



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2021 – 12:10 AM EDT

PDB ID : 6W03  
Title : Crystal Structure of HIV-1 BG505 DS-SOSIP.3mut Prefusion Env Trimer in Complex with Human Antibodies 3H109L and 35O22 at 3.3 Angstrom  
Authors : Lai, Y.-T.; Kwong, P.D.  
Deposited on : 2020-02-28  
Resolution : 2.40 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 : 2.23.2  
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) : 2.23.2

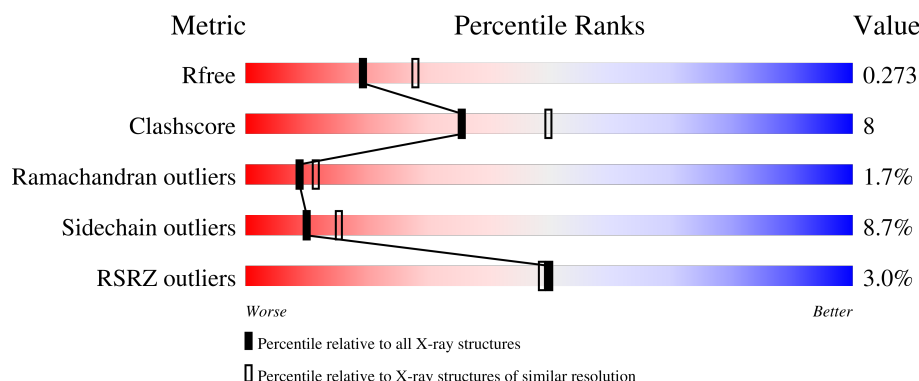
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	153	<div> <div>2%</div> <div>65%</div> <div>14%</div> <div>•</div> <div>19%</div> </div>
2	D	134	<div> <div>5%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>
3	E	114	<div> <div>10%</div> <div>75%</div> <div>22%</div> <div>• •</div> </div>
4	G	481	<div> <div>•</div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
5	H	244	<div> <div>2%</div> <div>67%</div> <div>22%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
6	L	217	
7	A	4	
8	C	2	
8	F	2	
8	I	2	
8	J	2	
8	K	2	
9	M	5	
10	N	4	
11	O	6	
12	P	10	

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	BMA	N	3	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	124	Total	C	N	O	S	0	0	0
			988	627	170	185	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 3 is a protein called 35O22 scFv light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	112	Total	C	N	O	S	0	0	0
			851	533	141	171	6			

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	427	Total	C	N	O	S	0	0	0
			3365	2121	592	622	30			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	145	ALA	ASN	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	329	PRO	ALA	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	508	ARG	-	expression tag	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	227	Total	C	N	O	S	0	0	0
			1721	1096	279	340	6			

- Molecule 6 is a protein called 3H109L Fab light chain.

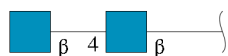
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

- Molecule 7 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.



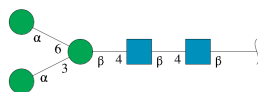
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



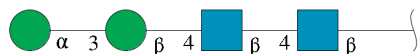
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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.



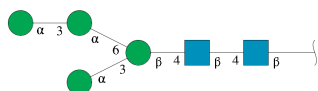
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



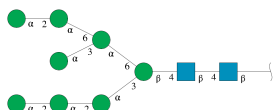
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 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.



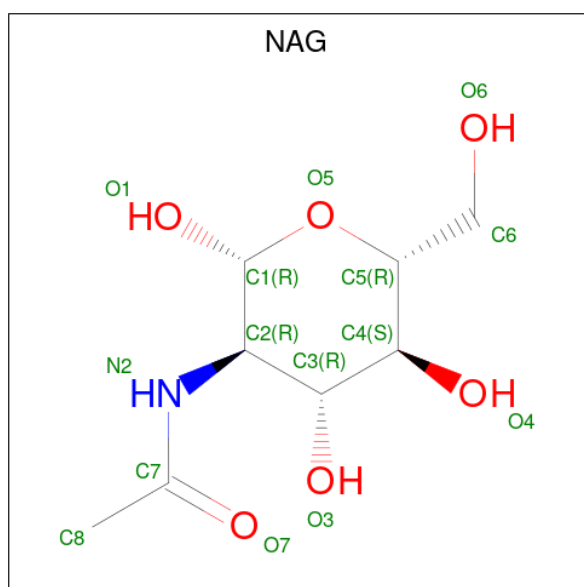
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
12	P	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 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
13	B	1	Total	C	N	O	0	0
			14	8	1	5		

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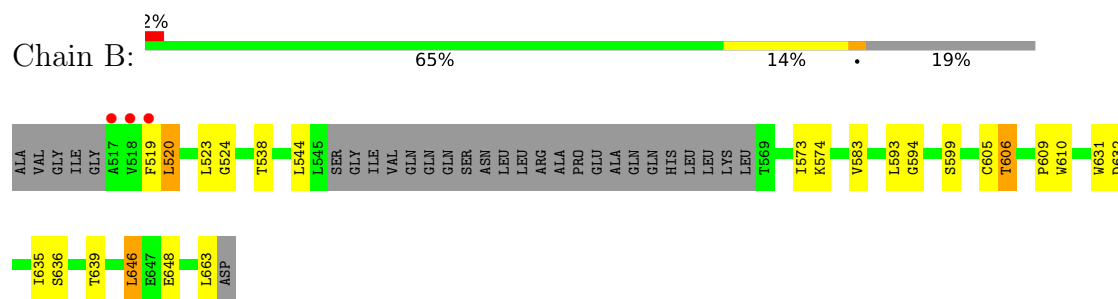
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		



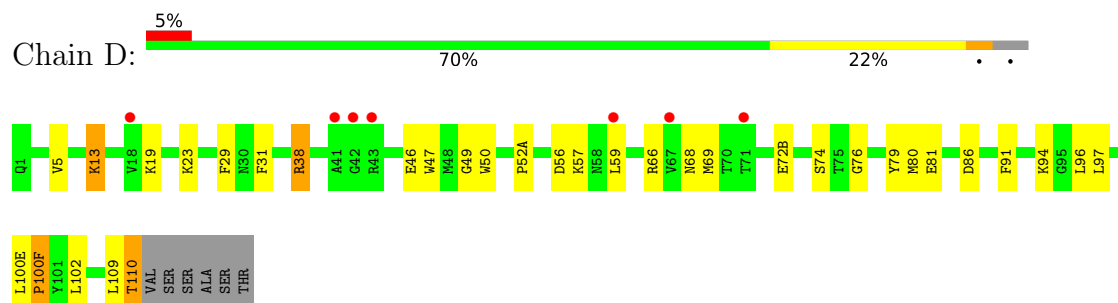
### 3 Residue-property plots [i](#)

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.

