



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:45 PM BST

PDB ID : 6OM1  
Title : Crystal structure of an atypical integrin  
Authors : Wang, J.C.; Springer, T.A.  
Deposited on : 2019-04-17  
Resolution : 2.66 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

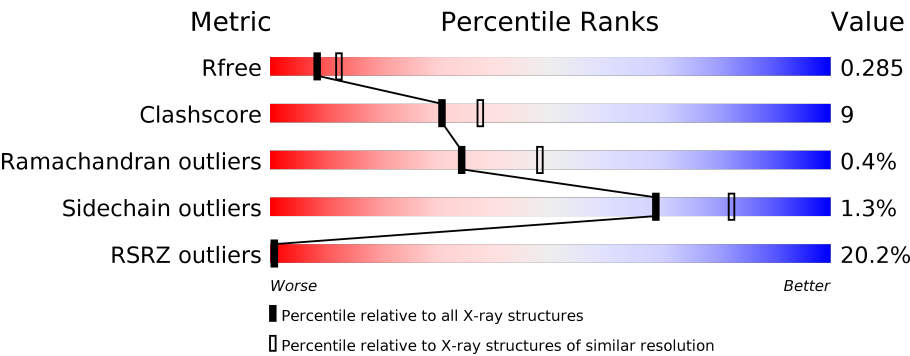
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	599	<div><div>6%</div><div><div></div><div>85%</div><div>13%</div><div>..</div></div></div>
1	C	599	<div><div>10%</div><div><div></div><div>85%</div><div>13%</div><div>..</div></div></div>
1	E	599	<div><div>18%</div><div><div></div><div>80%</div><div>18%</div><div>..</div></div></div>
1	G	599	<div><div>20%</div><div><div></div><div>85%</div><div>13%</div><div>..</div></div></div>
2	B	456	<div><div>17%</div><div><div></div><div>54%</div><div>18%</div><div>27%</div></div></div>
2	D	456	<div><div>25%</div><div><div></div><div>55%</div><div>13%</div><div>32%</div></div></div>

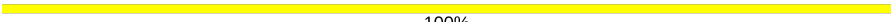

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Mol	Chain	Length	Quality of chain
2	F	456	
2	H	456	
3	I	4	
3	K	4	
3	O	4	
3	Q	4	
3	S	4	
3	a	4	
3	d	4	
4	J	5	
4	U	5	
4	X	5	
5	L	6	
6	M	2	
6	N	2	
6	T	2	
6	V	2	
6	Y	2	
6	Z	2	
6	e	2	
6	f	2	
6	g	2	
7	P	6	
7	R	6	
7	W	6	

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Mol	Chain	Length	Quality of chain
8	b	6	 100%
9	c	4	 75% 25%

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
10	NAG	C	601	-	-	-	X
10	NAG	C	626	-	-	-	X
10	NAG	F	501	-	-	-	X
10	NAG	G	2023	-	-	-	X
10	NAG	G	2024	-	-	-	X
12	EDO	C	629	-	-	-	X
3	NAG	I	1	-	-	-	X
3	NAG	I	2	-	-	X	-
3	BMA	I	3	-	-	X	-
3	MAN	I	4	-	-	-	X
3	BMA	Q	3	-	-	X	-
6	NAG	M	2	-	-	-	X
6	NAG	T	1	-	-	-	X
6	NAG	T	2	-	-	-	X
6	NAG	Z	2	-	-	-	X
6	NAG	e	1	-	-	-	X
6	NAG	e	2	-	-	-	X
6	NAG	g	2	-	-	-	X
7	BMA	R	3	-	-	X	-
7	BMA	W	3	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 57933 atoms, of which 27345 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	592	Total	C	H	N	O	S	0	0	0
			8954	2905	4374	776	878	21			
1	C	595	Total	C	H	N	O	S	0	0	0
			9011	2918	4409	780	883	21			
1	E	593	Total	C	H	N	O	S	0	0	0
			8984	2905	4399	778	881	21			
1	G	596	Total	C	H	N	O	S	0	0	0
			9006	2922	4395	783	885	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	engineered mutation	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
A	599	LEU	-	expression tag	UNP P06756
C	400	GLY	-	insertion	UNP P06756
C	401	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756
C	599	LEU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	engineered mutation	UNP P06756
E	596	THR	-	expression tag	UNP P06756
E	597	GLY	-	expression tag	UNP P06756
E	598	GLY	-	expression tag	UNP P06756
E	599	LEU	-	expression tag	UNP P06756
G	400	GLY	-	insertion	UNP P06756
G	401	CYS	MET	engineered mutation	UNP P06756
G	596	THR	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
G	597	GLY	-	expression tag	UNP P06756
G	598	GLY	-	expression tag	UNP P06756
G	599	LEU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	333	Total	C	H	N	O	S	0	0	0
			5068	1658	2455	447	491	17			
2	D	312	Total	C	H	N	O	S	0	0	0
			4742	1559	2291	416	462	14			
2	F	332	Total	C	H	N	O	S	0	0	0
			5069	1648	2470	448	488	15			
2	H	336	Total	C	H	N	O	S	0	0	0
			5181	1667	2552	453	491	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	CYS	VAL	engineered mutation	UNP P26012
D	259	CYS	VAL	engineered mutation	UNP P26012
F	259	CYS	VAL	engineered mutation	UNP P26012
H	259	CYS	VAL	engineered mutation	UNP P26012

- Molecule 3 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.



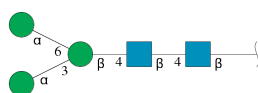
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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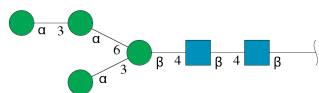
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	a	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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.



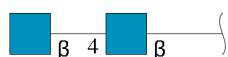
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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.



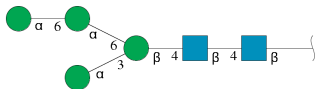
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



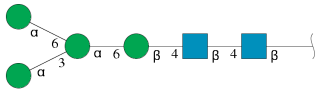
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called 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	P	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	R	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.





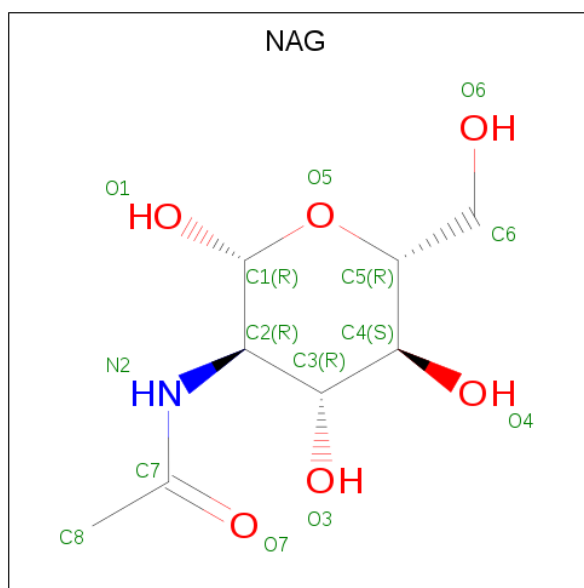
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	b	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 is an oligosaccharide called 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
9	c	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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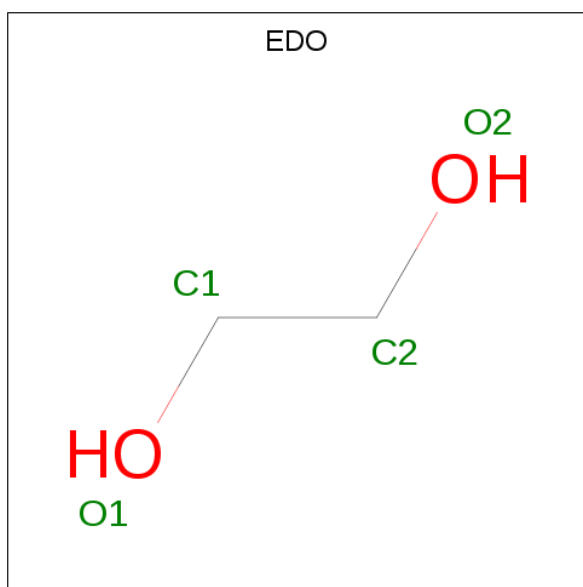
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	4	Total	Ca	0	0
			4	4		
11	D	1	Total	Ca	0	0
			1	1		
11	E	4	Total	Ca	0	0
			4	4		
11	H	1	Total	Ca	0	0
			1	1		
11	B	1	Total	Ca	0	0
			1	1		
11	C	4	Total	Ca	0	0
			4	4		
11	A	4	Total	Ca	0	0
			4	4		
11	F	1	Total	Ca	0	0
			1	1		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

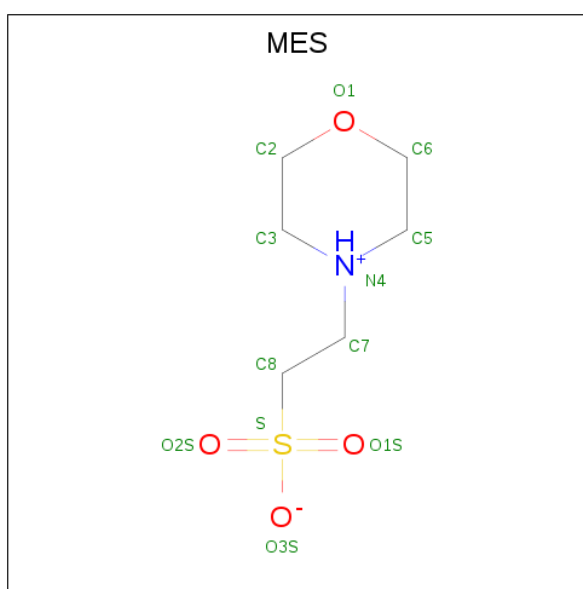


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	B	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	C	1	Total	C	O	0	0
			4	2	2		
12	E	1	Total	C	O	0	0
			4	2	2		
12	F	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	G	1	Total	C	O	0	0
			4	2	2		
12	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total Mg 1 1	0	0
13	B	1	Total Mg 1 1	0	0
13	D	1	Total Mg 1 1	0	0
13	F	1	Total Mg 1 1	0	0

- Molecule 14 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C N O S 12 6 1 4 1	0	0
14	D	1	Total C N O S 12 6 1 4 1	0	0
14	F	1	Total C N O S 12 6 1 4 1	0	0
14	H	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	137	Total O 137 137	0	0

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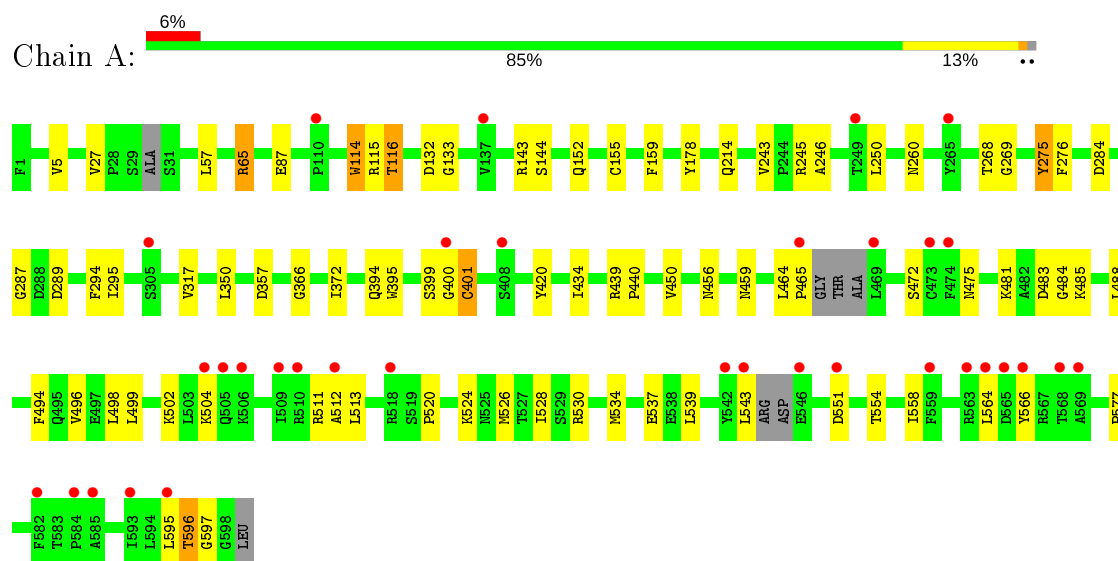
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	25	Total 25	O 25	0	0
15	C	108	Total 108	O 108	0	0
15	D	14	Total 14	O 14	0	0
15	E	47	Total 47	O 47	0	0
15	F	23	Total 23	O 23	0	0
15	G	62	Total 62	O 62	0	0
15	H	15	Total 15	O 15	0	0

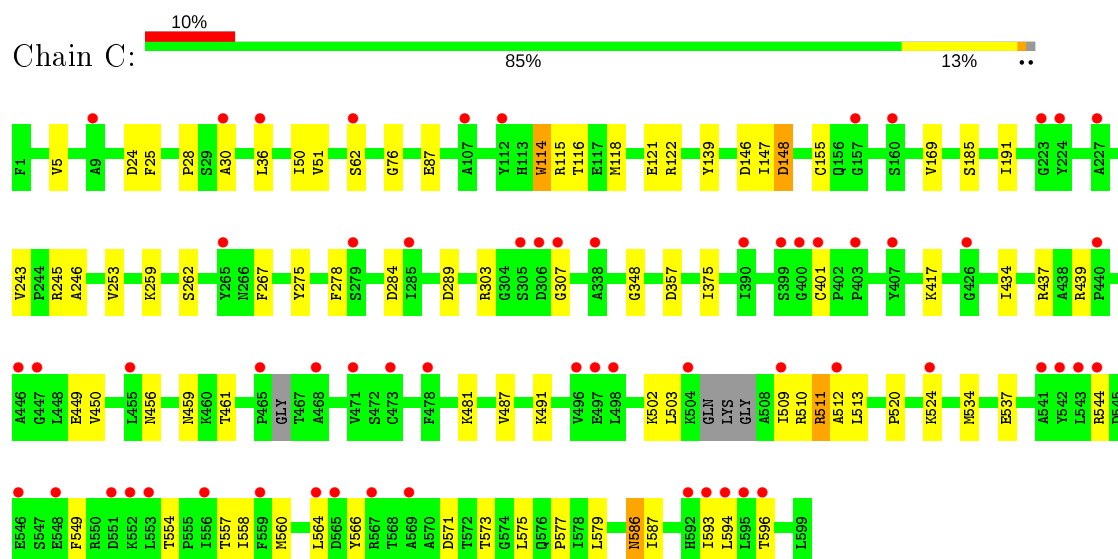
### 3 Residue-property plots [i](#)

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.

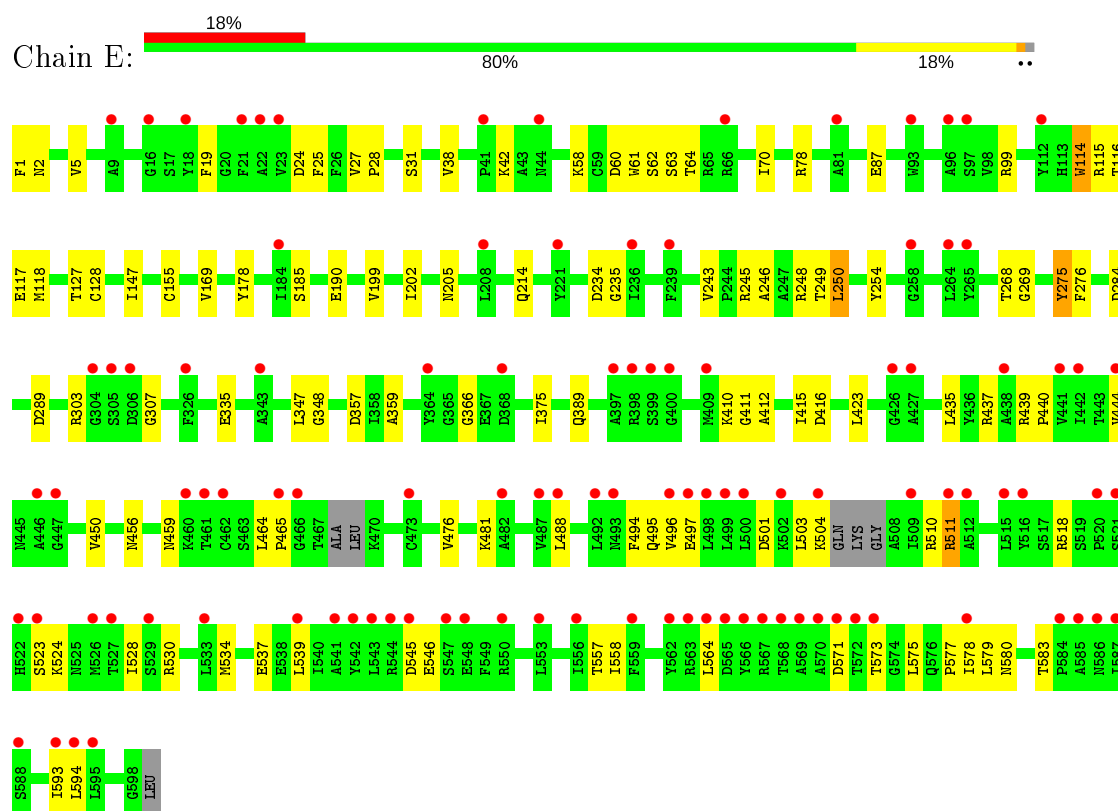
#### • Molecule 1: Integrin alpha-V



#### • Molecule 1: Integrin alpha-V



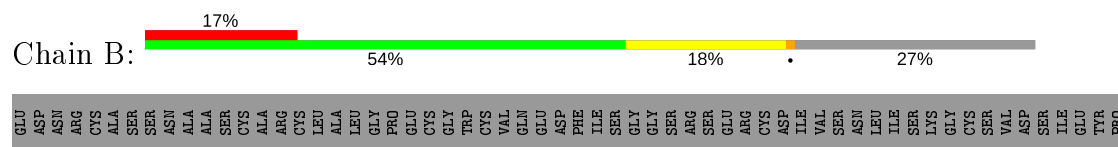
#### • Molecule 1: Integrin alpha-V

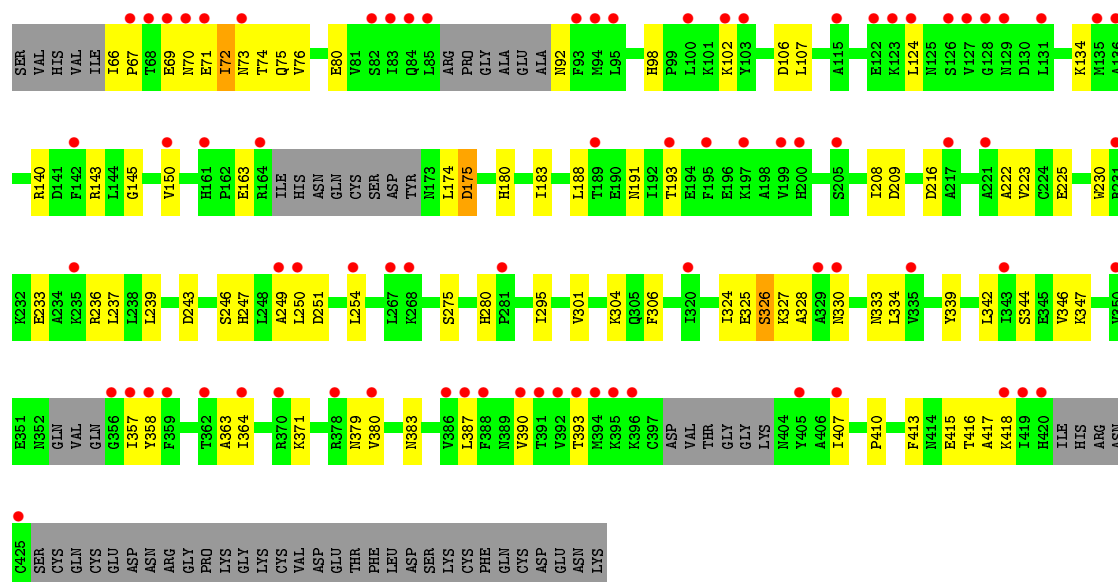


• Molecule 1: Integrin alpha-V

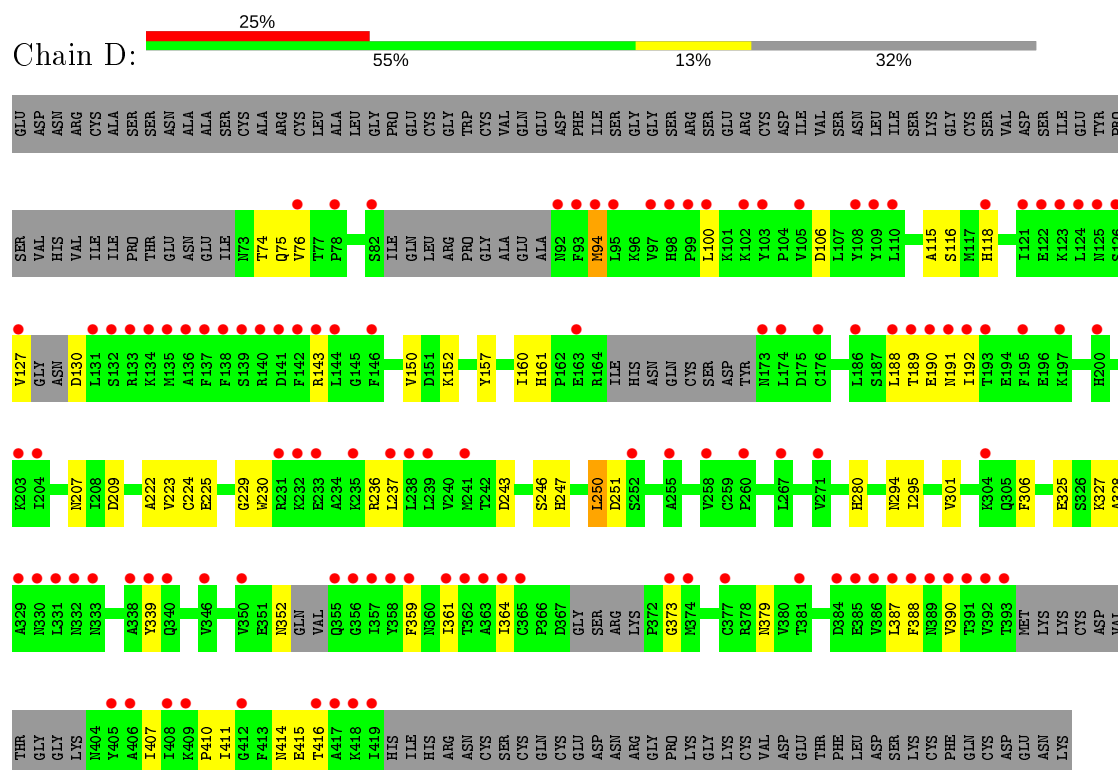


• Molecule 2: Integrin beta-8

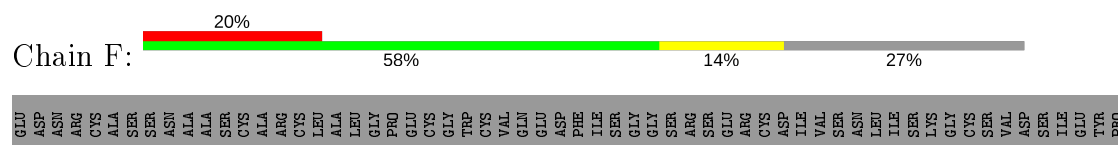




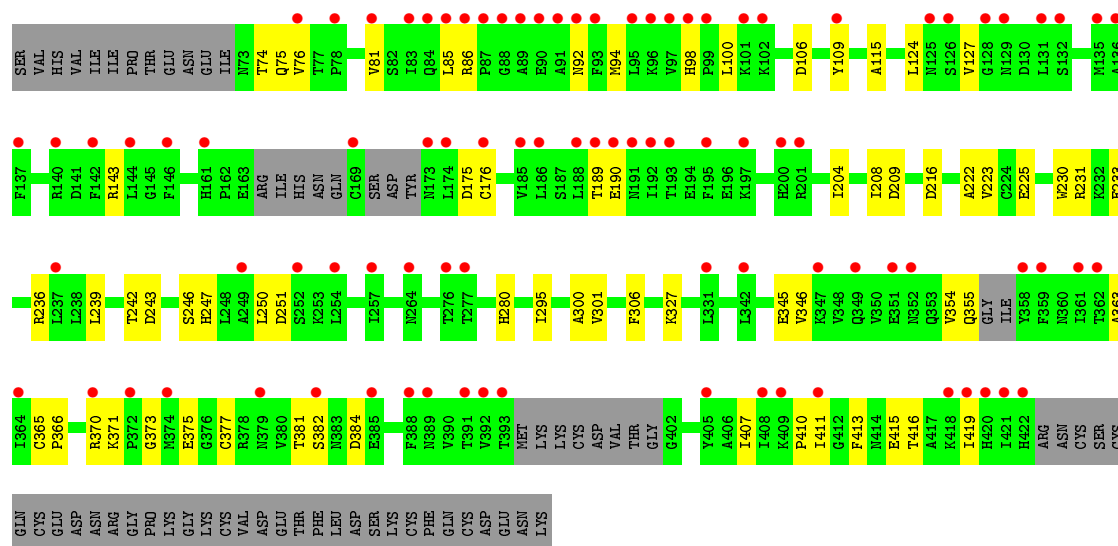
• Molecule 2: Integrin beta-8



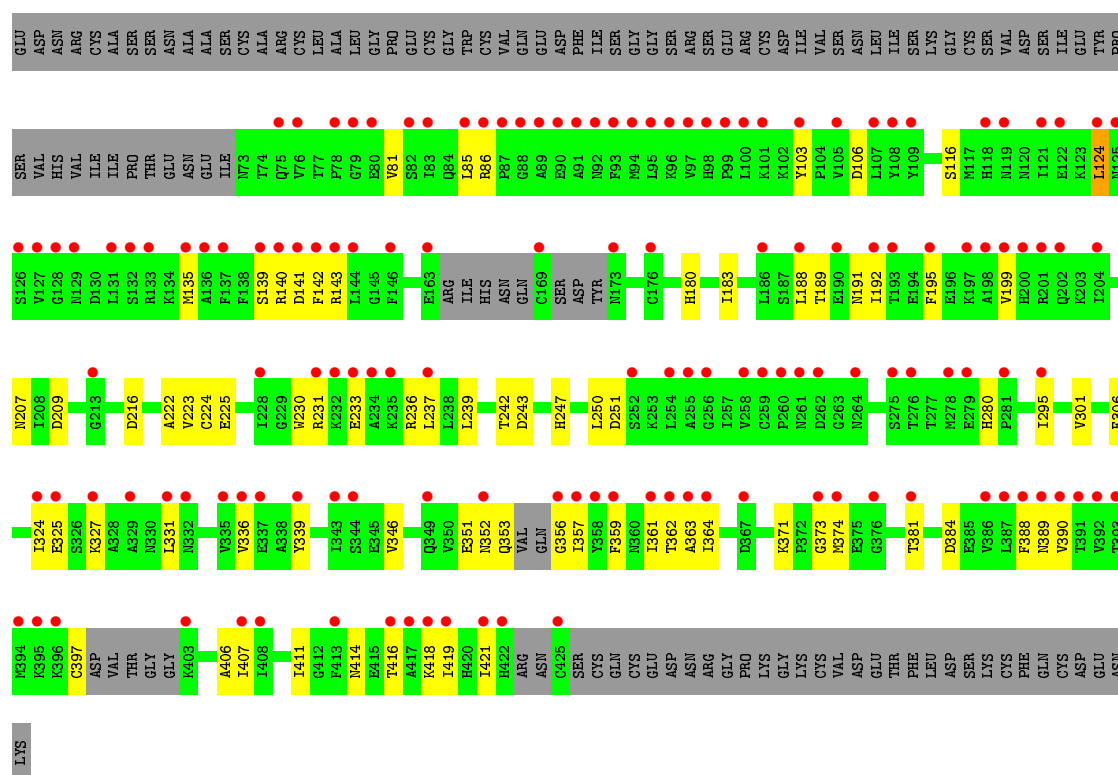
• Molecule 2: Integrin beta-8



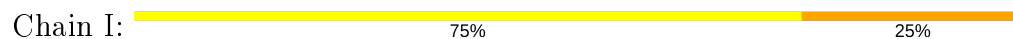




### • Molecule 2: Integrin beta-8



### • Molecule 3: 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




- Molecule 3: 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 K: 




- Molecule 3: 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 O: 



- Molecule 3: 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 Q: 



- Molecule 3: 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 S: 



- Molecule 3: 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 a: 



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

Chain d: 



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

Chain J:  60% 40%



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

Chain U:  40% 60%



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

Chain X:  20% 80%



- Molecule 5: 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 L:  17% 33% 50%



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

Chain M:  100%



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

Chain N:  100%



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

Chain T:  100%

MAG1  
MAG2

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

Chain V:  100%MAG1  
MAG2

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

Chain Y:  100%MAG1  
MAG2

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

Chain Z:  50% 50%MAG1  
MAG2

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

Chain e:  100%MAG1  
MAG2

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

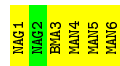
Chain f:  50% 50%MAG1  
MAG2

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

Chain g:  50% 50%MAG1  
MAG2

• Molecule 7: 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 P:  17% 83%



• Molecule 7: 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 R:  17% 17% 67%



• Molecule 7: 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 W:  50% 50%



• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 b:  100%



• Molecule 9: 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 c:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.24Å 55.07Å 175.07Å 90.37° 107.00° 90.01°	Depositor
Resolution (Å)	48.07 – 2.66 48.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.07-2.66) 95.3 (48.07-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.248 , 0.280 0.254 , 0.285	Depositor DCC
$R_{free}$ test set	2001 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 75.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	57933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

