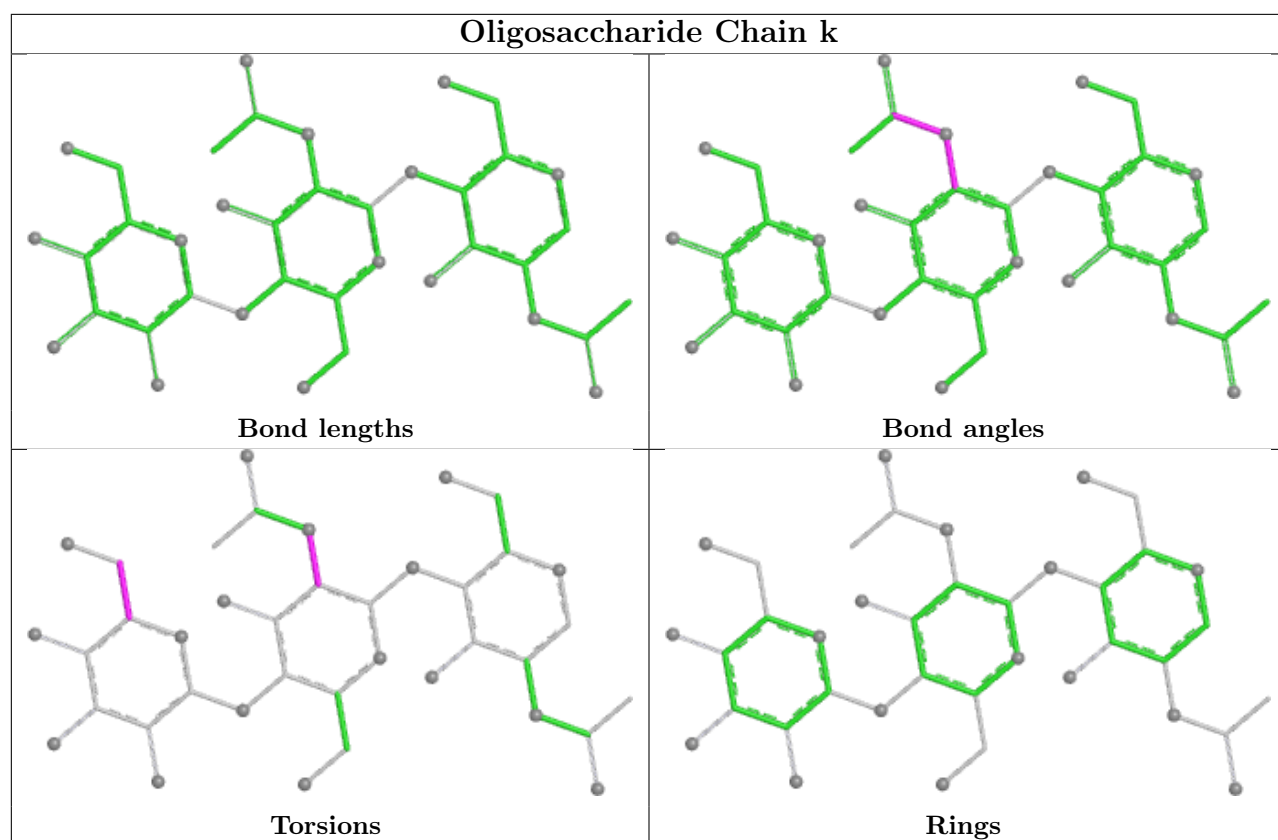
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	h	1	NAG	1	0
12	j	5	MAN	3	0
7	p	2	NAG	1	0
12	a	4	BMA	1	0
8	T	1	NAG	2	0
7	p	1	NAG	1	0
8	e	1	NAG	1	0
9	d	2	NAG	2	0
7	r	2	NAG	1	0
12	j	2	NAG	1	0
11	Z	1	NAG	1	0
13	s	3	BMA	1	0
8	e	2	NAG	1	0
7	n	3	BMA	1	0
10	m	3	BMA	1	0
9	h	3	BMA	2	0
9	h	4	MAN	1	0
13	s	5	MAN	2	0
7	n	1	NAG	4	0

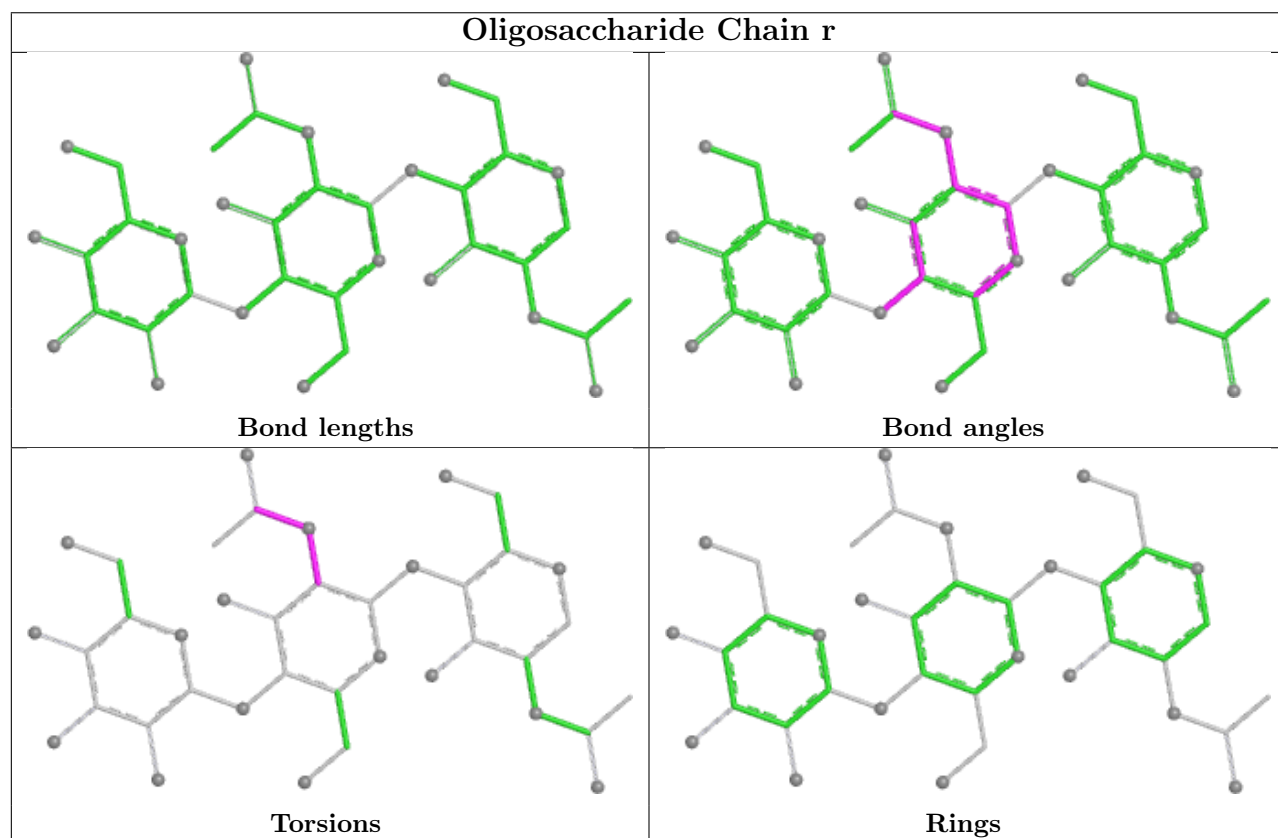
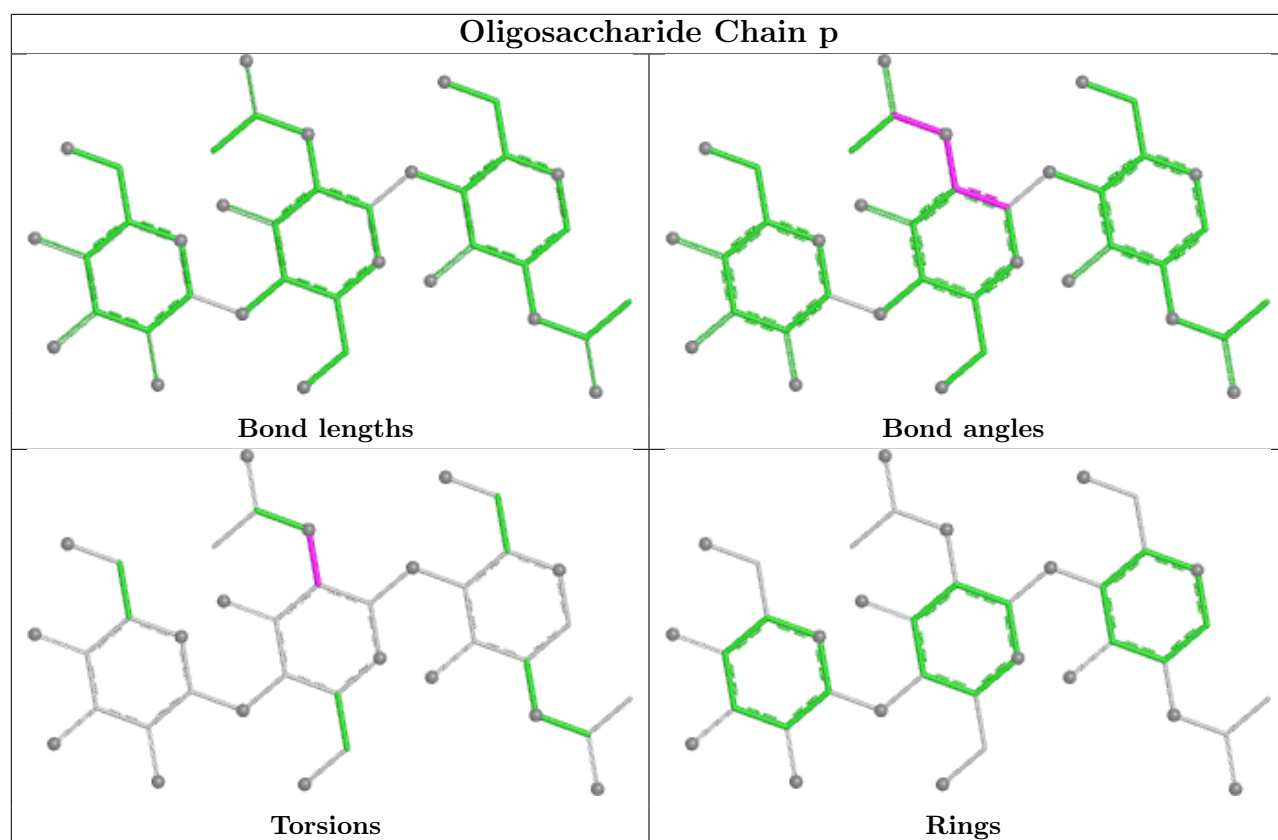
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

