



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 1ZPU / pdb_00001zpu
Title : Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import
Authors : Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.
Deposited on : 2005-05-17
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

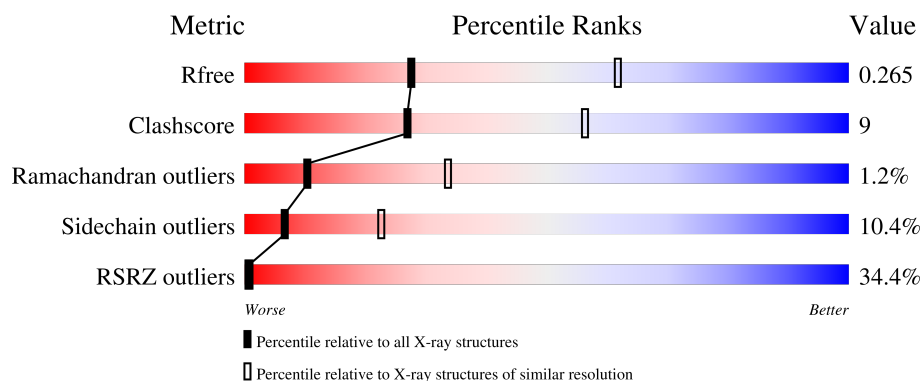
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	30% 72% 22% ..
1	B	534	13% 68% 26% 5% .
1	C	534	40% 71% 23% ..
1	D	534	25% 71% 24% ..
1	E	534	28% 75% 21% ..

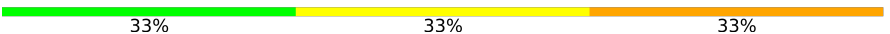
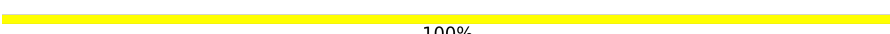
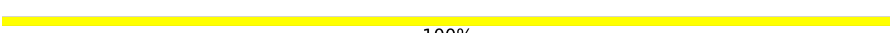
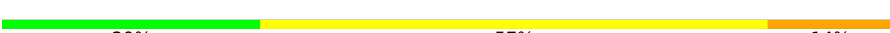
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	534	
2	G	5	
2	J	5	
2	M	5	
2	O	5	
2	S	5	
2	U	5	
2	Y	5	
2	a	5	
2	d	5	
2	f	5	
2	i	5	
2	k	5	
3	H	6	
3	N	6	
3	Z	6	
3	j	6	
4	I	2	
4	P	2	
4	Q	2	
4	V	2	
4	b	2	
4	g	2	
5	K	3	
5	L	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	W	3	
5	X	3	
5	c	3	
5	h	3	
5	l	3	
6	R	4	
7	T	7	
7	e	7	

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
2	NAG	a	1	X	-	-	-
2	NAG	f	1	X	-	-	-
3	NAG	H	1	X	-	-	-
3	NAG	N	1	X	-	-	-
3	NAG	Z	1	X	-	-	-
3	NAG	j	1	X	-	-	-
4	NAG	b	1	X	-	-	-
5	NAG	L	1	X	-	-	-
5	NAG	X	1	X	-	-	-
5	NAG	c	1	X	-	-	-
5	NAG	h	1	X	-	-	-
5	NAG	l	1	X	-	-	-
6	NAG	R	1	X	-	-	-
7	NAG	T	1	X	-	-	-
7	NAG	e	1	X	-	-	-
8	NAG	A	2006	X	-	-	-
8	NAG	A	2012	X	-	-	-
8	NAG	A	2018	X	-	-	-
8	NAG	B	2006	X	-	-	-
8	NAG	B	2012	X	-	-	-
8	NAG	B	2018	X	-	-	-
8	NAG	C	2012	X	-	-	-
8	NAG	C	2018	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	D	2006	X	-	-	-
8	NAG	E	2012	X	-	-	-
8	NAG	F	2005	X	-	-	-
8	NAG	F	2006	X	-	-	-
8	NAG	F	2009	X	-	-	-
8	NAG	F	2012	X	-	-	-

2 Entry composition [i](#)

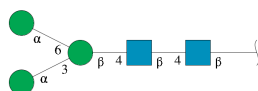
There are 9 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

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



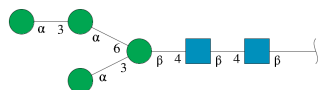
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	Y	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	d	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	f	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	i	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	k	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



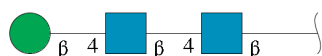
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	N	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	Z	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	j	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



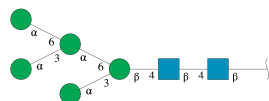
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	l	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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.



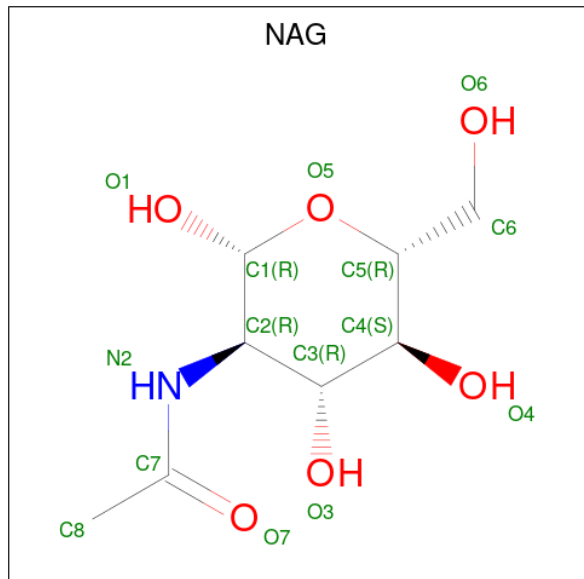
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
7	e	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

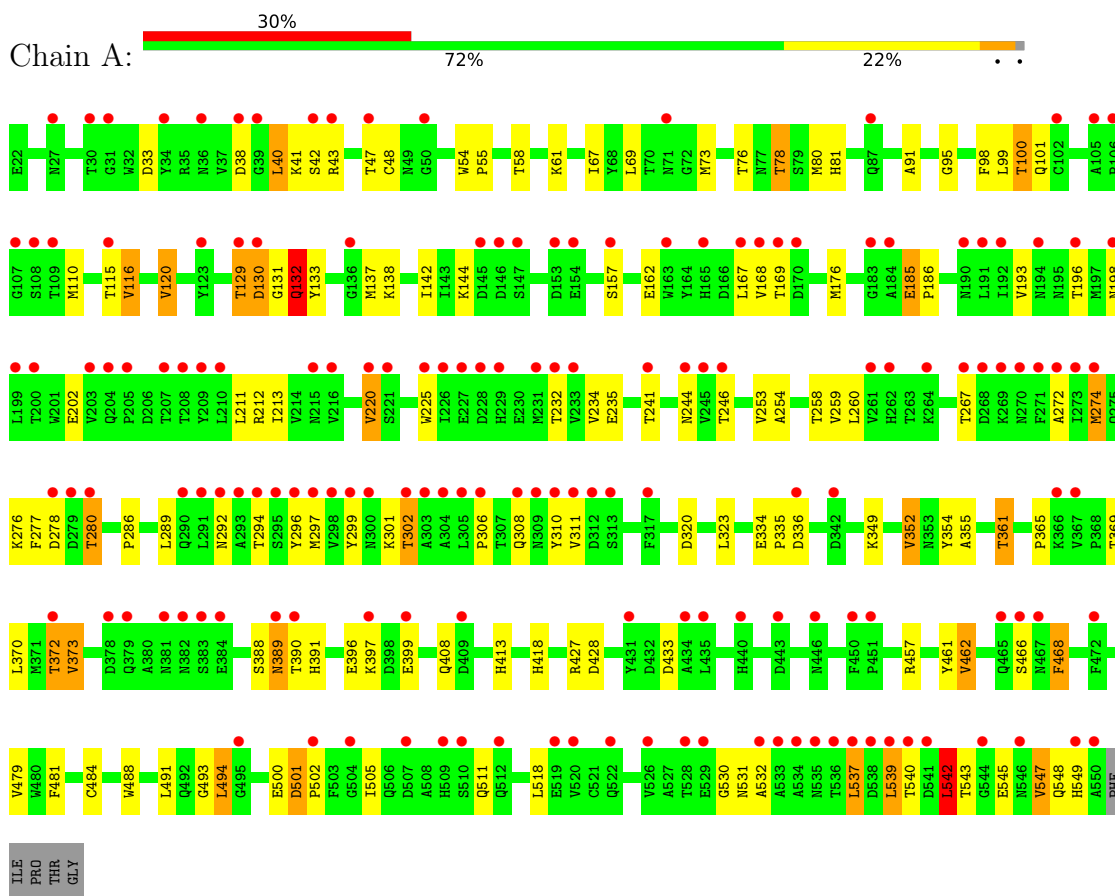
- Molecule 9 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cu	0	0
			4	4		
9	B	4	Total	Cu	0	0
			4	4		
9	C	4	Total	Cu	0	0
			4	4		
9	D	4	Total	Cu	0	0
			4	4		
9	E	4	Total	Cu	0	0
			4	4		
9	F	4	Total	Cu	0	0
			4	4		

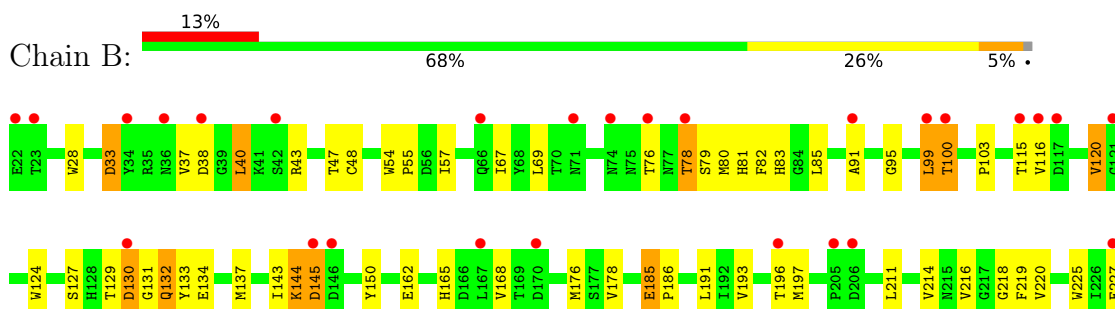
3 Residue-property plots

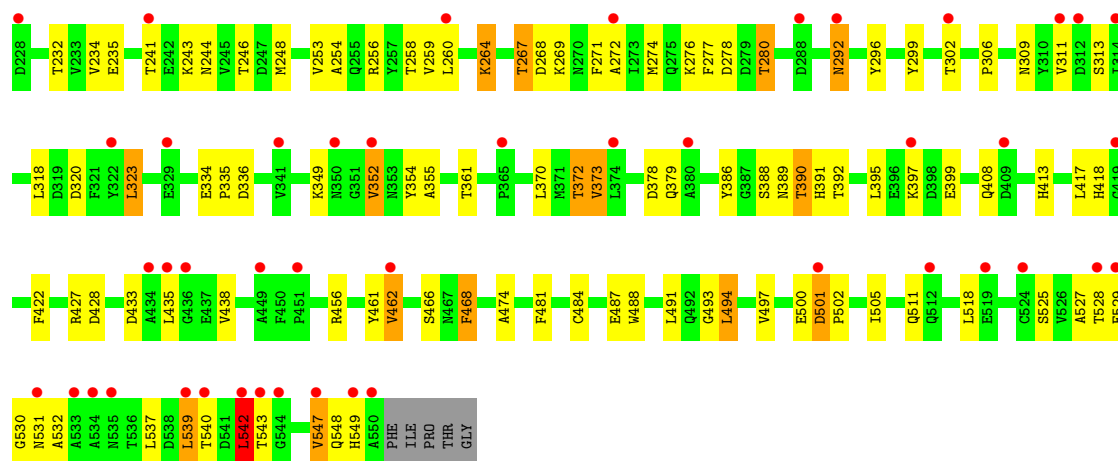
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Iron transport multicopper oxidase FET3

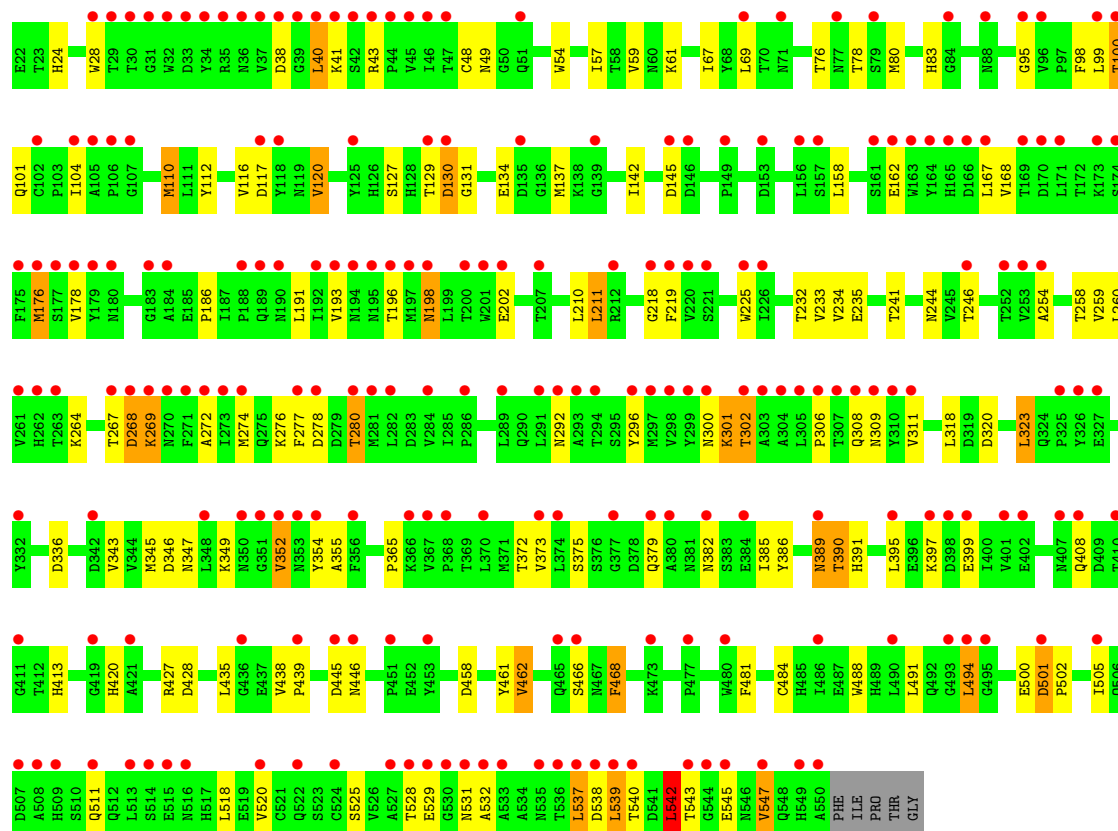
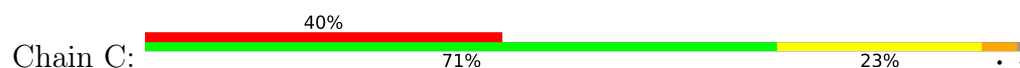


- Molecule 1: Iron transport multicopper oxidase FET3

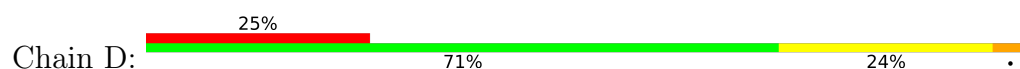


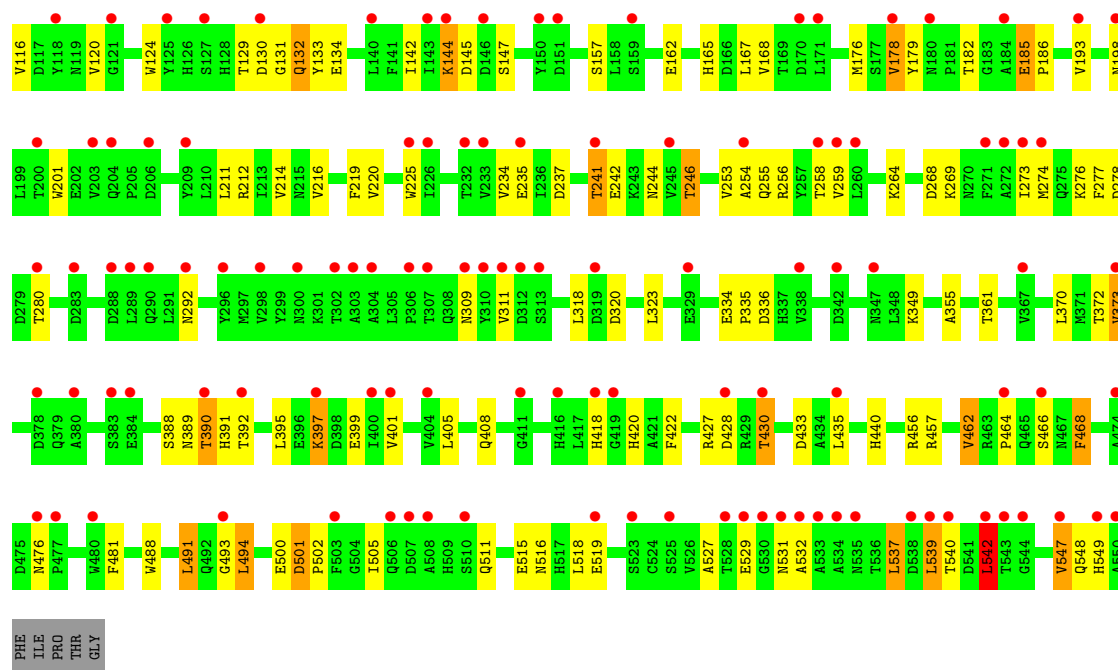


• Molecule 1: Iron transport multicopper oxidase FET3

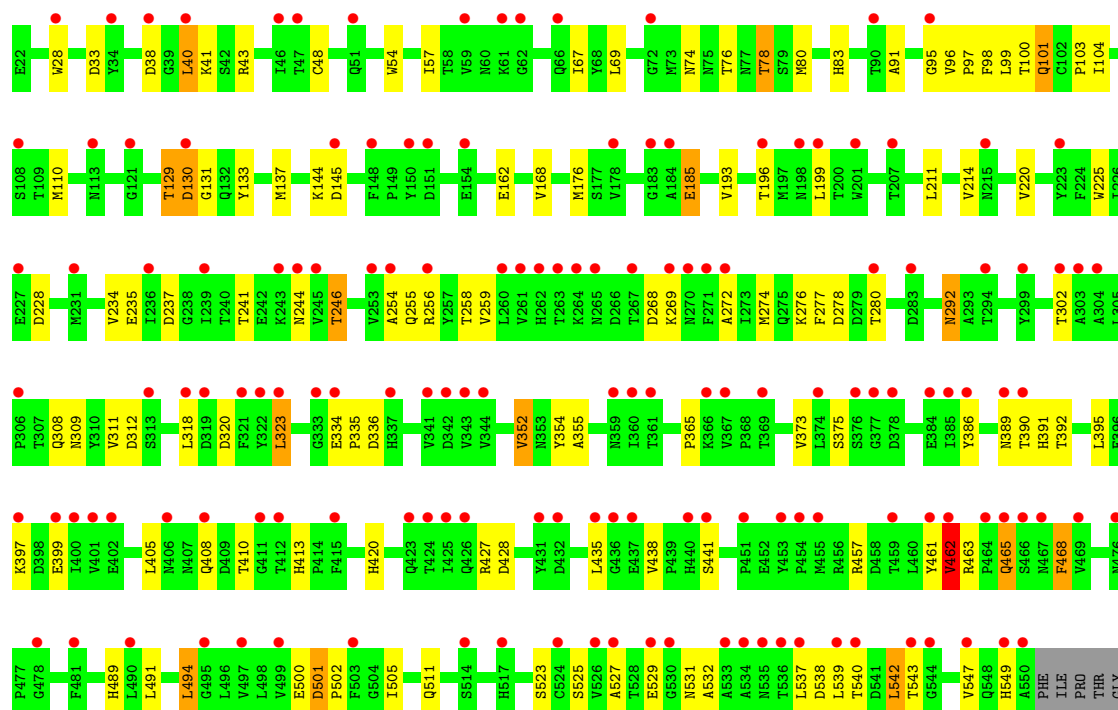
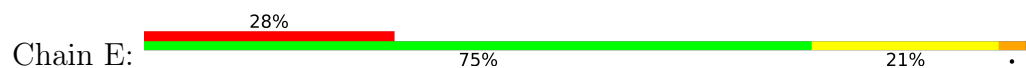


• Molecule 1: Iron transport multicopper oxidase FET3



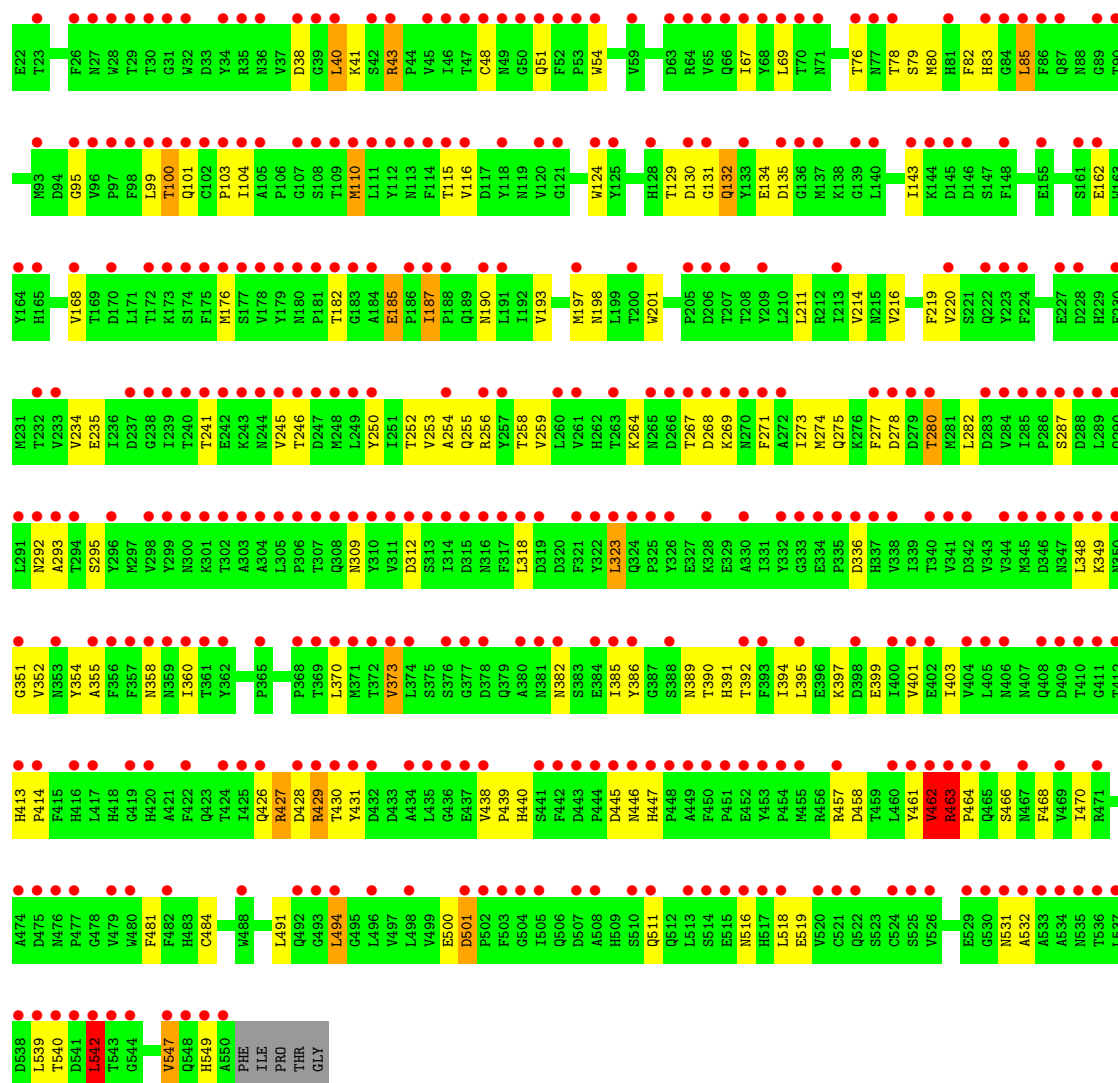


• Molecule 1: Iron transport multicopper oxidase FET3



• Molecule 1: Iron transport multicopper oxidase FET3





● Molecule 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 G: 60%

MAG1
MAG2
EWA3
MAN4
MAN5

● Molecule 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 J: 80%

MAG1
MAG2
EWA3
MAN4
MAN5

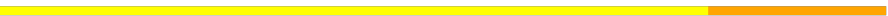
● Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

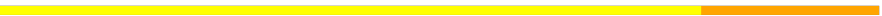
MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 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 O:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 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:  80% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 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 U:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 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 Y:  60% 40%

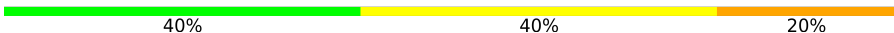
MAG1
MAG2
BMA3
MAN4
MAN5

• Molecule 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 a:  100%

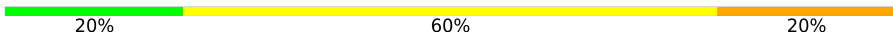
MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 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 d: 



- Molecule 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 f: 

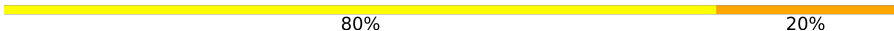


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 

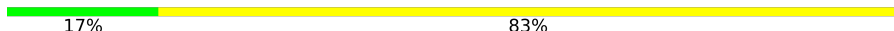


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 

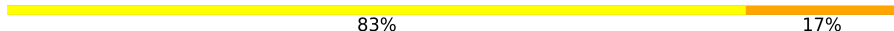


- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 



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

Chain N: 



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

Chain Z: 100%



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

Chain j: 83% 17%



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

Chain I: 50% 50%



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

Chain P: 50% 50%



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

Chain Q: 100%



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

Chain V: 100%

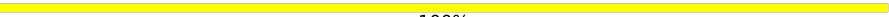
MAG1
MAG2

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

Chain b:  50% 50%

MAG1
MAG2

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

Chain g:  100%

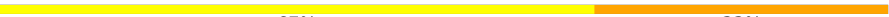
MAG1
MAG2

- Molecule 5: 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
BKA3

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

Chain L:  67% 33%

MAG1
MAG2
BKA3

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

Chain W:  33% 67%

MAG1
MAG2
BKA3

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

Chain X:  33% 33% 33%

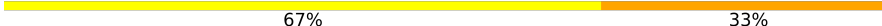
MAG1
MAG2
BKA3

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

Chain c:  33% 67%

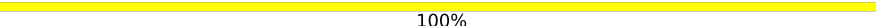
NAG1
NAG2
BMA3

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

Chain h:  67% 33%

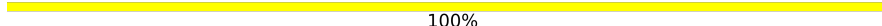
NAG1
NAG2
BMA3

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

Chain l:  100%

NAG1
NAG2
BMA3

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

Chain R:  100%

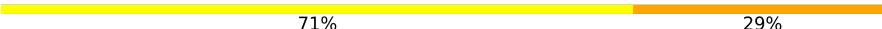
NAG1
NAG2
BMA3
MAN4

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  29% 57% 14%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  71% 29%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.257 0.235 , 0.265	Depositor DCC
R_{free} test set	6726 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, NAG, MAN, 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	0.59	0/4373	0.88	2/5981 (0.0%)
1	B	0.59	2/4373 (0.0%)	0.87	4/5981 (0.1%)
1	C	0.62	5/4373 (0.1%)	0.86	4/5981 (0.1%)
1	D	0.53	3/4373 (0.1%)	0.80	1/5981 (0.0%)
1	E	0.52	2/4373 (0.0%)	0.80	4/5981 (0.1%)
1	F	0.96	19/4373 (0.4%)	0.86	7/5981 (0.1%)
All	All	0.65	31/26238 (0.1%)	0.85	22/35886 (0.1%)

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

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	37.41	1.85	1.32
1	F	358	ASN	CG-OD1	12.49	1.47	1.23
1	F	445	ASP	CG-OD2	11.82	1.47	1.25
1	C	538	ASP	CG-OD2	11.39	1.47	1.25
1	F	312	ASP	CG-OD2	9.52	1.43	1.25
1	F	250	TYR	CG-CD2	9.40	1.59	1.39
1	F	426	GLN	CD-OE1	8.99	1.40	1.23
1	F	446	ASN	CG-OD1	8.78	1.40	1.23
1	F	250	TYR	CE2-CZ	8.61	1.58	1.38
1	E	549	HIS	CE1-NE2	8.60	1.41	1.32
1	D	35	ARG	CZ-NH1	8.34	1.44	1.32
1	F	429	ARG	NE-CZ	8.00	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	GLU	CD-OE1	7.96	1.40	1.25
1	F	463	ARG	CD-NE	7.86	1.57	1.46
1	F	312	ASP	CG-OD1	7.54	1.39	1.25
1	F	250	TYR	CE1-CZ	7.31	1.55	1.38
1	F	445	ASP	CG-OD1	7.20	1.39	1.25
1	F	463	ARG	NE-CZ	7.06	1.40	1.33
1	F	250	TYR	CG-CD1	6.94	1.53	1.39
1	C	379	GLN	CG-CD	6.36	1.68	1.52
1	C	379	GLN	CD-NE2	6.11	1.46	1.33
1	B	379	GLN	CD-OE1	5.83	1.34	1.23
1	C	538	ASP	CB-CG	5.77	1.66	1.52
1	F	426	GLN	CD-NE2	5.68	1.45	1.33
1	B	379	GLN	CD-NE2	5.63	1.45	1.33
1	E	549	HIS	CG-ND1	5.63	1.44	1.38
1	F	190	ASN	CG-ND2	5.53	1.44	1.33
1	C	445	ASP	CG-OD1	5.28	1.35	1.25
1	D	515	GLU	CD-OE2	5.25	1.35	1.25
1	F	431	TYR	CE1-CZ	5.24	1.50	1.38
1	F	190	ASN	CG-OD1	5.00	1.33	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	463	ARG	NE-CZ-NH2	-13.17	107.34	119.20
1	E	465	GLN	OE1-CD-NE2	-8.63	113.97	122.60
1	B	462	VAL	CB-CA-C	-7.61	100.79	111.21
1	C	458	ASP	CB-CA-C	-7.28	96.35	110.11
1	E	465	GLN	CG-CD-NE2	7.13	127.10	116.40
1	F	463	ARG	NH1-CZ-NH2	-6.80	110.46	119.30
1	F	358	ASN	OD1-CG-ND2	6.75	129.35	122.60
1	F	540	THR	N-CA-C	6.58	119.43	110.35
1	C	379	GLN	CG-CD-NE2	-6.50	106.64	116.40
1	A	462	VAL	CB-CA-C	-6.46	102.36	111.21
1	E	540	THR	N-CA-C	6.44	119.24	110.35
1	B	540	THR	N-CA-C	6.24	118.96	110.35
1	A	540	THR	N-CA-C	6.20	118.91	110.35
1	C	540	THR	N-CA-C	6.18	118.88	110.35
1	F	447	HIS	ND1-CG-CD2	6.16	112.26	106.10
1	F	462	VAL	CB-CA-C	-6.13	102.81	111.21
1	D	540	THR	N-CA-C	5.95	118.57	110.35
1	B	37	VAL	CA-C-N	5.40	127.83	120.54
1	B	37	VAL	C-N-CA	5.40	127.83	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	462	VAL	CB-CA-C	-5.24	104.03	111.21
1	F	447	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	C	390	THR	N-CA-C	-5.00	107.86	114.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4254	0	3960	78	0
1	B	4254	0	3960	99	0
1	C	4254	0	3961	83	0
1	D	4254	0	3960	79	0
1	E	4254	0	3962	69	0
1	F	4254	0	3960	82	0
2	G	61	0	52	1	0
2	J	61	0	52	1	0
2	M	61	0	52	0	0
2	O	61	0	52	1	0
2	S	61	0	52	1	0
2	U	61	0	52	0	0
2	Y	61	0	52	2	0
2	a	61	0	52	0	0
2	d	61	0	52	1	0
2	f	61	0	52	1	0
2	i	61	0	52	0	0
2	k	61	0	52	1	0
3	H	72	0	61	0	0
3	N	72	0	61	1	0
3	Z	72	0	61	0	0
3	j	72	0	61	1	0
4	I	28	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
4	b	28	0	25	0	0
4	g	28	0	25	0	0
5	K	39	0	34	0	0
5	L	39	0	34	2	0
5	W	39	0	34	3	0
5	X	39	0	34	1	0
5	c	39	0	34	0	0
5	h	39	0	34	1	0
5	l	39	0	34	0	0
6	R	50	0	43	0	0
7	T	83	0	70	1	0
7	e	83	0	70	2	0
8	A	70	0	65	0	0
8	B	70	0	65	3	0
8	C	70	0	65	2	0
8	D	70	0	64	2	0
8	E	70	0	65	2	0
8	F	84	0	78	4	0
9	A	4	0	0	0	0
9	B	4	0	0	0	0
9	C	4	0	0	0	0
9	D	4	0	0	0	0
9	E	4	0	0	0	0
9	F	4	0	0	0	0
All	All	27659	0	25604	491	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 9.