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

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	0.27	0/4681	0.46	0/6332
1	C	0.26	0/4704	0.46	0/6367
1	E	0.26	0/4687	0.45	0/6343
1	G	0.26	0/4713	0.45	0/6377
2	B	0.25	0/2662	0.42	0/3600
2	D	0.25	0/2497	0.42	0/3378
2	F	0.25	0/2650	0.41	0/3587
2	H	0.25	0/2679	0.44	0/3621
All	All	0.26	0/29273	0.44	0/39605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4580	4374	4429	64	1
1	C	4602	4409	4450	60	2
1	E	4585	4399	4427	82	0
1	G	4611	4395	4458	61	0
2	B	2613	2455	2600	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2451	2291	2431	51	0
2	F	2599	2470	2580	48	0
2	H	2629	2552	2615	54	0
3	I	50	0	43	11	1
3	K	50	0	43	2	0
3	O	50	0	43	2	0
3	Q	50	0	43	10	0
3	S	50	0	43	1	0
3	a	50	0	43	0	0
3	d	50	0	43	0	0
4	J	61	0	52	0	0
4	U	61	0	52	1	0
4	X	61	0	52	1	0
5	L	72	0	61	8	0
6	M	28	0	25	1	0
6	N	28	0	25	0	0
6	T	28	0	25	2	0
6	V	28	0	25	1	0
6	Y	28	0	25	4	0
6	Z	28	0	25	1	0
6	e	28	0	25	0	0
6	f	28	0	25	0	0
6	g	28	0	25	0	0
7	P	72	0	61	1	0
7	R	72	0	61	7	0
7	W	72	0	61	7	0
8	b	72	0	61	0	0
9	c	50	0	43	0	0
10	A	14	0	13	0	0
10	B	14	0	13	0	0
10	C	28	0	26	1	0
10	D	28	0	26	3	0
10	E	28	0	26	1	0
10	F	28	0	26	1	0
10	G	28	0	26	3	0
11	A	4	0	0	0	0
11	B	1	0	0	0	0
11	C	4	0	0	0	0
11	D	1	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
11	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1	0	0	0	0
12	A	4	0	6	0	0
12	B	8	0	12	0	0
12	C	12	0	18	0	0
12	E	4	0	6	0	0
12	F	4	0	6	0	0
12	G	16	0	24	2	0
12	H	4	0	6	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	H	1	0	0	0	0
14	B	12	0	13	3	0
14	D	12	0	13	3	0
14	F	12	0	13	4	0
14	H	12	0	13	2	0
15	A	137	0	0	3	1
15	B	25	0	0	5	0
15	C	108	0	0	4	1
15	D	14	0	0	1	0
15	E	47	0	0	3	0
15	F	23	0	0	1	0
15	G	62	0	0	3	1
15	H	15	0	0	2	1
All	All	30588	27345	29306	512	4

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 (512) 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)
2:D:325:GLU:HG2	2:D:327:LYS:HE2	1.26	1.12
3:I:2:NAG:O3	3:I:3:BMA:O5	1.78	1.02
2:B:66:ILE:HB	2:B:67:PRO:HD3	1.44	0.98
2:H:352:ASN:HB3	2:H:406:ALA:HB1	1.44	0.97
7:R:2:NAG:H61	7:R:3:BMA:H2	1.56	0.87
1:A:287:GLY:O	1:C:259:LYS:NZ	2.08	0.86
1:E:416:ASP:OD2	15:E:702:HOH:O	1.93	0.85
1:A:115:ARG:O	1:A:116:THR:OG1	1.97	0.83
2:B:66:ILE:HB	2:B:67:PRO:CD	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:243:ASP:OD1	15:H:601:HOH:O	1.97	0.82
2:B:70:ASN:ND2	15:B:2101:HOH:O	2.10	0.81
1:G:115:ARG:O	1:G:116:THR:OG1	1.97	0.81
2:D:325:GLU:HG3	2:D:327:LYS:HG2	1.61	0.81
15:C:701:HOH:O	3:Q:2:NAG:O7	1.99	0.81
1:C:115:ARG:O	1:C:116:THR:OG1	1.99	0.80
7:W:2:NAG:H61	7:W:3:BMA:O2	1.82	0.79
5:L:2:NAG:H61	5:L:3:BMA:H2	1.64	0.77
1:C:449:GLU:OE1	3:S:4:MAN:O4	2.01	0.77
2:F:208:ILE:O	14:F:510:MES:H31	1.83	0.77
3:I:1:NAG:H61	3:I:2:NAG:HN2	1.52	0.75
1:C:502:LYS:O	15:C:702:HOH:O	2.04	0.74
2:D:325:GLU:HG2	2:D:327:LYS:CE	2.11	0.74
2:D:325:GLU:CG	2:D:327:LYS:HG2	2.17	0.74
3:Q:2:NAG:H62	3:Q:3:BMA:H2	1.69	0.74
1:G:126:GLY:O	15:G:2101:HOH:O	2.06	0.73
1:C:459:ASN:OD1	1:C:461:THR:OG1	2.07	0.73
2:F:243:ASP:OD1	15:F:601:HOH:O	2.05	0.73
2:H:301:VAL:HG21	2:H:306:PHE:HA	1.70	0.73
1:E:495:GLN:OE1	10:E:624:NAG:O6	2.07	0.73
2:B:98:HIS:NE2	2:B:383:ASN:O	2.22	0.73
1:C:115:ARG:NH2	1:E:118:MET:O	2.23	0.72
1:E:456:ASN:HB3	1:E:459:ASN:HB2	1.70	0.72
3:Q:3:BMA:O2	3:Q:4:MAN:O5	2.07	0.71
1:E:444:VAL:N	15:E:703:HOH:O	2.19	0.71
2:B:208:ILE:O	14:B:2014:MES:H31	1.90	0.71
1:G:564:LEU:HD22	1:G:579:LEU:HD11	1.71	0.71
1:G:84:ASP:OD1	15:G:2102:HOH:O	2.09	0.71
1:E:275:TYR:OH	2:F:251:ASP:OD1	2.06	0.71
2:H:352:ASN:HB3	2:H:406:ALA:CB	2.18	0.70
1:G:31:SER:OG	15:G:2103:HOH:O	2.10	0.70
2:B:301:VAL:HG21	2:B:306:PHE:HA	1.73	0.70
1:G:511:ARG:NH2	1:G:554:THR:O	2.25	0.70
1:C:439:ARG:NH1	1:C:577:PRO:O	2.24	0.70
1:G:439:ARG:NH1	1:G:577:PRO:O	2.24	0.69
2:B:163:GLU:O	15:B:2102:HOH:O	2.11	0.69
2:D:209:ASP:OD2	2:D:247:HIS:NE2	2.26	0.68
1:E:465:PRO:O	1:E:518:ARG:NH1	2.27	0.68
2:F:100:LEU:HD22	6:Y:2:NAG:H81	1.74	0.68
1:G:450:VAL:HG21	1:G:558:ILE:HD12	1.76	0.68
2:H:362:THR:OG1	2:H:389:ASN:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:4:MAN:H2	5:L:5:MAN:H2	1.74	0.68
1:A:597:GLY:O	15:A:701:HOH:O	2.11	0.67
1:C:456:ASN:HB3	1:C:459:ASN:HB2	1.77	0.67
1:G:524:LYS:NZ	1:G:537:GLU:OE1	2.22	0.66
1:A:260:ASN:HD22	3:K:1:NAG:H83	1.59	0.66
1:E:61:TRP:O	1:E:62:SER:OG	2.13	0.66
2:F:363:ALA:HB2	2:F:373:GLY:HA2	1.78	0.65
1:C:284:ASP:OD2	1:C:289:ASP:N	2.30	0.65
2:B:106:ASP:OD1	2:B:143:ARG:NH1	2.30	0.64
1:C:586:ASN:OD1	10:C:601:NAG:N2	2.30	0.64
1:G:145:GLN:OE1	1:G:145:GLN:N	2.30	0.64
1:E:439:ARG:NH1	1:E:577:PRO:O	2.30	0.64
1:G:243:VAL:CG1	1:G:246:ALA:HB2	2.28	0.64
7:R:2:NAG:H61	7:R:3:BMA:C2	2.28	0.64
2:B:69:GLU:HG2	2:B:80:GLU:HB2	1.79	0.64
3:I:2:NAG:HO3	3:I:3:BMA:C1	2.06	0.64
1:E:178:TYR:CE1	14:F:510:MES:H22	2.33	0.63
1:A:394:GLN:OE1	1:A:394:GLN:N	2.31	0.63
2:H:361:ILE:HD12	2:H:390:VAL:HG22	1.79	0.63
2:B:72:ILE:HG13	2:B:73:ASN:H	1.63	0.62
1:E:450:VAL:HG21	1:E:558:ILE:HD12	1.82	0.62
2:F:365:CYS:HB3	2:F:366:PRO:HD2	1.82	0.62
2:H:374:MET:N	2:H:374:MET:SD	2.73	0.62
1:E:24:ASP:OD1	1:E:25:PHE:N	2.30	0.62
1:G:178:TYR:OH	14:H:510:MES:H22	2.00	0.62
1:C:560:MET:CE	1:C:587:ILE:HD11	2.31	0.61
2:F:233:GLU:HB2	6:Y:1:NAG:H4	1.82	0.61
1:A:512:ALA:O	1:A:513:LEU:HD23	1.99	0.60
1:A:596:THR:OG1	1:A:597:GLY:N	2.33	0.60
2:B:243:ASP:OD1	15:B:2105:HOH:O	2.15	0.60
1:G:308:LYS:NZ	2:H:351:GLU:OE1	2.34	0.60
14:D:507:MES:H22	15:D:609:HOH:O	2.00	0.60
2:F:233:GLU:N	2:F:233:GLU:OE2	2.33	0.60
7:W:3:BMA:O4	7:W:6:MAN:H3	2.00	0.60
1:G:144:SER:OG	1:G:152:GLN:OE1	2.19	0.60
1:A:420:TYR:OH	1:A:485:LYS:O	2.14	0.60
2:B:180:HIS:CD2	2:B:183:ILE:HD12	2.37	0.60
1:E:497:GLU:OE2	1:E:523:SER:OG	2.05	0.60
1:G:24:ASP:OD1	1:G:25:PHE:N	2.33	0.60
2:B:237:LEU:HD11	2:B:339:TYR:CD1	2.37	0.59
1:E:440:PRO:HB2	1:E:488:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ALA:HB3	2:B:371:LYS:H	1.67	0.59
2:D:106:ASP:HB3	2:D:188:LEU:HD13	1.83	0.59
1:G:24:ASP:OD2	1:G:99:ARG:NH1	2.35	0.59
2:D:115:ALA:O	2:D:118:HIS:ND1	2.31	0.59
2:H:301:VAL:O	2:H:324:ILE:N	2.35	0.59
1:A:357:ASP:O	15:A:702:HOH:O	2.17	0.59
1:A:485:LYS:HE2	3:Q:3:BMA:H61	1.84	0.59
1:E:214:GLN:HE21	7:W:3:BMA:H61	1.68	0.59
1:A:395:TRP:CZ3	1:A:434:ILE:HD11	2.37	0.58
2:F:371:LYS:HD2	2:F:375:GLU:CB	2.33	0.58
1:C:456:ASN:HA	1:C:594:LEU:HD23	1.85	0.58
2:F:301:VAL:HG21	2:F:306:PHE:HA	1.85	0.58
3:Q:3:BMA:H4	3:Q:4:MAN:H3	1.84	0.58
1:C:524:LYS:NZ	1:C:537:GLU:OE1	2.24	0.58
1:C:481:LYS:HB2	1:C:534:MET:HG2	1.86	0.58
1:C:564:LEU:HD21	1:C:566:TYR:CE1	2.38	0.58
2:D:301:VAL:HG21	2:D:306:PHE:HA	1.85	0.58
2:D:74:THR:HG23	2:D:415:GLU:HB3	1.86	0.58
1:E:524:LYS:NZ	1:E:537:GLU:OE1	2.31	0.57
2:H:81:VAL:HB	2:H:419:ILE:HG22	1.86	0.57
6:V:1:NAG:H62	6:V:2:NAG:C7	2.35	0.57
2:D:237:LEU:HD11	2:D:339:TYR:HD2	1.69	0.57
2:B:107:LEU:HD12	2:B:237:LEU:HB2	1.88	0.56
1:A:275:TYR:CG	2:B:250:LEU:HD12	2.40	0.56
3:I:2:NAG:C3	3:I:3:BMA:O5	2.53	0.56
2:B:275:SER:OG	15:B:2104:HOH:O	2.15	0.56
2:B:363:ALA:C	2:B:364:ILE:HD12	2.26	0.56
2:D:94:MET:HE1	10:D:502:NAG:O5	2.05	0.56
2:D:116:SER:OG	2:D:243:ASP:OD2	2.12	0.56
1:E:545:ASP:OD1	1:E:546:GLU:N	2.39	0.56
2:D:294:ASN:ND2	2:D:414:ASN:HA	2.20	0.56
2:B:222:ALA:HA	2:B:295:ILE:CD1	2.36	0.56
2:H:233:GLU:HA	2:H:414:ASN:HD22	1.70	0.56
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.36	0.56
3:I:1:NAG:O3	3:I:1:NAG:O7	2.18	0.56
1:G:505:GLN:HA	1:G:510:ARG:HE	1.70	0.55
3:I:2:NAG:HO3	3:I:3:BMA:C5	2.08	0.55
2:D:157:TYR:OH	2:D:251:ASP:O	2.24	0.55
1:E:2:ASN:O	1:E:439:ARG:N	2.36	0.55
1:E:504:LYS:O	1:E:510:ARG:NE	2.39	0.55
1:A:524:LYS:NZ	1:A:537:GLU:OE1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASP:OD1	1:C:25:PHE:N	2.38	0.55
2:F:370:ARG:O	2:F:371:LYS:HB2	2.06	0.55
7:R:2:NAG:H61	7:R:3:BMA:C1	2.36	0.55
1:C:564:LEU:H	1:C:564:LEU:HD23	1.72	0.55
1:G:243:VAL:HG12	1:G:246:ALA:HB2	1.87	0.55
2:H:362:THR:HG1	2:H:389:ASN:HB3	1.72	0.55
2:B:330:ASN:OD1	2:B:333:ASN:HB2	2.07	0.55
1:E:494:PHE:CE1	1:E:528:ILE:HD11	2.41	0.55
2:B:74:THR:OG1	15:B:2103:HOH:O	2.14	0.54
1:A:214:GLN:NE2	5:L:3:BMA:O5	2.38	0.54
5:L:4:MAN:H2	5:L:5:MAN:C2	2.37	0.54
1:A:456:ASN:HB3	1:A:459:ASN:HB2	1.89	0.54
1:E:214:GLN:NE2	7:W:3:BMA:H61	2.22	0.54
1:A:144:SER:OG	1:A:152:GLN:OE1	2.23	0.54
2:B:325:GLU:O	2:B:328:ALA:N	2.36	0.54
2:B:357:ILE:HD12	2:B:358:TYR:H	1.72	0.54
1:A:260:ASN:ND2	3:K:1:NAG:H83	2.22	0.54
1:E:24:ASP:OD2	1:E:99:ARG:NH1	2.38	0.54
1:E:464:LEU:HD12	1:E:465:PRO:HD2	1.88	0.54
2:H:116:SER:OG	2:H:243:ASP:OD2	2.18	0.54
2:F:74:THR:HB	2:F:415:GLU:HB3	1.88	0.54
3:Q:2:NAG:H62	3:Q:3:BMA:C2	2.36	0.54
1:C:245:ARG:NH2	2:D:246:SER:O	2.41	0.54
2:B:66:ILE:CB	2:B:67:PRO:HD3	2.27	0.54
2:H:230:TRP:HB3	2:H:236:ARG:NE	2.23	0.54
3:I:1:NAG:C6	3:I:2:NAG:HN2	2.20	0.53
2:B:75:GLN:N	2:B:415:GLU:OE1	2.39	0.53
1:E:63:SER:O	1:E:64:THR:OG1	2.23	0.53
1:G:138:GLU:OE2	1:G:143:ARG:NH2	2.39	0.53
2:F:371:LYS:HD2	2:F:375:GLU:HB3	1.90	0.53
1:E:115:ARG:HG3	1:E:116:THR:O	2.08	0.53
1:G:586:ASN:OD1	10:G:2024:NAG:N2	2.41	0.53
1:E:127:THR:HG22	1:E:128:CYS:N	2.24	0.53
7:R:2:NAG:C6	7:R:3:BMA:H2	2.35	0.53
1:E:501:ASP:OD2	1:E:511:ARG:NH1	2.42	0.53
2:F:216:ASP:OD1	2:F:280:HIS:ND1	2.40	0.53
2:H:106:ASP:OD2	2:H:143:ARG:NH2	2.41	0.52
1:A:513:LEU:HD22	1:A:520:PRO:HG3	1.90	0.52
2:H:223:VAL:O	2:H:225:GLU:N	2.42	0.52
2:B:69:GLU:HG3	2:B:80:GLU:O	2.09	0.52
2:F:76:VAL:HG11	2:F:410:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:3:BMA:HO2	3:Q:4:MAN:C1	2.21	0.52
1:C:510:ARG:O	1:C:544:ARG:NH1	2.43	0.52
2:H:209:ASP:OD2	2:H:247:HIS:NE2	2.39	0.52
2:D:94:MET:N	2:D:94:MET:SD	2.82	0.52
1:A:250:LEU:HD21	1:A:269:GLY:O	2.10	0.52
1:C:115:ARG:HA	1:C:121:GLU:O	2.09	0.52
2:D:76:VAL:HG23	2:D:76:VAL:O	2.09	0.52
2:B:216:ASP:OD1	2:B:280:HIS:ND1	2.41	0.52
2:D:76:VAL:HG11	2:D:410:PRO:HG2	1.90	0.52
6:Y:1:NAG:O4	6:Y:2:NAG:O7	2.28	0.52
2:D:222:ALA:HA	2:D:295:ILE:CD1	2.40	0.51
4:X:2:NAG:H62	4:X:3:BMA:C1	2.40	0.51
1:A:65:ARG:NH2	15:A:709:HOH:O	2.42	0.51
1:A:132:ASP:OD1	1:A:133:GLY:N	2.43	0.51
1:A:512:ALA:C	1:A:513:LEU:HD23	2.30	0.51
1:A:399:SER:O	1:A:401:CYS:N	2.43	0.51
1:C:511:ARG:NH2	1:C:554:THR:O	2.43	0.51
2:D:223:VAL:O	2:D:225:GLU:N	2.41	0.51
1:G:338:ALA:HB1	1:G:362:ALA:HB1	1.93	0.51
2:H:363:ALA:HB2	2:H:388:PHE:CE2	2.45	0.51
1:A:395:TRP:CH2	1:A:434:ILE:HD11	2.45	0.51
2:F:124:LEU:HG	2:F:127:VAL:HG22	1.91	0.51
1:A:250:LEU:CD2	1:A:268:THR:HG22	2.40	0.51
1:E:250:LEU:CD2	1:E:268:THR:HG22	2.41	0.51
2:F:85:LEU:HD23	2:F:86:ARG:O	2.10	0.51
5:L:4:MAN:C2	5:L:5:MAN:H2	2.38	0.51
1:E:250:LEU:HD21	1:E:269:GLY:O	2.11	0.51
2:F:407:ILE:HD11	2:F:416:THR:CG2	2.40	0.51
2:H:85:LEU:HD23	2:H:86:ARG:O	2.11	0.51
1:A:440:PRO:HB2	1:A:488:LEU:HD21	1.93	0.50
1:C:303:ARG:NE	1:C:307:GLY:O	2.41	0.50
1:G:464:LEU:HD23	1:G:465:PRO:HD2	1.93	0.50
2:B:66:ILE:CB	2:B:67:PRO:CD	2.85	0.50
1:C:147:ILE:HD12	1:C:148:ASP:HB2	1.92	0.50
2:B:209:ASP:OD2	2:B:247:HIS:NE2	2.39	0.50
1:E:564:LEU:HD23	1:E:564:LEU:H	1.75	0.50
1:G:5:VAL:HG12	1:G:5:VAL:O	2.12	0.50
1:A:564:LEU:H	1:A:564:LEU:HD23	1.75	0.50
2:F:124:LEU:HG	2:F:127:VAL:CG2	2.41	0.50
2:F:92:ASN:OD1	10:F:502:NAG:H2	2.12	0.50
1:G:314:GLN:NE2	1:G:332:ASN:OD1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:ASN:O	14:H:510:MES:H72	2.11	0.50
2:B:364:ILE:HD13	2:B:387:LEU:HD12	1.94	0.50
2:F:242:THR:O	2:F:301:VAL:HA	2.12	0.50
1:G:564:LEU:H	1:G:564:LEU:HD23	1.76	0.50
1:A:539:LEU:N	1:A:539:LEU:HD23	2.27	0.49
2:H:141:ASP:OD1	2:H:142:PHE:N	2.44	0.49
2:B:76:VAL:HG11	2:B:410:PRO:HG2	1.95	0.49
2:D:189:THR:HG22	2:D:190:GLU:N	2.27	0.49
1:E:199:VAL:O	1:E:202:ILE:HD11	2.12	0.49
1:E:78:ARG:HD3	1:E:87:GLU:OE1	2.12	0.49
1:G:525:ASN:CB	10:G:2023:NAG:O5	2.59	0.49
2:H:222:ALA:HA	2:H:295:ILE:CD1	2.43	0.49
1:A:564:LEU:HD21	1:A:566:TYR:CE1	2.47	0.49
2:B:357:ILE:HD11	2:B:393:THR:H	1.76	0.49
1:C:303:ARG:NH2	1:C:307:GLY:O	2.42	0.49
2:D:237:LEU:HD11	2:D:339:TYR:CD2	2.47	0.49
1:E:415:ILE:HG21	1:E:435:LEU:HD21	1.94	0.49
2:H:421:ILE:HD12	2:H:421:ILE:N	2.28	0.49
2:D:361:ILE:CD1	2:D:390:VAL:HG23	2.41	0.49
1:E:275:TYR:CG	2:F:250:LEU:HD12	2.48	0.49
2:H:363:ALA:N	2:H:371:LYS:O	2.39	0.49
1:A:115:ARG:O	1:A:116:THR:CB	2.61	0.49
1:A:243:VAL:HG12	1:A:246:ALA:HB2	1.95	0.49
2:D:94:MET:CG	2:D:387:LEU:HD13	2.42	0.49
2:B:92:ASN:HA	2:B:390:VAL:O	2.13	0.49
1:C:512:ALA:O	1:C:513:LEU:HD23	2.13	0.49
1:G:178:TYR:HB2	12:G:2025:EDO:H21	1.94	0.49
2:H:364:ILE:N	2:H:364:ILE:HD12	2.27	0.49
6:T:2:NAG:O3	6:T:2:NAG:O7	2.28	0.49
1:A:524:LYS:HZ3	1:A:526:MET:HG3	1.78	0.49
2:D:387:LEU:HD12	2:D:387:LEU:C	2.34	0.49
1:E:42:LYS:O	4:U:1:NAG:H82	2.11	0.49
1:A:178:TYR:HE2	14:B:2014:MES:H22	1.77	0.48
1:E:476:VAL:HG22	1:E:558:ILE:HD13	1.95	0.48
1:G:334:PHE:O	12:G:2026:EDO:H11	2.13	0.48
1:E:571:ASP:OD1	1:E:575:LEU:N	2.45	0.48
2:H:363:ALA:C	2:H:364:ILE:HD12	2.33	0.48
2:D:361:ILE:O	2:D:373:GLY:HA3	2.13	0.48
1:E:115:ARG:O	1:E:116:THR:HB	2.13	0.48
2:F:106:ASP:OD1	2:F:143:ARG:NH1	2.47	0.48
1:G:564:LEU:HD21	1:G:566:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:VAL:HG21	1:A:558:ILE:HD12	1.95	0.48
1:C:87:GLU:HA	1:C:114:TRP:HA	1.96	0.48
1:E:335:GLU:OE1	1:E:366:GLY:N	2.45	0.48
2:F:143:ARG:NH2	2:F:231:ARG:HG2	2.28	0.48
1:E:178:TYR:HE1	14:F:510:MES:H22	1.78	0.48
1:G:243:VAL:HG11	1:G:246:ALA:HB2	1.95	0.48
1:E:583:THR:HG21	15:E:703:HOH:O	2.13	0.48
2:H:192:ILE:O	2:H:195:PHE:N	2.44	0.48
1:A:496:VAL:HG12	1:A:498:LEU:CD1	2.44	0.47
1:E:284:ASP:OD2	1:E:289:ASP:N	2.43	0.47
6:Z:1:NAG:O7	6:Z:1:NAG:O3	2.24	0.47
1:A:543:LEU:N	1:A:543:LEU:HD12	2.28	0.47
1:C:513:LEU:HD22	1:C:520:PRO:HG3	1.96	0.47
2:D:207:ASN:ND2	14:D:507:MES:O1S	2.47	0.47
2:F:381:THR:OG1	2:F:384:ASP:OD2	2.32	0.47
3:O:1:NAG:H62	3:O:2:NAG:C1	2.43	0.47
1:C:564:LEU:HD22	1:C:579:LEU:HD11	1.96	0.47
1:E:1:PHE:HA	1:E:389:GLN:HB2	1.96	0.47
1:E:202:ILE:H	1:E:202:ILE:HD12	1.79	0.47
1:G:481:LYS:HB3	1:G:534:MET:HA	1.95	0.47
2:F:76:VAL:HG23	2:F:76:VAL:O	2.14	0.47
2:H:189:THR:HG22	2:H:191:ASN:H	1.79	0.47
5:L:3:BMA:H61	5:L:4:MAN:H2	1.56	0.47
1:C:262:SER:HB2	3:Q:1:NAG:HN2	1.79	0.47
2:D:94:MET:HG3	2:D:387:LEU:HD13	1.95	0.47
2:H:247:HIS:O	15:H:602:HOH:O	2.20	0.47
2:B:233:GLU:HG2	3:O:2:NAG:H61	1.96	0.47
2:B:237:LEU:HD11	2:B:339:TYR:HD1	1.79	0.47
1:C:51:VAL:HG13	7:P:1:NAG:H5	1.95	0.47
1:G:559:PHE:CE2	1:G:586:ASN:HB2	2.50	0.47
1:A:294:PHE:CE2	1:A:317:VAL:HG13	2.50	0.47
1:E:116:THR:HG22	1:E:117:GLU:N	2.29	0.47
2:H:124:LEU:HD12	2:H:331:LEU:HD12	1.96	0.47
1:A:595:LEU:O	1:A:597:GLY:N	2.47	0.47
1:E:348:GLY:O	1:E:357:ASP:N	2.41	0.47
1:E:580:ASN:HB3	1:E:583:THR:HG23	1.97	0.47
2:F:346:VAL:O	2:F:346:VAL:HG23	2.14	0.47
2:B:223:VAL:O	2:B:225:GLU:N	2.47	0.46
2:B:327:LYS:O	2:B:328:ALA:HB3	2.15	0.46
2:B:134:LYS:NZ	2:B:333:ASN:OD1	2.47	0.46
1:G:494:PHE:CE1	1:G:528:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:GLU:O	2:D:192:ILE:N	2.49	0.46
1:C:560:MET:HE2	1:C:587:ILE:HD11	1.97	0.46
2:D:352:ASN:HB3	2:D:359:PHE:CE1	2.51	0.46
2:D:75:GLN:HG3	2:D:100:LEU:HD11	1.98	0.46
2:B:357:ILE:HD12	2:B:358:TYR:N	2.31	0.46
1:E:234:ASP:OD1	1:E:235:GLY:N	2.49	0.46
2:F:223:VAL:O	2:F:225:GLU:N	2.49	0.46
2:D:387:LEU:HD12	2:D:388:PHE:N	2.31	0.46
2:D:74:THR:HG22	2:D:76:VAL:HG22	1.98	0.46
1:E:116:THR:HG21	1:E:147:ILE:HD13	1.98	0.46
6:T:1:NAG:H4	6:T:2:NAG:H2	1.83	0.46
1:C:118:MET:HA	1:E:118:MET:HA	1.96	0.46
1:E:27:VAL:O	1:E:27:VAL:HG13	2.15	0.46
2:H:124:LEU:HD23	2:H:199:VAL:HG11	1.98	0.46
2:D:222:ALA:HA	2:D:295:ILE:HD13	1.98	0.46
2:F:363:ALA:HB3	2:F:370:ARG:O	2.16	0.46
1:A:245:ARG:NH2	2:B:246:SER:O	2.48	0.45
2:D:230:TRP:HB3	2:D:236:ARG:NE	2.31	0.45
2:D:364:ILE:HD12	2:D:387:LEU:HD11	1.98	0.45
1:E:564:LEU:HD22	1:E:579:LEU:HD11	1.98	0.45
2:F:75:GLN:HG3	2:F:100:LEU:HD11	1.98	0.45
2:D:188:LEU:HD12	2:D:229:GLY:O	2.16	0.45
2:D:411:ILE:HD12	2:D:411:ILE:O	2.17	0.45
2:H:327:LYS:HA	2:H:327:LYS:HD2	1.75	0.45
3:I:2:NAG:O7	3:I:2:NAG:O3	2.33	0.45
1:A:5:VAL:HG12	1:A:5:VAL:O	2.17	0.45
1:A:178:TYR:CE2	14:B:2014:MES:H22	2.51	0.45
1:C:594:LEU:HD22	1:C:594:LEU:N	2.31	0.45
1:E:437:ARG:NH2	1:E:573:THR:OG1	2.44	0.45
1:G:437:ARG:NH2	1:G:573:THR:OG1	2.43	0.45
2:H:216:ASP:OD1	2:H:280:HIS:ND1	2.44	0.45
6:M:1:NAG:H61	6:M:2:NAG:H82	1.98	0.45
1:G:275:TYR:OH	2:H:251:ASP:OD1	2.20	0.45
1:A:350:LEU:N	1:A:357:ASP:OD2	2.50	0.45
1:E:243:VAL:CG1	1:E:246:ALA:HB2	2.47	0.45
1:E:60:ASP:OD1	1:E:61:TRP:N	2.48	0.45
1:G:418:ASN:ND2	1:G:438:ALA:O	2.50	0.45
1:E:410:LYS:O	1:E:423:LEU:HD12	2.17	0.45
7:W:3:BMA:O4	7:W:6:MAN:H5	2.16	0.45
6:Y:1:NAG:O3	6:Y:2:NAG:O5	2.17	0.45
2:B:74:THR:HG22	2:B:76:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:LEU:HD11	1:E:359:ALA:HB2	1.98	0.45
2:H:407:ILE:HD11	2:H:416:THR:CG2	2.47	0.45
1:A:483:ASP:OD1	1:A:484:GLY:N	2.45	0.44
2:D:75:GLN:N	2:D:415:GLU:OE1	2.31	0.44
2:F:109:TYR:CE2	2:F:124:LEU:HD11	2.53	0.44
1:G:275:TYR:CG	2:H:250:LEU:HD12	2.52	0.44
2:F:222:ALA:HA	2:F:295:ILE:CD1	2.46	0.44
2:F:346:VAL:HG12	2:F:413:PHE:CE1	2.51	0.44
2:B:357:ILE:HD11	2:B:393:THR:N	2.32	0.44
1:C:122:ARG:CD	2:D:160:ILE:HG13	2.47	0.44
2:D:327:LYS:O	2:D:328:ALA:HB3	2.17	0.44
2:F:81:VAL:HB	2:F:419:ILE:HG22	1.98	0.44
1:A:439:ARG:NH1	1:A:577:PRO:O	2.51	0.44
1:A:511:ARG:NH2	1:A:554:THR:O	2.50	0.44
1:C:481:LYS:CB	1:C:534:MET:HG2	2.47	0.44
1:G:543:LEU:CD2	1:G:593:ILE:HD11	2.47	0.44
7:R:4:MAN:H61	7:R:5:MAN:H2	1.40	0.44
1:A:494:PHE:CE1	1:A:528:ILE:HD11	2.53	0.44
1:G:115:ARG:HA	1:G:121:GLU:O	2.18	0.44
1:A:27:VAL:O	1:A:27:VAL:HG13	2.18	0.44
1:A:276:PHE:CZ	1:A:295:ILE:HG21	2.52	0.44
2:F:209:ASP:OD2	2:F:247:HIS:NE2	2.50	0.44
2:F:98:HIS:NE2	2:F:382:SER:O	2.50	0.44
1:G:464:LEU:HB3	1:G:465:PRO:HD2	2.00	0.44
5:L:2:NAG:H61	5:L:3:BMA:C2	2.42	0.44
2:B:346:VAL:HG23	2:B:346:VAL:O	2.17	0.44
1:E:115:ARG:O	1:E:116:THR:CB	2.66	0.44
2:F:115:ALA:N	14:F:510:MES:O2S	2.40	0.44
2:D:143:ARG:HB3	2:D:188:LEU:HB3	1.98	0.43
1:E:190:GLU:OE1	1:E:205:ASN:N	2.51	0.43
2:F:230:TRP:HB3	2:F:236:ARG:NE	2.34	0.43
2:H:346:VAL:O	2:H:346:VAL:HG23	2.18	0.43
2:F:189:THR:HG22	2:F:190:GLU:N	2.32	0.43
2:H:242:THR:O	2:H:301:VAL:HA	2.18	0.43
1:A:488:LEU:HB2	1:A:530:ARG:NH1	2.33	0.43
2:B:230:TRP:HB3	2:B:236:ARG:NE	2.32	0.43
2:B:380:VAL:HG13	2:B:380:VAL:O	2.17	0.43
1:E:593:ILE:HG22	1:E:594:LEU:H	1.83	0.43
2:F:411:ILE:O	2:F:411:ILE:HD12	2.19	0.43
1:G:372:ILE:HG22	1:G:373:VAL:N	2.34	0.43
7:R:3:BMA:O4	7:R:6:MAN:H2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:VAL:HG13	1:C:487:VAL:O	2.17	0.43
1:G:539:LEU:HD23	1:G:539:LEU:N	2.34	0.43
1:E:116:THR:HG23	1:E:147:ILE:HG21	2.00	0.43
1:G:411:GLY:O	1:G:412:ALA:HB3	2.18	0.43
1:G:471:VAL:HG21	1:G:542:TYR:CG	2.54	0.43
5:L:4:MAN:C2	5:L:5:MAN:C2	2.96	0.43
2:B:344:SER:O	2:B:379:ASN:N	2.52	0.43
1:C:571:ASP:OD1	1:C:575:LEU:N	2.48	0.43
1:G:60:ASP:OD1	1:G:61:TRP:N	2.51	0.43
1:A:87:GLU:HA	1:A:114:TRP:HA	2.00	0.43
2:B:416:THR:HG22	2:B:417:ALA:N	2.34	0.43
2:B:71:GLU:O	2:B:72:ILE:C	2.57	0.43
2:B:72:ILE:HG13	2:B:73:ASN:N	2.31	0.43
2:D:127:VAL:O	2:D:130:ASP:N	2.52	0.43
1:C:278:PHE:CD1	2:D:250:LEU:CD1	3.02	0.43
2:H:237:LEU:HD11	2:H:339:TYR:CD1	2.54	0.43
1:C:28:PRO:HB2	1:C:30:ALA:O	2.19	0.43
2:D:94:MET:HE1	10:D:502:NAG:O3	2.19	0.43
1:E:243:VAL:HG12	1:E:246:ALA:HB2	2.01	0.43
1:A:481:LYS:HB3	1:A:534:MET:HA	2.00	0.43
1:C:593:ILE:HG22	1:C:594:LEU:N	2.34	0.43
2:H:356:GLY:O	2:H:357:ILE:HG23	2.19	0.43
1:A:464:LEU:HG	1:A:465:PRO:HD2	2.00	0.42
1:C:278:PHE:CD1	2:D:250:LEU:HD12	2.54	0.42
1:C:459:ASN:HB3	15:C:705:HOH:O	2.18	0.42
1:E:503:LEU:HD21	1:E:557:THR:HG23	2.00	0.42
1:C:243:VAL:CG1	1:C:246:ALA:HB2	2.49	0.42
1:G:27:VAL:O	1:G:27:VAL:HG13	2.20	0.42
2:D:325:GLU:O	2:D:328:ALA:N	2.48	0.42
1:G:375:ILE:N	1:G:375:ILE:HD12	2.35	0.42
2:B:239:LEU:HD23	2:B:239:LEU:C	2.39	0.42
1:C:139:TYR:CD1	1:C:191:ILE:HG12	2.54	0.42
1:C:450:VAL:HG21	1:C:558:ILE:HD12	2.01	0.42
1:G:143:ARG:NE	1:G:200:TYR:O	2.51	0.42
1:C:434:ILE:HD12	1:C:434:ILE:N	2.34	0.42
1:G:278:PHE:CD1	2:H:250:LEU:HD13	2.54	0.42
1:G:571:ASP:OD1	1:G:575:LEU:N	2.52	0.42
2:H:231:ARG:C	2:H:236:ARG:HH11	2.23	0.42
3:I:1:NAG:C6	3:I:2:NAG:N2	2.83	0.42
1:E:450:VAL:CG2	1:E:558:ILE:HD12	2.49	0.42
1:G:553:LEU:N	1:G:553:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:ILE:HD13	2:B:418:LYS:HG2	2.00	0.42
1:E:481:LYS:HB2	1:E:534:MET:CB	2.50	0.42
7:R:3:BMA:H62	7:R:4:MAN:H2	1.82	0.42
7:W:3:BMA:H3	7:W:6:MAN:H2	1.30	0.42
1:C:5:VAL:O	1:C:5:VAL:HG12	2.19	0.42
1:E:375:ILE:N	1:E:375:ILE:HD12	2.35	0.42
1:G:494:PHE:HE1	1:G:528:ILE:HD11	1.84	0.42
3:Q:3:BMA:H4	3:Q:4:MAN:H5	2.02	0.42
1:A:284:ASP:OD2	1:A:289:ASP:N	2.49	0.42
1:A:472:SER:HB3	1:A:543:LEU:HD13	2.02	0.42
2:B:249:ALA:HA	2:B:280:HIS:HB2	2.02	0.42
2:H:135:MET:O	2:H:139:SER:N	2.52	0.42
1:E:303:ARG:NH1	1:E:307:GLY:O	2.52	0.41
2:B:191:ASN:OD1	2:B:193:THR:HG22	2.20	0.41
2:B:347:LYS:O	2:B:410:PRO:HA	2.20	0.41
2:F:354:VAL:O	2:F:355:GLN:C	2.58	0.41
1:G:525:ASN:HD21	10:G:2023:NAG:C7	2.33	0.41
2:H:239:LEU:C	2:H:239:LEU:HD23	2.40	0.41
1:A:57:LEU:N	1:A:57:LEU:HD12	2.36	0.41
1:C:594:LEU:O	1:C:596:THR:N	2.49	0.41
1:E:539:LEU:HD23	1:E:539:LEU:N	2.36	0.41
2:F:76:VAL:HG11	2:F:410:PRO:CG	2.49	0.41
2:H:180:HIS:ND1	2:H:183:ILE:HD12	2.35	0.41
2:H:411:ILE:HD12	2:H:411:ILE:O	2.20	0.41
1:C:169:VAL:O	1:C:185:SER:HA	2.20	0.41
1:E:411:GLY:O	1:E:412:ALA:HB3	2.20	0.41
2:F:239:LEU:HD11	2:F:300:ALA:HB2	2.02	0.41
1:C:36:LEU:HD12	1:C:36:LEU:N	2.36	0.41
1:C:503:LEU:HD21	1:C:557:THR:HG23	2.02	0.41
1:E:248:ARG:O	1:E:249:THR:OG1	2.36	0.41
1:E:28:PRO:HB2	1:E:31:SER:HB3	2.02	0.41
1:E:439:ARG:NH2	1:E:578:ILE:HD13	2.35	0.41
1:E:564:LEU:HD22	1:E:579:LEU:CD1	2.51	0.41
1:G:85:PRO:O	1:G:115:ARG:HD2	2.21	0.41
1:G:496:VAL:HG12	1:G:524:LYS:O	2.21	0.41
2:B:145:GLY:N	2:B:188:LEU:HD23	2.35	0.41
1:C:121:GLU:OE2	2:D:161:HIS:HB2	2.20	0.41
1:E:87:GLU:HA	1:E:114:TRP:HA	2.02	0.41
1:G:284:ASP:OD2	1:G:289:ASP:N	2.50	0.41
3:Q:3:BMA:C4	3:Q:4:MAN:H3	2.51	0.41
1:A:275:TYR:CB	2:B:250:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LYS:HZ3	2:D:280:HIS:CE1	2.39	0.41
2:F:345:GLU:HA	2:F:377:CYS:O	2.20	0.41
1:G:1:PHE:HA	1:G:389:GLN:HB2	2.02	0.41
2:H:407:ILE:HD13	2:H:418:LYS:HD2	2.02	0.41
1:E:254:TYR:OH	7:W:1:NAG:H62	2.21	0.41
1:A:464:LEU:C	1:A:464:LEU:HD23	2.42	0.41
1:A:504:LYS:NZ	1:A:551:ASP:OD2	2.52	0.41
1:A:275:TYR:OH	2:B:251:ASP:OD1	2.29	0.41
2:B:74:THR:CG2	2:B:76:VAL:HG22	2.51	0.41
1:C:146:ASP:OD1	15:C:703:HOH:O	2.21	0.41
1:G:564:LEU:HD21	1:G:566:TYR:HE1	1.85	0.41
2:H:361:ILE:O	2:H:373:GLY:N	2.45	0.41
1:A:143:ARG:O	1:A:143:ARG:CG	2.69	0.41
1:A:159:PHE:CE1	2:B:254:LEU:HD23	2.55	0.41
1:A:499:LEU:CD1	1:A:502:LYS:HB2	2.51	0.41
1:C:503:LEU:HD22	1:C:557:THR:OG1	2.20	0.41
2:H:135:MET:SD	2:H:336:VAL:HG12	2.61	0.41
2:H:106:ASP:HB3	2:H:188:LEU:HD13	2.03	0.41
2:H:351:GLU:HB3	2:H:407:ILE:HG23	2.03	0.41
2:H:381:THR:OG1	2:H:384:ASP:OD2	2.39	0.41
2:B:102:LYS:HB2	2:B:140:ARG:HG3	2.03	0.41
2:B:174:LEU:O	2:B:175:ASP:C	2.59	0.41
2:B:346:VAL:HG12	2:B:413:PHE:CE1	2.56	0.41
1:C:253:VAL:HB	1:C:267:PHE:HB2	2.03	0.41
1:E:496:VAL:HG12	1:E:524:LYS:O	2.21	0.41
2:F:115:ALA:HA	2:F:204:ILE:HG21	2.03	0.41
2:H:357:ILE:HB	2:H:359:PHE:CE1	2.56	0.41
1:E:58:LYS:HB2	1:E:70:ILE:HD11	2.02	0.40
1:A:366:GLY:CA	1:A:372:ILE:HD11	2.52	0.40
2:B:325:GLU:O	2:B:326:SER:C	2.60	0.40
2:B:334:LEU:C	2:B:334:LEU:HD23	2.42	0.40
1:C:348:GLY:O	1:C:357:ASP:N	2.42	0.40
1:C:375:ILE:N	1:C:375:ILE:HD12	2.37	0.40
1:C:50:ILE:HD11	1:C:76:GLY:HA2	2.03	0.40
2:D:379:ASN:OD1	10:D:501:NAG:H2	2.20	0.40
2:D:407:ILE:HD11	2:D:416:THR:CG2	2.51	0.40
1:E:116:THR:HG21	1:E:147:ILE:CD1	2.52	0.40
2:F:231:ARG:C	2:F:236:ARG:HH11	2.24	0.40
3:I:2:NAG:O3	3:I:3:BMA:H61	2.20	0.40
2:B:301:VAL:O	2:B:324:ILE:N	2.32	0.40
1:C:509:ILE:HD11	1:C:549:PHE:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PHE:CZ	1:E:38:VAL:HG11	2.57	0.40
2:F:175:ASP:OD1	2:F:176:CYS:N	2.55	0.40
1:E:5:VAL:HG12	1:E:5:VAL:O	2.20	0.40
1:G:234:ASP:OD1	1:G:235:GLY:N	2.54	0.40
1:G:57:LEU:HD12	1:G:57:LEU:N	2.37	0.40
1:C:437:ARG:NH2	1:C:573:THR:OG1	2.48	0.40
14:D:507:MES:H82	14:D:507:MES:H51	1.75	0.40
1:E:169:VAL:O	1:E:185:SER:HA	2.22	0.40
1:E:245:ARG:NH2	2:F:246:SER:O	2.54	0.40
1:G:224:TYR:OH	2:H:250:LEU:O	2.39	0.40
3:I:1:NAG:HO3	3:I:1:NAG:C7	2.25	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:809:HOH:O	15:C:731:HOH:O[1_545]	2.01	0.19
15:G:2123:HOH:O	15:H:603:HOH:O[1_565]	2.07	0.13
1:A:530:ARG:O	1:C:417:LYS:NZ[1_545]	2.08	0.12
1:C:491:LYS:NZ	3:I:3:BMA:O6[1_565]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	584/599 (98%)	550 (94%)	31 (5%)	3 (0%)	29	43
1	C	589/599 (98%)	556 (94%)	32 (5%)	1 (0%)	47	64
1	E	587/599 (98%)	538 (92%)	48 (8%)	1 (0%)	47	64
1	G	590/599 (98%)	546 (92%)	43 (7%)	1 (0%)	47	64
2	B	322/456 (71%)	290 (90%)	28 (9%)	4 (1%)	13	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	298/456 (65%)	266 (89%)	29 (10%)	3 (1%)	15	23
2	F	323/456 (71%)	288 (89%)	35 (11%)	0	100	100
2	H	326/456 (72%)	293 (90%)	31 (10%)	2 (1%)	25	37
All	All	3619/4220 (86%)	3327 (92%)	277 (8%)	15 (0%)	34	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	GLY
2	B	326	SER
1	A	596	THR
2	B	72	ILE
2	B	175	ASP
2	D	191	ASN
1	C	62	SER
2	D	150	VAL
2	D	224	CYS
1	G	465	PRO
2	H	140	ARG
2	H	224	CYS
1	A	116	THR
1	E	276	PHE
2	B	150	VAL