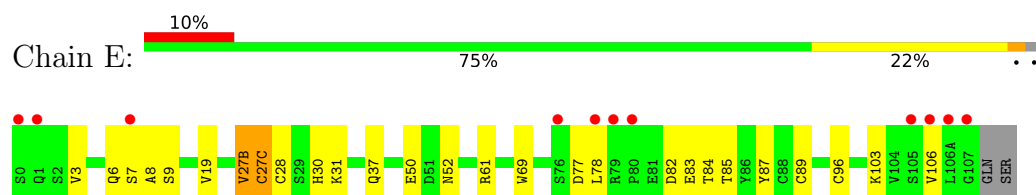
- Molecule 1: Envelope glycoprotein gp41



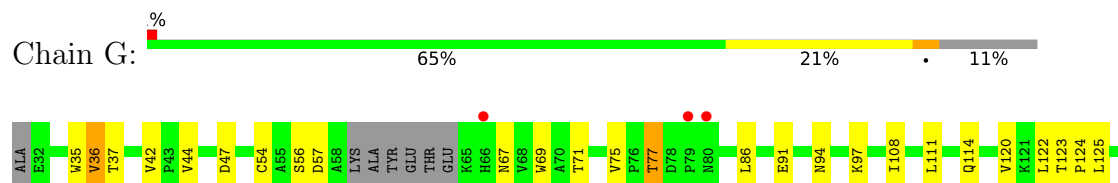
- Molecule 2: 35O22 scFv heavy chain

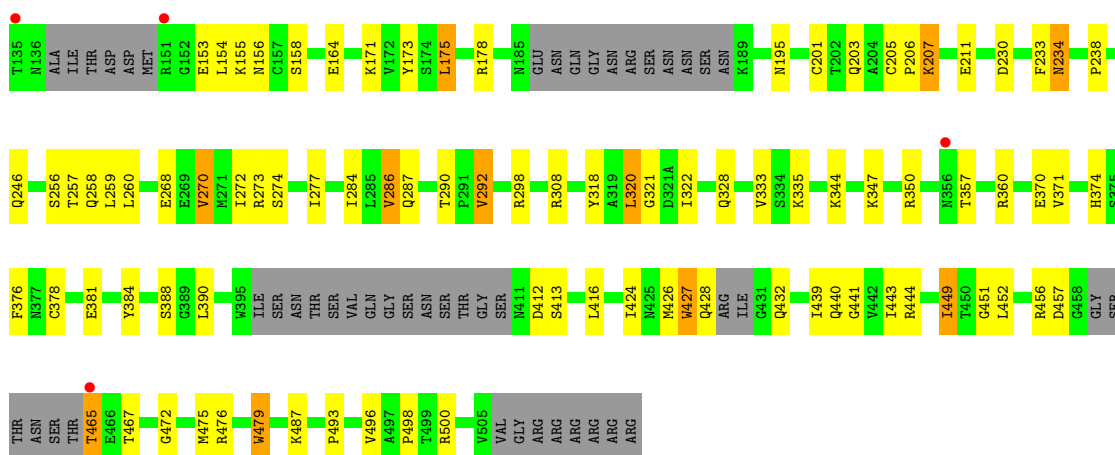


- Molecule 3: 35O22 scFv light chain

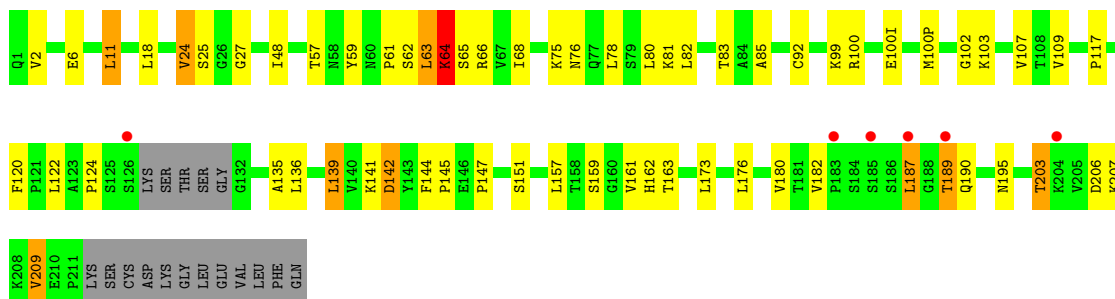


- Molecule 4: Envelope glycoprotein gp160

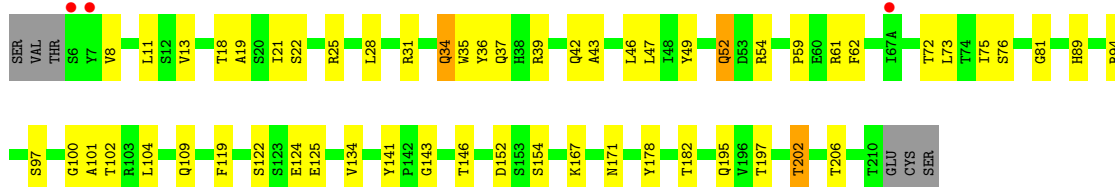




• Molecule 5: 3H109L Fab heavy chain



• Molecule 6: 3H109L Fab light chain



• Molecule 7: 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



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





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

Chain F:  100%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain K:  100%



- Molecule 9: 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 M:  60% 40%



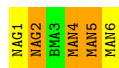
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  25% 75%

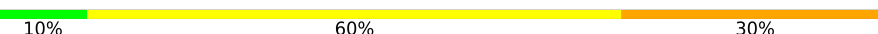


- Molecule 11:  $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain O:  17% 33% 50%



- Molecule 12:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -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 P:  10% 60% 30%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.39Å 131.39Å 315.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.80 – 2.40 45.50 – 2.37	Depositor EDS
% Data completeness (in resolution range)	29.4 (39.80-2.40) 29.4 (45.50-2.37)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.230 , 0.273 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	1837 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 23.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: BMA, NAG, 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	B	0.23	0/1006	0.39	0/1365
2	D	0.24	0/1021	0.47	0/1390
3	E	0.25	0/875	0.45	0/1195
4	G	0.24	0/3435	0.45	0/4658
5	H	0.26	0/1764	0.48	0/2405
6	L	0.24	0/1647	0.44	0/2247
All	All	0.24	0/9748	0.45	0/13260