All (491) 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)
8:F:2006:NAG:C7	8:F:2006:NAG:C8	1.80	1.60
1:F:463:ARG:CZ	1:F:463:ARG:NH1	1.85	1.37
8:F:2005:NAG:O6	8:F:2005:NAG:C6	1.74	1.32
5:W:3:BMA:O6	5:W:3:BMA:C6	1.75	1.32
1:F:427:ARG:HD2	1:F:463:ARG:NH1	1.56	1.20
1:C:246:THR:HG21	1:C:318:LEU:HB2	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:HG21	1:F:318:LEU:HB2	1.44	0.98
1:F:427:ARG:HD2	1:F:463:ARG:HH11	1.12	0.95
1:D:78:THR:HG23	1:D:132:GLN:OE1	1.70	0.91
1:F:427:ARG:CD	1:F:463:ARG:HH11	1.82	0.91
1:E:131:GLY:HA3	1:E:168:VAL:HG11	1.52	0.90
1:A:78:THR:HG23	1:A:132:GLN:OE1	1.71	0.90
1:E:420:HIS:NE2	1:E:500:GLU:OE1	2.05	0.90
1:B:131:GLY:HA3	1:B:168:VAL:HG11	1.51	0.89
1:C:244:ASN:HD22	8:C:2005:NAG:H83	1.38	0.89
1:A:131:GLY:HA3	1:A:168:VAL:HG11	1.56	0.87
1:A:302:THR:HG23	1:B:55:PRO:HB3	1.55	0.86
1:D:131:GLY:HA3	1:D:168:VAL:HG11	1.55	0.86
1:A:272:ALA:HB1	1:A:274:MET:HE1	1.59	0.85
1:F:131:GLY:HA3	1:F:168:VAL:HG11	1.59	0.84
1:A:176:MET:HE1	1:A:491:LEU:HB3	1.61	0.82
1:B:78:THR:HG23	1:B:132:GLN:OE1	1.79	0.82
1:C:131:GLY:HA3	1:C:168:VAL:HG11	1.60	0.82
1:B:395:LEU:HD12	1:B:500:GLU:HG3	1.63	0.81
1:A:129:THR:HG22	1:A:130:ASP:H	1.45	0.80
1:D:246:THR:HG21	1:D:318:LEU:HB2	1.63	0.79
1:B:67:ILE:HG21	1:B:80:MET:HE1	1.63	0.79
1:A:244:ASN:HD22	4:I:1:NAG:H83	1.48	0.78
1:A:278:ASP:OD2	1:A:280:THR:HB	1.84	0.77
1:C:272:ALA:HB1	1:C:274:MET:HE1	1.66	0.77
1:B:272:ALA:HB1	1:B:274:MET:HE1	1.68	0.76
1:C:395:LEU:HD12	1:C:500:GLU:HG3	1.68	0.75
1:B:38:ASP:OD2	1:B:165:HIS:NE2	2.19	0.74
1:C:276:LYS:HG3	1:C:292:ASN:HB3	1.68	0.74
1:B:235:GLU:HB3	1:B:258:THR:HB	1.70	0.73
1:D:274:MET:HE3	1:D:309:ASN:H	1.54	0.72
1:B:278:ASP:OD2	1:B:280:THR:HB	1.91	0.71
1:F:176:MET:HE1	1:F:491:LEU:HB3	1.73	0.71
1:B:129:THR:HG22	1:B:130:ASP:H	1.56	0.70
1:A:302:THR:CG2	1:B:55:PRO:HB3	2.21	0.70
1:C:129:THR:HG22	1:C:130:ASP:H	1.56	0.69
1:B:246:THR:HG21	1:B:318:LEU:HB2	1.72	0.69
1:D:116:VAL:HG12	1:D:116:VAL:O	1.93	0.69
1:C:67:ILE:HG21	1:C:80:MET:HE1	1.74	0.69
1:B:67:ILE:HG21	1:B:80:MET:CE	2.24	0.68
1:F:395:LEU:HD12	1:F:500:GLU:HG3	1.75	0.68
1:F:80:MET:HE3	1:F:82:PHE:CZ	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ALA:HB1	1:A:274:MET:CE	2.23	0.68
1:D:178:VAL:HG11	1:F:440:HIS:CD2	2.29	0.68
1:B:116:VAL:HG12	1:B:116:VAL:O	1.94	0.67
1:B:349:LYS:HD2	1:B:547:VAL:HG23	1.77	0.67
1:D:388:SER:H	1:D:542:LEU:HD21	1.59	0.67
1:F:274:MET:HE3	1:F:309:ASN:H	1.61	0.66
1:A:129:THR:HG22	1:A:130:ASP:N	2.11	0.66
1:D:349:LYS:HD2	1:D:547:VAL:HG23	1.76	0.66
1:F:542:LEU:HD13	1:F:542:LEU:H	1.61	0.65
1:B:185:GLU:HG3	1:B:219:PHE:CZ	2.31	0.65
1:E:246:THR:HG21	1:E:318:LEU:HB2	1.77	0.65
1:E:274:MET:HE3	1:E:309:ASN:H	1.62	0.65
1:B:505:ILE:HG23	1:B:511:GLN:HG2	1.78	0.65
1:F:116:VAL:HG11	1:F:143:ILE:HD13	1.78	0.65
1:C:272:ALA:HB1	1:C:274:MET:CE	2.27	0.64
1:A:505:ILE:HG23	1:A:511:GLN:HG2	1.79	0.64
1:A:38:ASP:HB3	1:A:40:LEU:H	1.63	0.64
1:D:235:GLU:HB3	1:D:258:THR:HB	1.77	0.64
1:B:372:THR:HB	1:B:530:GLY:HA2	1.80	0.64
1:D:167:LEU:HD12	1:D:167:LEU:H	1.62	0.64
1:C:296:TYR:HD2	1:C:306:PRO:HG2	1.62	0.64
1:C:116:VAL:HG12	1:C:116:VAL:O	1.97	0.64
1:D:395:LEU:HD12	1:D:500:GLU:HG3	1.81	0.63
1:E:67:ILE:HG21	1:E:80:MET:HE1	1.80	0.63
1:D:220:VAL:HG21	1:D:277:PHE:HD2	1.63	0.63
1:B:244:ASN:HD22	8:B:2005:NAG:H83	1.64	0.62
1:D:274:MET:CE	1:D:309:ASN:H	2.13	0.62
1:C:38:ASP:HB3	1:C:40:LEU:H	1.63	0.62
1:D:185:GLU:HG3	1:D:219:PHE:CZ	2.35	0.61
1:D:225:TRP:CZ2	1:D:274:MET:HG2	2.36	0.61
1:B:38:ASP:HB3	1:B:40:LEU:H	1.64	0.61
1:A:537:LEU:HD23	1:A:539:LEU:HB2	1.83	0.61
1:F:116:VAL:HG11	1:F:143:ILE:CD1	2.30	0.61
1:C:244:ASN:HD22	8:C:2005:NAG:C8	2.10	0.60
1:C:278:ASP:OD2	1:C:280:THR:HB	2.01	0.60
1:A:116:VAL:CG1	1:A:116:VAL:O	2.49	0.60
2:G:3:BMA:H3	2:G:4:MAN:H3	1.83	0.60
1:A:234:VAL:C	1:A:241:THR:HG22	2.26	0.60
1:C:420:HIS:NE2	1:C:500:GLU:OE1	2.27	0.60
1:E:278:ASP:OD2	1:E:280:THR:HB	2.01	0.60
1:F:318:LEU:HD21	1:F:323:LEU:HD11	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASP:HB3	1:B:466:SER:OG	2.01	0.60
1:F:427:ARG:CD	1:F:463:ARG:NH1	2.45	0.59
1:C:134:GLU:OE2	1:C:218:GLY:HA3	2.01	0.59
1:B:234:VAL:C	1:B:241:THR:HG22	2.28	0.59
1:D:95:GLY:H	1:D:100:THR:HG21	1.67	0.59
1:F:274:MET:CE	1:F:309:ASN:H	2.15	0.59
1:C:235:GLU:HB3	1:C:258:THR:HB	1.84	0.59
1:A:95:GLY:H	1:A:100:THR:HG21	1.67	0.59
1:B:129:THR:HG22	1:B:130:ASP:N	2.18	0.58
1:F:78:THR:HG23	1:F:132:GLN:OE1	2.02	0.58
1:C:48:CYS:HB2	1:C:54:TRP:CD2	2.38	0.58
1:C:100:THR:HG22	1:C:101:GLN:HG2	1.86	0.58
1:B:176:MET:HE1	1:B:491:LEU:HB3	1.85	0.58
1:D:430:THR:HG23	1:D:464:PRO:HD2	1.84	0.58
1:F:235:GLU:HB3	1:F:258:THR:HB	1.86	0.58
1:F:360:ILE:HD11	8:F:2012:NAG:H82	1.86	0.58
1:A:116:VAL:O	1:A:116:VAL:HG12	2.03	0.58
1:C:176:MET:HE1	1:C:491:LEU:HB3	1.86	0.58
1:F:78:THR:HG22	1:F:79:SER:H	1.67	0.58
1:B:134:GLU:OE2	1:B:218:GLY:HA3	2.04	0.57
1:F:67:ILE:HG21	1:F:80:MET:HE1	1.87	0.57
1:F:214:VAL:HG13	1:F:256:ARG:HG3	1.87	0.57
1:F:220:VAL:HG21	1:F:277:PHE:HD2	1.69	0.57
5:W:3:BMA:O6	5:W:3:BMA:C5	2.51	0.57
1:E:352:VAL:HG22	1:E:354:TYR:CE1	2.39	0.57
1:A:95:GLY:HA2	1:A:101:GLN:OE1	2.04	0.57
1:C:202:GLU:OE1	1:C:301:LYS:HD3	2.05	0.57
1:F:403:ILE:HD12	1:F:470:ILE:HD11	1.87	0.57
1:A:361:THR:HG22	1:A:493:GLY:HA3	1.87	0.57
1:B:103:PRO:HG2	2:O:1:NAG:H61	1.87	0.57
1:D:23:THR:HG23	1:D:64:ARG:HG2	1.87	0.56
1:E:104:ILE:HG12	1:E:110:MET:HE2	1.86	0.56
1:A:157:SER:OG	1:A:212:ARG:HD2	2.04	0.56
1:A:267:THR:HG22	1:A:267:THR:O	2.05	0.56
1:B:99:LEU:HD13	1:B:497:VAL:HG13	1.86	0.56
1:E:308:GLN:HE22	5:h:1:NAG:H2	1.68	0.56
1:E:438:VAL:HG21	1:F:351:GLY:HA3	1.87	0.56
1:B:355:ALA:HB1	1:B:494:LEU:HG	1.88	0.56
1:B:390:THR:HG23	1:B:392:THR:OG1	2.05	0.56
1:D:395:LEU:HD13	1:D:401:VAL:HG21	1.88	0.56
1:A:235:GLU:HB3	1:A:258:THR:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TRP:CE3	1:D:216:VAL:HG12	2.41	0.56
1:B:468:PHE:C	1:B:468:PHE:CD2	2.84	0.56
1:B:527:ALA:HB1	1:B:529:GLU:HG3	1.86	0.56
1:A:61:LYS:HD3	1:A:120:VAL:HG23	1.88	0.55
1:C:129:THR:HG22	1:C:130:ASP:N	2.19	0.55
1:A:48:CYS:HB2	1:A:54:TRP:CD2	2.41	0.55
1:A:211:LEU:HD22	1:A:213:ILE:CG1	2.37	0.55
1:B:81:HIS:CE1	1:B:418:HIS:CE1	2.94	0.55
1:D:176:MET:HE1	1:D:491:LEU:HB3	1.87	0.55
1:F:78:THR:HG22	1:F:79:SER:N	2.21	0.55
1:F:95:GLY:H	1:F:100:THR:HG21	1.70	0.55
1:A:296:TYR:HD2	1:A:306:PRO:HG2	1.70	0.55
1:A:276:LYS:HG3	1:A:292:ASN:HB3	1.87	0.55
1:B:276:LYS:HG3	1:B:292:ASN:HB3	1.89	0.55
1:D:537:LEU:HD23	1:D:539:LEU:HB2	1.89	0.55
1:C:267:THR:HG22	1:C:267:THR:O	2.07	0.55
1:F:386:TYR:O	1:F:390:THR:HG21	2.07	0.55
1:C:300:ASN:OD1	1:C:302:THR:HG22	2.06	0.55
1:A:225:TRP:CZ2	1:A:274:MET:HG2	2.42	0.54
1:D:100:THR:HG22	1:D:101:GLN:HG2	1.90	0.54
8:F:2005:NAG:O6	8:F:2005:NAG:C5	2.54	0.54
1:B:48:CYS:HB2	1:B:54:TRP:CD2	2.42	0.54
1:D:38:ASP:OD2	1:D:165:HIS:NE2	2.34	0.54
1:B:95:GLY:H	1:B:100:THR:HG21	1.73	0.54
1:B:244:ASN:HD22	8:B:2005:NAG:C8	2.19	0.54
1:F:131:GLY:CA	1:F:168:VAL:HG11	2.35	0.54
1:E:274:MET:CE	1:E:309:ASN:H	2.20	0.54
1:B:276:LYS:HE2	1:B:292:ASN:HD22	1.73	0.54
1:E:386:TYR:O	1:E:390:THR:HG21	2.07	0.54
1:B:388:SER:H	1:B:542:LEU:HD21	1.72	0.54
1:C:349:LYS:HD2	1:C:547:VAL:HG23	1.89	0.54
1:B:83:HIS:CE1	1:B:254:ALA:HB1	2.42	0.54
1:B:120:VAL:HG21	1:B:145:ASP:HB3	1.89	0.54
1:B:272:ALA:HB1	1:B:274:MET:CE	2.36	0.54
1:F:336:ASP:HB2	1:F:399:GLU:HB2	1.90	0.54
1:B:468:PHE:C	1:B:468:PHE:HD2	2.16	0.54
1:D:48:CYS:HB2	1:D:54:TRP:CD2	2.43	0.53
1:B:28:TRP:HH2	1:B:57:ILE:HD11	1.73	0.53
1:D:361:THR:HG23	1:D:493:GLY:HA3	1.89	0.53
1:C:95:GLY:H	1:C:100:THR:HG21	1.73	0.53
1:D:101:GLN:NE2	1:D:110:MET:HE1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:GLY:HA2	1:E:101:GLN:OE1	2.09	0.53
1:B:78:THR:HG21	1:B:137:MET:HE1	1.91	0.53
1:F:462:VAL:HG22	1:F:468:PHE:CE1	2.44	0.53
1:A:244:ASN:HD22	4:I:1:NAG:C8	2.19	0.53
1:E:355:ALA:HB1	1:E:494:LEU:HG	1.90	0.53
1:F:429:ARG:HA	1:F:463:ARG:HD2	1.90	0.53
1:D:142:ILE:HD12	2:Y:2:NAG:H81	1.90	0.52
1:F:104:ILE:HG12	1:F:110:MET:HE3	1.91	0.52
1:D:48:CYS:HB2	1:D:54:TRP:CE2	2.43	0.52
1:E:438:VAL:HG21	1:F:351:GLY:CA	2.40	0.52
1:E:95:GLY:H	1:E:100:THR:HG21	1.75	0.52
1:B:244:ASN:HB2	8:B:2005:NAG:H83	1.92	0.52
1:B:120:VAL:CG2	1:B:145:ASP:HB3	2.40	0.52
1:C:468:PHE:C	1:C:468:PHE:CD2	2.88	0.52
1:B:214:VAL:HG13	1:B:256:ARG:HG3	1.90	0.52
1:C:352:VAL:HG22	1:C:354:TYR:CE1	2.45	0.52
1:C:537:LEU:HD23	1:C:539:LEU:HB2	1.91	0.52
1:A:211:LEU:HD22	1:A:213:ILE:HG13	1.92	0.51
1:B:78:THR:CG2	1:B:132:GLN:OE1	2.54	0.51
1:D:167:LEU:HD12	1:D:167:LEU:N	2.24	0.51
1:C:110:MET:HB2	1:C:520:VAL:HG21	1.91	0.51
1:C:462:VAL:HG13	1:C:468:PHE:CD1	2.46	0.51
1:A:428:ASP:HB3	1:A:466:SER:OG	2.11	0.51
1:D:157:SER:OG	1:D:212:ARG:HD2	2.10	0.51
1:E:244:ASN:HB2	8:E:2005:NAG:H83	1.93	0.51
1:D:186:PRO:HG2	1:D:488:TRP:CZ2	2.45	0.51
1:B:130:ASP:O	1:B:487:GLU:OE1	2.28	0.51
1:D:502:PRO:HA	1:D:505:ILE:HD12	1.93	0.51
1:A:308:GLN:OE1	5:L:1:NAG:H83	2.11	0.51
1:A:349:LYS:HD2	1:A:547:VAL:HG23	1.93	0.51
1:E:199:LEU:HD21	2:d:1:NAG:H82	1.92	0.51
1:B:225:TRP:CZ2	1:B:274:MET:HG2	2.46	0.50
1:E:272:ALA:HB1	1:E:274:MET:CE	2.40	0.50
1:E:276:LYS:HG3	1:E:292:ASN:HB3	1.93	0.50
1:C:336:ASP:HB2	1:C:399:GLU:HB2	1.93	0.50
1:E:237:ASP:OD1	1:E:457:ARG:HB2	2.11	0.50
1:C:274:MET:CE	1:C:309:ASN:H	2.24	0.50
1:B:386:TYR:O	1:B:390:THR:HG21	2.12	0.50
1:A:389:ASN:OD1	1:A:545:GLU:HG2	2.12	0.50
1:B:274:MET:HE3	1:B:309:ASN:HB3	1.94	0.50
1:B:370:LEU:HA	1:B:373:VAL:HG13	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLY:HA2	1:C:101:GLN:OE1	2.10	0.50
1:D:220:VAL:HG21	1:D:277:PHE:CD2	2.45	0.50
1:F:348:LEU:HD12	1:F:354:TYR:CD1	2.47	0.50
1:A:352:VAL:HG22	1:A:354:TYR:CE1	2.46	0.50
1:D:22:GLU:OE1	1:D:24:HIS:NE2	2.45	0.50
1:F:95:GLY:N	1:F:100:THR:HG21	2.26	0.50
1:B:33:ASP:HB2	1:B:47:THR:HG21	1.94	0.50
1:F:103:PRO:HG2	2:k:1:NAG:H61	1.93	0.50
1:A:370:LEU:HA	1:A:373:VAL:HG13	1.93	0.49
1:F:100:THR:HG22	1:F:101:GLN:HG2	1.92	0.49
1:A:186:PRO:HG2	1:A:488:TRP:CZ2	2.48	0.49
1:B:78:THR:HG22	1:B:79:SER:H	1.77	0.49
1:D:179:TYR:HE2	1:F:428:ASP:OD2	1.95	0.49
1:A:67:ILE:HG21	1:A:80:MET:HE1	1.93	0.49
1:A:468:PHE:C	1:A:468:PHE:CD2	2.90	0.49
1:D:276:LYS:HE2	1:D:292:ASN:HD22	1.77	0.49
1:E:527:ALA:HB1	1:E:529:GLU:HG3	1.94	0.49
1:D:78:THR:HG22	1:D:79:SER:H	1.75	0.49
1:F:82:PHE:HB3	1:F:85:LEU:HD22	1.93	0.49
1:E:390:THR:HG23	1:E:392:THR:OG1	2.12	0.49
1:A:484:CYS:HB2	1:A:494:LEU:HD13	1.94	0.49
1:B:197:MET:HB2	3:N:1:NAG:HN2	1.77	0.49
1:F:220:VAL:HG11	1:F:277:PHE:CE2	2.48	0.49
1:D:278:ASP:OD2	1:D:280:THR:HB	2.12	0.49
1:A:253:VAL:O	1:A:254:ALA:HB3	2.13	0.48
1:C:505:ILE:HG23	1:C:511:GLN:HG2	1.94	0.48
1:C:274:MET:HE3	1:C:309:ASN:H	1.77	0.48
1:B:227:GLU:HG2	1:B:271:PHE:HD2	1.78	0.48
1:B:336:ASP:HB2	1:B:399:GLU:HB2	1.95	0.48
1:C:83:HIS:CE1	1:C:254:ALA:HB1	2.49	0.48
1:A:91:ALA:N	1:A:511:GLN:OE1	2.46	0.48
1:C:413:HIS:O	1:C:461:TYR:HA	2.13	0.48
1:A:502:PRO:HA	1:A:505:ILE:HD12	1.96	0.48
1:B:186:PRO:HG2	1:B:488:TRP:CZ2	2.49	0.48
1:E:48:CYS:HB2	1:E:54:TRP:CD2	2.49	0.48
1:E:176:MET:HE1	1:E:491:LEU:HB3	1.95	0.48
1:A:372:THR:HB	1:A:530:GLY:HA2	1.95	0.48
1:C:225:TRP:CZ2	1:C:274:MET:HG2	2.49	0.48
1:B:413:HIS:O	1:B:461:TYR:HA	2.14	0.47
1:C:274:MET:HE3	1:C:309:ASN:HB3	1.96	0.47
1:F:430:THR:HG23	1:F:464:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PHE:HB3	1:B:85:LEU:HD22	1.96	0.47
1:B:296:TYR:HD2	1:B:306:PRO:HG2	1.78	0.47
1:C:127:SER:HB2	1:C:137:MET:SD	2.54	0.47
1:D:38:ASP:HB3	1:D:40:LEU:H	1.79	0.47
1:C:134:GLU:OE2	1:C:218:GLY:CA	2.61	0.47
1:D:237:ASP:OD1	1:D:457:ARG:HB2	2.14	0.47
1:F:255:GLN:HB2	1:F:457:ARG:NH2	2.29	0.47
1:F:355:ALA:HB1	1:F:494:LEU:HG	1.97	0.47
1:D:67:ILE:HG21	1:D:80:MET:HE1	1.97	0.47
1:A:388:SER:H	1:A:542:LEU:HD21	1.78	0.47
1:B:124:TRP:CE3	1:B:216:VAL:HG12	2.50	0.47
1:C:48:CYS:HB2	1:C:54:TRP:CE2	2.49	0.47
1:D:516:ASN:O	1:D:519:GLU:HB3	2.15	0.47
1:F:278:ASP:OD2	1:F:280:THR:HB	2.14	0.47
1:A:98:PHE:HB3	1:A:365:PRO:HD2	1.97	0.47
1:B:352:VAL:HG22	1:B:354:TYR:CE1	2.50	0.47
1:F:390:THR:HG23	1:F:392:THR:OG1	2.14	0.47
2:J:2:NAG:H83	2:J:2:NAG:H3	1.97	0.47
1:C:158:LEU:HG	1:C:211:LEU:HD21	1.95	0.47
1:E:104:ILE:CG1	1:E:110:MET:HE2	2.44	0.47
1:F:234:VAL:C	1:F:241:THR:HG22	2.40	0.47
1:F:413:HIS:O	1:F:461:TYR:HA	2.15	0.47
1:A:55:PRO:HB3	1:C:302:THR:HG23	1.97	0.47
1:B:191:LEU:HG	1:B:277:PHE:CE1	2.50	0.47
1:D:468:PHE:C	1:D:468:PHE:CD2	2.93	0.47
1:D:234:VAL:C	1:D:241:THR:HG22	2.40	0.46
1:F:48:CYS:HB2	1:F:54:TRP:CD2	2.51	0.46
1:A:542:LEU:HB2	1:A:543:THR:H	1.33	0.46
1:C:61:LYS:HD3	1:C:120:VAL:HG23	1.97	0.46
1:E:185:GLU:OE2	1:E:489:HIS:NE2	2.47	0.46
1:B:28:TRP:CH2	1:B:57:ILE:HD11	2.49	0.46
1:E:78:THR:CG2	1:E:137:MET:HE1	2.45	0.46
1:C:110:MET:HG2	1:C:112:TYR:CE1	2.51	0.46
1:D:390:THR:HG23	1:D:392:THR:OG1	2.16	0.46
1:E:225:TRP:CZ2	1:E:274:MET:HG2	2.50	0.46
1:F:80:MET:HE3	1:F:82:PHE:HZ	1.79	0.46
1:B:388:SER:H	1:B:542:LEU:CD2	2.28	0.46
1:C:542:LEU:HB2	1:C:543:THR:H	1.52	0.46
1:D:505:ILE:HG23	1:D:511:GLN:HG2	1.96	0.46
1:F:201:TRP:HE3	1:F:273:ILE:HD11	1.80	0.46
1:A:396:GLU:H	1:A:399:GLU:CD	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:HIS:O	1:A:461:TYR:HA	2.15	0.46
1:C:24:HIS:CD2	1:C:59:VAL:HG12	2.50	0.46
1:E:129:THR:HG22	1:E:130:ASP:H	1.80	0.46
5:W:2:NAG:O3	5:W:2:NAG:H83	2.15	0.46
1:A:101:GLN:NE2	1:A:110:MET:HE1	2.30	0.46
1:E:91:ALA:O	1:E:100:THR:HG23	2.16	0.46
1:C:428:ASP:HB3	1:C:466:SER:OG	2.15	0.46
1:D:500:GLU:O	1:D:501:ASP:C	2.59	0.46
1:E:501:ASP:HA	1:E:502:PRO:HD2	1.72	0.46
1:A:336:ASP:HB2	1:A:399:GLU:HB2	1.97	0.46
1:D:244:ASN:HB2	8:D:2005:NAG:H83	1.97	0.46
1:D:336:ASP:HB2	1:D:399:GLU:HB2	1.98	0.46
1:D:476:ASN:HB2	8:D:2008:NAG:H82	1.96	0.46
1:F:48:CYS:HB2	1:F:54:TRP:CE2	2.51	0.46
1:E:336:ASP:HB2	1:E:399:GLU:HB2	1.97	0.45
1:E:468:PHE:C	1:E:468:PHE:CD2	2.94	0.45
1:A:500:GLU:O	1:A:501:ASP:C	2.59	0.45
1:B:134:GLU:OE2	1:B:218:GLY:CA	2.64	0.45
1:B:500:GLU:O	1:B:501:ASP:C	2.58	0.45
1:C:500:GLU:O	1:C:501:ASP:C	2.60	0.45
1:A:95:GLY:N	1:A:100:THR:HG21	2.31	0.45
1:B:248:MET:HE1	1:B:313:SER:O	2.17	0.45
1:C:198:ASN:OD1	7:T:1:NAG:H83	2.16	0.45
1:C:232:THR:HB	1:C:260:LEU:HB2	1.98	0.45
1:F:197:MET:HB2	3:j:1:NAG:HN2	1.79	0.45
1:F:395:LEU:HD22	1:F:401:VAL:HG21	1.97	0.45
1:A:297:MET:HE2	1:A:299:TYR:CE1	2.52	0.45
1:A:369:THR:HB	1:A:479:VAL:HG11	1.98	0.45
1:C:219:PHE:CD1	1:C:219:PHE:C	2.93	0.45
1:E:131:GLY:CA	1:E:168:VAL:HG11	2.36	0.45
1:E:395:LEU:HD12	1:E:500:GLU:HG2	1.97	0.45
1:F:104:ILE:CG1	1:F:110:MET:HE3	2.47	0.45
1:A:355:ALA:HB1	1:A:494:LEU:HG	1.97	0.45
1:B:116:VAL:HG11	1:B:143:ILE:HD13	1.99	0.45
1:C:167:LEU:H	1:C:167:LEU:HD12	1.82	0.45
1:C:355:ALA:HB1	1:C:494:LEU:HG	1.98	0.45
1:E:375:SER:OG	1:E:529:GLU:O	2.33	0.45
1:D:355:ALA:HB1	1:D:494:LEU:HG	1.98	0.45
8:E:2006:NAG:H5	8:E:2006:NAG:O7	2.17	0.44
1:B:116:VAL:CG1	1:B:143:ILE:HD13	2.47	0.44
1:A:286:PRO:HG2	1:A:289:LEU:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ASP:OD2	1:D:457:ARG:NH1	2.50	0.44
1:C:142:ILE:HD12	2:S:2:NAG:H81	1.98	0.44
1:D:28:TRP:HH2	1:D:57:ILE:HD11	1.82	0.44
1:E:235:GLU:HB3	1:E:258:THR:HB	1.99	0.44
1:E:500:GLU:O	1:E:501:ASP:C	2.61	0.44
1:D:167:LEU:H	1:D:167:LEU:CD1	2.30	0.44
1:E:40:LEU:HB3	7:e:2:NAG:H61	1.99	0.44
1:E:48:CYS:HB2	1:E:54:TRP:CE2	2.53	0.44
1:B:267:THR:HG22	1:B:299:TYR:O	2.17	0.44
1:E:272:ALA:HB1	1:E:274:MET:HE1	1.99	0.44
1:F:382:ASN:O	1:F:385:ILE:HG12	2.18	0.44
1:F:500:GLU:O	1:F:501:ASP:C	2.60	0.44
1:B:484:CYS:HB2	1:B:494:LEU:HD13	2.00	0.44
1:C:308:GLN:HE22	5:X:1:NAG:H2	1.82	0.44
1:F:187:ILE:HG23	1:F:282:LEU:HD22	1.99	0.44
1:B:232:THR:HB	1:B:260:LEU:HB2	1.99	0.44
1:B:417:LEU:HD23	1:B:422:PHE:HD1	1.83	0.44
1:A:185:GLU:H	1:A:185:GLU:HG2	1.25	0.43
1:A:334:GLU:HA	1:A:335:PRO:HD3	1.83	0.43
1:A:388:SER:H	1:A:542:LEU:CD2	2.31	0.43
1:B:537:LEU:HD23	1:B:539:LEU:HB2	2.00	0.43
1:F:414:PRO:HD2	1:F:484:CYS:SG	2.57	0.43
1:B:91:ALA:N	1:B:511:GLN:OE1	2.41	0.43
1:D:527:ALA:HB1	1:D:529:GLU:HG3	2.00	0.43
1:C:386:TYR:O	1:C:390:THR:HG21	2.18	0.43
1:D:468:PHE:C	1:D:468:PHE:HD2	2.26	0.43
1:C:382:ASN:O	1:C:385:ILE:HG12	2.18	0.43
1:C:501:ASP:HA	1:C:502:PRO:HD2	1.80	0.43
1:D:214:VAL:HG13	1:D:256:ARG:HG3	2.00	0.43
1:E:83:HIS:CE1	1:E:254:ALA:HB1	2.54	0.43
1:E:98:PHE:HB3	1:E:365:PRO:HD2	2.01	0.43
1:E:214:VAL:HG13	1:E:256:ARG:HG3	2.01	0.43
1:F:116:VAL:CG1	1:F:143:ILE:HD13	2.47	0.43
1:F:516:ASN:O	1:F:519:GLU:HB3	2.19	0.43
1:A:167:LEU:HD12	1:A:167:LEU:H	1.84	0.43
1:B:361:THR:HG23	1:B:493:GLY:HA3	2.00	0.43
1:D:255:GLN:HB2	1:D:457:ARG:NH2	2.34	0.43
1:D:542:LEU:HD12	1:D:542:LEU:H	1.84	0.43
1:F:253:VAL:O	1:F:254:ALA:HB3	2.17	0.43
1:F:511:GLN:HA	1:F:511:GLN:OE1	2.18	0.43
1:A:78:THR:CG2	1:A:137:MET:HE1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:O	1:A:138:LYS:HD3	2.18	0.43
1:C:98:PHE:HB3	1:C:365:PRO:HD2	2.00	0.43
1:D:95:GLY:N	1:D:100:THR:HG21	2.31	0.43
1:E:144:LYS:HE2	1:E:144:LYS:HB2	1.70	0.43
1:E:255:GLN:HB2	1:E:457:ARG:HH21	1.82	0.43
1:E:320:ASP:HA	1:E:323:LEU:HD22	2.00	0.43
1:E:505:ILE:HG23	1:E:511:GLN:HG2	2.01	0.43
1:B:144:LYS:HB2	1:B:144:LYS:HE2	1.75	0.43
1:E:334:GLU:HA	1:E:335:PRO:HD3	1.83	0.43
1:F:370:LEU:HA	1:F:373:VAL:HG13	2.01	0.43
1:B:253:VAL:O	1:B:254:ALA:HB3	2.18	0.43
1:D:405:LEU:HD22	1:D:462:VAL:HG21	2.01	0.43
1:E:103:PRO:HG2	2:f:1:NAG:H61	2.01	0.43
1:A:274:MET:HE1	1:A:294:THR:HG23	2.00	0.42
1:C:28:TRP:HH2	1:C:57:ILE:HD11	1.83	0.42
1:D:428:ASP:HB3	1:D:466:SER:OG	2.19	0.42
1:F:185:GLU:H	1:F:185:GLU:HG2	1.62	0.42
1:F:386:TYR:HE1	1:F:394:ILE:HD11	1.83	0.42
1:D:370:LEU:HA	1:D:373:VAL:HG13	2.01	0.42
1:E:220:VAL:HG21	1:E:277:PHE:HD2	1.85	0.42
1:A:310:TYR:HE2	5:L:1:NAG:H82	1.85	0.42
1:B:127:SER:HB2	1:B:137:MET:SD	2.60	0.42
1:D:144:LYS:NZ	2:Y:5:MAN:H2	2.34	0.42
1:E:40:LEU:N	1:E:40:LEU:HD23	2.33	0.42
1:A:220:VAL:HG11	1:A:277:PHE:CD2	2.54	0.42
1:B:474:ALA:HB1	1:B:500:GLU:HG2	2.01	0.42
1:B:150:TYR:CD2	1:B:243:LYS:HE3	2.54	0.42
1:B:220:VAL:HG21	1:B:277:PHE:HD2	1.85	0.42
1:E:38:ASP:HB3	1:E:40:LEU:H	1.83	0.42
1:B:81:HIS:CE1	1:B:418:HIS:ND1	2.88	0.42
1:F:43:ARG:NH2	1:F:135:ASP:OD1	2.52	0.42
1:A:320:ASP:OD2	1:A:457:ARG:NH1	2.49	0.42
1:B:318:LEU:HD21	1:B:323:LEU:HD11	2.02	0.42
1:C:49:ASN:HD22	1:E:302:THR:HA	1.85	0.42
1:D:95:GLY:HA2	1:D:101:GLN:OE1	2.19	0.42
1:D:234:VAL:HA	1:D:241:THR:HG22	2.00	0.42
1:D:241:THR:HG23	1:D:242:GLU:O	2.19	0.42
1:D:253:VAL:O	1:D:254:ALA:HB3	2.19	0.42
1:F:395:LEU:HD12	1:F:500:GLU:CG	2.47	0.42
1:B:422:PHE:O	1:B:456:ARG:HA	2.19	0.42
1:B:537:LEU:C	1:B:539:LEU:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ASP:OD1	1:C:269:LYS:HB2	2.19	0.42
1:D:176:MET:HE2	1:D:176:MET:HB2	1.93	0.42
1:E:91:ALA:N	1:E:511:GLN:OE1	2.51	0.42
1:C:191:LEU:HG	1:C:277:PHE:CE1	2.54	0.42
1:C:233:VAL:HG21	1:C:318:LEU:HD22	2.01	0.42
1:A:232:THR:HB	1:A:260:LEU:HB2	2.02	0.42
1:C:28:TRP:CH2	1:C:57:ILE:HD11	2.55	0.42
1:C:468:PHE:C	1:C:468:PHE:HD2	2.27	0.42
1:E:413:HIS:O	1:E:461:TYR:HA	2.20	0.42
1:F:438:VAL:HB	1:F:439:PRO:CD	2.49	0.42
1:B:320:ASP:HA	1:B:323:LEU:HD22	2.02	0.41
1:B:542:LEU:HB2	1:B:543:THR:H	1.51	0.41
1:C:134:GLU:OE2	1:C:218:GLY:N	2.53	0.41
1:C:186:PRO:HG2	1:C:488:TRP:CZ2	2.55	0.41
1:D:201:TRP:HE3	1:D:273:ILE:HD11	1.85	0.41
1:B:334:GLU:HA	1:B:335:PRO:HD3	1.85	0.41
1:C:389:ASN:OD1	1:C:545:GLU:HG2	2.21	0.41
1:D:420:HIS:NE2	1:D:500:GLU:OE1	2.42	0.41
1:E:185:GLU:H	1:E:185:GLU:HG2	1.23	0.41
1:F:255:GLN:HB2	1:F:457:ARG:HH21	1.85	0.41
1:F:428:ASP:OD1	1:F:429:ARG:N	2.52	0.41
1:C:375:SER:OG	1:C:529:GLU:O	2.37	0.41
1:E:28:TRP:CH2	1:E:57:ILE:HD11	2.56	0.41
1:A:33:ASP:HB2	1:A:47:THR:HG21	2.01	0.41
1:F:264:LYS:HD2	1:F:271:PHE:CZ	2.56	0.41
1:E:410:THR:HA	1:E:465:GLN:HG3	2.03	0.41
1:F:124:TRP:CE3	1:F:216:VAL:HG12	2.55	0.41
1:C:234:VAL:C	1:C:241:THR:HG22	2.45	0.41
1:F:95:GLY:HA2	1:F:101:GLN:OE1	2.21	0.41
1:F:185:GLU:HG3	1:F:219:PHE:CZ	2.56	0.41
1:F:349:LYS:HD2	1:F:547:VAL:HG23	2.02	0.41
1:B:178:VAL:HG11	1:D:440:HIS:NE2	2.35	0.41
1:B:361:THR:CG2	1:B:493:GLY:HA3	2.50	0.41
1:C:95:GLY:N	1:C:100:THR:HG21	2.34	0.41
1:C:543:THR:HG23	1:C:543:THR:O	2.21	0.41
1:D:234:VAL:CA	1:D:241:THR:HG22	2.50	0.41
1:E:101:GLN:NE2	1:E:110:MET:HE1	2.35	0.41
1:E:537:LEU:C	1:E:539:LEU:H	2.28	0.41
1:A:48:CYS:HB2	1:A:54:TRP:CE2	2.55	0.41
1:B:48:CYS:HB2	1:B:54:TRP:CE2	2.55	0.41
1:B:131:GLY:HA2	1:B:487:GLU:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:HIS:CE1	1:F:254:ALA:HB1	2.55	0.41
1:F:220:VAL:HG21	1:F:277:PHE:CD2	2.53	0.41
1:F:275:GLN:HG3	1:F:293:ALA:HB3	2.03	0.41
7:e:1:NAG:H62	7:e:2:NAG:HN2	1.86	0.41
1:B:33:ASP:HB2	1:B:47:THR:CG2	2.50	0.41
1:B:501:ASP:HA	1:B:502:PRO:HD2	1.83	0.41
1:D:81:HIS:CE1	1:D:418:HIS:CE1	3.09	0.41
1:D:334:GLU:HA	1:D:335:PRO:HD3	1.81	0.41
1:D:537:LEU:C	1:D:539:LEU:H	2.29	0.41
1:E:234:VAL:C	1:E:241:THR:HG22	2.46	0.41
1:E:405:LEU:HD22	1:E:462:VAL:HG21	2.03	0.41
1:E:428:ASP:O	1:E:463:ARG:NH1	2.53	0.41
1:A:73:MET:HE3	1:A:73:MET:HB2	1.80	0.41
1:C:346:ASP:OD2	1:C:347:ASN:N	2.54	0.41
1:C:484:CYS:HB2	1:C:494:LEU:HD13	2.02	0.41
1:D:91:ALA:N	1:D:511:GLN:OE1	2.52	0.41
1:A:202:GLU:OE1	1:A:301:LYS:HD3	2.20	0.40
1:A:468:PHE:C	1:A:468:PHE:HD2	2.27	0.40
1:B:264:LYS:HB3	1:B:264:LYS:HE2	1.90	0.40
1:C:104:ILE:HD11	1:C:110:MET:HE3	2.02	0.40
1:E:255:GLN:HB2	1:E:457:ARG:NH2	2.36	0.40
1:A:58:THR:CG2	1:A:144:LYS:HD2	2.51	0.40
1:A:537:LEU:C	1:A:539:LEU:H	2.29	0.40
1:E:542:LEU:HD23	1:E:542:LEU:H	1.86	0.40
1:C:320:ASP:HA	1:C:323:LEU:HD22	2.02	0.40
1:C:343:VAL:HG13	1:C:494:LEU:HD21	2.02	0.40
1:C:438:VAL:HB	1:C:439:PRO:CD	2.51	0.40
1:C:537:LEU:C	1:C:539:LEU:H	2.29	0.40
1:F:38:ASP:HB3	1:F:40:LEU:H	1.86	0.40
1:D:422:PHE:O	1:D:456:ARG:HA	2.22	0.40
1:E:96:VAL:HA	1:E:97:PRO:HD2	1.90	0.40
1:A:81:HIS:CE1	1:A:418:HIS:CE1	3.08	0.40
1:E:302:THR:O	1:E:302:THR:HG22	2.21	0.40
1:F:484:CYS:HB2	1:F:494:LEU:HD13	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	9	31
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	11	36
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	14	41
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	8	28
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	11	36
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	11	36
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	10	34

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP
1	E	531	ASN
1	F	130	ASP
1	A	531	ASN
1	B	130	ASP
1	B	542	LEU
1	C	531	ASN
1	D	531	ASN
1	D	542	LEU
1	F	531	ASN
1	A	542	LEU
1	C	542	LEU
1	E	542	LEU
1	F	542	LEU
1	A	132	GLN
1	A	501	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	501	ASP
1	B	532	ALA
1	C	501	ASP
1	D	501	ASP
1	E	501	ASP
1	E	532	ALA
1	F	501	ASP
1	B	132	GLN
1	C	532	ALA
1	D	129	THR
1	D	132	GLN
1	D	397	LYS
1	D	532	ALA
1	E	129	THR
1	F	532	ALA
1	A	129	THR
1	A	532	ALA
1	F	129	THR

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 X-ray entries followed by that with respect to entries of similar resolution.

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	477/481 (99%)	427 (90%)	50 (10%)	6	22
1	B	477/481 (99%)	424 (89%)	53 (11%)	6	20
1	C	477/481 (99%)	426 (89%)	51 (11%)	6	21
1	D	477/481 (99%)	422 (88%)	55 (12%)	5	18
1	E	477/481 (99%)	434 (91%)	43 (9%)	9	28
1	F	477/481 (99%)	430 (90%)	47 (10%)	7	24
All	All	2862/2886 (99%)	2563 (90%)	299 (10%)	7	22

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	41	LYS
1	A	42	SER
1	A	43	ARG
1	A	69	LEU
1	A	76	THR
1	A	78	THR
1	A	99	LEU
1	A	100	THR
1	A	115	THR
1	A	116	VAL
1	A	120	VAL
1	A	132	GLN
1	A	142	ILE
1	A	162	GLU
1	A	169	THR
1	A	185	GLU
1	A	193	VAL
1	A	196	THR
1	A	198	ASN
1	A	220	VAL
1	A	246	THR
1	A	259	VAL
1	A	274	MET
1	A	280	THR
1	A	302	THR
1	A	311	VAL
1	A	323	LEU
1	A	352	VAL
1	A	361	THR
1	A	372	THR
1	A	373	VAL
1	A	389	ASN
1	A	390	THR
1	A	391	HIS
1	A	397	LYS
1	A	408	GLN
1	A	427	ARG
1	A	433	ASP
1	A	462	VAL
1	A	468	PHE
1	A	481	PHE
1	A	494	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	LEU
1	A	537	LEU
1	A	539	LEU
1	A	542	LEU
1	A	547	VAL
1	A	548	GLN
1	A	549	HIS
1	B	33	ASP
1	B	40	LEU
1	B	43	ARG
1	B	69	LEU
1	B	76	THR
1	B	78	THR
1	B	99	LEU
1	B	100	THR
1	B	115	THR
1	B	120	VAL
1	B	133	TYR
1	B	144	LYS
1	B	145	ASP
1	B	162	GLU
1	B	185	GLU
1	B	193	VAL
1	B	196	THR
1	B	211	LEU
1	B	259	VAL
1	B	264	LYS
1	B	267	THR
1	B	268	ASP
1	B	269	LYS
1	B	280	THR
1	B	292	ASN
1	B	302	THR
1	B	311	VAL
1	B	323	LEU
1	B	352	VAL
1	B	372	THR
1	B	373	VAL
1	B	378	ASP
1	B	389	ASN
1	B	390	THR
1	B	391	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	397	LYS
1	B	408	GLN
1	B	427	ARG
1	B	433	ASP
1	B	435	LEU
1	B	438	VAL
1	B	462	VAL
1	B	468	PHE
1	B	481	PHE
1	B	494	LEU
1	B	518	LEU
1	B	525	SER
1	B	528	THR
1	B	539	LEU
1	B	542	LEU
1	B	547	VAL
1	B	548	GLN
1	B	549	HIS
1	C	40	LEU
1	C	41	LYS
1	C	43	ARG
1	C	69	LEU
1	C	76	THR
1	C	78	THR
1	C	99	LEU
1	C	100	THR
1	C	110	MET
1	C	117	ASP
1	C	120	VAL
1	C	145	ASP
1	C	162	GLU
1	C	176	MET
1	C	178	VAL
1	C	193	VAL
1	C	196	THR
1	C	198	ASN
1	C	210	LEU
1	C	211	LEU
1	C	259	VAL
1	C	264	LYS
1	C	268	ASP
1	C	269	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	280	THR
1	C	301	LYS
1	C	302	THR
1	C	311	VAL
1	C	323	LEU
1	C	345	MET
1	C	352	VAL
1	C	372	THR
1	C	373	VAL
1	C	389	ASN
1	C	391	HIS
1	C	397	LYS
1	C	408	GLN
1	C	427	ARG
1	C	435	LEU
1	C	446	ASN
1	C	462	VAL
1	C	468	PHE
1	C	481	PHE
1	C	494	LEU
1	C	518	LEU
1	C	525	SER
1	C	528	THR
1	C	537	LEU
1	C	539	LEU
1	C	542	LEU
1	C	547	VAL
1	D	40	LEU
1	D	41	LYS
1	D	64	ARG
1	D	69	LEU
1	D	74	ASN
1	D	76	THR
1	D	78	THR
1	D	99	LEU
1	D	100	THR
1	D	110	MET
1	D	115	THR
1	D	120	VAL
1	D	133	TYR
1	D	134	GLU
1	D	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	145	ASP
1	D	147	SER
1	D	162	GLU
1	D	178	VAL
1	D	182	THR
1	D	185	GLU
1	D	193	VAL
1	D	198	ASN
1	D	211	LEU
1	D	241	THR
1	D	246	THR
1	D	259	VAL
1	D	264	LYS
1	D	268	ASP
1	D	269	LYS
1	D	311	VAL
1	D	323	LEU
1	D	372	THR
1	D	373	VAL
1	D	389	ASN
1	D	390	THR
1	D	391	HIS
1	D	397	LYS
1	D	408	GLN
1	D	427	ARG
1	D	430	THR
1	D	433	ASP
1	D	435	LEU
1	D	462	VAL
1	D	468	PHE
1	D	481	PHE
1	D	491	LEU
1	D	494	LEU
1	D	518	LEU
1	D	537	LEU
1	D	539	LEU
1	D	542	LEU
1	D	547	VAL
1	D	548	GLN
1	D	549	HIS
1	E	33	ASP
1	E	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	41	LYS
1	E	43	ARG
1	E	69	LEU
1	E	74	ASN
1	E	76	THR
1	E	78	THR
1	E	99	LEU
1	E	101	GLN
1	E	133	TYR
1	E	145	ASP
1	E	162	GLU
1	E	185	GLU
1	E	193	VAL
1	E	196	THR
1	E	211	LEU
1	E	228	ASP
1	E	246	THR
1	E	259	VAL
1	E	268	ASP
1	E	269	LYS
1	E	292	ASN
1	E	311	VAL
1	E	312	ASP
1	E	323	LEU
1	E	352	VAL
1	E	373	VAL
1	E	389	ASN
1	E	391	HIS
1	E	397	LYS
1	E	408	GLN
1	E	427	ARG
1	E	435	LEU
1	E	441	SER
1	E	462	VAL
1	E	468	PHE
1	E	494	LEU
1	E	523	SER
1	E	525	SER
1	E	538	ASP
1	E	543	THR
1	E	547	VAL
1	F	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	41	LYS
1	F	43	ARG
1	F	51	GLN
1	F	69	LEU
1	F	76	THR
1	F	85	LEU
1	F	99	LEU
1	F	100	THR
1	F	110	MET
1	F	115	THR
1	F	132	GLN
1	F	134	GLU
1	F	162	GLU
1	F	182	THR
1	F	185	GLU
1	F	187	ILE
1	F	193	VAL
1	F	198	ASN
1	F	211	LEU
1	F	245	VAL
1	F	252	THR
1	F	259	VAL
1	F	267	THR
1	F	268	ASP
1	F	269	LYS
1	F	280	THR
1	F	287	SER
1	F	292	ASN
1	F	295	SER
1	F	323	LEU
1	F	352	VAL
1	F	373	VAL
1	F	389	ASN
1	F	391	HIS
1	F	397	LYS
1	F	427	ARG
1	F	458	ASP
1	F	462	VAL
1	F	466	SER
1	F	481	PHE
1	F	494	LEU
1	F	518	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	539	LEU
1	F	542	LEU
1	F	547	VAL
1	F	549	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	60	ASN
1	A	87	GLN
1	A	190	ASN
1	A	255	GLN
1	A	324	GLN
1	A	347	ASN
1	A	440	HIS
1	A	535	ASN
1	B	255	GLN
1	B	275	GLN
1	B	324	GLN
1	B	347	ASN
1	B	440	HIS
1	B	546	ASN
1	C	51	GLN
1	C	347	ASN
1	C	353	ASN
1	C	391	HIS
1	C	465	GLN
1	C	492	GLN
1	C	517	HIS
1	C	522	GLN
1	D	324	GLN
1	D	347	ASN
1	D	353	ASN
1	D	391	HIS
1	D	446	ASN
1	D	465	GLN
1	D	492	GLN
1	E	60	ASN
1	E	195	ASN
1	E	347	ASN
1	E	465	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	549	HIS
1	F	51	GLN
1	F	87	GLN
1	F	204	GLN
1	F	255	GLN
1	F	275	GLN
1	F	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

135 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	2,1	14,14,15	0.71	0	17,19,21	1.37	3 (17%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.07	2 (11%)
2	BMA	G	3	2	11,11,12	0.81	0	15,15,17	1.71	2 (13%)
2	MAN	G	4	2	11,11,12	0.58	0	15,15,17	1.33	1 (6%)
2	MAN	G	5	2	11,11,12	0.73	0	15,15,17	2.09	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.78	0	17,19,21	2.11	4 (23%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.85	0
3	BMA	H	3	3	11,11,12	0.73	0	15,15,17	1.82	3 (20%)
3	MAN	H	4	3	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
3	MAN	H	5	3	11,11,12	0.71	0	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	H	6	3	11,11,12	0.67	0	15,15,17	1.54	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.63	0	17,19,21	2.17	5 (29%)
4	NAG	I	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.32	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.72	0	17,19,21	1.73	4 (23%)
2	NAG	J	2	2	14,14,15	0.62	0	17,19,21	2.05	3 (17%)
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	1.30	2 (13%)
2	MAN	J	4	2	11,11,12	0.72	0	15,15,17	1.59	2 (13%)
2	MAN	J	5	2	11,11,12	0.69	0	15,15,17	1.74	1 (6%)
5	NAG	K	1	5,1	14,14,15	0.51	0	17,19,21	2.04	3 (17%)
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.94	0
5	BMA	K	3	5	11,11,12	0.92	0	15,15,17	1.07	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.49	0	17,19,21	1.88	5 (29%)
5	NAG	L	2	5	14,14,15	0.54	0	17,19,21	1.14	2 (11%)
5	BMA	L	3	5	11,11,12	0.63	0	15,15,17	1.92	2 (13%)
2	NAG	M	1	2,1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
2	NAG	M	2	2	14,14,15	0.60	0	17,19,21	1.10	1 (5%)
2	BMA	M	3	2	11,11,12	0.75	0	15,15,17	0.92	1 (6%)
2	MAN	M	4	2	11,11,12	0.70	0	15,15,17	2.65	5 (33%)
2	MAN	M	5	2	11,11,12	0.45	0	15,15,17	1.34	3 (20%)
3	NAG	N	1	3,1	14,14,15	0.69	0	17,19,21	1.53	4 (23%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
3	BMA	N	3	3	11,11,12	0.75	0	15,15,17	1.37	2 (13%)
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	2.08	2 (13%)
3	MAN	N	5	3	11,11,12	0.54	0	15,15,17	1.22	1 (6%)
3	MAN	N	6	3	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.56	0	17,19,21	1.68	3 (17%)
2	NAG	O	2	2	14,14,15	0.74	0	17,19,21	1.28	3 (17%)
2	BMA	O	3	2	11,11,12	0.75	0	15,15,17	1.51	4 (26%)
2	MAN	O	4	2	11,11,12	0.61	0	15,15,17	1.93	5 (33%)
2	MAN	O	5	2	11,11,12	1.67	2 (18%)	15,15,17	2.23	4 (26%)
4	NAG	P	1	4,1	14,14,15	0.56	0	17,19,21	0.96	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.47	0	17,19,21	1.87	4 (23%)
4	NAG	Q	2	4	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	NAG	R	1	6,1	14,14,15	0.73	0	17,19,21	1.61	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	R	2	6	14,14,15	0.62	0	17,19,21	1.21	2 (11%)
6	BMA	R	3	6	11,11,12	0.54	0	15,15,17	0.90	1 (6%)
6	MAN	R	4	6	11,11,12	0.53	0	15,15,17	2.04	4 (26%)
2	NAG	S	1	2,1	14,14,15	0.74	0	17,19,21	1.37	5 (29%)
2	NAG	S	2	2	14,14,15	0.61	0	17,19,21	1.36	3 (17%)
2	BMA	S	3	2	11,11,12	0.56	0	15,15,17	1.77	3 (20%)
2	MAN	S	4	2	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
2	MAN	S	5	2	11,11,12	0.62	0	15,15,17	1.18	1 (6%)
7	NAG	T	1	7,1	14,14,15	0.91	1 (7%)	17,19,21	2.10	7 (41%)
7	NAG	T	2	7	14,14,15	0.44	0	17,19,21	0.94	0
7	BMA	T	3	7	11,11,12	0.58	0	15,15,17	1.80	3 (20%)
7	MAN	T	4	7	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
7	MAN	T	5	7	11,11,12	0.70	0	15,15,17	0.75	0
7	MAN	T	6	7	11,11,12	0.55	0	15,15,17	2.10	1 (6%)
7	MAN	T	7	7	11,11,12	0.75	0	15,15,17	1.72	3 (20%)
2	NAG	U	1	2,1	14,14,15	0.48	0	17,19,21	1.98	2 (11%)
2	NAG	U	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.30	4 (23%)
2	BMA	U	3	2	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
2	MAN	U	4	2	11,11,12	0.77	0	15,15,17	1.43	3 (20%)
2	MAN	U	5	2	11,11,12	0.59	0	15,15,17	1.61	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
4	NAG	V	2	4	14,14,15	1.20	2 (14%)	17,19,21	1.46	2 (11%)
5	NAG	W	1	5,1	14,14,15	1.99	3 (21%)	17,19,21	0.92	0
5	NAG	W	2	5	14,14,15	1.77	3 (21%)	17,19,21	2.25	4 (23%)
5	BMA	W	3	5	11,11,12	2.48	1 (9%)	15,15,17	1.70	4 (26%)
5	NAG	X	1	5,1	14,14,15	0.49	0	17,19,21	1.80	5 (29%)
5	NAG	X	2	5	14,14,15	0.42	0	17,19,21	1.21	2 (11%)
5	BMA	X	3	5	11,11,12	0.66	0	15,15,17	0.88	0
2	NAG	Y	1	2,1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	Y	2	2	14,14,15	0.58	0	17,19,21	1.23	3 (17%)
2	BMA	Y	3	2	11,11,12	0.57	0	15,15,17	1.29	2 (13%)
2	MAN	Y	4	2	11,11,12	0.57	0	15,15,17	1.25	1 (6%)
2	MAN	Y	5	2	11,11,12	0.62	0	15,15,17	1.08	1 (6%)
3	NAG	Z	1	3,1	14,14,15	0.62	0	17,19,21	1.77	3 (17%)
3	NAG	Z	2	3	14,14,15	0.69	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	Z	3	3	11,11,12	0.70	0	15,15,17	1.75	4 (26%)
3	MAN	Z	4	3	11,11,12	0.59	0	15,15,17	1.09	1 (6%)
3	MAN	Z	5	3	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
3	MAN	Z	6	3	11,11,12	1.07	1 (9%)	15,15,17	1.83	3 (20%)
2	NAG	a	1	2,1	14,14,15	0.40	0	17,19,21	1.23	1 (5%)
2	NAG	a	2	2	14,14,15	0.57	0	17,19,21	1.01	2 (11%)
2	BMA	a	3	2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
2	MAN	a	4	2	11,11,12	0.54	0	15,15,17	1.46	1 (6%)
2	MAN	a	5	2	11,11,12	0.60	0	15,15,17	1.53	2 (13%)
4	NAG	b	1	4,1	14,14,15	1.38	2 (14%)	17,19,21	1.66	3 (17%)
4	NAG	b	2	4	14,14,15	0.50	0	17,19,21	0.69	0
5	NAG	c	1	5,1	14,14,15	0.53	0	17,19,21	1.38	2 (11%)
5	NAG	c	2	5	14,14,15	0.54	0	17,19,21	0.82	0
5	BMA	c	3	5	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	d	1	2,1	14,14,15	0.60	0	17,19,21	1.11	1 (5%)
2	NAG	d	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	d	3	2	11,11,12	0.76	0	15,15,17	1.91	4 (26%)
2	MAN	d	4	2	11,11,12	0.59	0	15,15,17	0.61	0
2	MAN	d	5	2	11,11,12	0.54	0	15,15,17	1.38	1 (6%)
7	NAG	e	1	7,1	14,14,15	0.56	0	17,19,21	1.08	1 (5%)
7	NAG	e	2	7	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
7	BMA	e	3	7	11,11,12	0.61	0	15,15,17	1.41	4 (26%)
7	MAN	e	4	7	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	MAN	e	5	7	11,11,12	0.55	0	15,15,17	0.98	1 (6%)
7	MAN	e	6	7	11,11,12	0.70	0	15,15,17	1.54	2 (13%)
7	MAN	e	7	7	11,11,12	0.52	0	15,15,17	1.52	1 (6%)
2	NAG	f	1	2,1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
2	NAG	f	2	2	14,14,15	0.50	0	17,19,21	0.95	0
2	BMA	f	3	2	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
2	MAN	f	4	2	11,11,12	0.56	0	15,15,17	1.34	1 (6%)
2	MAN	f	5	2	11,11,12	0.56	0	15,15,17	1.37	1 (6%)
4	NAG	g	1	4,1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
4	NAG	g	2	4	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
5	NAG	h	1	5,1	14,14,15	0.60	0	17,19,21	1.68	4 (23%)
5	NAG	h	2	5	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
5	BMA	h	3	5	11,11,12	0.86	0	15,15,17	1.78	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	i	1	2,1	14,14,15	0.60	0	17,19,21	0.96	0
2	NAG	i	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	i	3	2	11,11,12	0.64	0	15,15,17	1.31	3 (20%)
2	MAN	i	4	2	11,11,12	0.64	0	15,15,17	1.79	3 (20%)
2	MAN	i	5	2	11,11,12	0.49	0	15,15,17	1.57	1 (6%)
3	NAG	j	1	3,1	14,14,15	0.63	0	17,19,21	1.49	3 (17%)
3	NAG	j	2	3	14,14,15	0.75	0	17,19,21	1.50	2 (11%)
3	BMA	j	3	3	11,11,12	0.78	0	15,15,17	0.90	2 (13%)
3	MAN	j	4	3	11,11,12	1.19	1 (9%)	15,15,17	1.42	2 (13%)
3	MAN	j	5	3	11,11,12	0.94	1 (9%)	15,15,17	0.92	1 (6%)
3	MAN	j	6	3	11,11,12	0.58	0	15,15,17	1.55	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
2	NAG	k	2	2	14,14,15	0.55	0	17,19,21	1.07	2 (11%)
2	BMA	k	3	2	11,11,12	0.69	0	15,15,17	1.22	1 (6%)
2	MAN	k	4	2	11,11,12	0.66	0	15,15,17	0.87	1 (6%)
2	MAN	k	5	2	11,11,12	1.57	1 (9%)	15,15,17	1.70	2 (13%)
5	NAG	l	1	5,1	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
5	NAG	l	2	5	14,14,15	0.57	0	17,19,21	1.52	4 (23%)
5	BMA	l	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.98	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
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	1/1/1/1
3	NAG	H	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	5/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	MAN	J	4	2	-	2/2/19/22	0/1/1/1
2	MAN	J	5	2	-	1/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	NAG	L	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	MAN	M	4	2	-	1/2/19/22	0/1/1/1
2	MAN	M	5	2	-	1/2/19/22	1/1/1/1
3	NAG	N	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1
3	MAN	N	6	3	-	2/2/19/22	0/1/1/1
2	NAG	O	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	2/2/19/22	0/1/1/1
2	MAN	O	5	2	-	2/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
6	NAG	R	1	6,1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	R	2	6	-	1/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	j	1	3,1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	j	2	3	-	5/6/23/26	0/1/1/1
3	BMA	j	3	3	-	2/2/19/22	0/1/1/1
3	MAN	j	4	3	-	2/2/19/22	0/1/1/1
3	MAN	j	5	3	-	1/2/19/22	0/1/1/1
3	MAN	j	6	3	-	2/2/19/22	0/1/1/1
2	NAG	k	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	k	2	2	-	5/6/23/26	0/1/1/1
2	BMA	k	3	2	-	0/2/19/22	0/1/1/1
2	MAN	k	4	2	-	2/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	1/1/1/1
5	NAG	l	1	5,1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
5	BMA	l	3	5	-	2/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	O6-C6	7.78	1.75	1.42
2	k	5	MAN	O6-C6	4.89	1.63	1.42
5	l	3	BMA	O6-C6	4.81	1.62	1.42
5	W	1	NAG	C8-C7	4.59	1.60	1.50
5	W	2	NAG	C8-C7	4.54	1.60	1.50
5	W	1	NAG	O7-C7	4.47	1.33	1.23
4	b	1	NAG	C8-C7	4.04	1.58	1.50
2	O	5	MAN	O6-C6	3.83	1.58	1.42
3	j	4	MAN	O6-C6	3.54	1.57	1.42
5	W	2	NAG	O7-C7	3.40	1.30	1.23
2	O	5	MAN	C2-C3	3.17	1.57	1.52
5	W	1	NAG	O6-C6	3.11	1.55	1.42
5	W	2	NAG	C7-N2	2.91	1.43	1.34
3	Z	6	MAN	O6-C6	2.83	1.54	1.42
4	V	2	NAG	O7-C7	2.61	1.29	1.23
3	j	5	MAN	O6-C6	2.61	1.53	1.42
4	V	2	NAG	C8-C7	2.60	1.55	1.50
4	b	1	NAG	O7-C7	2.54	1.28	1.23
4	I	2	NAG	C1-C2	2.52	1.55	1.52
5	l	3	BMA	C4-C3	2.52	1.58	1.52
7	T	1	NAG	O5-C1	-2.13	1.40	1.43
2	U	2	NAG	O7-C7	2.02	1.27	1.23