### 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	485/489 (99%)	479 (99%)	6 (1%)	71	84
1	C	487/489 (100%)	480 (99%)	7 (1%)	67	81
1	E	485/489 (99%)	479 (99%)	6 (1%)	71	84
1	G	488/489 (100%)	480 (98%)	8 (2%)	62	78
2	B	296/402 (74%)	293 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	277/402 (69%)	275 (99%)	2 (1%)	84	91
2	F	292/402 (73%)	290 (99%)	2 (1%)	84	91
2	H	296/402 (74%)	291 (98%)	5 (2%)	60	77
All	All	3106/3564 (87%)	3067 (99%)	39 (1%)	69	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	114	TRP
1	A	155	CYS
1	A	275	TYR
1	A	401	CYS
1	A	475	ASN
2	B	124	LEU
2	B	304	LYS
2	B	342	LEU
1	C	114	TRP
1	C	148	ASP
1	C	155	CYS
1	C	275	TYR
1	C	401	CYS
1	C	511	ARG
1	C	586	ASN
2	D	94	MET
2	D	250	LEU
1	E	114	TRP
1	E	155	CYS
1	E	250	LEU
1	E	275	TYR
1	E	511	ARG
1	E	530	ARG
2	F	94	MET
2	F	327	LYS
1	G	114	TRP
1	G	155	CYS
1	G	275	TYR
1	G	401	CYS
1	G	463	SER
1	G	464	LEU
1	G	475	ASN

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Mol	Chain	Res	Type
1	G	511	ARG
2	H	103	TYR
2	H	124	LEU
2	H	325	GLU
2	H	353	GLN
2	H	397	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	180	HIS
2	D	294	ASN
2	H	383	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 ⓘ

95 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	$\# Z  > 2$
3	NAG	I	1	1,3	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.50	0
3	BMA	I	3	3	11,11,12	0.51	0	15,15,17	1.33	2 (13%)
3	MAN	I	4	3	11,11,12	0.86	1 (9%)	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	J	1	1,4	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	BMA	J	3	4	11,11,12	0.56	0	15,15,17	0.89	0
4	MAN	J	4	4	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
4	MAN	J	5	4	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.38	0
3	BMA	K	3	3	11,11,12	0.70	0	15,15,17	1.08	1 (6%)
3	MAN	K	4	3	11,11,12	0.77	0	15,15,17	1.41	3 (20%)
5	NAG	L	1	1,5	14,14,15	0.34	0	17,19,21	0.41	0
5	NAG	L	2	5	14,14,15	0.24	0	17,19,21	0.47	0
5	BMA	L	3	5	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
5	MAN	L	4	5	11,11,12	1.16	1 (9%)	15,15,17	1.56	4 (26%)
5	MAN	L	5	5	11,11,12	0.80	1 (9%)	15,15,17	1.18	3 (20%)
5	MAN	L	6	5	11,11,12	1.33	1 (9%)	15,15,17	0.91	1 (6%)
6	NAG	M	1	2,6	14,14,15	0.19	0	17,19,21	0.44	0
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	N	1	2,6	14,14,15	0.18	0	17,19,21	0.39	0
6	NAG	N	2	6	14,14,15	0.26	0	17,19,21	0.36	0
3	NAG	O	1	3,2	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.28	0	17,19,21	0.41	0
3	BMA	O	3	3	11,11,12	0.50	0	15,15,17	0.90	0
3	MAN	O	4	3	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
7	NAG	P	1	1,7	14,14,15	0.46	0	17,19,21	0.43	0
7	NAG	P	2	7	14,14,15	0.35	0	17,19,21	0.39	0
7	BMA	P	3	7	11,11,12	0.94	1 (9%)	15,15,17	0.95	0
7	MAN	P	4	7	11,11,12	0.65	0	15,15,17	1.37	3 (20%)
7	MAN	P	5	7	11,11,12	0.79	1 (9%)	15,15,17	0.84	1 (6%)
7	MAN	P	6	7	11,11,12	0.75	0	15,15,17	1.07	2 (13%)
3	NAG	Q	1	1,3	14,14,15	0.43	0	17,19,21	0.41	0
3	NAG	Q	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	BMA	Q	3	3	11,11,12	0.70	0	15,15,17	0.95	0
3	MAN	Q	4	3	11,11,12	1.18	1 (9%)	15,15,17	2.32	4 (26%)
7	NAG	R	1	1,7	14,14,15	0.45	0	17,19,21	0.50	0
7	NAG	R	2	7	14,14,15	0.28	0	17,19,21	0.44	0
7	BMA	R	3	7	11,11,12	0.80	1 (9%)	15,15,17	1.16	1 (6%)
7	MAN	R	4	7	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
7	MAN	R	5	7	11,11,12	0.77	0	15,15,17	1.00	1 (6%)
7	MAN	R	6	7	11,11,12	1.14	1 (9%)	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	S	1	1,3	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	S	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	BMA	S	3	3	11,11,12	0.93	1 (9%)	15,15,17	1.19	1 (6%)
3	MAN	S	4	3	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
6	NAG	T	1	2,6	14,14,15	0.29	0	17,19,21	0.52	0
6	NAG	T	2	6	14,14,15	0.26	0	17,19,21	0.37	0
4	NAG	U	1	1,4	14,14,15	0.40	0	17,19,21	0.46	0
4	NAG	U	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	BMA	U	3	4	11,11,12	0.53	0	15,15,17	0.93	0
4	MAN	U	4	4	11,11,12	0.63	0	15,15,17	1.13	2 (13%)
4	MAN	U	5	4	11,11,12	0.82	1 (9%)	15,15,17	1.43	3 (20%)
6	NAG	V	1	1,6	14,14,15	0.33	0	17,19,21	0.44	0
6	NAG	V	2	6	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	W	1	1,7	14,14,15	0.59	1 (7%)	17,19,21	0.49	0
7	NAG	W	2	7	14,14,15	0.56	0	17,19,21	0.50	0
7	BMA	W	3	7	11,11,12	1.21	1 (9%)	15,15,17	2.02	4 (26%)
7	MAN	W	4	7	11,11,12	0.78	1 (9%)	15,15,17	1.05	2 (13%)
7	MAN	W	5	7	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
7	MAN	W	6	7	11,11,12	1.53	2 (18%)	15,15,17	1.79	3 (20%)
4	NAG	X	1	1,4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	X	2	4	14,14,15	0.26	0	17,19,21	0.47	0
4	BMA	X	3	4	11,11,12	0.82	0	15,15,17	0.87	0
4	MAN	X	4	4	11,11,12	0.72	0	15,15,17	1.03	2 (13%)
4	MAN	X	5	4	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
6	NAG	Y	1	2,6	14,14,15	0.26	0	17,19,21	0.46	0
6	NAG	Y	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	Z	1	2,6	14,14,15	0.37	0	17,19,21	0.62	0
6	NAG	Z	2	6	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	a	1	1,3	14,14,15	0.53	0	17,19,21	0.46	0
3	NAG	a	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	a	3	3	11,11,12	0.53	0	15,15,17	1.09	1 (6%)
3	MAN	a	4	3	11,11,12	0.71	0	15,15,17	1.11	2 (13%)
8	NAG	b	1	1,8	14,14,15	0.82	1 (7%)	17,19,21	0.63	1 (5%)
8	NAG	b	2	8	14,14,15	0.79	1 (7%)	17,19,21	1.59	3 (17%)
8	BMA	b	3	8	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
8	MAN	b	4	8	11,11,12	1.35	2 (18%)	15,15,17	1.23	4 (26%)
8	MAN	b	5	8	11,11,12	0.89	1 (9%)	15,15,17	1.30	2 (13%)
8	MAN	b	6	8	11,11,12	1.52	3 (27%)	15,15,17	1.85	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	c	1	1,9	14,14,15	0.39	0	17,19,21	0.44	0
9	NAG	c	2	9	14,14,15	0.24	0	17,19,21	0.43	0
9	BMA	c	3	9	11,11,12	0.60	0	15,15,17	0.76	0
9	MAN	c	4	9	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
3	NAG	d	1	1,3	14,14,15	0.54	0	17,19,21	0.50	0
3	NAG	d	2	3	14,14,15	0.41	0	17,19,21	0.42	0
3	BMA	d	3	3	11,11,12	0.75	0	15,15,17	0.69	0
3	MAN	d	4	3	11,11,12	0.78	0	15,15,17	1.03	1 (6%)
6	NAG	e	1	2,6	14,14,15	0.55	0	17,19,21	0.46	0
6	NAG	e	2	6	14,14,15	0.24	0	17,19,21	0.55	0
6	NAG	f	1	2,6	14,14,15	0.36	0	17,19,21	0.54	0
6	NAG	f	2	6	14,14,15	0.18	0	17,19,21	0.74	1 (5%)
6	NAG	g	1	2,6	14,14,15	0.59	1 (7%)	17,19,21	0.51	0
6	NAG	g	2	6	14,14,15	0.29	0	17,19,21	0.58	0

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	BMA	W	3	7	-	2/2/19/22	0/1/1/1
7	MAN	W	4	7	-	0/2/19/22	0/1/1/1
7	MAN	W	5	7	-	1/2/19/22	0/1/1/1
7	MAN	W	6	7	-	0/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	BMA	X	3	4	-	2/2/19/22	0/1/1/1
4	MAN	X	4	4	-	2/2/19/22	0/1/1/1
4	MAN	X	5	4	-	2/2/19/22	0/1/1/1
6	NAG	Y	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Z	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	BMA	a	3	3	-	2/2/19/22	0/1/1/1
3	MAN	a	4	3	-	0/2/19/22	1/1/1/1
8	NAG	b	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	2/2/19/22	0/1/1/1
8	MAN	b	4	8	-	2/2/19/22	0/1/1/1
8	MAN	b	5	8	-	2/2/19/22	0/1/1/1
8	MAN	b	6	8	-	0/2/19/22	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
3	NAG	d	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	d	2	3	-	3/6/23/26	0/1/1/1
3	BMA	d	3	3	-	0/2/19/22	0/1/1/1
3	MAN	d	4	3	-	1/2/19/22	0/1/1/1
6	NAG	e	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	3/6/23/26	0/1/1/1
6	NAG	f	1	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	4/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	6	MAN	O5-C1	-3.91	1.37	1.43
7	W	6	MAN	C2-C3	3.58	1.57	1.52
7	R	6	MAN	O5-C1	-2.90	1.39	1.43
8	b	6	MAN	C4-C5	2.77	1.58	1.53
7	W	6	MAN	C1-C2	2.65	1.58	1.52
8	b	2	NAG	O5-C1	-2.63	1.39	1.43
3	Q	4	MAN	C1-C2	2.63	1.58	1.52
5	L	4	MAN	O5-C1	-2.59	1.39	1.43
8	b	4	MAN	O5-C1	-2.58	1.39	1.43
8	b	6	MAN	O5-C5	2.57	1.48	1.43
3	I	4	MAN	O5-C1	-2.53	1.39	1.43
8	b	6	MAN	C2-C3	-2.46	1.48	1.52
7	P	3	BMA	O5-C1	-2.38	1.39	1.43
5	L	5	MAN	C1-C2	2.38	1.57	1.52
8	b	1	NAG	O5-C1	2.33	1.47	1.43
8	b	5	MAN	C1-C2	2.22	1.57	1.52
8	b	4	MAN	C2-C3	2.21	1.55	1.52
7	W	3	BMA	C1-C2	2.21	1.57	1.52
7	W	1	NAG	O5-C1	-2.17	1.40	1.43
4	U	5	MAN	C1-C2	2.16	1.57	1.52
6	g	1	NAG	O5-C1	-2.13	1.40	1.43
3	S	3	BMA	O5-C1	-2.12	1.40	1.43
7	R	3	BMA	O5-C1	-2.08	1.40	1.43
7	W	4	MAN	O5-C1	-2.05	1.40	1.43
7	P	5	MAN	O5-C1	-2.02	1.40	1.43