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	B	988	0	969	11	0
2	D	994	0	953	19	0
3	E	851	0	801	10	0
4	G	3365	0	3303	59	0
5	H	1721	0	1690	36	0
6	L	1604	0	1551	30	0
7	A	50	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	28	0	25	0	0
8	F	28	0	25	0	0
8	I	28	0	25	2	0
8	J	28	0	25	0	0
8	K	28	0	25	0	0
9	M	61	0	52	0	0
10	N	50	0	43	1	0
11	O	72	0	61	6	0
12	P	116	0	96	3	0
13	B	28	0	26	0	0
13	G	56	0	52	1	0
All	All	10096	0	9765	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (161) 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)
5:H:24:VAL:HG22	5:H:76:ASN:HB3	1.68	0.76
4:G:333:VAL:HG21	4:G:390:LEU:HD21	1.68	0.74
4:G:154:LEU:HD11	4:G:322:ILE:HD11	1.70	0.71
4:G:335:LYS:HB3	4:G:412:ASP:HB3	1.72	0.70
2:D:57:LYS:NZ	2:D:69:MET:O	2.26	0.69
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.75	0.69
6:L:122:SER:HB3	6:L:125:GLU:HG2	1.75	0.69
4:G:205:CYS:HB3	4:G:207:LYS:HD2	1.75	0.68
4:G:292:VAL:HG13	4:G:449:ILE:HG23	1.77	0.67
4:G:298:ARG:NH2	4:G:441:GLY:O	2.29	0.66
1:B:605:CYS:HA	4:G:37:THR:HG22	1.78	0.66
4:G:230:ASP:HB3	4:G:233:PHE:HB2	1.77	0.65
3:E:78:LEU:HD13	3:E:106:VAL:HG23	1.79	0.65
5:H:99:LYS:HB3	12:P:9:MAN:H62	1.79	0.65
5:H:151:SER:HB2	5:H:195:ASN:HB2	1.80	0.63
4:G:270:VAL:HG11	4:G:344:LYS:HB3	1.80	0.62
1:B:520:LEU:HB3	1:B:524:GLY:HA3	1.80	0.62
4:G:439:ILE:HB	4:G:443:ILE:HD11	1.81	0.62
3:E:37:GLN:HG3	3:E:84:THR:HG21	1.82	0.61
4:G:164:GLU:OE2	4:G:308:ARG:NH1	2.33	0.61
5:H:120:PHE:HE2	5:H:141:LYS:HE2	1.66	0.61
4:G:94:ASN:HB3	4:G:97:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:LEU:HG	2:D:97:LEU:HG	1.84	0.60
4:G:69:TRP:HZ3	4:G:108:ILE:HG23	1.67	0.59
4:G:277:ILE:HD11	8:I:1:NAG:H81	1.84	0.59
5:H:100:ARG:NH1	6:L:31:ARG:O	2.36	0.59
5:H:195:ASN:ND2	5:H:206:ASP:OD2	2.35	0.59
5:H:63:LEU:O	5:H:65:SER:N	2.35	0.58
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.85	0.58
4:G:350:ARG:NH2	4:G:357:THR:O	2.36	0.58
6:L:59:PRO:HB2	6:L:61:ARG:HG2	1.85	0.58
5:H:100:ARG:NH2	12:P:4:MAN:O6	2.36	0.58
5:H:59:TYR:HB2	5:H:64:LYS:HD2	1.86	0.57
6:L:119:PHE:HB2	6:L:134:VAL:HG23	1.86	0.57
6:L:197:THR:HA	6:L:202:THR:HA	1.85	0.57
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.41	0.56
11:O:2:NAG:H83	11:O:2:NAG:H3	1.87	0.56
5:H:27:GLY:O	5:H:76:ASN:ND2	2.39	0.56
6:L:54:ARG:NH2	6:L:62:PHE:O	2.27	0.56
4:G:69:TRP:HA	4:G:111:LEU:HD13	1.88	0.56
5:H:117:PRO:HD2	5:H:203:THR:HG21	1.87	0.56
6:L:19:ALA:HB3	6:L:75:ILE:HB	1.88	0.56
4:G:370:GLU:HG3	4:G:384:TYR:HE2	1.71	0.56
5:H:139:LEU:HD22	5:H:141:LYS:HG2	1.88	0.55
1:B:544:LEU:HD21	4:G:493:PRO:HG3	1.88	0.55
1:B:609:PRO:HA	4:G:35:TRP:HA	1.89	0.54
4:G:259:LEU:HD23	4:G:449:ILE:HD12	1.89	0.54
2:D:68:ASN:HB3	2:D:81:GLU:HB2	1.90	0.54
5:H:6:GLU:N	5:H:6:GLU:OE1	2.40	0.54
4:G:156:ASN:HA	4:G:175:LEU:HD12	1.89	0.53
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	1.90	0.53
4:G:286:VAL:HG13	4:G:452:LEU:HB3	1.89	0.53
4:G:457:ASP:OD1	4:G:467:THR:OG1	2.27	0.53
6:L:34:GLN:NE2	6:L:49:TYR:O	2.42	0.52
5:H:11:LEU:HD12	5:H:145:PRO:HD3	1.91	0.52
4:G:122:LEU:HD11	4:G:203:GLN:HB2	1.92	0.52
2:D:109:LEU:HG	2:D:110:THR:H	1.75	0.52
3:E:83:GLU:HG3	3:E:106:VAL:HG12	1.91	0.52
5:H:92:CYS:O	5:H:102:GLY:N	2.40	0.51
5:H:61:PRO:HA	5:H:64:LYS:HG2	1.91	0.51
4:G:298:ARG:NH1	4:G:381:GLU:OE2	2.43	0.51
6:L:124:GLU:N	6:L:124:GLU:OE1	2.44	0.51
4:G:370:GLU:N	4:G:370:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:91:GLU:OE1	4:G:487:LYS:NZ	2.45	0.50
5:H:136:LEU:HD13	5:H:209:VAL:HG21	1.92	0.50
6:L:22:SER:HA	6:L:72:THR:HG22	1.94	0.50
2:D:5:VAL:HG23	2:D:23:LYS:HE3	1.93	0.49
5:H:124:PRO:HG3	5:H:136:LEU:HD23	1.94	0.49
2:D:38:ARG:HD2	2:D:46:GLU:HB3	1.93	0.49
3:E:84:THR:OG1	3:E:85:THR:N	2.46	0.49
6:L:13:VAL:HG22	6:L:104:LEU:HD11	1.94	0.49
6:L:109:GLN:HB2	6:L:141:TYR:CE1	2.47	0.49
2:D:13:LYS:HD2	2:D:13:LYS:HA	1.53	0.49
5:H:68:ILE:HG23	5:H:81:LYS:HB2	1.93	0.49
5:H:161:VAL:HA	5:H:180:VAL:HG22	1.95	0.49
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.95	0.49
4:G:155:LYS:HE3	4:G:178:ARG:HD2	1.95	0.49
6:L:8:VAL:HA	6:L:101:ALA:HB3	1.94	0.48
6:L:39:ARG:NH1	6:L:81:GLY:O	2.41	0.48
4:G:357:THR:HG1	4:G:465:THR:N	2.11	0.48
3:E:103:LYS:HD2	3:E:103:LYS:H	1.78	0.48
2:D:56:ASP:OD2	11:O:4:MAN:O4	2.24	0.48
12:P:1:NAG:H83	12:P:1:NAG:H3	1.94	0.48
4:G:274:SER:HB2	4:G:284:ILE:HA	1.95	0.48
4:G:390:LEU:HG	4:G:416:LEU:HD21	1.95	0.48
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.48	0.48
5:H:64:LYS:HD2	5:H:64:LYS:HA	1.56	0.48
5:H:124:PRO:HD3	5:H:136:LEU:HB3	1.95	0.48
4:G:175:LEU:HB2	4:G:320:LEU:HB3	1.97	0.47
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.96	0.47
6:L:46:LEU:HD21	6:L:49:TYR:HB3	1.96	0.47
6:L:134:VAL:HG12	6:L:178:TYR:CD2	2.49	0.47
1:B:632:ASP:O	1:B:636:SER:OG	2.23	0.47
1:B:610:TRP:HE3	4:G:36:VAL:HG12	1.79	0.47
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.68	0.47
4:G:123:THR:N	4:G:124:PRO:HD2	2.30	0.47
4:G:427:TRP:HE1	4:G:475:MET:HG2	1.78	0.47
4:G:171:LYS:HE2	13:G:607:NAG:H83	1.97	0.47
5:H:18:LEU:HD11	5:H:107:VAL:HG11	1.97	0.47
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.50	0.47
4:G:256:SER:OG	4:G:259:LEU:O	2.28	0.47
5:H:163:THR:HG23	5:H:176:LEU:HD21	1.96	0.47
6:L:21:ILE:HG23	6:L:102:THR:HG21	1.97	0.47
2:D:50:TRP:HH2	11:O:4:MAN:H62	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:83:THR:HG23	5:H:85:ALA:H	1.80	0.46
1:B:606:THR:HG21	1:B:646:LEU:HD12	1.98	0.46
6:L:18:THR:HG22	6:L:76:SER:HA	1.97	0.46
4:G:344:LYS:HA	4:G:347:LYS:HD2	1.97	0.46
1:B:631:TRP:CE2	1:B:635:ILE:HG13	2.51	0.46
4:G:258:GLN:NE2	4:G:371:VAL:O	2.46	0.45
2:D:50:TRP:CH2	11:O:4:MAN:H62	2.50	0.45
5:H:83:THR:O	5:H:109:VAL:HG21	2.15	0.45
1:B:594:GLY:HA2	1:B:599:SER:HB3	1.99	0.45
6:L:42:GLN:HG2	6:L:43:ALA:H	1.82	0.45
4:G:273:ARG:O	4:G:274:SER:HB3	2.17	0.45
11:O:4:MAN:O4	11:O:5:MAN:H5	2.17	0.44
5:H:103:LYS:N	5:H:103:LYS:HD2	2.33	0.44
2:D:66:ARG:NH1	2:D:86:ASP:OD2	2.51	0.44
4:G:206:PRO:HG3	4:G:318:TYR:CE1	2.51	0.44
5:H:189:THR:O	5:H:189:THR:OG1	2.25	0.44
2:D:29:PHE:CG	2:D:76:GLY:HA3	2.53	0.43
4:G:69:TRP:HB2	4:G:71:THR:HG23	2.00	0.43
3:E:7:SER:O	3:E:9:SER:N	2.51	0.43
1:B:523:LEU:O	4:G:86:LEU:HD22	2.18	0.43
4:G:56:SER:O	4:G:77:THR:N	2.35	0.43
3:E:6:GLN:OE1	3:E:87:TYR:HA	2.18	0.42
2:D:19:LYS:HD2	2:D:81:GLU:HG3	1.99	0.42
2:D:31:PHE:HA	11:O:1:NAG:H62	2.01	0.42
6:L:167:LYS:HE2	6:L:171:ASN:HA	2.01	0.42
3:E:61:ARG:NH2	3:E:82:ASP:OD2	2.53	0.42
4:G:256:SER:OG	4:G:257:THR:N	2.52	0.42
4:G:234:ASN:OD1	8:I:1:NAG:N2	2.52	0.42
6:L:36:TYR:HE1	6:L:46:LEU:HD13	1.83	0.42
4:G:158:SER:HA	4:G:173:TYR:HA	2.02	0.42
4:G:376:PHE:CE2	4:G:378:CYS:HB2	2.55	0.42
4:G:67:ASN:HD22	4:G:69:TRP:HD1	1.67	0.42
6:L:52:GLN:N	6:L:52:GLN:OE1	2.53	0.42
2:D:29:PHE:CE2	2:D:52(A):PRO:HB3	2.55	0.41
4:G:122:LEU:HD13	4:G:125:LEU:HD12	2.02	0.41
5:H:157:LEU:HD21	5:H:180:VAL:HG11	2.03	0.41
6:L:36:TYR:CE1	6:L:46:LEU:HD13	2.55	0.41
5:H:2:VAL:HA	5:H:25:SER:O	2.20	0.41
4:G:360:ARG:HB3	4:G:467:THR:HG22	2.02	0.41
5:H:124:PRO:HG3	5:H:187:LEU:HD11	2.02	0.41
4:G:42:VAL:HG23	4:G:44:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:28:LEU:HB2	6:L:94:ARG:HB2	2.02	0.41
6:L:119:PHE:HB2	6:L:134:VAL:CG2	2.48	0.41
2:D:72(B):GLU:HB2	2:D:74:SER:HB2	2.02	0.41
4:G:211:GLU:OE2	7:A:2:NAG:H5	2.20	0.41
4:G:270:VAL:HG23	4:G:287:GLN:O	2.21	0.41
4:G:500:ARG:H	4:G:500:ARG:HG2	1.72	0.41
5:H:122:LEU:HB3	6:L:119:PHE:CD2	2.56	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.84	0.41
5:H:124:PRO:HB3	5:H:135:ALA:O	2.21	0.41
3:E:50:GLU:O	3:E:52:ASN:N	2.52	0.40
6:L:35:TRP:CD2	6:L:73:LEU:HB2	2.57	0.40
5:H:142:ASP:HB3	5:H:173:LEU:HD22	2.02	0.40
5:H:66:ARG:CZ	5:H:82:LEU:HD21	2.52	0.40
2:D:19:LYS:HE3	2:D:79:TYR:HB3	2.03	0.40
4:G:376:PHE:HE2	4:G:378:CYS:HB2	1.86	0.40
10:N:1:NAG:H62	10:N:2:NAG:H82	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	120/153 (78%)	108 (90%)	12 (10%)	0	100	100
2	D	126/134 (94%)	112 (89%)	13 (10%)	1 (1%)	19	29
3	E	110/114 (96%)	90 (82%)	17 (16%)	3 (3%)	5	5
4	G	413/481 (86%)	375 (91%)	29 (7%)	9 (2%)	6	7
5	H	223/244 (91%)	205 (92%)	14 (6%)	4 (2%)	8	10
6	L	209/217 (96%)	194 (93%)	12 (6%)	3 (1%)	11	15
All	All	1201/1343 (89%)	1084 (90%)	97 (8%)	20 (2%)	9	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	64	LYS
3	E	8	ALA
5	H	48	ILE
5	H	142	ASP
6	L	152	ASP
4	G	426	MET
4	G	427	TRP
4	G	153	GLU
4	G	321	GLY
6	L	100	GLY
3	E	77	ASP
4	G	413	SER
4	G	268	GLU
4	G	374	HIS
4	G	472	GLY
6	L	143	GLY
3	E	27(B)	VAL
2	D	100(F)	PRO
4	G	238	PRO
5	H	147	PRO