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MAN	C1-O5-C5	7.27	121.93	112.19
2	M	4	MAN	C1-O5-C5	7.15	121.77	112.19
2	O	5	MAN	C1-O5-C5	6.84	121.35	112.19
2	U	1	NAG	C1-O5-C5	6.74	121.22	112.19
7	T	6	MAN	C1-O5-C5	6.61	121.04	112.19
2	J	2	NAG	C2-N2-C7	6.51	131.63	122.90
3	N	4	MAN	C1-O5-C5	6.43	120.80	112.19
5	W	2	NAG	C2-N2-C7	-6.34	114.40	122.90
2	J	5	MAN	C1-O5-C5	6.17	120.46	112.19
7	e	7	MAN	C1-O5-C5	5.58	119.67	112.19
2	k	5	MAN	C1-O5-C5	5.50	119.56	112.19
6	R	4	MAN	C1-O5-C5	5.45	119.48	112.19
5	L	3	BMA	C1-O5-C5	5.30	119.29	112.19
2	i	5	MAN	C1-O5-C5	5.30	119.29	112.19
3	H	1	NAG	C2-N2-C7	5.22	129.90	122.90
4	Q	1	NAG	C2-N2-C7	5.13	129.77	122.90
7	T	1	NAG	O5-C1-C2	-5.10	103.40	111.29
5	L	1	NAG	C1-O5-C5	4.95	118.81	112.19
3	Z	1	NAG	C2-N2-C7	4.91	129.48	122.90
2	M	4	MAN	C3-C4-C5	4.85	119.03	110.23
2	O	1	NAG	C1-O5-C5	4.84	118.67	112.19
5	K	1	NAG	C2-N2-C7	4.84	129.38	122.90
2	d	5	MAN	C1-O5-C5	4.81	118.63	112.19
3	Z	6	MAN	C1-C2-C3	4.81	116.64	109.64
2	d	3	BMA	C1-C2-C3	4.76	116.58	109.64
4	b	1	NAG	C2-N2-C7	4.75	129.27	122.90
4	I	1	NAG	O5-C1-C2	-4.69	104.04	111.29
2	i	4	MAN	C1-O5-C5	4.65	118.42	112.19
6	R	1	NAG	O5-C1-C2	-4.63	104.13	111.29
3	j	6	MAN	C1-O5-C5	4.54	118.27	112.19
5	W	2	NAG	O7-C7-N2	-4.54	113.95	121.98
4	I	1	NAG	C4-C3-C2	4.54	117.67	111.02
7	T	4	MAN	C1-O5-C5	4.52	118.25	112.19
5	X	1	NAG	O5-C1-C2	-4.47	104.38	111.29
2	S	3	BMA	C1-C2-C3	4.44	116.11	109.64
3	j	4	MAN	C1-O5-C5	4.42	118.11	112.19
2	J	1	NAG	C1-O5-C5	4.36	118.03	112.19
5	K	1	NAG	C1-C2-N2	4.34	117.28	110.43
5	L	3	BMA	C1-C2-C3	4.34	115.96	109.64
3	Z	3	BMA	O3-C3-C2	4.28	118.79	110.05
2	G	3	BMA	C3-C4-C5	4.28	117.99	110.23
3	H	1	NAG	O5-C1-C2	-4.25	104.72	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	4	MAN	C1-C2-C3	-4.22	103.50	109.64
2	U	5	MAN	C1-O5-C5	4.17	117.78	112.19
2	f	5	MAN	C1-O5-C5	4.16	117.76	112.19
3	j	1	NAG	O5-C1-C2	-4.16	104.86	111.29
5	h	1	NAG	C1-O5-C5	4.15	117.75	112.19
2	a	1	NAG	C1-O5-C5	4.15	117.75	112.19
4	V	2	NAG	C4-C3-C2	4.14	117.09	111.02
7	T	3	BMA	O3-C3-C2	4.09	118.40	110.05
2	a	5	MAN	C1-O5-C5	4.06	117.63	112.19
3	H	3	BMA	O3-C3-C2	4.05	118.32	110.05
2	G	4	MAN	C1-O5-C5	4.03	117.59	112.19
2	f	4	MAN	C1-O5-C5	4.02	117.57	112.19
2	O	4	MAN	C1-C2-C3	-4.01	103.81	109.64
7	T	7	MAN	C3-C4-C5	3.98	117.45	110.23
3	N	1	NAG	O5-C1-C2	-3.93	105.21	111.29
2	k	1	NAG	C1-O5-C5	3.93	117.45	112.19
4	I	2	NAG	C2-N2-C7	3.83	128.03	122.90
7	e	6	MAN	C3-C4-C5	3.79	117.10	110.23
2	i	4	MAN	C3-C4-C5	3.79	117.10	110.23
3	j	2	NAG	C4-C3-C2	3.78	116.56	111.02
5	c	1	NAG	O5-C1-C2	-3.75	105.50	111.29
2	J	4	MAN	C1-C2-C3	-3.74	104.20	109.64
5	h	3	BMA	C3-C4-C5	3.69	116.93	110.23
2	i	2	NAG	C1-O5-C5	3.67	117.11	112.19
3	N	4	MAN	C3-C4-C5	3.63	116.81	110.23
3	N	5	MAN	C1-O5-C5	3.60	117.01	112.19
2	O	3	BMA	O3-C3-C2	-3.60	102.71	110.05
4	Q	1	NAG	O5-C1-C2	-3.59	105.73	111.29
5	W	3	BMA	O6-C6-C5	-3.58	99.13	111.33
2	S	3	BMA	O5-C5-C6	3.57	114.61	107.66
2	U	4	MAN	C1-C2-C3	-3.53	104.50	109.64
7	T	3	BMA	C1-O5-C5	3.51	116.89	112.19
5	X	2	NAG	C1-O5-C5	3.48	116.85	112.19
3	H	3	BMA	O3-C3-C4	3.47	118.56	110.38
5	K	1	NAG	O5-C1-C2	-3.46	105.94	111.29
3	N	3	BMA	O3-C3-C2	3.45	117.10	110.05
2	J	3	BMA	C1-C2-C3	3.44	114.66	109.64
2	O	1	NAG	C2-N2-C7	-3.42	118.31	122.90
6	R	4	MAN	C1-C2-C3	3.42	114.62	109.64
2	Y	4	MAN	C3-C4-C5	3.41	116.42	110.23
5	h	3	BMA	C1-C2-C3	3.39	114.58	109.64
3	H	6	MAN	C3-C4-C5	3.37	116.34	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	5	MAN	C1-O5-C5	3.36	116.69	112.19
7	e	4	MAN	C1-O5-C5	3.35	116.68	112.19
5	h	3	BMA	C2-C3-C4	3.35	116.75	110.86
5	W	3	BMA	C1-C2-C3	3.32	114.48	109.64
2	G	3	BMA	C1-C2-C3	3.30	114.45	109.64
2	S	2	NAG	O4-C4-C3	-3.28	102.65	110.38
4	I	1	NAG	C2-N2-C7	3.27	127.29	122.90
2	d	3	BMA	C2-C3-C4	3.27	116.61	110.86
3	j	6	MAN	C1-C2-C3	3.26	114.40	109.64
4	b	1	NAG	C1-C2-N2	3.24	115.55	110.43
4	V	1	NAG	C1-O5-C5	3.24	116.53	112.19
2	f	1	NAG	C4-C3-C2	3.22	115.74	111.02
2	O	4	MAN	C1-O5-C5	3.21	116.49	112.19
3	j	2	NAG	C2-N2-C7	3.21	127.20	122.90
3	Z	4	MAN	C1-O5-C5	3.21	116.49	112.19
3	Z	1	NAG	C1-O5-C5	3.20	116.47	112.19
2	S	4	MAN	C3-C4-C5	3.18	115.99	110.23
5	l	2	NAG	C1-O5-C5	3.17	116.44	112.19
5	X	1	NAG	C8-C7-N2	3.17	121.38	116.12
2	J	2	NAG	C8-C7-N2	3.17	121.38	116.12
2	k	3	BMA	C3-C4-C5	3.17	115.97	110.23
3	H	3	BMA	C3-C4-C5	-3.14	104.53	110.23
7	T	1	NAG	C2-N2-C7	3.13	127.09	122.90
2	U	5	MAN	C3-C4-C5	3.11	115.87	110.23
2	a	5	MAN	C3-C4-C5	3.09	115.84	110.23
2	M	2	NAG	C1-O5-C5	3.09	116.33	112.19
2	S	2	NAG	C2-N2-C7	-3.09	118.76	122.90
3	H	5	MAN	C1-O5-C5	3.06	116.29	112.19
2	Y	2	NAG	C1-O5-C5	3.04	116.26	112.19
2	O	5	MAN	C3-C4-C5	3.02	115.72	110.23
5	W	2	NAG	O7-C7-C8	3.01	127.42	122.05
2	O	4	MAN	C3-C4-C5	3.00	115.68	110.23
2	G	1	NAG	C1-O5-C5	2.98	116.18	112.19
2	d	3	BMA	C3-C4-C5	2.98	115.63	110.23
3	Z	6	MAN	C2-C3-C4	2.97	116.08	110.86
2	U	1	NAG	C2-N2-C7	-2.97	118.92	122.90
2	J	2	NAG	O5-C1-C2	-2.94	106.75	111.29
4	Q	2	NAG	C1-O5-C5	2.93	116.12	112.19
5	h	1	NAG	C2-N2-C7	2.92	126.82	122.90
7	T	7	MAN	O5-C1-C2	-2.92	103.82	110.79
2	U	2	NAG	C1-C2-N2	2.92	115.03	110.43
5	L	1	NAG	C3-C4-C5	-2.91	104.95	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	6	MAN	C1-O5-C5	2.90	116.08	112.19
4	g	2	NAG	C4-C3-C2	2.90	115.27	111.02
7	e	6	MAN	C1-O5-C5	2.88	116.04	112.19
7	e	2	NAG	C1-O5-C5	2.86	116.02	112.19
2	J	1	NAG	O5-C5-C6	2.85	113.20	107.66
2	M	4	MAN	O5-C5-C4	2.84	117.74	110.83
5	l	2	NAG	O5-C1-C2	-2.84	106.90	111.29
7	e	5	MAN	C1-O5-C5	2.83	115.98	112.19
7	e	3	BMA	O3-C3-C2	2.81	115.79	110.05
5	K	3	BMA	C1-C2-C3	2.80	113.72	109.64
3	Z	3	BMA	C3-C4-C5	-2.80	105.15	110.23
3	H	4	MAN	C1-O5-C5	2.80	115.94	112.19
5	X	1	NAG	C3-C4-C5	-2.77	105.22	110.23
7	T	1	NAG	C4-C3-C2	2.76	115.06	111.02
5	l	2	NAG	C2-N2-C7	-2.75	119.21	122.90
3	j	5	MAN	C1-O5-C5	2.74	115.86	112.19
7	T	3	BMA	O3-C3-C4	2.73	116.82	110.38
2	i	3	BMA	C1-O5-C5	2.72	115.83	112.19
2	S	5	MAN	C1-C2-C3	-2.70	105.71	109.64
2	k	2	NAG	C4-C3-C2	2.70	114.97	111.02
5	h	2	NAG	C4-C3-C2	2.70	114.97	111.02
2	J	4	MAN	O2-C2-C1	2.69	115.39	109.22
2	M	4	MAN	O5-C1-C2	2.69	117.20	110.79
2	a	3	BMA	O3-C3-C2	-2.68	104.58	110.05
4	I	1	NAG	C8-C7-N2	2.68	120.56	116.12
4	b	1	NAG	O5-C1-C2	-2.66	107.18	111.29
5	L	1	NAG	O5-C1-C2	-2.66	107.18	111.29
7	T	1	NAG	C3-C4-C5	-2.64	105.45	110.23
5	l	1	NAG	C1-O5-C5	2.64	115.72	112.19
2	d	1	NAG	O5-C1-C2	-2.64	107.21	111.29
5	L	2	NAG	C1-O5-C5	2.63	115.72	112.19
2	a	3	BMA	O3-C3-C4	2.63	116.57	110.38
3	Z	6	MAN	C1-O5-C5	2.62	115.70	112.19
3	Z	3	BMA	O3-C3-C4	2.62	116.55	110.38
3	Z	5	MAN	C1-O5-C5	2.61	115.69	112.19
7	e	3	BMA	C1-C2-C3	-2.61	105.85	109.64
2	O	2	NAG	O7-C7-N2	2.60	126.58	121.98
6	R	4	MAN	C3-C4-C5	2.60	114.95	110.23
7	e	4	MAN	C1-C2-C3	2.58	113.40	109.64
2	i	3	BMA	C1-C2-C3	2.58	113.40	109.64
4	Q	1	NAG	C1-O5-C5	2.58	115.64	112.19
2	M	4	MAN	C2-C3-C4	2.58	115.39	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	2.58	115.64	112.19
5	h	1	NAG	C8-C7-N2	2.57	120.38	116.12
2	O	2	NAG	C4-C3-C2	2.57	114.78	111.02
2	i	3	BMA	C3-C4-C5	2.57	114.89	110.23
3	j	1	NAG	C2-N2-C7	2.56	126.33	122.90
5	X	1	NAG	O7-C7-C8	-2.56	117.50	122.05
3	H	6	MAN	O5-C1-C2	-2.55	104.71	110.79
2	O	5	MAN	C1-C2-C3	2.55	113.35	109.64
2	J	3	BMA	O3-C3-C2	-2.54	104.86	110.05
3	Z	3	BMA	C1-O5-C5	2.54	115.59	112.19
2	Y	3	BMA	C1-C2-C3	2.52	113.32	109.64
2	S	1	NAG	O7-C7-C8	-2.52	117.57	122.05
2	U	3	BMA	O3-C3-C2	-2.51	104.92	110.05
7	T	1	NAG	C6-C5-C4	2.50	119.15	113.02
2	O	4	MAN	O2-C2-C1	2.49	114.93	109.22
2	J	1	NAG	C1-C2-N2	2.49	114.36	110.43
6	R	4	MAN	O5-C5-C6	2.49	112.50	107.66
2	k	5	MAN	C1-C2-C3	2.48	113.25	109.64
3	j	1	NAG	C8-C7-N2	2.47	120.22	116.12
2	Y	3	BMA	O5-C5-C6	2.46	112.45	107.66
6	R	2	NAG	O4-C4-C3	-2.46	104.58	110.38
5	W	3	BMA	C2-C3-C4	2.45	115.16	110.86
2	M	5	MAN	C2-C3-C4	-2.44	106.57	110.86
2	a	2	NAG	O5-C1-C2	-2.44	107.52	111.29
2	U	3	BMA	C1-C2-C3	2.44	113.19	109.64
2	S	1	NAG	O5-C1-C2	-2.43	107.53	111.29
2	O	3	BMA	O3-C3-C4	2.43	116.11	110.38
2	O	1	NAG	O5-C5-C6	2.42	112.37	107.66
3	H	1	NAG	C8-C7-N2	2.41	120.12	116.12
2	Y	1	NAG	O5-C1-C2	-2.41	107.56	111.29
7	T	1	NAG	C8-C7-N2	2.39	120.08	116.12
2	f	1	NAG	C3-C4-C5	2.38	114.56	110.23
7	e	1	NAG	O5-C1-C2	-2.36	107.64	111.29
2	f	1	NAG	C1-C2-N2	-2.35	106.72	110.43
7	e	3	BMA	O3-C3-C4	2.35	115.92	110.38
4	g	1	NAG	C2-N2-C7	2.34	126.04	122.90
2	U	2	NAG	O5-C1-C2	-2.34	107.67	111.29
2	G	1	NAG	C6-C5-C4	-2.34	107.28	113.02
5	l	2	NAG	C4-C3-C2	-2.34	107.59	111.02
2	U	2	NAG	C1-O5-C5	2.32	115.30	112.19
3	N	1	NAG	C2-N2-C7	2.32	126.01	122.90
2	G	5	MAN	O5-C5-C6	2.31	112.16	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	4	MAN	C3-C4-C5	2.31	114.42	110.23
5	c	1	NAG	C8-C7-N2	2.30	119.93	116.12
5	X	1	NAG	C1-O5-C5	2.30	115.26	112.19
4	V	2	NAG	C3-C4-C5	2.30	114.39	110.23
2	k	2	NAG	C2-N2-C7	2.29	125.97	122.90
2	G	2	NAG	O5-C1-C2	-2.29	107.75	111.29
2	S	1	NAG	C4-C3-C2	2.28	114.36	111.02
2	S	2	NAG	C1-O5-C5	2.28	115.25	112.19
7	T	1	NAG	O5-C5-C4	-2.28	105.28	110.83
4	g	1	NAG	C1-C2-N2	2.28	114.02	110.43
5	W	3	BMA	C1-O5-C5	2.27	115.23	112.19
2	M	5	MAN	O5-C5-C6	2.26	112.07	107.66
6	R	2	NAG	C1-O5-C5	-2.26	109.16	112.19
2	Y	5	MAN	C3-C4-C5	2.26	114.33	110.23
3	N	6	MAN	C1-O5-C5	2.26	115.21	112.19
3	Z	2	NAG	C1-O5-C5	2.25	115.21	112.19
4	P	2	NAG	C3-C4-C5	2.22	114.27	110.23
5	L	1	NAG	O7-C7-C8	-2.22	118.09	122.05
3	Z	1	NAG	O5-C1-C2	-2.22	107.86	111.29
5	h	1	NAG	O7-C7-C8	-2.22	118.11	122.05
5	X	2	NAG	O5-C1-C2	-2.22	107.86	111.29
2	O	5	MAN	O5-C5-C4	2.21	116.21	110.83
2	M	3	BMA	C1-O5-C5	2.21	115.15	112.19
4	Q	1	NAG	C1-C2-N2	2.20	113.89	110.43
2	J	1	NAG	C2-N2-C7	-2.20	119.96	122.90
2	U	2	NAG	C2-N2-C7	2.20	125.84	122.90
2	i	4	MAN	O5-C5-C4	2.19	116.14	110.83
2	Y	2	NAG	O4-C4-C3	-2.18	105.25	110.38
5	L	2	NAG	O5-C1-C2	-2.16	107.96	111.29
7	T	7	MAN	C2-C3-C4	2.15	114.65	110.86
3	N	3	BMA	O3-C3-C4	2.15	115.45	110.38
3	j	3	BMA	C1-O5-C5	2.14	115.06	112.19
6	R	3	BMA	C1-C2-C3	2.14	112.76	109.64
2	O	3	BMA	O5-C5-C6	2.13	111.81	107.66
2	d	3	BMA	O5-C5-C6	2.13	111.81	107.66
2	k	4	MAN	O5-C5-C6	2.12	111.79	107.66
4	I	1	NAG	O4-C4-C3	-2.12	105.38	110.38
2	O	3	BMA	C3-C4-C5	2.09	114.03	110.23
2	U	4	MAN	O2-C2-C1	2.09	114.01	109.22
2	a	2	NAG	C3-C4-C5	2.09	114.02	110.23
3	j	4	MAN	C3-C4-C5	2.08	114.00	110.23
3	N	1	NAG	C8-C7-N2	2.07	119.56	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	O5-C1-C2	-2.07	108.08	111.29
5	c	3	BMA	C1-O5-C5	2.06	114.95	112.19
7	e	2	NAG	C3-C4-C5	2.06	113.97	110.23
3	H	1	NAG	C3-C4-C5	-2.06	106.50	110.23
6	R	1	NAG	C2-N2-C7	-2.06	120.15	122.90
2	O	2	NAG	C8-C7-N2	-2.05	112.72	116.12
3	N	1	NAG	C1-O5-C5	2.05	114.93	112.19
2	f	3	BMA	O3-C3-C2	-2.05	105.87	110.05
4	I	2	NAG	C4-C3-C2	2.05	114.02	111.02
3	j	3	BMA	C1-C2-C3	2.04	112.61	109.64
5	W	2	NAG	C1-O5-C5	2.04	114.92	112.19
2	O	4	MAN	O3-C3-C2	-2.04	105.90	110.05
3	N	2	NAG	C2-N2-C7	2.03	125.62	122.90
2	U	4	MAN	O5-C5-C6	2.03	111.61	107.66
2	S	1	NAG	C1-C2-N2	2.03	113.63	110.43
2	S	4	MAN	C1-C2-C3	-2.03	106.69	109.64
2	S	3	BMA	O3-C3-C2	-2.03	105.92	110.05
7	e	3	BMA	C1-O5-C5	2.03	114.90	112.19
2	S	1	NAG	O4-C4-C3	-2.01	105.63	110.38
2	M	1	NAG	O7-C7-C8	-2.01	118.47	122.05
2	Y	2	NAG	C4-C3-C2	2.01	113.96	111.02
5	L	1	NAG	O4-C4-C5	2.00	114.25	109.32

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	a	1	NAG	C1
2	f	1	NAG	C1
3	H	1	NAG	C1
3	N	1	NAG	C1
3	Z	1	NAG	C1
3	j	1	NAG	C1
4	b	1	NAG	C1
5	L	1	NAG	C1
5	X	1	NAG	C1
5	c	1	NAG	C1
5	h	1	NAG	C1
5	l	1	NAG	C1
6	R	1	NAG	C1
7	T	1	NAG	C1
7	e	1	NAG	C1

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
2	k	1	NAG	C8-C7-N2-C2
2	k	1	NAG	O7-C7-N2-C2
2	k	2	NAG	C3-C2-N2-C7
2	k	2	NAG	C8-C7-N2-C2
2	k	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	Q	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C1-C2-N2-C7
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	c	1	NAG	C8-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
2	J	4	MAN	C4-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	U	4	MAN	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
2	U	4	MAN	C4-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
3	Z	6	MAN	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
2	G	4	MAN	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	d	4	MAN	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	e	4	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	S	3	BMA	O5-C5-C6-O6
2	a	5	MAN	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	d	5	MAN	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
3	j	3	BMA	O5-C5-C6-O6
5	h	3	BMA	O5-C5-C6-O6
2	a	2	NAG	C4-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
2	Y	3	BMA	O5-C5-C6-O6
7	T	7	MAN	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
2	Y	4	MAN	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	f	5	MAN	C4-C5-C6-O6
3	Z	6	MAN	C4-C5-C6-O6
3	N	6	MAN	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	k	4	MAN	O5-C5-C6-O6
7	T	6	MAN	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	d	5	MAN	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
7	e	6	MAN	O5-C5-C6-O6
2	d	3	BMA	C4-C5-C6-O6
3	N	6	MAN	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
3	j	3	BMA	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	j	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	T	1	NAG	C8-C7-N2-C2
2	S	3	BMA	C4-C5-C6-O6
2	Y	3	BMA	C4-C5-C6-O6
2	Y	4	MAN	C4-C5-C6-O6
2	d	4	MAN	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
2	O	5	MAN	C4-C5-C6-O6
2	i	4	MAN	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
2	k	4	MAN	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
5	l	3	BMA	C4-C5-C6-O6
7	T	6	MAN	C4-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
2	U	5	MAN	C4-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
7	e	7	MAN	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	j	4	MAN	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	a	4	MAN	O5-C5-C6-O6
3	j	6	MAN	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
3	Z	5	MAN	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
2	f	5	MAN	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
3	j	4	MAN	O5-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	h	3	BMA	C4-C5-C6-O6
7	e	4	MAN	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
2	a	3	BMA	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
2	U	3	BMA	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	a	5	MAN	C4-C5-C6-O6
2	f	3	BMA	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	M	4	MAN	O5-C5-C6-O6
5	l	3	BMA	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	Z	5	MAN	O5-C5-C6-O6
7	T	7	MAN	C4-C5-C6-O6
2	i	2	NAG	C8-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
2	O	4	MAN	O5-C5-C6-O6
2	S	5	MAN	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	M	5	MAN	O5-C5-C6-O6
4	P	2	NAG	O7-C7-N2-C2
2	Y	5	MAN	O5-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
2	U	5	MAN	O5-C5-C6-O6
5	W	1	NAG	O7-C7-N2-C2
2	i	5	MAN	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
5	l	1	NAG	C8-C7-N2-C2
2	J	2	NAG	C3-C2-N2-C7
2	f	4	MAN	O5-C5-C6-O6
2	S	4	MAN	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
2	i	2	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	c	2	NAG	C8-C7-N2-C2
2	G	3	BMA	O5-C5-C6-O6
2	f	3	BMA	O5-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
5	l	1	NAG	O7-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
2	a	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
4	P	1	NAG	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
3	j	2	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
7	e	7	MAN	C4-C5-C6-O6
2	a	3	BMA	C4-C5-C6-O6
3	j	5	MAN	C4-C5-C6-O6
3	j	6	MAN	C4-C5-C6-O6
5	K	2	NAG	O7-C7-N2-C2
2	i	2	NAG	C1-C2-N2-C7
4	b	1	NAG	C1-C2-N2-C7
2	G	5	MAN	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
2	O	4	MAN	C4-C5-C6-O6
7	e	6	MAN	C4-C5-C6-O6
2	U	3	BMA	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6

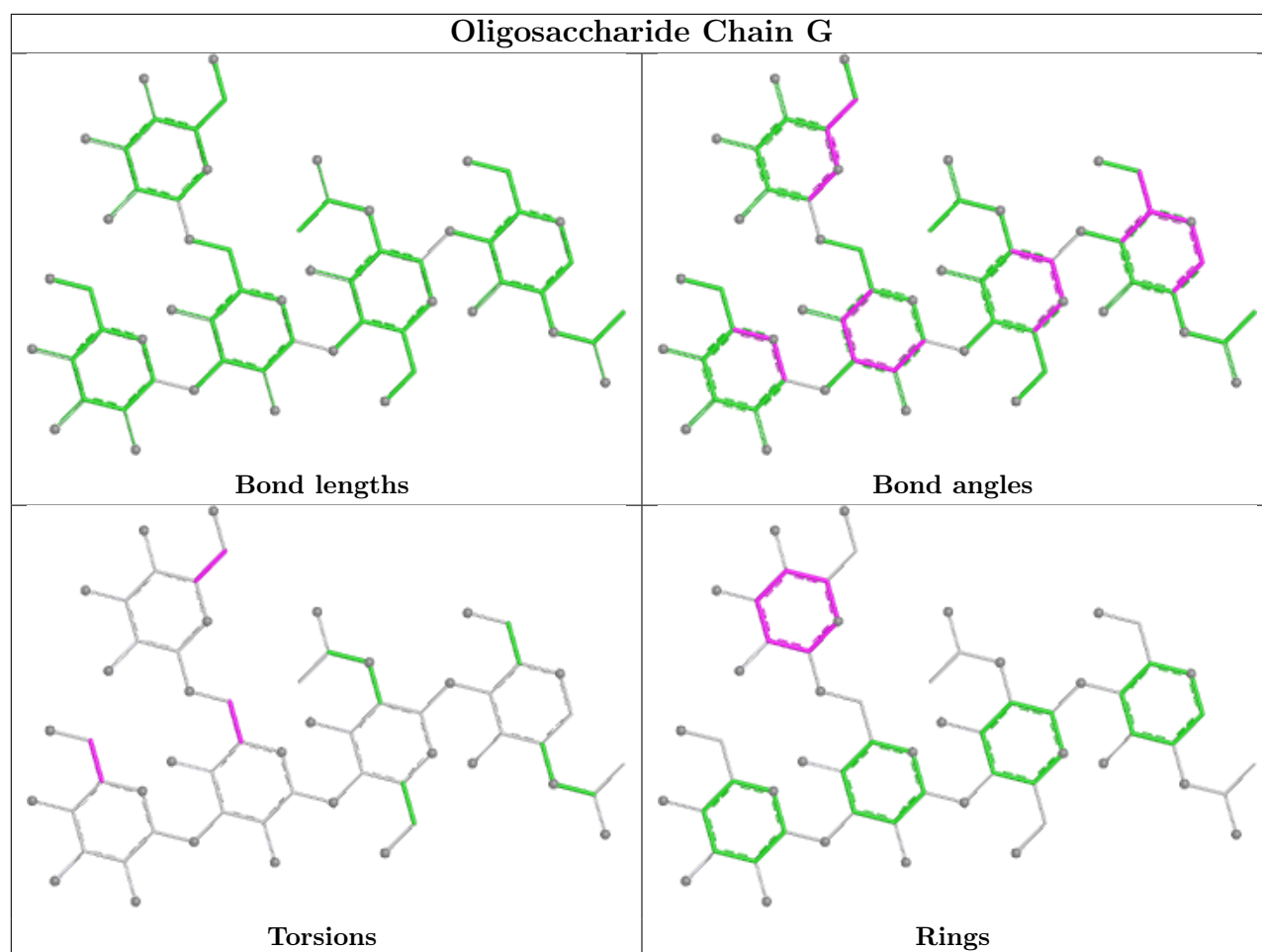
All (5) ring outliers are listed below:

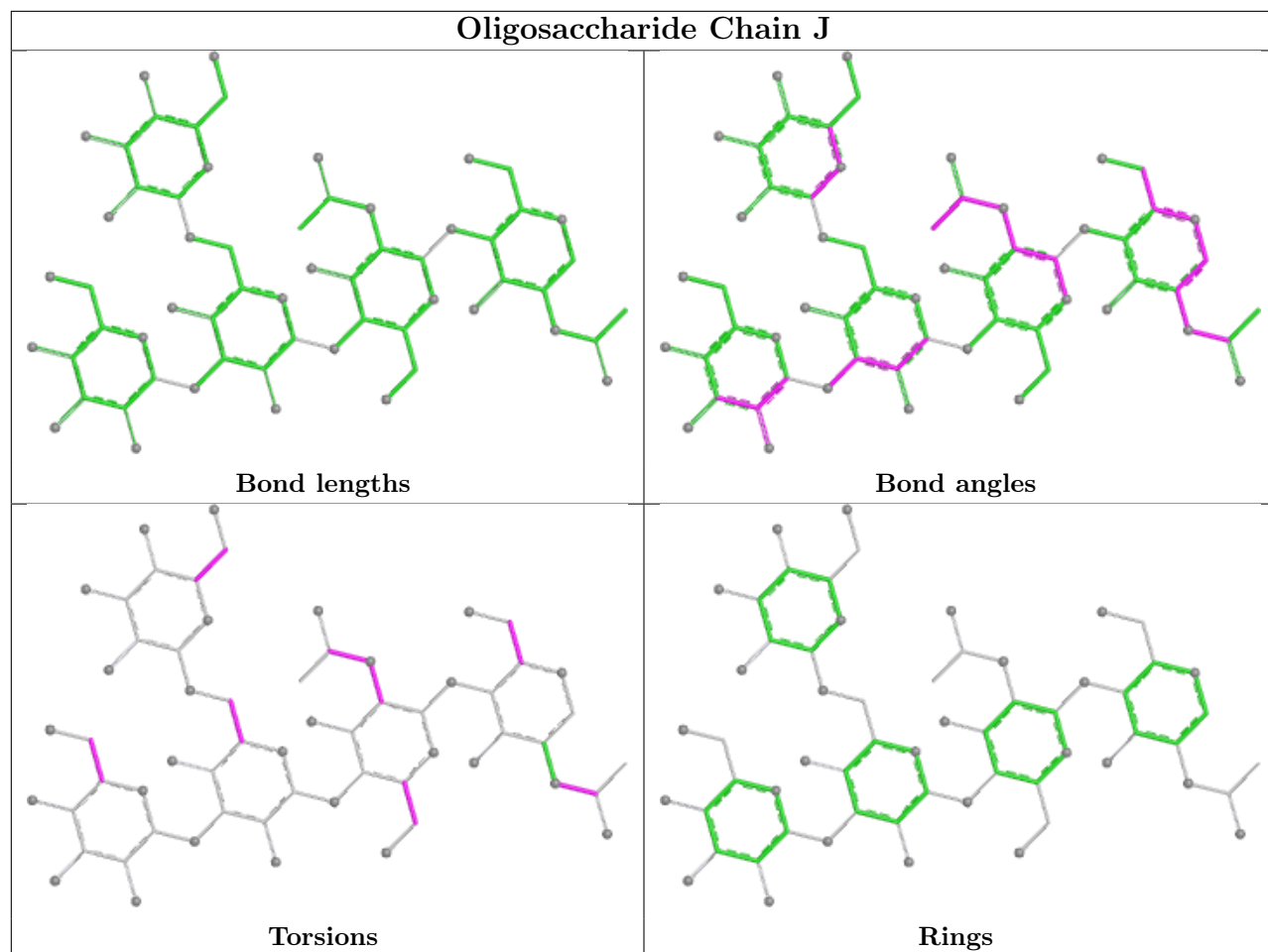
Mol	Chain	Res	Type	Atoms
2	G	5	MAN	C1-C2-C3-C4-C5-O5
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	f	4	MAN	C1-C2-C3-C4-C5-O5
2	i	5	MAN	C1-C2-C3-C4-C5-O5
2	M	5	MAN	C1-C2-C3-C4-C5-O5

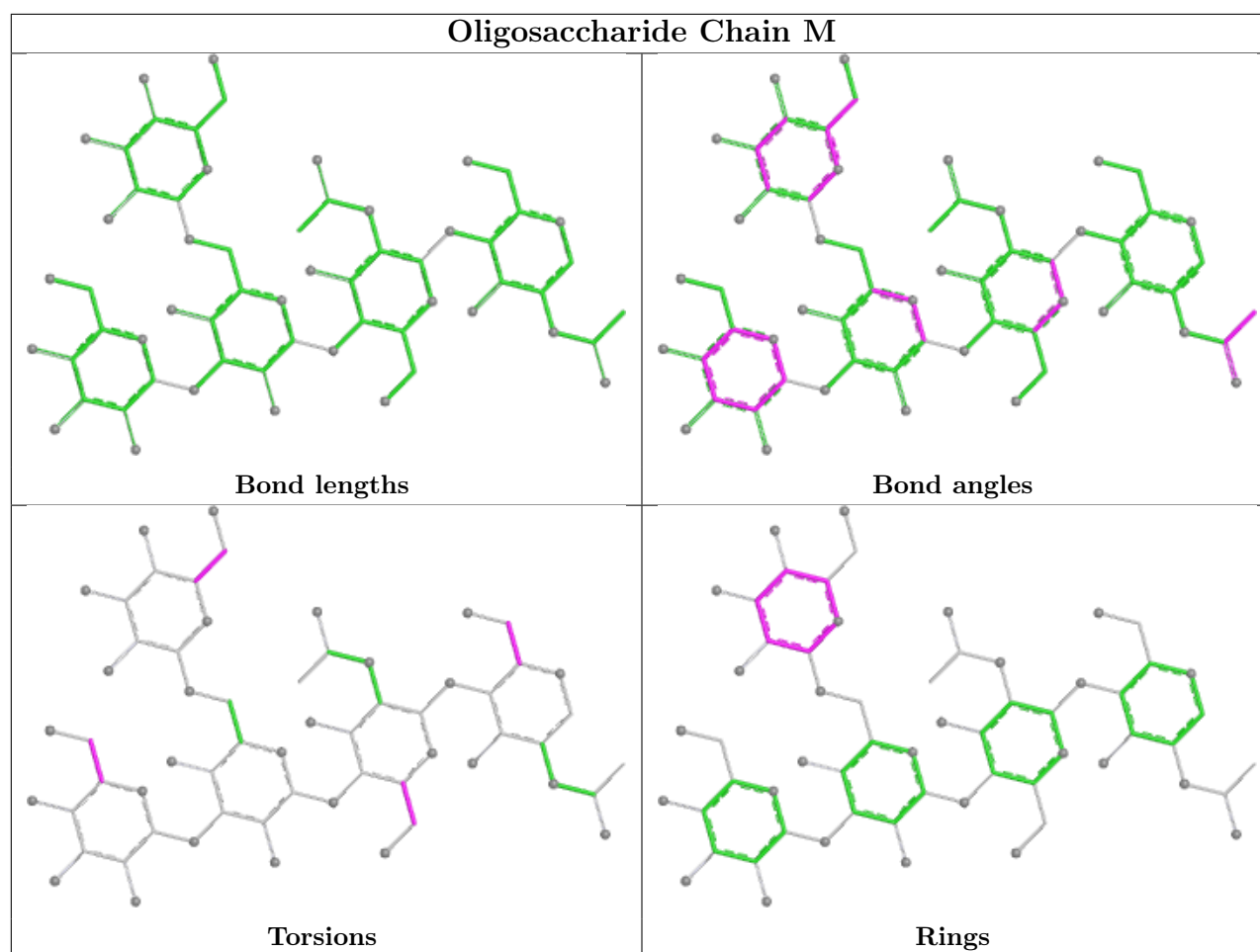
21 monomers are involved in 23 short contacts:

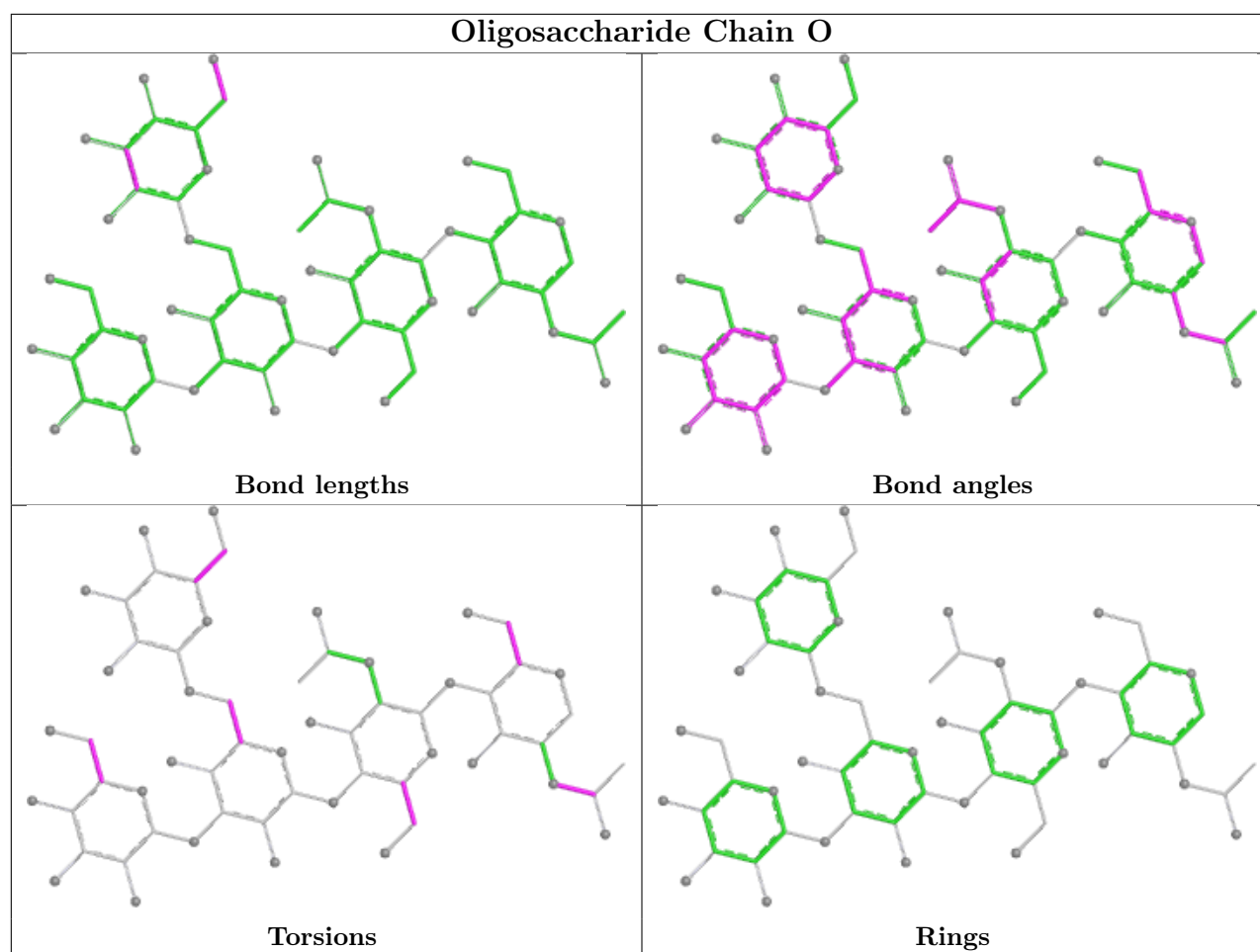
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	BMA	1	0
3	j	1	NAG	1	0
2	G	4	MAN	1	0
2	J	2	NAG	1	0
3	N	1	NAG	1	0
5	W	2	NAG	1	0
4	I	1	NAG	2	0
7	e	1	NAG	1	0
5	L	1	NAG	2	0
2	S	2	NAG	1	0
5	W	3	BMA	2	0
2	Y	2	NAG	1	0
2	Y	5	MAN	1	0
2	k	1	NAG	1	0
7	e	2	NAG	2	0
2	d	1	NAG	1	0
2	f	1	NAG	1	0
7	T	1	NAG	1	0
5	X	1	NAG	1	0
2	O	1	NAG	1	0
5	h	1	NAG	1	0

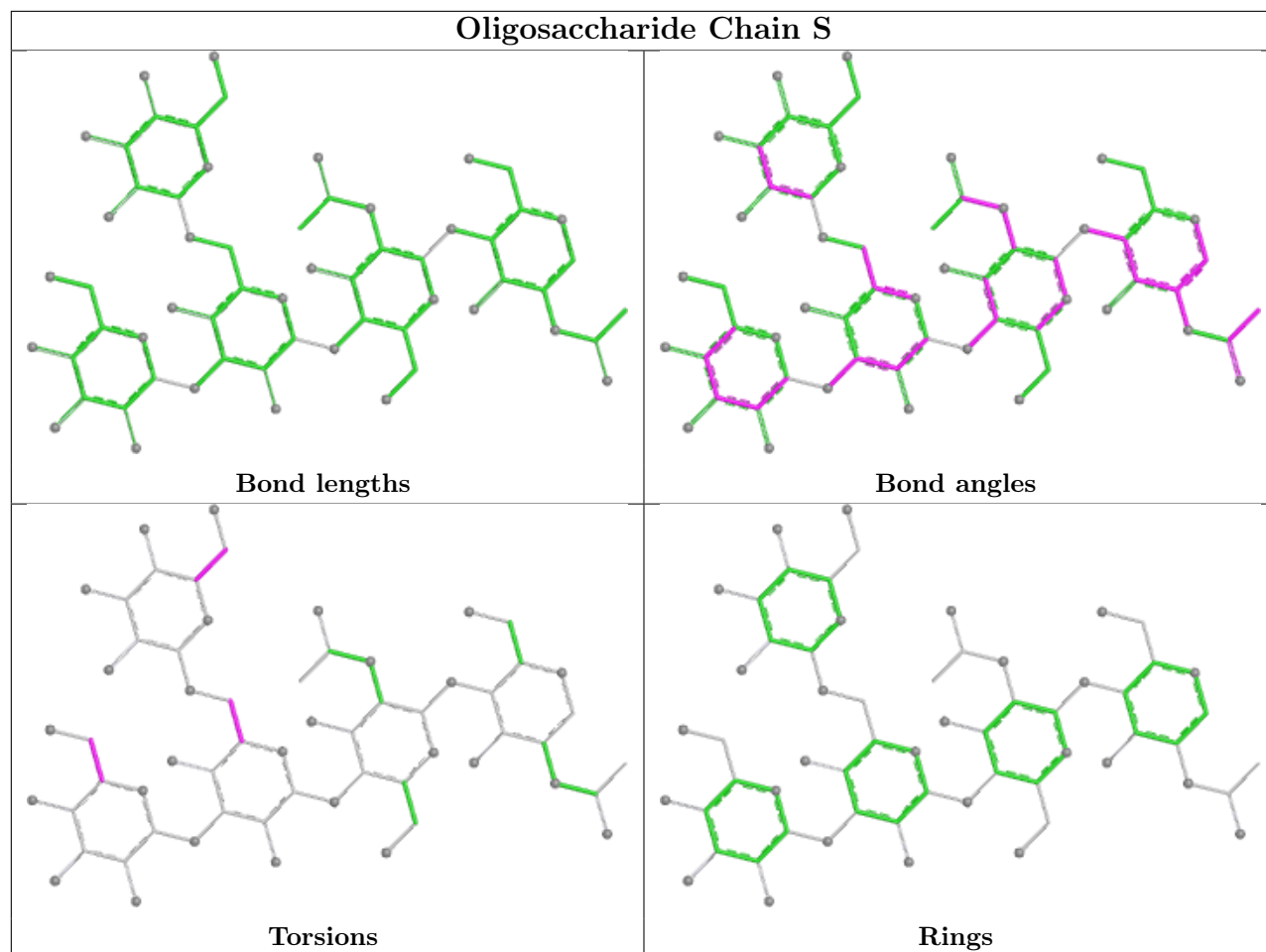
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