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	4	MAN	C1-O5-C5	6.06	120.40	112.19
7	W	3	BMA	C1-C2-C3	5.21	116.07	109.67
3	Q	4	MAN	O5-C1-C2	4.95	118.41	110.77
8	b	6	MAN	C1-O5-C5	4.53	118.32	112.19
3	I	3	BMA	C1-O5-C5	4.37	118.12	112.19
7	W	6	MAN	C1-C2-C3	4.19	114.81	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	2	NAG	O4-C4-C5	-3.94	99.52	109.30
7	W	3	BMA	O5-C1-C2	3.79	116.62	110.77
8	b	5	MAN	O5-C1-C2	3.73	116.53	110.77
8	b	2	NAG	C3-C4-C5	3.70	116.83	110.24
8	b	6	MAN	C1-C2-C3	-3.64	105.19	109.67
7	P	4	MAN	C1-O5-C5	3.49	116.92	112.19
5	L	4	MAN	C1-O5-C5	3.42	116.83	112.19
7	R	6	MAN	C1-C2-C3	-3.40	105.49	109.67
7	W	6	MAN	O5-C1-C2	3.34	115.92	110.77
7	R	4	MAN	C1-O5-C5	3.32	116.68	112.19
3	K	4	MAN	C1-O5-C5	2.93	116.16	112.19
4	U	4	MAN	C1-O5-C5	2.92	116.15	112.19
4	U	5	MAN	O5-C1-C2	2.90	115.25	110.77
3	S	4	MAN	C1-O5-C5	2.85	116.05	112.19
4	U	5	MAN	C1-O5-C5	2.73	115.89	112.19
5	L	5	MAN	O5-C1-C2	2.65	114.86	110.77
3	a	4	MAN	C1-O5-C5	2.60	115.71	112.19
3	K	4	MAN	O5-C1-C2	2.57	114.74	110.77
4	J	5	MAN	C1-O5-C5	2.54	115.64	112.19
7	W	5	MAN	C1-O5-C5	2.52	115.61	112.19
5	L	4	MAN	O6-C6-C5	-2.52	102.64	111.29
7	W	3	BMA	O2-C2-C3	-2.51	105.10	110.14
3	S	3	BMA	C1-C2-C3	2.51	112.75	109.67
8	b	4	MAN	C1-O5-C5	2.50	115.58	112.19
8	b	2	NAG	O4-C4-C3	-2.45	104.70	110.35
7	P	6	MAN	C1-O5-C5	2.43	115.49	112.19
4	X	4	MAN	C1-O5-C5	2.43	115.48	112.19
6	f	2	NAG	C1-O5-C5	2.40	115.45	112.19
4	X	5	MAN	C1-O5-C5	2.39	115.43	112.19
5	L	4	MAN	O3-C3-C2	2.39	114.57	109.99
7	P	4	MAN	O2-C2-C3	-2.38	105.38	110.14
7	R	3	BMA	C1-O5-C5	2.38	115.41	112.19
5	L	5	MAN	C1-O5-C5	2.37	115.41	112.19
7	W	3	BMA	O5-C5-C4	-2.37	105.06	110.83
3	Q	4	MAN	C3-C4-C5	-2.34	106.06	110.24
7	R	4	MAN	O2-C2-C3	-2.33	105.46	110.14
5	L	5	MAN	O2-C2-C3	-2.31	105.51	110.14
4	X	5	MAN	O2-C2-C3	-2.30	105.52	110.14
3	O	4	MAN	O2-C2-C3	-2.30	105.53	110.14
3	d	4	MAN	O2-C2-C3	-2.29	105.55	110.14
3	K	3	BMA	C1-C2-C3	2.29	112.48	109.67
3	Q	4	MAN	O2-C2-C3	-2.29	105.56	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	4	MAN	C1-O5-C5	2.25	115.25	112.19
8	b	6	MAN	C3-C4-C5	2.25	114.25	110.24
7	W	6	MAN	O5-C5-C4	-2.24	105.39	110.83
8	b	1	NAG	C1-O5-C5	2.23	115.22	112.19
4	X	4	MAN	O2-C2-C3	-2.23	105.67	110.14
7	P	6	MAN	O2-C2-C3	-2.23	105.68	110.14
8	b	6	MAN	O2-C2-C3	-2.22	105.68	110.14
9	c	4	MAN	C1-O5-C5	2.21	115.19	112.19
7	W	5	MAN	O2-C2-C3	-2.21	105.72	110.14
7	R	6	MAN	O2-C2-C3	-2.19	105.75	110.14
7	P	5	MAN	O2-C2-C3	-2.18	105.76	110.14
3	a	4	MAN	O2-C2-C3	-2.18	105.76	110.14
4	J	4	MAN	C1-O5-C5	2.18	115.15	112.19
3	S	4	MAN	O2-C2-C3	-2.18	105.77	110.14
4	J	5	MAN	O2-C2-C3	-2.17	105.79	110.14
7	W	4	MAN	C1-O5-C5	2.15	115.11	112.19
3	I	4	MAN	O2-C2-C3	-2.15	105.84	110.14
4	J	4	MAN	O2-C2-C3	-2.13	105.86	110.14
5	L	4	MAN	O2-C2-C3	-2.11	105.90	110.14
8	b	4	MAN	O2-C2-C3	-2.11	105.90	110.14
7	W	4	MAN	O2-C2-C3	-2.11	105.92	110.14
4	U	5	MAN	O2-C2-C3	-2.08	105.97	110.14
5	L	6	MAN	O2-C2-C3	-2.08	105.97	110.14
3	a	3	BMA	O5-C1-C2	2.07	113.97	110.77
8	b	5	MAN	O2-C2-C3	-2.07	106.00	110.14
4	U	4	MAN	O2-C2-C3	-2.07	106.00	110.14
5	L	3	BMA	C1-O5-C5	2.06	114.98	112.19
7	R	5	MAN	O2-C2-C3	-2.05	106.03	110.14
9	c	4	MAN	O2-C2-C3	-2.04	106.05	110.14
8	b	4	MAN	C1-C2-C3	2.04	112.17	109.67
7	P	4	MAN	O5-C1-C2	2.03	113.91	110.77
3	I	3	BMA	O2-C2-C3	-2.03	106.07	110.14
3	K	4	MAN	O2-C2-C3	-2.03	106.07	110.14
8	b	3	BMA	C1-O5-C5	2.01	114.91	112.19
8	b	4	MAN	O3-C3-C2	2.01	113.83	109.99

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	2	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	L	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C1-C2-N2-C7
7	P	1	NAG	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
5	L	3	BMA	C4-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	X	4	MAN	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	L	6	MAN	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C1-C2-N2-C7
6	Z	1	NAG	C1-C2-N2-C7
3	d	2	NAG	C4-C5-C6-O6
3	O	4	MAN	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	Z	1	NAG	C4-C5-C6-O6
8	b	5	MAN	O5-C5-C6-O6
8	b	4	MAN	O5-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
6	g	2	NAG	C8-C7-N2-C2
6	g	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
6	e	2	NAG	C8-C7-N2-C2
6	e	2	NAG	O7-C7-N2-C2
7	R	3	BMA	O5-C5-C6-O6
7	R	6	MAN	C4-C5-C6-O6
5	L	6	MAN	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
3	a	3	BMA	C4-C5-C6-O6
4	X	5	MAN	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
3	S	4	MAN	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
8	b	3	BMA	C4-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
7	R	3	BMA	C4-C5-C6-O6
7	W	3	BMA	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
3	a	3	BMA	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	U	5	MAN	C4-C5-C6-O6
7	R	6	MAN	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
8	b	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
4	U	5	MAN	O5-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
4	X	2	NAG	C4-C5-C6-O6
3	d	4	MAN	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
4	X	5	MAN	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
7	R	4	MAN	O5-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6
3	S	4	MAN	C4-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
8	b	4	MAN	C4-C5-C6-O6
4	U	3	BMA	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
3	d	2	NAG	C3-C2-N2-C7
3	d	1	NAG	O5-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
8	b	5	MAN	C4-C5-C6-O6
4	U	3	BMA	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
7	P	6	MAN	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
6	g	2	NAG	C3-C2-N2-C7
6	Y	2	NAG	C3-C2-N2-C7
6	Z	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C3-C2-N2-C7
6	e	2	NAG	C3-C2-N2-C7
7	W	5	MAN	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
9	c	4	MAN	C4-C5-C6-O6
6	T	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
4	U	4	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	4	MAN	C1-C2-C3-C4-C5-O5
3	a	4	MAN	C1-C2-C3-C4-C5-O5

37 monomers are involved in 61 short contacts:

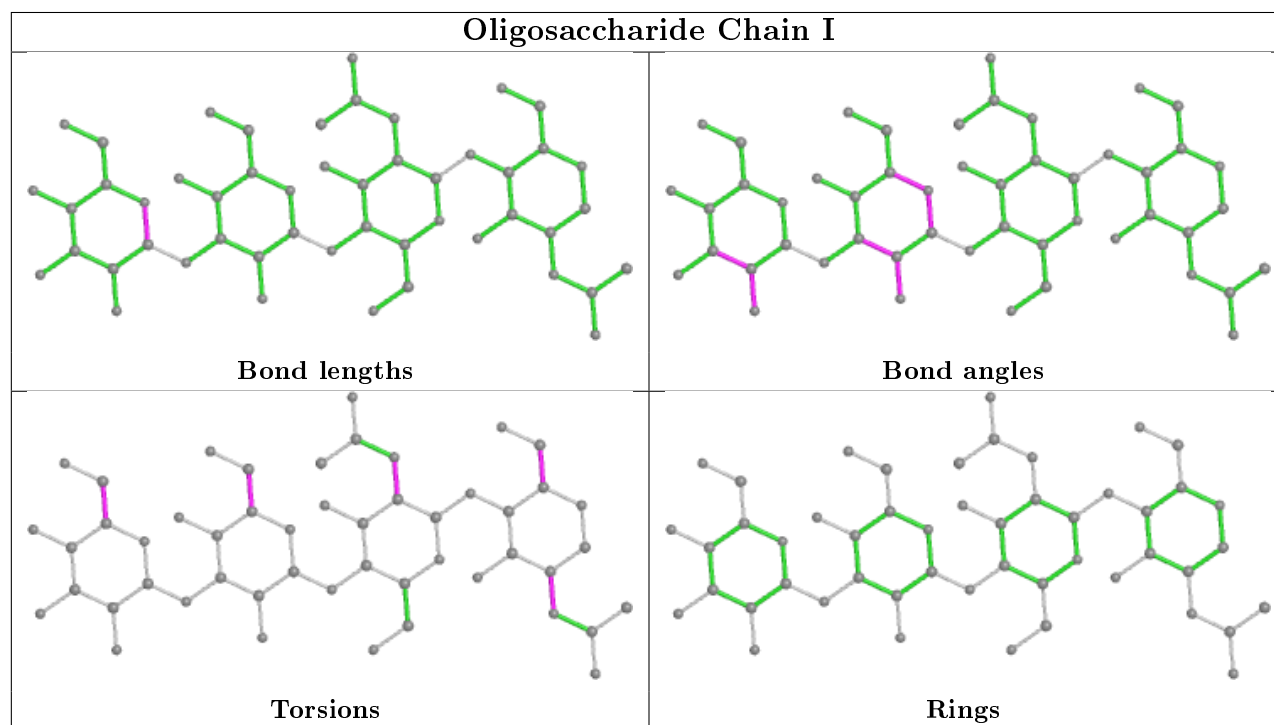
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	4	MAN	5	0
3	I	1	NAG	5	0
6	T	2	NAG	2	0
3	Q	4	MAN	5	0
3	Q	1	NAG	1	0
7	W	6	MAN	3	0
4	X	3	BMA	1	0
7	R	3	BMA	6	0
5	L	5	MAN	4	0
7	W	2	NAG	1	0
6	M	2	NAG	1	0
6	T	1	NAG	1	0
3	K	1	NAG	2	0
3	I	3	BMA	5	1
7	R	4	MAN	2	0
6	V	2	NAG	1	0
3	O	2	NAG	2	0
6	V	1	NAG	1	0
7	R	2	NAG	4	0
6	M	1	NAG	1	0
7	R	6	MAN	1	0
6	Y	1	NAG	3	0
7	W	1	NAG	1	0
4	U	1	NAG	1	0

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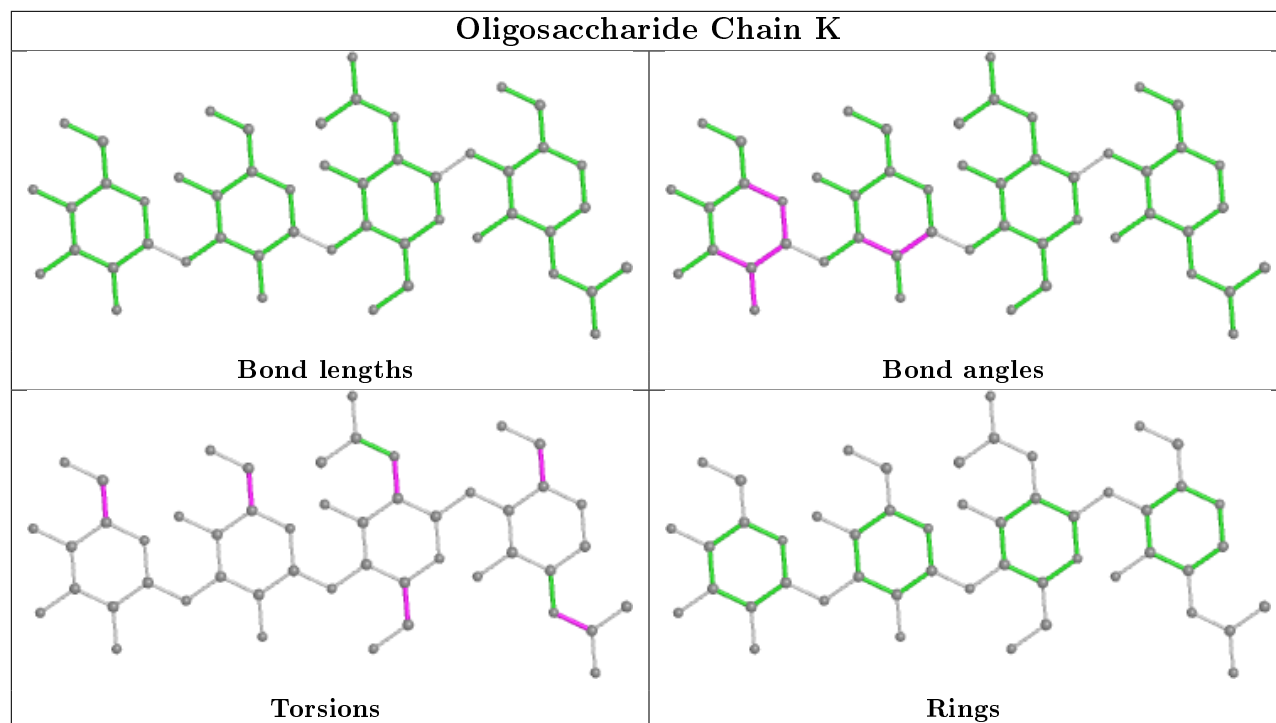
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	1	0
7	P	1	NAG	1	0
6	Y	2	NAG	3	0
3	S	4	MAN	1	0
7	W	3	BMA	6	0
3	Q	3	BMA	8	0
5	L	2	NAG	2	0
6	Z	1	NAG	1	0
3	Q	2	NAG	3	0
7	R	5	MAN	1	0
4	X	2	NAG	1	0
3	I	2	NAG	9	0
5	L	3	BMA	4	0

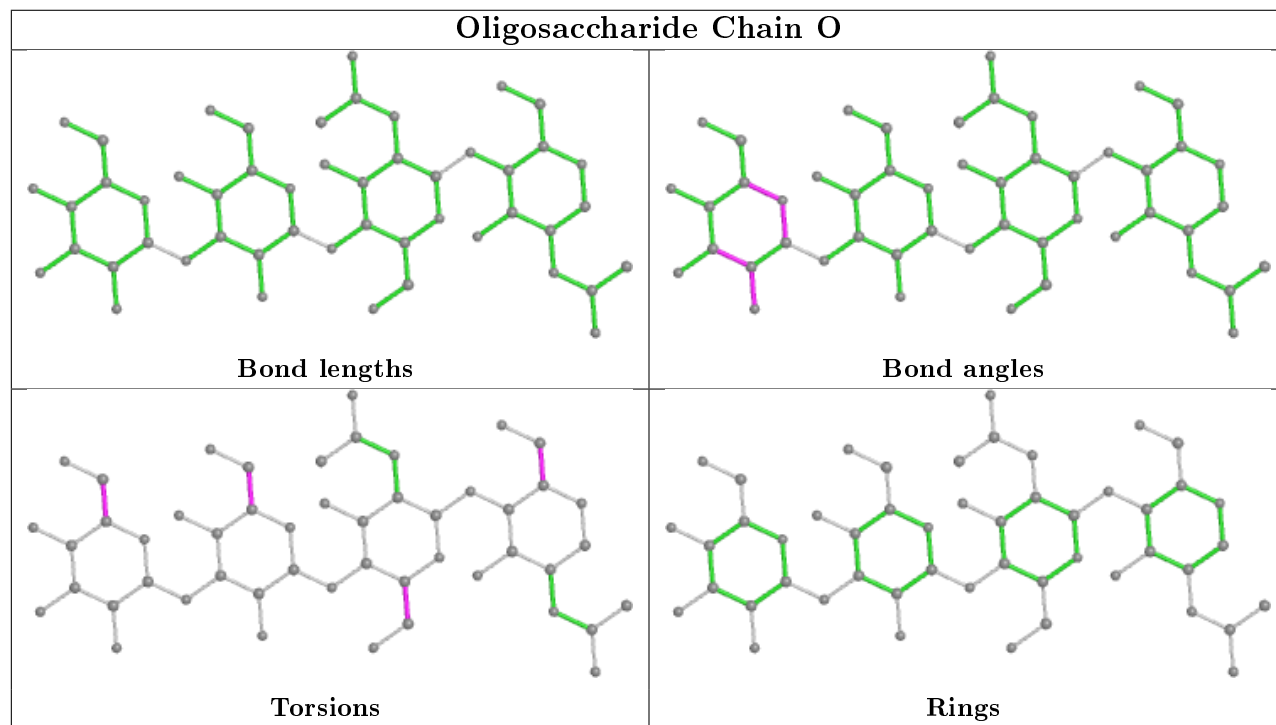
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