### 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	B	106/129 (82%)	94 (89%)	12 (11%)	6	8
2	D	107/112 (96%)	99 (92%)	8 (8%)	13	21
3	E	98/100 (98%)	89 (91%)	9 (9%)	9	13
4	G	382/429 (89%)	350 (92%)	32 (8%)	11	16
5	H	197/212 (93%)	176 (89%)	21 (11%)	6	9
6	L	175/181 (97%)	164 (94%)	11 (6%)	18	28
All	All	1065/1163 (92%)	972 (91%)	93 (9%)	10	15

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	PHE
1	B	520	LEU
1	B	538	THR
1	B	573	ILE
1	B	574	LYS
1	B	583	VAL
1	B	593	LEU
1	B	606	THR
1	B	639	THR
1	B	646	LEU
1	B	648	GLU
1	B	663	LEU
2	D	13	LYS
2	D	38	ARG
2	D	59	LEU
2	D	80	MET
2	D	91	PHE
2	D	94	LYS
2	D	102	LEU
2	D	110	THR
3	E	3	VAL
3	E	19	VAL
3	E	27(B)	VAL
3	E	27(C)	CYS
3	E	30	HIS
3	E	31	LYS
3	E	69	TRP
3	E	89	CYS
3	E	96	CYS
4	G	36	VAL
4	G	47	ASP
4	G	54	CYS
4	G	57	ASP
4	G	75	VAL
4	G	77	THR
4	G	114	GLN
4	G	120	VAL
4	G	175	LEU
4	G	195	ASN
4	G	201	CYS
4	G	207	LYS
4	G	234	ASN