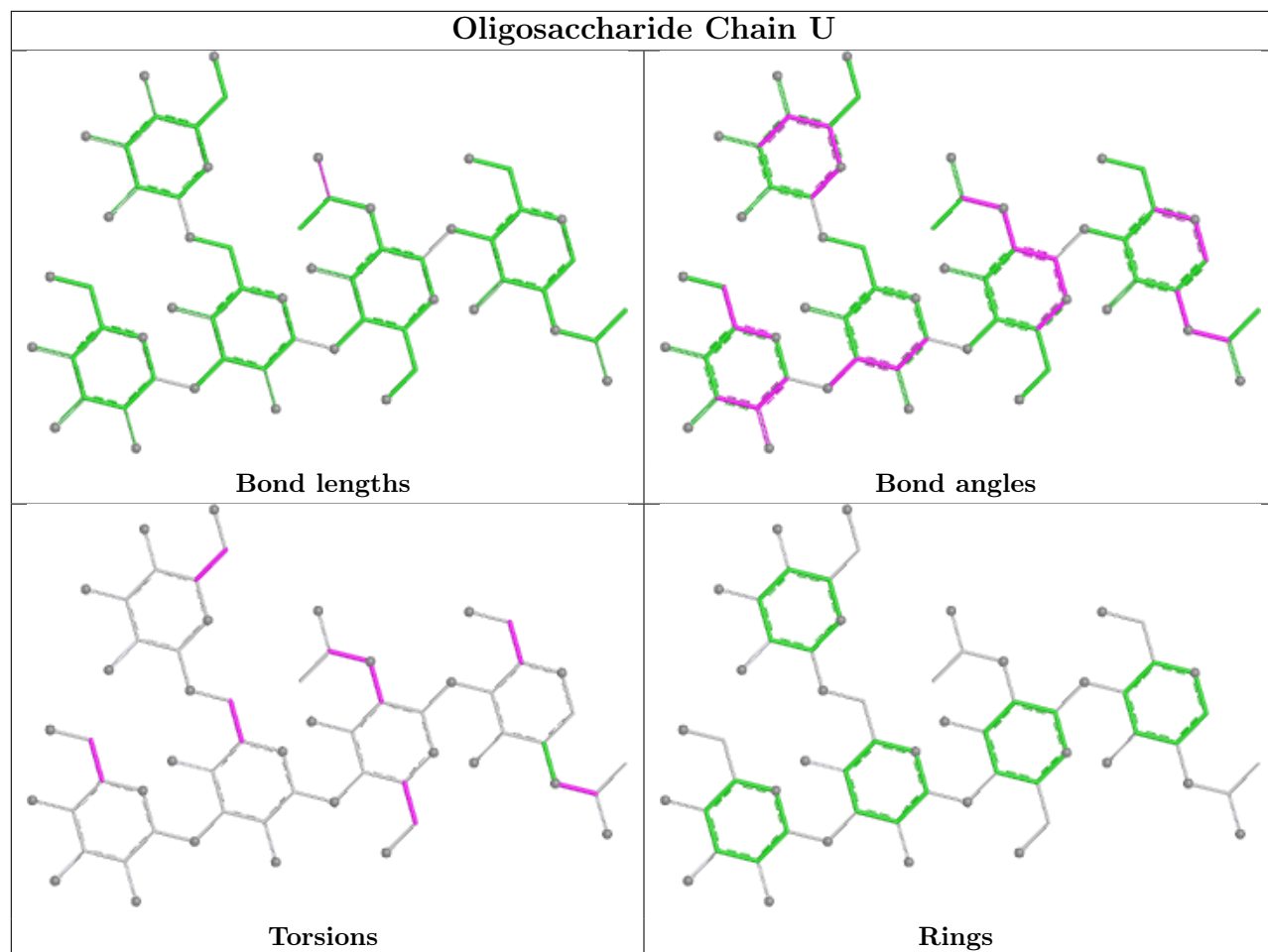


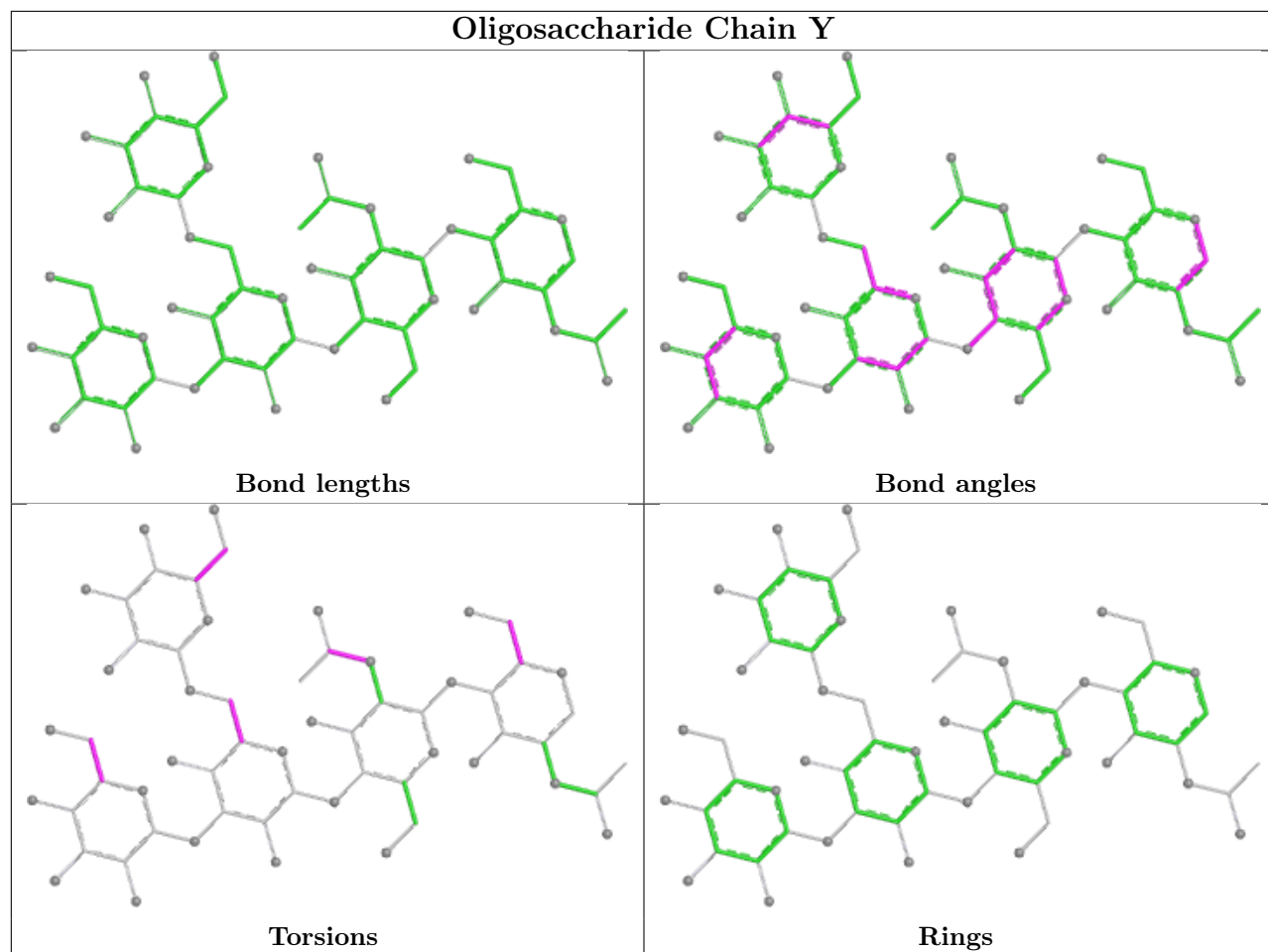


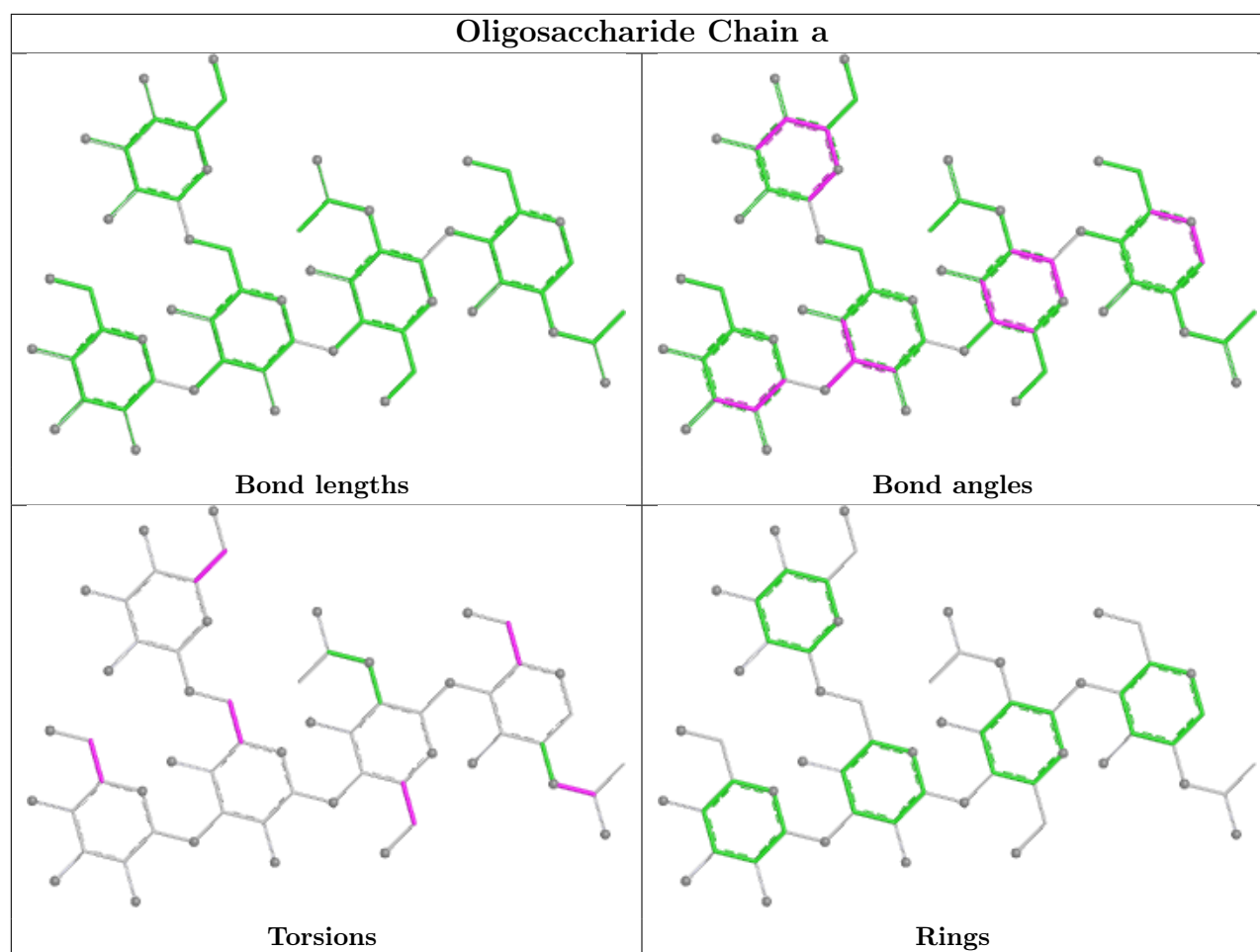


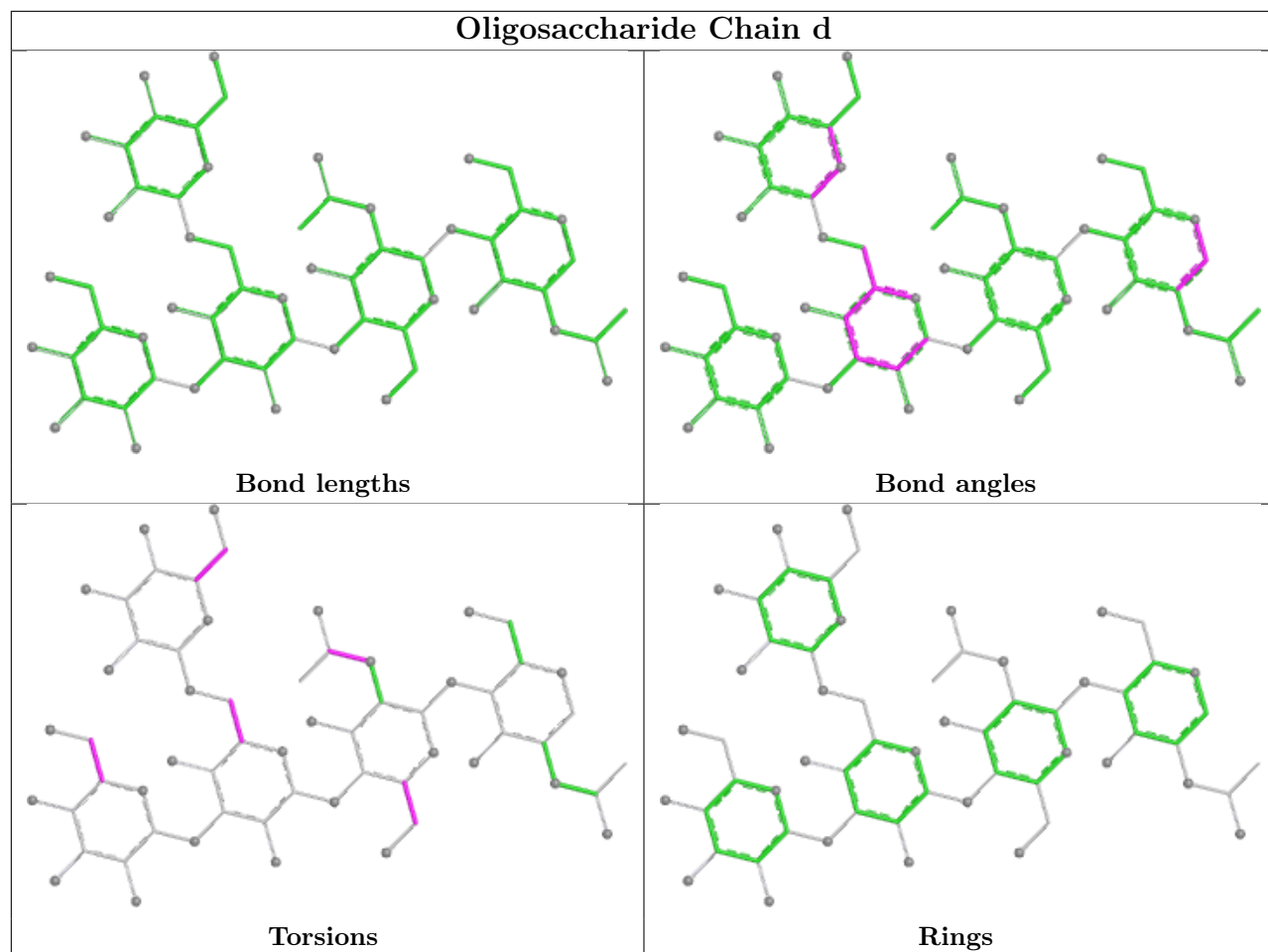


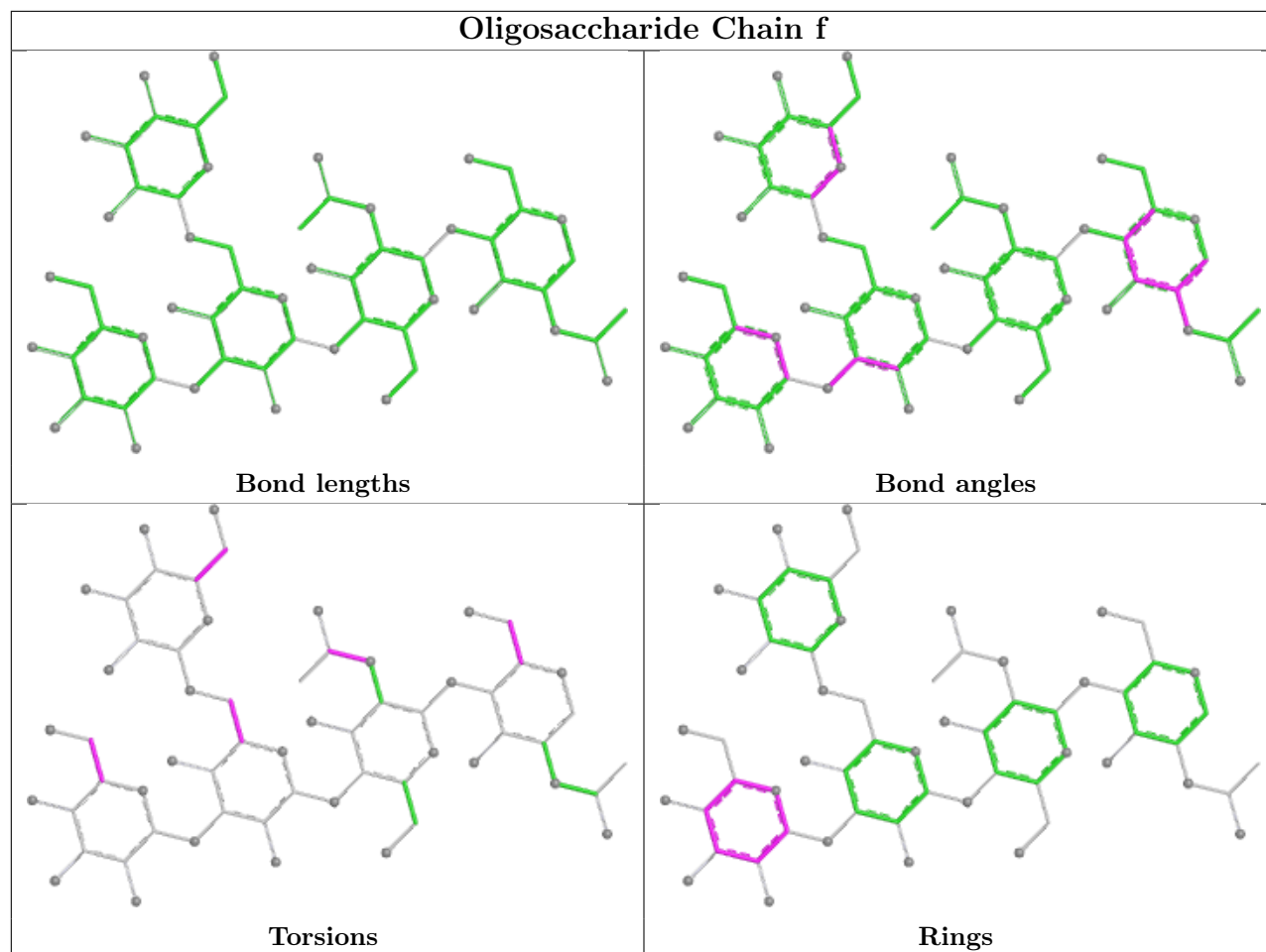


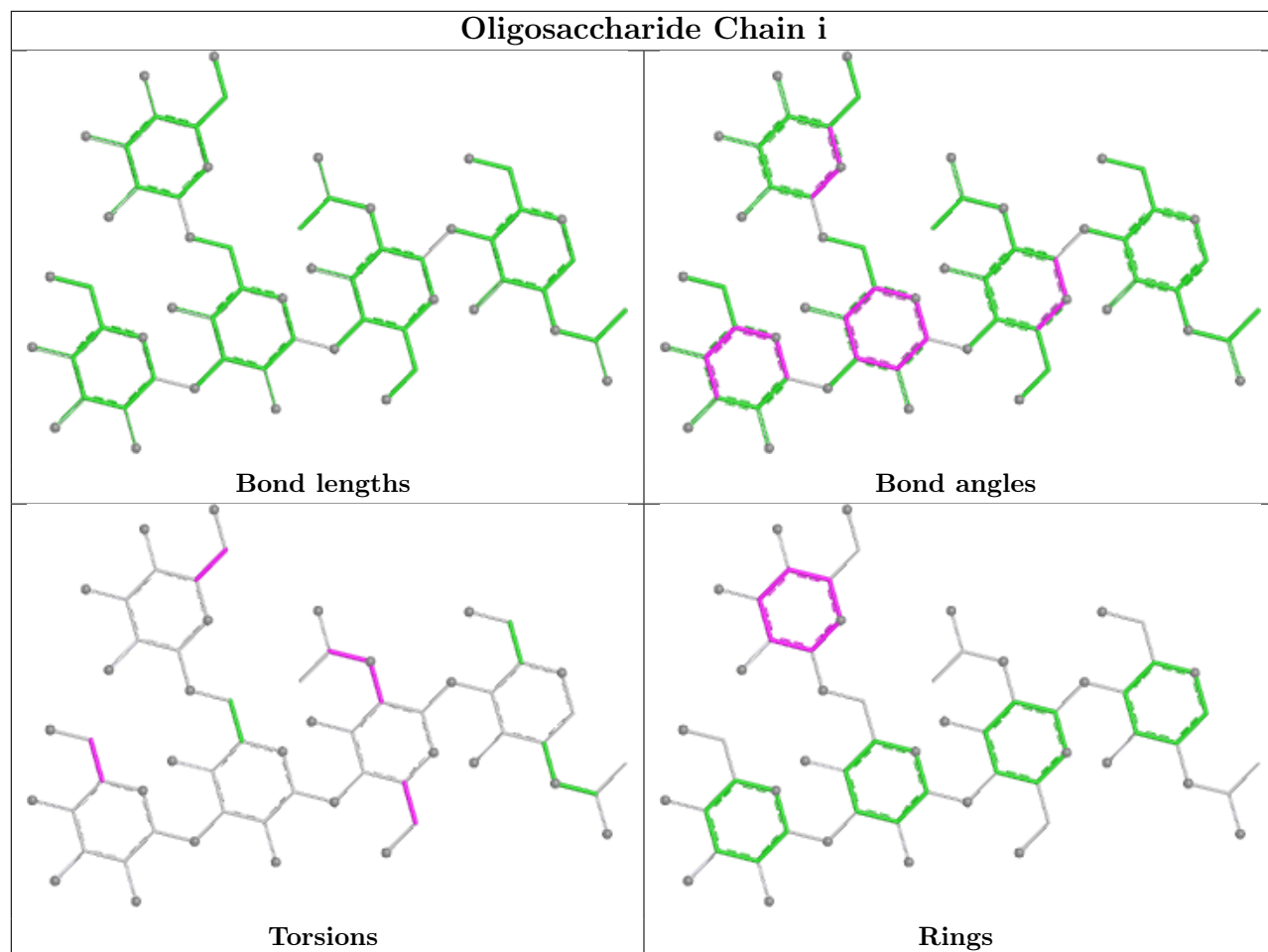


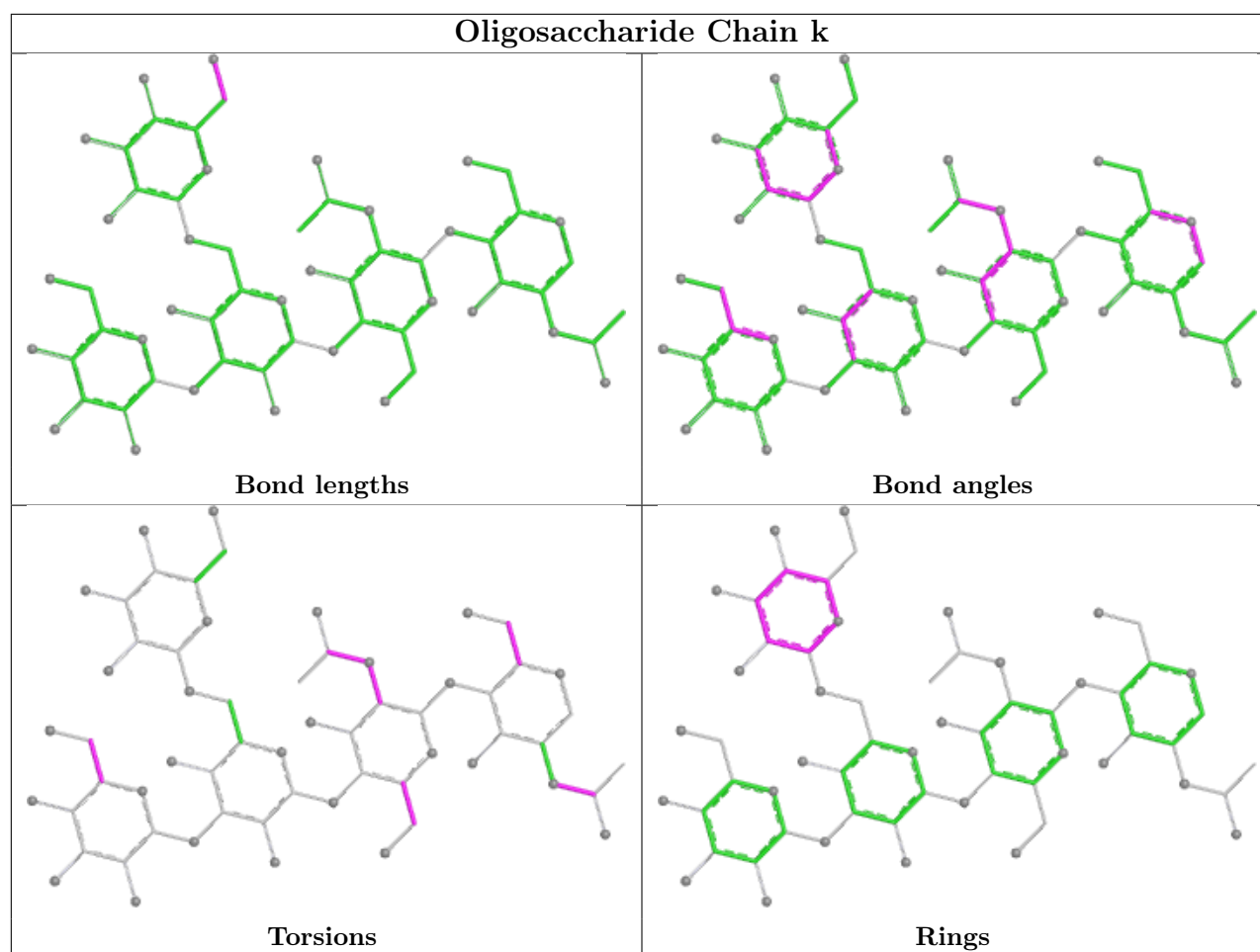


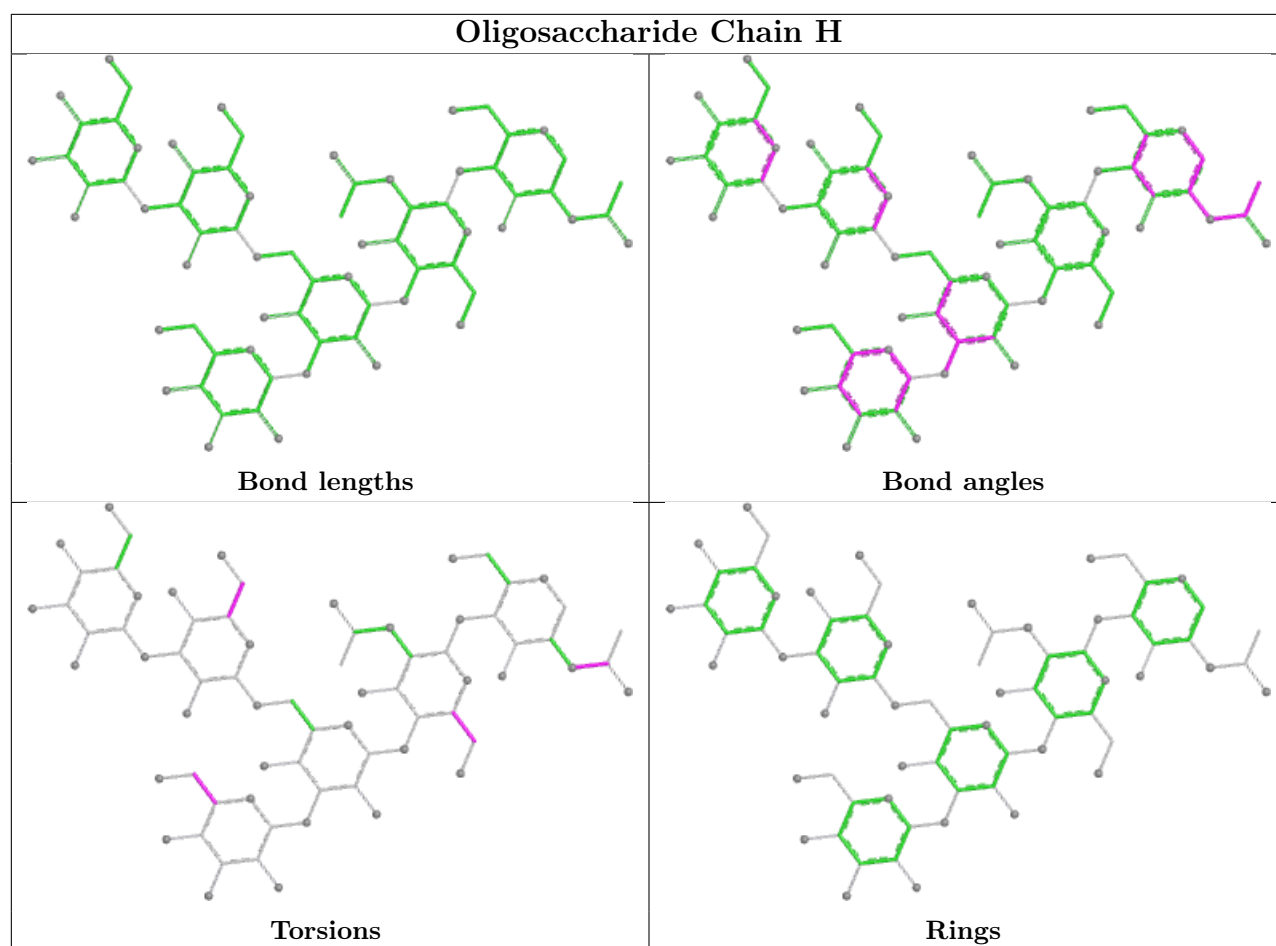


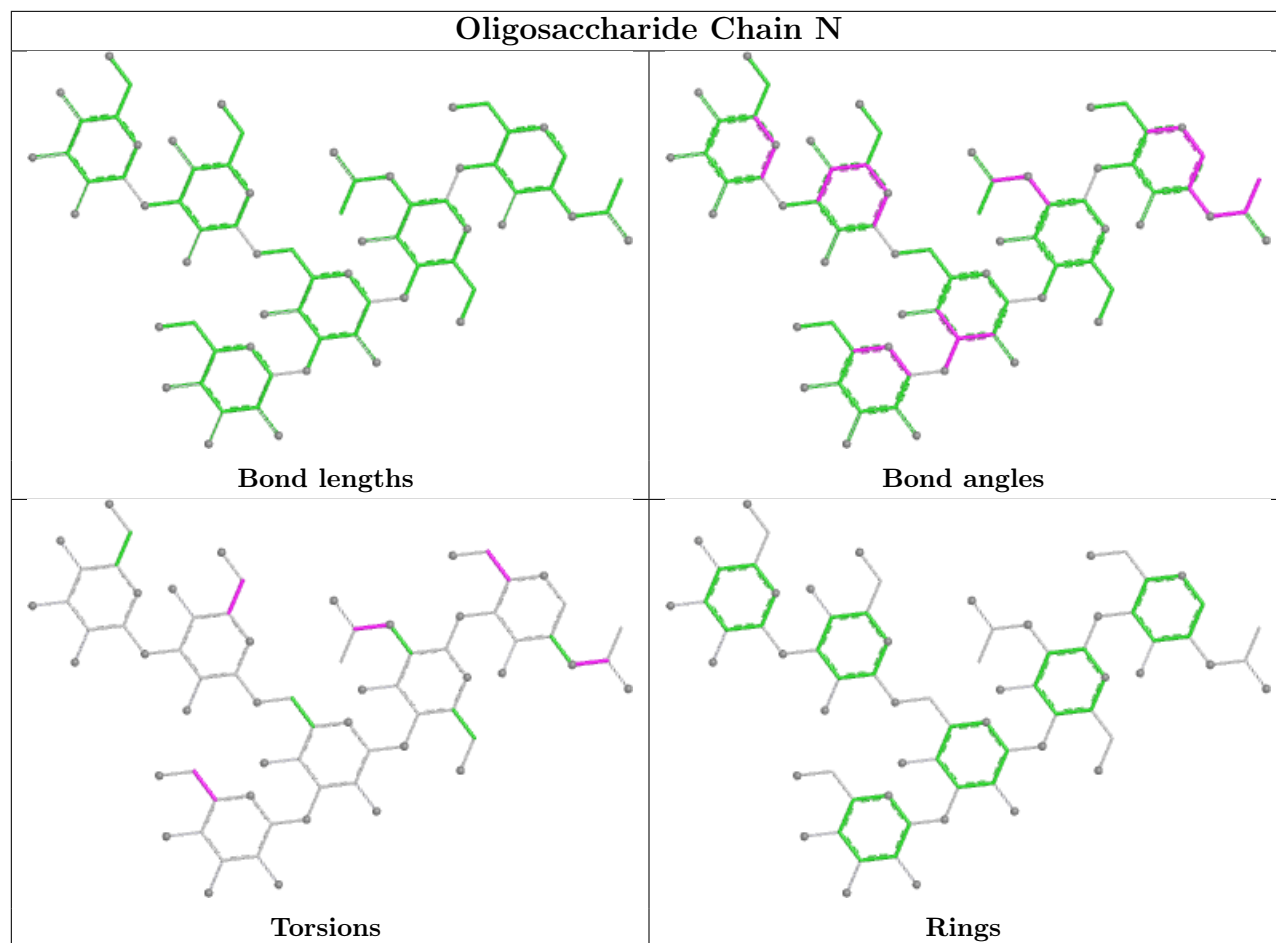


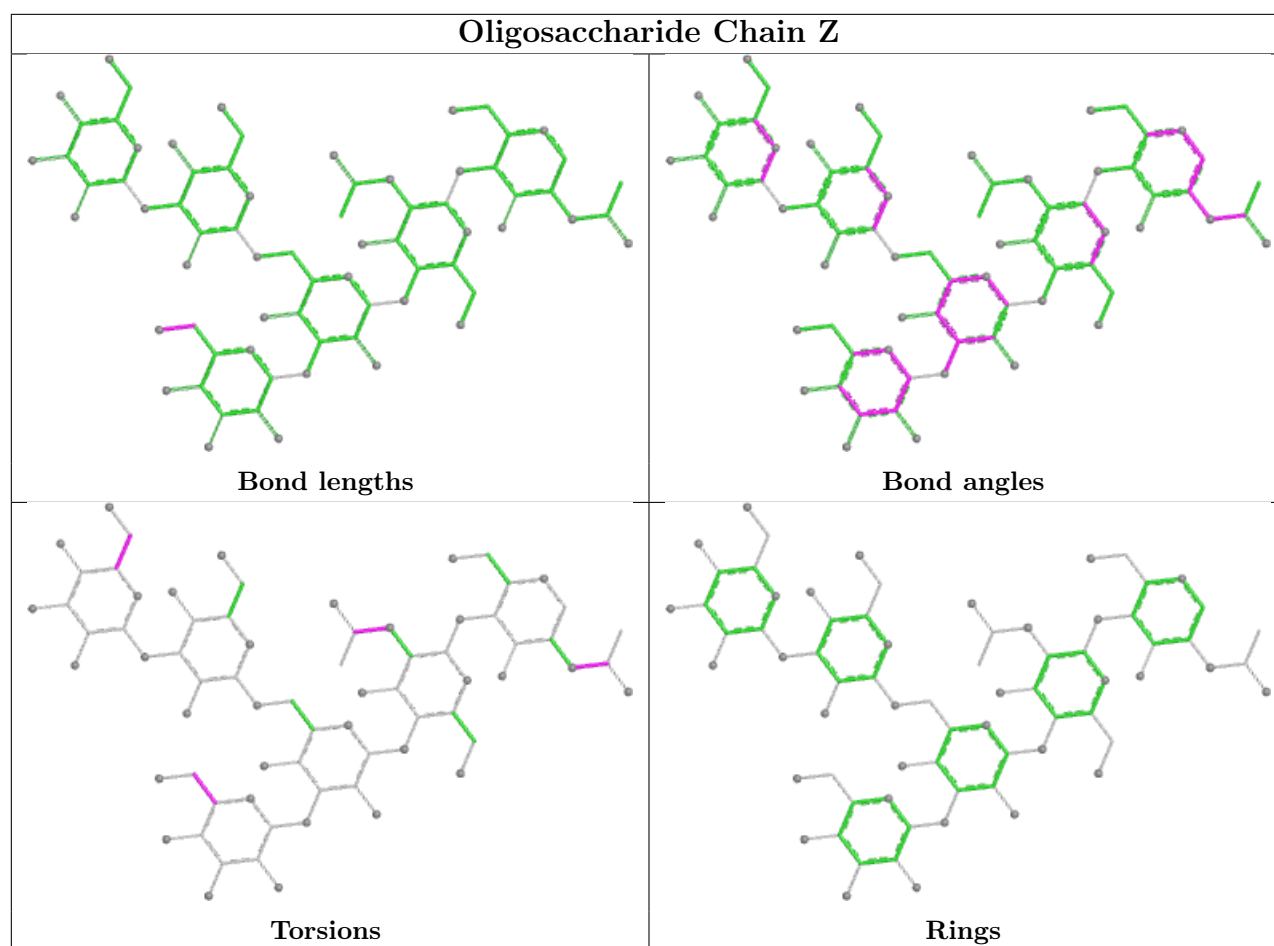


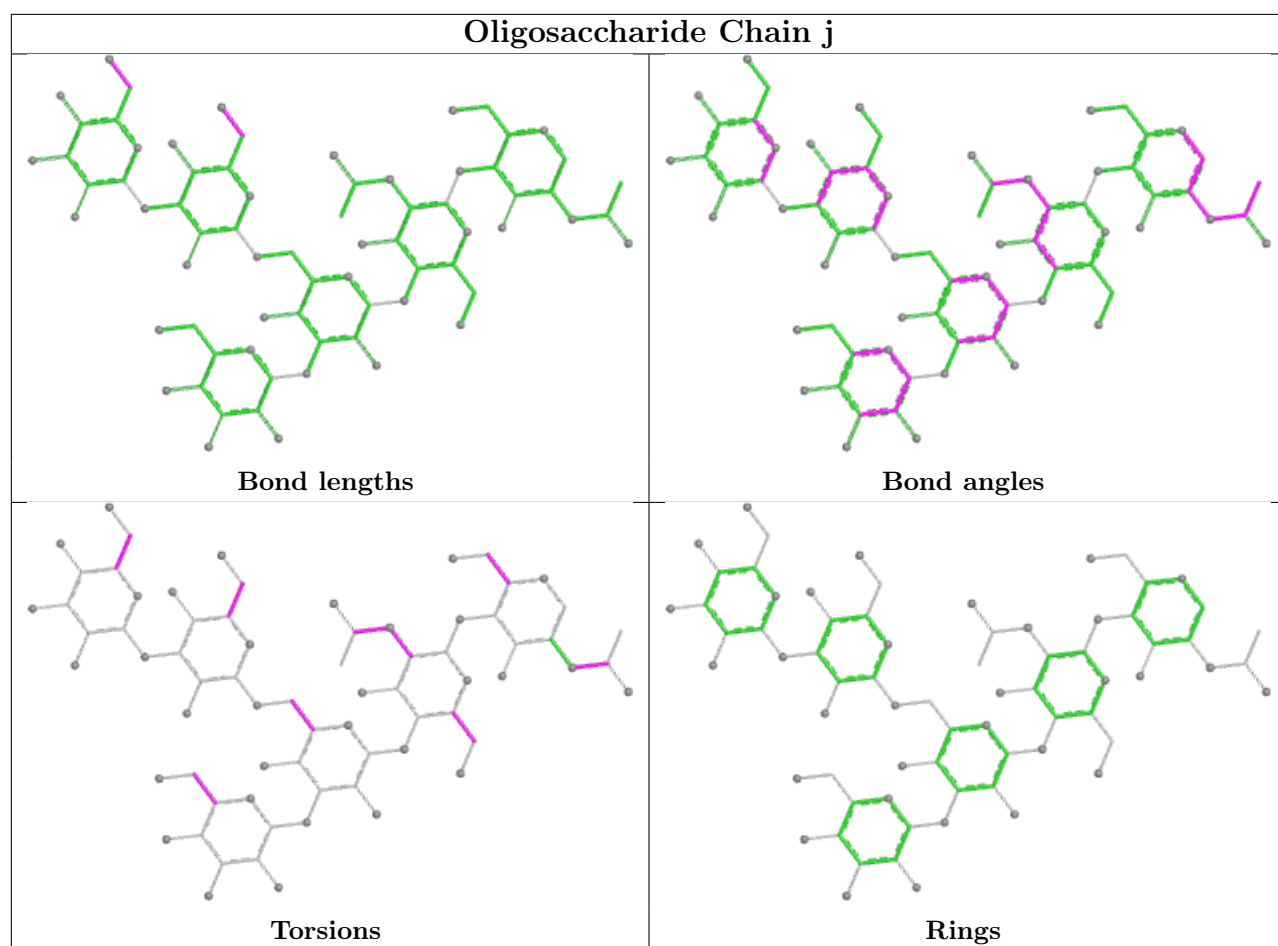


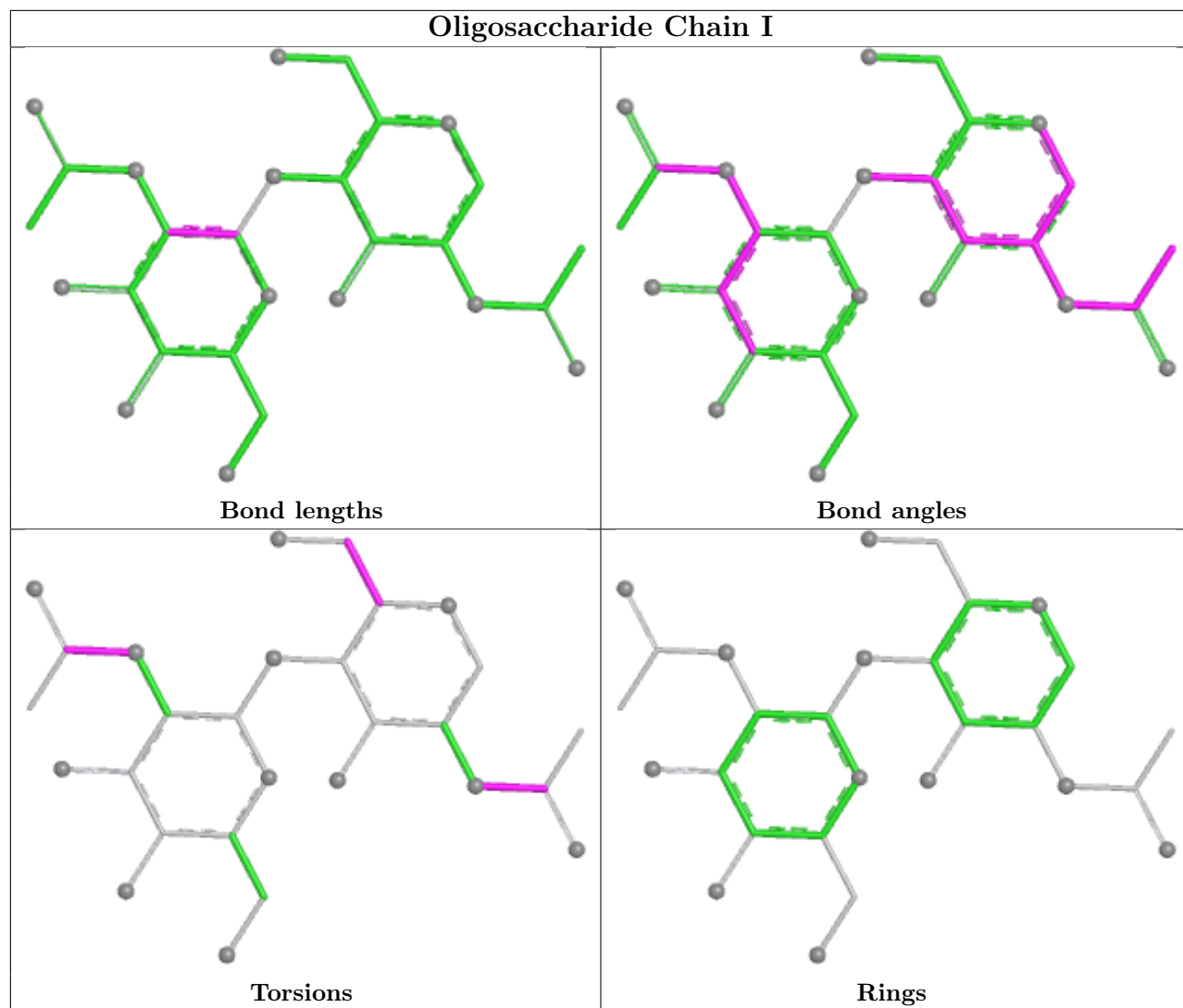