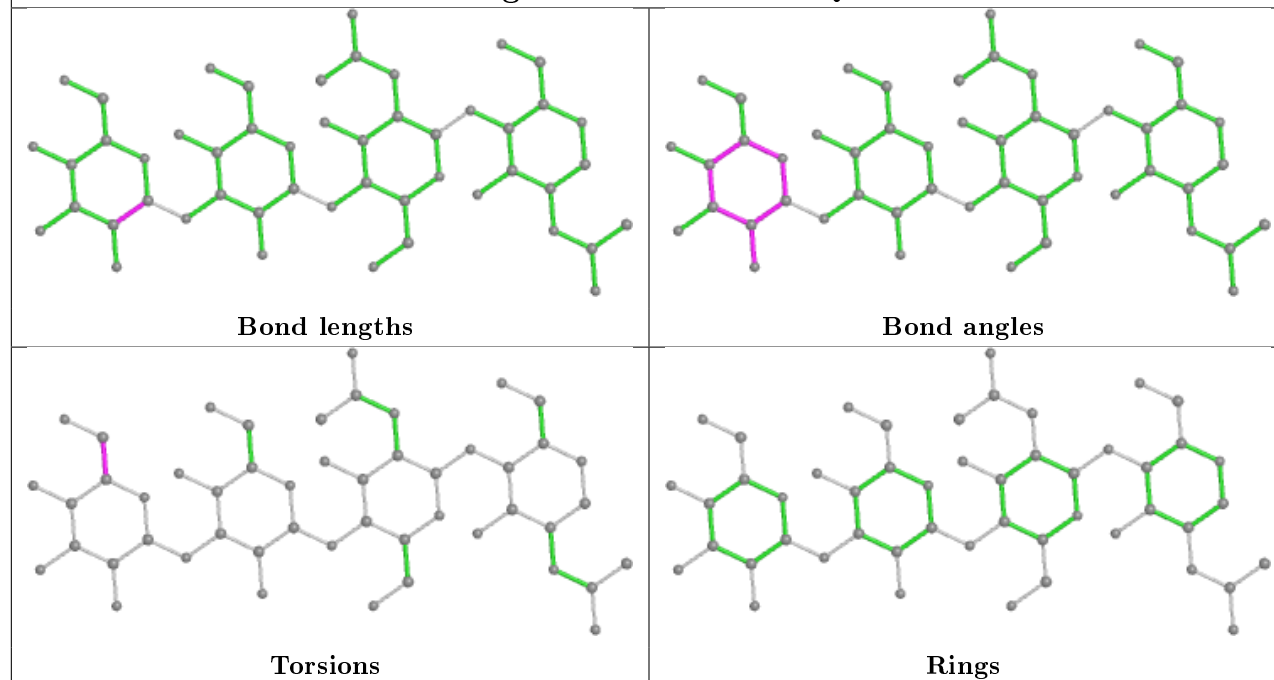
## Oligosaccharide Chain K



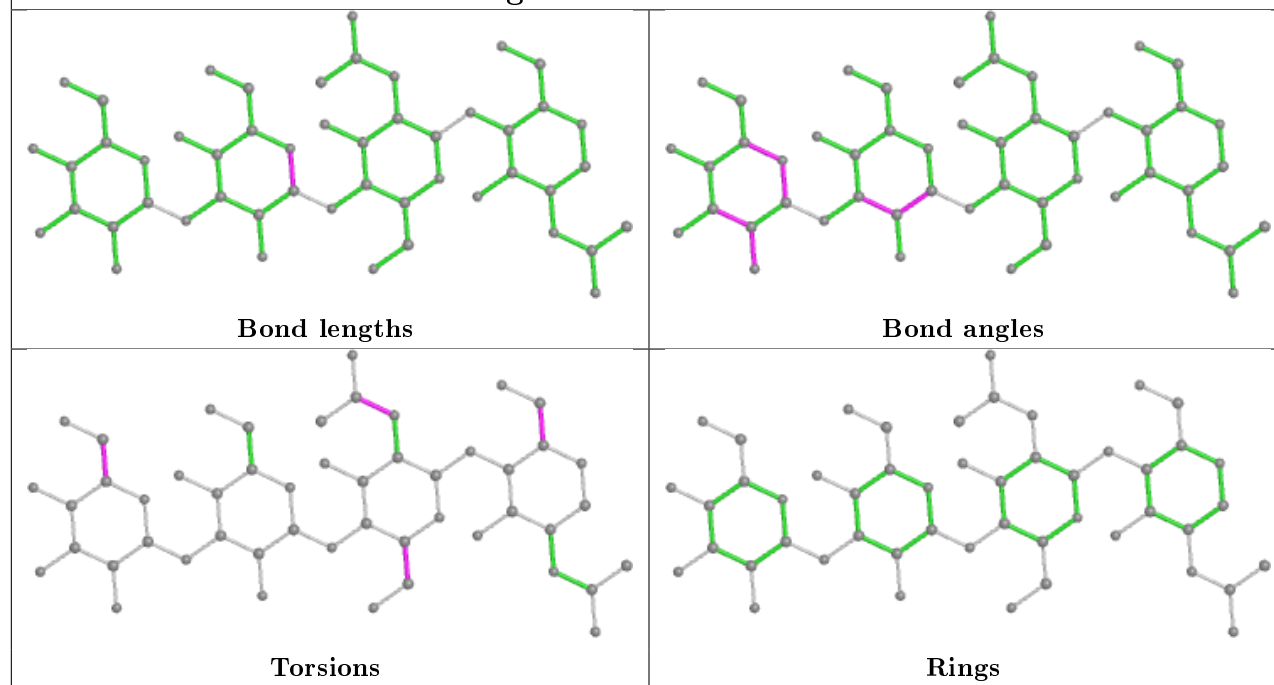
## Oligosaccharide Chain O



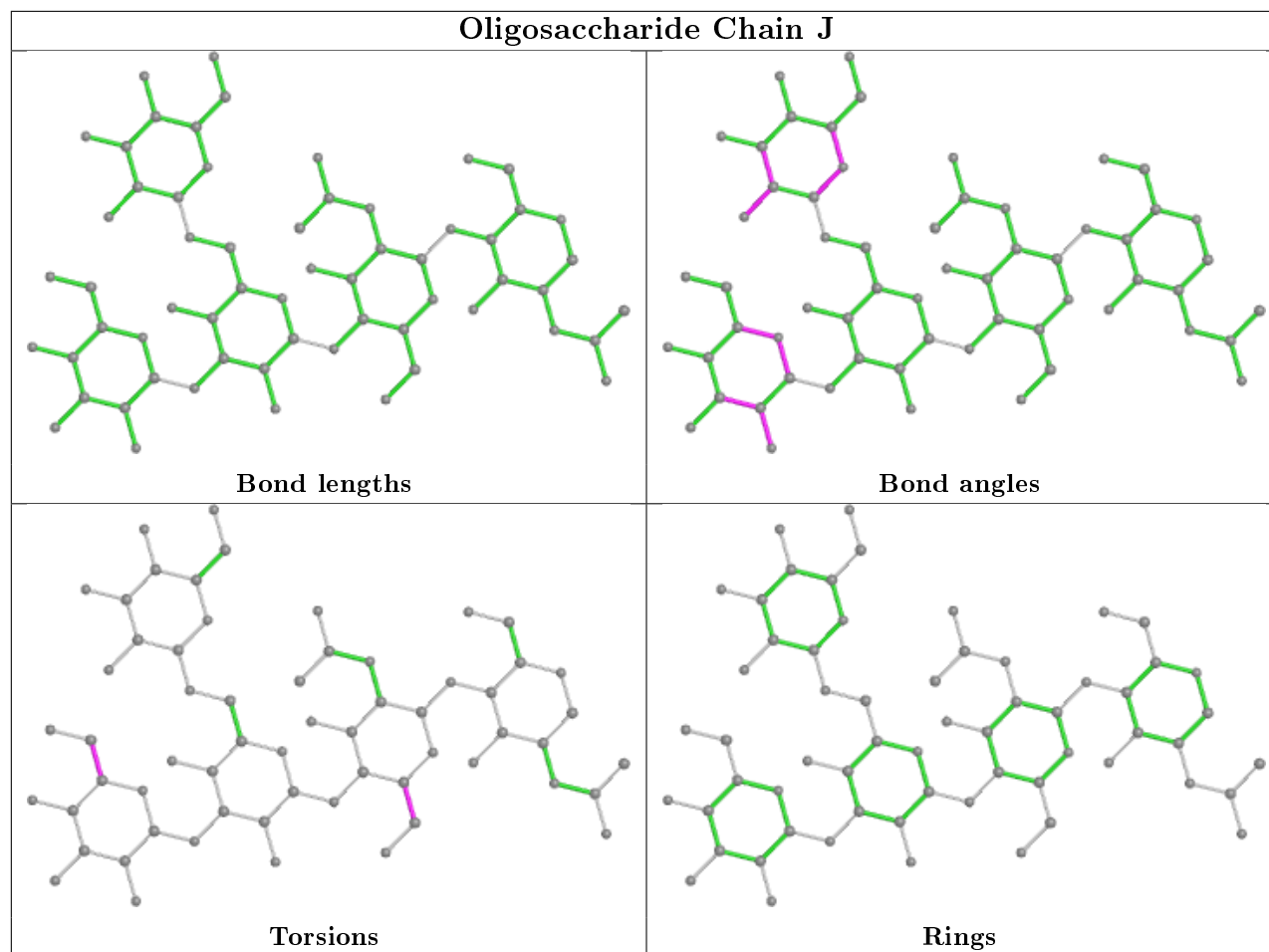
## Oligosaccharide Chain Q

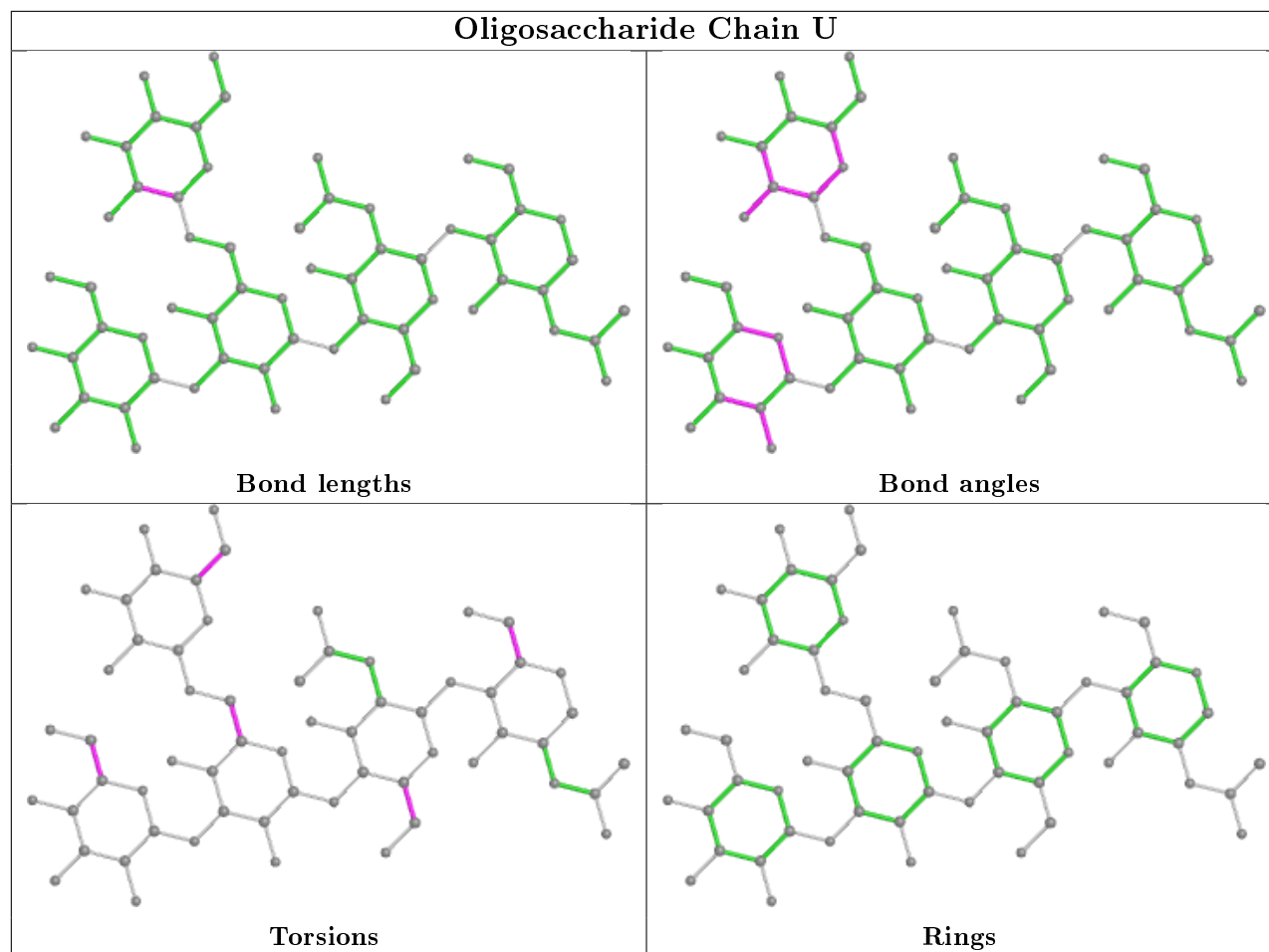


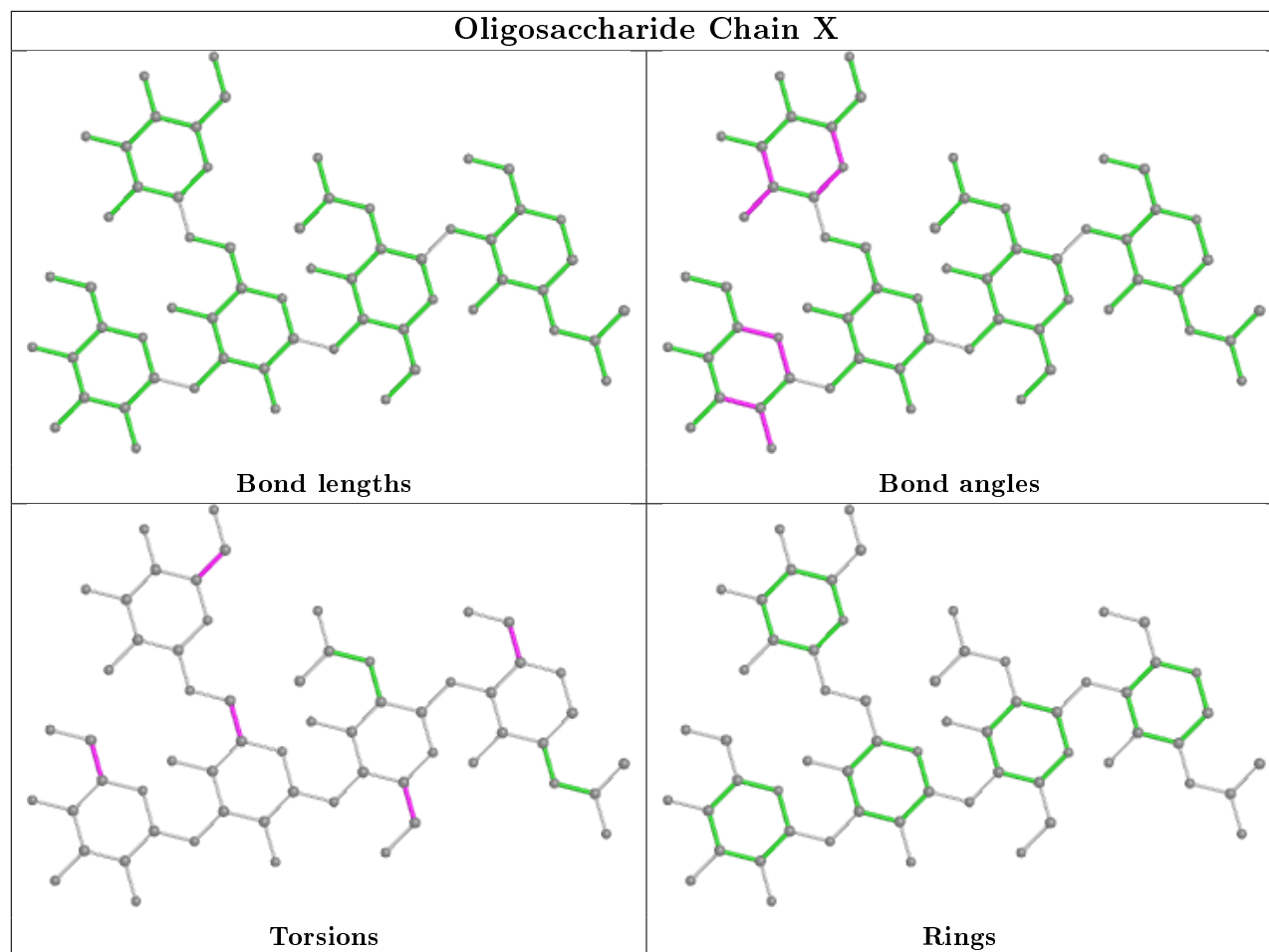
## Oligosaccharide Chain S

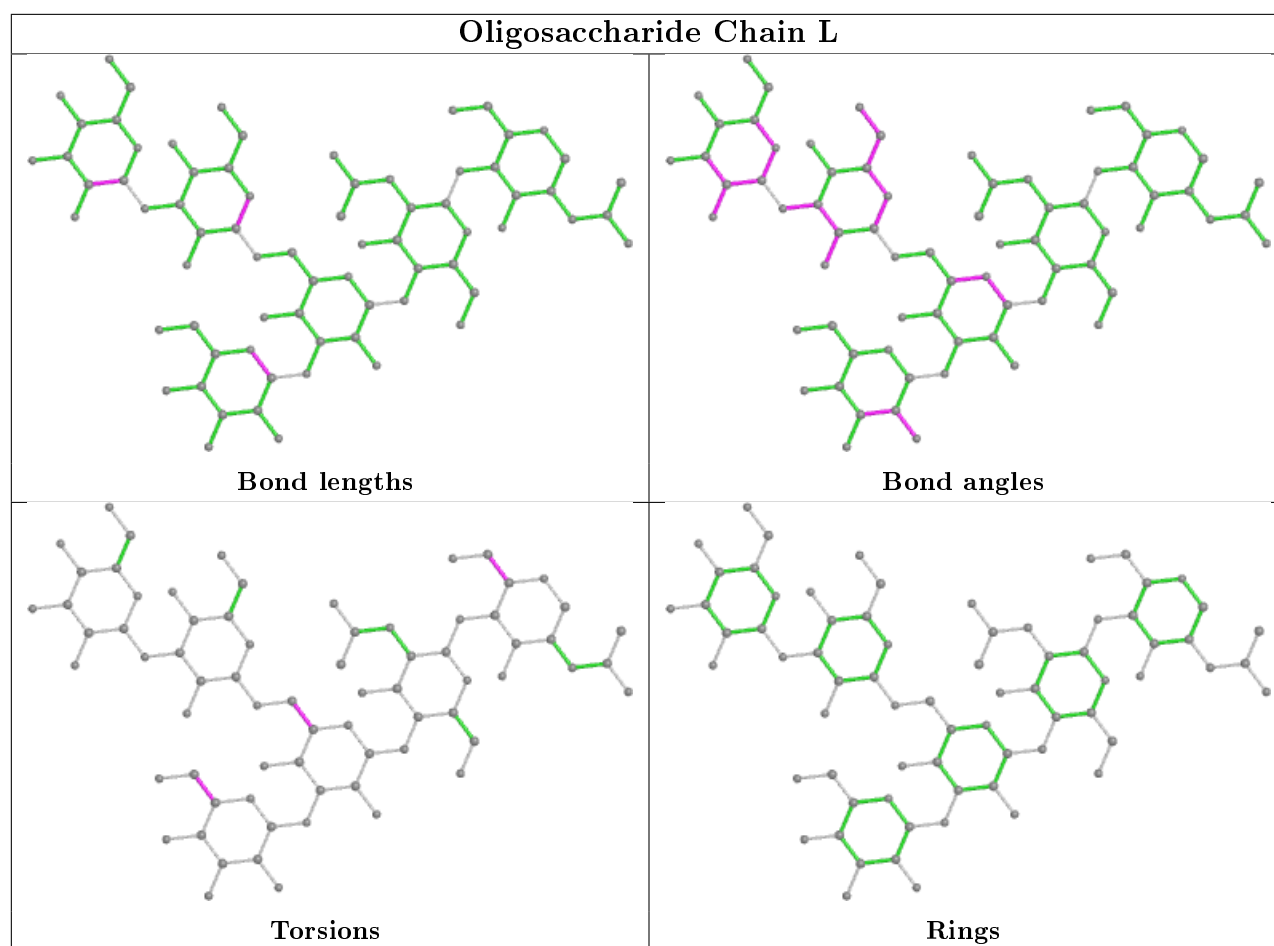


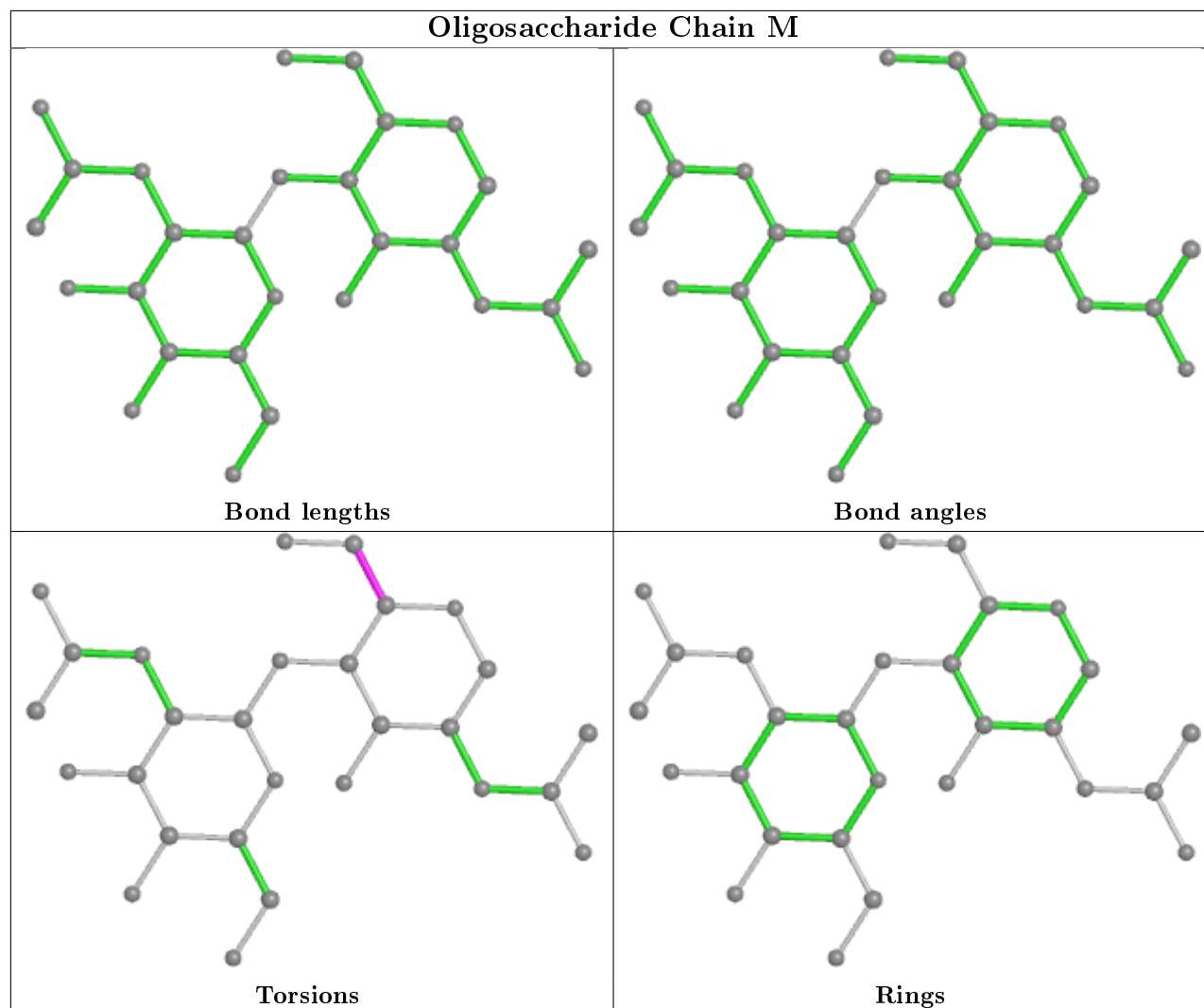


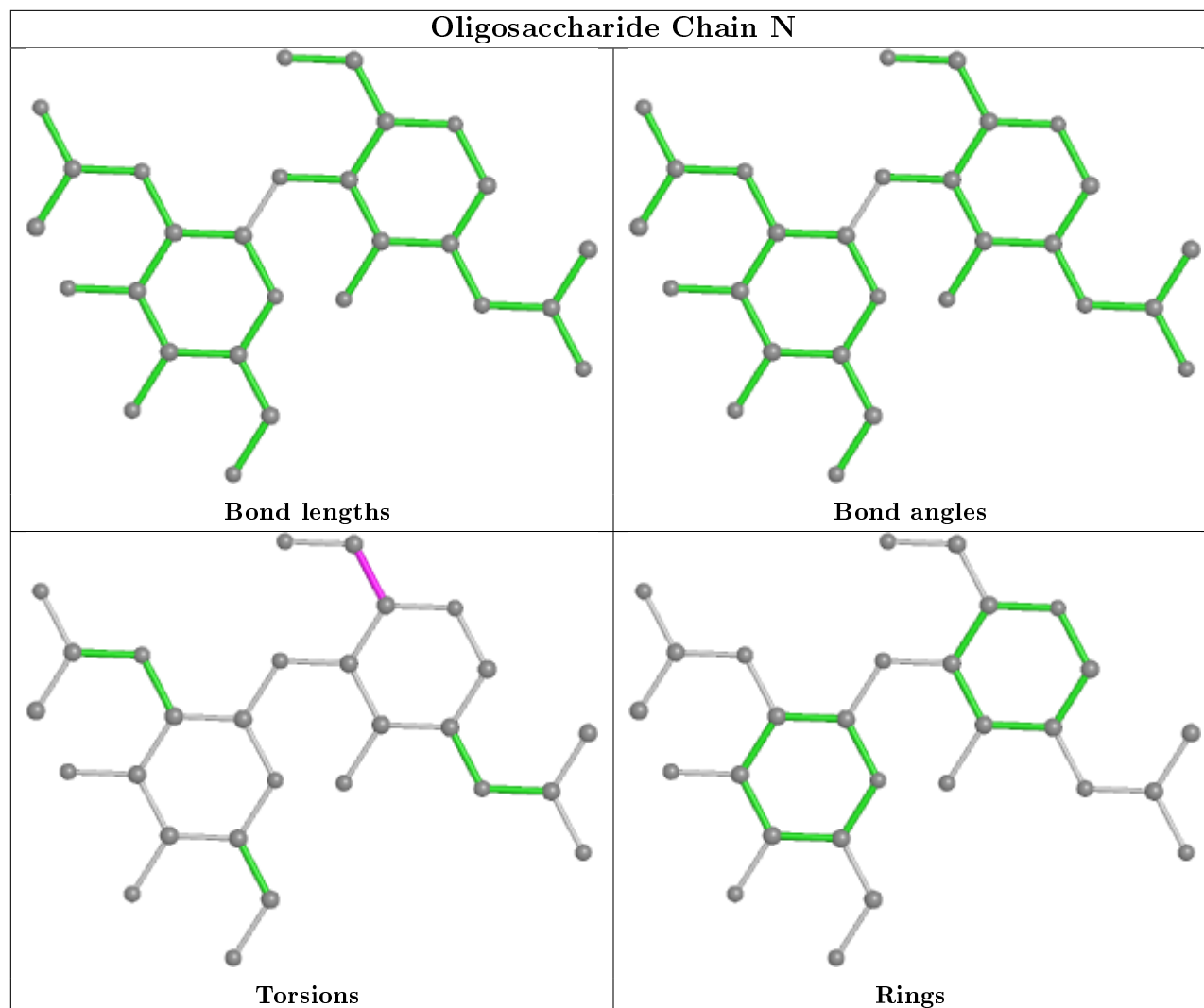


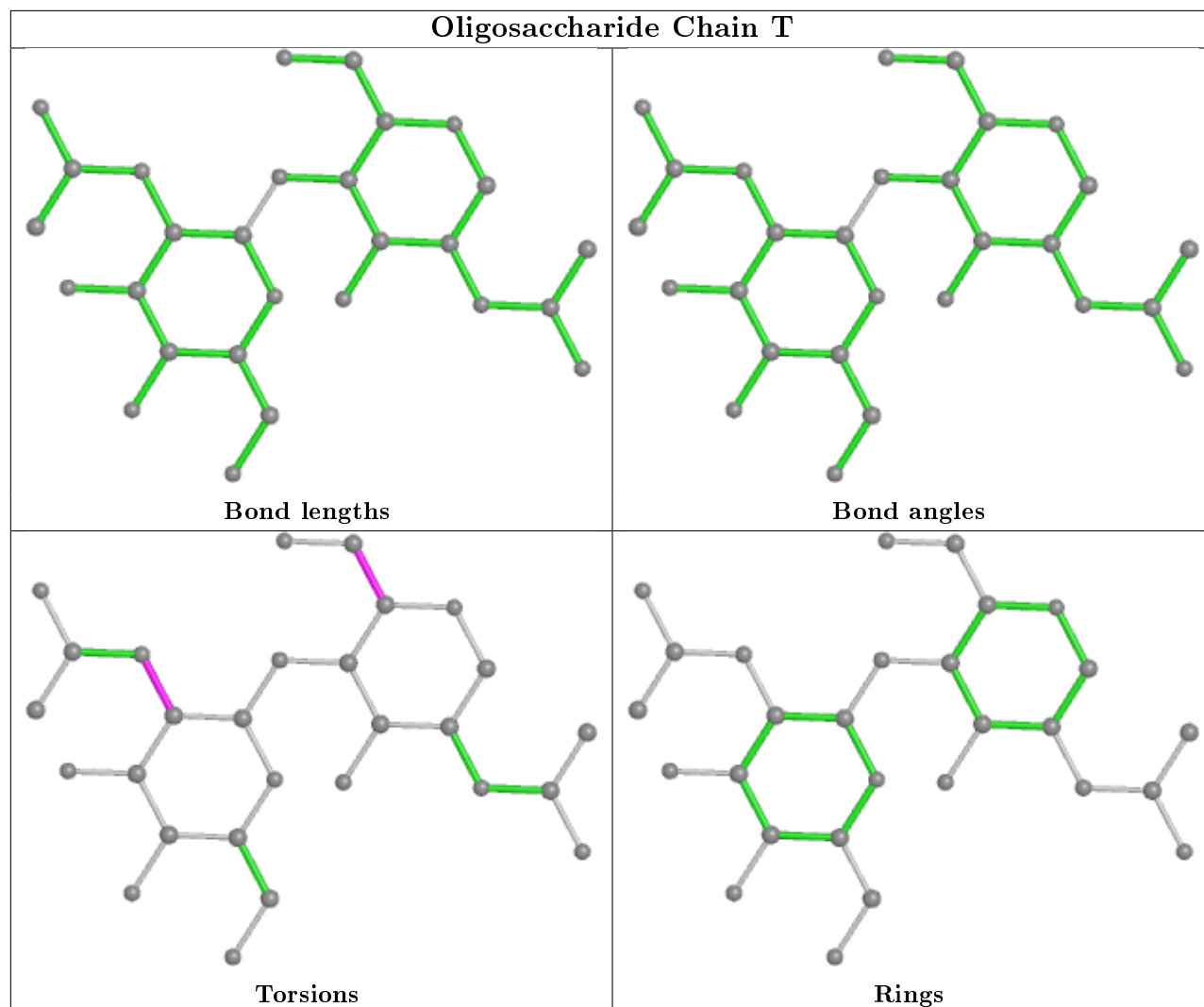


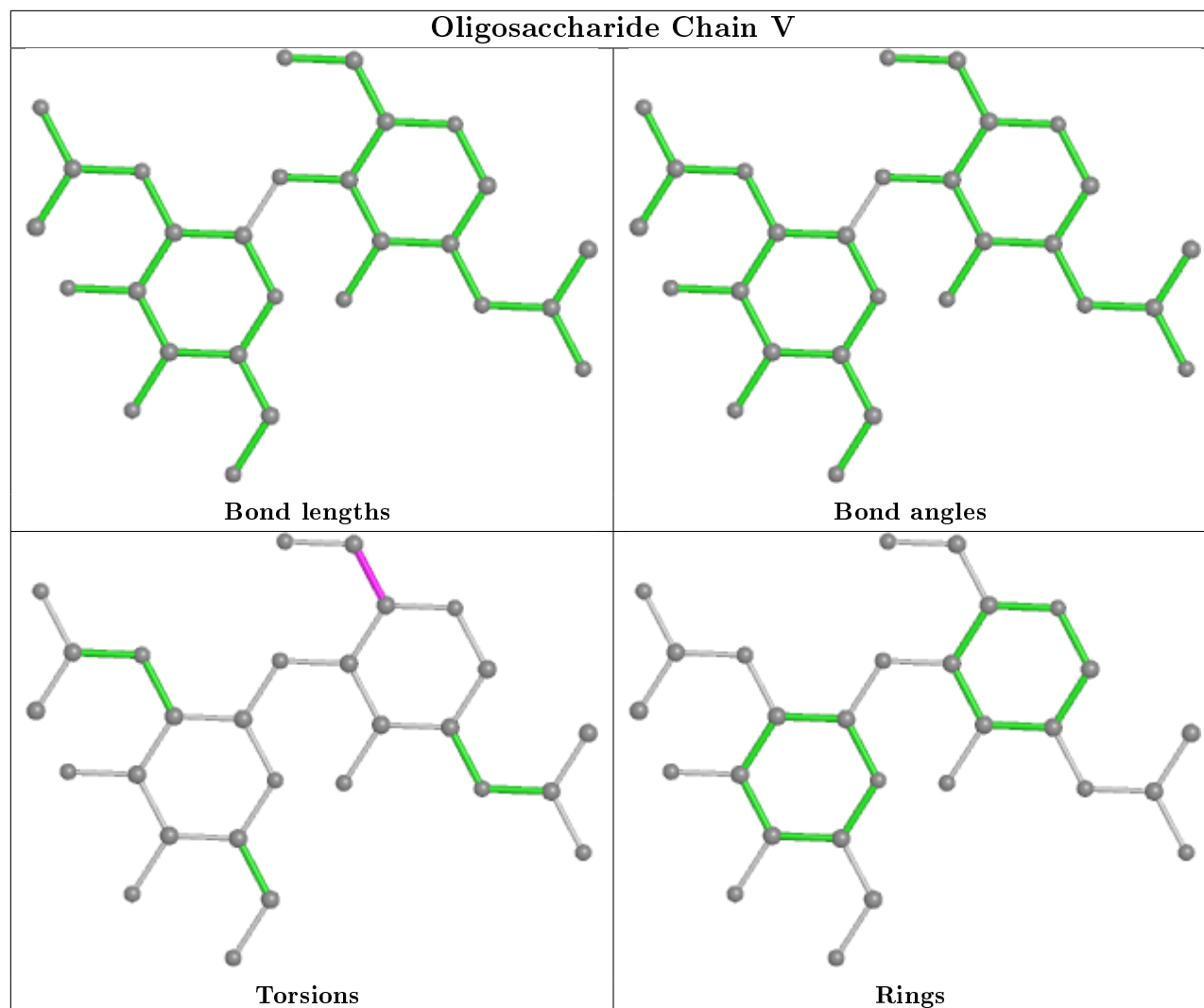




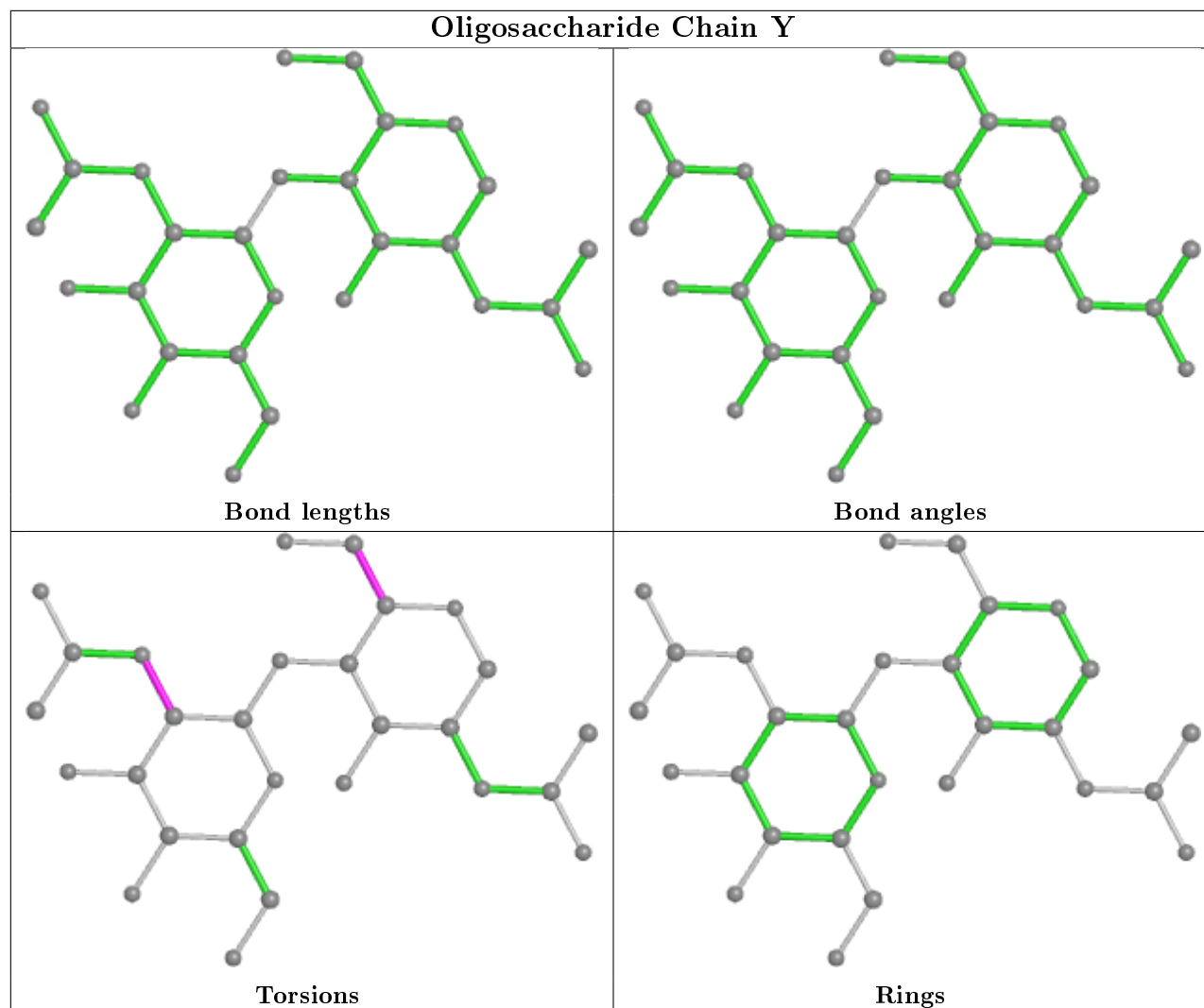


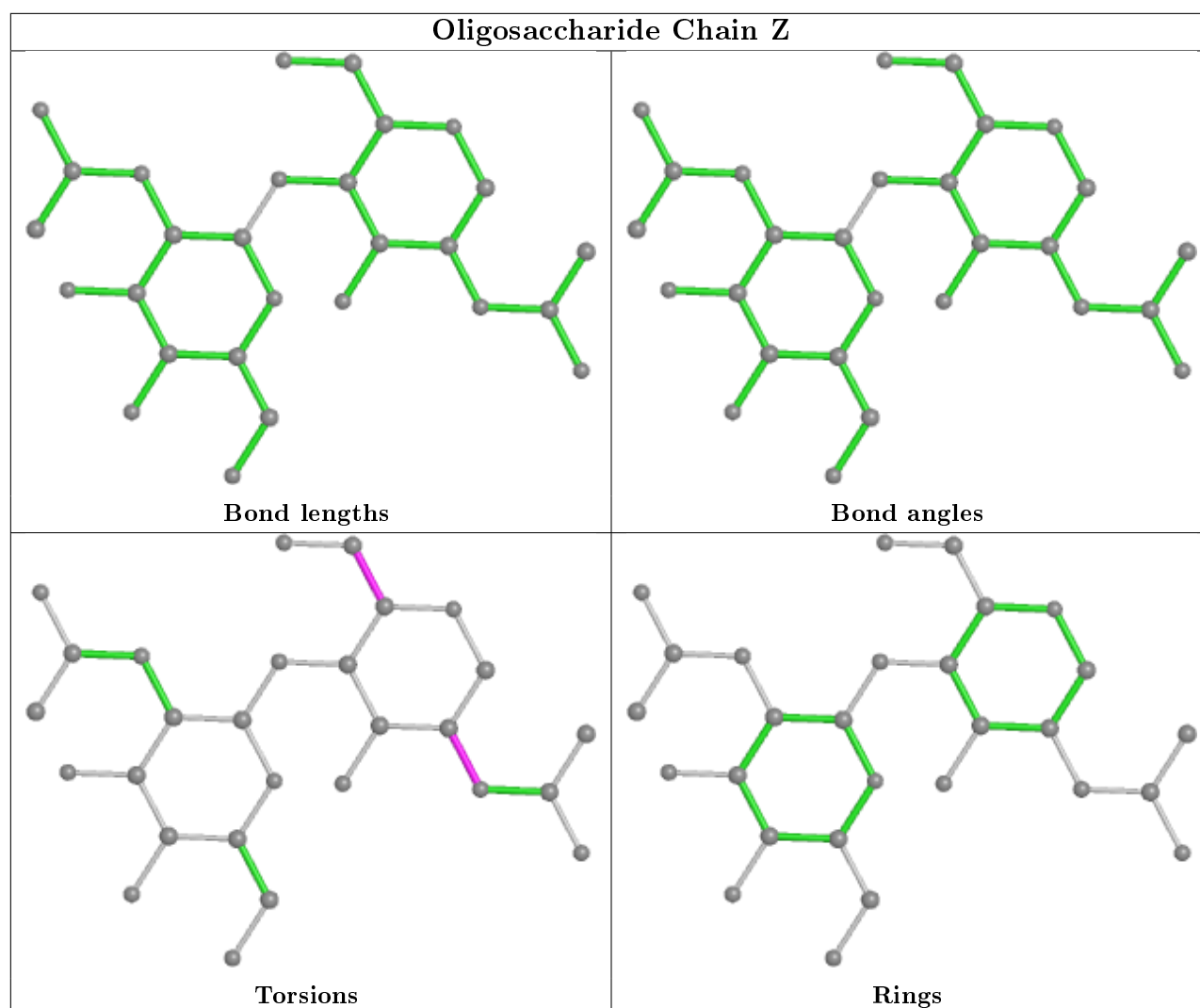


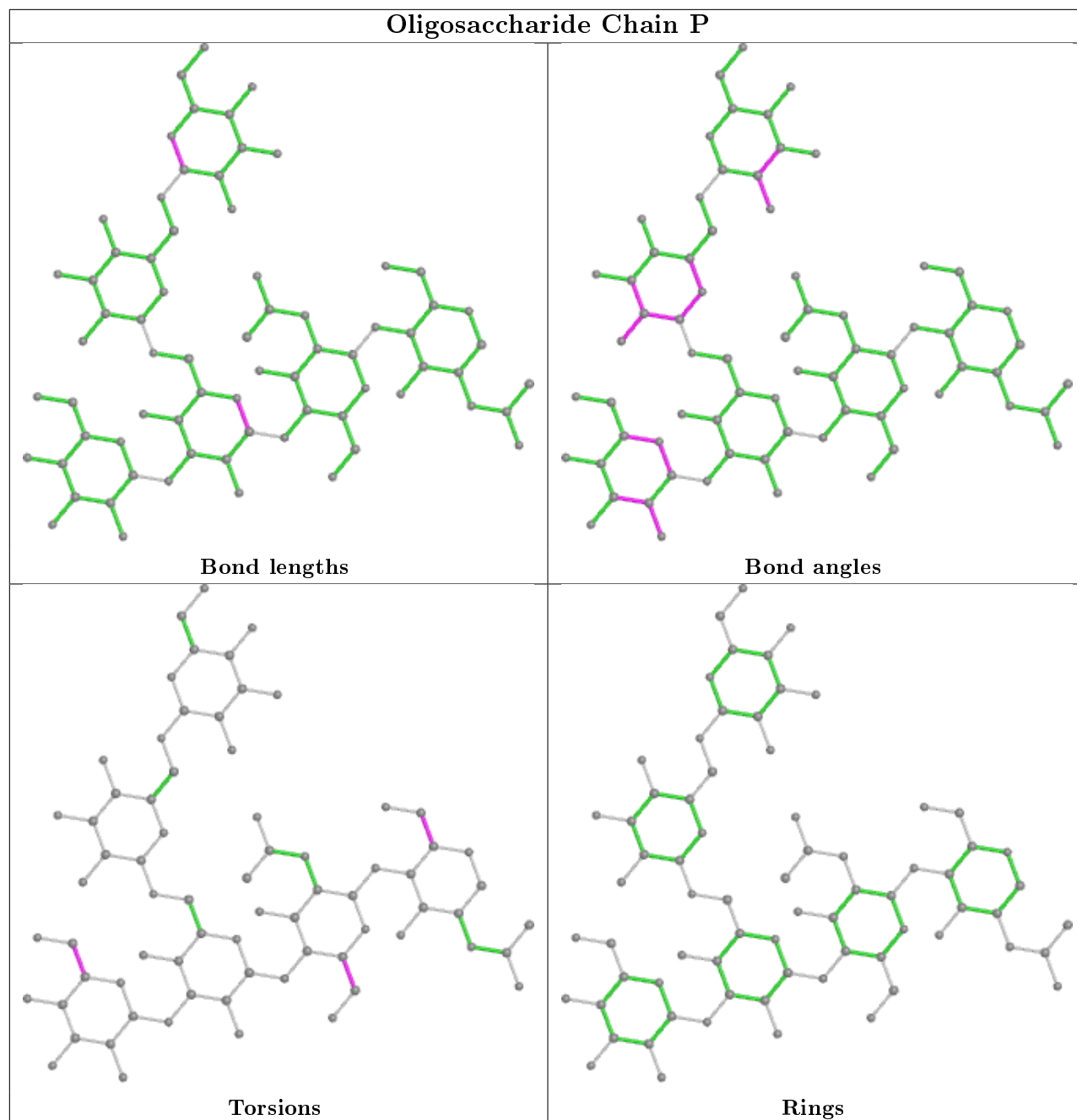


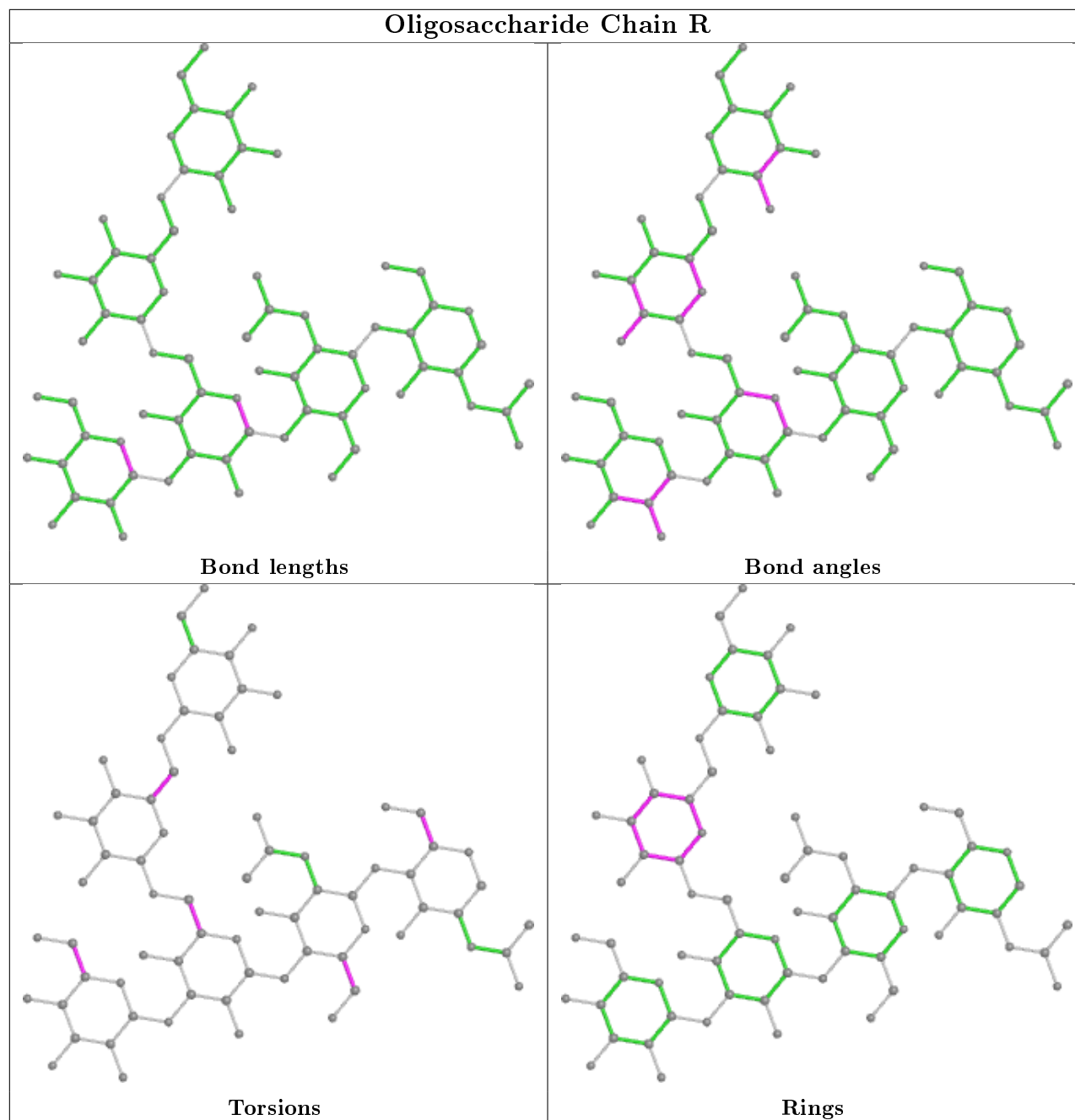


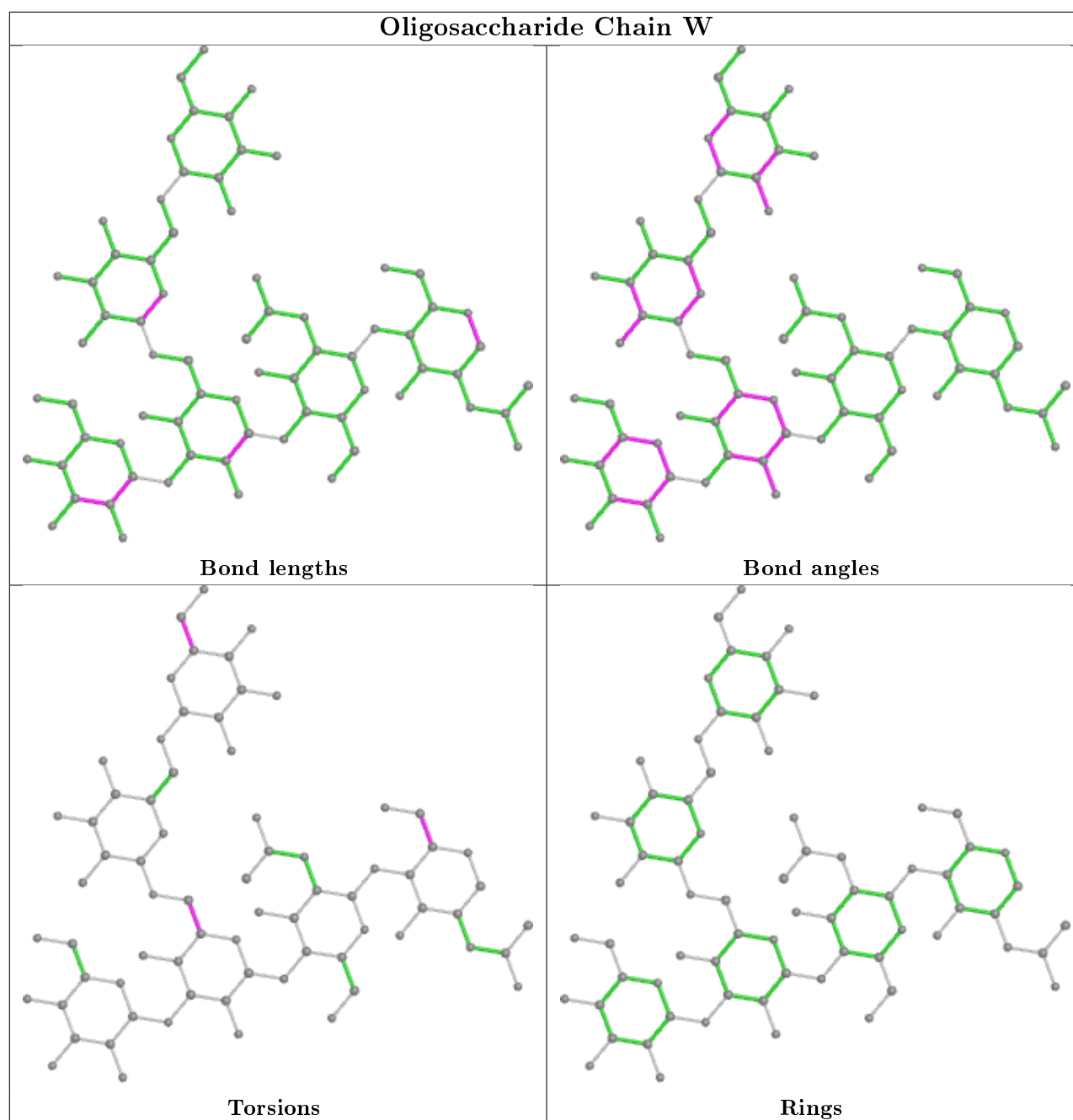












## 5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 24 are monoatomic - leaving 29 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
12	EDO	C	629	-	3,3,3	0.44	0	2,2,2	0.36	0
10	NAG	G	2023	1	14,14,15	0.25	0	17,19,21	0.41	0
10	NAG	E	624	1	14,14,15	0.28	0	17,19,21	0.49	0
12	EDO	A	625	-	3,3,3	0.47	0	2,2,2	0.29	0
10	NAG	A	601	1	14,14,15	0.22	0	17,19,21	0.41	0
14	MES	B	2014	13	12,12,12	1.67	2 (16%)	14,16,16	1.96	4 (28%)
10	NAG	F	502	2	14,14,15	0.30	0	17,19,21	0.34	0
12	EDO	G	2026	-	3,3,3	0.46	0	2,2,2	0.29	0
12	EDO	G	2028	-	3,3,3	0.46	0	2,2,2	0.35	0
12	EDO	F	509	-	3,3,3	0.47	0	2,2,2	0.30	0
10	NAG	G	2024	1	14,14,15	0.32	0	17,19,21	0.33	0
12	EDO	H	509	-	3,3,3	0.47	0	2,2,2	0.31	0
12	EDO	B	2012	-	3,3,3	0.46	0	2,2,2	0.33	0
12	EDO	B	2013	-	3,3,3	0.47	0	2,2,2	0.34	0
14	MES	H	510	13	12,12,12	1.67	3 (25%)	14,16,16	1.96	4 (28%)
10	NAG	C	626	1	14,14,15	0.40	0	17,19,21	0.50	0
10	NAG	D	501	2	14,14,15	0.26	0	17,19,21	0.64	1 (5%)
10	NAG	F	501	2	14,14,15	0.18	0	17,19,21	0.37	0
10	NAG	D	502	2	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
10	NAG	B	2005	2	14,14,15	0.24	0	17,19,21	0.38	0
12	EDO	C	627	-	3,3,3	0.45	0	2,2,2	0.34	0
12	EDO	G	2027	-	3,3,3	0.45	0	2,2,2	0.34	0
12	EDO	C	628	-	3,3,3	0.45	0	2,2,2	0.36	0
12	EDO	E	625	-	3,3,3	0.45	0	2,2,2	0.35	0
14	MES	F	510	13	12,12,12	1.59	3 (25%)	14,16,16	1.93	4 (28%)
10	NAG	E	601	-	14,14,15	0.95	1 (7%)	17,19,21	1.46	2 (11%)
10	NAG	C	601	1	14,14,15	0.28	0	17,19,21	0.46	0
12	EDO	G	2025	-	3,3,3	0.46	0	2,2,2	0.31	0
14	MES	D	507	13	12,12,12	1.62	2 (16%)	14,16,16	1.99	4 (28%)

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
12	EDO	C	629	-	-	0/1/1/1	-
10	NAG	G	2023	1	-	1/6/23/26	0/1/1/1
10	NAG	E	624	1	-	2/6/23/26	0/1/1/1
12	EDO	A	625	-	-	0/1/1/1	-
10	NAG	A	601	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MES	B	2014	13	-	4/6/14/14	0/1/1/1
10	NAG	F	502	2	-	2/6/23/26	0/1/1/1
12	EDO	G	2026	-	-	0/1/1/1	-
12	EDO	G	2028	-	-	0/1/1/1	-
12	EDO	F	509	-	-	0/1/1/1	-
10	NAG	G	2024	1	-	2/6/23/26	0/1/1/1
12	EDO	H	509	-	-	0/1/1/1	-
12	EDO	B	2012	-	-	0/1/1/1	-
12	EDO	B	2013	-	-	0/1/1/1	-
14	MES	H	510	13	-	3/6/14/14	0/1/1/1
10	NAG	C	626	1	-	2/6/23/26	0/1/1/1
10	NAG	D	501	2	-	4/6/23/26	0/1/1/1
10	NAG	F	501	2	-	0/6/23/26	0/1/1/1
10	NAG	D	502	2	-	3/6/23/26	0/1/1/1
10	NAG	B	2005	2	-	0/6/23/26	0/1/1/1
12	EDO	C	627	-	-	0/1/1/1	-
12	EDO	G	2027	-	-	0/1/1/1	-
12	EDO	C	628	-	-	0/1/1/1	-
12	EDO	E	625	-	-	0/1/1/1	-
14	MES	F	510	13	-	0/6/14/14	0/1/1/1
10	NAG	E	601	-	-	4/6/23/26	0/1/1/1
10	NAG	C	601	1	-	2/6/23/26	0/1/1/1
12	EDO	G	2025	-	-	0/1/1/1	-