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Mol	Chain	Res	Type
4	G	246	GLN
4	G	270	VAL
4	G	272	ILE
4	G	286	VAL
4	G	290	THR
4	G	292	VAL
4	G	320	LEU
4	G	328	GLN
4	G	388	SER
4	G	424	ILE
4	G	428	GLN
4	G	432	GLN
4	G	440	GLN
4	G	444	ARG
4	G	449	ILE
4	G	456	ARG
4	G	465	THR
4	G	479	TRP
4	G	496	VAL
5	H	11	LEU
5	H	24	VAL
5	H	57	THR
5	H	62	SER
5	H	63	LEU
5	H	64	LYS
5	H	75	LYS
5	H	78	LEU
5	H	80	LEU
5	H	100(I)	GLU
5	H	100(P)	MET
5	H	139	LEU
5	H	159	SER
5	H	162	HIS
5	H	182	VAL
5	H	187	LEU
5	H	189	THR
5	H	190	GLN
5	H	203	THR
5	H	207	LYS
5	H	209	VAL
6	L	11	LEU
6	L	25	ARG

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Mol	Chain	Res	Type
6	L	34	GLN
6	L	52	GLN
6	L	97	SER
6	L	146	THR
6	L	154	SER
6	L	182	THR
6	L	195	GLN
6	L	202	THR
6	L	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	428	GLN
6	L	34	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	A	1	7,4	14,14,15	0.26	0	17,19,21	0.50	0
7	NAG	A	2	7	14,14,15	0.25	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	A	3	7	11,11,12	1.09	1 (9%)	15,15,17	1.16	2 (13%)
7	MAN	A	4	7	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
8	NAG	C	1	8,4	14,14,15	0.94	1 (7%)	17,19,21	1.66	1 (5%)
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	F	1	8,4	14,14,15	0.25	0	17,19,21	0.44	0
8	NAG	F	2	8	14,14,15	0.27	0	17,19,21	0.38	0
8	NAG	I	1	8,4	14,14,15	0.30	0	17,19,21	0.45	0
8	NAG	I	2	8	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	J	1	8,4	14,14,15	0.29	0	17,19,21	0.48	0
8	NAG	J	2	8	14,14,15	0.27	0	17,19,21	0.37	0
8	NAG	K	1	8,4	14,14,15	0.21	0	17,19,21	0.48	0
8	NAG	K	2	8	14,14,15	0.24	0	17,19,21	0.47	0
9	NAG	M	1	9,4	14,14,15	0.25	0	17,19,21	0.41	0
9	NAG	M	2	9	14,14,15	0.22	0	17,19,21	0.37	0
9	BMA	M	3	9	11,11,12	0.76	0	15,15,17	0.88	0
9	MAN	M	4	9	11,11,12	0.84	1 (9%)	15,15,17	1.24	2 (13%)
9	MAN	M	5	9	11,11,12	0.78	1 (9%)	15,15,17	1.19	2 (13%)
10	NAG	N	1	10,4	14,14,15	0.33	0	17,19,21	0.45	0
10	NAG	N	2	10	14,14,15	0.21	0	17,19,21	0.50	0
10	BMA	N	3	10	11,11,12	0.66	0	15,15,17	0.78	0
10	MAN	N	4	10	11,11,12	1.08	1 (9%)	15,15,17	1.57	4 (26%)
11	NAG	O	1	11,4	14,14,15	0.30	0	17,19,21	0.44	0
11	NAG	O	2	11	14,14,15	0.43	0	17,19,21	1.28	1 (5%)
11	BMA	O	3	11	11,11,12	0.64	0	15,15,17	0.72	0
11	MAN	O	4	11	11,11,12	1.14	1 (9%)	15,15,17	1.33	3 (20%)
11	MAN	O	5	11	11,11,12	1.56	1 (9%)	15,15,17	1.79	3 (20%)
11	MAN	O	6	11	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
12	NAG	P	1	12,4	14,14,15	0.36	0	17,19,21	1.47	2 (11%)
12	MAN	P	10	12	11,11,12	0.97	0	15,15,17	1.14	1 (6%)
12	NAG	P	2	12	14,14,15	0.25	0	17,19,21	0.47	0
12	BMA	P	3	12	11,11,12	0.95	1 (9%)	15,15,17	0.87	0
12	MAN	P	4	12	11,11,12	0.76	1 (9%)	15,15,17	1.44	2 (13%)
12	MAN	P	5	12	11,11,12	0.85	0	15,15,17	1.12	2 (13%)
12	MAN	P	6	12	11,11,12	0.79	0	15,15,17	0.86	1 (6%)
12	MAN	P	7	12	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
12	MAN	P	8	12	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
12	MAN	P	9	12	11,11,12	0.78	1 (9%)	15,15,17	1.30	2 (13%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	4/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	NAG	I	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	NAG	K	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
9	NAG	M	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	2/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	2/2/19/22	0/1/1/1
10	NAG	N	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	1/6/23/26	0/1/1/1
10	BMA	N	3	10	-	0/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
11	NAG	O	1	11,4	-	0/6/23/26	0/1/1/1
11	NAG	O	2	11	-	5/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	2/2/19/22	0/1/1/1
11	MAN	O	5	11	-	1/2/19/22	0/1/1/1
11	MAN	O	6	11	-	0/2/19/22	0/1/1/1
12	NAG	P	1	12,4	-	3/6/23/26	0/1/1/1
12	MAN	P	10	12	-	2/2/19/22	0/1/1/1
12	NAG	P	2	12	-	2/6/23/26	0/1/1/1
12	BMA	P	3	12	-	0/2/19/22	0/1/1/1
12	MAN	P	4	12	-	2/2/19/22	0/1/1/1
12	MAN	P	5	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	P	6	12	-	0/2/19/22	0/1/1/1
12	MAN	P	7	12	-	0/2/19/22	0/1/1/1
12	MAN	P	8	12	-	2/2/19/22	0/1/1/1
12	MAN	P	9	12	-	2/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	5	MAN	C1-C2	4.35	1.62	1.52
8	C	1	NAG	O5-C1	3.38	1.49	1.43
10	N	4	MAN	C1-C2	2.97	1.59	1.52
11	O	4	MAN	O5-C1	-2.58	1.39	1.43
9	M	4	MAN	C1-C2	2.44	1.57	1.52
12	P	9	MAN	C1-C2	2.29	1.57	1.52
9	M	5	MAN	C1-C2	2.27	1.57	1.52
12	P	4	MAN	C1-C2	2.05	1.56	1.52
7	A	3	BMA	C4-C3	2.04	1.57	1.52
12	P	3	BMA	O5-C1	-2.04	1.40	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	NAG	C1-O5-C5	6.44	120.92	112.19
12	P	1	NAG	C2-N2-C7	4.59	129.43	122.90
11	O	2	NAG	C2-N2-C7	4.31	129.04	122.90
11	O	5	MAN	C1-C2-C3	4.17	114.80	109.67
11	O	5	MAN	C1-O5-C5	4.00	117.61	112.19
12	P	4	MAN	C1-O5-C5	3.99	117.59	112.19
12	P	9	MAN	C1-O5-C5	3.74	117.27	112.19
10	N	4	MAN	C1-O5-C5	3.63	117.11	112.19
11	O	4	MAN	C3-C4-C5	2.92	115.45	110.24
9	M	5	MAN	C1-O5-C5	2.90	116.12	112.19
12	P	8	MAN	C1-O5-C5	2.78	115.96	112.19
10	N	4	MAN	C1-C2-C3	2.77	113.07	109.67
9	M	4	MAN	C1-O5-C5	2.71	115.86	112.19
7	A	4	MAN	C1-O5-C5	2.66	115.80	112.19
7	A	3	BMA	C2-C3-C4	2.53	115.27	110.89
12	P	1	NAG	C1-C2-N2	2.50	114.76	110.49
12	P	5	MAN	O2-C2-C3	-2.49	105.16	110.14
12	P	4	MAN	O2-C2-C3	-2.43	105.27	110.14
11	O	6	MAN	C1-O5-C5	2.34	115.36	112.19
10	N	4	MAN	O5-C1-C2	2.32	114.36	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	4	MAN	O2-C2-C3	-2.29	105.54	110.14
12	P	7	MAN	C1-O5-C5	2.29	115.30	112.19
12	P	10	MAN	O2-C2-C3	-2.28	105.57	110.14
11	O	5	MAN	O2-C2-C3	-2.28	105.58	110.14
7	A	4	MAN	O2-C2-C3	-2.25	105.62	110.14
12	P	9	MAN	O2-C2-C3	-2.25	105.64	110.14
11	O	6	MAN	O2-C2-C3	-2.21	105.70	110.14
10	N	4	MAN	O2-C2-C3	-2.19	105.74	110.14
12	P	7	MAN	O2-C2-C3	-2.18	105.77	110.14
9	M	5	MAN	O2-C2-C3	-2.17	105.80	110.14
7	A	3	BMA	C3-C4-C5	2.13	114.05	110.24
9	M	4	MAN	O2-C2-C3	-2.13	105.88	110.14
12	P	5	MAN	C1-C2-C3	2.06	112.20	109.67
12	P	6	MAN	O2-C2-C3	-2.04	106.05	110.14
11	O	4	MAN	C2-C3-C4	2.03	114.41	110.89