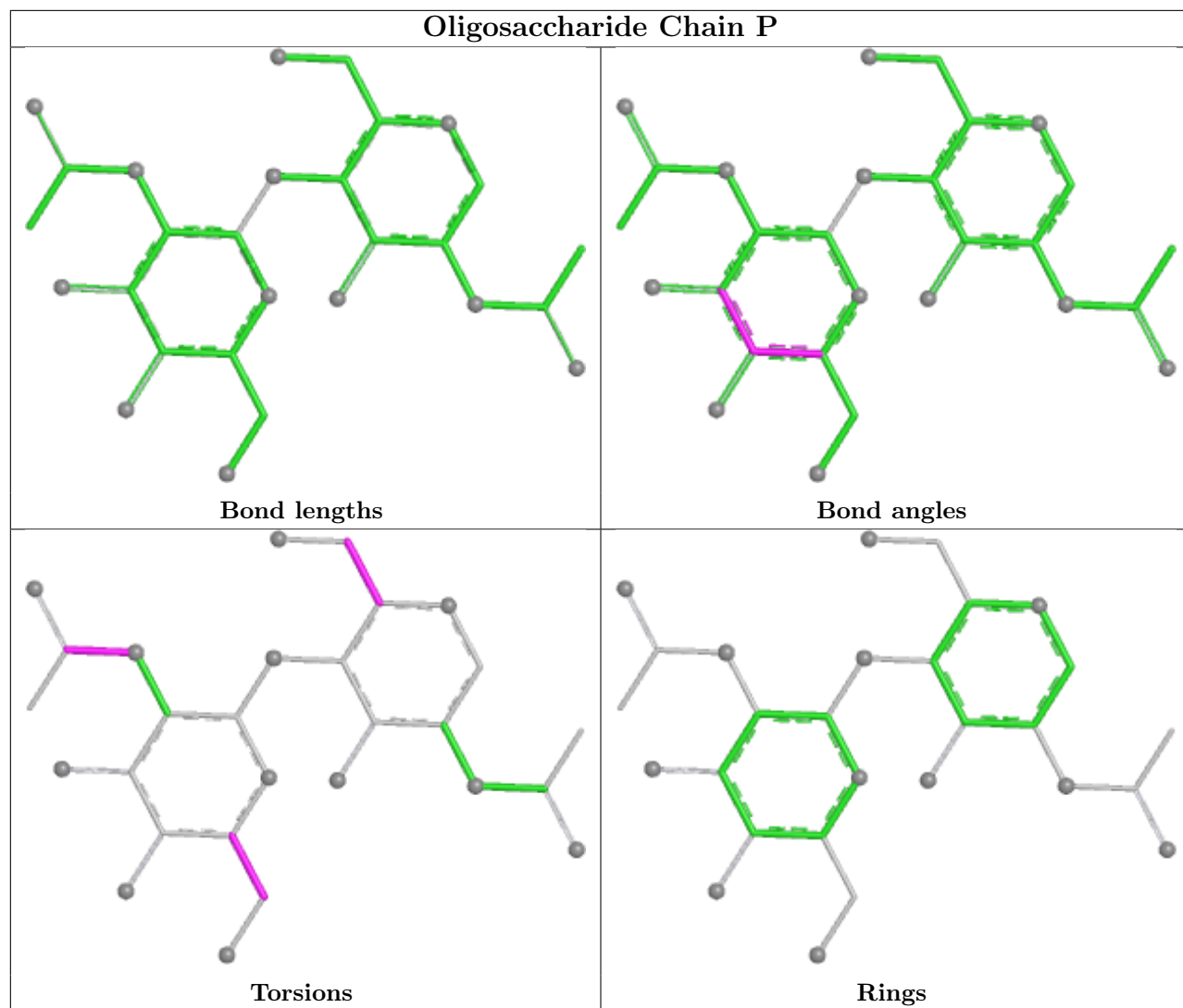


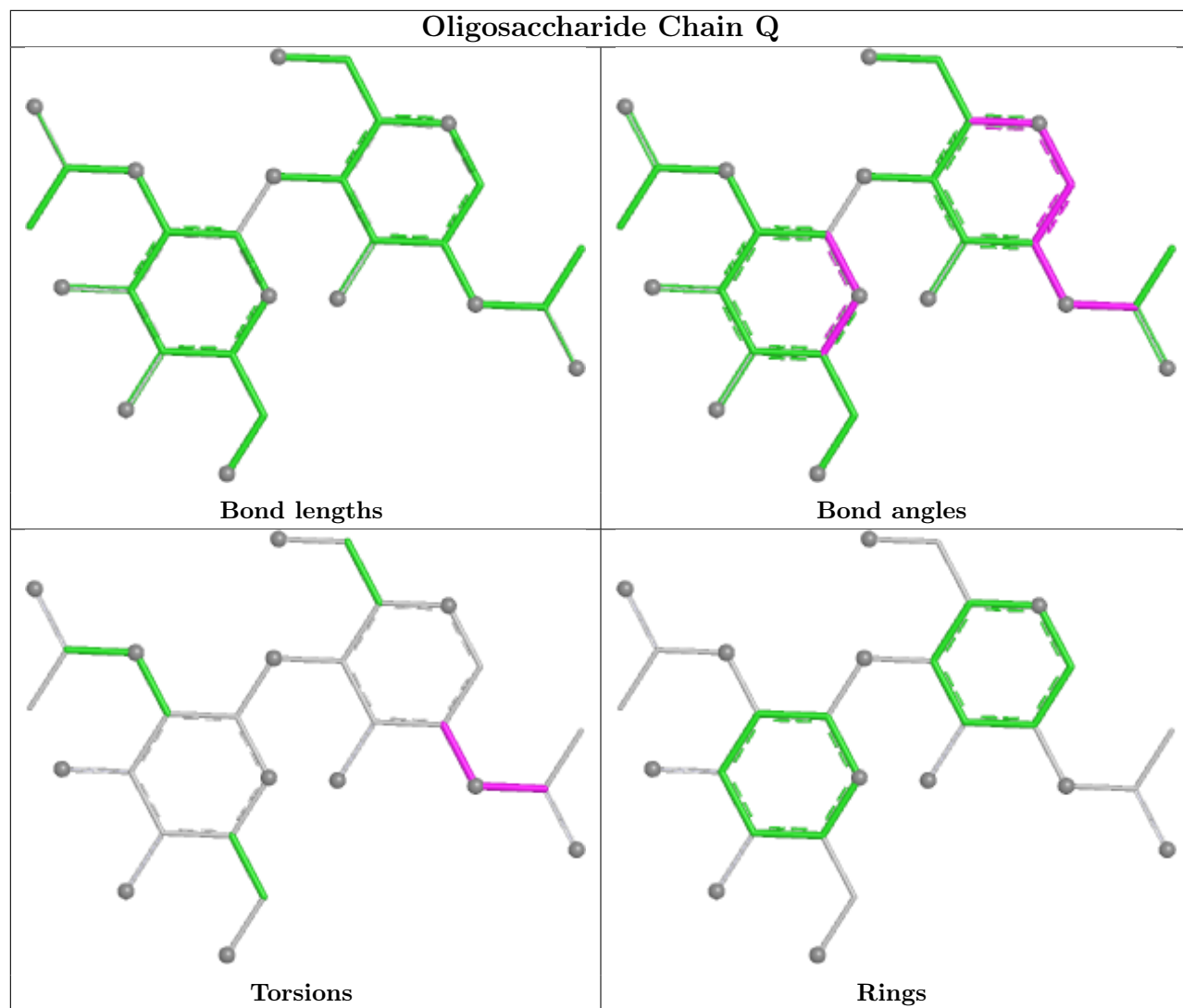


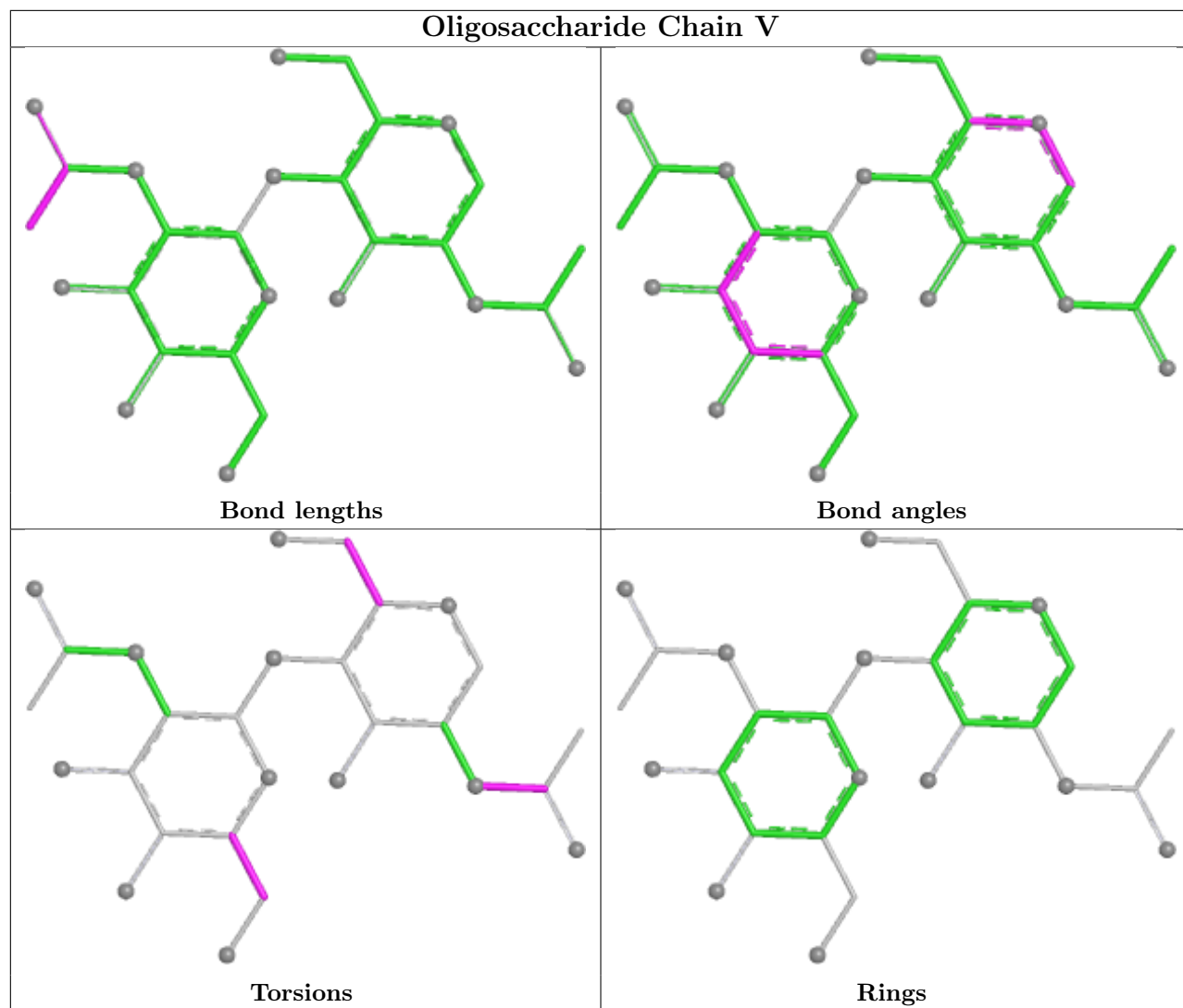


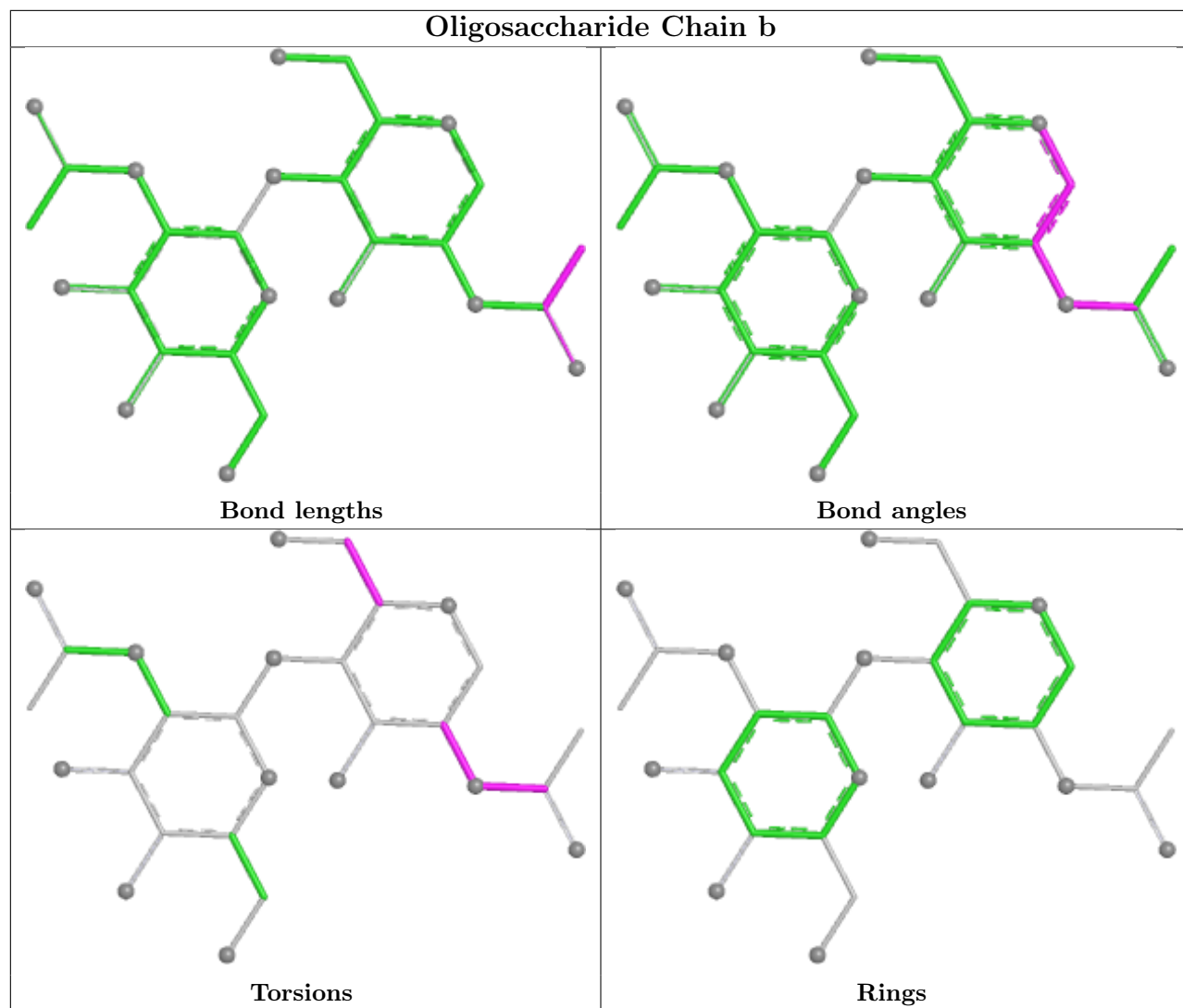


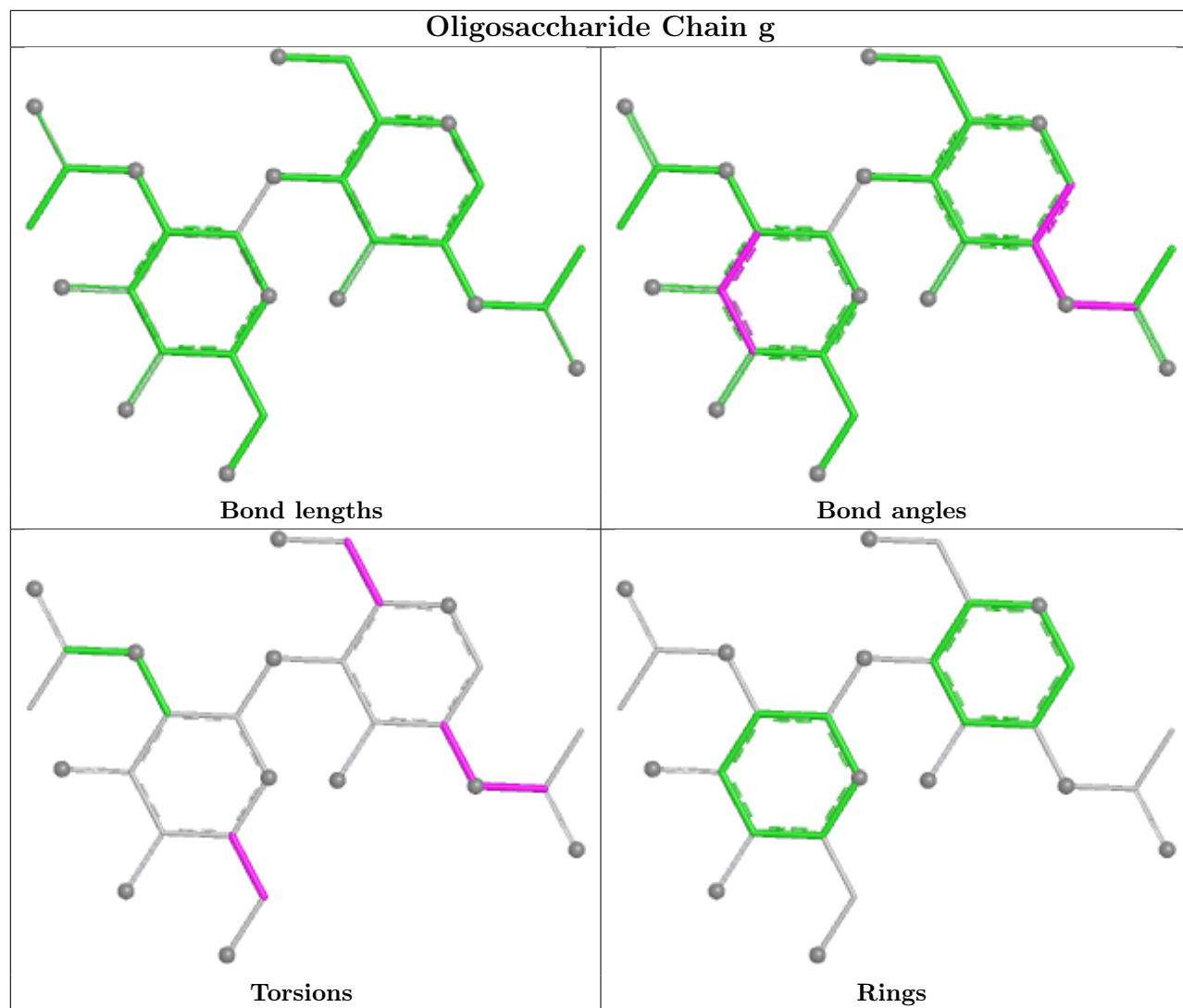


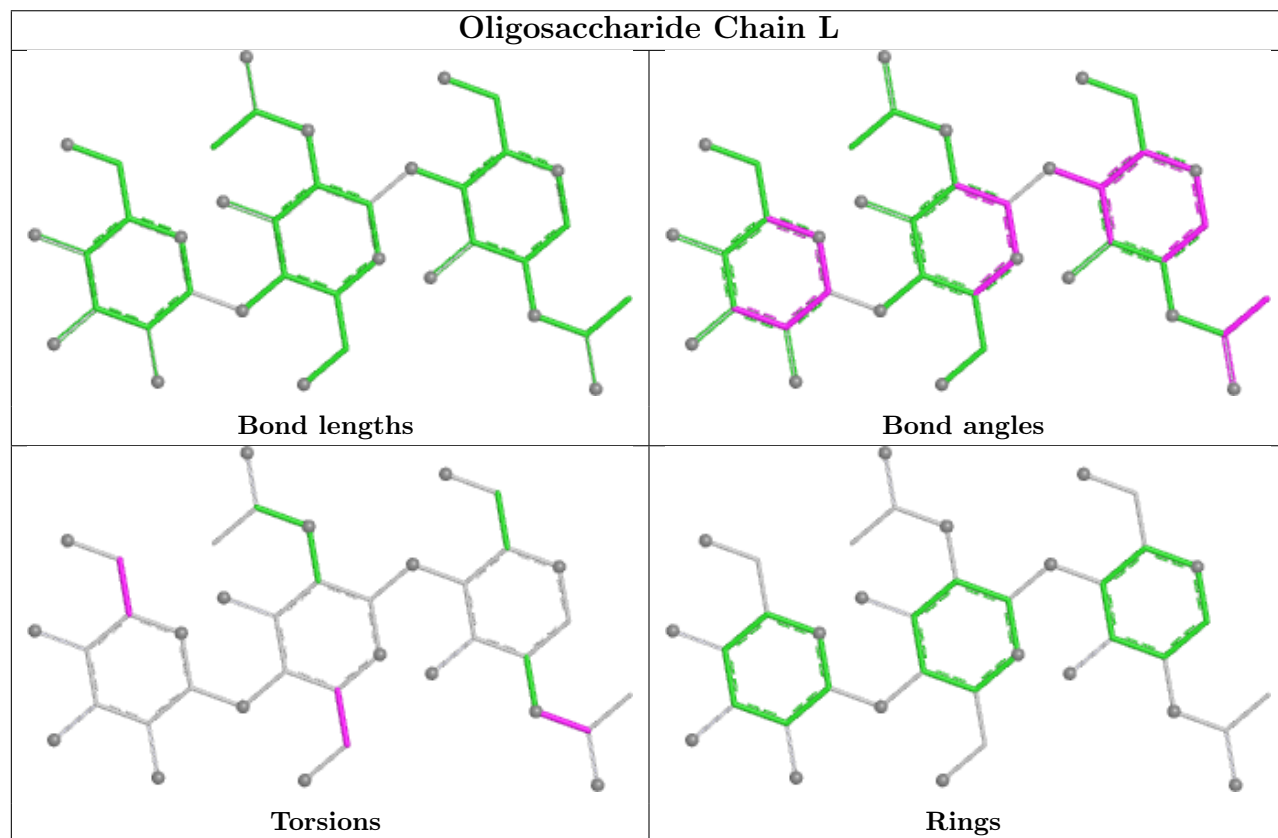
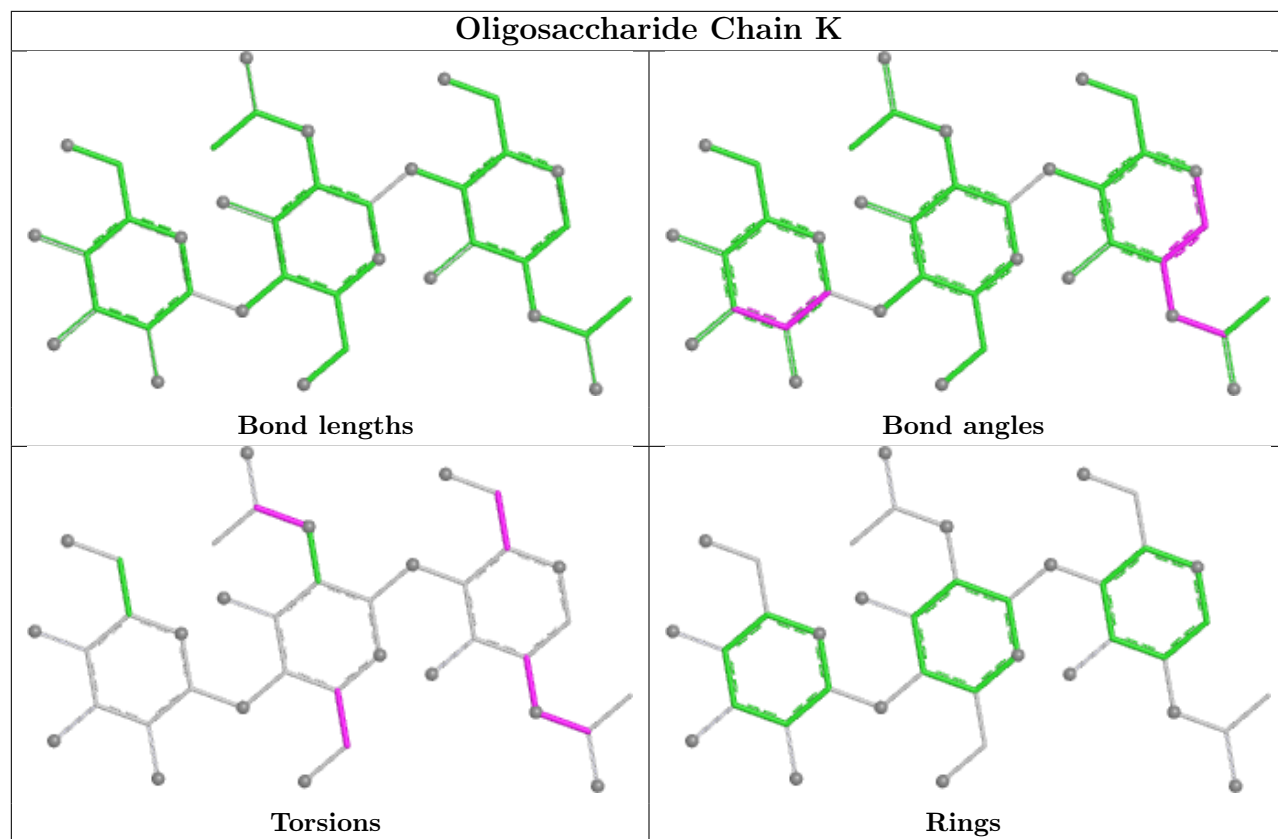


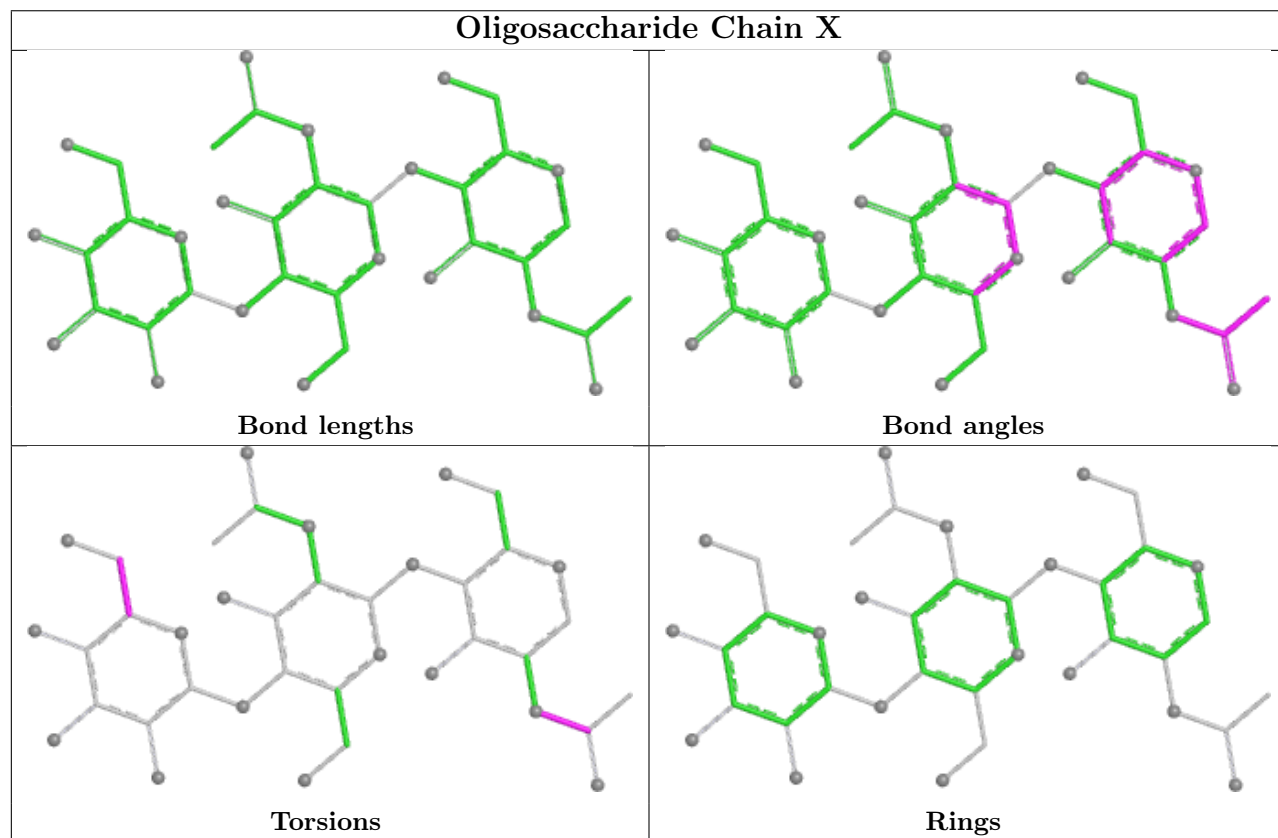
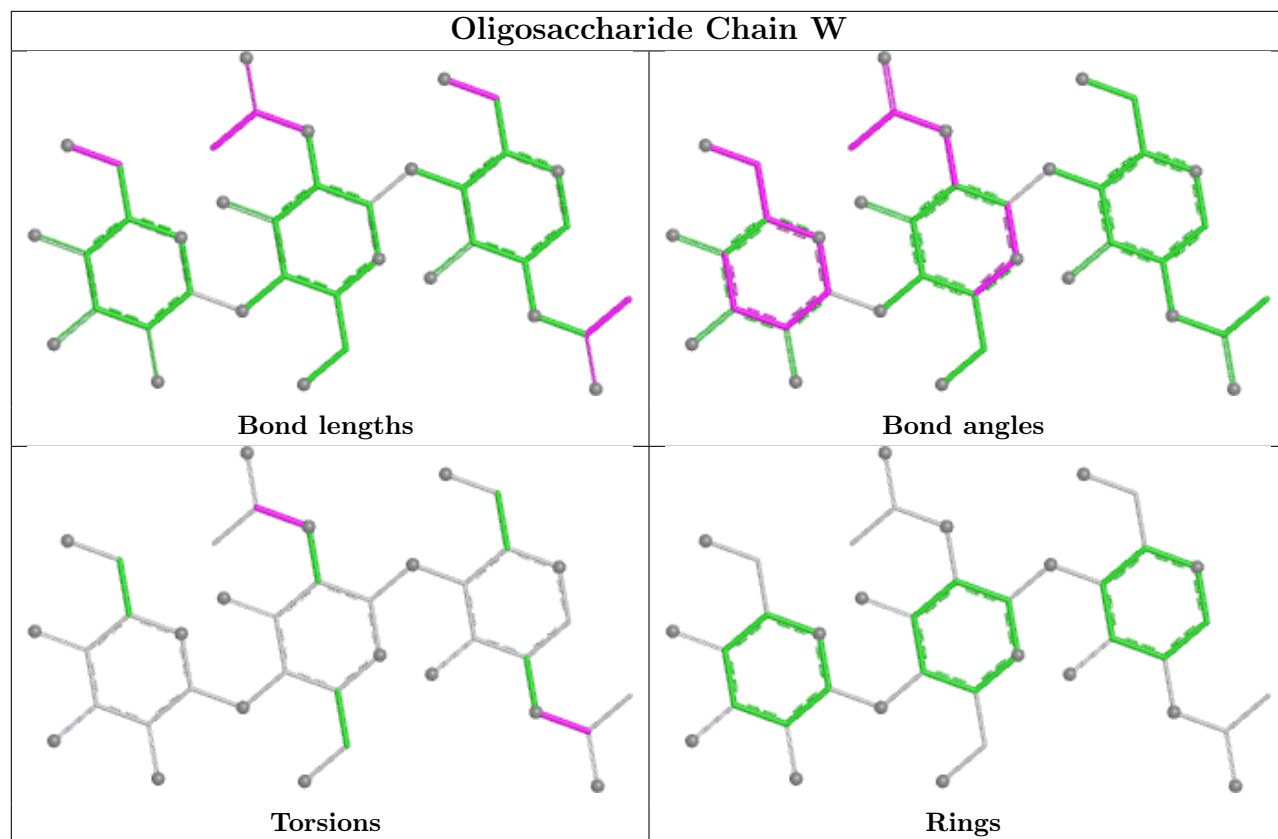


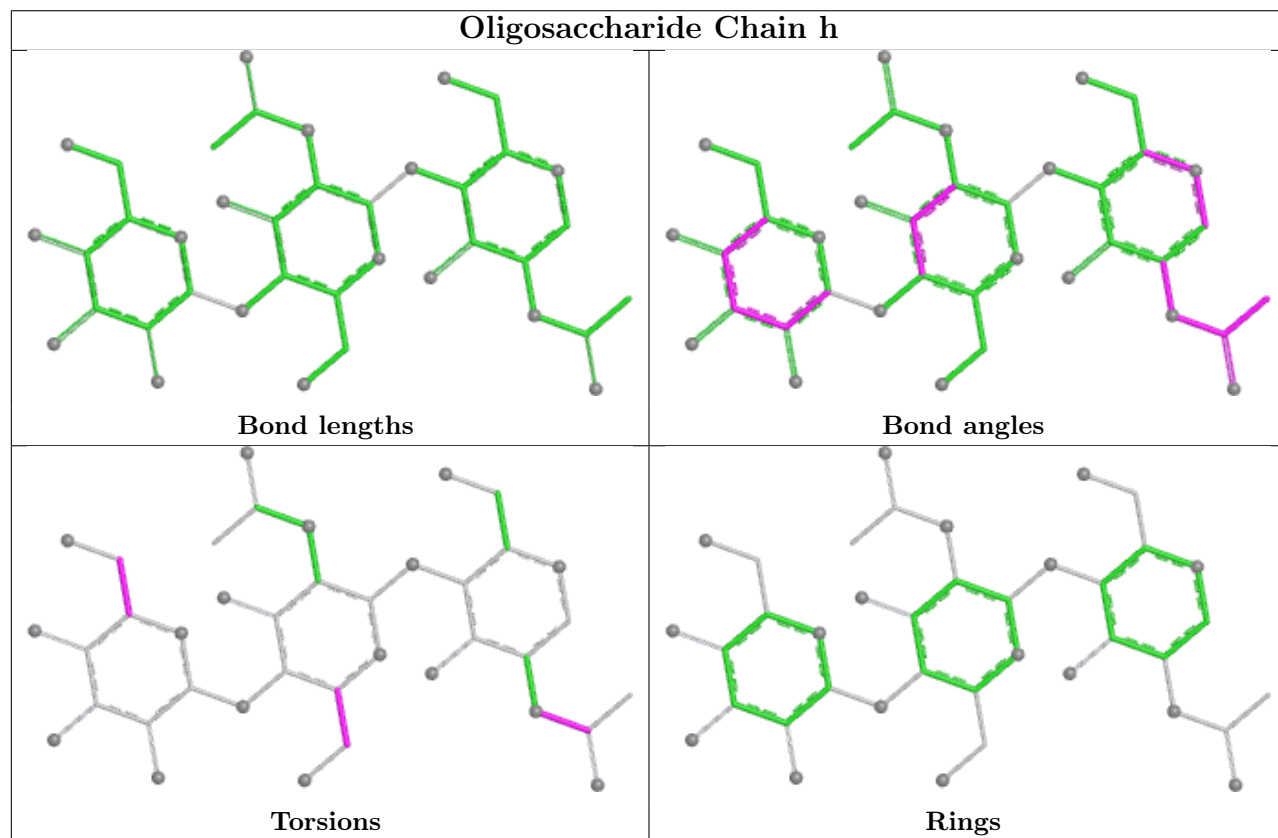
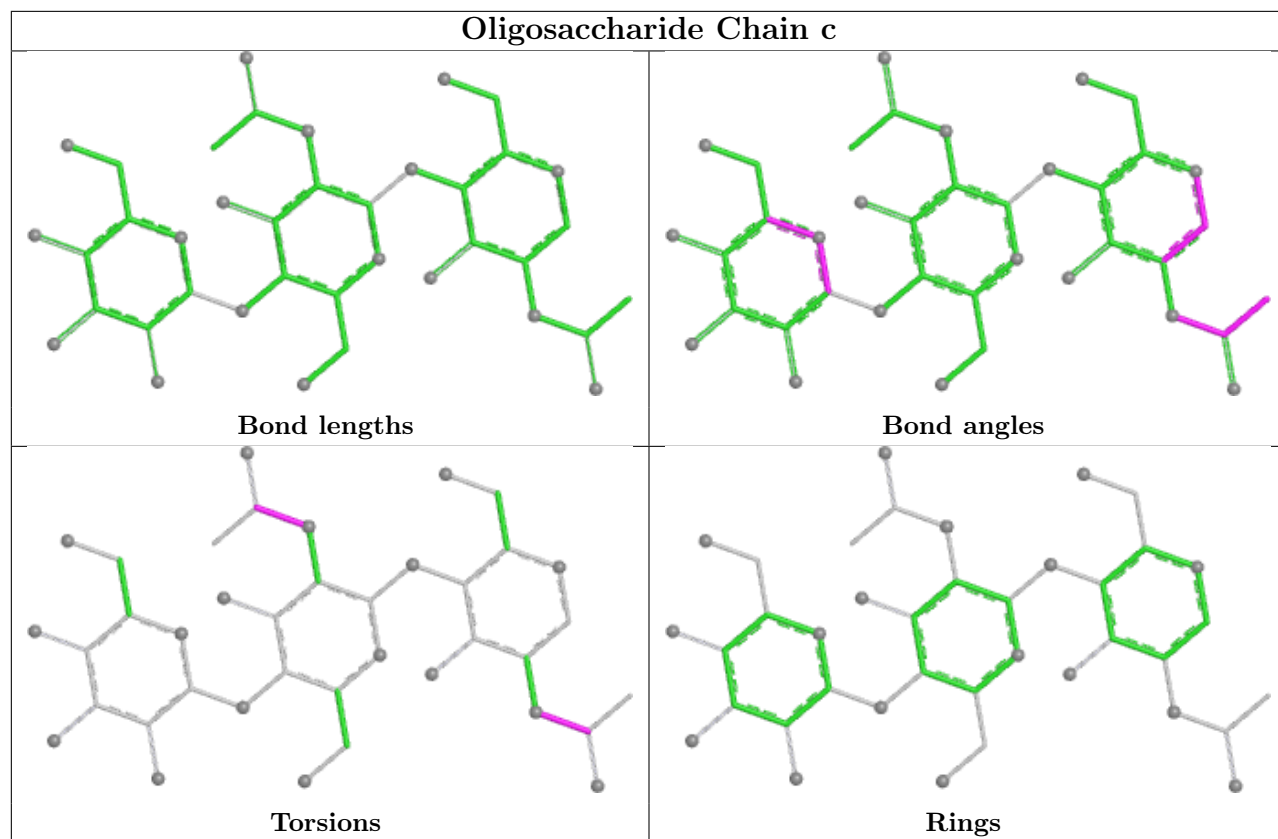


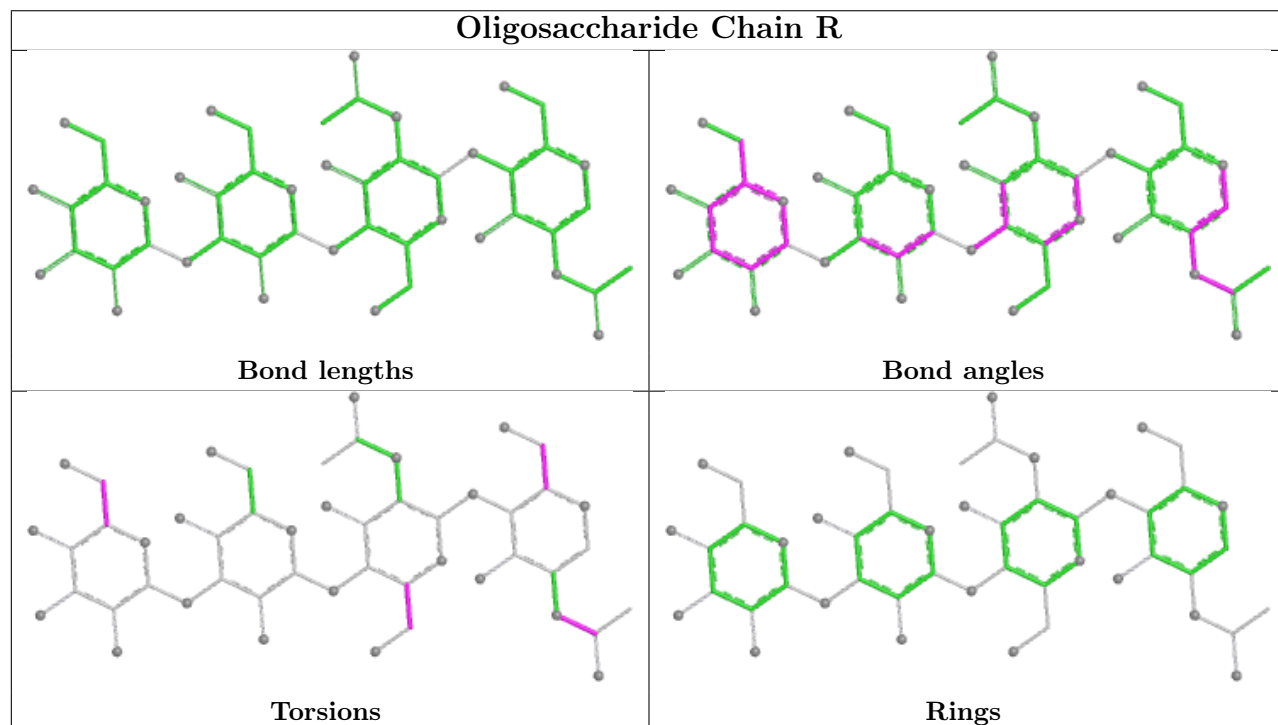
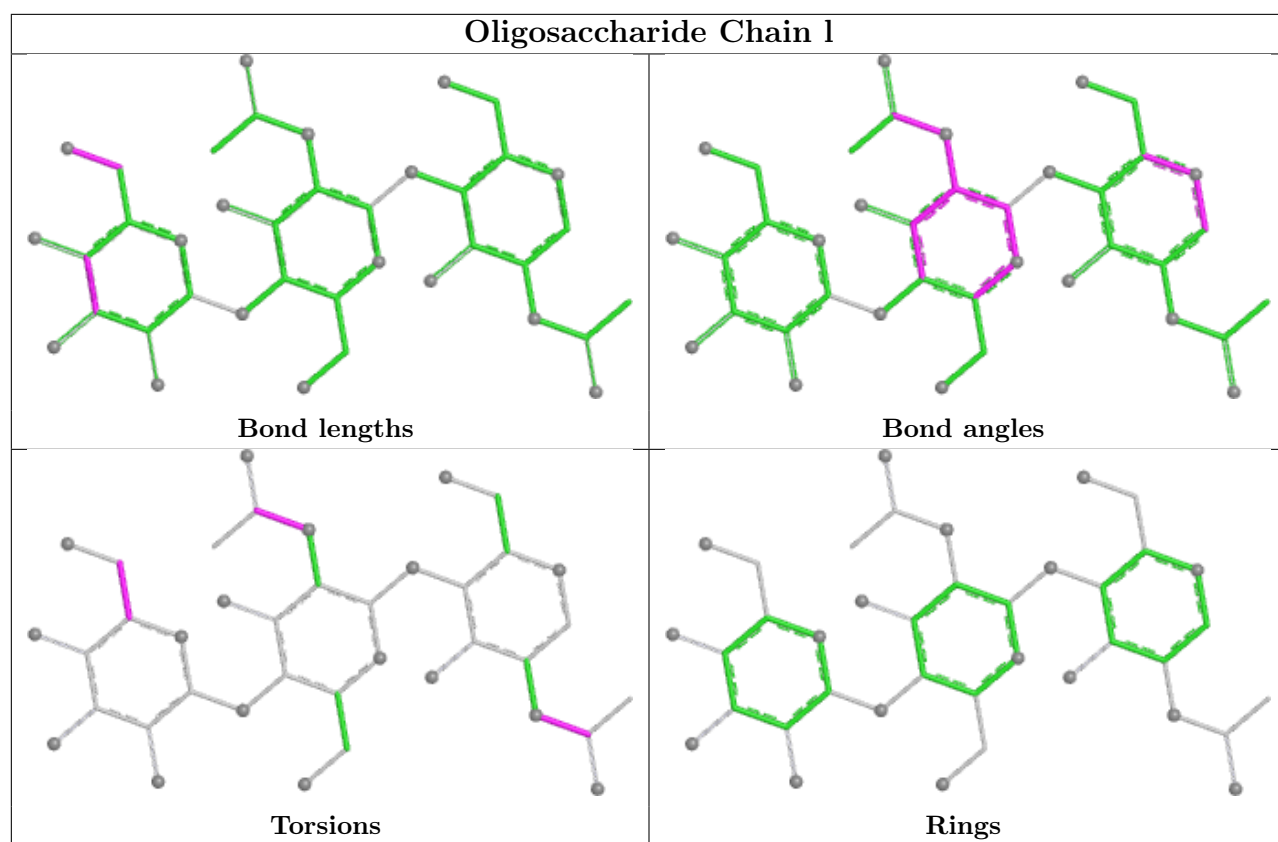