14	MES	D	507	13	-	2/6/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2014	MES	C8-S	3.65	1.82	1.77
14	D	507	MES	C8-S	3.50	1.82	1.77
14	H	510	MES	C8-S	3.45	1.82	1.77
14	F	510	MES	C8-S	3.08	1.81	1.77
14	H	510	MES	O2S-S	2.87	1.53	1.45
14	B	2014	MES	O1S-S	2.84	1.53	1.45
14	F	510	MES	O2S-S	2.79	1.53	1.45
14	H	510	MES	O1S-S	2.61	1.52	1.45
14	D	507	MES	O1S-S	2.60	1.52	1.45
14	F	510	MES	O1S-S	2.57	1.52	1.45
10	E	601	NAG	C2-N2	-2.11	1.42	1.46
10	D	502	NAG	O5-C1	-2.00	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	510	MES	O3S-S-O1S	-4.05	101.39	111.27
14	B	2014	MES	O3S-S-O2S	-4.02	101.46	111.27
14	H	510	MES	O3S-S-O1S	-3.78	102.04	111.27
10	E	601	NAG	C2-N2-C7	-3.77	117.53	122.90
14	D	507	MES	O2S-S-O1S	-3.77	100.91	113.95
14	B	2014	MES	O2S-S-C8	3.67	111.34	106.92
14	B	2014	MES	O3S-S-C8	3.66	111.69	105.77
14	D	507	MES	O2S-S-C8	3.55	111.19	106.92
14	H	510	MES	O1S-S-C8	3.50	111.13	106.92
14	D	507	MES	O1S-S-C8	3.44	111.05	106.92
14	H	510	MES	O3S-S-C8	3.34	111.17	105.77
14	F	510	MES	O1S-S-C8	3.18	110.74	106.92
14	F	510	MES	O3S-S-C8	3.08	110.76	105.77
14	D	507	MES	O3S-S-C8	2.95	110.53	105.77
14	F	510	MES	O2S-S-C8	2.93	110.44	106.92
10	E	601	NAG	C4-C3-C2	2.64	114.89	111.02
14	H	510	MES	O2S-S-C8	2.45	109.87	106.92
10	D	501	NAG	C1-O5-C5	2.27	115.27	112.19
14	B	2014	MES	O1S-S-C8	2.05	109.38	106.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	2014	MES	N4-C7-C8-S
14	H	510	MES	C8-C7-N4-C5
14	H	510	MES	N4-C7-C8-S
14	D	507	MES	C8-C7-N4-C5
10	E	601	NAG	C8-C7-N2-C2
10	E	601	NAG	O7-C7-N2-C2
10	C	626	NAG	O5-C5-C6-O6
10	D	501	NAG	O5-C5-C6-O6
10	C	626	NAG	C4-C5-C6-O6
10	D	502	NAG	O5-C5-C6-O6
10	D	502	NAG	C1-C2-N2-C7
10	D	501	NAG	C4-C5-C6-O6
10	C	601	NAG	O5-C5-C6-O6
10	E	601	NAG	O5-C5-C6-O6
10	G	2024	NAG	C4-C5-C6-O6
10	E	624	NAG	O5-C5-C6-O6
14	B	2014	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
10	C	601	NAG	C4-C5-C6-O6
10	D	501	NAG	C1-C2-N2-C7
10	G	2024	NAG	O5-C5-C6-O6
10	E	601	NAG	C4-C5-C6-O6
10	D	502	NAG	C4-C5-C6-O6
10	E	624	NAG	C4-C5-C6-O6
10	F	502	NAG	C1-C2-N2-C7
14	B	2014	MES	C7-C8-S-O1S
14	B	2014	MES	C7-C8-S-O2S
10	D	501	NAG	C3-C2-N2-C7
14	D	507	MES	C8-C7-N4-C3
10	F	502	NAG	C3-C2-N2-C7
14	H	510	MES	C8-C7-N4-C3
10	G	2023	NAG	C4-C5-C6-O6

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	2023	NAG	2	0
10	E	624	NAG	1	0
14	B	2014	MES	3	0
10	F	502	NAG	1	0
12	G	2026	EDO	1	0
10	G	2024	NAG	1	0
14	H	510	MES	2	0
10	D	501	NAG	1	0
10	D	502	NAG	2	0
14	F	510	MES	4	0
10	C	601	NAG	1	0
12	G	2025	EDO	1	0
14	D	507	MES	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	592/599 (98%)	0.83	34 (5%) 23 20	49, 78, 135, 172	0
1	C	595/599 (99%)	0.98	61 (10%) 6 4	50, 78, 148, 197	0
1	E	593/599 (98%)	1.18	106 (17%) 1 1	62, 100, 158, 204	0
1	G	596/599 (99%)	1.31	118 (19%) 1 1	72, 104, 152, 190	0
2	B	333/456 (73%)	1.31	79 (23%) 0 0	61, 122, 165, 244	0
2	D	312/456 (68%)	1.85	114 (36%) 0 0	58, 133, 178, 237	0
2	F	332/456 (72%)	1.57	91 (27%) 0 0	67, 128, 174, 206	0
2	H	336/456 (73%)	1.95	142 (42%) 0 0	75, 135, 181, 249	0
All	All	3689/4220 (87%)	1.29	745 (20%) 1 1	49, 101, 165, 249	0

All (745) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	358	TYR	10.7
2	D	135	MET	10.6
2	D	95	LEU	9.5
1	E	570	ALA	9.1
1	C	553	LEU	9.1
2	F	422	HIS	8.3
2	D	358	TYR	8.0
2	H	418	LYS	7.9
2	D	357	ILE	7.7
2	H	95	LEU	7.6
2	H	136	ALA	7.6
2	B	364	ILE	7.5
2	F	421	ILE	7.5
2	D	136	ALA	7.3
2	H	142	PHE	7.2
2	D	82	SER	7.1