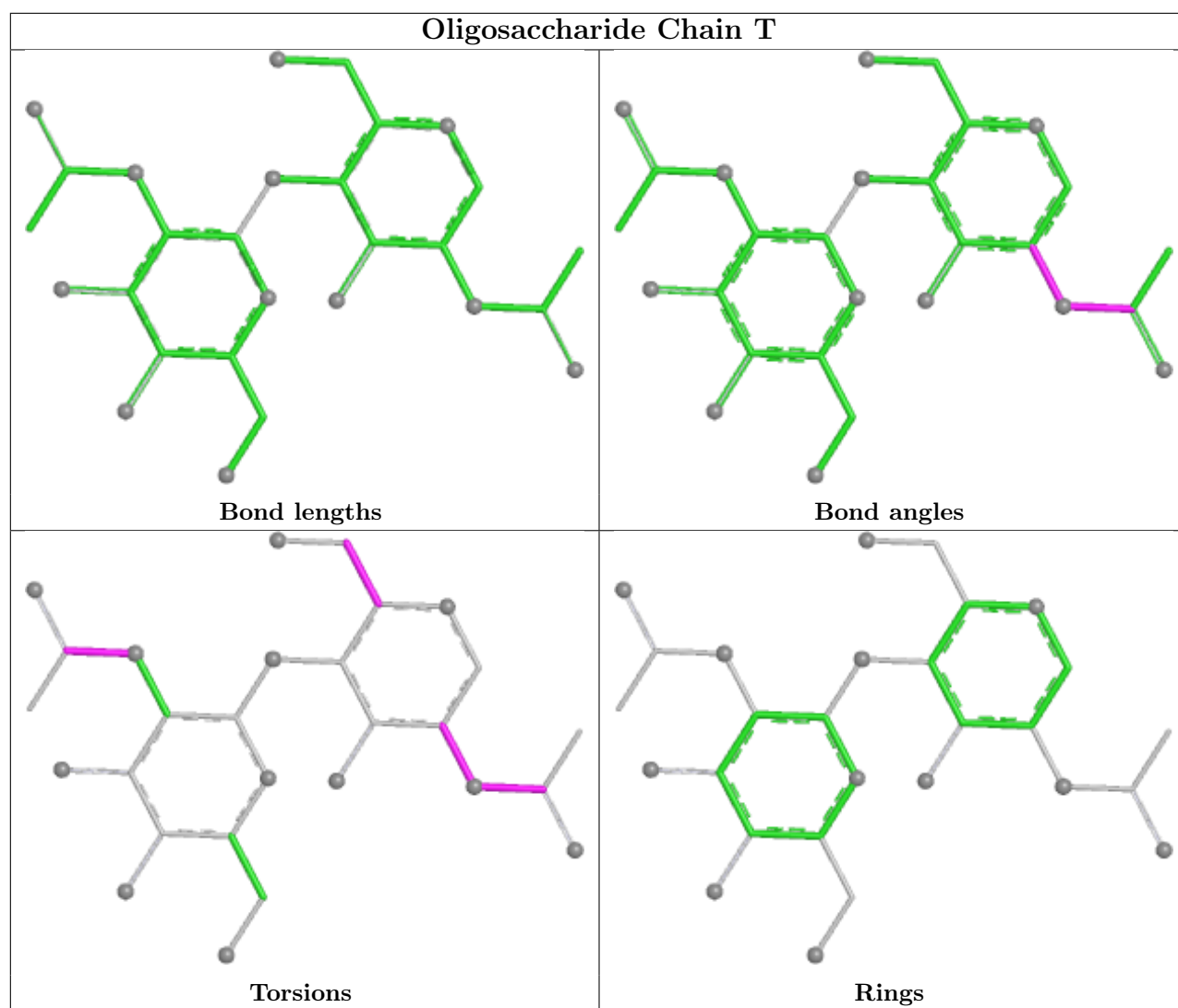


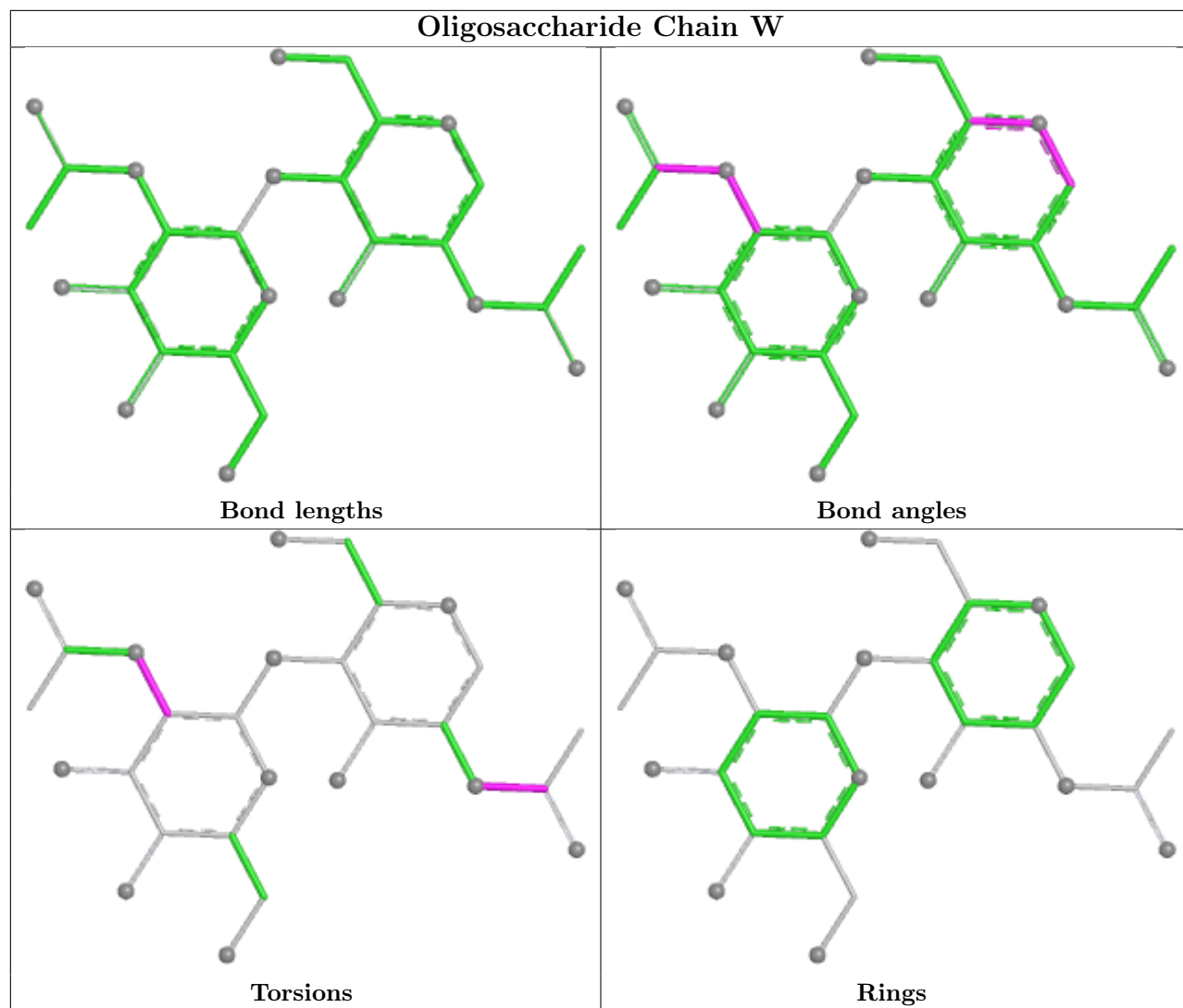


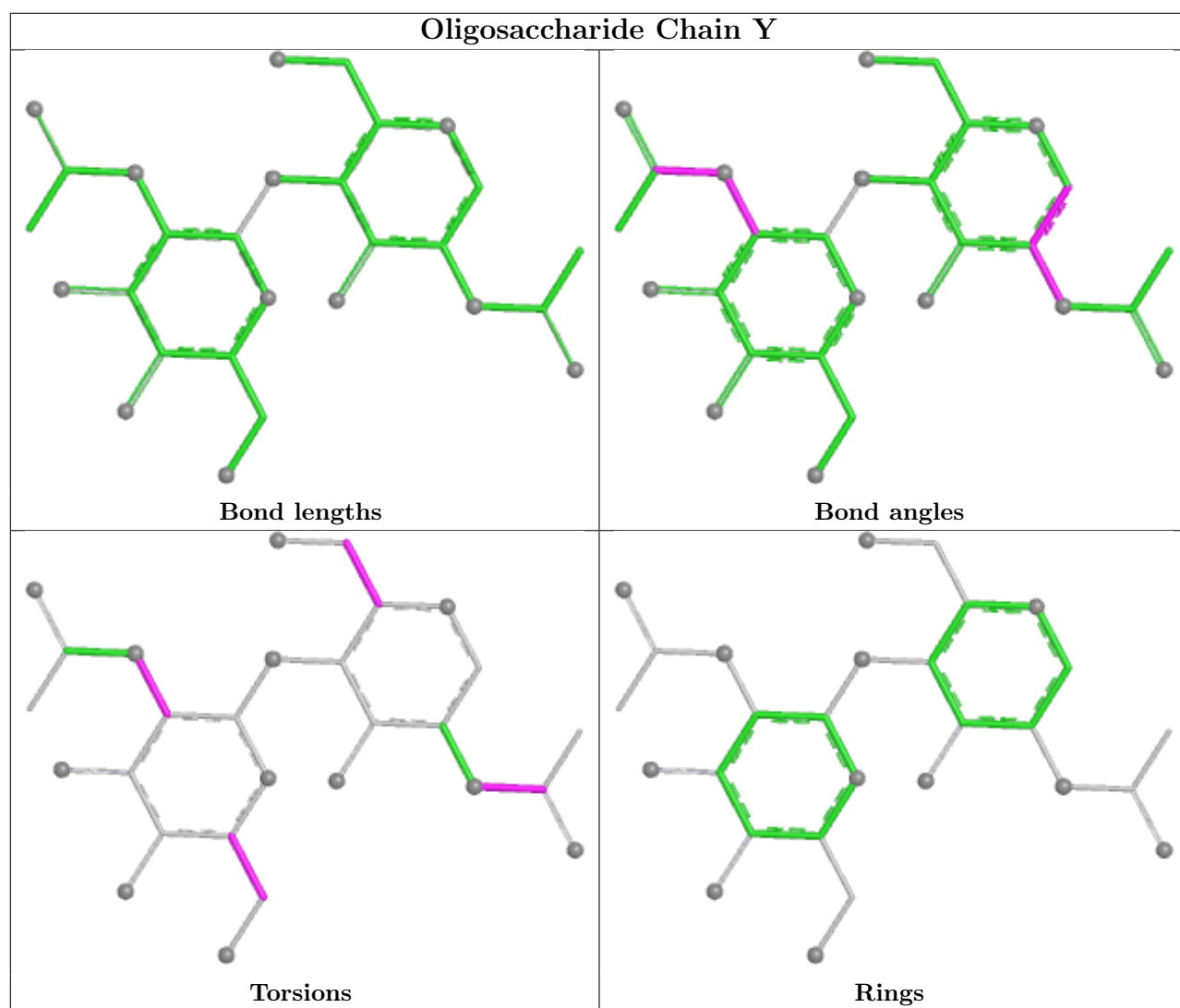


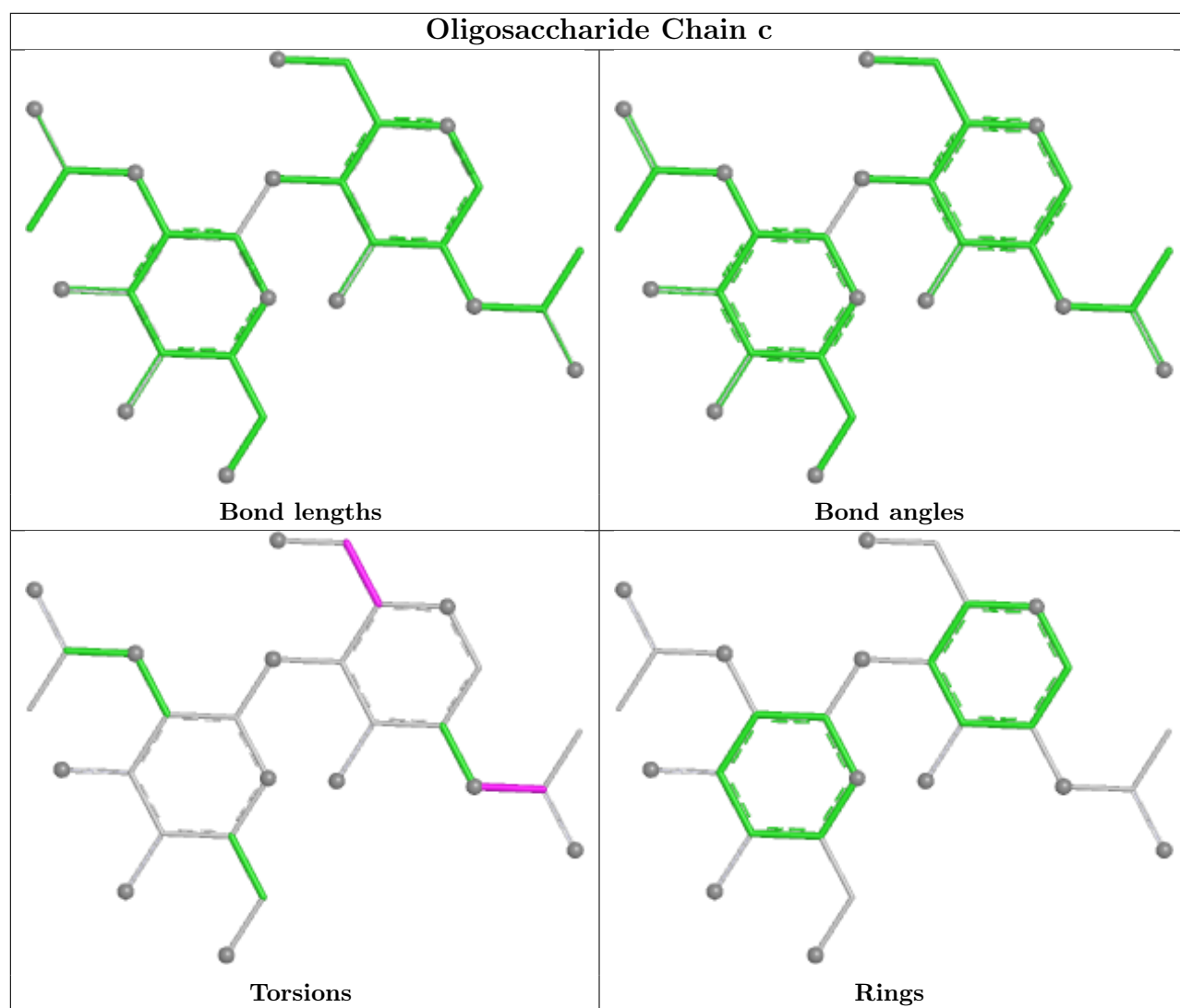


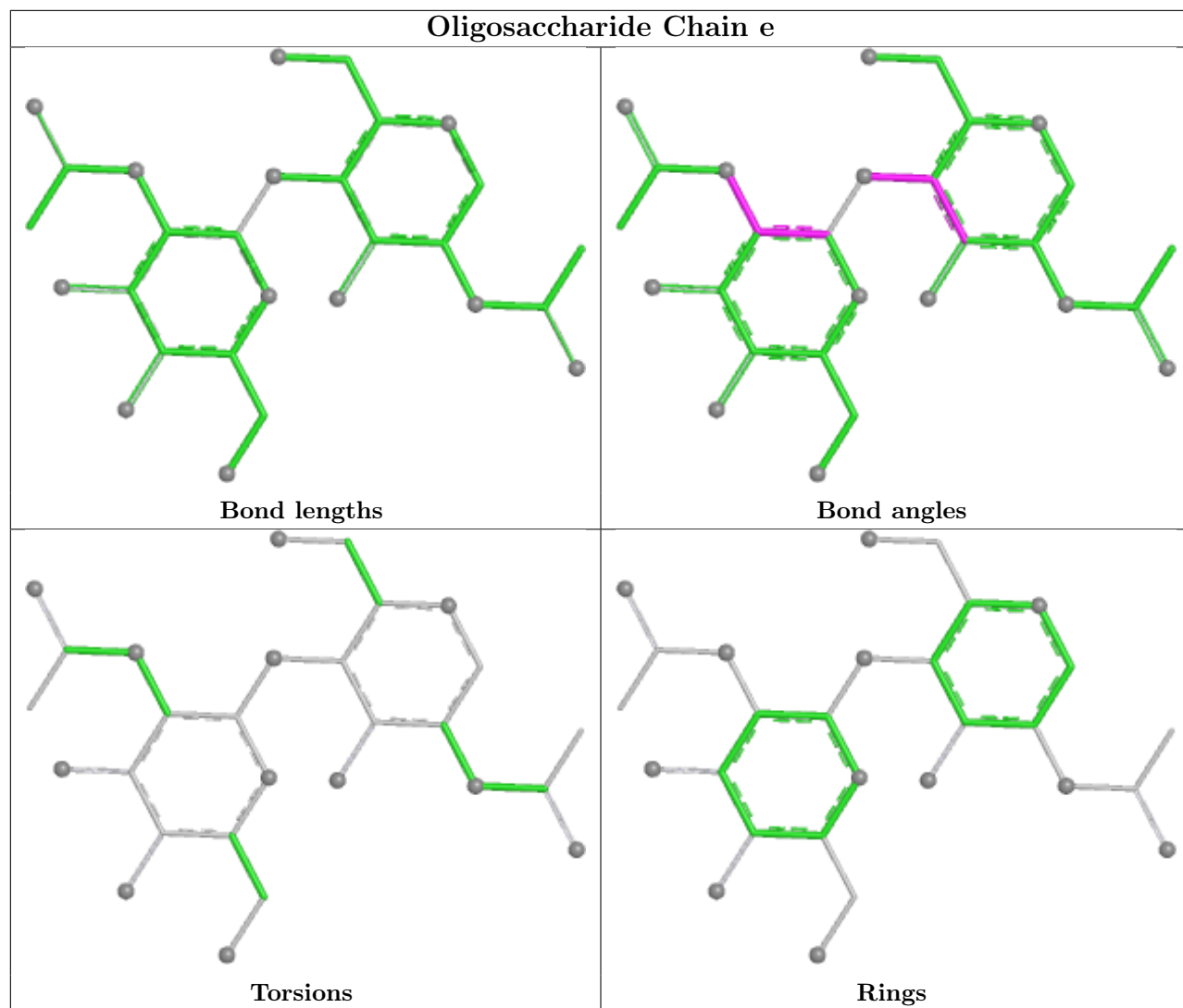