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	O	2	NAG	O5-C5-C6-O6
8	K	2	NAG	O5-C5-C6-O6
11	O	3	BMA	O5-C5-C6-O6
9	M	3	BMA	C4-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
8	K	2	NAG	C4-C5-C6-O6
11	O	2	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	J	1	NAG	O5-C5-C6-O6
11	O	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
9	M	3	BMA	O5-C5-C6-O6
8	J	1	NAG	C4-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
12	P	4	MAN	O5-C5-C6-O6
8	C	1	NAG	C8-C7-N2-C2
8	C	1	NAG	O7-C7-N2-C2
11	O	2	NAG	C8-C7-N2-C2
11	O	2	NAG	O7-C7-N2-C2
12	P	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	P	1	NAG	O7-C7-N2-C2
7	A	4	MAN	C4-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
12	P	4	MAN	C4-C5-C6-O6
9	M	5	MAN	C4-C5-C6-O6
11	O	4	MAN	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
9	M	5	MAN	O5-C5-C6-O6
12	P	10	MAN	C4-C5-C6-O6
12	P	8	MAN	O5-C5-C6-O6
8	K	1	NAG	C4-C5-C6-O6
8	K	1	NAG	O5-C5-C6-O6
12	P	10	MAN	O5-C5-C6-O6
11	O	5	MAN	O5-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
8	F	1	NAG	O5-C5-C6-O6
12	P	9	MAN	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
12	P	8	MAN	C4-C5-C6-O6
11	O	2	NAG	C3-C2-N2-C7
12	P	1	NAG	C3-C2-N2-C7
12	P	9	MAN	O5-C5-C6-O6

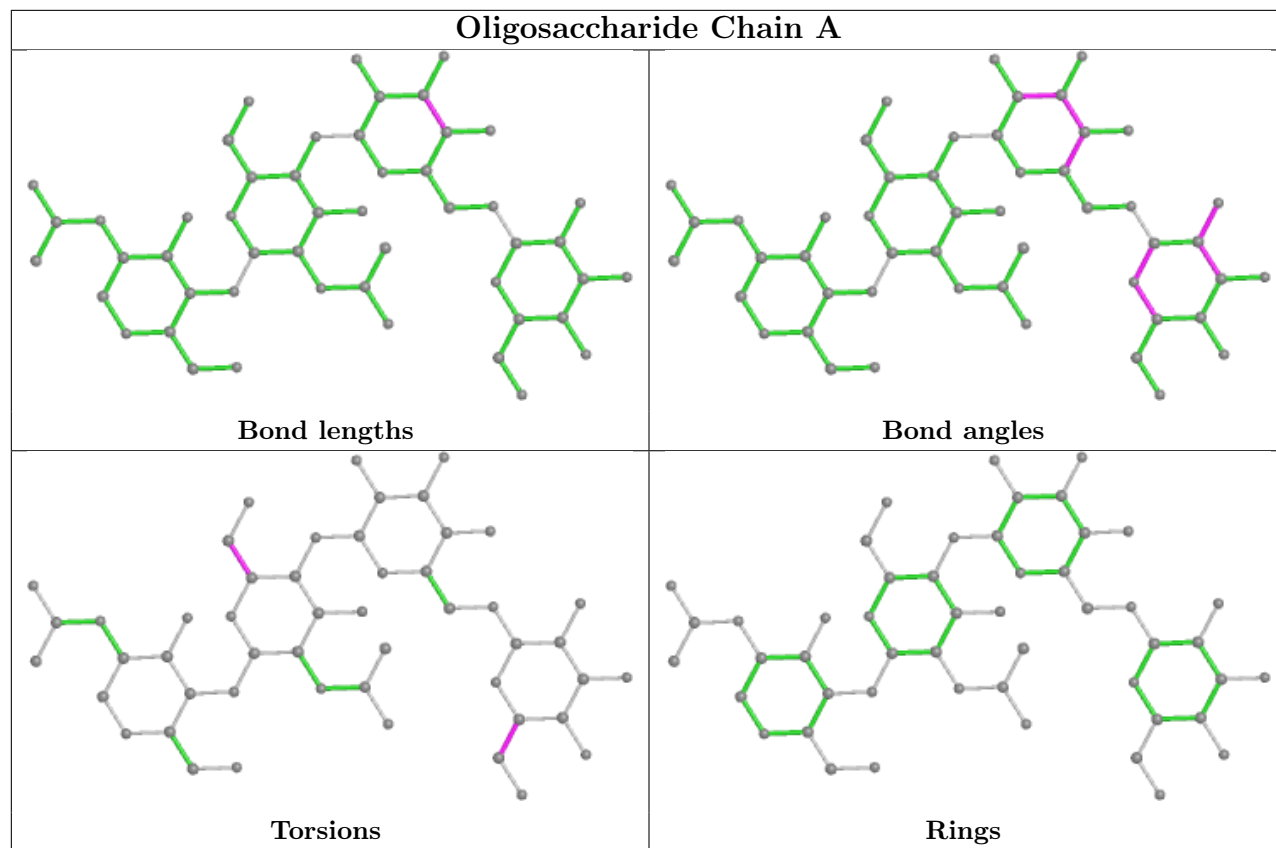
There are no ring outliers.