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Mol	Chain	Res	Type	RSRZ
2	H	126	SER	6.8
2	D	97	VAL	6.7
2	H	393	THR	6.6
1	E	305	SER	6.6
2	D	364	ILE	6.4
1	G	562	TYR	6.4
2	H	421	ILE	6.4
2	H	144	LEU	6.3
1	C	593	ILE	6.3
1	E	499	LEU	6.3
2	H	99	PRO	6.3
2	D	93	PHE	6.3
2	H	133	ARG	6.2
2	B	136	ALA	6.2
1	G	305	SER	6.2
1	E	462	CYS	6.2
2	B	83	ILE	6.2
2	H	78	PRO	6.2
1	G	446	ALA	6.1
2	D	374	MET	6.1
2	H	395	LYS	6.1
2	D	392	VAL	6.0
2	F	364	ILE	5.9
2	D	231	ARG	5.9
2	D	405	TYR	5.9
1	E	509	ILE	5.9
2	H	392	VAL	5.8
1	A	465	PRO	5.8
2	H	135	MET	5.8
2	H	361	ILE	5.7
2	H	85	LEU	5.7
2	F	131	LEU	5.6
2	F	95	LEU	5.6
2	F	173	ASN	5.6
2	B	135	MET	5.5
2	F	197	LYS	5.5
2	H	331	LEU	5.5
2	H	388	PHE	5.5
2	H	97	VAL	5.5
2	H	233	GLU	5.5
2	D	190	GLU	5.5
2	H	83	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	400	GLY	5.5
2	F	93	PHE	5.4
2	D	92	ASN	5.4
2	H	137	PHE	5.4
1	E	512	ALA	5.3
2	F	392	VAL	5.3
2	B	394	MET	5.3
2	D	143	ARG	5.3
1	E	487	VAL	5.3
1	A	566	TYR	5.2
2	F	352	ASN	5.2
1	C	468	ALA	5.2
2	F	91	ALA	5.2
1	G	466	GLY	5.2
1	G	510	ARG	5.2
2	B	358	TYR	5.2
2	D	189	THR	5.1
1	G	399	SER	5.1
2	F	97	VAL	5.1
2	F	136	ALA	5.1
2	H	105	VAL	5.0
2	B	95	LEU	5.0
2	D	359	PHE	5.0
2	H	339	TYR	5.0
2	H	87	PRO	5.0
1	E	482	ALA	5.0
1	E	566	TYR	5.0
2	H	146	PHE	4.9
1	G	552	LYS	4.9
2	D	203	LYS	4.9
2	D	142	PHE	4.9
1	G	564	LEU	4.9
2	H	173	ASN	4.9
2	F	135	MET	4.9
1	G	585	ALA	4.8
1	C	564	LEU	4.8
2	F	83	ILE	4.8
2	H	140	ARG	4.8
1	G	467	THR	4.8
2	F	109	TYR	4.8
2	D	188	LEU	4.8
2	B	93	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	387	LEU	4.8
2	D	144	LEU	4.7
2	D	361	ILE	4.7
2	D	387	LEU	4.7
2	D	137	PHE	4.7
2	D	94	MET	4.7
2	H	91	ALA	4.7
2	F	393	THR	4.6
2	D	377	CYS	4.6
2	B	393	THR	4.6
2	D	385	GLU	4.6
2	F	359	PHE	4.6
1	C	465	PRO	4.6
2	F	126	SER	4.6
1	G	551	ASP	4.5
1	E	553	LEU	4.5
2	D	195	PHE	4.5
2	D	127	VAL	4.5
1	C	305	SER	4.5
1	E	542	TYR	4.5
2	F	90	GLU	4.5
2	B	195	PHE	4.5
2	D	105	VAL	4.5
2	H	82	SER	4.5
1	C	595	LEU	4.5
2	H	390	VAL	4.5
1	G	441	VAL	4.5
2	F	188	LEU	4.4
2	H	124	LEU	4.4
2	H	79	GLY	4.4
2	D	123	LYS	4.4
2	D	350	VAL	4.4
2	H	195	PHE	4.4
1	E	544	ARG	4.4
2	F	76	VAL	4.4
1	G	566	TYR	4.4
1	G	482	ALA	4.4
2	F	351	GLU	4.4
2	H	417	ALA	4.3
1	G	400	GLY	4.3
2	D	141	ASP	4.3
2	H	129	ASN	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	267	LEU	4.3
2	D	174	LEU	4.3
1	A	542	TYR	4.3
1	G	593	ILE	4.3
1	A	504	LYS	4.3
1	C	552	LYS	4.3
1	E	567	ARG	4.3
1	A	595	LEU	4.3
1	E	587	ILE	4.3
2	D	331	LEU	4.2
2	H	128	GLY	4.2
2	H	352	ASN	4.2
2	D	124	LEU	4.2
2	H	394	MET	4.2
2	H	204	ILE	4.2
2	H	188	LEU	4.2
1	E	504	LYS	4.2
2	F	358	TYR	4.2
2	H	76	VAL	4.2
2	B	395	LYS	4.2
1	G	495	GLN	4.2
2	D	232	LYS	4.1
2	D	408	ILE	4.1
2	D	173	ASN	4.1
2	D	346	VAL	4.1
2	D	386	VAL	4.1
2	B	82	SER	4.1
2	D	406	ALA	4.1
2	H	88	GLY	4.1
1	C	569	ALA	4.1
2	B	164	ARG	4.0
1	G	569	ALA	4.0
1	E	588	SER	4.0
2	B	161	HIS	4.0
1	E	594	LEU	4.0
2	H	396	LYS	4.0
2	H	141	ASP	3.9
2	H	92	ASN	3.9
2	H	343	ILE	3.9
1	G	550	ARG	3.9
1	G	487	VAL	3.9
1	G	544	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	551	ASP	3.9
2	F	92	ASN	3.9
2	D	329	ALA	3.8
2	F	137	PHE	3.8
2	D	131	LEU	3.8
2	F	408	ILE	3.8
2	H	422	HIS	3.8
2	B	387	LEU	3.8
2	D	333	ASN	3.8
2	B	392	VAL	3.8
2	B	391	THR	3.8
1	G	584	PRO	3.8
1	E	521	SER	3.8
2	D	365	CYS	3.7
2	F	89	ALA	3.7
2	B	71	GLU	3.7
2	B	94	MET	3.7
1	G	492	LEU	3.7
2	D	391	THR	3.7
2	H	362	THR	3.7
2	B	73	ASN	3.7
2	F	102	LYS	3.7
2	H	94	MET	3.7
2	D	132	SER	3.7
1	C	471	VAL	3.7
2	F	87	PRO	3.7
1	E	543	LEU	3.7
1	E	562	TYR	3.7
2	D	381	THR	3.7
2	H	359	PHE	3.7
1	E	265	TYR	3.7
2	H	259	CYS	3.6
1	E	556	ILE	3.6
1	G	442	ILE	3.6
2	D	109	TYR	3.6
2	H	127	VAL	3.6
1	E	573	THR	3.6
2	H	193	THR	3.6
2	H	132	SER	3.6
2	F	85	LEU	3.6
2	F	195	PHE	3.6
2	D	390	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	305	SER	3.6
1	E	569	ALA	3.6
2	F	99	PRO	3.6
2	D	330	ASN	3.6
1	C	9	ALA	3.6
1	G	500	LEU	3.6
1	E	304	GLY	3.6
2	D	78	PRO	3.6
2	D	393	THR	3.6
2	D	356	GLY	3.6
2	F	372	PRO	3.6
1	G	542	TYR	3.6
2	B	69	GLU	3.6
1	C	542	TYR	3.6
2	D	163	GLU	3.5
1	E	442	ILE	3.5
2	B	85	LEU	3.5
2	F	144	LEU	3.5
1	A	569	ALA	3.5
2	B	357	ILE	3.5
2	F	192	ILE	3.5
2	H	103	TYR	3.5
1	G	401	CYS	3.5
2	B	370	ARG	3.5
2	F	86	ARG	3.5
2	B	126	SER	3.5
2	H	381	THR	3.5
2	D	338	ALA	3.5
2	H	192	ILE	3.5
1	G	579	LEU	3.5
1	G	512	ALA	3.5
2	F	189	THR	3.5
2	D	98	HIS	3.4
1	E	399	SER	3.4
1	E	112	TYR	3.4
1	C	543	LEU	3.4
2	H	324	ILE	3.4
2	H	169	CYS	3.4
2	D	191	ASN	3.4
2	D	389	ASN	3.4
2	F	370	ARG	3.4
1	E	465	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	336	VAL	3.4
2	H	356	GLY	3.4
2	F	191	ASN	3.4
2	H	125	ASN	3.4
1	E	496	VAL	3.4
1	G	509	ILE	3.4
2	D	126	SER	3.4
2	B	419	ILE	3.4
2	B	330	ASN	3.3
2	D	332	ASN	3.3
1	G	471	VAL	3.3
2	B	231	ARG	3.3
2	D	388	PHE	3.3
1	E	264	LEU	3.3
2	H	100	LEU	3.3
2	D	409	LYS	3.3
2	B	362	THR	3.3
2	D	193	THR	3.3
2	B	396	LYS	3.3
2	D	125	ASN	3.3
1	A	584	PRO	3.3
1	G	496	VAL	3.3
2	F	132	SER	3.3
2	H	86	ARG	3.3
1	E	593	ILE	3.3
2	D	176	CYS	3.3
2	H	349	GLN	3.3
2	H	357	ILE	3.3
2	H	186	LEU	3.3
1	G	429	GLY	3.2
1	C	565	ASP	3.2
2	H	416	THR	3.2
2	H	201	ARG	3.2
2	H	374	MET	3.2
2	H	98	HIS	3.2
2	B	329	ALA	3.2
1	A	510	ARG	3.2
2	F	347	LYS	3.2
1	A	509	ILE	3.2
1	C	512	ALA	3.2
1	A	543	LEU	3.2
2	F	342	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	70	ASN	3.2
2	F	391	THR	3.2
1	G	304	GLY	3.2
2	F	361	ILE	3.2
1	G	364	TYR	3.1
2	H	425	CYS	3.1
1	G	402	PRO	3.1
2	H	260	PRO	3.1
2	B	193	THR	3.1
2	F	88	GLY	3.1
1	E	466	GLY	3.1
2	H	337	GLU	3.1
1	C	556	ILE	3.1
1	G	517	SER	3.1
2	B	124	LEU	3.1
2	F	146	PHE	3.1
2	D	239	LEU	3.1
1	C	509	ILE	3.1
2	B	388	PHE	3.1
1	E	523	SER	3.1
1	E	564	LEU	3.1
2	H	228	ILE	3.0
2	B	103	TYR	3.0
2	D	76	VAL	3.0
2	H	344	SER	3.0
2	B	197	LYS	3.0
2	F	418	LYS	3.0
1	E	572	THR	3.0
1	A	546	GLU	3.0
1	C	455	LEU	3.0
1	G	498	LEU	3.0
2	H	200	HIS	3.0
2	F	264	ASN	3.0
1	C	497	GLU	3.0
1	G	539	LEU	3.0
2	F	419	ILE	2.9
2	H	119	ASN	2.9
1	G	582	PHE	2.9
2	F	201	ARG	2.9
2	H	89	ALA	2.9
1	G	558	ILE	2.9
1	G	3	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	128	GLY	2.9
1	A	585	ALA	2.9
2	D	122	GLU	2.9
1	G	21	PHE	2.9
1	G	543	LEU	2.9
2	B	267	LEU	2.9
1	C	157	GLY	2.9
1	E	447	GLY	2.9
1	G	474	PHE	2.9
1	E	208	LEU	2.9
2	D	186	LEU	2.9
2	F	174	LEU	2.9
1	G	407	TYR	2.9
2	B	84	GLN	2.9
1	A	559	PHE	2.9
2	F	142	PHE	2.9
2	H	190	GLU	2.9
2	D	99	PRO	2.9
1	E	571	ASP	2.9
1	G	358	ILE	2.8
2	B	420	HIS	2.8
1	C	559	PHE	2.8
1	G	505	GLN	2.8
1	C	446	ALA	2.8
1	G	447	GLY	2.8
1	C	551	ASP	2.8
2	D	241	MET	2.8
2	D	103	TYR	2.8
1	E	184	ILE	2.8
2	D	192	ILE	2.8
1	A	469	LEU	2.8
1	E	488	LEU	2.8
2	F	388	PHE	2.8
1	E	568	THR	2.8
2	B	123	LYS	2.8
1	E	548	GLU	2.8
1	E	500	LEU	2.8
2	D	237	LEU	2.8
1	E	586	ASN	2.8
1	G	553	LEU	2.8
1	E	81	ALA	2.7
2	H	255	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	374	MET	2.7
2	B	418	LYS	2.7
1	E	493	ASN	2.7
1	G	563	ARG	2.7
1	C	548	GLU	2.7
2	H	197	LYS	2.7
2	F	129	ASN	2.7
1	C	504	LYS	2.7
1	G	462	CYS	2.7
2	D	139	SER	2.7
2	D	304	LYS	2.7
2	H	96	LYS	2.7
1	C	567	ARG	2.7
1	E	498	LEU	2.7
1	E	515	LEU	2.7
1	E	550	ARG	2.7
1	C	62	SER	2.7
1	E	397	ALA	2.7
2	H	386	VAL	2.7
2	B	425	CYS	2.7
2	F	98	HIS	2.7
1	A	518	ARG	2.7
1	A	474	PHE	2.7
1	E	595	LEU	2.7
2	D	134	LYS	2.7
2	F	101	LYS	2.7
2	H	419	ILE	2.7
1	E	529	SER	2.7
1	A	137	VAL	2.7
2	H	367	ASP	2.7
2	H	276	THR	2.7
1	E	9	ALA	2.7
2	B	128	GLY	2.7
2	F	405	TYR	2.7
2	H	121	ILE	2.7
1	G	368	ASP	2.7
2	D	133	ARG	2.7
2	D	417	ALA	2.7
1	E	522	HIS	2.7
2	H	256	GLY	2.7
1	C	544	ARG	2.7
1	C	524	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	23	VAL	2.6
1	E	364	TYR	2.6
2	H	408	ILE	2.6
1	G	9	ALA	2.6
2	H	163	GLU	2.6
2	D	140	ARG	2.6
2	D	355	GLN	2.6
1	A	593	ILE	2.6
1	E	516	TYR	2.6
1	E	473	CYS	2.6
2	D	197	LYS	2.6
2	H	403	LYS	2.6
2	H	281	PRO	2.6
2	H	391	THR	2.6
1	G	22	ALA	2.6
2	F	379	ASN	2.6
2	H	252	SER	2.6
1	G	105	ILE	2.6
1	G	274	ALA	2.6
1	G	363	PRO	2.6
1	E	565	ASP	2.6
2	D	235	LYS	2.6
1	E	584	PRO	2.6
1	G	528	ILE	2.6
1	G	20	GLY	2.6
2	B	359	PHE	2.6
2	H	376	GLY	2.6
1	C	592	HIS	2.6
2	B	343	ILE	2.5
2	D	121	ILE	2.5
1	E	539	LEU	2.5
2	B	199	VAL	2.5
1	E	426	GLY	2.5
2	B	205	SER	2.5
1	G	591	ALA	2.5
2	F	362	THR	2.5
1	E	492	LEU	2.5
2	F	81	VAL	2.5
1	E	326	PHE	2.5
1	C	401	CYS	2.5
1	G	479	CYS	2.5
1	G	497	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	122	GLU	2.5
1	G	435	LEU	2.5
2	D	373	GLY	2.5
2	F	140	ARG	2.5
1	G	514	PHE	2.5
2	F	389	ASN	2.5
1	A	512	ALA	2.5
2	D	200	HIS	2.5
2	D	204	ILE	2.5
2	D	418	LYS	2.5
2	H	373	GLY	2.5
2	H	108	TYR	2.5
1	E	398	ARG	2.5
1	E	541	ALA	2.5
2	B	131	LEU	2.5
2	F	186	LEU	2.5
2	H	122	GLU	2.5
2	F	409	LYS	2.5
1	G	403	PRO	2.5
1	A	568	THR	2.5
1	G	468	ALA	2.5
1	G	578	ILE	2.5
2	F	200	HIS	2.5
1	C	473	CYS	2.5
1	C	112	TYR	2.5
1	G	428	PHE	2.5
2	H	264	ASN	2.5
1	A	400	GLY	2.5
2	F	161	HIS	2.5
2	H	234	ALA	2.5
2	H	325	GLU	2.5
1	E	578	ILE	2.5
1	G	408	SER	2.5
2	D	108	TYR	2.5
1	E	22	ALA	2.4
2	H	327	LYS	2.4
1	C	498	LEU	2.4
2	B	320	ILE	2.4
1	G	220	SER	2.4
2	H	258	VAL	2.4
2	D	339	TYR	2.4
2	H	363	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	448	LEU	2.4
2	B	100	LEU	2.4
2	D	384	ASP	2.4
2	F	84	GLN	2.4
2	H	75	GLN	2.4
1	G	488	LEU	2.4
2	H	80	GLU	2.4
2	H	279	GLU	2.4
2	H	335	VAL	2.4
2	H	202	GLN	2.4
1	G	438	ALA	2.4
1	C	546	GLU	2.4
2	F	411	ILE	2.4
1	A	565	ASP	2.4
2	B	129	ASN	2.4
2	H	199	VAL	2.4
1	C	447	GLY	2.4
1	G	420	TYR	2.4
1	E	41	PRO	2.4
2	F	277	THR	2.4
1	C	306	ASP	2.4
2	H	364	ILE	2.4
2	D	271	VAL	2.4
2	F	190	GLU	2.4
2	H	118	HIS	2.4
1	A	564	LEU	2.4
1	E	461	THR	2.4
2	F	276	THR	2.4
1	G	294	PHE	2.4
2	H	413	PHE	2.4
1	E	502	LYS	2.4
1	E	18	TYR	2.4
1	G	383	LEU	2.4
1	G	549	PHE	2.4
1	C	224	TYR	2.3
2	B	281	PRO	2.3
1	C	107	ALA	2.3
2	F	382	SER	2.3
2	H	389	ASN	2.3
2	H	407	ILE	2.3
1	E	444	VAL	2.3
2	B	335	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	118	HIS	2.3
2	H	254	LEU	2.3
2	F	385	GLU	2.3
2	D	419	ILE	2.3
1	C	478	PHE	2.3
2	B	150	VAL	2.3
2	D	340	GLN	2.3
2	H	176	CYS	2.3
1	G	308	LYS	2.3
1	C	403	PRO	2.3
2	H	278	MET	2.3
1	E	16	GLY	2.3
2	F	252	SER	2.3
1	E	527	THR	2.3
2	B	386	VAL	2.3
2	H	232	LYS	2.3
1	E	306	ASP	2.3
2	F	254	LEU	2.3
2	F	193	THR	2.3
1	E	559	PHE	2.3
1	C	440	PRO	2.3
1	E	585	ALA	2.3
2	H	90	GLU	2.3
2	B	115	ALA	2.3
2	B	142	PHE	2.3
2	B	217	ALA	2.3
1	C	265	TYR	2.3
2	B	68	THR	2.3
2	H	109	TYR	2.3
1	G	25	PHE	2.3
1	G	504	LYS	2.3
2	B	380	VAL	2.3
1	G	279	SER	2.2
1	C	594	LEU	2.2
1	E	409	MET	2.2
1	C	596	THR	2.2
2	B	378	ARG	2.2
2	H	143	ARG	2.2
1	G	110	PRO	2.2
2	D	252	SER	2.2
1	A	563	ARG	2.2
1	E	221	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	161	ILE	2.2
1	C	36	LEU	2.2
2	B	268	LYS	2.2
2	D	100	LEU	2.2
1	E	343	ALA	2.2
1	G	221	TYR	2.2
1	G	265	TYR	2.2
2	B	405	TYR	2.2
1	C	390	ILE	2.2
1	E	497	GLU	2.2
1	C	160	SER	2.2
1	E	44	ASN	2.2
1	G	339	ARG	2.2
1	G	469	LEU	2.2
2	B	250	LEU	2.2
2	D	238	LEU	2.2
2	D	255	ALA	2.2
1	A	265	TYR	2.2
1	G	159	PHE	2.2
2	D	146	PHE	2.2
1	C	285	ILE	2.2
2	B	407	ILE	2.2
2	D	110	LEU	2.2
2	D	260	PRO	2.2
2	F	176	CYS	2.2
2	D	412	GLY	2.2
1	E	239	PHE	2.2
1	G	445	ASN	2.2
2	B	390	VAL	2.2
2	D	258	VAL	2.2
1	G	575	LEU	2.2
2	B	200	HIS	2.2
2	F	331	LEU	2.2
1	G	203	LYS	2.2
2	D	102	LYS	2.2
2	F	96	LYS	2.2
1	C	541	ALA	2.2
1	A	582	PHE	2.2
1	E	21	PHE	2.2
1	E	511	ARG	2.2
2	H	93	PHE	2.2
2	H	139	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	295	ILE	2.2
2	B	102	LYS	2.2
2	F	349	GLN	2.2
1	E	96	ALA	2.2
2	D	416	THR	2.2
1	C	399	SER	2.1
2	B	127	VAL	2.1
1	G	244	PRO	2.1
1	G	465	PRO	2.1
1	C	400	GLY	2.1
1	C	426	GLY	2.1
1	C	227	ALA	2.1
1	E	446	ALA	2.1
1	E	526	MET	2.1
1	E	563	ARG	2.1
2	F	169	CYS	2.1
1	E	520	PRO	2.1
1	E	533	LEU	2.1
1	E	545	ASP	2.1
1	G	41	PRO	2.1
2	B	356	GLY	2.1
1	G	96	ALA	2.1
1	G	570	ALA	2.1
2	H	198	ALA	2.1
2	B	254	LEU	2.1
2	F	420	HIS	2.1
2	H	235	LYS	2.1
1	C	30	ALA	2.1
2	B	249	ALA	2.1
2	D	233	GLU	2.1
2	F	249	ALA	2.1
2	H	329	ALA	2.1
2	F	125	ASN	2.1
1	C	279	SER	2.1
1	G	264	LEU	2.1
1	G	398	ARG	2.1
1	A	249	THR	2.1
1	G	342	SER	2.1
2	B	235	LYS	2.1
2	H	101	LYS	2.1
1	G	125	VAL	2.1
2	F	237	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	107	LEU	2.1
1	C	338	ALA	2.1
1	G	345	ALA	2.1
2	H	261	ASN	2.1
1	G	499	LEU	2.1
1	A	473	CYS	2.1
1	G	8	PRO	2.1
2	F	78	PRO	2.1
1	A	506	LYS	2.1
2	H	332	ASN	2.1
2	H	231	ARG	2.1
2	D	138	PHE	2.1
1	G	130	LEU	2.1
1	E	66	ARG	2.1
1	C	223	GLY	2.1
1	E	93	TRP	2.1
1	E	97	SER	2.1
1	G	97	SER	2.1
1	G	153	GLY	2.1
2	H	213	GLY	2.1
1	E	460	LYS	2.0
2	H	237	LEU	2.0
1	C	496	VAL	2.0
1	E	441	VAL	2.0
1	G	56	VAL	2.0
1	G	174	PRO	2.0
2	B	350	VAL	2.0
2	F	257	ILE	2.0
1	E	438	ALA	2.0
1	G	273	ALA	2.0
1	G	338	ALA	2.0
1	E	547	SER	2.0
2	B	189	THR	2.0
1	G	298	PRO	2.0
2	B	67	PRO	2.0
2	F	185	VAL	2.0
1	C	407	TYR	2.0
2	D	363	ALA	2.0
1	C	307	GLY	2.0
1	E	258	GLY	2.0
1	E	368	ASP	2.0
2	H	262	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	275	SER	2.0
1	A	505	GLN	2.0
1	A	110	PRO	2.0
1	E	236	ILE	2.0
1	E	427	ALA	2.0
2	B	221	ALA	2.0
1	A	408	SER	2.0
1	G	554	THR	2.0
1	G	568	THR	2.0
2	D	362	THR	2.0
1	G	276	PHE	2.0
1	G	409	MET	2.0
1	G	391	LEU	2.0
2	H	131	LEU	2.0
1	G	23	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	NAG	e	2	14/15	0.38	0.52	157,165,176,176	0
8	MAN	b	6	11/12	0.41	0.40	155,160,164,164	0
8	MAN	b	4	11/12	0.41	0.27	157,161,164,165	0
3	MAN	I	4	11/12	0.44	0.53	187,189,190,191	0
4	MAN	U	5	11/12	0.47	0.39	140,143,149,151	0
6	NAG	M	2	14/15	0.60	0.69	153,159,169,172	0
3	NAG	I	2	14/15	0.61	0.39	169,174,179,181	0
6	NAG	f	2	14/15	0.65	0.29	165,166,177,178	0
6	NAG	g	2	14/15	0.66	0.45	161,168,174,175	0
3	MAN	a	4	11/12	0.66	0.30	149,157,160,165	0
7	MAN	P	4	11/12	0.66	0.20	133,136,141,141	0
8	MAN	b	5	11/12	0.68	0.38	156,159,161,163	0
3	NAG	S	1	14/15	0.70	0.26	94,108,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	BMA	b	3	11/12	0.70	0.18	144,148,156,159	0
3	BMA	I	3	11/12	0.71	0.24	142,178,189,201	0
7	BMA	P	3	11/12	0.72	0.19	106,117,127,130	0
6	NAG	M	1	14/15	0.73	0.31	115,130,138,144	0
3	MAN	Q	4	11/12	0.73	0.27	142,144,145,147	0
6	NAG	T	1	14/15	0.74	0.48	146,163,166,171	0
7	BMA	W	3	11/12	0.74	0.18	110,118,123,126	0
6	NAG	e	1	14/15	0.75	0.44	128,147,150,156	0
3	BMA	Q	3	11/12	0.75	0.37	136,142,143,143	0
7	MAN	P	5	11/12	0.75	0.29	133,135,139,142	0
6	NAG	N	1	14/15	0.75	0.30	127,151,154,156	0
3	BMA	d	3	11/12	0.76	0.18	120,127,133,135	0
6	NAG	g	1	14/15	0.76	0.24	126,146,152,161	0
3	NAG	I	1	14/15	0.76	0.41	122,139,150,159	0
9	BMA	c	3	11/12	0.76	0.19	94,100,106,110	0
8	NAG	b	2	14/15	0.76	0.29	141,145,153,156	0
6	NAG	Z	2	14/15	0.76	0.45	143,150,154,157	0
6	NAG	T	2	14/15	0.77	0.48	175,180,185,186	0
7	MAN	R	5	11/12	0.77	0.28	130,131,134,135	0
6	NAG	Y	2	14/15	0.77	0.27	135,140,144,148	0
5	BMA	L	3	11/12	0.77	0.15	104,108,115,118	0
3	MAN	S	4	11/12	0.77	0.17	78,96,105,106	0
5	MAN	L	4	11/12	0.78	0.22	123,128,133,135	0
4	MAN	X	5	11/12	0.78	0.18	130,134,141,142	0
3	BMA	S	3	11/12	0.79	0.14	108,111,118,121	0
5	MAN	L	5	11/12	0.79	0.22	124,131,133,134	0
9	MAN	c	4	11/12	0.79	0.20	109,113,116,117	0
7	BMA	R	3	11/12	0.80	0.14	98,103,109,111	0
7	MAN	R	4	11/12	0.80	0.18	111,113,124,128	0
7	MAN	W	5	11/12	0.80	0.16	92,109,119,121	0
4	MAN	U	4	11/12	0.81	0.29	136,144,147,149	0
4	BMA	U	3	11/12	0.81	0.22	113,124,133,137	0
3	NAG	K	2	14/15	0.82	0.30	116,122,125,131	0
4	BMA	J	3	11/12	0.82	0.16	119,125,127,128	0
3	NAG	Q	2	14/15	0.82	0.27	110,118,130,138	0
3	BMA	a	3	11/12	0.83	0.16	126,133,138,142	0
7	MAN	P	6	11/12	0.83	0.17	128,130,134,136	0
3	BMA	O	3	11/12	0.83	0.18	143,144,150,150	0
7	MAN	W	6	11/12	0.83	0.18	113,118,122,126	0
5	MAN	L	6	11/12	0.83	0.15	101,106,114,116	0
7	NAG	W	1	14/15	0.84	0.19	62,77,80,86	0
3	BMA	K	3	11/12	0.84	0.21	115,122,125,126	0

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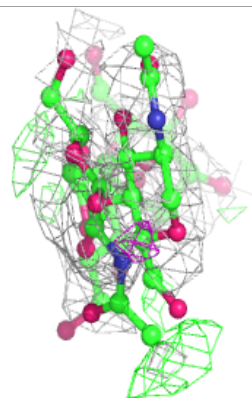
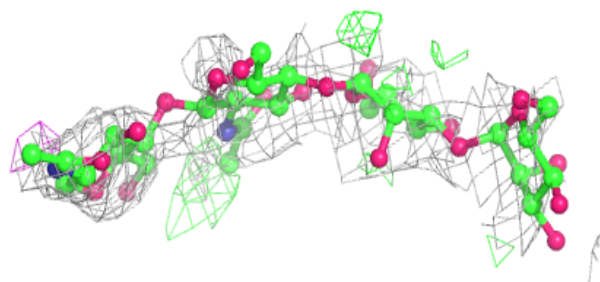
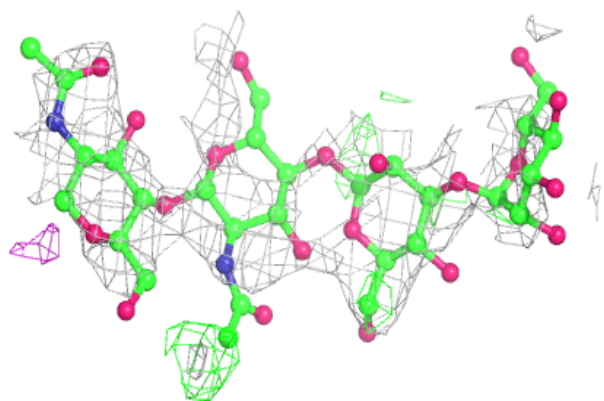
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	N	2	14/15	0.84	0.25	154,157,161,164	0
3	MAN	d	4	11/12	0.84	0.16	124,127,130,130	0
5	NAG	L	2	14/15	0.85	0.19	80,84,88,96	0
7	MAN	W	4	11/12	0.85	0.17	116,120,127,129	0
3	NAG	Q	1	14/15	0.85	0.16	65,79,89,105	0
8	NAG	b	1	14/15	0.85	0.20	87,107,115,129	0
4	MAN	J	5	11/12	0.85	0.15	111,114,116,118	0
3	NAG	d	2	14/15	0.85	0.18	136,141,150,150	0
3	NAG	O	2	14/15	0.85	0.21	130,134,142,148	0
3	MAN	O	4	11/12	0.85	0.27	148,149,151,152	0
4	NAG	X	1	14/15	0.86	0.18	87,106,114,114	0
7	MAN	R	6	11/12	0.86	0.16	114,117,125,127	0
3	NAG	K	1	14/15	0.86	0.15	82,94,109,110	0
6	NAG	f	1	14/15	0.86	0.22	143,159,177,178	0
4	MAN	X	4	11/12	0.86	0.18	108,111,114,116	0
6	NAG	Z	1	14/15	0.86	0.40	124,136,138,139	0
6	NAG	V	2	14/15	0.86	0.29	114,121,128,130	0
9	NAG	c	1	14/15	0.87	0.17	56,67,71,75	0
4	BMA	X	3	11/12	0.87	0.17	106,117,121,125	0
3	NAG	S	2	14/15	0.87	0.21	116,119,124,130	0
3	NAG	d	1	14/15	0.87	0.21	97,120,127,128	0
4	NAG	J	2	14/15	0.88	0.20	99,105,115,120	0
3	NAG	O	1	14/15	0.88	0.27	102,124,127,132	0
7	NAG	W	2	14/15	0.89	0.16	70,84,91,100	0
4	NAG	X	2	14/15	0.89	0.15	117,120,122,124	0
4	MAN	J	4	11/12	0.89	0.17	131,137,142,142	0
3	NAG	a	2	14/15	0.90	0.20	89,99,106,115	0
6	NAG	V	1	14/15	0.90	0.26	93,106,119,120	0
4	NAG	U	2	14/15	0.90	0.23	81,86,96,102	0
3	MAN	K	4	11/12	0.90	0.17	75,91,104,105	0
6	NAG	Y	1	14/15	0.90	0.26	106,129,133,138	0
7	NAG	R	2	14/15	0.91	0.14	63,76,83,90	0
4	NAG	J	1	14/15	0.92	0.19	52,70,78,84	0
3	NAG	a	1	14/15	0.92	0.25	62,81,89,90	0
7	NAG	P	2	14/15	0.92	0.18	87,93,97,101	0
9	NAG	c	2	14/15	0.92	0.15	58,74,83,91	0
7	NAG	R	1	14/15	0.92	0.20	46,58,68,71	0
7	NAG	P	1	14/15	0.93	0.13	55,75,81,82	0
4	NAG	U	1	14/15	0.94	0.23	53,69,82,82	0
5	NAG	L	1	14/15	0.94	0.15	51,60,67,76	0

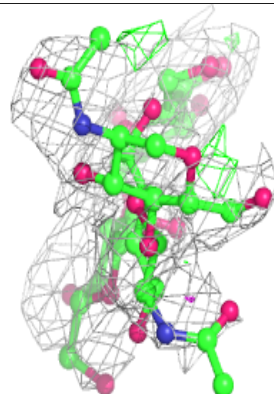
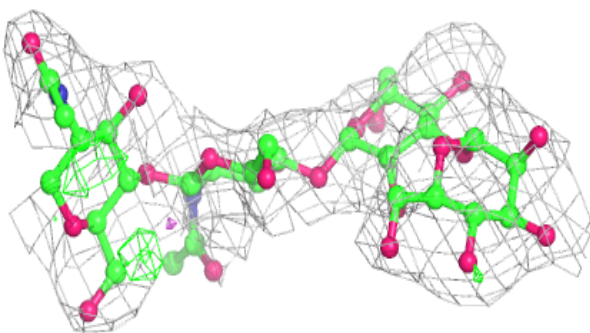
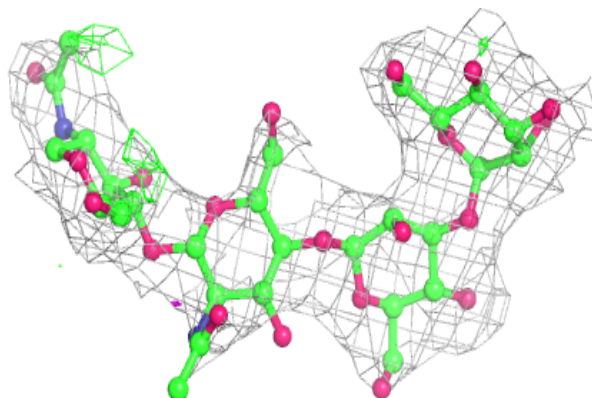
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain I:**

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

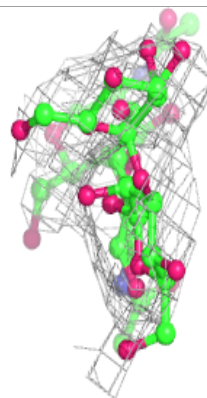
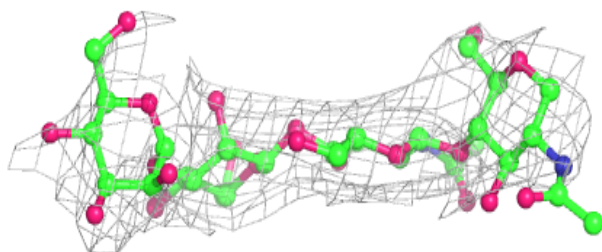
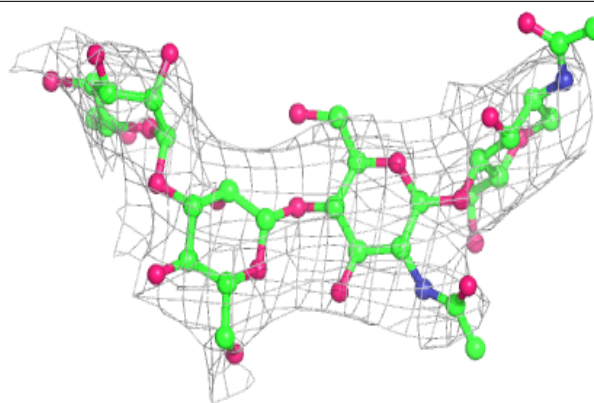
**Electron density around Chain K:**

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

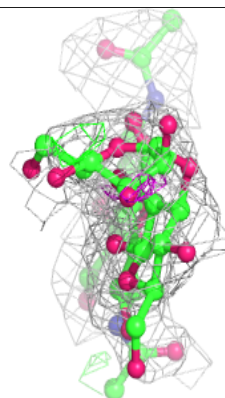
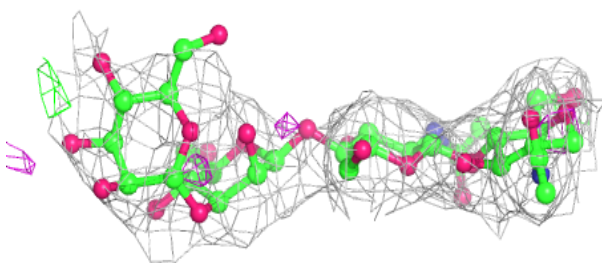
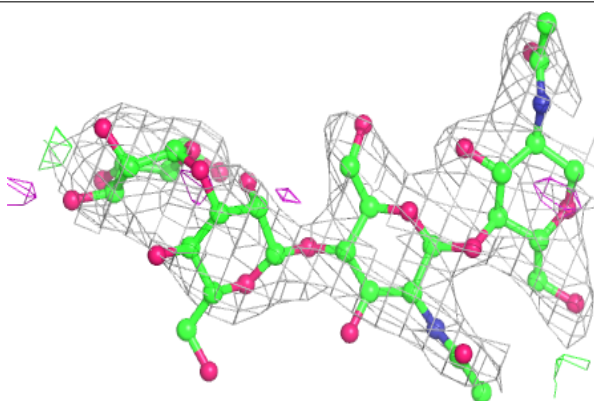