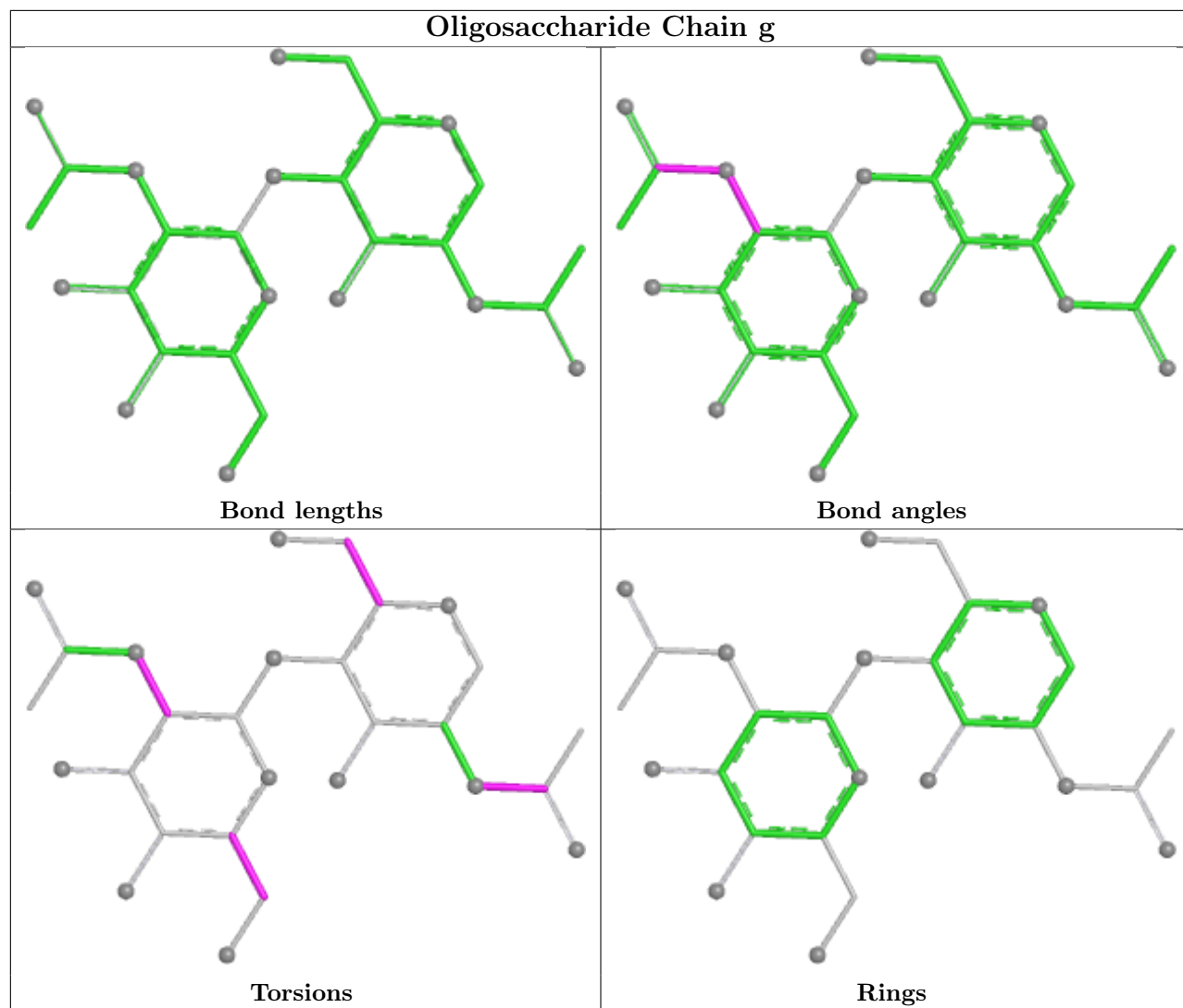


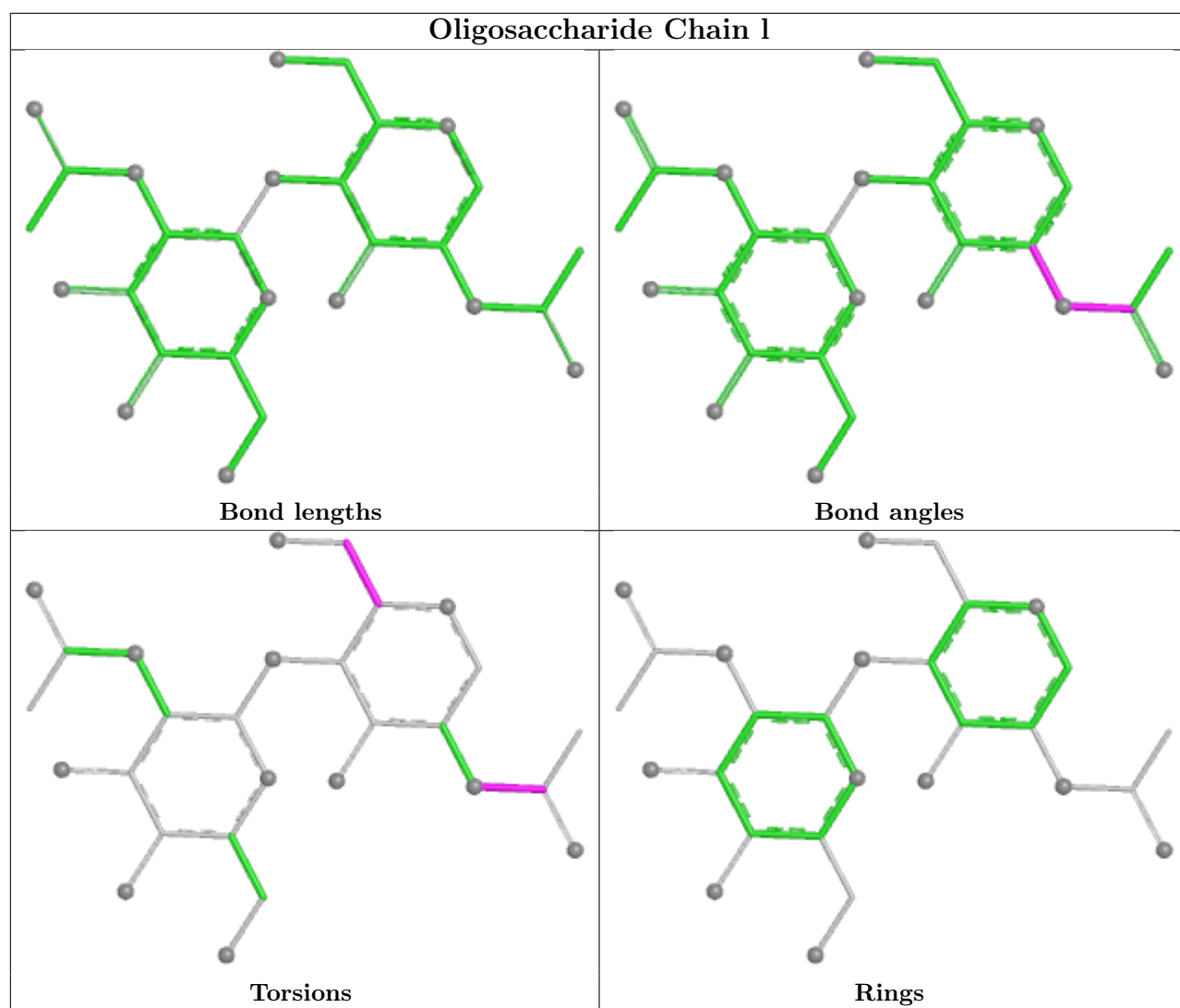


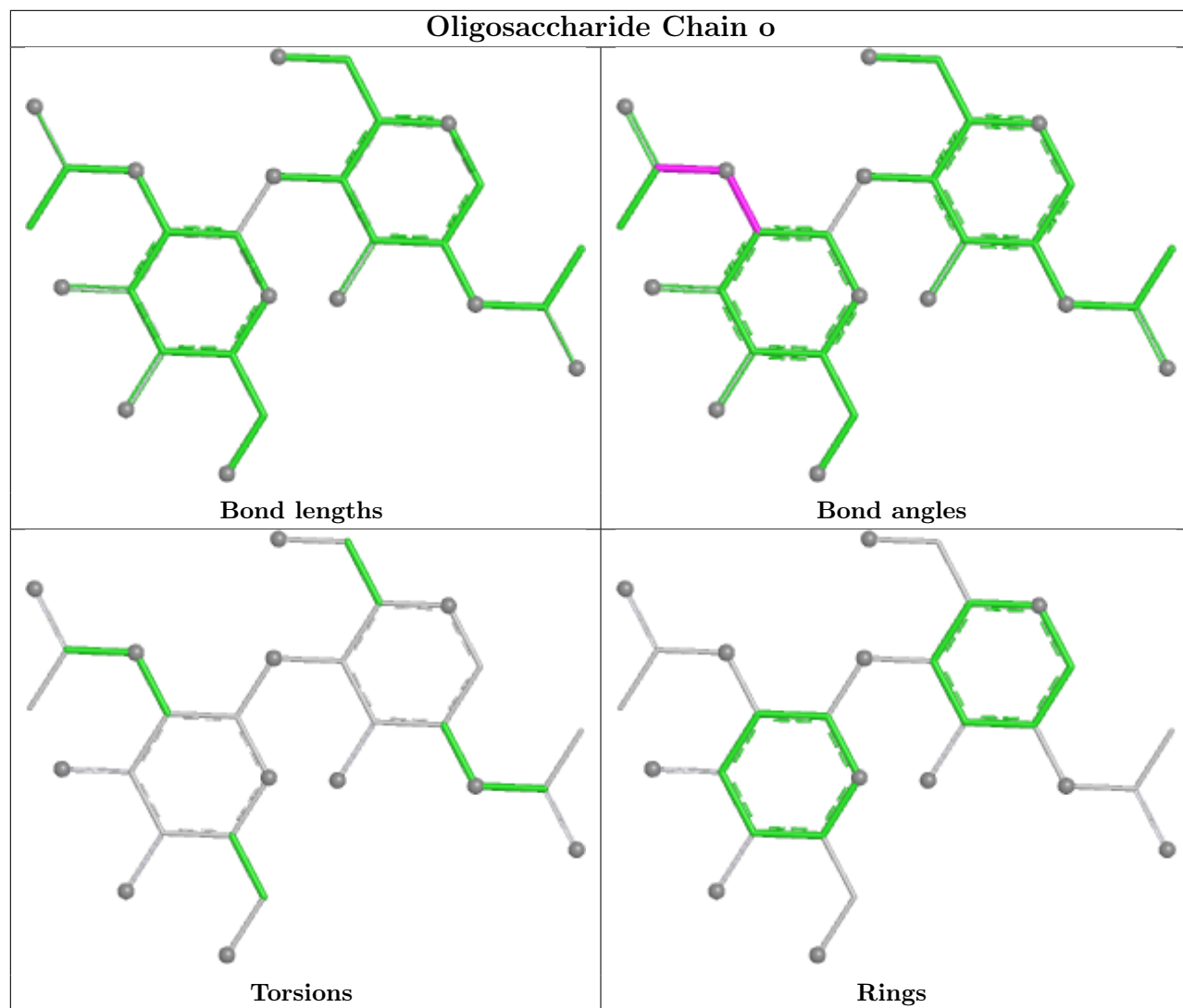


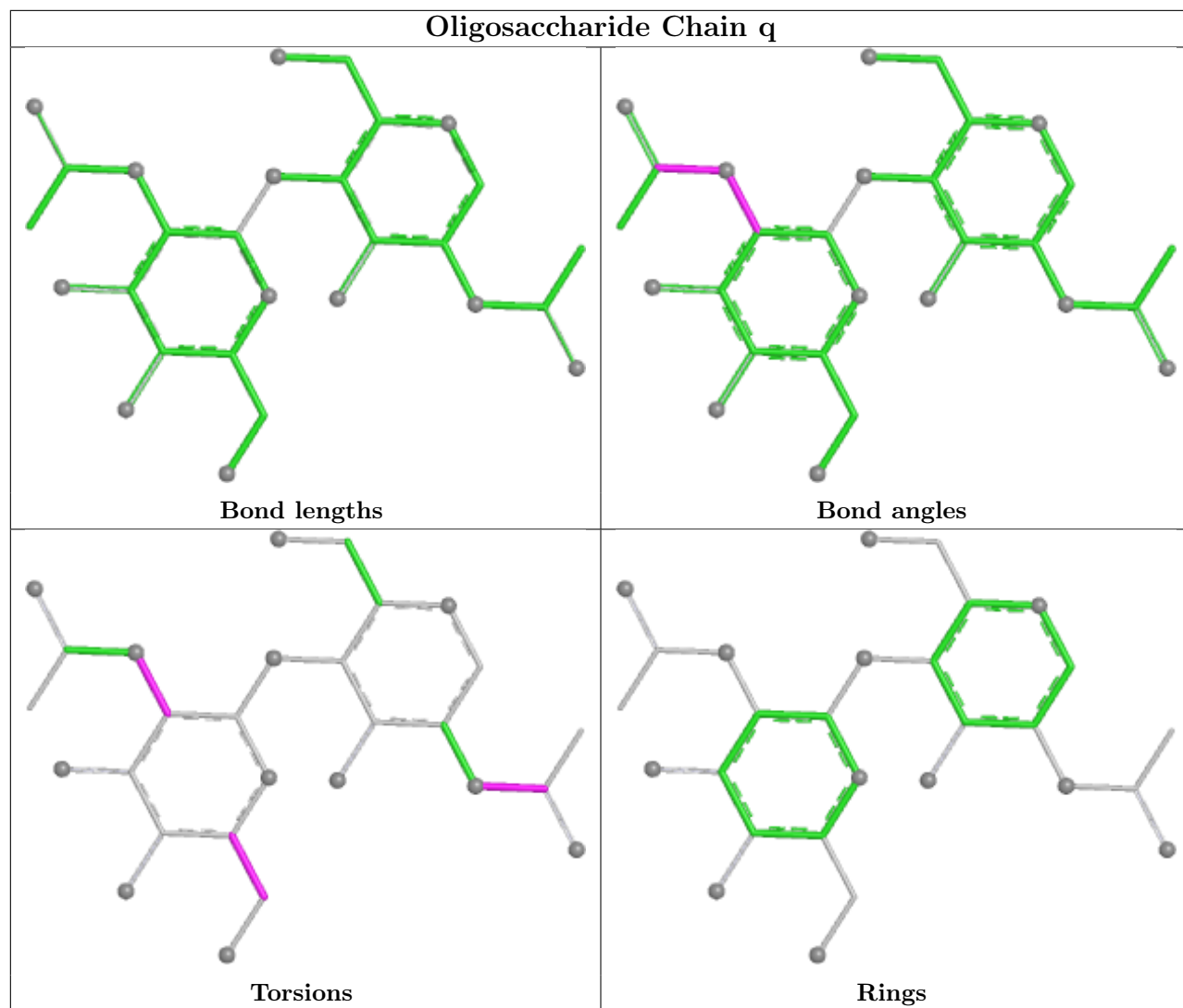


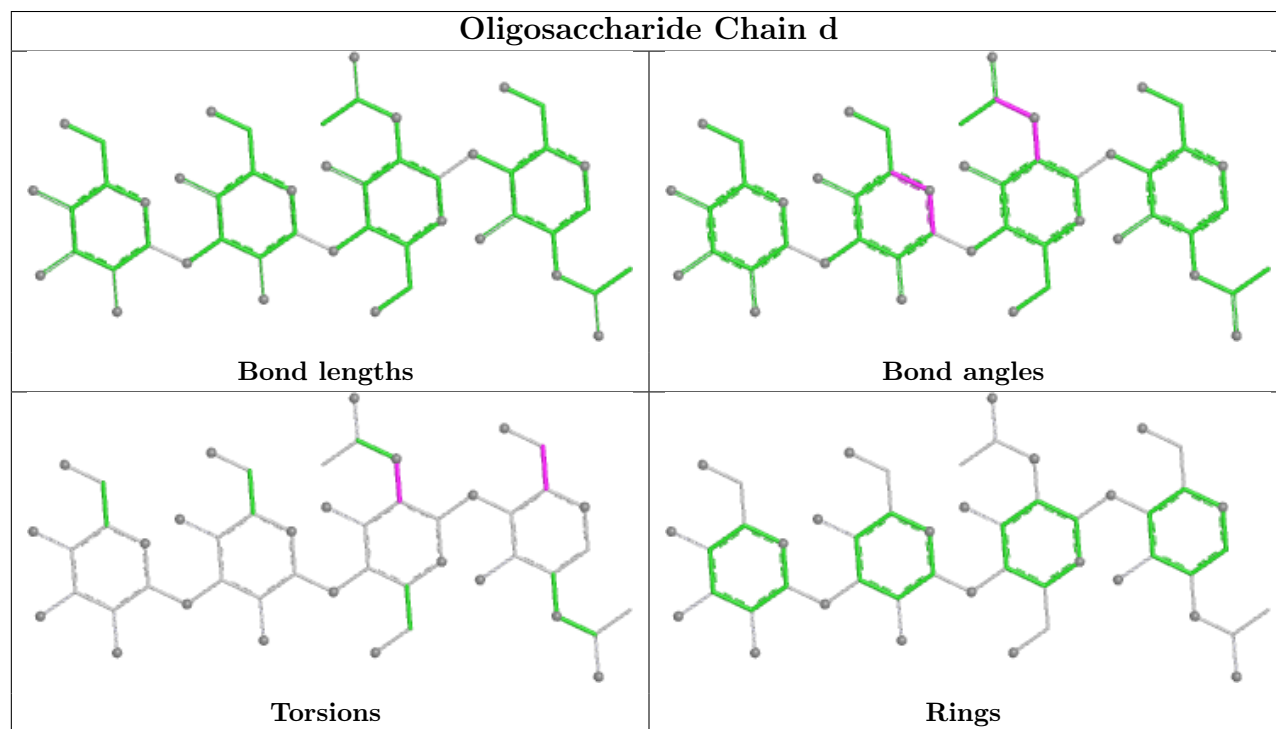