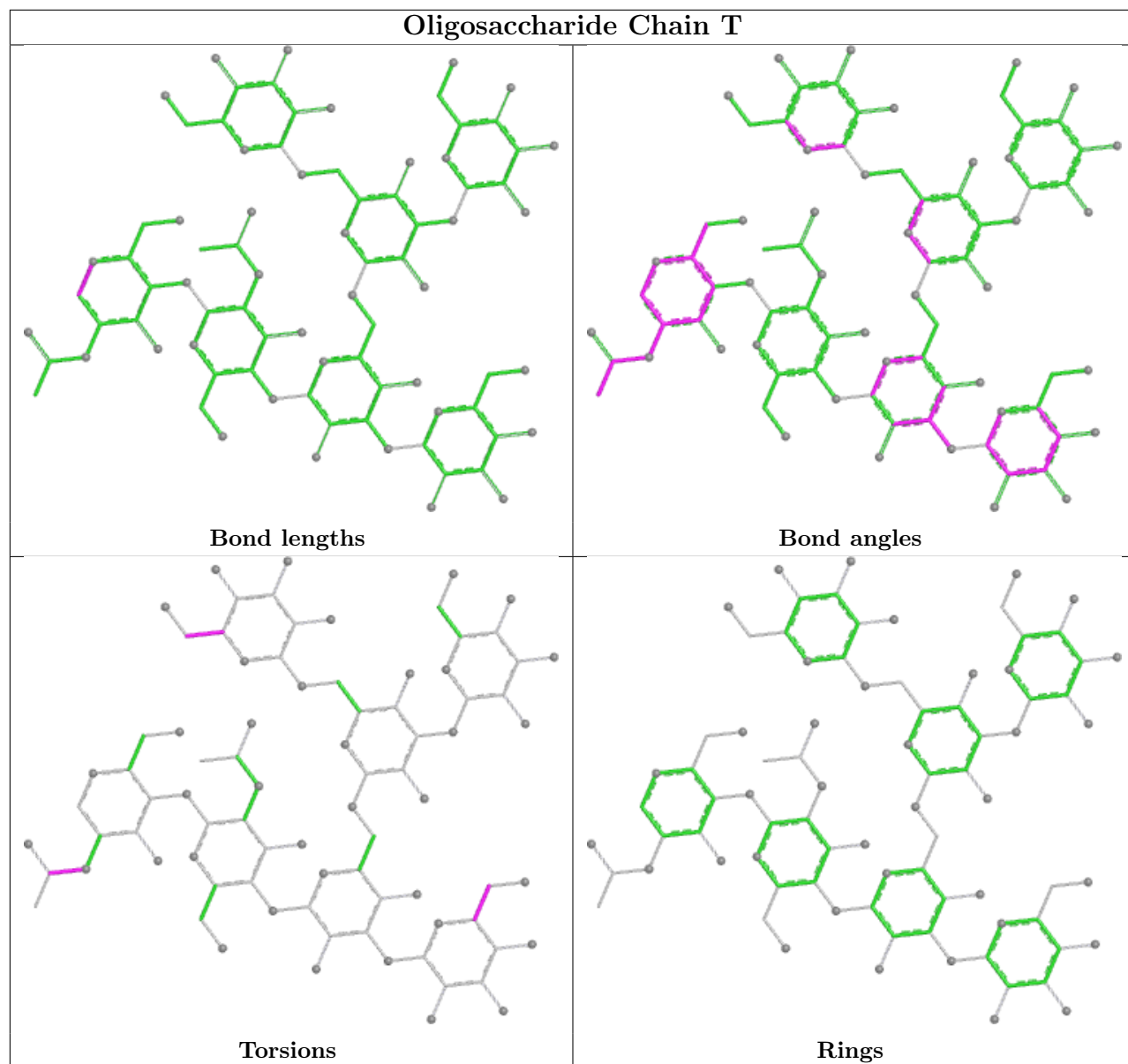


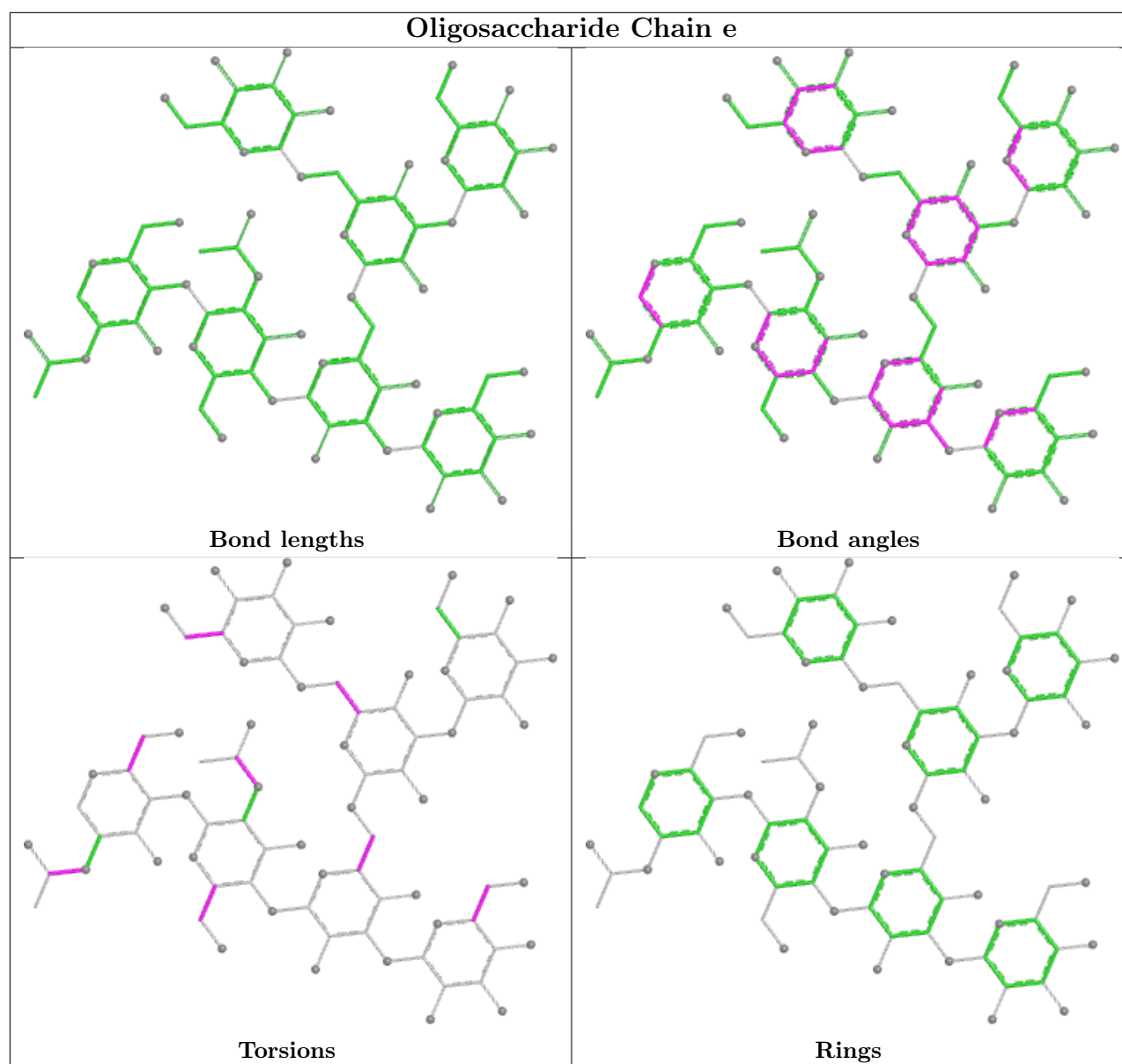












5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	2006	1	14,14,15	0.47	0	17,19,21	1.45	1 (5%)
8	NAG	E	2006	1	14,14,15	0.68	0	17,19,21	1.88	4 (23%)
8	NAG	F	2005	1	14,14,15	4.26	4 (28%)	17,19,21	1.96	4 (23%)
8	NAG	E	2008	1	14,14,15	0.52	0	17,19,21	0.94	0
8	NAG	E	2012	1	14,14,15	3.43	2 (14%)	17,19,21	1.50	3 (17%)
8	NAG	D	2014	1	14,14,15	0.52	0	17,19,21	0.91	0
8	NAG	D	2006	1	14,14,15	3.86	3 (21%)	17,19,21	2.07	4 (23%)
8	NAG	B	2005	1	14,14,15	0.58	0	17,19,21	1.00	2 (11%)
8	NAG	A	2014	1	14,14,15	0.64	0	17,19,21	1.08	0
8	NAG	A	2006	1	14,14,15	0.88	0	17,19,21	1.17	3 (17%)
8	NAG	D	2012	1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
8	NAG	E	2014	1	14,14,15	0.47	0	17,19,21	1.86	2 (11%)
8	NAG	F	2014	1	14,14,15	0.46	0	17,19,21	1.28	2 (11%)
8	NAG	A	2018	1	14,14,15	0.70	0	17,19,21	1.55	2 (11%)
8	NAG	F	2006	1	14,14,15	4.11	4 (28%)	17,19,21	1.98	4 (23%)
8	NAG	D	2008	1	14,14,15	0.48	0	17,19,21	1.09	1 (5%)
8	NAG	C	2018	1	14,14,15	5.07	3 (21%)	17,19,21	2.19	4 (23%)
8	NAG	C	2005	1	14,14,15	0.54	0	17,19,21	1.70	4 (23%)
8	NAG	C	2012	1	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
8	NAG	E	2005	1	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
8	NAG	B	2014	1	14,14,15	0.46	0	17,19,21	2.00	3 (17%)
8	NAG	B	2006	1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
8	NAG	A	2008	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
8	NAG	B	2018	1	14,14,15	0.80	1 (7%)	17,19,21	1.26	1 (5%)
8	NAG	B	2012	1	14,14,15	0.53	0	17,19,21	1.21	1 (5%)
8	NAG	F	2008	1	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
8	NAG	F	2012	1	14,14,15	0.48	0	17,19,21	1.39	2 (11%)
8	NAG	D	2005	1	14,14,15	0.52	0	17,19,21	1.17	2 (11%)
8	NAG	C	2014	1	14,14,15	0.54	0	17,19,21	1.82	3 (17%)
8	NAG	A	2012	1	14,14,15	0.54	0	17,19,21	1.21	1 (5%)
8	NAG	F	2009	1	14,14,15	0.88	0	17,19,21	1.59	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
8	NAG	E	2006	1	-	3/6/23/26	0/1/1/1
8	NAG	F	2005	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	E	2008	1	-	2/6/23/26	0/1/1/1
8	NAG	D	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	B	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	D	2012	1	-	5/6/23/26	0/1/1/1
8	NAG	E	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	F	2014	1	-	2/6/23/26	0/1/1/1
8	NAG	A	2018	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2006	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	2012	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	D	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	E	2005	1	-	2/6/23/26	0/1/1/1
8	NAG	B	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	B	2006	1	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	B	2018	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	B	2012	1	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
8	NAG	F	2012	1	1/1/5/7	5/6/23/26	0/1/1/1
8	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
8	NAG	C	2014	1	-	4/6/23/26	0/1/1/1
8	NAG	A	2012	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	F	2009	1	1/1/5/7	5/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2018	NAG	O7-C7	14.52	1.55	1.23
8	F	2006	NAG	C8-C7	14.37	1.80	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2006	NAG	O7-C7	11.91	1.49	1.23
8	C	2018	NAG	C8-C7	11.45	1.74	1.50
8	E	2012	NAG	C8-C7	10.37	1.72	1.50
8	F	2005	NAG	C8-C7	9.16	1.69	1.50
8	F	2005	NAG	C1-C2	8.45	1.63	1.52
8	F	2005	NAG	O6-C6	7.65	1.74	1.42
8	E	2012	NAG	O7-C7	7.31	1.39	1.23
8	D	2006	NAG	C8-C7	6.64	1.64	1.50
8	F	2005	NAG	C2-N2	5.27	1.55	1.46
8	F	2006	NAG	O7-C7	-3.42	1.15	1.23
8	F	2006	NAG	C7-N2	2.99	1.44	1.34
8	C	2018	NAG	O6-C6	2.99	1.55	1.42
8	D	2006	NAG	C1-C2	2.49	1.55	1.52
8	B	2018	NAG	C1-C2	2.28	1.55	1.52
8	F	2006	NAG	C1-C2	2.22	1.55	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2014	NAG	C1-O5-C5	6.36	120.71	112.19
8	C	2014	NAG	C1-O5-C5	5.97	120.19	112.19
8	F	2005	NAG	C1-O5-C5	5.46	119.51	112.19
8	D	2006	NAG	C8-C7-N2	-5.31	107.31	116.12
8	B	2014	NAG	C1-O5-C5	5.25	119.22	112.19
8	C	2018	NAG	O7-C7-N2	-5.14	112.90	121.98
8	C	2012	NAG	C1-O5-C5	4.65	118.41	112.19
8	F	2006	NAG	O7-C7-N2	-4.62	113.82	121.98
8	A	2018	NAG	C4-C3-C2	4.60	117.77	111.02
8	E	2006	NAG	C1-O5-C5	4.55	118.28	112.19
8	C	2018	NAG	C4-C3-C2	4.45	117.54	111.02
8	C	2018	NAG	O7-C7-C8	4.38	129.86	122.05
8	F	2006	NAG	C2-N2-C7	-4.22	117.24	122.90
8	C	2006	NAG	C1-O5-C5	4.05	117.61	112.19
8	B	2018	NAG	C4-C3-C2	4.01	116.89	111.02
8	F	2012	NAG	C2-N2-C7	3.93	128.17	122.90
8	C	2005	NAG	C2-N2-C7	3.90	128.13	122.90
8	B	2014	NAG	O5-C1-C2	-3.65	105.64	111.29
8	E	2012	NAG	O7-C7-C8	3.61	128.48	122.05
8	F	2009	NAG	C2-N2-C7	3.55	127.66	122.90
8	F	2008	NAG	C1-O5-C5	3.54	116.92	112.19
8	C	2005	NAG	C8-C7-N2	3.47	121.88	116.12
8	F	2005	NAG	O6-C6-C5	-3.46	99.55	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2006	NAG	O5-C1-C2	3.44	116.61	111.29
8	B	2012	NAG	C1-O5-C5	3.40	116.75	112.19
8	D	2006	NAG	C2-N2-C7	-3.33	118.44	122.90
8	C	2005	NAG	C1-O5-C5	3.32	116.64	112.19
8	F	2014	NAG	C1-O5-C5	3.24	116.53	112.19
8	F	2009	NAG	C1-C2-N2	3.18	115.44	110.43
8	A	2012	NAG	C1-O5-C5	3.16	116.42	112.19
8	B	2006	NAG	O5-C1-C2	-3.13	106.45	111.29
8	F	2005	NAG	O7-C7-N2	-3.05	116.59	121.98
8	F	2006	NAG	O5-C1-C2	-3.03	106.60	111.29
8	F	2006	NAG	O7-C7-C8	3.02	127.43	122.05
8	E	2006	NAG	C2-N2-C7	3.00	126.93	122.90
8	F	2009	NAG	C1-O5-C5	2.88	116.05	112.19
8	C	2018	NAG	C3-C4-C5	2.86	115.42	110.23
8	D	2008	NAG	O5-C1-C2	-2.66	107.18	111.29
8	D	2006	NAG	C1-O5-C5	2.60	115.67	112.19
8	E	2006	NAG	C4-C3-C2	2.59	114.81	111.02
8	C	2012	NAG	C4-C3-C2	2.59	114.81	111.02
8	F	2012	NAG	C1-O5-C5	2.58	115.64	112.19
8	E	2012	NAG	C8-C7-N2	-2.53	111.91	116.12
8	E	2012	NAG	C1-O5-C5	2.53	115.58	112.19
8	D	2006	NAG	O5-C1-C2	-2.47	107.46	111.29
8	B	2005	NAG	O5-C1-C2	-2.47	107.47	111.29
8	A	2006	NAG	O5-C5-C4	-2.44	104.90	110.83
8	A	2018	NAG	C3-C4-C5	2.40	114.58	110.23
8	F	2005	NAG	O5-C1-C2	-2.32	107.70	111.29
8	B	2014	NAG	C1-C2-N2	2.29	114.05	110.43
8	C	2014	NAG	O5-C5-C4	2.28	116.38	110.83
8	A	2008	NAG	O5-C1-C2	-2.27	107.78	111.29
8	D	2005	NAG	C8-C7-N2	2.27	119.88	116.12
8	A	2006	NAG	C4-C3-C2	2.23	114.29	111.02
8	D	2005	NAG	O5-C1-C2	-2.21	107.87	111.29
8	F	2014	NAG	O5-C1-C2	-2.20	107.88	111.29
8	C	2014	NAG	C6-C5-C4	-2.16	107.71	113.02
8	A	2006	NAG	O5-C1-C2	-2.16	107.96	111.29
8	C	2005	NAG	O7-C7-C8	-2.15	118.22	122.05
8	E	2014	NAG	C6-C5-C4	-2.13	107.79	113.02
8	F	2009	NAG	O5-C1-C2	-2.11	108.03	111.29
8	B	2005	NAG	C8-C7-N2	2.09	119.58	116.12
8	E	2005	NAG	C8-C7-N2	2.04	119.51	116.12
8	D	2012	NAG	O5-C1-C2	2.02	114.41	111.29

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	2006	NAG	C1
8	A	2012	NAG	C1
8	A	2018	NAG	C1
8	B	2006	NAG	C1
8	B	2012	NAG	C1
8	B	2018	NAG	C1
8	C	2012	NAG	C1
8	C	2018	NAG	C1
8	D	2006	NAG	C1
8	E	2012	NAG	C1
8	F	2005	NAG	C1
8	F	2006	NAG	C1
8	F	2009	NAG	C1
8	F	2012	NAG	C1

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2012	NAG	C8-C7-N2-C2
8	A	2012	NAG	O7-C7-N2-C2
8	A	2014	NAG	O7-C7-N2-C2
8	B	2005	NAG	C8-C7-N2-C2
8	B	2005	NAG	O7-C7-N2-C2
8	B	2012	NAG	O7-C7-N2-C2
8	B	2014	NAG	C8-C7-N2-C2
8	B	2014	NAG	O7-C7-N2-C2
8	B	2018	NAG	C8-C7-N2-C2
8	B	2018	NAG	O7-C7-N2-C2
8	C	2018	NAG	C8-C7-N2-C2
8	C	2018	NAG	O7-C7-N2-C2
8	D	2005	NAG	C8-C7-N2-C2
8	D	2005	NAG	O7-C7-N2-C2
8	D	2006	NAG	C8-C7-N2-C2
8	D	2012	NAG	C8-C7-N2-C2
8	D	2012	NAG	O7-C7-N2-C2
8	D	2014	NAG	C8-C7-N2-C2
8	D	2014	NAG	O7-C7-N2-C2
8	E	2005	NAG	C8-C7-N2-C2
8	E	2005	NAG	O7-C7-N2-C2
8	E	2006	NAG	C1-C2-N2-C7
8	E	2006	NAG	C8-C7-N2-C2
8	E	2006	NAG	O7-C7-N2-C2
8	F	2005	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	F	2005	NAG	C8-C7-N2-C2
8	F	2005	NAG	O7-C7-N2-C2
8	F	2006	NAG	C8-C7-N2-C2
8	F	2006	NAG	O7-C7-N2-C2
8	F	2009	NAG	C8-C7-N2-C2
8	F	2009	NAG	O7-C7-N2-C2
8	F	2012	NAG	C3-C2-N2-C7
8	F	2012	NAG	C8-C7-N2-C2
8	F	2012	NAG	O7-C7-N2-C2
8	F	2014	NAG	C8-C7-N2-C2
8	F	2014	NAG	O7-C7-N2-C2
8	A	2006	NAG	O7-C7-N2-C2
8	A	2014	NAG	C8-C7-N2-C2
8	B	2012	NAG	C8-C7-N2-C2
8	D	2006	NAG	O7-C7-N2-C2
8	C	2018	NAG	O5-C5-C6-O6
8	C	2012	NAG	O5-C5-C6-O6
8	E	2014	NAG	O5-C5-C6-O6
8	A	2006	NAG	C8-C7-N2-C2
8	B	2006	NAG	C8-C7-N2-C2
8	B	2006	NAG	O7-C7-N2-C2
8	C	2006	NAG	C8-C7-N2-C2
8	C	2006	NAG	O7-C7-N2-C2
8	E	2012	NAG	O7-C7-N2-C2
8	B	2005	NAG	O5-C5-C6-O6
8	D	2014	NAG	C4-C5-C6-O6
8	F	2009	NAG	C4-C5-C6-O6
8	C	2005	NAG	O5-C5-C6-O6
8	D	2005	NAG	O5-C5-C6-O6
8	F	2012	NAG	O5-C5-C6-O6
8	B	2014	NAG	O5-C5-C6-O6
8	B	2018	NAG	O5-C5-C6-O6
8	E	2012	NAG	O5-C5-C6-O6
8	C	2012	NAG	C4-C5-C6-O6
8	C	2018	NAG	C4-C5-C6-O6
8	C	2014	NAG	O5-C5-C6-O6
8	B	2005	NAG	C4-C5-C6-O6
8	E	2012	NAG	C8-C7-N2-C2
8	E	2014	NAG	C4-C5-C6-O6
8	F	2009	NAG	O5-C5-C6-O6
8	C	2005	NAG	C4-C5-C6-O6
8	D	2005	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	B	2014	NAG	C4-C5-C6-O6
8	D	2014	NAG	O5-C5-C6-O6
8	B	2018	NAG	C4-C5-C6-O6
8	C	2014	NAG	C4-C5-C6-O6
8	C	2005	NAG	C8-C7-N2-C2
8	C	2005	NAG	O7-C7-N2-C2
8	E	2008	NAG	O5-C5-C6-O6
8	B	2012	NAG	O5-C5-C6-O6
8	F	2012	NAG	C4-C5-C6-O6
8	A	2006	NAG	O5-C5-C6-O6
8	A	2006	NAG	C4-C5-C6-O6
8	A	2012	NAG	O5-C5-C6-O6
8	F	2005	NAG	C3-C2-N2-C7
8	F	2006	NAG	C4-C5-C6-O6
8	E	2012	NAG	C4-C5-C6-O6
8	A	2018	NAG	C8-C7-N2-C2
8	E	2008	NAG	C4-C5-C6-O6
8	A	2018	NAG	O7-C7-N2-C2
8	C	2014	NAG	C8-C7-N2-C2
8	F	2009	NAG	C3-C2-N2-C7
8	F	2006	NAG	O5-C5-C6-O6
8	C	2014	NAG	O7-C7-N2-C2
8	D	2012	NAG	C3-C2-N2-C7
8	A	2018	NAG	C4-C5-C6-O6
8	D	2012	NAG	O5-C5-C6-O6
8	B	2012	NAG	C4-C5-C6-O6
8	D	2012	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	2006	NAG	1	0
8	F	2005	NAG	2	0
8	B	2005	NAG	3	0
8	F	2006	NAG	1	0
8	D	2008	NAG	1	0
8	C	2005	NAG	2	0
8	E	2005	NAG	1	0
8	F	2012	NAG	1	0
8	D	2005	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	529/534 (99%)	1.66	161 (30%) 1 1	67, 69, 71, 74	0
1	B	529/534 (99%)	1.21	72 (13%) 7 5	67, 69, 71, 74	0
1	C	529/534 (99%)	1.84	216 (40%) 0 0	67, 69, 71, 74	0
1	D	529/534 (99%)	1.57	131 (24%) 2 1	67, 69, 71, 73	0
1	E	529/534 (99%)	1.63	150 (28%) 1 1	68, 69, 71, 73	0
1	F	529/534 (99%)	2.67	363 (68%) 0 0	68, 69, 71, 73	0
All	All	3174/3204 (99%)	1.76	1093 (34%) 1 1	67, 69, 71, 74	0

All (1093) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	550	ALA	7.6
1	F	436	GLY	7.3
1	D	533	ALA	6.5
1	F	533	ALA	6.5
1	F	454	PRO	6.4
1	A	397	LYS	6.2
1	F	435	LEU	6.0
1	A	533	ALA	6.0
1	F	376	SER	6.0
1	F	313	SER	5.9
1	F	549	HIS	5.9
1	F	87	GLN	5.9
1	F	108	SER	5.8
1	F	105	ALA	5.8
1	F	38	ASP	5.8
1	F	266	ASP	5.7
1	F	446	ASN	5.7
1	F	109	THR	5.6
1	F	372	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	503	PHE	5.5
1	C	540	THR	5.4
1	F	96	VAL	5.4
1	C	493	GLY	5.4
1	F	526	VAL	5.3
1	C	533	ALA	5.3
1	F	307	THR	5.3
1	F	291	LEU	5.3
1	F	444	PRO	5.3
1	F	99	LEU	5.2
1	D	312	ASP	5.2
1	F	504	GLY	5.2
1	F	306	PRO	5.1
1	C	177	SER	5.1
1	D	535	ASN	5.1
1	F	536	THR	5.0
1	B	535	ASN	5.0
1	B	540	THR	5.0
1	F	188	PRO	5.0
1	F	453	TYR	5.0
1	F	294	THR	4.9
1	F	355	ALA	4.9
1	F	302	THR	4.9
1	F	543	THR	4.9
1	A	272	ALA	4.9
1	C	352	VAL	4.9
1	F	287	SER	4.9
1	F	286	PRO	4.9
1	F	309	ASN	4.8
1	F	385	ILE	4.8
1	D	534	ALA	4.8
1	D	290	GLN	4.8
1	E	184	ALA	4.8
1	F	206	ASP	4.8
1	F	514	SER	4.7
1	A	540	THR	4.7
1	F	312	ASP	4.7
1	F	474	ALA	4.7
1	F	428	ASP	4.7
1	B	529	GLU	4.7
1	F	164	TYR	4.6
1	F	325	PRO	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	196	THR	4.6
1	F	178	VAL	4.6
1	D	241	THR	4.6
1	F	347	ASN	4.6
1	F	542	LEU	4.5
1	F	303	ALA	4.5
1	A	302	THR	4.4
1	F	508	ALA	4.4
1	C	102	CYS	4.4
1	E	535	ASN	4.4
1	A	549	HIS	4.4
1	F	451	PRO	4.4
1	C	179	TYR	4.4
1	F	425	ILE	4.4
1	E	540	THR	4.4
1	C	39	GLY	4.4
1	F	84	GLY	4.4
1	F	530	GLY	4.4
1	F	290	GLN	4.4
1	A	228	ASP	4.4
1	E	454	PRO	4.3
1	F	103	PRO	4.3
1	F	520	VAL	4.3
1	F	529	GLU	4.3
1	F	28	TRP	4.3
1	E	269	LYS	4.3
1	F	59	VAL	4.3
1	F	361	THR	4.3
1	B	533	ALA	4.3
1	C	304	ALA	4.3
1	F	184	ALA	4.3
1	A	372	THR	4.3
1	C	198	ASN	4.3
1	F	353	ASN	4.3
1	C	40	LEU	4.2
1	C	538	ASP	4.2
1	F	305	LEU	4.2
1	A	198	ASN	4.2
1	A	299	TYR	4.2
1	C	178	VAL	4.2
1	C	38	ASP	4.2
1	D	549	HIS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	349	LYS	4.2
1	A	303	ALA	4.2
1	B	146	ASP	4.2
1	E	465	GLN	4.2
1	F	308	GLN	4.2
1	F	539	LEU	4.2
1	E	333	GLY	4.2
1	F	400	ILE	4.2
1	F	359	ASN	4.1
1	F	131	GLY	4.1
1	A	245	VAL	4.1
1	E	549	HIS	4.1
1	F	462	VAL	4.1
1	F	507	ASP	4.1
1	F	513	LEU	4.1
1	E	113	ASN	4.1
1	F	265	ASN	4.1
1	C	515	GLU	4.1
1	C	524	CYS	4.1
1	E	262	HIS	4.0
1	F	181	PRO	4.0
1	E	400	ILE	4.0
1	F	118	TYR	4.0
1	C	539	LEU	4.0
1	F	443	ASP	4.0
1	A	270	ASN	4.0
1	C	370	LEU	4.0
1	B	205	PRO	4.0
1	A	36	ASN	3.9
1	E	435	LEU	3.9
1	F	301	LYS	3.9
1	A	534	ALA	3.9
1	F	237	ASP	3.9
1	F	445	ASP	3.9
1	C	300	ASN	3.9
1	F	322	TYR	3.9
1	F	100	THR	3.9
1	F	136	GLY	3.9
1	F	431	TYR	3.9
1	A	311	VAL	3.9
1	C	298	VAL	3.9
1	F	548	GLN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	307	THR	3.9
1	A	378	ASP	3.9
1	F	227	GLU	3.9
1	C	36	ASN	3.9
1	C	292	ASN	3.9
1	A	298	VAL	3.9
1	E	261	VAL	3.9
1	F	434	ALA	3.9
1	F	493	GLY	3.8
1	F	323	LEU	3.8
1	F	342	ASP	3.8
1	F	244	ASN	3.8
1	E	299	TYR	3.8
1	F	209	TYR	3.8
1	F	296	TYR	3.8
1	D	272	ALA	3.8
1	F	98	PHE	3.8
1	A	294	THR	3.8
1	E	547	VAL	3.8
1	F	475	ASP	3.8
1	F	191	LEU	3.8
1	A	536	THR	3.8
1	F	360	ILE	3.8
1	F	101	GLN	3.8
1	A	292	ASN	3.8
1	D	71	ASN	3.7
1	B	42	SER	3.7
1	C	34	TYR	3.7
1	C	531	ASN	3.7
1	F	345	MET	3.7
1	A	550	ALA	3.7
1	F	48	CYS	3.7
1	F	270	ASN	3.7
1	F	310	TYR	3.7
1	F	540	THR	3.7
1	F	505	ILE	3.7
1	F	388	SER	3.7
1	B	228	ASP	3.7
1	E	130	ASP	3.7
1	F	180	ASN	3.7
1	C	169	THR	3.7
1	F	29	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	534	ALA	3.6
1	A	130	ASP	3.6
1	E	378	ASP	3.6
1	D	503	PHE	3.6
1	F	77	ASN	3.6
1	F	476	ASN	3.6
1	A	226	ILE	3.6
1	F	104	ILE	3.6
1	F	419	GLY	3.6
1	E	51	GLN	3.6
1	E	304	ALA	3.6
1	C	175	PHE	3.6
1	C	501	ASP	3.6
1	B	292	ASN	3.6
1	F	406	ASN	3.6
1	D	539	LEU	3.6
1	E	431	TYR	3.6
1	C	289	LEU	3.6
1	F	31	GLY	3.5
1	A	227	GLU	3.5
1	F	338	VAL	3.5
1	C	163	TRP	3.5
1	D	38	ASP	3.5
1	E	455	MET	3.5
1	D	540	THR	3.5
1	D	254	ALA	3.5
1	D	380	ALA	3.5
1	C	33	ASP	3.5
1	F	288	ASP	3.5
1	F	346	ASP	3.5
1	F	179	TYR	3.5
1	E	544	GLY	3.5
1	F	374	LEU	3.5
1	F	205	PRO	3.5
1	C	508	ALA	3.5
1	D	508	ALA	3.5
1	E	497	VAL	3.5
1	E	526	VAL	3.5
1	F	311	VAL	3.5
1	C	513	LEU	3.5
1	F	405	LEU	3.5
1	C	445	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	ASN	3.5
1	F	496	LEU	3.4
1	F	525	SER	3.4
1	F	70	THR	3.4
1	F	437	GLU	3.4
1	C	262	HIS	3.4
1	A	207	THR	3.4
1	B	130	ASP	3.4
1	F	34	TYR	3.4
1	A	535	ASN	3.4
1	C	190	ASN	3.4
1	F	356	PHE	3.4
1	F	518	LEU	3.4
1	A	105	ALA	3.4
1	A	304	ALA	3.4
1	F	46	ILE	3.4
1	F	340	THR	3.4
1	D	506	GLN	3.4
1	D	367	VAL	3.4
1	D	329	GLU	3.4
1	C	549	HIS	3.4
1	F	510	SER	3.4
1	C	29	THR	3.4
1	C	100	THR	3.4
1	D	390	THR	3.4
1	A	537	LEU	3.3
1	C	305	LEU	3.3
1	E	384	GLU	3.3
1	E	527	ALA	3.3
1	F	248	MET	3.3
1	F	78	THR	3.3
1	D	180	ASN	3.3
1	F	429	ARG	3.3
1	E	154	GLU	3.3
1	F	521	CYS	3.3
1	A	200	THR	3.3
1	F	116	VAL	3.3
1	A	39	GLY	3.3
1	C	31	GLY	3.3
1	A	309	ASN	3.3
1	C	529	GLU	3.3
1	E	503	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	482	PHE	3.3
1	A	47	THR	3.3
1	C	389	ASN	3.3
1	F	455	MET	3.3
1	D	400	ILE	3.3
1	F	420	HIS	3.3
1	C	291	LEU	3.3
1	A	196	THR	3.3
1	D	258	THR	3.3
1	C	41	LYS	3.2
1	E	265	ASN	3.2
1	F	448	PRO	3.2
1	A	532	ALA	3.2
1	B	549	HIS	3.2
1	F	65	VAL	3.2
1	D	530	GLY	3.2
1	E	183	GLY	3.2
1	E	207	THR	3.2
1	D	466	SER	3.2
1	E	150	TYR	3.2
1	D	538	ASP	3.2
1	D	292	ASN	3.2
1	D	306	PRO	3.2
1	F	67	ILE	3.2
1	F	298	VAL	3.2
1	C	302	THR	3.2
1	F	241	THR	3.2
1	D	313	SER	3.2
1	F	531	ASN	3.2
1	F	40	LEU	3.2
1	F	89	GLY	3.2
1	F	412	THR	3.2
1	F	32	TRP	3.2
1	F	133	TYR	3.2
1	B	117	ASP	3.2
1	F	27	ASN	3.2
1	F	71	ASN	3.2
1	F	494	LEU	3.2
1	F	492	GLN	3.2
1	C	107	GLY	3.2
1	C	377	GLY	3.2
1	F	182	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	402	GLU	3.2
1	C	164	TYR	3.1
1	A	295	SER	3.1
1	C	254	ALA	3.1
1	E	389	ASN	3.1
1	E	550	ALA	3.1
1	F	413	HIS	3.1
1	F	50	GLY	3.1
1	A	30	THR	3.1
1	C	536	THR	3.1
1	F	30	THR	3.1
1	F	186	PRO	3.1
1	D	310	TYR	3.1
1	A	269	LYS	3.1
1	F	449	ALA	3.1
1	A	38	ASP	3.1
1	D	130	ASP	3.1
1	F	26	PHE	3.1
1	F	321	PHE	3.1
1	A	203	VAL	3.1
1	C	439	PRO	3.1
1	E	90	THR	3.1
1	F	43	ARG	3.1
1	F	471	ARG	3.1
1	A	102	CYS	3.1
1	C	253	VAL	3.1
1	F	358	ASN	3.1
1	F	501	ASP	3.1
1	F	452	GLU	3.1
1	C	99	LEU	3.1
1	C	306	PRO	3.1
1	C	356	PHE	3.1
1	D	259	VAL	3.1
1	D	373	VAL	3.1
1	F	450	PHE	3.1
1	D	342	ASP	3.1
1	C	43	ARG	3.1
1	F	260	LEU	3.1
1	D	78	THR	3.1
1	C	299	TYR	3.0
1	A	146	ASP	3.0
1	C	170	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	428	ASP	3.0
1	F	49	ASN	3.0
1	F	130	ASP	3.0
1	F	64	ARG	3.0
1	A	115	THR	3.0
1	A	271	PHE	3.0
1	D	311	VAL	3.0
1	E	440	HIS	3.0
1	F	233	VAL	3.0
1	F	480	TRP	3.0
1	C	77	ASN	3.0
1	D	288	ASP	3.0
1	F	279	ASP	3.0
1	F	173	LYS	3.0
1	F	187	ILE	3.0
1	F	289	LEU	3.0
1	B	329	GLU	3.0
1	C	307	THR	3.0
1	F	430	THR	3.0
1	F	83	HIS	3.0
1	C	530	GLY	3.0
1	F	51	GLN	3.0
1	F	537	LEU	3.0
1	A	154	GLU	3.0
1	F	230	GLU	3.0
1	F	197	MET	3.0
1	C	165	HIS	3.0
1	A	512	GLN	3.0
1	C	351	GLY	3.0
1	D	121	GLY	3.0
1	D	493	GLY	3.0
1	E	408	GLN	3.0
1	A	342	ASP	3.0
1	A	446	ASN	3.0
1	C	507	ASP	3.0
1	D	300	ASN	3.0
1	D	476	ASN	3.0
1	C	44	PRO	3.0
1	C	201	TRP	2.9
1	F	68	TYR	2.9
1	A	107	GLY	2.9
1	F	368	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	541	ASP	2.9
1	A	293	ALA	2.9
1	E	272	ALA	2.9
1	A	129	THR	2.9
1	F	442	PHE	2.9
1	E	385	ILE	2.9
1	E	537	LEU	2.9
1	B	419	GLY	2.9
1	C	145	ASP	2.9
1	F	247	ASP	2.9
1	A	233	VAL	2.9
1	C	272	ALA	2.9
1	C	303	ALA	2.9
1	C	30	THR	2.9
1	D	543	THR	2.9
1	E	524	CYS	2.9
1	A	273	ILE	2.9
1	A	34	TYR	2.9
1	C	453	TYR	2.9
1	C	130	ASP	2.9
1	C	353	ASN	2.9
1	D	550	ALA	2.9
1	F	404	VAL	2.9
1	F	532	ALA	2.9
1	E	239	ILE	2.9
1	F	488	TRP	2.9
1	D	477	PRO	2.9
1	C	421	ALA	2.9
1	D	146	ASP	2.9
1	E	38	ASP	2.9
1	E	533	ALA	2.9
1	F	315	ASP	2.9
1	E	108	SER	2.9
1	A	509	HIS	2.9
1	C	47	THR	2.9
1	F	240	THR	2.9
1	B	539	LEU	2.9
1	F	95	GLY	2.8
1	A	274	MET	2.8
1	C	408	GLN	2.8
1	F	477	PRO	2.8
1	F	461	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	220	VAL	2.8
1	C	71	ASN	2.8
1	C	105	ALA	2.8
1	F	272	ALA	2.8
1	F	463	ARG	2.8
1	B	206	ASP	2.8
1	B	312	ASP	2.8
1	C	117	ASP	2.8
1	F	165	HIS	2.8
1	A	539	LEU	2.8
1	C	543	THR	2.8
1	E	536	THR	2.8
1	D	84	GLY	2.8
1	F	114	PHE	2.8
1	D	309	ASN	2.8
1	C	104	ILE	2.8
1	C	342	ASP	2.8
1	F	69	LEU	2.8
1	F	460	LEU	2.8
1	C	42	SER	2.8
1	F	410	THR	2.8
1	D	144	LYS	2.8
1	F	269	LYS	2.8
1	E	451	PRO	2.8
1	A	296	TYR	2.8
1	C	37	VAL	2.8
1	E	245	VAL	2.8
1	F	299	TYR	2.8
1	B	435	LEU	2.8
1	C	309	ASN	2.8
1	A	278	ASP	2.8
1	A	42	SER	2.8
1	E	361	THR	2.8
1	E	466	SER	2.8
1	F	115	THR	2.8
1	F	392	THR	2.8
1	A	264	LYS	2.8
1	C	218	GLY	2.8
1	C	544	GLY	2.8
1	F	402	GLU	2.8
1	F	112	TYR	2.8
1	F	326	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	395	LEU	2.8
1	F	111	LEU	2.8
1	F	370	LEU	2.8
1	F	517	HIS	2.8
1	A	382	ASN	2.8
1	C	270	ASN	2.8
1	A	507	ASP	2.8
1	B	78	THR	2.8
1	E	397	LYS	2.8
1	F	137	MET	2.8
1	F	232	THR	2.8
1	F	424	THR	2.8
1	E	495	GLY	2.8
1	F	351	GLY	2.8
1	A	451	PRO	2.8
1	F	426	GLN	2.7
1	F	148	PHE	2.7
1	F	175	PHE	2.7
1	E	514	SER	2.7
1	C	522	GLN	2.7
1	C	284	VAL	2.7
1	F	45	VAL	2.7
1	B	380	ALA	2.7
1	F	271	PHE	2.7
1	A	229	HIS	2.7
1	F	243	LYS	2.7
1	C	411	GLY	2.7
1	E	530	GLY	2.7
1	F	377	GLY	2.7
1	F	335	PRO	2.7
1	A	147	SER	2.7
1	C	514	SER	2.7
1	E	334	GLU	2.7
1	D	338	VAL	2.7
1	E	253	VAL	2.7
1	E	462	VAL	2.7
1	C	527	ALA	2.7
1	D	474	ALA	2.7
1	E	40	LEU	2.7
1	A	310	TYR	2.7
1	C	294	THR	2.7
1	C	350	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	246	THR	2.7
1	F	467	ASN	2.7
1	D	544	GLY	2.7
1	F	319	ASP	2.7
1	E	441	SER	2.7
1	F	42	SER	2.7
1	F	161	SER	2.7
1	F	174	SER	2.7
1	F	438	VAL	2.7
1	B	542	LEU	2.7
1	C	167	LEU	2.7
1	E	481	PHE	2.7
1	B	34	TYR	2.7
1	C	310	TYR	2.7
1	B	74	ASN	2.7
1	B	241	THR	2.7
1	D	392	THR	2.7
1	D	411	GLY	2.7
1	F	200	THR	2.7
1	F	280	THR	2.7
1	F	544	GLY	2.7
1	A	261	VAL	2.7
1	C	79	SER	2.7
1	C	490	LEU	2.7
1	A	366	LYS	2.6
1	D	397	LYS	2.6
1	F	357	PHE	2.6
1	E	62	GLY	2.6
1	D	25	THR	2.6
1	A	145	ASP	2.6
1	A	199	LEU	2.6
1	A	409	ASP	2.6
1	C	520	VAL	2.6
1	D	170	ASP	2.6
1	F	242	GLU	2.6
1	F	268	ASP	2.6
1	F	110	MET	2.6
1	F	277	PHE	2.6
1	E	322	TYR	2.6
1	F	102	CYS	2.6
1	A	169	THR	2.6
1	E	294	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	76	THR	2.6
1	A	220	VAL	2.6
1	A	367	VAL	2.6
1	B	531	ASN	2.6
1	D	74	ASN	2.6
1	F	85	LEU	2.6
1	D	235	GLU	2.6
1	F	81	HIS	2.6
1	A	106	PRO	2.6
1	C	286	PRO	2.6
1	A	208	THR	2.6
1	C	311	VAL	2.6
1	D	226	ILE	2.6
1	E	148	PHE	2.6
1	E	271	PHE	2.6
1	F	317	PHE	2.6
1	A	262	HIS	2.6
1	C	28	TRP	2.6
1	A	183	GLY	2.6
1	C	188	PRO	2.6
1	C	326	TYR	2.6
1	C	473	LYS	2.6
1	F	333	GLY	2.6
1	F	502	PRO	2.6
1	D	435	LEU	2.6
1	A	241	THR	2.6
1	E	196	THR	2.6
1	F	93	MET	2.6
1	F	143	ILE	2.6
1	F	239	ILE	2.6
1	F	401	VAL	2.6
1	F	479	VAL	2.6
1	C	399	GLU	2.6
1	A	190	ASN	2.6
1	C	532	ALA	2.6
1	E	406	ASN	2.6
1	B	288	ASP	2.6
1	C	161	SER	2.5
1	C	139	GLY	2.5
1	E	377	GLY	2.5
1	F	97	PRO	2.5
1	F	121	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	2.5
1	C	274	MET	2.5
1	C	367	VAL	2.5
1	C	547	VAL	2.5
1	D	298	VAL	2.5
1	F	176	MET	2.5
1	F	341	VAL	2.5
1	B	22	GLU	2.5
1	C	263	THR	2.5
1	E	267	THR	2.5
1	F	465	GLN	2.5
1	D	184	ALA	2.5
1	D	532	ALA	2.5
1	F	304	ALA	2.5
1	A	244	ASN	2.5
1	C	180	ASN	2.5
1	E	270	ASN	2.5
1	F	381	ASN	2.5
1	C	268	ASP	2.5
1	E	283	ASP	2.5
1	F	432	ASP	2.5
1	A	108	SER	2.5
1	F	144	LYS	2.5
1	A	205	PRO	2.5
1	C	477	PRO	2.5
1	C	32	TRP	2.5
1	D	171	LEU	2.5
1	D	289	LEU	2.5
1	F	498	LEU	2.5
1	D	104	ILE	2.5
1	E	499	VAL	2.5
1	F	332	TYR	2.5
1	A	384	GLU	2.5
1	D	528	THR	2.5
1	F	47	THR	2.5
1	C	184	ALA	2.5
1	E	303	ALA	2.5
1	A	300	ASN	2.5
1	B	36	ASN	2.5
1	C	173	LYS	2.5
1	C	397	LYS	2.5
1	D	151	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	432	ASP	2.5
1	F	63	ASP	2.5
1	F	398	ASP	2.5
1	F	371	MET	2.5
1	B	352	VAL	2.5
1	F	257	TYR	2.5
1	D	529	GLU	2.5
1	A	184	ALA	2.5
1	A	522	GLN	2.5
1	C	267	THR	2.5
1	D	302	THR	2.5
1	F	457	ARG	2.5
1	B	397	LYS	2.5
1	C	269	LYS	2.5
1	F	36	ASN	2.5
1	F	113	ASN	2.5
1	F	292	ASN	2.5
1	A	268	ASP	2.5
1	C	398	ASP	2.5
1	E	151	ASP	2.5
1	F	170	ASP	2.5
1	C	297	MET	2.5
1	A	157	SER	2.5
1	C	325	PRO	2.5
1	A	544	GLY	2.5
1	D	127	SER	2.5
1	C	384	GLU	2.5
1	B	66	GLN	2.5
1	F	66	GLN	2.5
1	E	390	THR	2.5
1	D	27	ASN	2.5
1	F	300	ASN	2.5
1	F	316	ASN	2.5
1	A	336	ASP	2.4
1	E	374	LEU	2.4
1	D	419	GLY	2.4
1	E	95	GLY	2.4
1	A	221	SER	2.4
1	D	159	SER	2.4
1	F	344	VAL	2.4
1	C	202	GLU	2.4
1	E	227	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	256	ARG	2.4
1	F	515	GLU	2.4
1	D	105	ALA	2.4
1	D	296	TYR	2.4
1	D	303	ALA	2.4
1	F	522	GLN	2.4
1	F	23	THR	2.4
1	A	194	ASN	2.4
1	A	389	ASN	2.4
1	E	198	ASN	2.4
1	A	167	LEU	2.4
1	A	170	ASP	2.4
1	A	538	ASP	2.4
1	C	226	ILE	2.4
1	C	486	ILE	2.4
1	D	507	ASP	2.4
1	C	84	GLY	2.4
1	C	436	GLY	2.4
1	E	469	VAL	2.4
1	F	245	VAL	2.4
1	F	411	GLY	2.4
1	D	510	SER	2.4
1	E	61	LYS	2.4
1	C	480	TRP	2.4
1	A	308	GLN	2.4
1	C	379	GLN	2.4
1	C	465	GLN	2.4
1	C	550	ALA	2.4
1	E	254	ALA	2.4
1	A	280	THR	2.4
1	C	129	THR	2.4
1	C	410	THR	2.4
1	F	337	HIS	2.4
1	C	171	LEU	2.4
1	D	274	MET	2.4
1	E	231	MET	2.4
1	F	348	LEU	2.4
1	D	531	ASN	2.4
1	A	443	ASP	2.4
1	B	38	ASP	2.4
1	B	145	ASP	2.4
1	C	95	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	238	GLY	2.4
1	F	373	VAL	2.4
1	F	547	VAL	2.4
1	A	399	GLU	2.4
1	E	437	GLU	2.4
1	F	177	SER	2.4
1	A	225	TRP	2.4
1	B	449	ALA	2.4
1	A	379	GLN	2.4
1	C	225	TRP	2.4
1	A	528	THR	2.4
1	B	543	THR	2.4
1	D	23	THR	2.4
1	F	267	THR	2.4
1	E	517	HIS	2.4
1	B	99	LEU	2.4
1	D	260	LEU	2.4
1	A	381	ASN	2.4
1	A	502	PRO	2.4
1	A	546	ASN	2.4
1	F	120	VAL	2.4
1	D	378	ASP	2.4
1	E	342	ASP	2.4
1	F	283	ASP	2.4
1	C	308	GLN	2.4
1	F	408	GLN	2.4
1	C	280	THR	2.4
1	F	369	THR	2.4
1	A	192	ILE	2.4
1	C	192	ILE	2.4
1	F	314	ILE	2.4
1	D	464	PRO	2.4
1	E	464	PRO	2.4
1	C	373	VAL	2.3
1	E	467	ASN	2.3
1	C	419	GLY	2.3
1	F	183	GLY	2.3
1	D	271	PHE	2.3
1	F	52	PHE	2.3
1	F	278	ASP	2.3
1	F	393	PHE	2.3
1	F	538	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	434	ALA	2.3
1	B	534	ALA	2.3
1	F	330	ALA	2.3
1	F	334	GLU	2.3
1	E	66	GLN	2.3
1	C	221	SER	2.3
1	D	383	SER	2.3
1	A	291	LEU	2.3
1	E	412	THR	2.3
1	F	172	THR	2.3
1	C	46	ILE	2.3
1	E	425	ILE	2.3
1	C	368	PRO	2.3
1	F	414	PRO	2.3
1	D	401	VAL	2.3
1	A	31	GLY	2.3
1	F	535	ASN	2.3
1	C	146	ASP	2.3
1	C	545	GLU	2.3
1	F	145	ASP	2.3
1	F	336	ASP	2.3
1	D	304	ALA	2.3
1	F	380	ALA	2.3
1	C	466	SER	2.3
1	D	85	LEU	2.3
1	E	318	LEU	2.3
1	E	490	LEU	2.3
1	C	509	HIS	2.3
1	C	273	ILE	2.3
1	C	354	TYR	2.3
1	E	47	THR	2.3
1	E	386	TYR	2.3
1	F	213	ILE	2.3
1	B	311	VAL	2.3
1	F	469	VAL	2.3
1	C	183	GLY	2.3
1	A	467	ASN	2.3
1	C	516	ASN	2.3
1	D	198	ASN	2.3
1	F	350	ASN	2.3
1	C	162	GLU	2.3
1	C	293	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	402	GLU	2.3
1	A	541	ASP	2.3
1	B	501	ASP	2.3
1	A	204	GLN	2.3
1	B	512	GLN	2.3
1	E	28	TRP	2.3
1	B	528	THR	2.3
1	F	90	THR	2.3
1	D	34	TYR	2.3
1	D	118	TYR	2.3
1	E	256	ARG	2.3
1	C	106	PRO	2.3
1	C	401	VAL	2.3
1	E	215	ASN	2.3
1	A	297	MET	2.3
1	C	327	GLU	2.3
1	E	529	GLU	2.3
1	F	254	ALA	2.3
1	C	189	GLN	2.3
1	F	324	GLN	2.3
1	F	409	ASP	2.3
1	D	416	HIS	2.3
1	A	43	ARG	2.3
1	A	313	SER	2.3
1	E	302	THR	2.3
1	F	441	SER	2.3
1	A	526	VAL	2.3
1	B	341	VAL	2.3
1	E	344	VAL	2.3
1	F	261	VAL	2.3
1	E	436	GLY	2.3
1	A	519	GLU	2.2
1	B	550	ALA	2.2
1	A	210	LEU	2.2
1	F	395	LEU	2.2
1	C	166	ASP	2.2
1	B	314	ILE	2.2
1	E	337	HIS	2.2
1	F	524	CYS	2.2
1	A	232	THR	2.2
1	A	267	THR	2.2
1	A	306	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	451	PRO	2.2
1	E	313	SER	2.2
1	F	250	TYR	2.2
1	F	107	GLY	2.2
1	B	260	LEU	2.2
1	C	69	LEU	2.2
1	D	384	GLU	2.2
1	F	384	GLU	2.2
1	E	264	LYS	2.2
1	C	511	GLN	2.2
1	D	204	GLN	2.2
1	F	222	GLN	2.2
1	A	279	ASP	2.2
1	D	418	HIS	2.2
1	E	145	ASP	2.2
1	F	447	HIS	2.2
1	B	302	THR	2.2
1	C	193	VAL	2.2
1	D	32	TRP	2.2
1	D	547	VAL	2.2
1	E	543	THR	2.2
1	F	365	PRO	2.2
1	A	431	TYR	2.2
1	D	150	TYR	2.2
1	E	223	TYR	2.2
1	E	376	SER	2.2
1	C	197	MET	2.2
1	A	450	PHE	2.2
1	C	271	PHE	2.2
1	C	348	LEU	2.2
1	C	366	LYS	2.2
1	E	323	LEU	2.2
1	F	162	GLU	2.2
1	F	249	LEU	2.2
1	F	382	ASN	2.2
1	F	416	HIS	2.2
1	B	409	ASP	2.2
1	C	261	VAL	2.2
1	D	404	VAL	2.2
1	E	367	VAL	2.2
1	A	163	TRP	2.2
1	C	200	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	280	THR	2.2
1	F	263	THR	2.2
1	A	136	GLY	2.2
1	A	510	SER	2.2
1	C	296	TYR	2.2
1	D	525	SER	2.2
1	C	494	LEU	2.2
1	B	227	GLU	2.2
1	C	380	ALA	2.2
1	C	505	ILE	2.2
1	A	290	GLN	2.2
1	D	66	GLN	2.2
1	A	440	HIS	2.2
1	A	168	VAL	2.2
1	B	547	VAL	2.2
1	C	278	ASP	2.2
1	E	59	VAL	2.2
1	F	146	ASP	2.2
1	F	168	VAL	2.2
1	A	390	THR	2.2
1	B	23	THR	2.2
1	D	100	THR	2.2
1	A	50	GLY	2.2
1	B	544	GLY	2.2
1	D	480	TRP	2.2
1	E	201	TRP	2.2
1	E	366	LYS	2.2
1	F	139	GLY	2.2
1	A	209	TYR	2.2
1	C	332	TYR	2.2
1	F	125	TYR	2.2
1	D	542	LEU	2.2
1	F	140	LEU	2.2
1	D	143	ILE	2.1
1	A	465	GLN	2.1
1	E	423	GLN	2.1
1	A	27	ASN	2.1
1	C	407	ASN	2.1
1	E	476	ASN	2.1
1	B	451	PRO	2.1
1	E	341	VAL	2.1
1	E	401	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	281	MET	2.1
1	F	378	ASP	2.1
1	B	115	THR	2.1
1	C	207	THR	2.1
1	C	495	GLY	2.1
1	D	232	THR	2.1
1	E	263	THR	2.1
1	E	411	GLY	2.1
1	F	39	GLY	2.1
1	F	318	LEU	2.1
1	F	422	PHE	2.1
1	B	322	TYR	2.1
1	C	125	TYR	2.1
1	D	125	TYR	2.1
1	E	461	TYR	2.1
1	C	157	SER	2.1
1	F	285	ILE	2.1
1	A	87	GLN	2.1
1	C	51	GLN	2.1
1	F	511	GLN	2.1
1	F	128	HIS	2.1
1	D	347	ASN	2.1
1	B	462	VAL	2.1
1	A	231	MET	2.1
1	F	464	PRO	2.1
1	C	153	ASP	2.1
1	A	109	THR	2.1
1	B	196	THR	2.1
1	B	436	GLY	2.1
1	F	207	THR	2.1
1	A	305	LEU	2.1
1	C	277	PHE	2.1
1	C	282	LEU	2.1
1	D	86	PHE	2.1
1	F	86	PHE	2.1
1	F	54	TRP	2.1
1	A	434	ALA	2.1
1	C	35	ARG	2.1
1	E	534	ALA	2.1
1	A	383	SER	2.1
1	A	466	SER	2.1
1	E	46	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	426	GLN	2.1
1	A	216	VAL	2.1
1	B	116	VAL	2.1
1	C	195	ASN	2.1
1	C	535	ASN	2.1
1	D	245	VAL	2.1
1	F	190	ASN	2.1
1	F	328	LYS	2.1
1	D	140	LEU	2.1
1	A	246	THR	2.1
1	A	312	ASP	2.1
1	B	121	GLY	2.1
1	C	135	ASP	2.1
1	E	478	GLY	2.1
1	E	539	LEU	2.1
1	C	219	PHE	2.1
1	C	528	THR	2.1
1	E	280	THR	2.1
1	E	319	ASP	2.1
1	F	224	PHE	2.1
1	F	228	ASP	2.1
1	C	212	ARG	2.1
1	B	272	ALA	2.1
1	A	529	GLU	2.1
1	D	178	VAL	2.1
1	E	178	VAL	2.1
1	F	220	VAL	2.1
1	C	149	PRO	2.1
1	E	306	PRO	2.1
1	C	194	ASN	2.1
1	A	191	LEU	2.1
1	C	156	LEU	2.1
1	C	374	LEU	2.1
1	E	260	LEU	2.1
1	F	417	LEU	2.1
1	A	472	PHE	2.1
1	E	321	PHE	2.1
1	B	76	THR	2.1
1	C	252	THR	2.1
1	D	200	THR	2.1
1	F	35	ARG	2.1
1	B	91	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	225	TRP	2.1
1	E	360	ILE	2.1
1	B	519	GLU	2.1
1	D	22	GLU	2.1
1	E	453	TYR	2.1
1	F	386	TYR	2.1
1	C	176	MET	2.0
1	A	165	HIS	2.0
1	B	365	PRO	2.0
1	F	53	PRO	2.0
1	A	435	LEU	2.0
1	B	71	ASN	2.0
1	B	167	LEU	2.0
1	B	350	ASN	2.0
1	C	88	ASN	2.0
1	C	446	ASN	2.0
1	E	199	LEU	2.0
1	E	359	ASN	2.0
1	E	121	GLY	2.0
1	E	415	PHE	2.0
1	B	100	THR	2.0
1	B	170	ASP	2.0
1	D	273	ILE	2.0
1	E	236	ILE	2.0
1	E	424	THR	2.0
1	D	283	ASP	2.0
1	D	319	ASP	2.0
1	D	209	TYR	2.0
1	E	34	TYR	2.0
1	E	243	LYS	2.0
1	F	223	TYR	2.0
1	F	362	TYR	2.0
1	C	96	VAL	2.0
1	C	174	SER	2.0
1	D	193	VAL	2.0
1	D	523	SER	2.0
1	F	284	VAL	2.0
1	B	524	CYS	2.0
1	B	374	LEU	2.0
1	C	537	LEU	2.0
1	A	215	ASN	2.0
1	C	382	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	244	ASN	2.0
1	F	516	ASN	2.0
1	A	317	PHE	2.0
1	A	495	GLY	2.0
1	A	504	GLY	2.0
1	E	72	GLY	2.0
1	C	246	THR	2.0
1	D	430	THR	2.0
1	E	369	THR	2.0
1	E	459	THR	2.0
1	F	293	ALA	2.0
1	A	153	ASP	2.0
1	D	206	ASP	2.0
1	D	519	GLU	2.0
1	E	399	GLU	2.0
1	F	135	ASP	2.0
1	F	155	GLU	2.0
1	F	124	TRP	2.0
1	A	123	TYR	2.0
1	C	118	TYR	2.0
1	A	520	VAL	2.0
1	D	203	VAL	2.0
1	D	233	VAL	2.0
1	E	343	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	Z	6	11/12	0.34	0.27	73,75,76,76	0
5	BMA	L	3	11/12	0.36	0.24	78,80,81,81	0
2	MAN	U	4	11/12	0.42	0.24	82,84,86,86	0
5	BMA	X	3	11/12	0.42	0.21	78,80,81,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	R	3	11/12	0.43	0.21	82,84,85,87	0
4	NAG	V	2	14/15	0.44	0.21	82,83,84,85	0
2	MAN	J	5	11/12	0.46	0.24	77,78,79,79	0
4	NAG	I	2	14/15	0.46	0.25	92,95,96,96	0
2	MAN	Y	5	11/12	0.46	0.21	77,78,78,78	0
6	MAN	R	4	11/12	0.46	0.19	88,88,89,89	0
2	MAN	O	4	11/12	0.47	0.22	70,73,74,75	0
2	MAN	Y	4	11/12	0.48	0.27	78,78,79,79	0
2	MAN	J	4	11/12	0.50	0.23	74,76,77,78	0
2	MAN	M	4	11/12	0.52	0.21	91,92,93,94	0
5	NAG	W	2	14/15	0.53	0.22	52,53,54,55	0
3	MAN	H	6	11/12	0.53	0.22	98,100,100,100	0
2	MAN	S	4	11/12	0.55	0.17	96,97,98,99	0
2	MAN	U	5	11/12	0.58	0.21	89,90,91,91	0
5	NAG	W	1	14/15	0.58	0.20	58,62,65,66	0
5	BMA	K	3	11/12	0.58	0.20	73,74,75,75	0
2	NAG	U	1	14/15	0.60	0.20	69,73,76,76	0
4	NAG	P	2	14/15	0.63	0.20	89,90,92,93	0
2	MAN	S	5	11/12	0.65	0.20	95,95,96,96	0
5	NAG	K	2	14/15	0.65	0.19	73,73,74,76	0
2	NAG	O	2	14/15	0.65	0.18	68,71,71,72	0
2	NAG	J	1	14/15	0.66	0.20	74,76,80,83	0
5	BMA	W	3	11/12	0.67	0.18	47,49,50,50	0
7	MAN	T	7	11/12	0.67	0.20	92,95,96,97	0
2	MAN	O	5	11/12	0.68	0.18	74,75,75,75	0
3	MAN	N	6	11/12	0.70	0.20	96,100,100,100	0
4	NAG	V	1	14/15	0.71	0.20	75,77,78,80	0
2	BMA	O	3	11/12	0.71	0.20	71,72,73,74	0
2	MAN	G	5	11/12	0.71	0.23	90,91,94,94	0
2	MAN	G	4	11/12	0.71	0.16	92,93,94,95	0
2	NAG	U	2	14/15	0.72	0.20	76,78,80,80	0
2	NAG	a	1	14/15	-	-	73,75,78,78	0
2	NAG	a	2	14/15	-	-	71,74,75,77	0
2	BMA	a	3	11/12	-	-	78,78,80,81	0
2	MAN	a	4	11/12	-	-	74,76,76,77	0
2	MAN	a	5	11/12	-	-	81,82,83,83	0
2	NAG	d	1	14/15	-	-	70,71,73,75	0
2	NAG	d	2	14/15	-	-	75,77,79,79	0
2	BMA	d	3	11/12	-	-	81,83,86,87	0
2	MAN	d	4	11/12	-	-	87,88,89,89	0
2	MAN	d	5	11/12	-	-	88,89,89,90	0
2	NAG	f	1	14/15	-	-	72,73,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	f	2	14/15	-	-	73,74,74,74	0
2	BMA	f	3	11/12	-	-	75,76,77,78	0
2	MAN	f	4	11/12	-	-	74,76,76,76	0
2	MAN	f	5	11/12	-	-	78,79,79,79	0
2	NAG	i	1	14/15	-	-	70,71,72,72	0
2	NAG	i	2	14/15	-	-	71,71,74,75	0
2	BMA	i	3	11/12	-	-	76,77,79,82	0
2	MAN	i	4	11/12	-	-	77,78,79,79	0
2	MAN	i	5	11/12	-	-	82,84,84,85	0
2	NAG	k	1	14/15	-	-	71,72,75,76	0
2	NAG	k	2	14/15	-	-	68,70,70,71	0
2	BMA	k	3	11/12	-	-	66,67,68,68	0
2	MAN	k	4	11/12	-	-	63,65,65,65	0
2	MAN	k	5	11/12	-	-	67,69,69,69	0
4	NAG	Q	1	14/15	0.72	0.17	70,71,73,74	0
4	NAG	Q	2	14/15	0.72	0.17	74,76,77,78	0
3	NAG	Z	2	14/15	0.73	0.21	67,68,69,71	0
2	NAG	O	1	14/15	0.73	0.19	74,77,81,84	0
6	NAG	R	2	14/15	0.75	0.19	73,75,76,79	0
7	MAN	T	6	11/12	0.75	0.15	86,87,88,90	0
5	NAG	K	1	14/15	0.75	0.16	64,69,71,72	0
3	MAN	Z	4	11/12	0.76	0.22	67,68,69,69	0
2	BMA	J	3	11/12	0.77	0.19	73,74,75,77	0
2	BMA	U	3	11/12	0.77	0.18	81,83,86,88	0
2	MAN	M	5	11/12	0.77	0.16	93,94,95,95	0
2	BMA	Y	3	11/12	0.78	0.17	75,76,77,77	0
2	NAG	J	2	14/15	0.78	0.18	71,73,75,75	0
3	BMA	Z	3	11/12	0.78	0.19	70,72,73,73	0
6	NAG	R	1	14/15	0.80	0.16	68,69,71,72	0
4	NAG	P	1	14/15	0.80	0.17	76,79,81,86	0
2	BMA	S	3	11/12	0.80	0.16	87,90,93,94	0
3	NAG	Z	1	14/15	0.82	0.18	64,68,70,71	0
3	NAG	j	1	14/15	-	-	78,81,83,83	0
3	NAG	j	2	14/15	-	-	82,83,85,85	0
3	BMA	j	3	11/12	-	-	80,82,82,83	0
3	MAN	j	4	11/12	-	-	76,78,79,79	0
3	MAN	j	5	11/12	-	-	75,76,77,77	0
3	MAN	j	6	11/12	-	-	80,80,81,82	0
5	NAG	X	2	14/15	0.82	0.18	68,71,75,76	0
3	MAN	N	4	11/12	0.82	0.15	73,77,78,79	0
3	BMA	N	3	11/12	0.83	0.14	79,85,88,92	0
7	NAG	T	1	14/15	0.84	0.17	69,70,76,79	0