**Electron density around Chain O:**

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

**Electron density around Chain Q:**

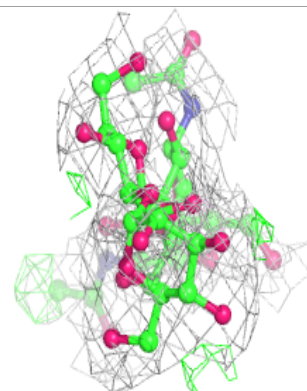
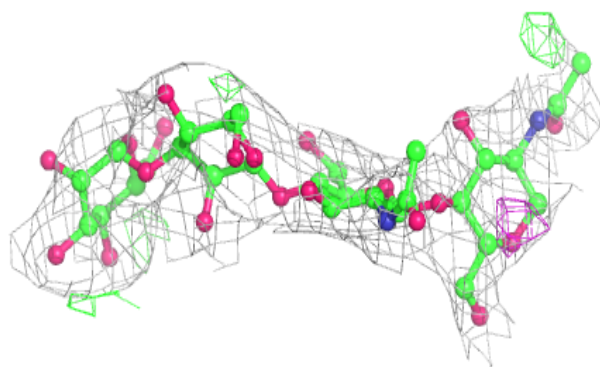
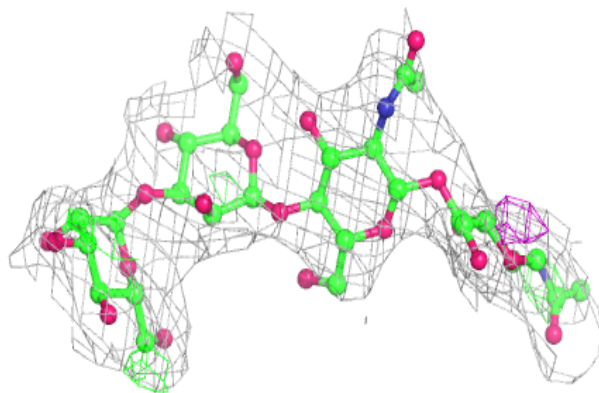
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



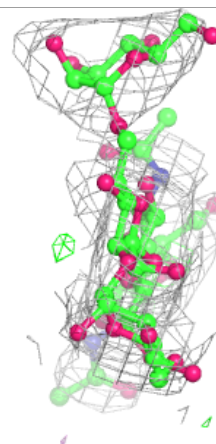
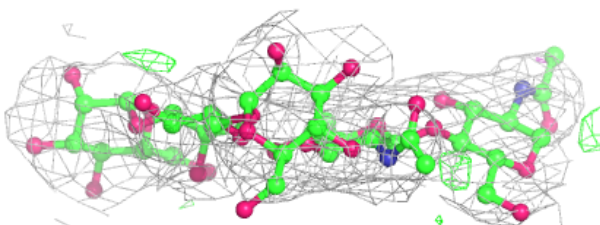
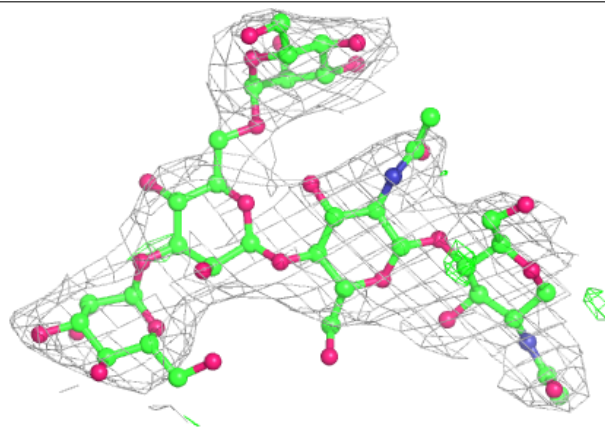


**Electron density around Chain S:**

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

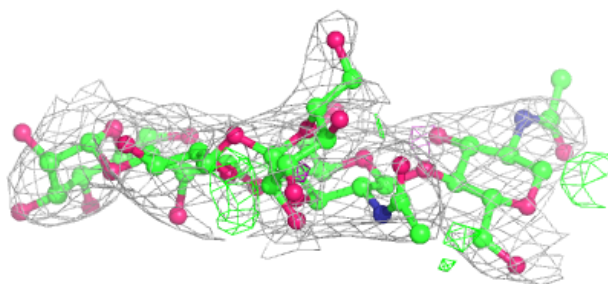
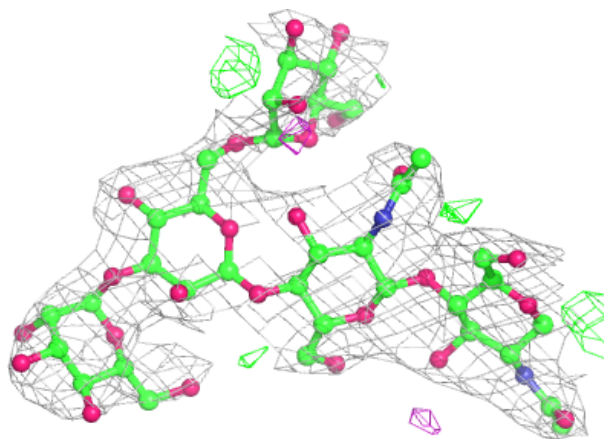
**Electron density around Chain J:**

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



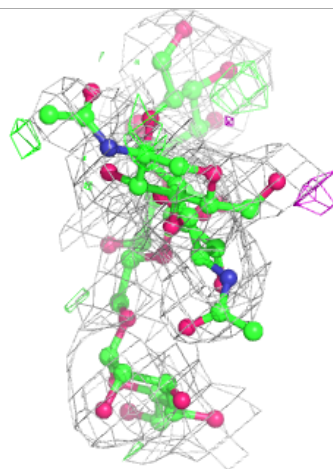
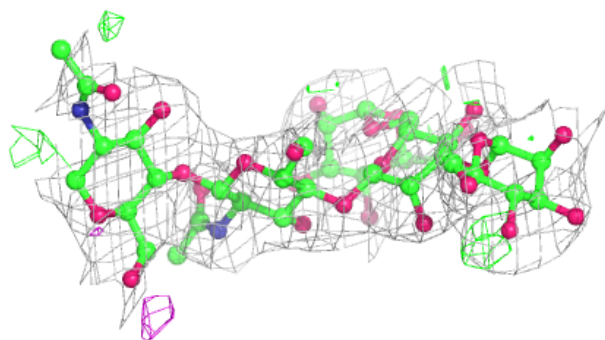
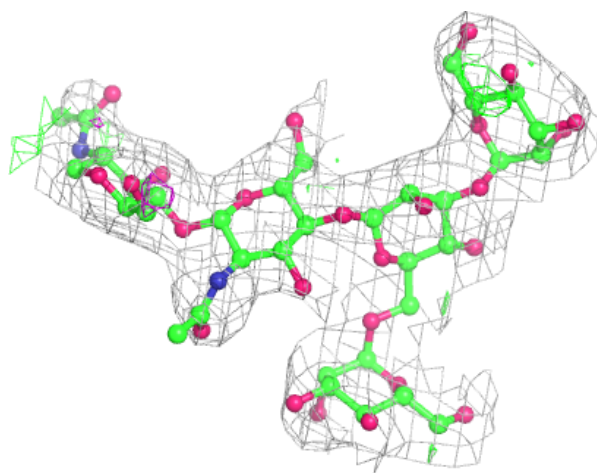
**Electron density around Chain U:**

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



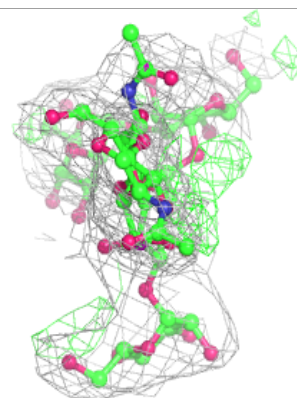
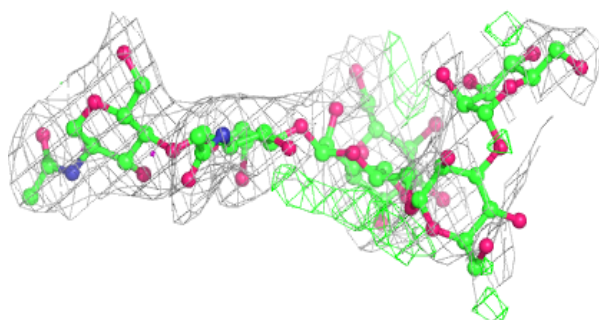
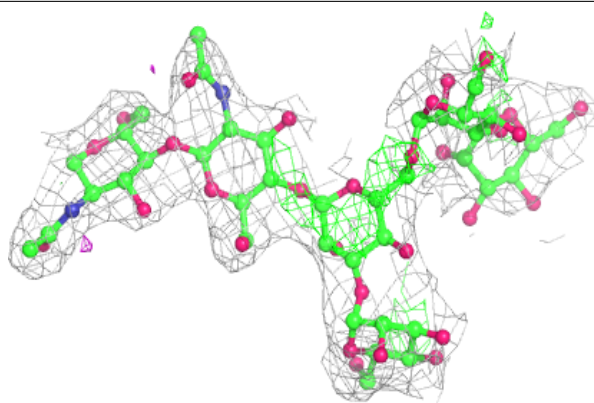
**Electron density around Chain X:**

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

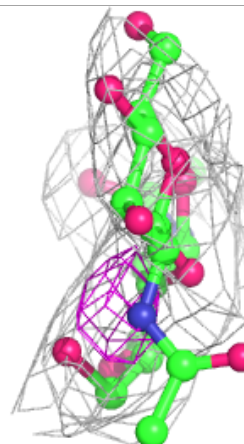
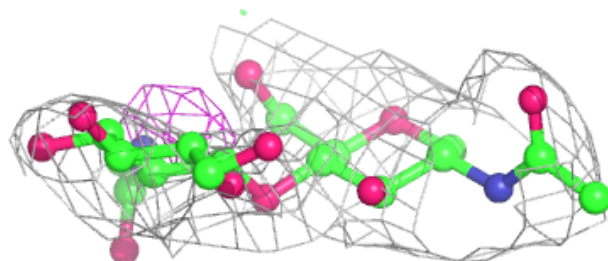
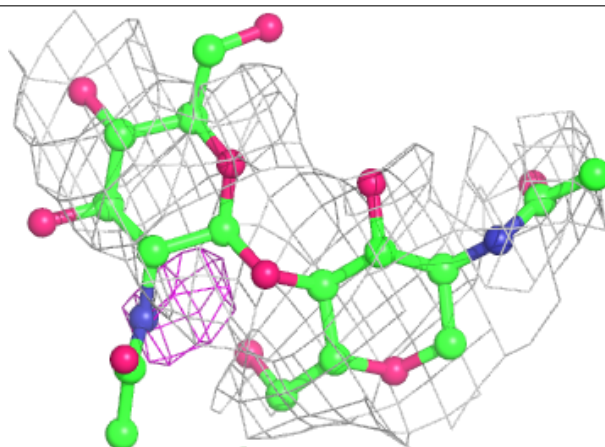


**Electron density around Chain L:**

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

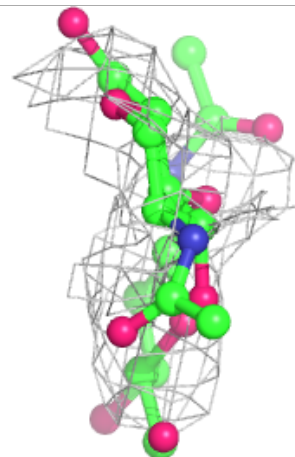
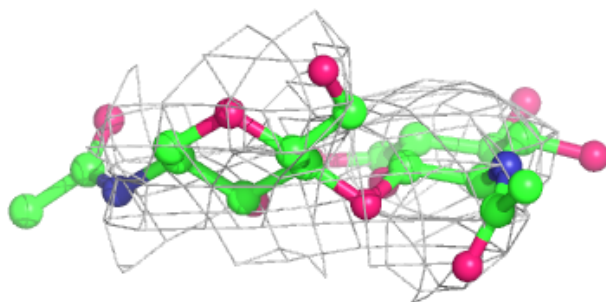
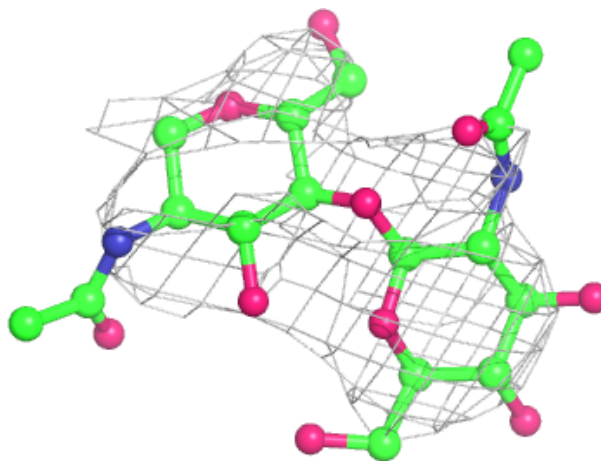
**Electron density around Chain M:**

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



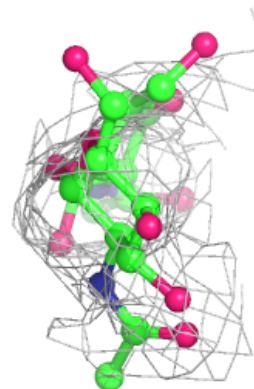
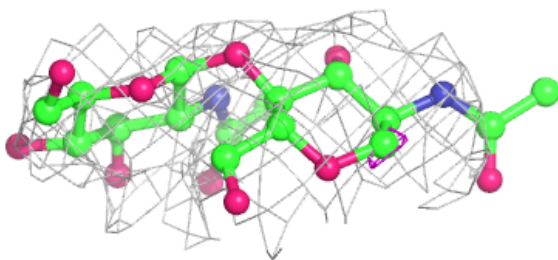
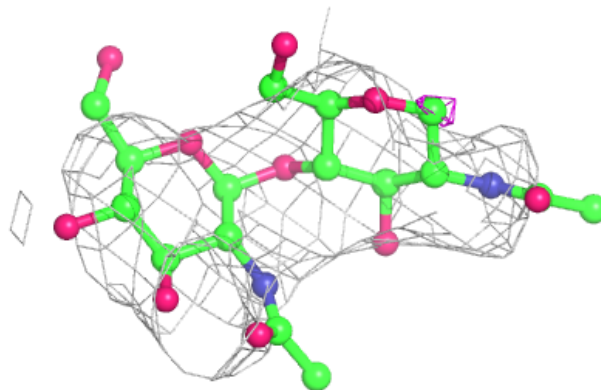
**Electron density around Chain N:**

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



**Electron density around Chain T:**

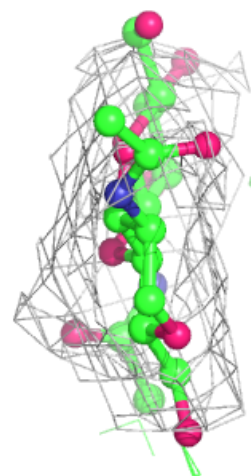
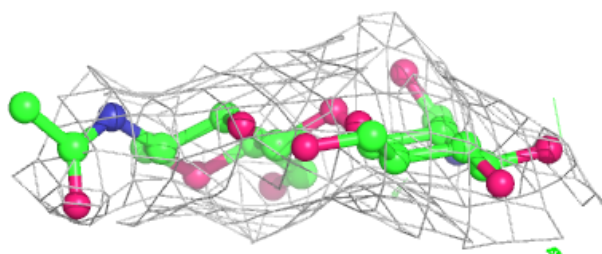
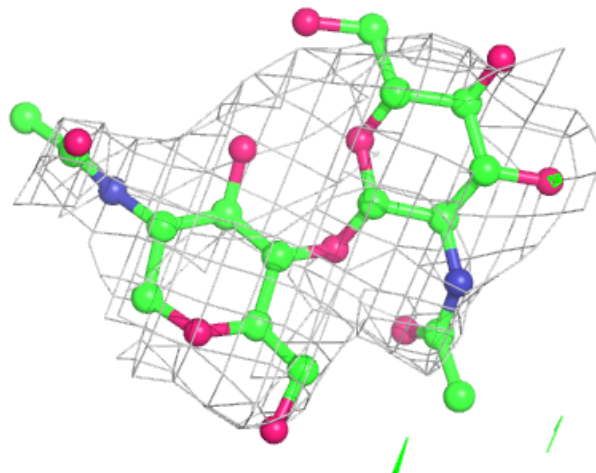
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





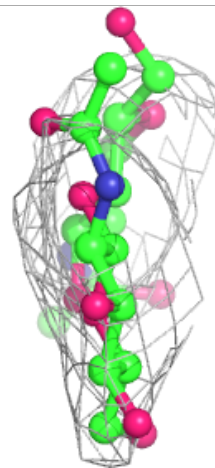
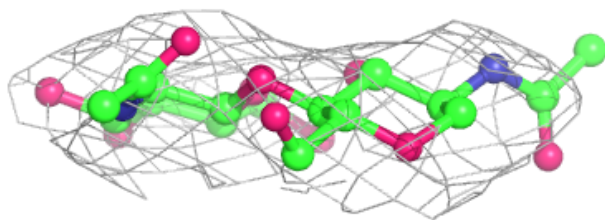
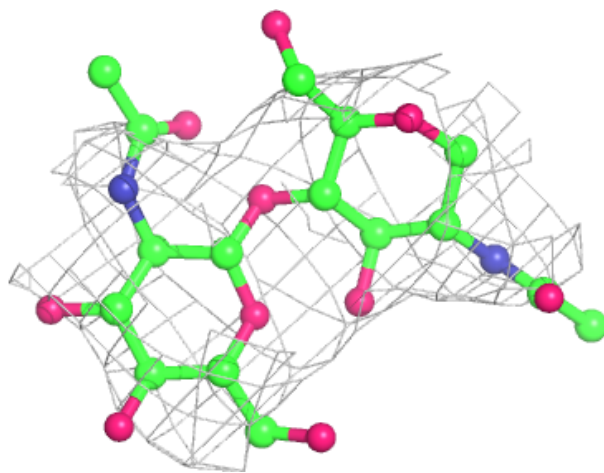
**Electron density around Chain V:**

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



**Electron density around Chain Y:**

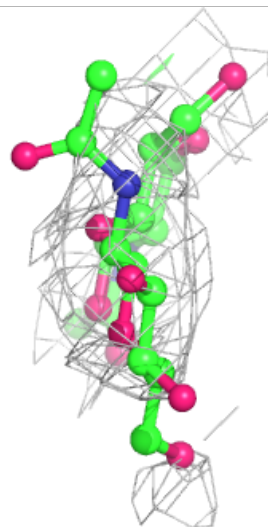
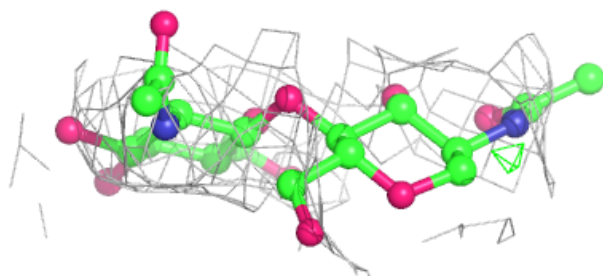
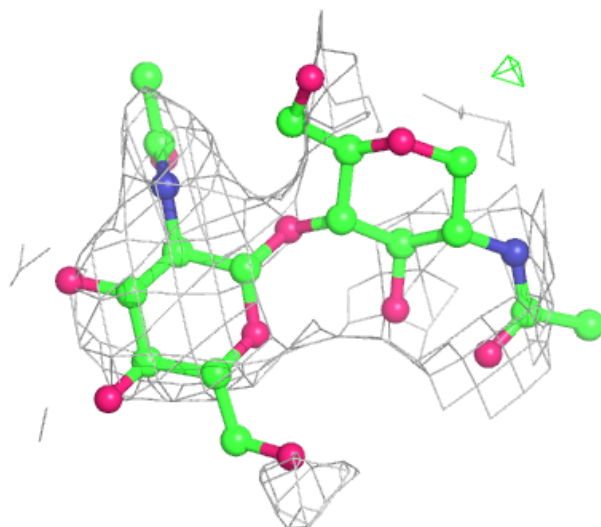
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





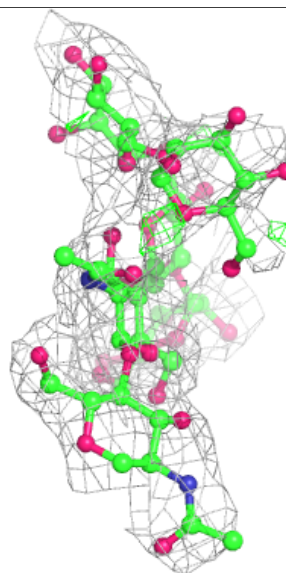
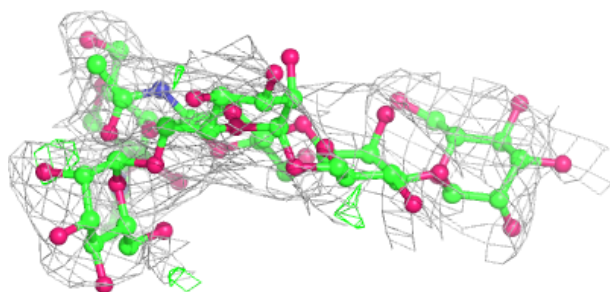
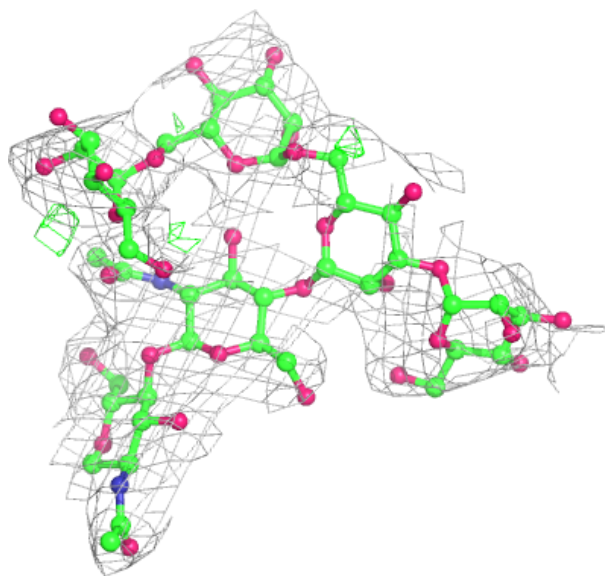
**Electron density around Chain Z:**

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



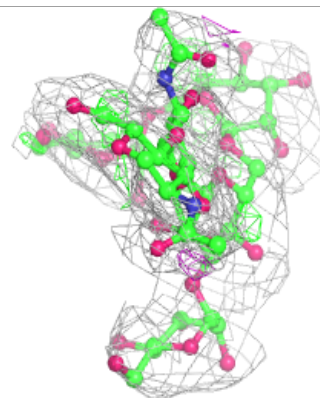
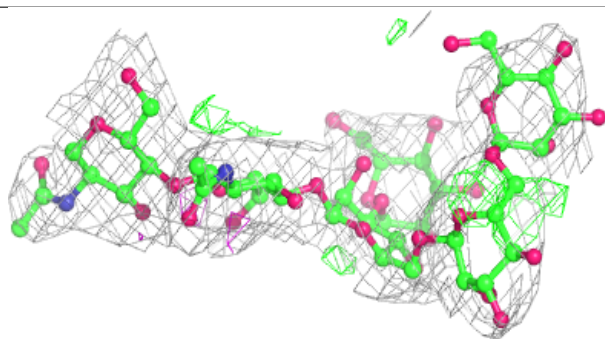
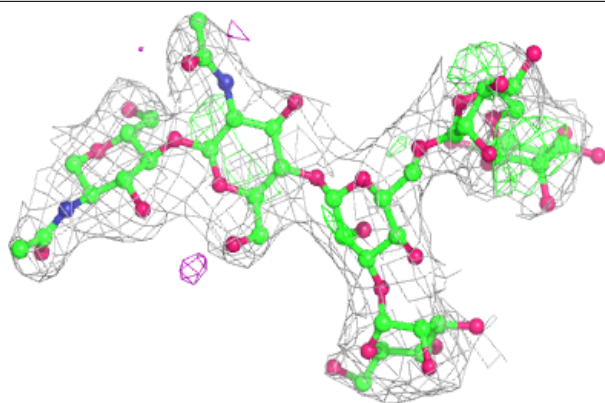
**Electron density around Chain P:**

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

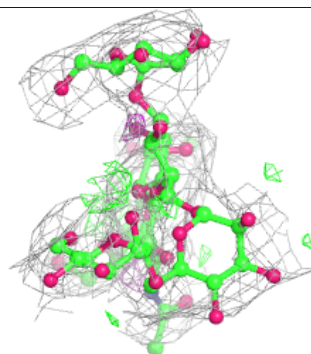
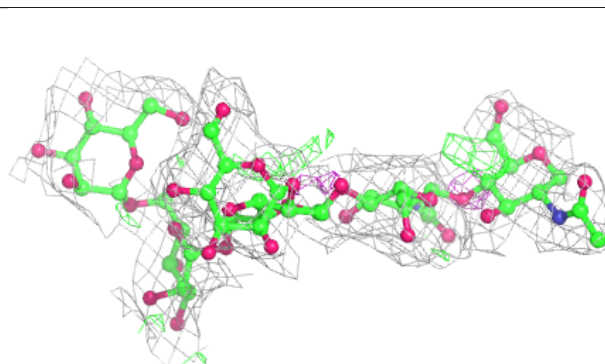
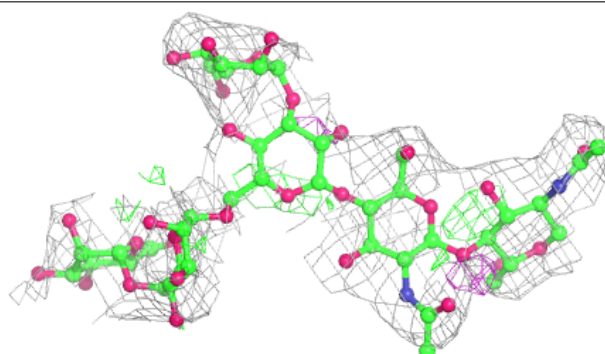


**Electron density around Chain R:**

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

**Electron density around Chain W:**

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



## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	NAG	F	501	14/15	0.38	0.68	125,142,159,163	0
10	NAG	G	2023	14/15	0.52	0.55	125,140,148,155	0
12	EDO	F	509	4/4	0.57	0.36	95,97,98,99	0
10	NAG	G	2024	14/15	0.60	0.44	140,153,166,169	0
12	EDO	G	2027	4/4	0.62	0.31	84,86,89,91	0
12	EDO	G	2028	4/4	0.69	0.22	85,88,89,90	0
12	EDO	C	628	4/4	0.69	0.12	86,88,93,97	0
10	NAG	D	501	14/15	0.71	0.30	134,158,162,162	0
11	CA	B	2002	1/1	0.73	0.16	77,77,77,77	0
12	EDO	A	625	4/4	0.73	0.19	80,82,82,83	0
12	EDO	G	2026	4/4	0.76	0.32	88,89,92,94	0
10	NAG	E	624	14/15	0.76	0.25	111,128,144,145	0
12	EDO	C	629	4/4	0.76	0.43	85,85,85,86	0
12	EDO	C	627	4/4	0.77	0.18	89,90,90,92	0
10	NAG	A	601	14/15	0.77	0.28	95,105,115,118	0
10	NAG	C	601	14/15	0.77	0.45	111,129,131,131	0
10	NAG	B	2005	14/15	0.78	0.38	103,123,133,135	0
10	NAG	C	626	14/15	0.79	0.46	113,129,138,138	0
12	EDO	B	2012	4/4	0.80	0.21	82,83,84,85	0
10	NAG	F	502	14/15	0.81	0.43	118,136,146,146	0
13	MG	F	505	1/1	0.83	0.11	82,82,82,82	0
12	EDO	H	509	4/4	0.83	0.22	95,98,102,105	0
10	NAG	D	502	14/15	0.84	0.40	118,133,138,141	0
14	MES	D	507	12/12	0.87	0.17	82,91,100,100	0
14	MES	F	510	12/12	0.87	0.24	89,99,109,111	0
12	EDO	E	625	4/4	0.88	0.18	58,59,63,67	0
12	EDO	G	2025	4/4	0.88	0.21	78,80,80,80	0
13	MG	B	2001	1/1	0.90	0.06	57,57,57,57	0
11	CA	E	603	1/1	0.90	0.10	84,84,84,84	0
11	CA	D	504	1/1	0.90	0.10	60,60,60,60	0
13	MG	D	503	1/1	0.91	0.06	66,66,66,66	0
11	CA	G	2002	1/1	0.91	0.10	61,61,61,61	0
11	CA	G	2001	1/1	0.92	0.10	82,82,82,82	0
14	MES	B	2014	12/12	0.94	0.22	73,103,110,111	0
14	MES	H	510	12/12	0.94	0.23	75,89,91,91	0
12	EDO	B	2013	4/4	0.95	0.43	62,65,66,68	0
11	CA	G	2004	1/1	0.95	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	CA	C	605	1/1	0.95	0.10	58,58,58,58	0
11	CA	E	604	1/1	0.95	0.14	98,98,98,98	0
11	CA	F	506	1/1	0.95	0.08	53,53,53,53	0
11	CA	G	2003	1/1	0.95	0.07	63,63,63,63	0
11	CA	A	607	1/1	0.96	0.13	54,54,54,54	0
11	CA	A	606	1/1	0.96	0.14	61,61,61,61	0
11	CA	E	602	1/1	0.96	0.09	82,82,82,82	0
11	CA	A	609	1/1	0.96	0.13	55,55,55,55	0
10	NAG	E	601	14/15	0.96	0.32	20,20,20,20	0
11	CA	C	604	1/1	0.97	0.11	69,69,69,69	0
13	MG	H	505	1/1	0.97	0.03	60,60,60,60	0
11	CA	E	605	1/1	0.97	0.11	102,102,102,102	0
11	CA	H	506	1/1	0.98	0.11	68,68,68,68	0
11	CA	A	608	1/1	0.98	0.14	44,44,44,44	0
11	CA	C	602	1/1	0.98	0.15	62,62,62,62	0
11	CA	C	603	1/1	0.98	0.08	56,56,56,56	0

## 6.5 Other polymers

There are no such residues in this entry.