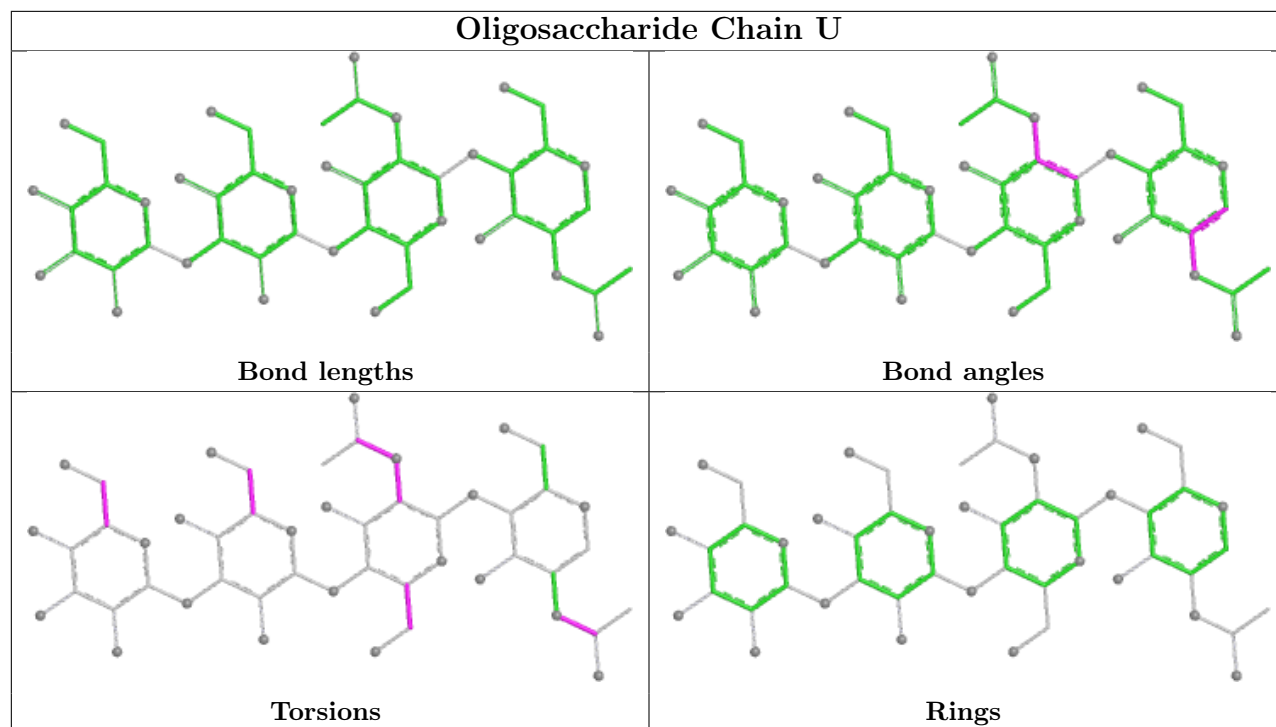


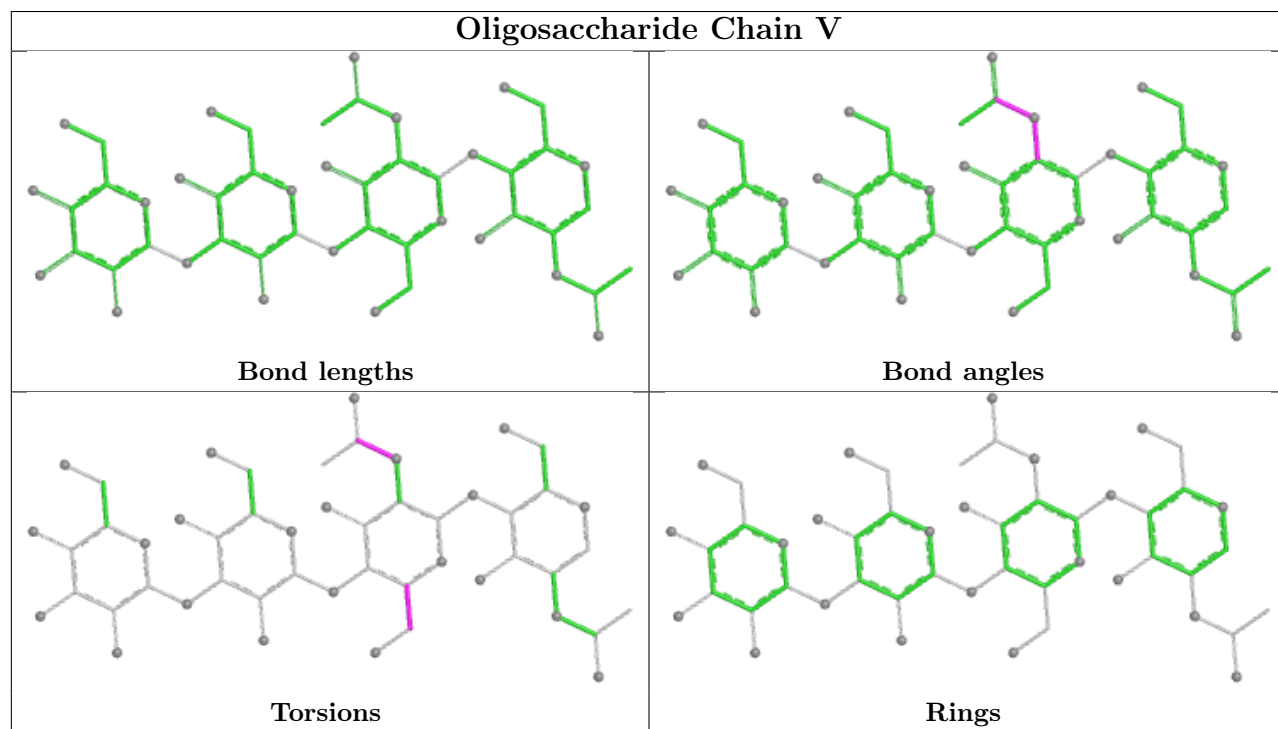
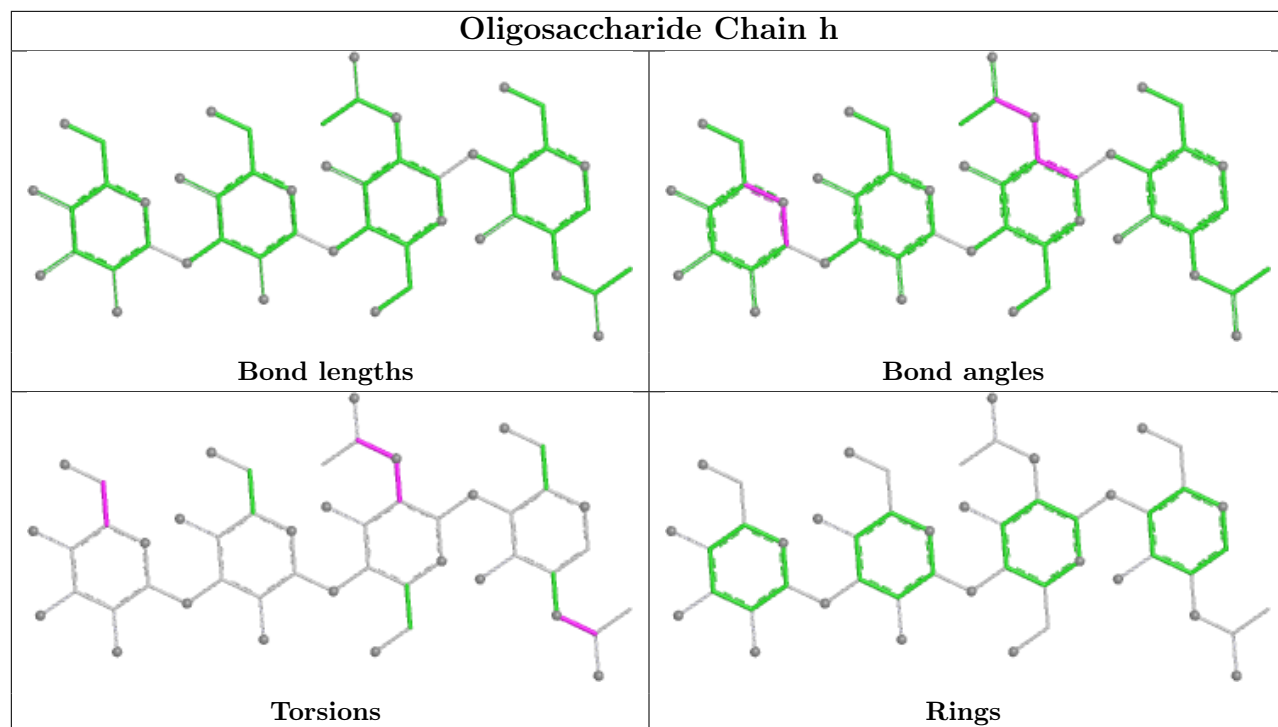


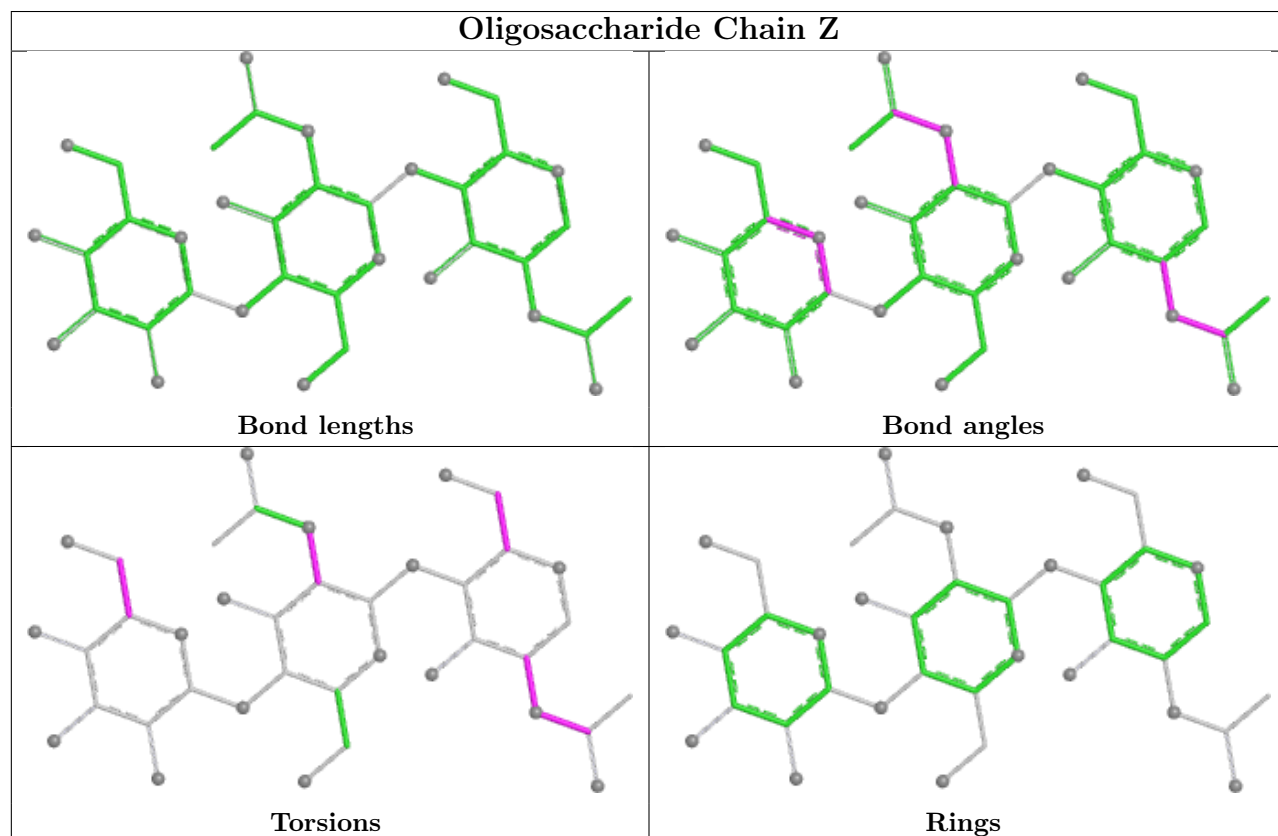
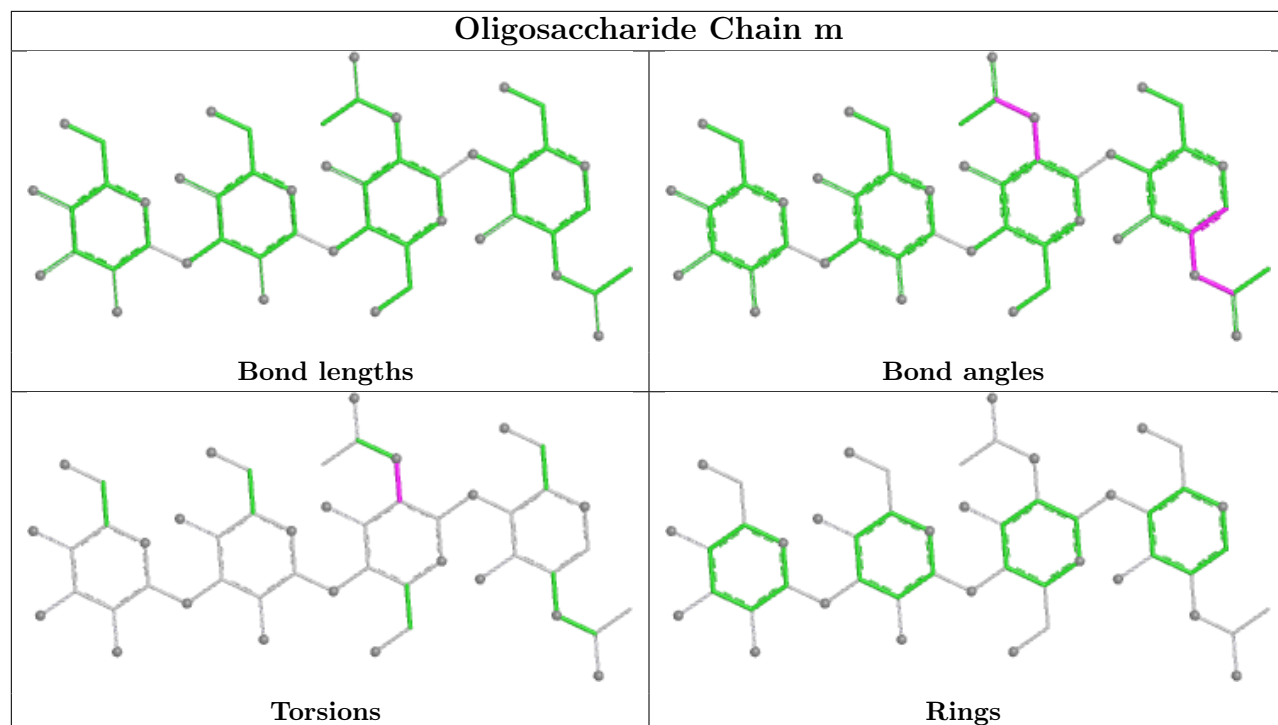