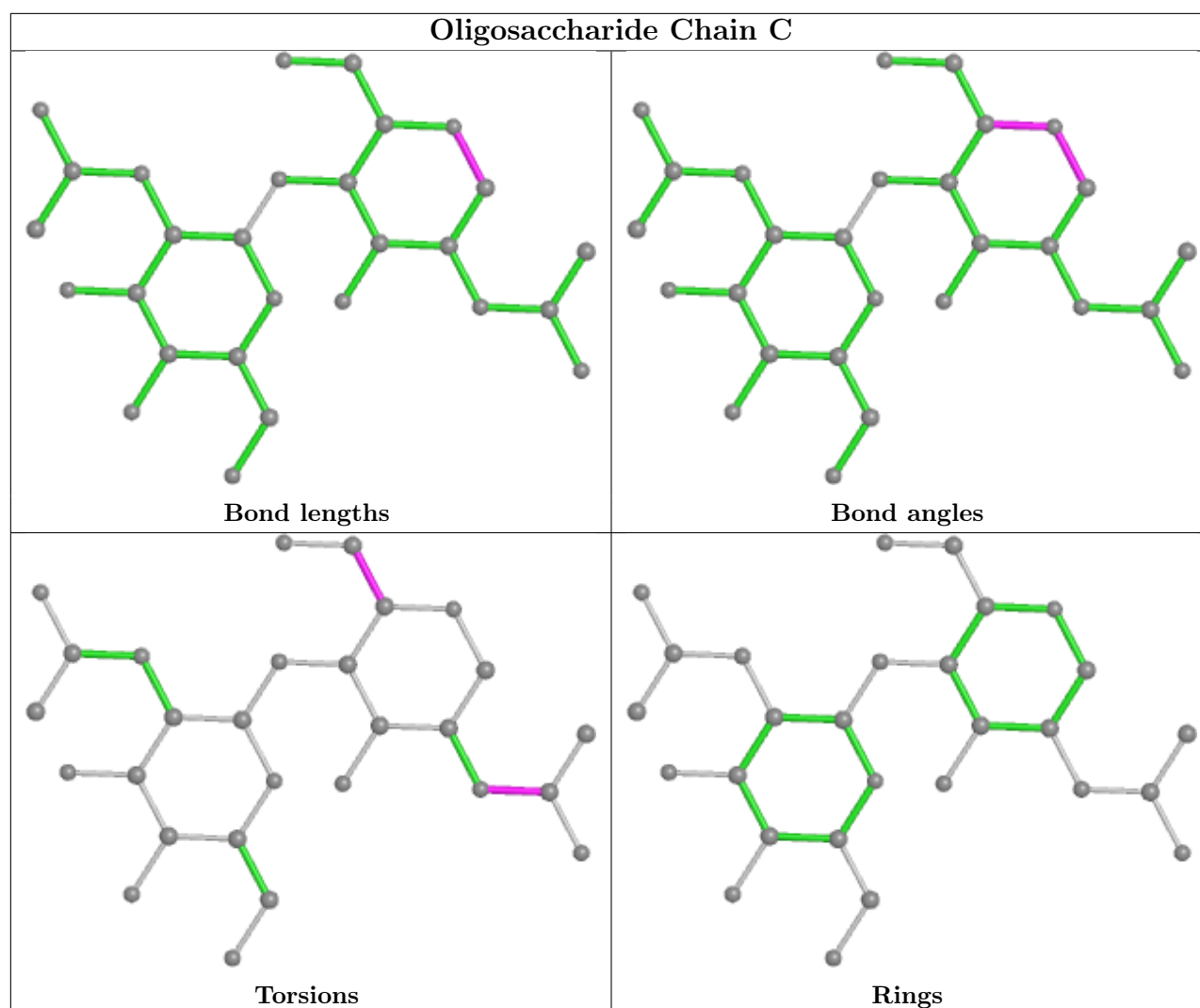
11 monomers are involved in 13 short contacts:

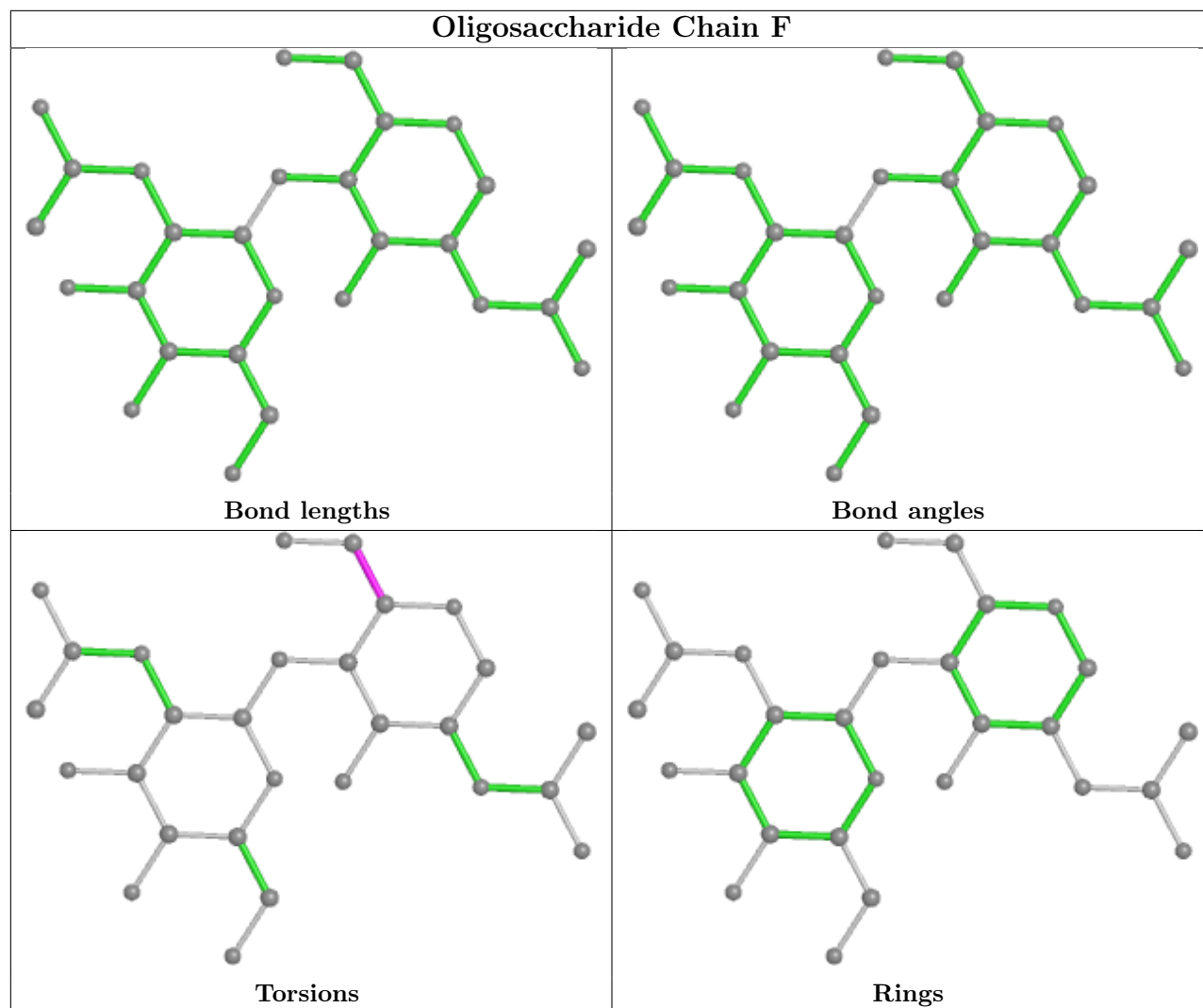
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	9	MAN	1	0
8	I	1	NAG	2	0
11	O	5	MAN	1	0
10	N	1	NAG	1	0
7	A	2	NAG	1	0
11	O	1	NAG	1	0
11	O	4	MAN	4	0
12	P	1	NAG	1	0
12	P	4	MAN	1	0
10	N	2	NAG	1	0
11	O	2	NAG	1	0