Continued on next page...

Continued from previous page...

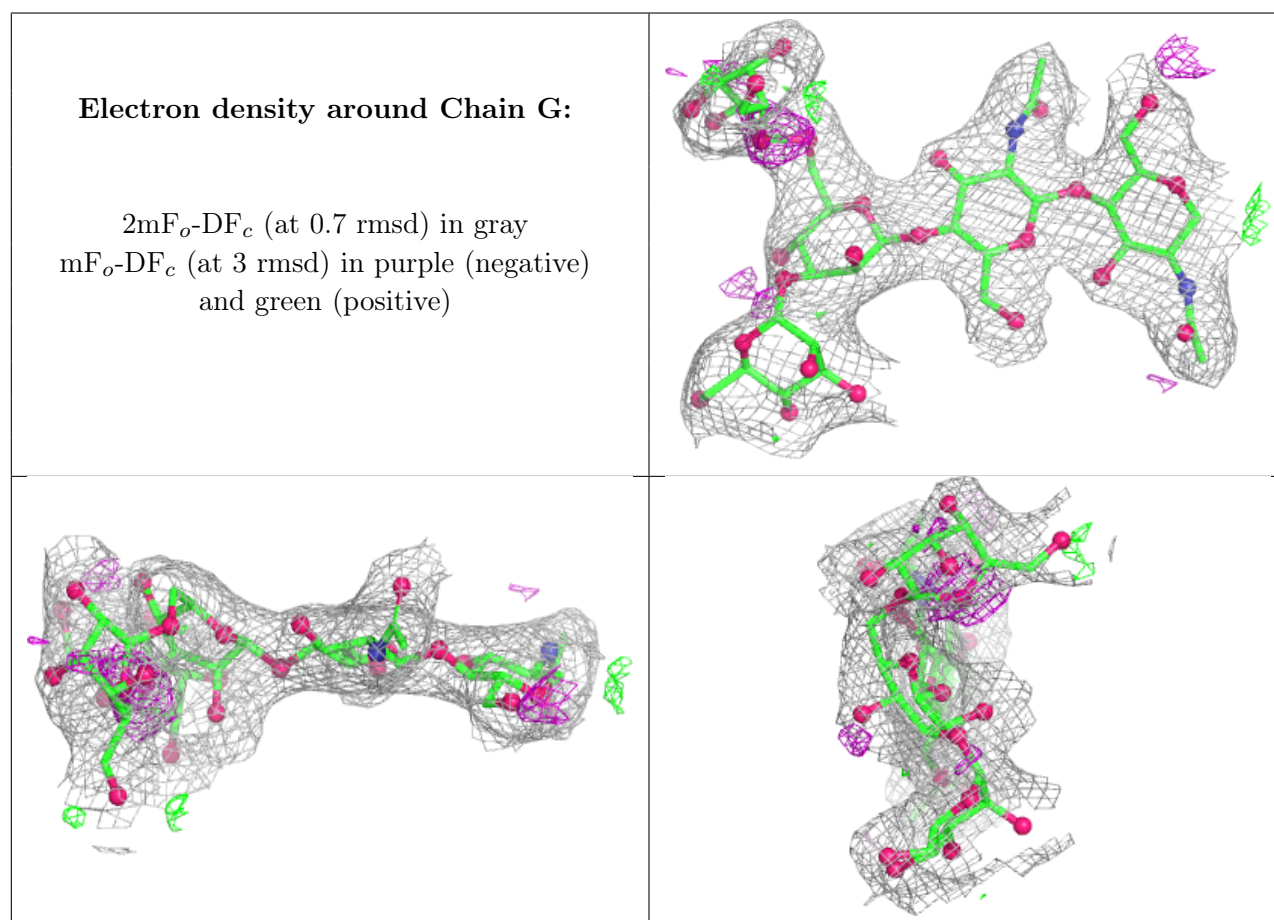
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	M	3	11/12	0.85	0.15	82,85,89,90	0
3	MAN	Z	5	11/12	0.85	0.16	63,64,65,65	0
5	NAG	X	1	14/15	0.86	0.13	62,64,67,68	0
2	BMA	G	3	11/12	0.86	0.14	80,84,88,89	0
4	NAG	b	1	14/15	-	-	68,69,70,72	0
4	NAG	b	2	14/15	-	-	73,74,75,76	0
4	NAG	g	1	14/15	-	-	65,67,67,67	0
4	NAG	g	2	14/15	-	-	64,65,66,66	0
4	NAG	I	1	14/15	0.87	0.14	71,76,80,87	0
7	BMA	T	3	11/12	0.88	0.14	77,81,85,88	0
2	NAG	Y	2	14/15	0.88	0.14	70,72,74,74	0
5	NAG	L	2	14/15	0.88	0.15	71,72,73,75	0
3	NAG	N	1	14/15	0.89	0.14	70,74,77,77	0
5	NAG	L	1	14/15	0.89	0.13	64,67,69,70	0
3	MAN	H	4	11/12	0.90	0.13	74,77,78,79	0
2	NAG	S	2	14/15	0.90	0.12	71,74,78,82	0
2	NAG	Y	1	14/15	0.90	0.12	68,69,69,71	0
7	MAN	T	4	11/12	0.90	0.13	72,76,80,83	0
3	NAG	H	1	14/15	0.90	0.14	67,72,78,80	0
3	BMA	H	3	11/12	0.90	0.11	80,86,89,93	0
5	NAG	c	1	14/15	-	-	72,73,75,76	0
5	NAG	c	2	14/15	-	-	75,76,76,78	0
5	BMA	c	3	11/12	-	-	80,80,80,81	0
5	NAG	h	1	14/15	-	-	63,66,69,69	0
5	NAG	h	2	14/15	-	-	65,65,66,66	0
5	BMA	h	3	11/12	-	-	65,66,66,66	0
5	NAG	l	1	14/15	-	-	75,76,77,77	0
5	NAG	l	2	14/15	-	-	77,78,79,81	0
5	BMA	l	3	11/12	-	-	81,82,82,83	0
2	NAG	S	1	14/15	0.91	0.12	67,69,71,72	0
3	NAG	N	2	14/15	0.92	0.15	78,79,80,82	0
7	NAG	T	2	14/15	0.93	0.13	72,75,77,79	0
2	NAG	M	1	14/15	0.93	0.12	67,68,70,71	0
3	NAG	H	2	14/15	0.93	0.14	79,82,86,86	0
2	NAG	G	1	14/15	0.93	0.11	63,65,68,68	0
3	MAN	N	5	11/12	0.93	0.11	68,70,71,73	0
3	MAN	H	5	11/12	0.94	0.10	67,72,73,75	0
2	NAG	M	2	14/15	0.94	0.10	72,74,76,79	0
2	NAG	G	2	14/15	0.95	0.11	70,72,73,77	0
7	MAN	T	5	11/12	0.95	0.09	64,65,66,67	0
7	NAG	e	1	14/15	-	-	76,77,79,79	0
7	NAG	e	2	14/15	-	-	80,82,82,83	0

Continued on next page...

Continued from previous page...

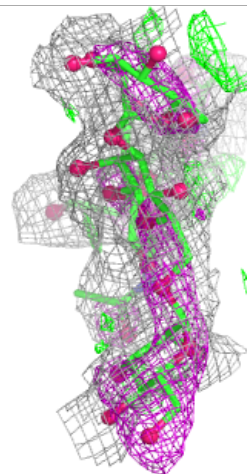
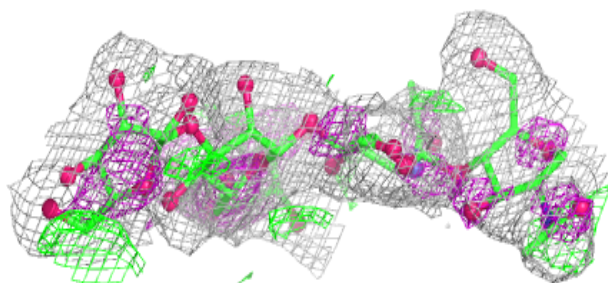
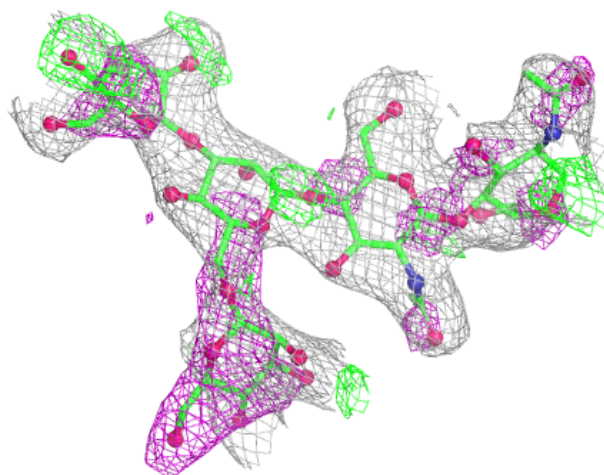
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BMA	e	3	11/12	-	-	82,86,89,92	0
7	MAN	e	4	11/12	-	-	76,80,82,84	0
7	MAN	e	5	11/12	-	-	71,72,73,73	0
7	MAN	e	6	11/12	-	-	83,85,86,87	0
7	MAN	e	7	11/12	-	-	95,97,97,97	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



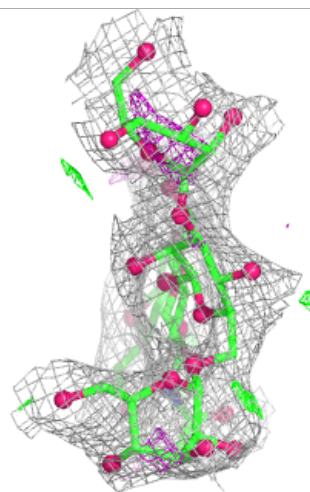
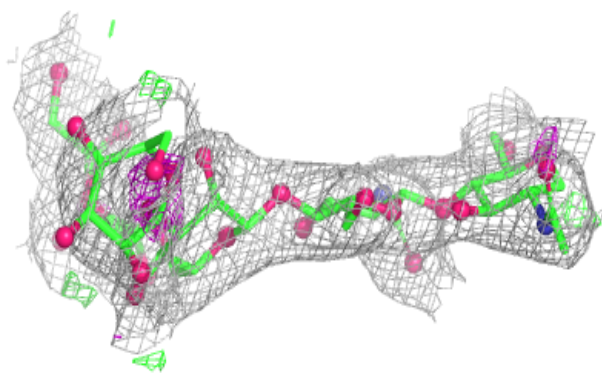
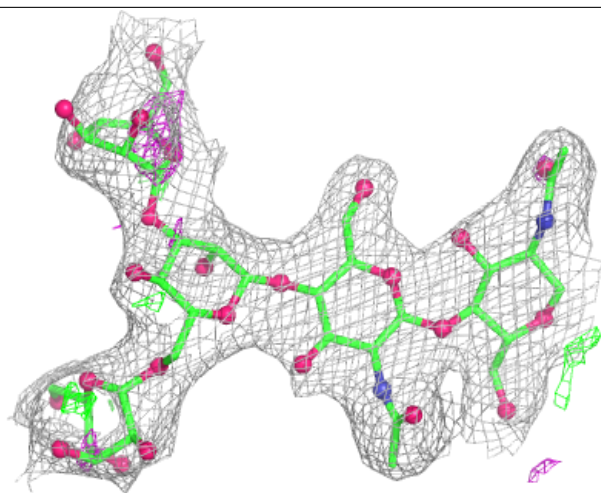
Electron density around Chain J:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



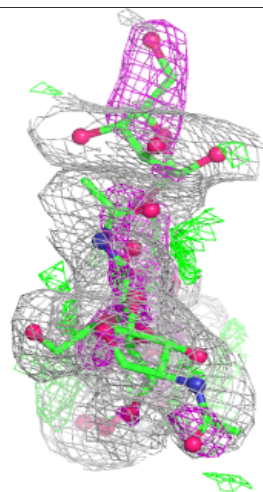
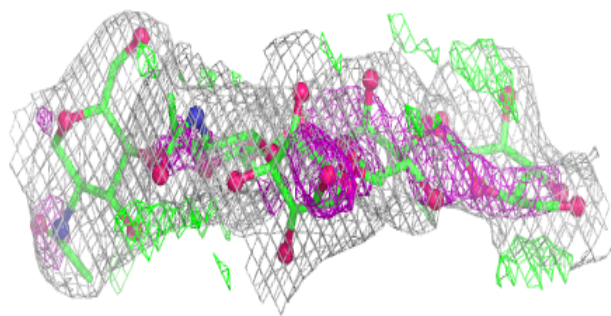
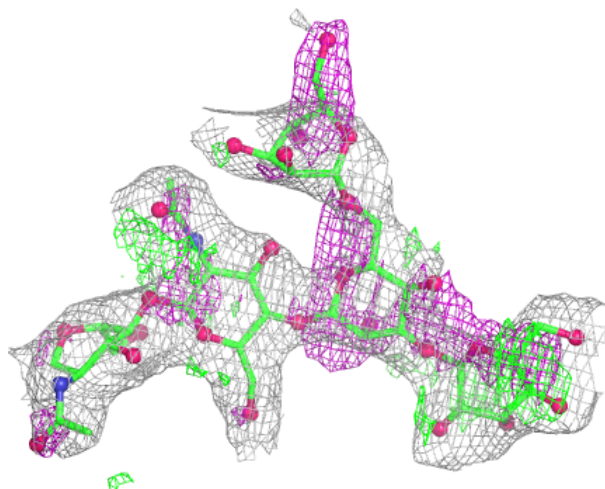
Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



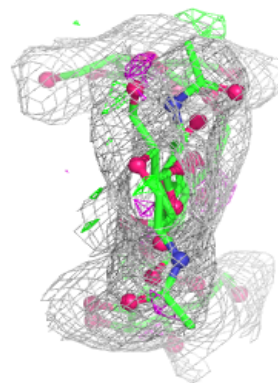
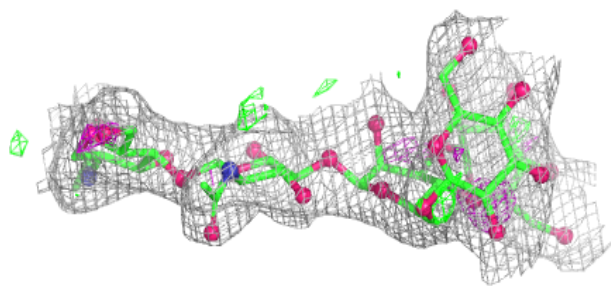
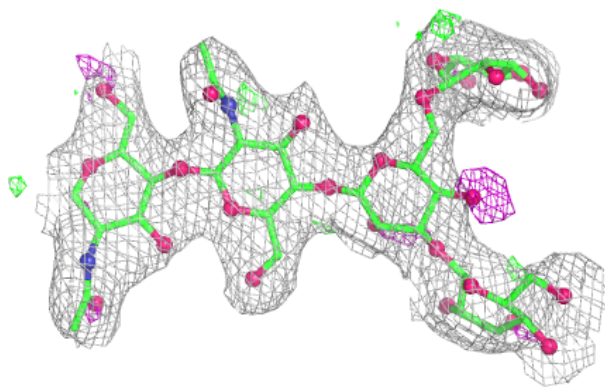
Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

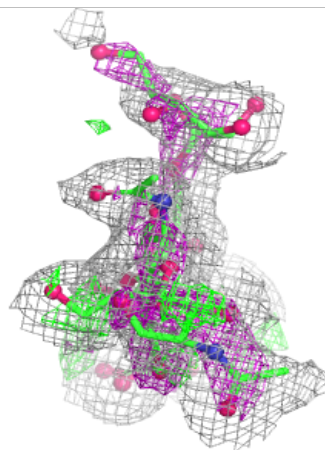
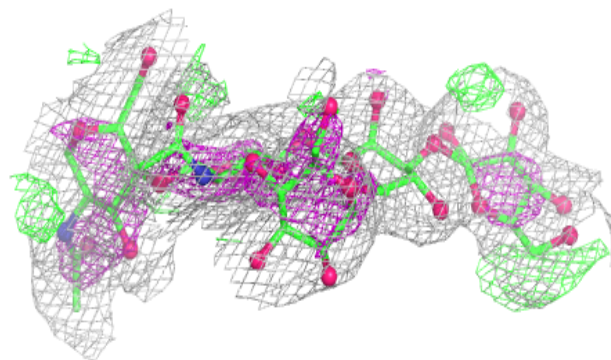
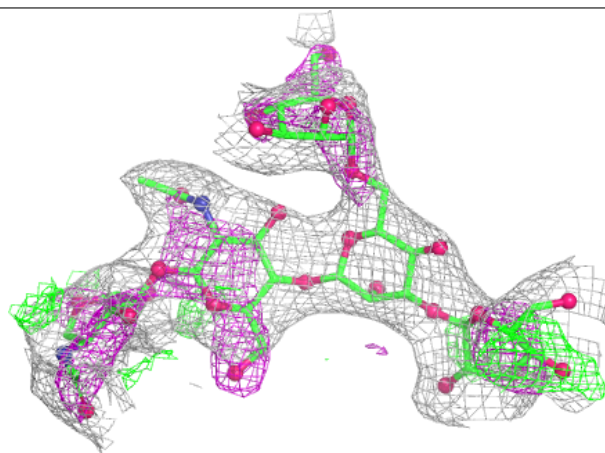


Electron density around Chain S:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

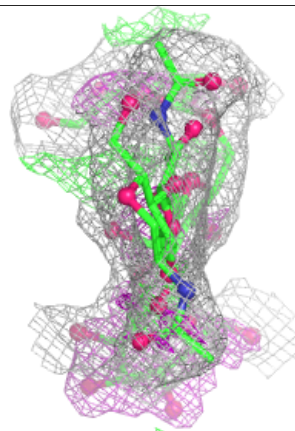
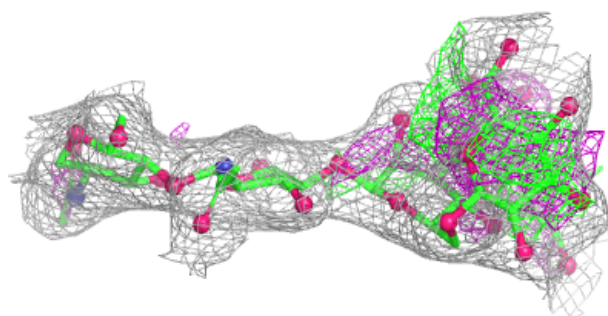
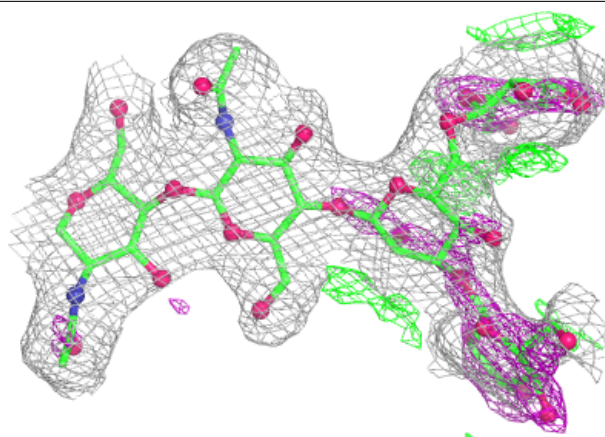
**Electron density around Chain U:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

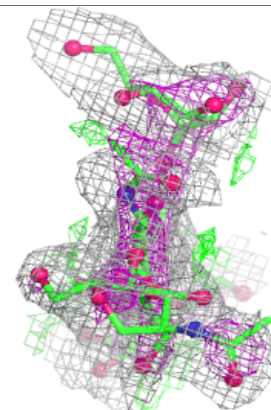
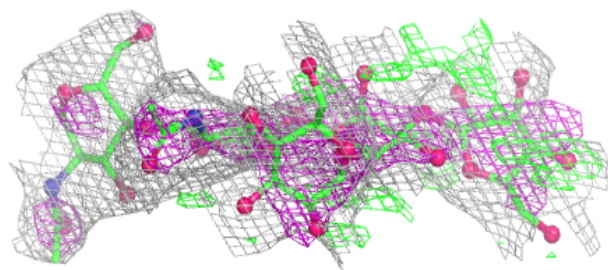
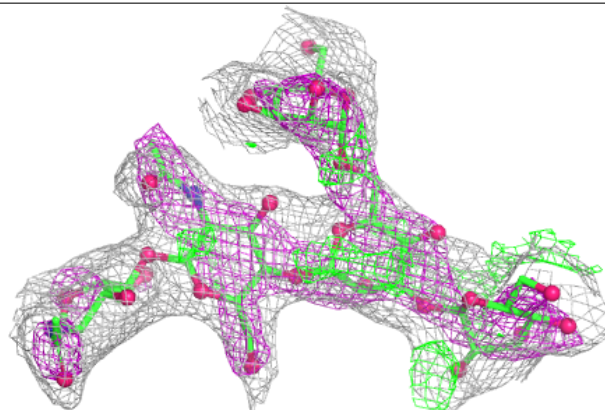


Electron density around Chain Y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

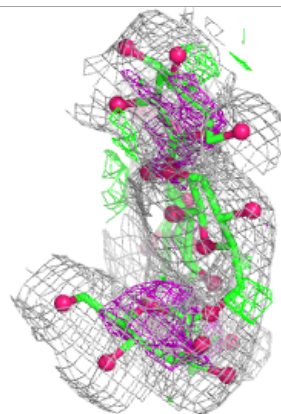
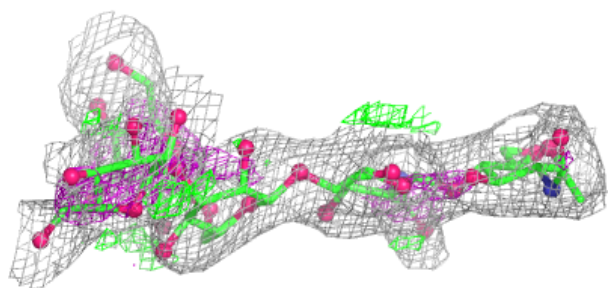
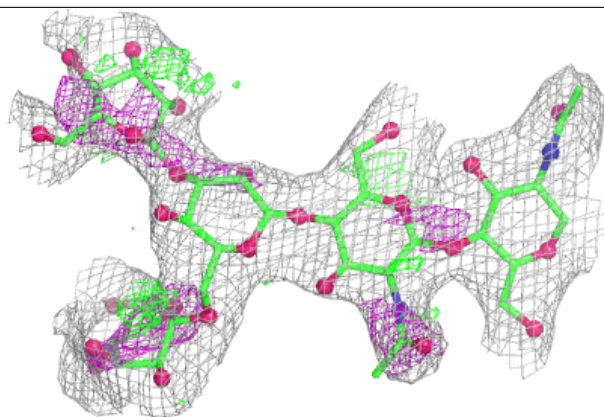
**Electron density around Chain a:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

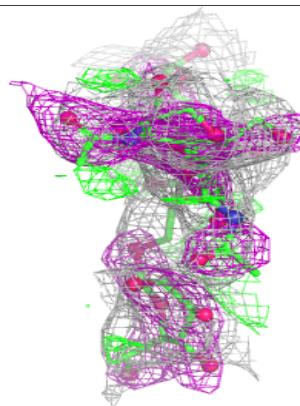
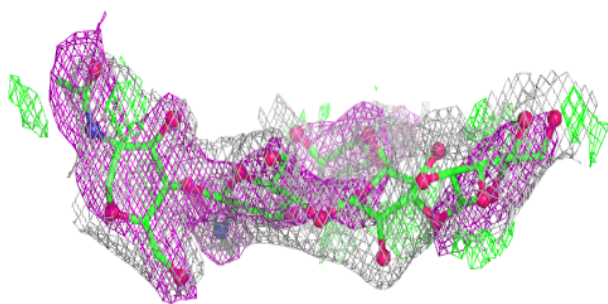
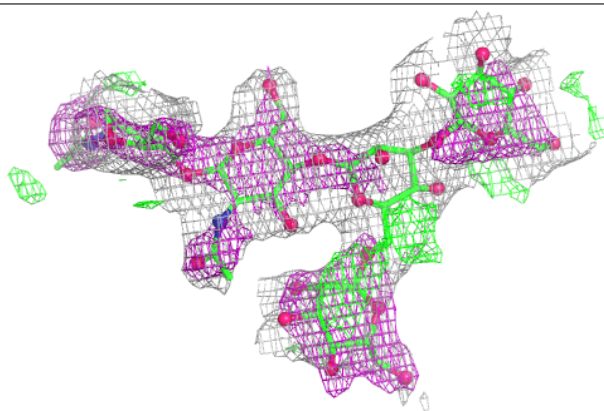


Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

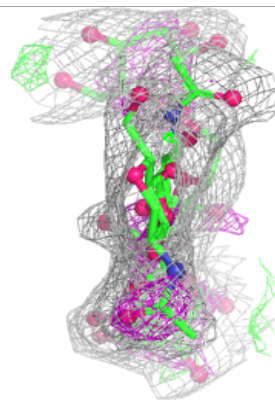
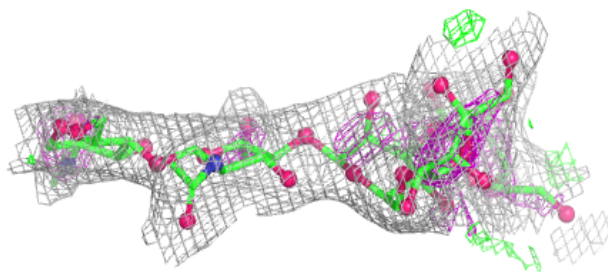
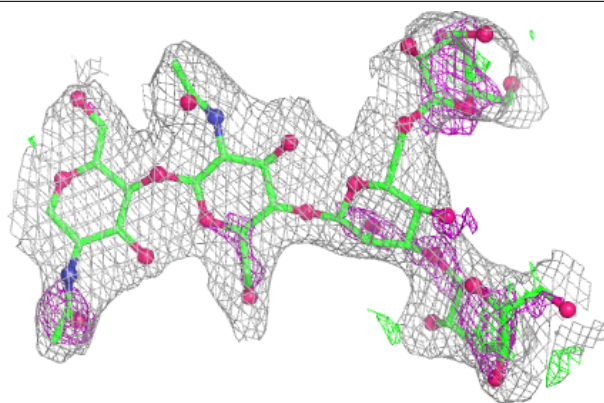
**Electron density around Chain f:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



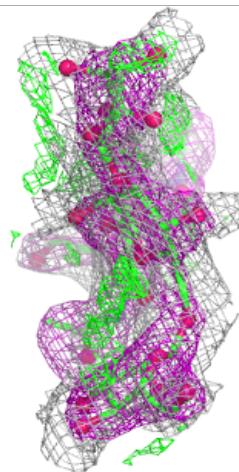
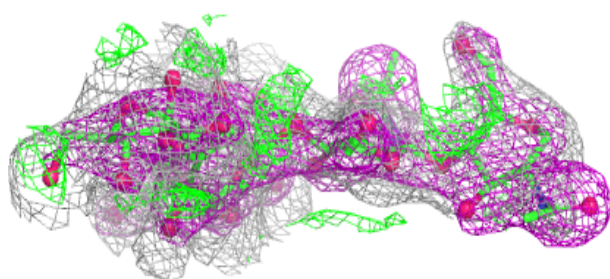
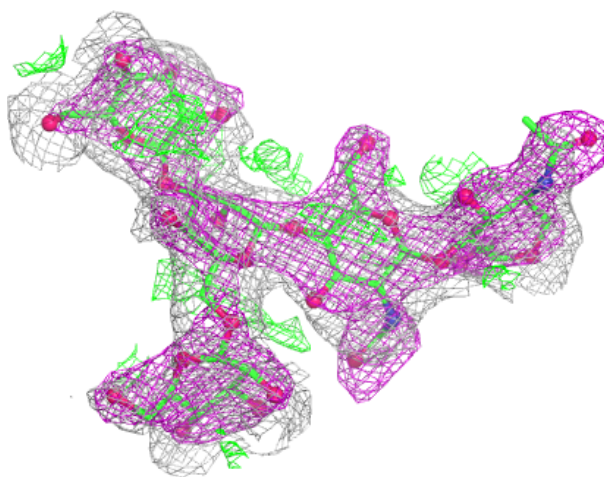
Electron density around Chain i:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