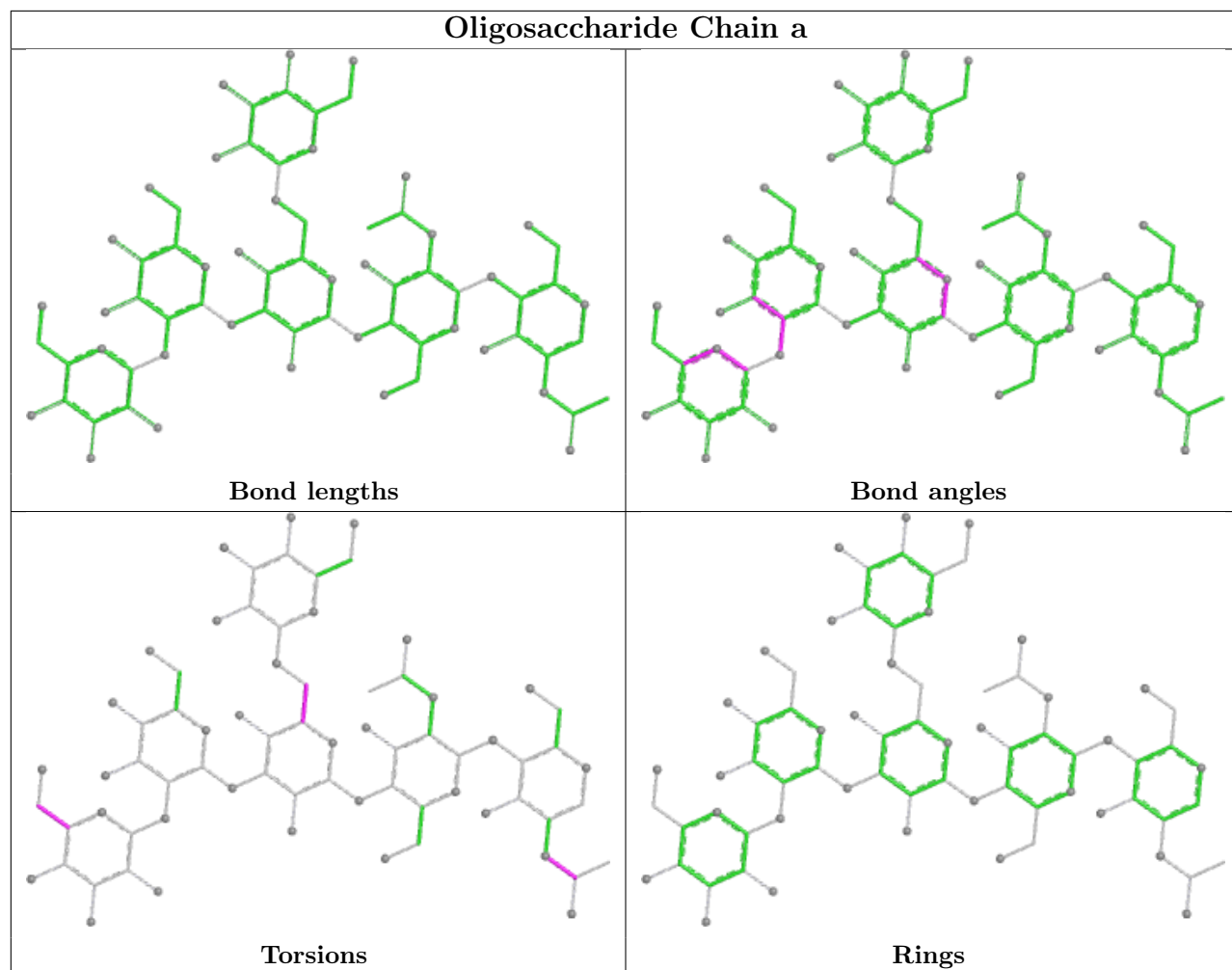


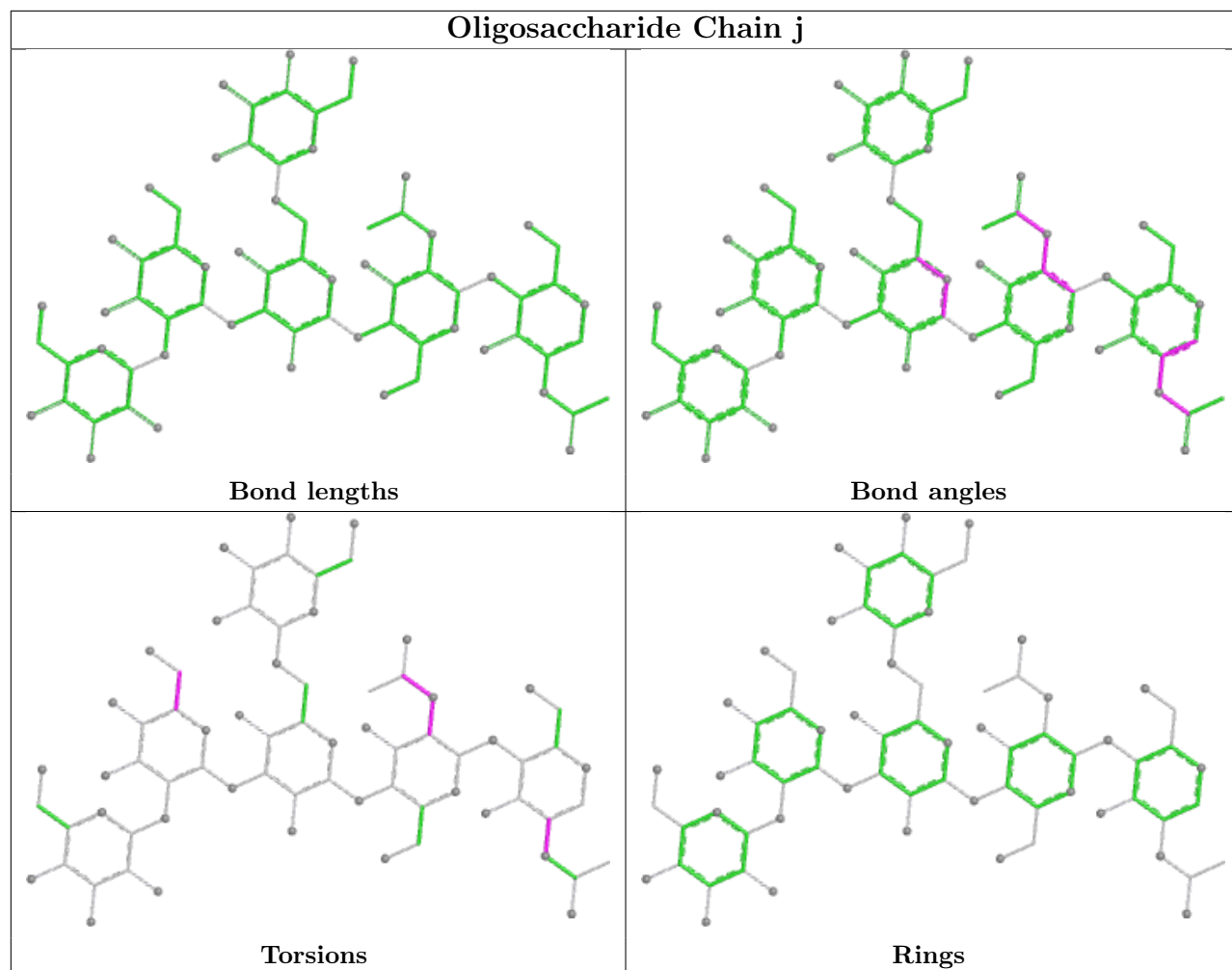


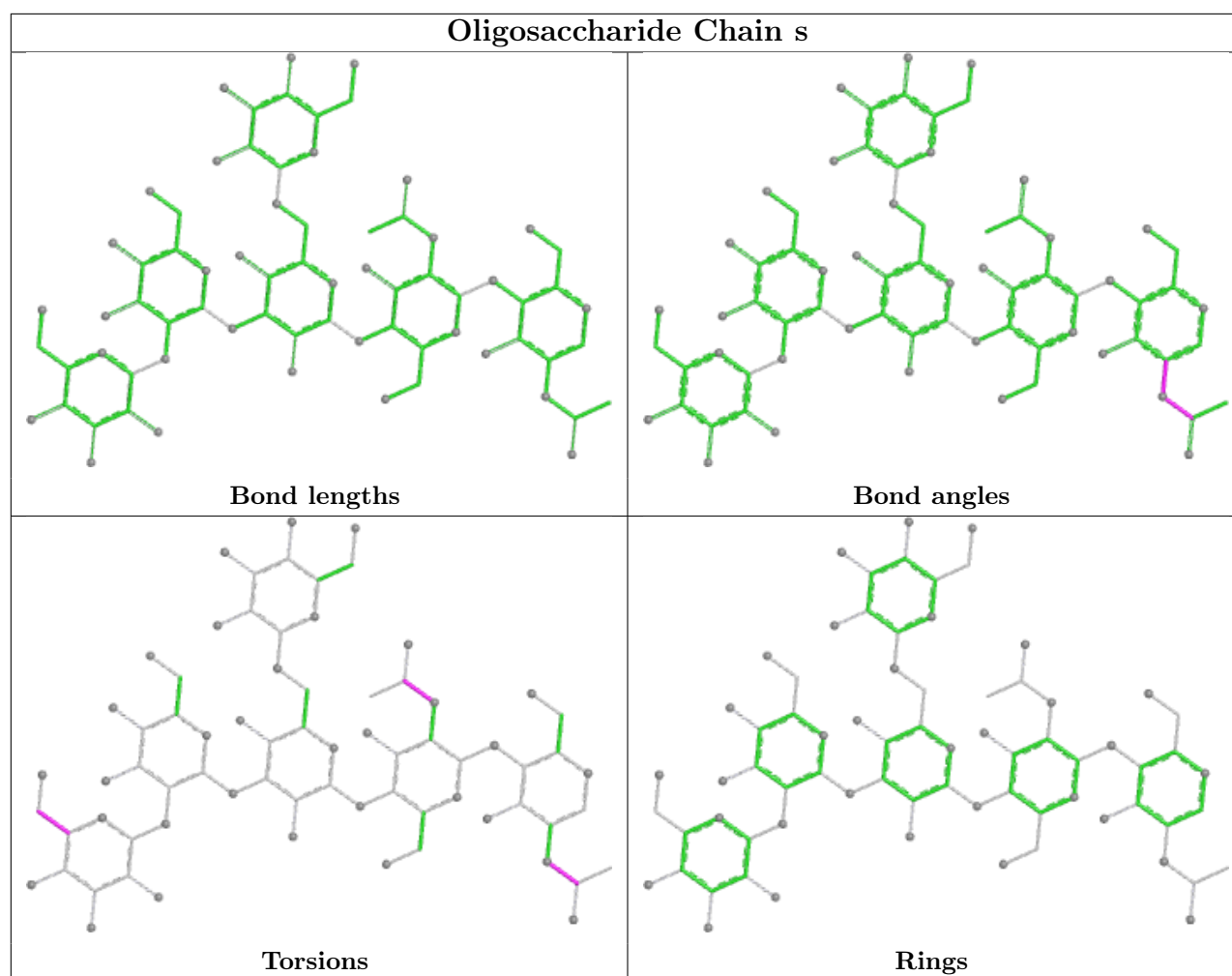












5.6 Ligand geometry [i](#)

27 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	$\# Z > 2$
14	NAG	C	603	1	14,14,15	0.40	0	17,19,21	0.99	1 (5%)
14	NAG	D	701	2	14,14,15	0.37	0	17,19,21	0.46	0
14	NAG	A	607	1	14,14,15	0.39	0	17,19,21	0.46	0
14	NAG	A	606	1	14,14,15	0.36	0	17,19,21	1.06	2 (11%)
14	NAG	B	604	1	14,14,15	0.38	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	A	601	1	14,14,15	0.39	0	17,19,21	0.51	0
14	NAG	D	702	2	14,14,15	0.38	0	17,19,21	0.48	0
14	NAG	B	605	1	14,14,15	0.39	0	17,19,21	0.59	0
14	NAG	E	701	2	14,14,15	0.38	0	17,19,21	0.44	0
14	NAG	C	602	1	14,14,15	0.39	0	17,19,21	0.59	0
14	NAG	E	702	2	14,14,15	0.38	0	17,19,21	0.48	0
14	NAG	A	603	1	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	C	604	1	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
14	NAG	A	605	1	14,14,15	0.38	0	17,19,21	0.35	0
14	NAG	B	602	1	14,14,15	0.39	0	17,19,21	0.60	0
14	NAG	B	601	1	14,14,15	0.38	0	17,19,21	0.44	0
14	NAG	C	605	1	14,14,15	0.38	0	17,19,21	0.47	0
14	NAG	C	606	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
14	NAG	C	607	1	14,14,15	0.38	0	17,19,21	0.46	0
14	NAG	B	603	1	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
14	NAG	C	601	1	14,14,15	0.38	0	17,19,21	0.38	0
14	NAG	A	604	1	14,14,15	0.39	0	17,19,21	1.20	2 (11%)
14	NAG	F	701	2	14,14,15	0.38	0	17,19,21	0.48	0
14	NAG	B	606	1	14,14,15	0.38	0	17,19,21	0.48	0
14	NAG	B	607	1	14,14,15	0.38	0	17,19,21	0.51	0
14	NAG	A	602	1	14,14,15	0.41	0	17,19,21	0.81	1 (5%)
14	NAG	F	702	2	14,14,15	0.39	0	17,19,21	0.72	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
14	NAG	C	603	1	-	2/6/23/26	0/1/1/1
14	NAG	D	701	2	-	0/6/23/26	0/1/1/1
14	NAG	A	607	1	-	3/6/23/26	0/1/1/1
14	NAG	A	606	1	-	2/6/23/26	0/1/1/1
14	NAG	B	604	1	-	0/6/23/26	0/1/1/1
14	NAG	A	601	1	-	0/6/23/26	0/1/1/1
14	NAG	D	702	2	-	2/6/23/26	0/1/1/1
14	NAG	B	605	1	-	0/6/23/26	0/1/1/1
14	NAG	E	701	2	-	0/6/23/26	0/1/1/1
14	NAG	C	602	1	-	0/6/23/26	0/1/1/1
14	NAG	E	702	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	A	603	1	-	4/6/23/26	0/1/1/1
14	NAG	C	604	1	1/1/5/7	0/6/23/26	0/1/1/1
14	NAG	A	605	1	-	0/6/23/26	0/1/1/1
14	NAG	B	602	1	-	3/6/23/26	0/1/1/1
14	NAG	B	601	1	-	0/6/23/26	0/1/1/1
14	NAG	C	605	1	-	1/6/23/26	0/1/1/1
14	NAG	C	606	1	-	0/6/23/26	0/1/1/1
14	NAG	C	607	1	-	3/6/23/26	0/1/1/1
14	NAG	B	603	1	-	1/6/23/26	0/1/1/1
14	NAG	C	601	1	-	0/6/23/26	0/1/1/1
14	NAG	A	604	1	-	3/6/23/26	0/1/1/1
14	NAG	F	701	2	-	0/6/23/26	0/1/1/1
14	NAG	B	606	1	-	1/6/23/26	0/1/1/1
14	NAG	B	607	1	-	3/6/23/26	0/1/1/1
14	NAG	A	602	1	-	0/6/23/26	0/1/1/1
14	NAG	F	702	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	603	NAG	C2-N2-C7	3.71	127.87	122.90
14	A	606	NAG	C2-N2-C7	3.36	127.40	122.90
14	C	603	NAG	C2-N2-C7	3.34	127.37	122.90
14	A	604	NAG	C1-C2-N2	3.28	115.60	110.43
14	A	604	NAG	C2-N2-C7	3.13	127.09	122.90
14	C	606	NAG	C2-N2-C7	2.43	126.16	122.90
14	F	702	NAG	C1-C2-N2	2.37	114.17	110.43
14	A	602	NAG	C2-N2-C7	-2.34	119.76	122.90
14	A	606	NAG	C1-C2-N2	-2.10	107.12	110.43
14	C	604	NAG	C1-O5-C5	2.00	114.87	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	604	NAG	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	603	NAG	C8-C7-N2-C2
14	A	603	NAG	O7-C7-N2-C2
14	A	604	NAG	C1-C2-N2-C7
14	A	604	NAG	C8-C7-N2-C2
14	A	604	NAG	O7-C7-N2-C2
14	B	602	NAG	C8-C7-N2-C2
14	B	602	NAG	O7-C7-N2-C2
14	F	702	NAG	C8-C7-N2-C2
14	F	702	NAG	O7-C7-N2-C2
14	A	606	NAG	C8-C7-N2-C2
14	B	607	NAG	C8-C7-N2-C2
14	D	702	NAG	C8-C7-N2-C2
14	D	702	NAG	O7-C7-N2-C2
14	E	702	NAG	C8-C7-N2-C2
14	E	702	NAG	O7-C7-N2-C2
14	C	607	NAG	C8-C7-N2-C2
14	A	603	NAG	C4-C5-C6-O6
14	B	607	NAG	O7-C7-N2-C2
14	A	606	NAG	O7-C7-N2-C2
14	C	607	NAG	O7-C7-N2-C2
14	A	603	NAG	O5-C5-C6-O6
14	B	602	NAG	O5-C5-C6-O6
14	B	606	NAG	O5-C5-C6-O6
14	C	607	NAG	O5-C5-C6-O6
14	C	603	NAG	O5-C5-C6-O6
14	B	607	NAG	O5-C5-C6-O6
14	A	607	NAG	O5-C5-C6-O6
14	B	603	NAG	C3-C2-N2-C7
14	C	603	NAG	C3-C2-N2-C7
14	A	607	NAG	C8-C7-N2-C2
14	C	605	NAG	C8-C7-N2-C2
14	A	607	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	603	NAG	1	0
14	A	607	NAG	1	0
14	C	602	NAG	2	0
14	B	602	NAG	2	0
14	B	601	NAG	1	0
14	C	607	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	603	NAG	2	0
14	A	604	NAG	1	0
14	B	606	NAG	1	0
14	A	602	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

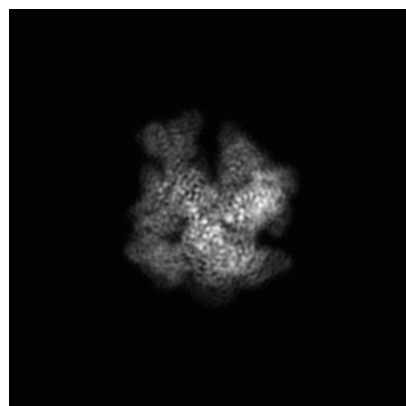
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48059. These allow visual inspection of the internal detail of the map and identification of artifacts.

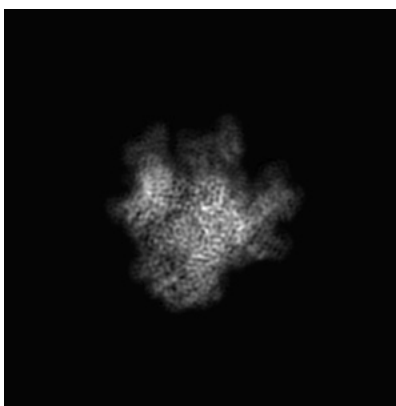
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

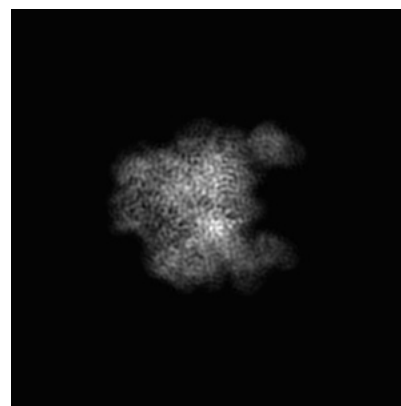
6.1.1 Primary map



X

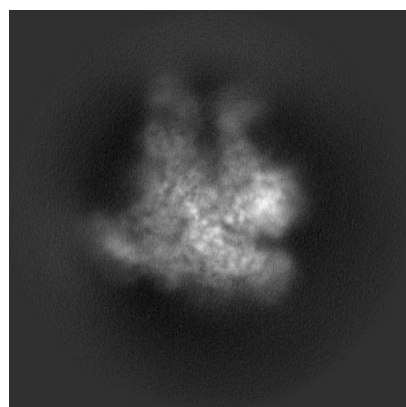


Y

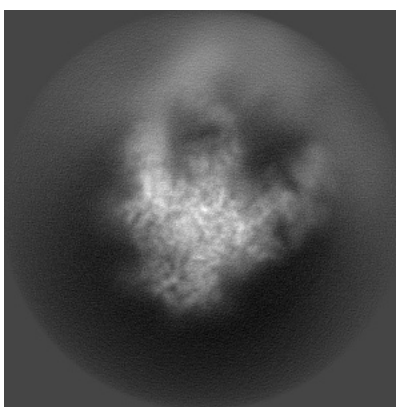


Z

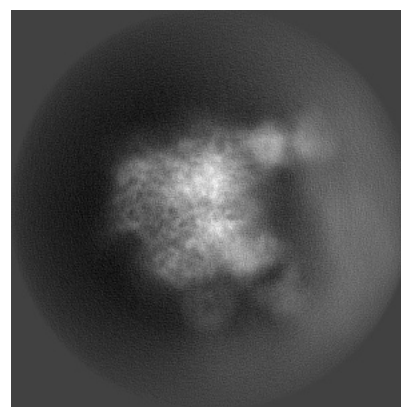
6.1.2 Raw map



X



Y

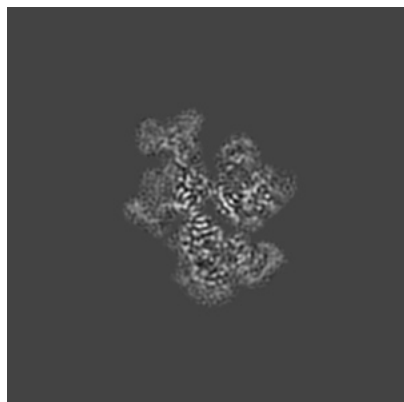


Z

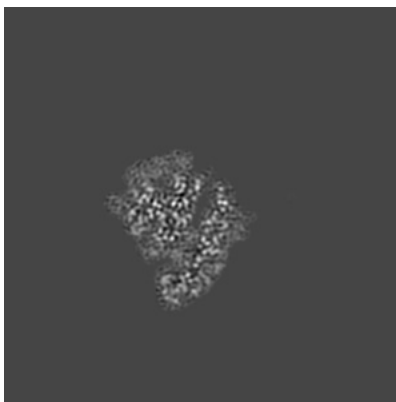
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

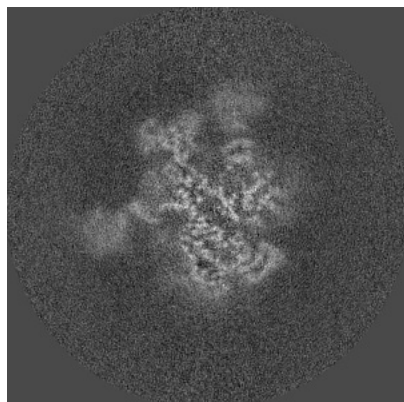


Y Index: 180

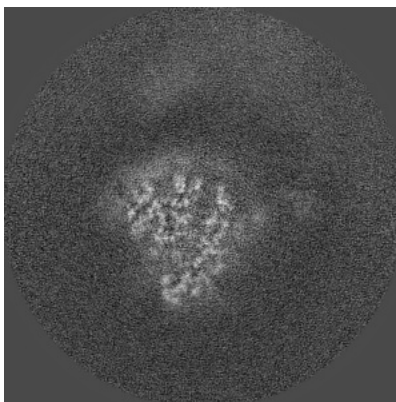


Z Index: 180

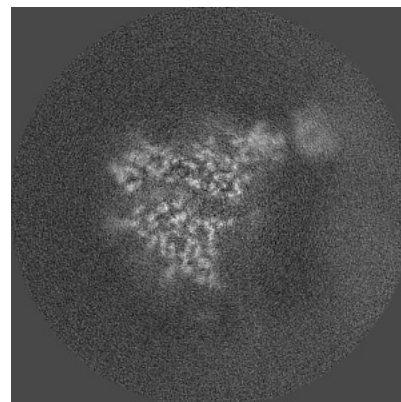
6.2.2 Raw map



X Index: 180



Y Index: 180

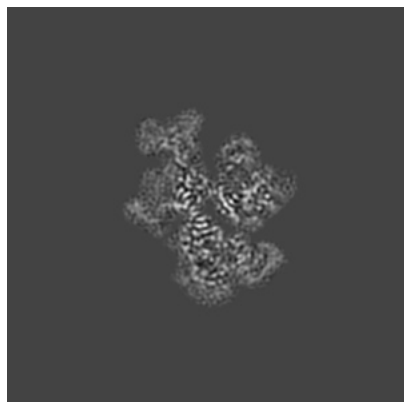


Z Index: 180

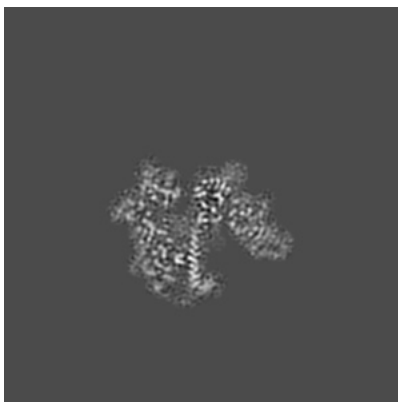
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 180