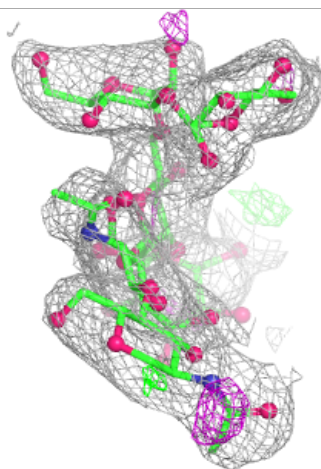
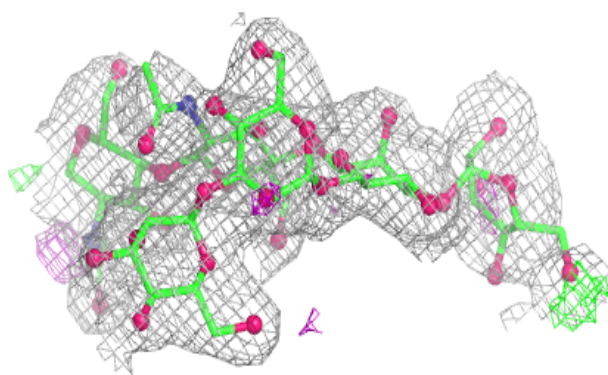
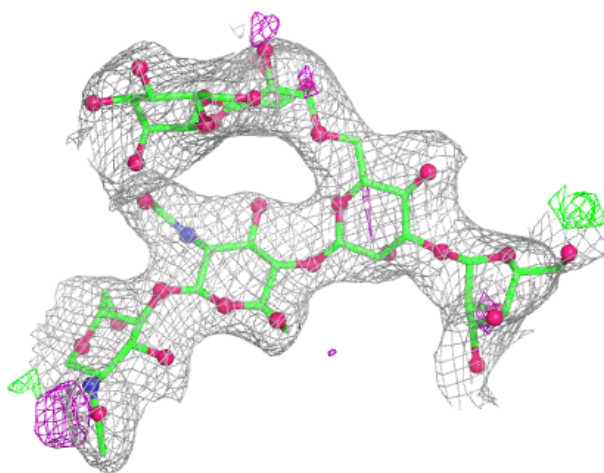
Electron density around Chain k:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



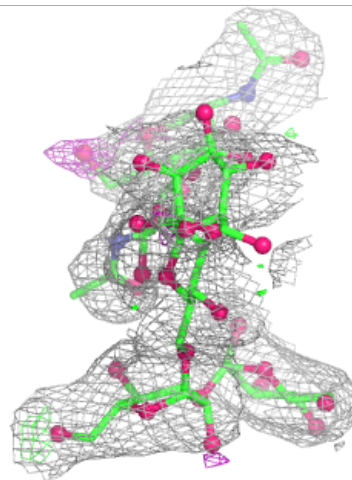
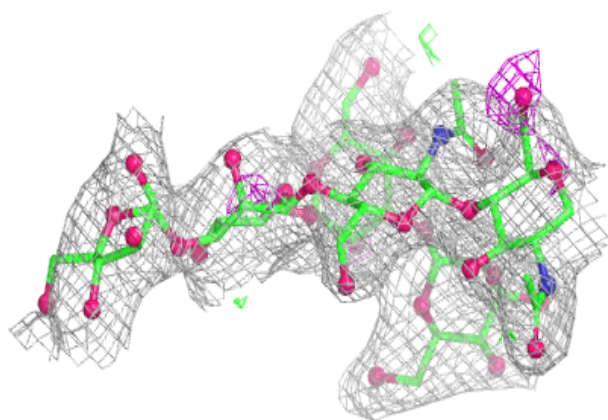
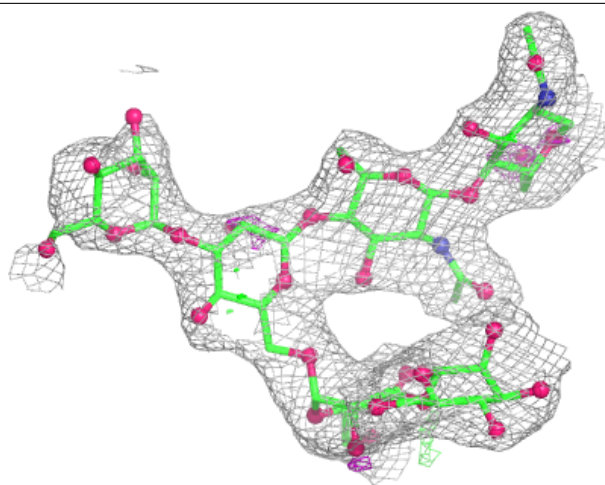
Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



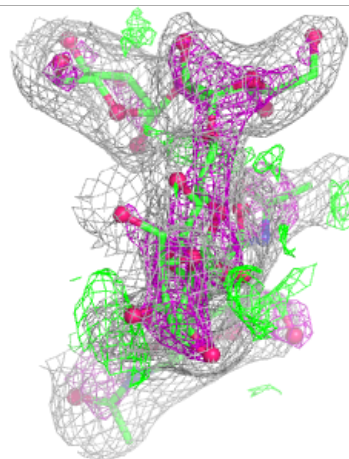
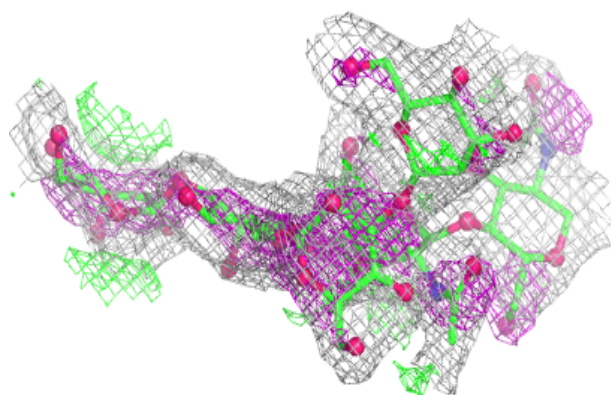
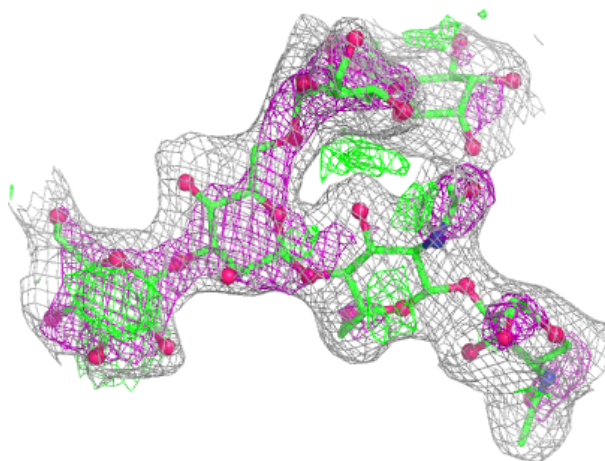
Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



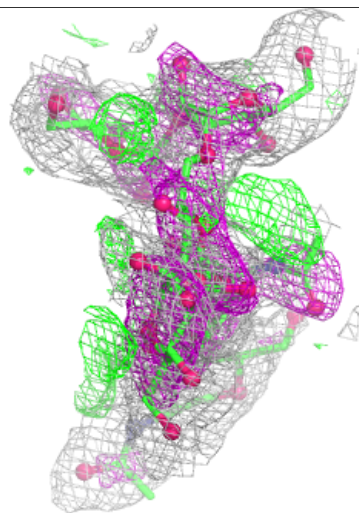
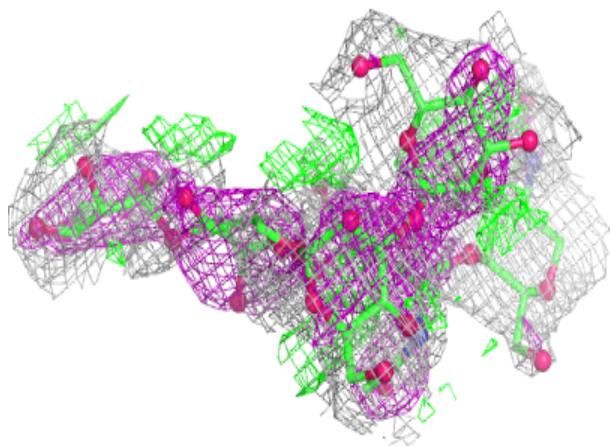
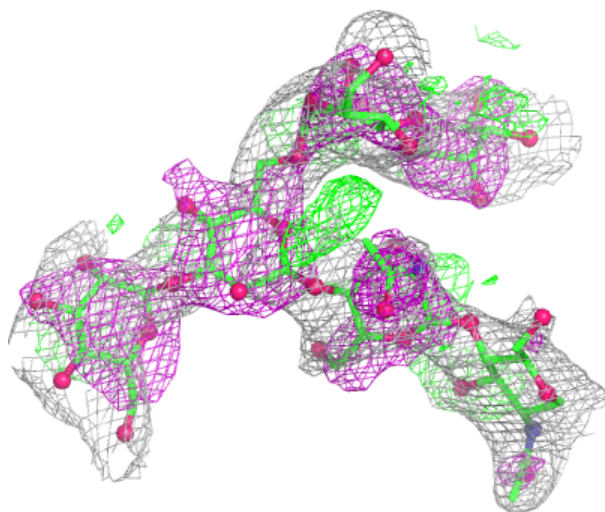
Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



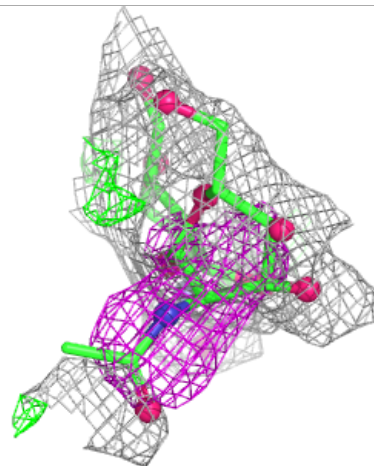
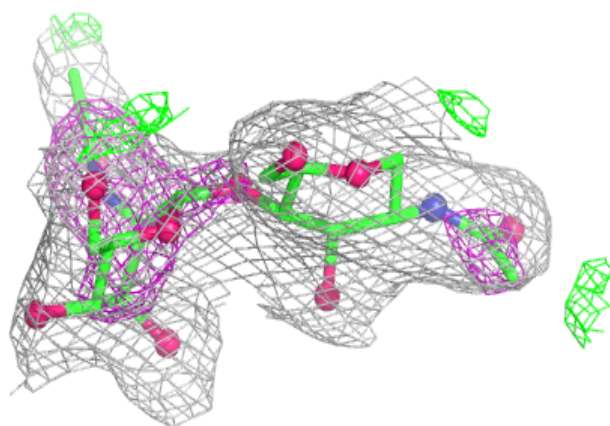
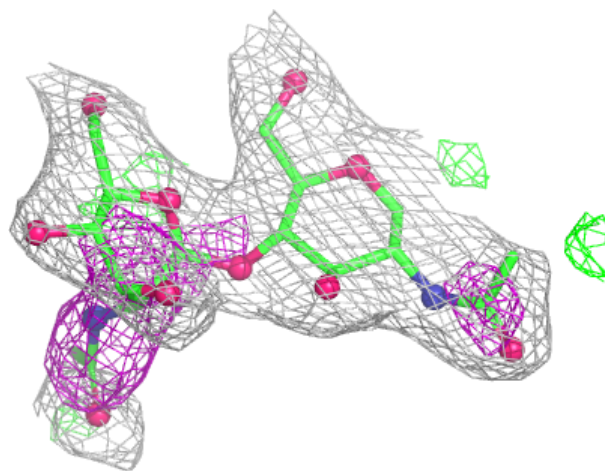
Electron density around Chain j:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



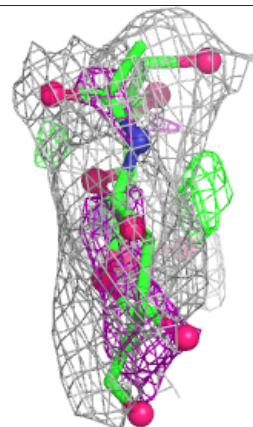
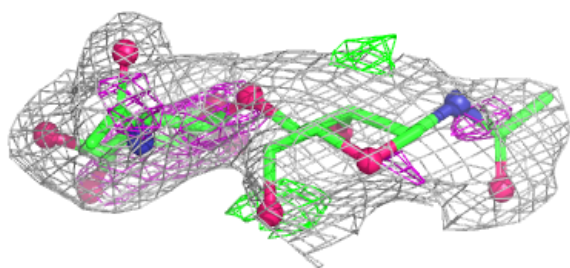
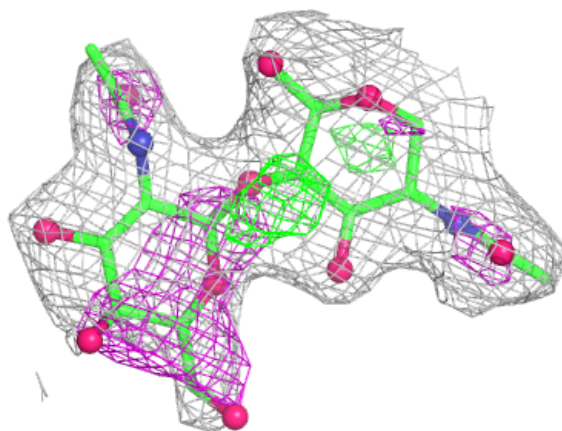
Electron density around Chain I:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



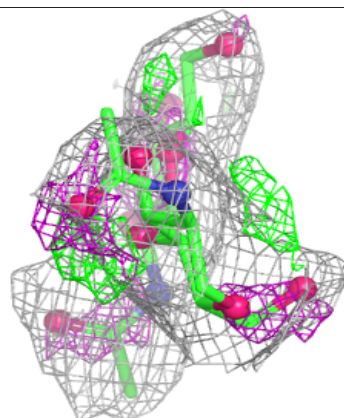
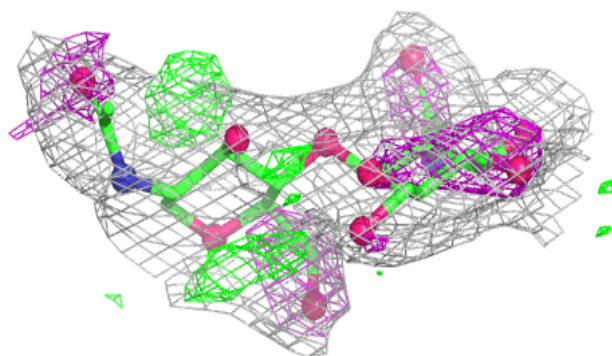
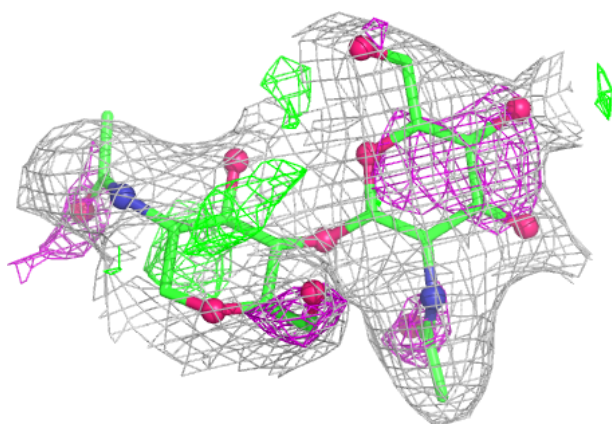
Electron density around Chain P:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

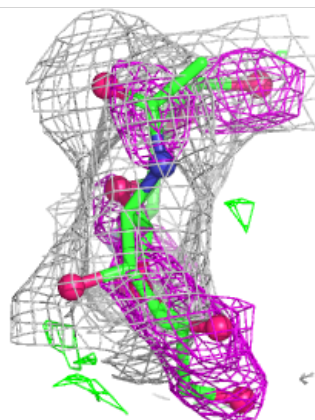
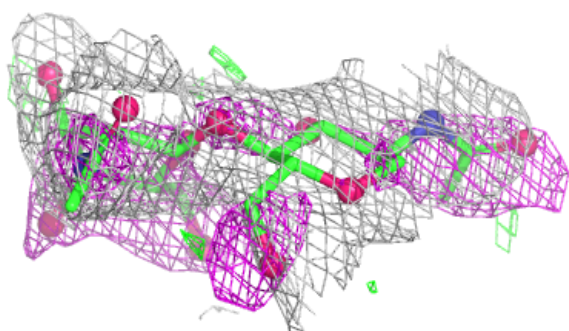
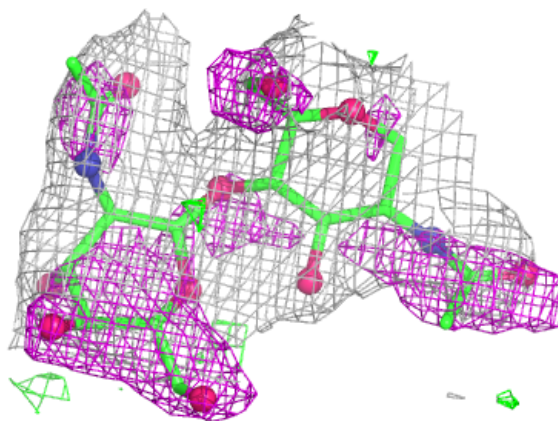


Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

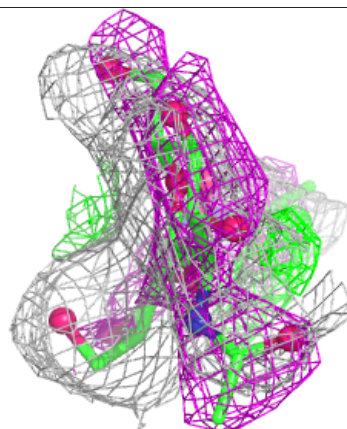
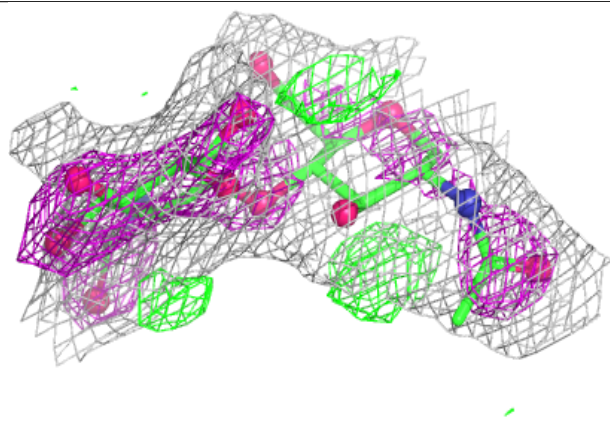
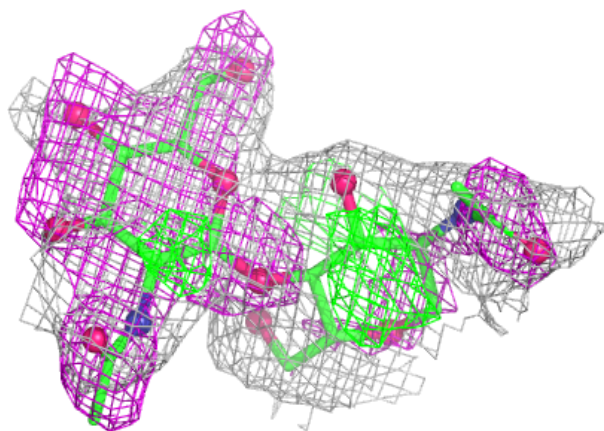
**Electron density around Chain V:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



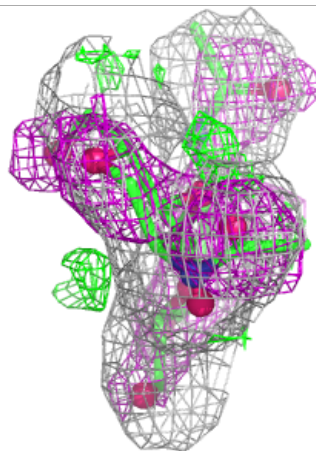
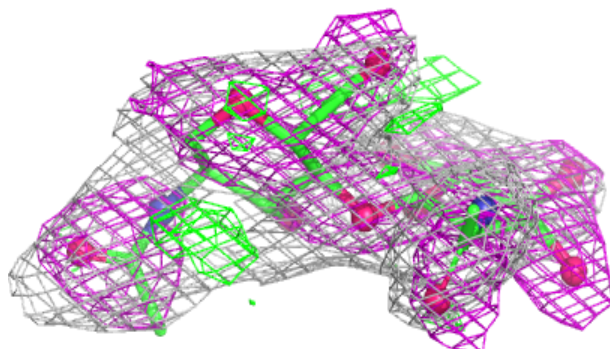
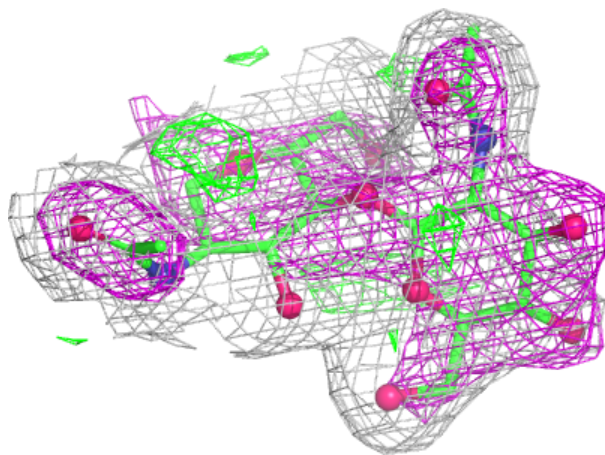
Electron density around Chain b:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



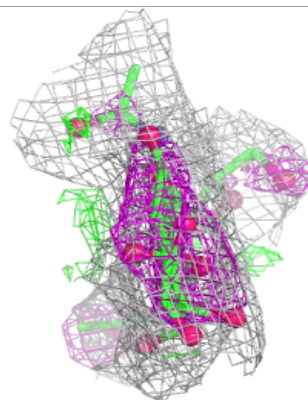
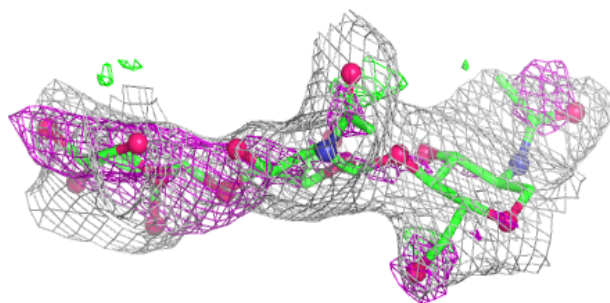
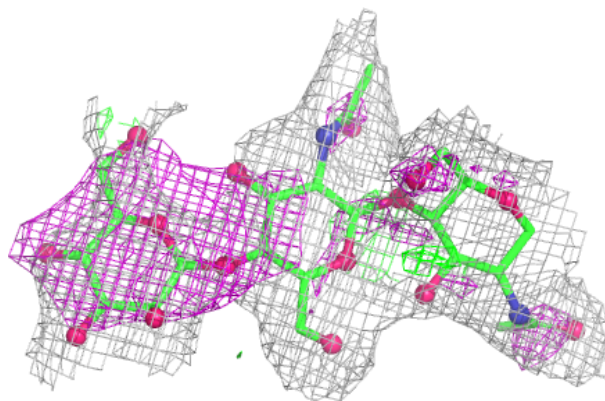
Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

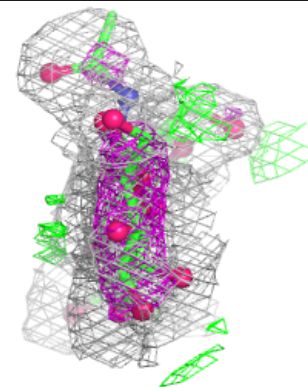
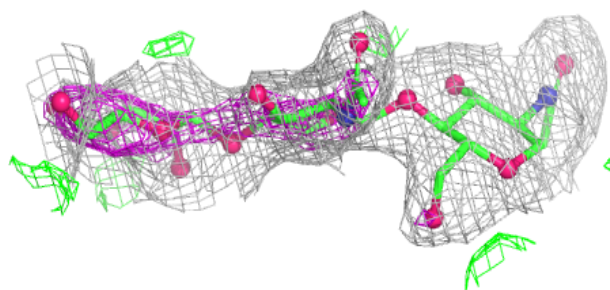
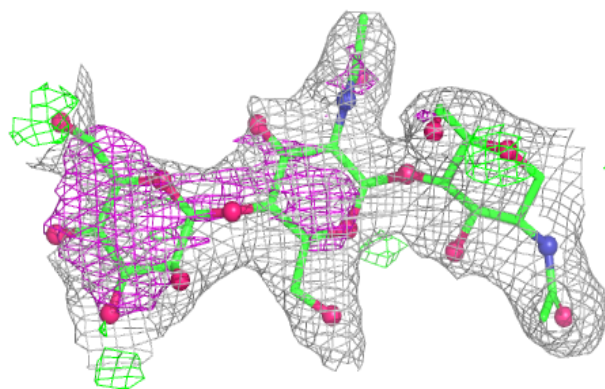


Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

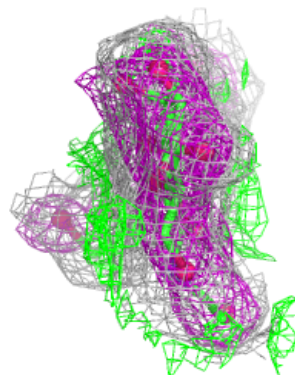
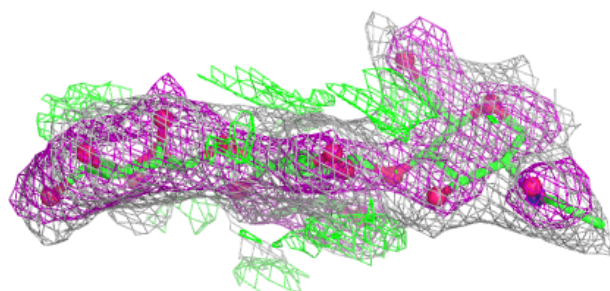
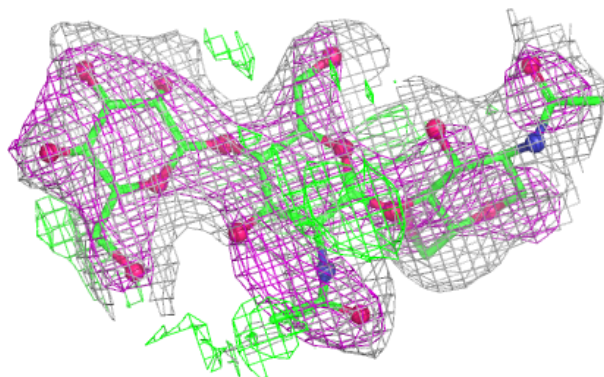
**Electron density around Chain L:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

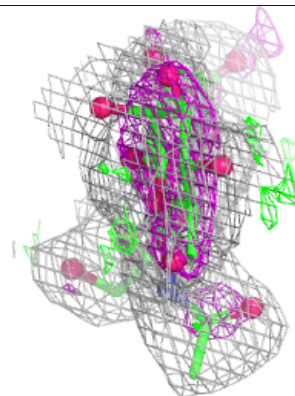
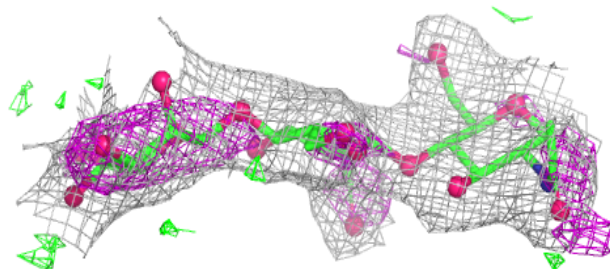
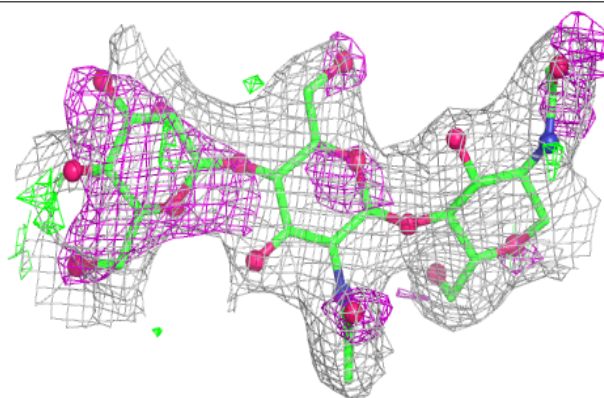


Electron density around Chain W:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

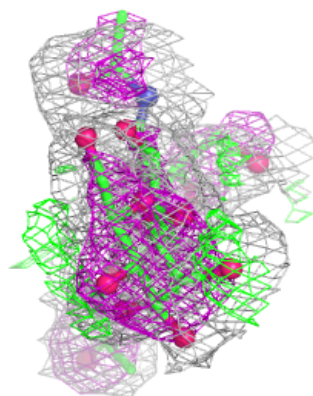
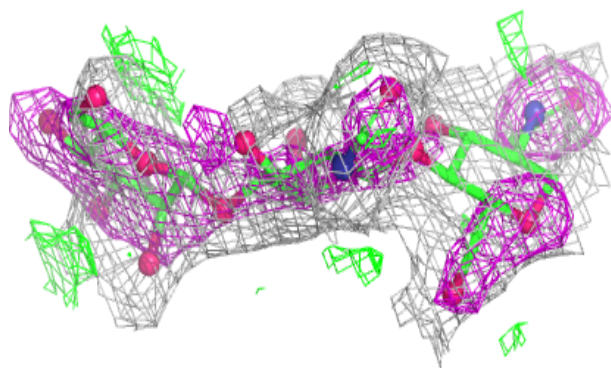
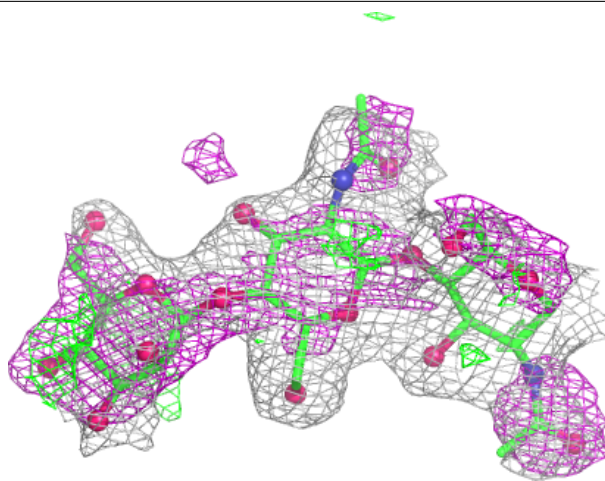
**Electron density around Chain X:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



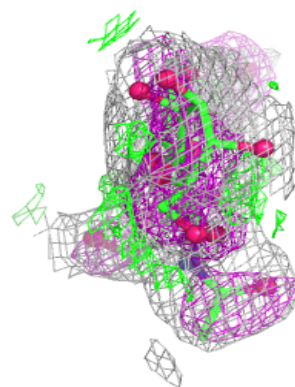
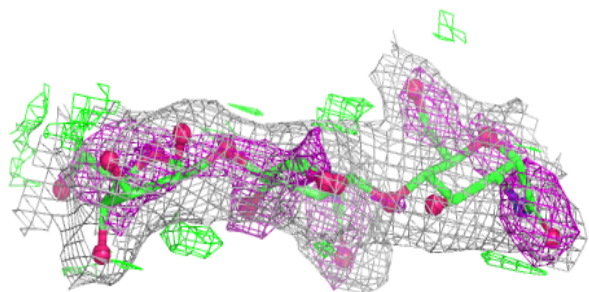
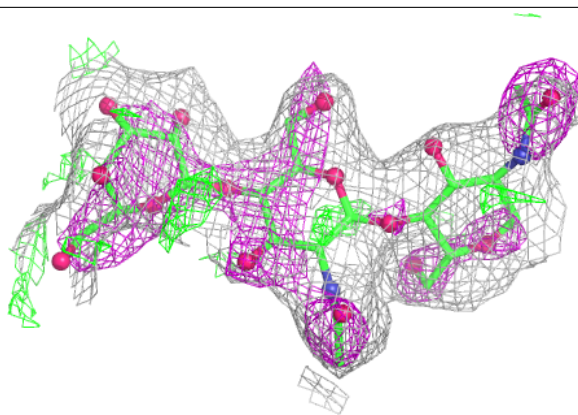
Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

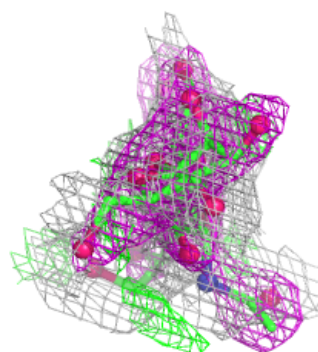
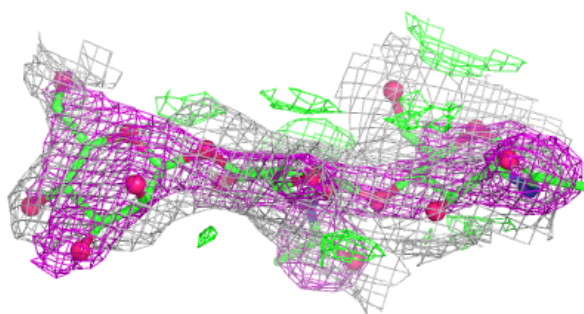
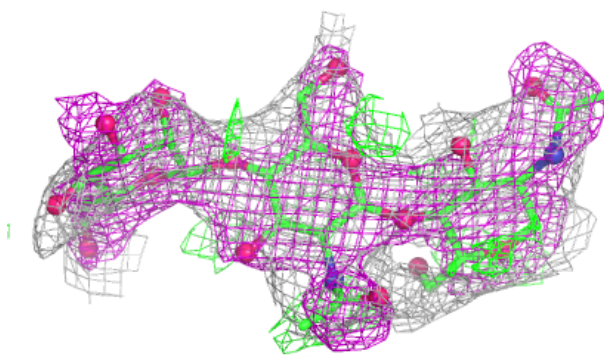


Electron density around Chain h:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

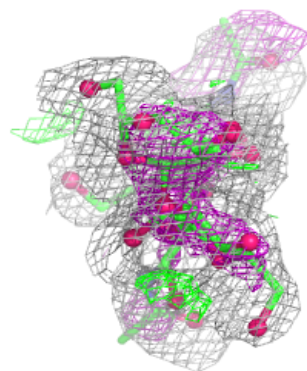
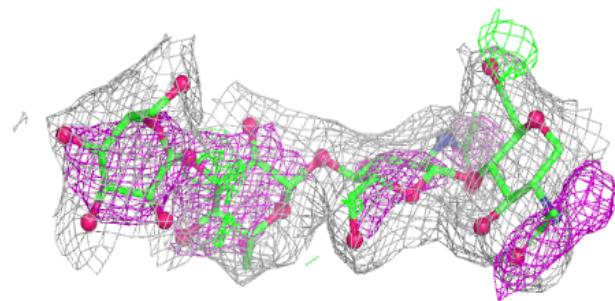
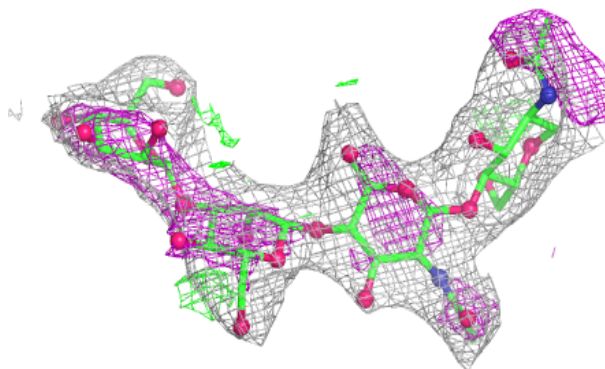
**Electron density around Chain l:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



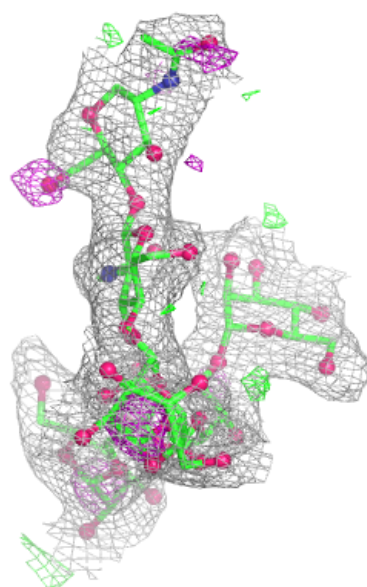
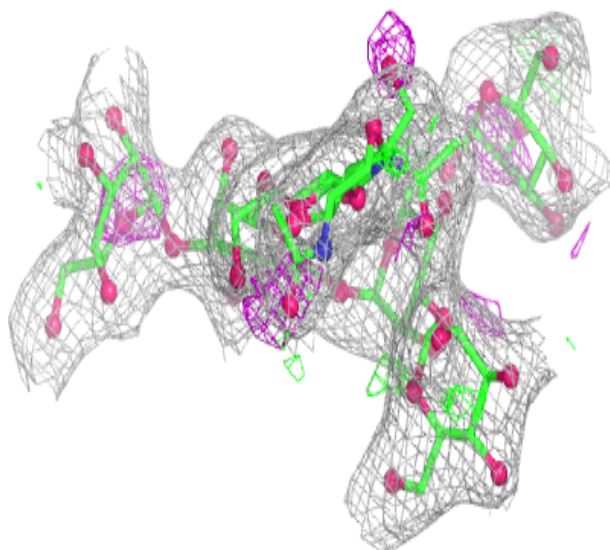
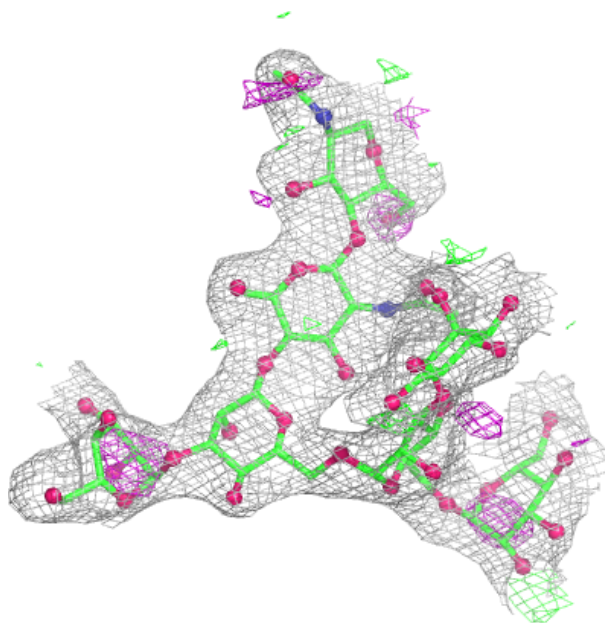
Electron density around Chain R:

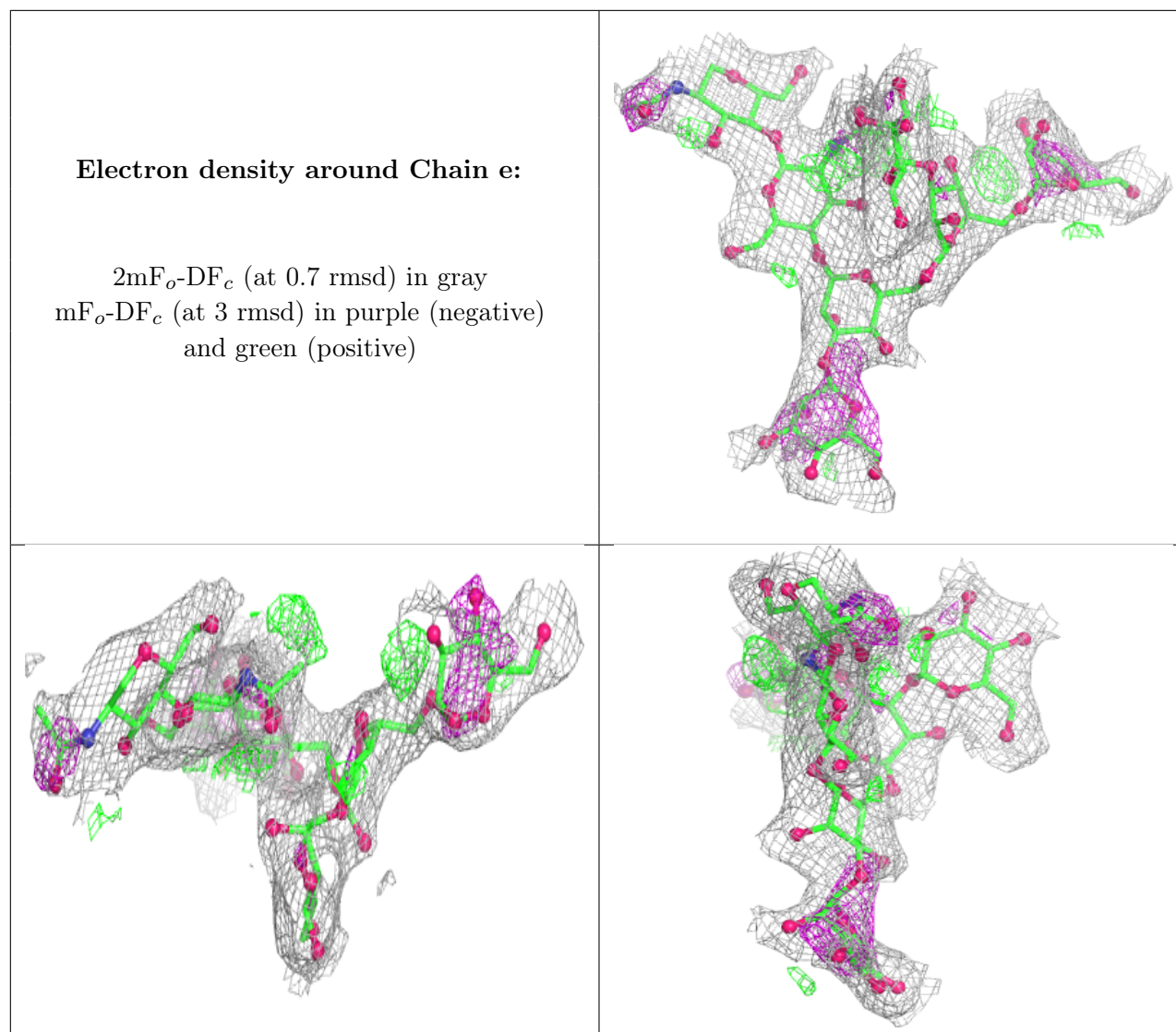
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	E	2005	14/15	0.29	0.23	70,71,71,71	0
8	NAG	E	2012	14/15	0.35	0.23	73,74,77,77	0
8	NAG	F	2012	14/15	0.35	0.22	72,73,75,75	0
8	NAG	F	2006	14/15	0.37	0.23	67,68,70,70	0
8	NAG	C	2018	14/15	0.52	0.19	74,76,77,78	0
8	NAG	E	2008	14/15	0.53	0.22	72,72,73,73	0
8	NAG	A	2018	14/15	0.53	0.20	78,80,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	D	2014	14/15	0.54	0.21	65,66,67,67	0
8	NAG	E	2006	14/15	0.55	0.22	73,74,75,76	0
8	NAG	F	2008	14/15	0.56	0.23	71,71,72,72	0
8	NAG	B	2014	14/15	0.56	0.22	67,70,71,71	0
8	NAG	B	2018	14/15	0.60	0.18	80,83,83,83	0
8	NAG	F	2005	14/15	0.61	0.18	67,70,71,72	0
8	NAG	F	2009	14/15	0.61	0.19	66,69,69,69	0
8	NAG	C	2006	14/15	0.61	0.19	74,76,77,78	0
8	NAG	D	2006	14/15	0.63	0.18	65,68,70,71	0
8	NAG	A	2006	14/15	0.64	0.19	71,73,74,74	0
8	NAG	C	2012	14/15	0.69	0.18	75,77,79,80	0
8	NAG	A	2012	14/15	0.71	0.18	76,79,80,81	0
8	NAG	D	2012	14/15	0.72	0.16	73,74,76,77	0
8	NAG	D	2008	14/15	0.73	0.19	70,71,73,73	0
8	NAG	D	2005	14/15	0.73	0.18	71,72,74,75	0
8	NAG	F	2014	14/15	0.74	0.16	59,62,63,64	0
8	NAG	B	2006	14/15	0.76	0.14	74,76,78,79	0
8	NAG	A	2014	14/15	0.79	0.16	67,67,71,72	0
8	NAG	B	2012	14/15	0.79	0.15	74,75,79,79	0
8	NAG	B	2005	14/15	0.83	0.14	64,67,69,70	0
8	NAG	C	2005	14/15	0.83	0.16	64,68,70,70	0
8	NAG	E	2014	14/15	0.84	0.13	52,56,57,58	0
8	NAG	A	2008	14/15	0.86	0.15	68,69,70,70	0
8	NAG	C	2014	14/15	0.88	0.12	53,55,57,58	0
9	CU1	F	1001	1/1	0.88	0.19	90,90,90,90	0
9	CU1	D	1004	1/1	0.91	0.19	100,100,100,100	0
9	CU1	F	1004	1/1	0.94	0.17	100,100,100,100	0
9	CU1	F	1003	1/1	0.95	0.14	91,91,91,91	0
9	CU1	A	1004	1/1	0.95	0.12	100,100,100,100	0
9	CU1	E	1003	1/1	0.96	0.14	99,99,99,99	0
9	CU1	E	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	C	1004	1/1	0.96	0.15	100,100,100,100	0
9	CU1	F	1002	1/1	0.96	0.10	96,96,96,96	0
9	CU1	C	1001	1/1	0.96	0.07	85,85,85,85	0
9	CU1	E	1001	1/1	0.96	0.14	88,88,88,88	0
9	CU1	D	1003	1/1	0.97	0.07	89,89,89,89	0
9	CU1	B	1004	1/1	0.97	0.07	100,100,100,100	0
9	CU1	D	1001	1/1	0.97	0.05	86,86,86,86	0
9	CU1	E	1002	1/1	0.97	0.16	93,93,93,93	0
9	CU1	D	1002	1/1	0.97	0.07	87,87,87,87	0
9	CU1	C	1003	1/1	0.98	0.05	83,83,83,83	0
9	CU1	B	1002	1/1	0.98	0.09	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CU1	B	1003	1/1	0.99	0.09	87,87,87,87	0
9	CU1	A	1003	1/1	0.99	0.10	89,89,89,89	0
9	CU1	A	1001	1/1	0.99	0.03	82,82,82,82	0
9	CU1	C	1002	1/1	0.99	0.04	85,85,85,85	0
9	CU1	B	1001	1/1	0.99	0.05	87,87,87,87	0
9	CU1	A	1002	1/1	0.99	0.09	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.