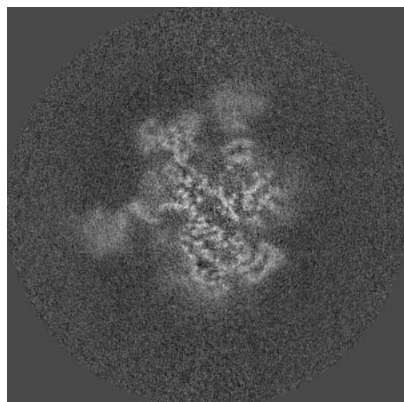


Y Index: 198

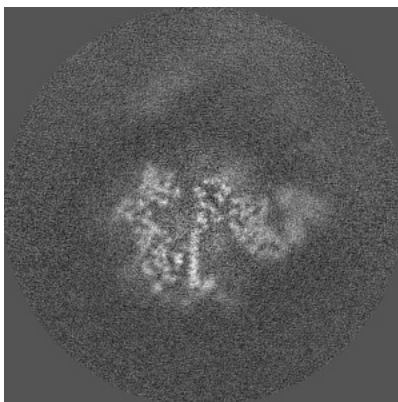


Z Index: 179

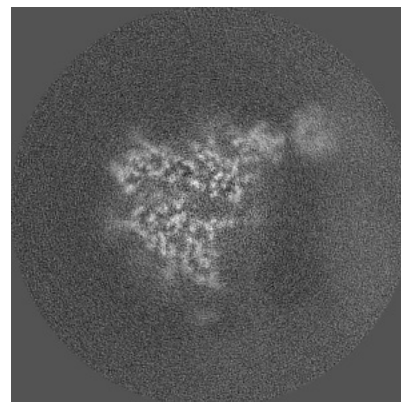
6.3.2 Raw map



X Index: 180



Y Index: 199

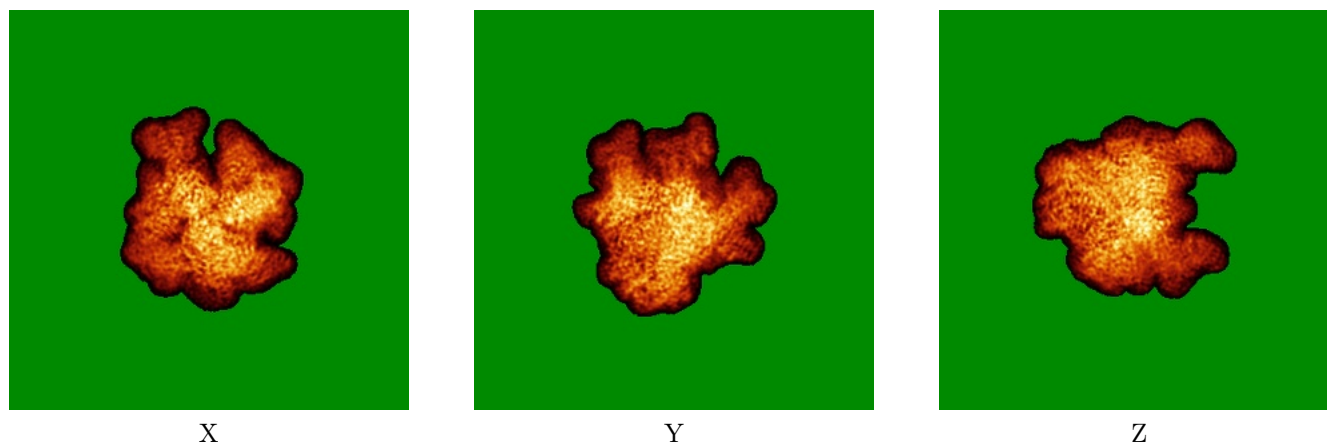


Z Index: 179

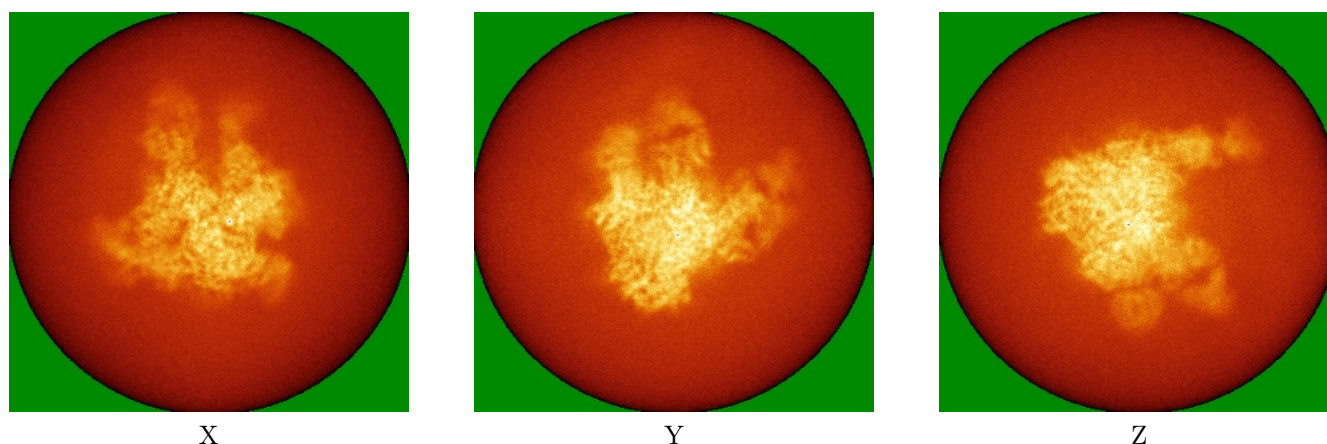
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

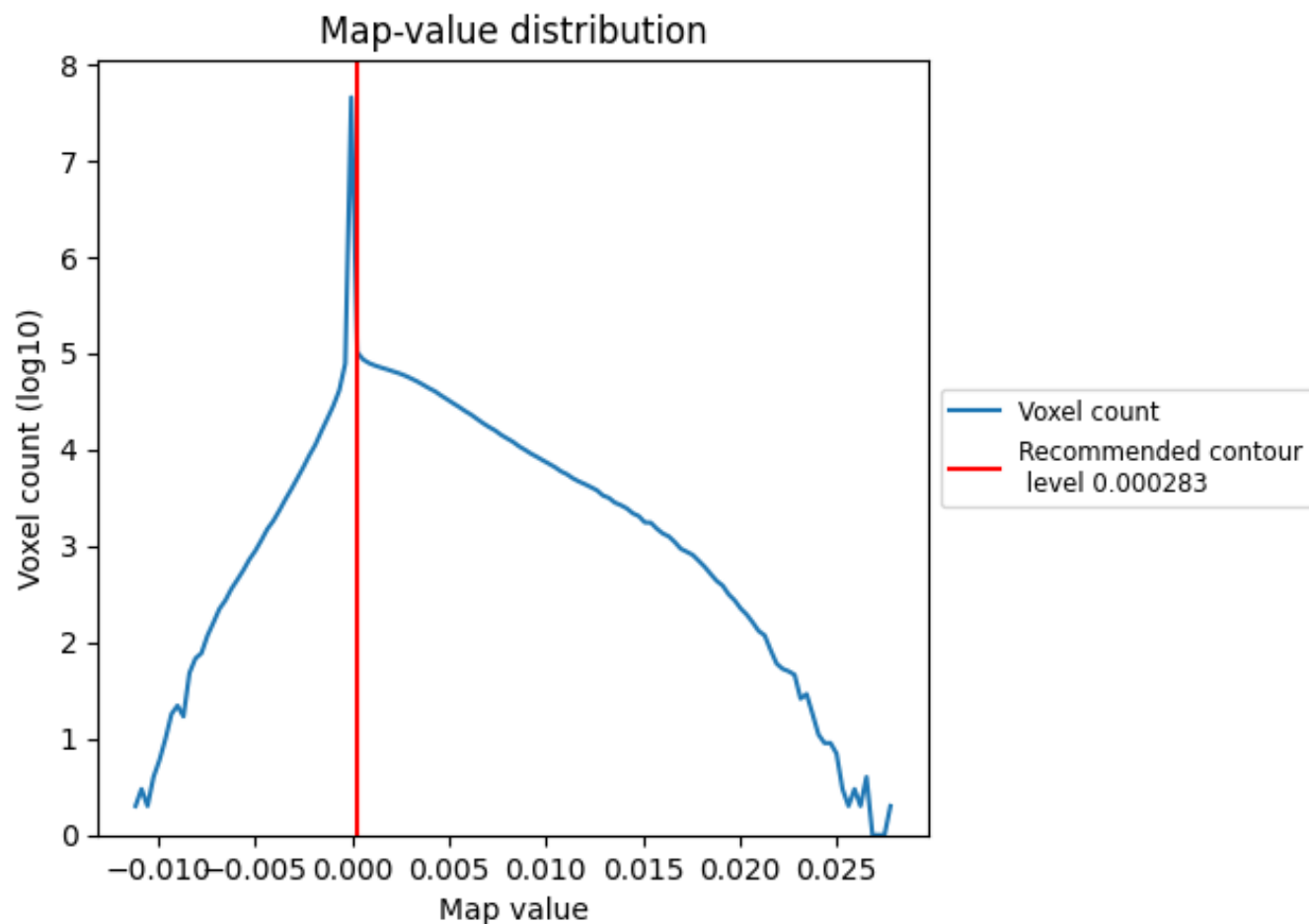
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

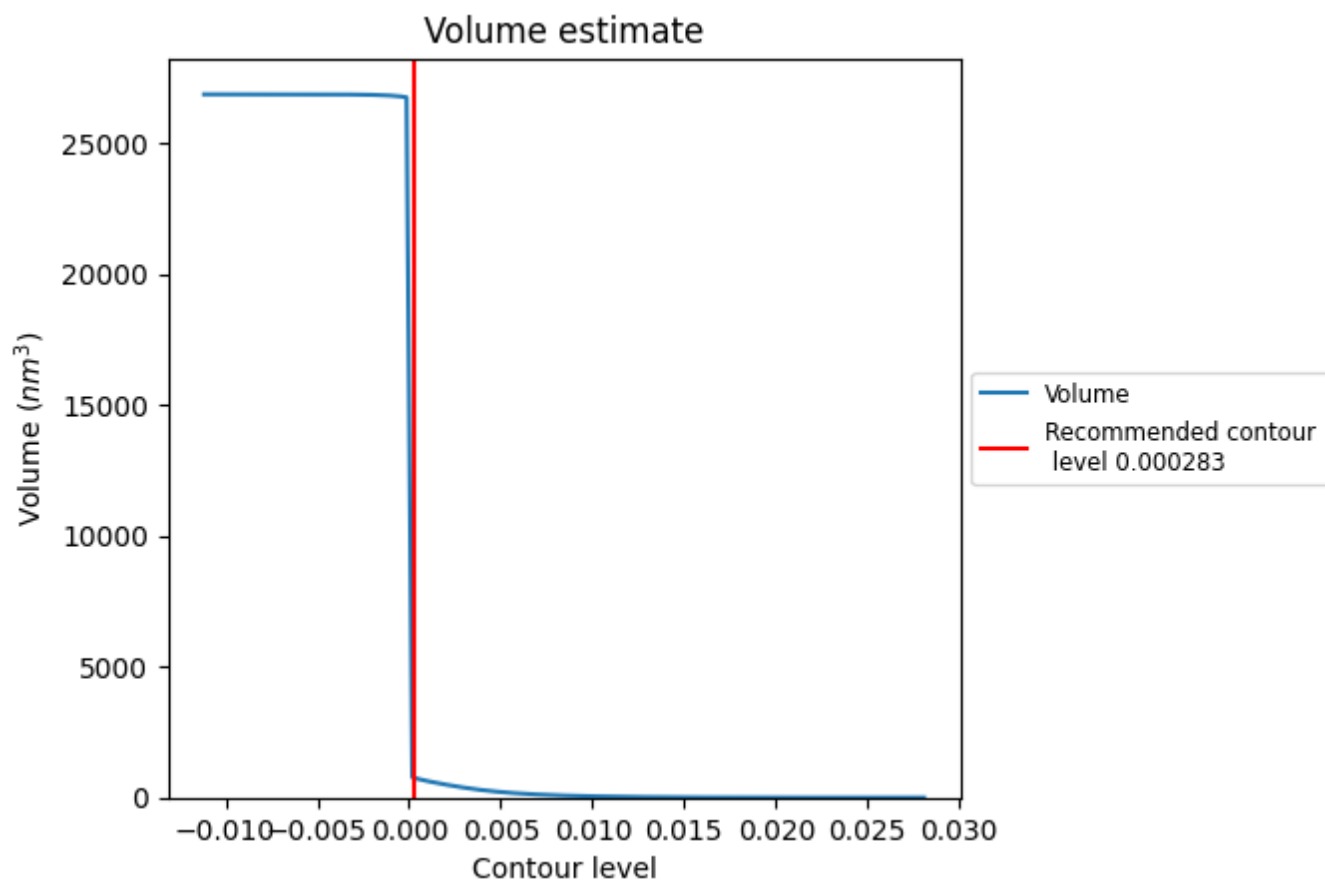
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

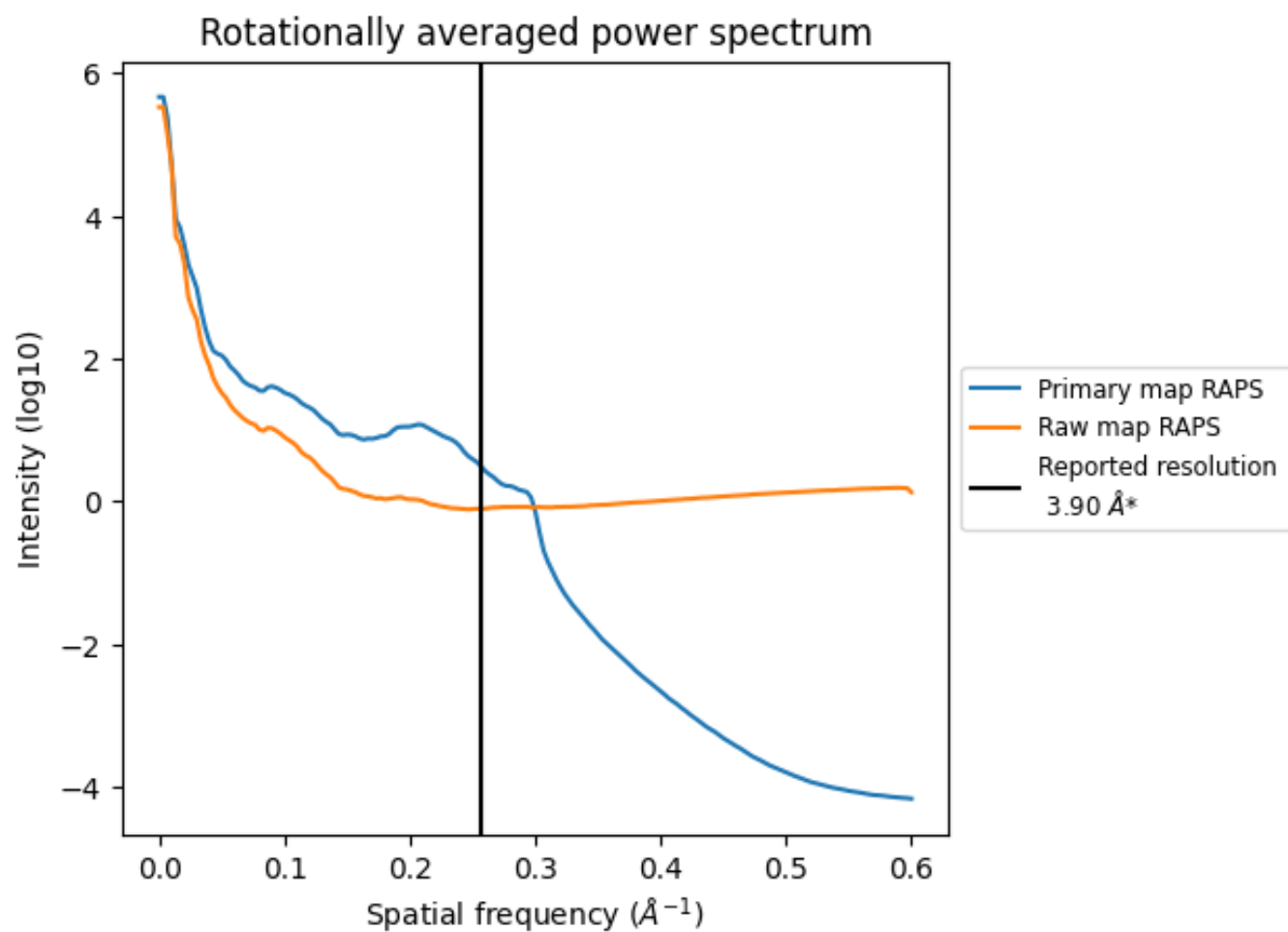
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 755 nm³; this corresponds to an approximate mass of 682 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 ⓘ

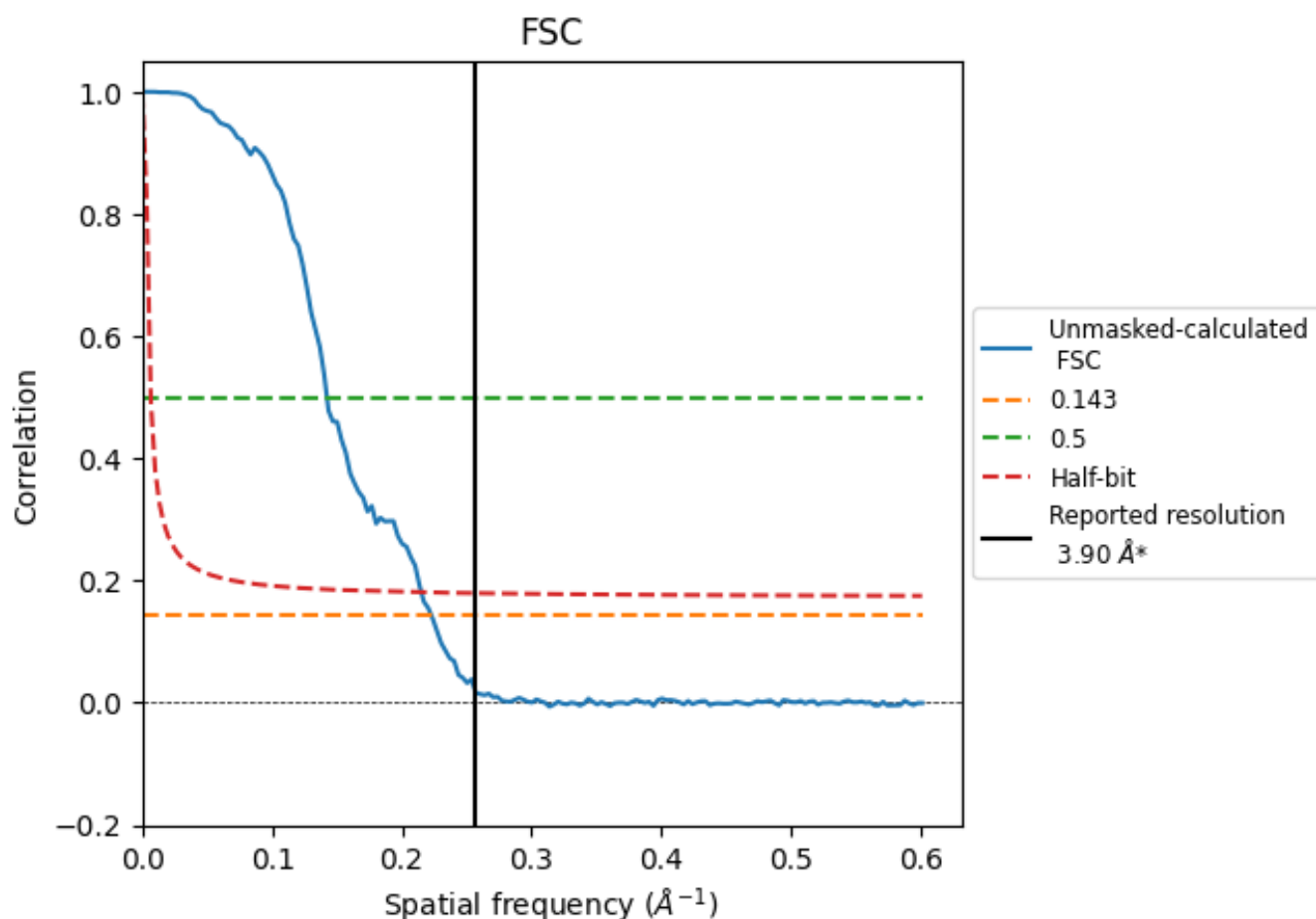


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

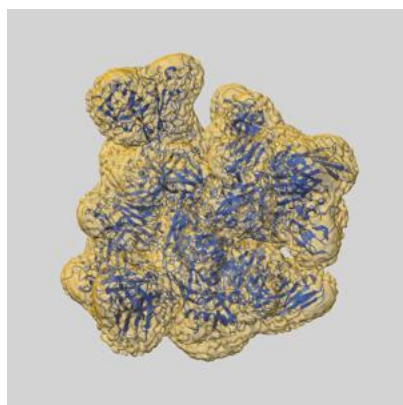
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	7.03	4.65

*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 4.49 differs from the reported value 3.9 by more than 10 %

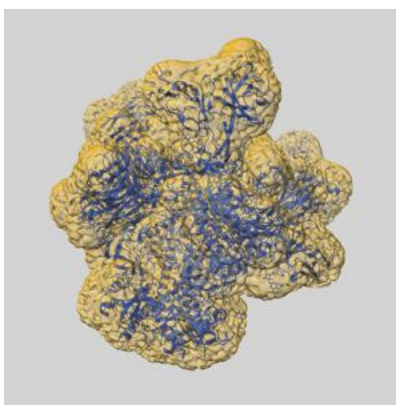
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48059 and PDB model 9EHL. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

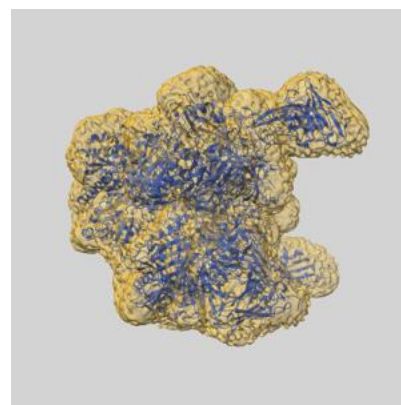
9.1 Map-model overlay [i](#)



X



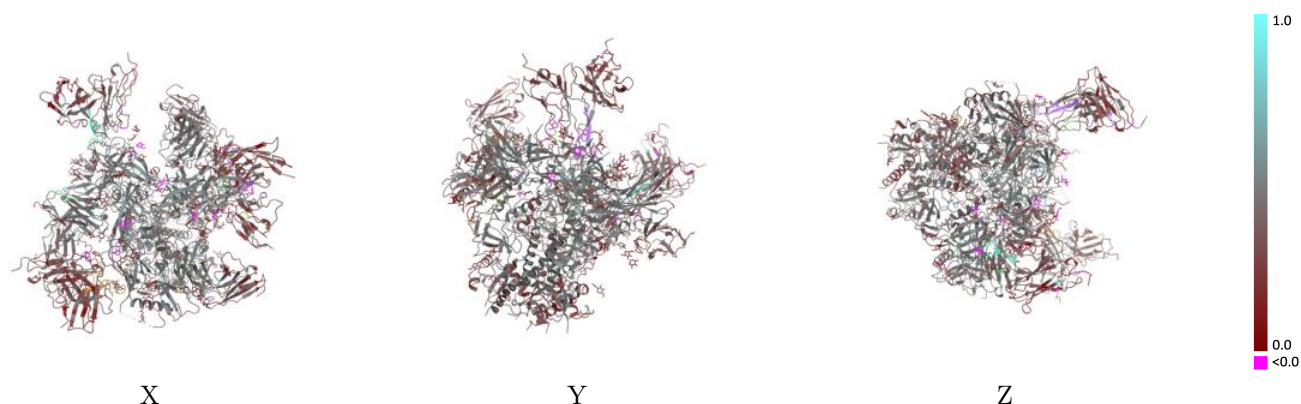
Y



Z

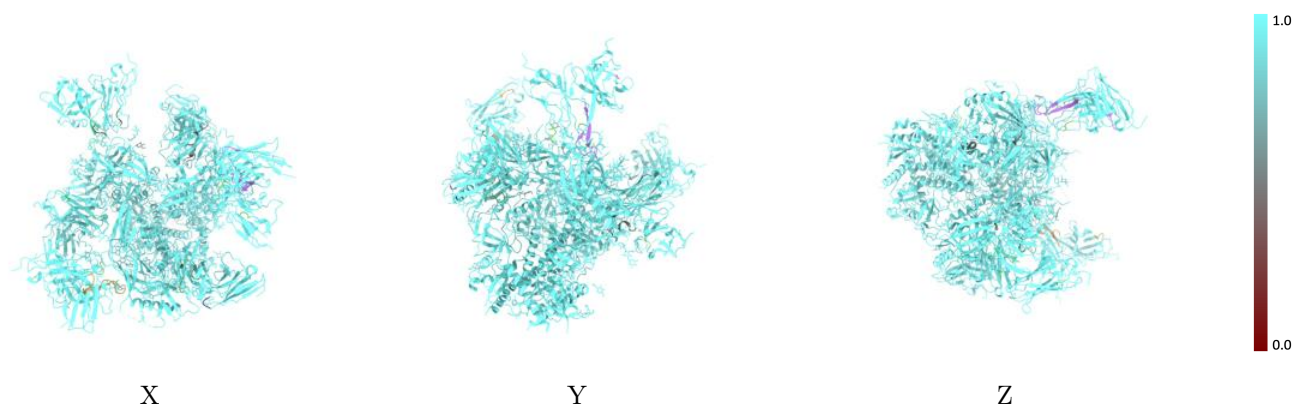
The images above show the 3D surface view of the map at the recommended contour level 0.000283 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



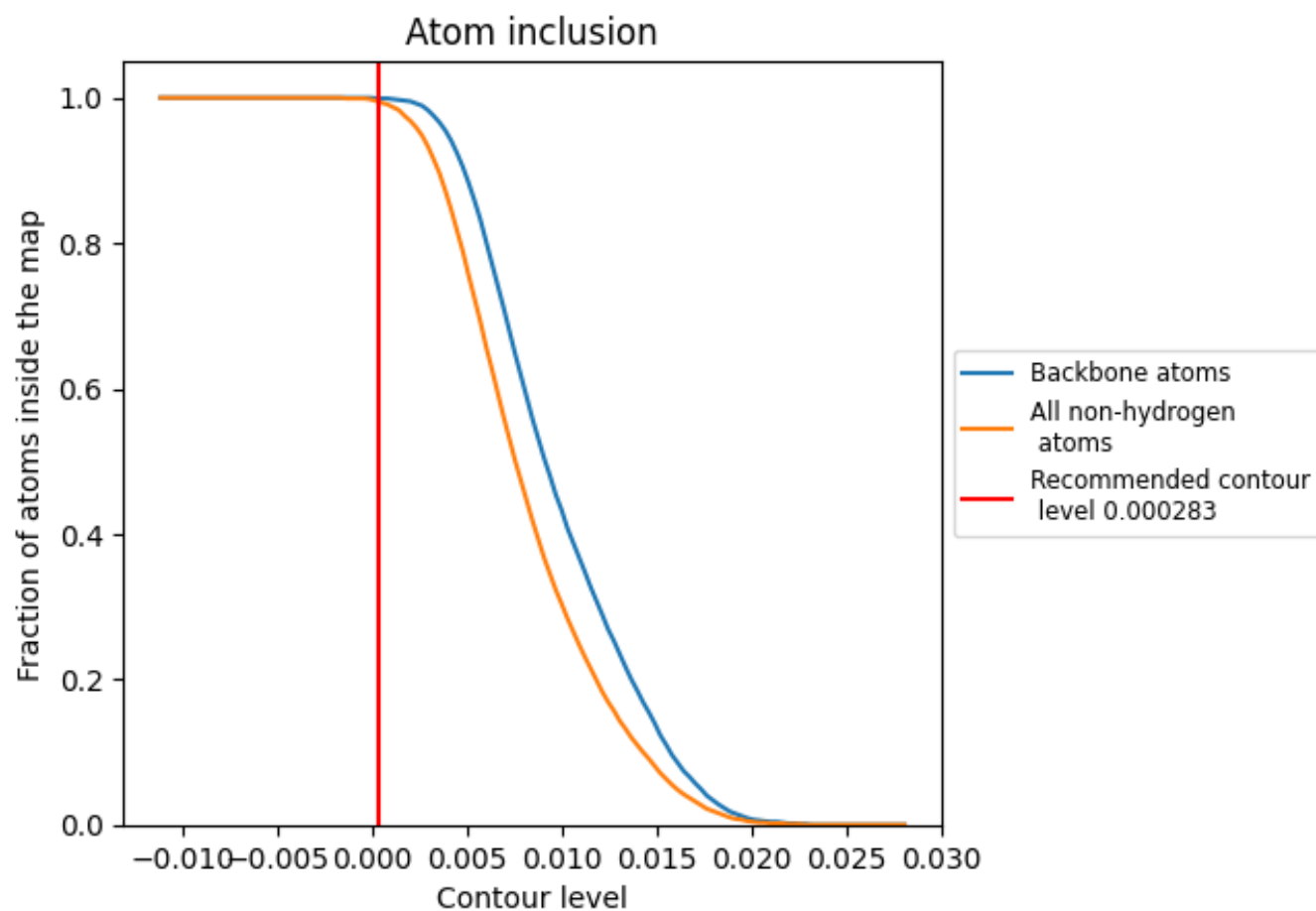
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



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 (0.000283).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.000283) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.3980
A	 0.9970	 0.4500
B	 0.9960	 0.4400
C	 0.9940	 0.4400
D	 0.9960	 0.3890
E	 0.9970	 0.3820
F	 0.9970	 0.3970
G	 0.9960	 0.4480
H	 0.9970	 0.4560
I	 1.0000	 0.4520
J	 0.9920	 0.3820
K	 0.9910	 0.3530
L	 0.9990	 0.3850
M	 0.9980	 0.3160
N	 0.9970	 0.3170
O	 0.9950	 0.3150
P	 0.9990	 0.3560
Q	 1.0000	 0.3580
R	 0.9950	 0.3420
S	 0.9230	 0.2420
T	 0.7860	 0.0680
U	 0.9800	 0.3370
V	 0.9400	 0.1240
W	 0.9290	 -0.0470
X	 1.0000	 0.2080
Y	 1.0000	 0.2800
Z	 1.0000	 0.0790
a	 1.0000	 0.2910
b	 0.9230	 0.1210
c	 0.9290	 0.1510
d	 1.0000	 0.1590
e	 1.0000	 0.3470
f	 1.0000	 0.1450
g	 1.0000	 0.3960
h	 1.0000	 0.3440



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 1.0000	 0.2140
j	 0.9580	 0.2640
k	 0.8720	 0.1950
l	 0.9290	 0.1890
m	 0.9600	 0.1740
n	 0.9740	 0.1680
o	 1.0000	 0.2720
p	 1.0000	 0.2310
q	 1.0000	 0.3450
r	 1.0000	 0.2000
s	 0.9580	 0.3420