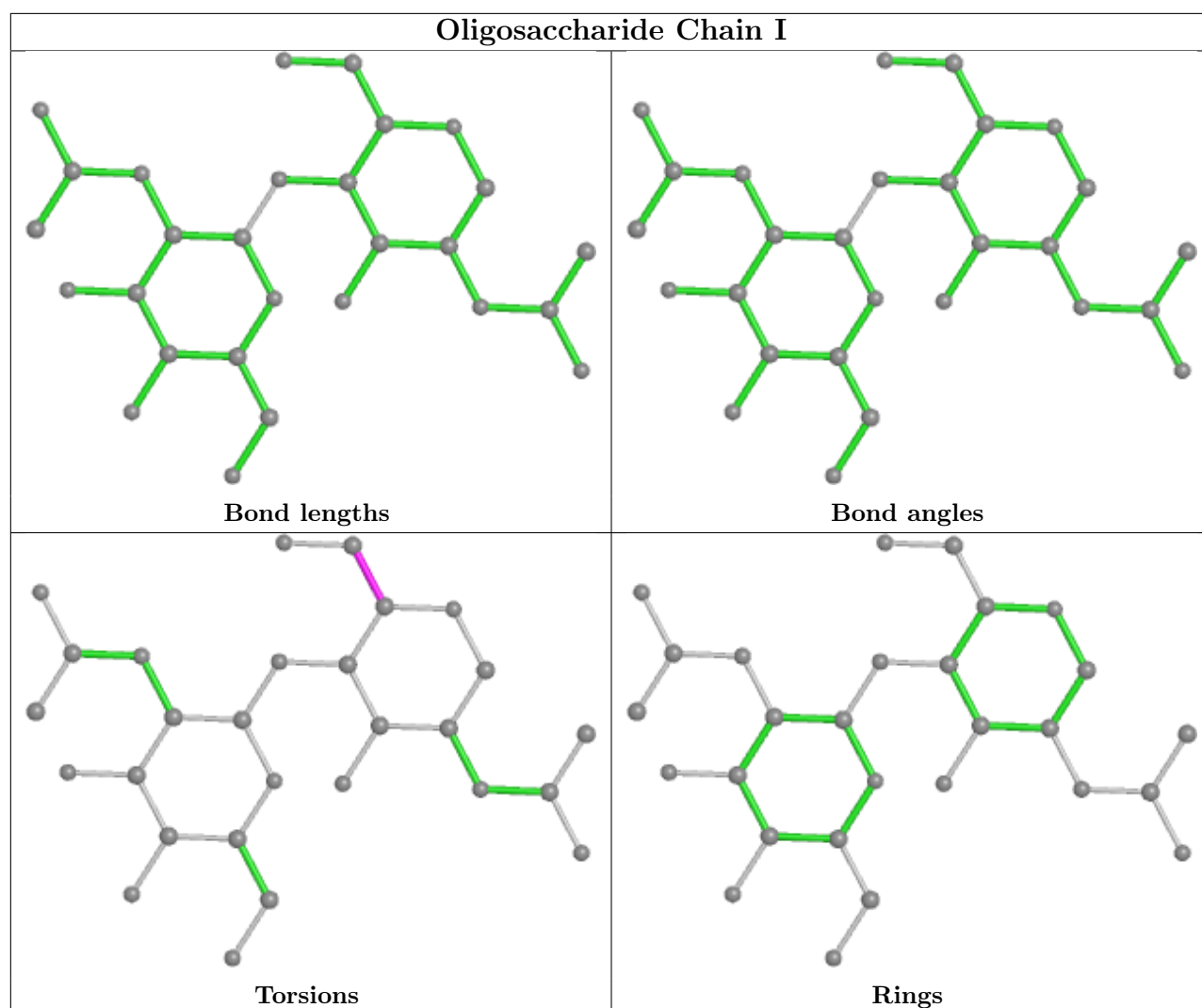
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

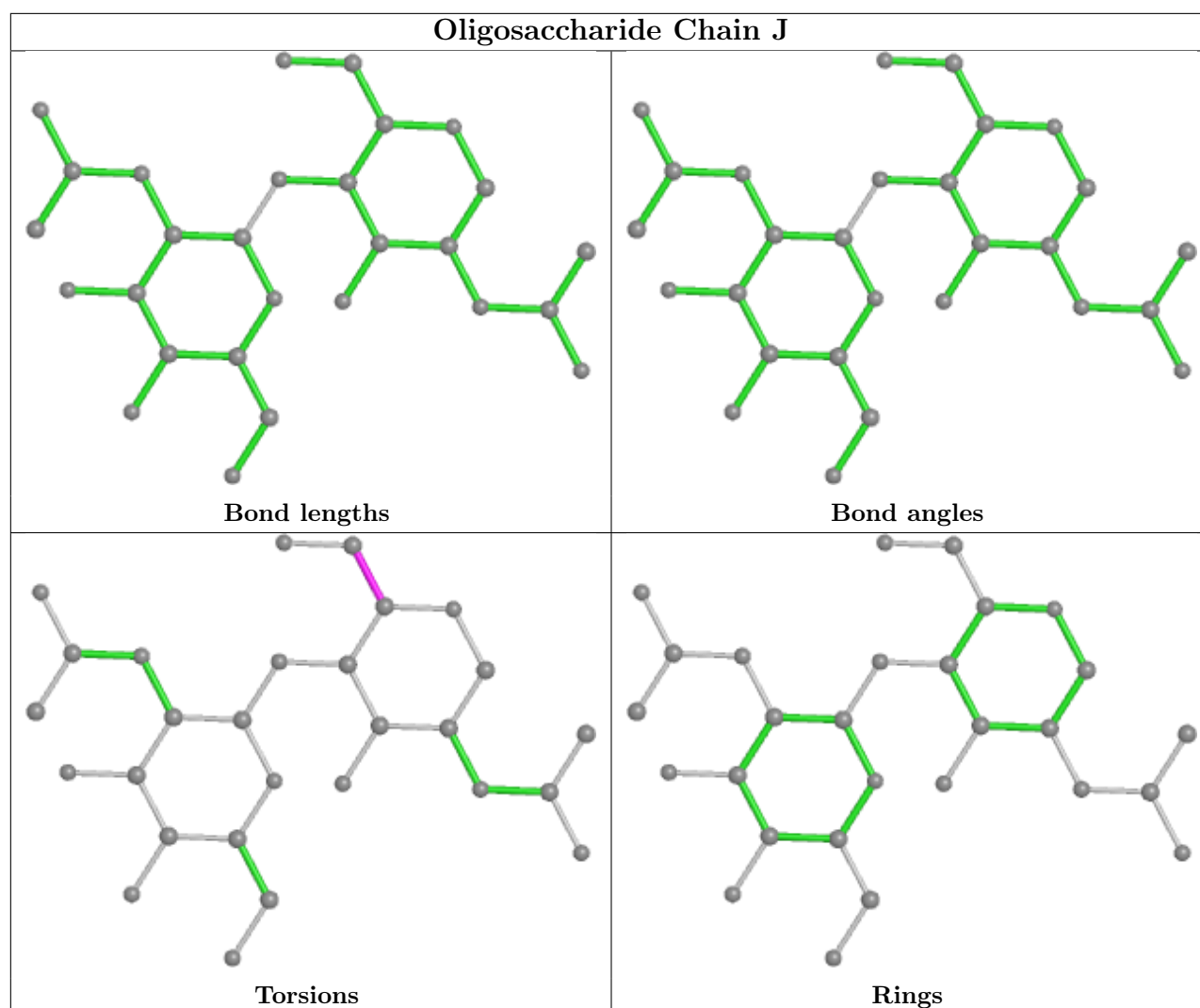


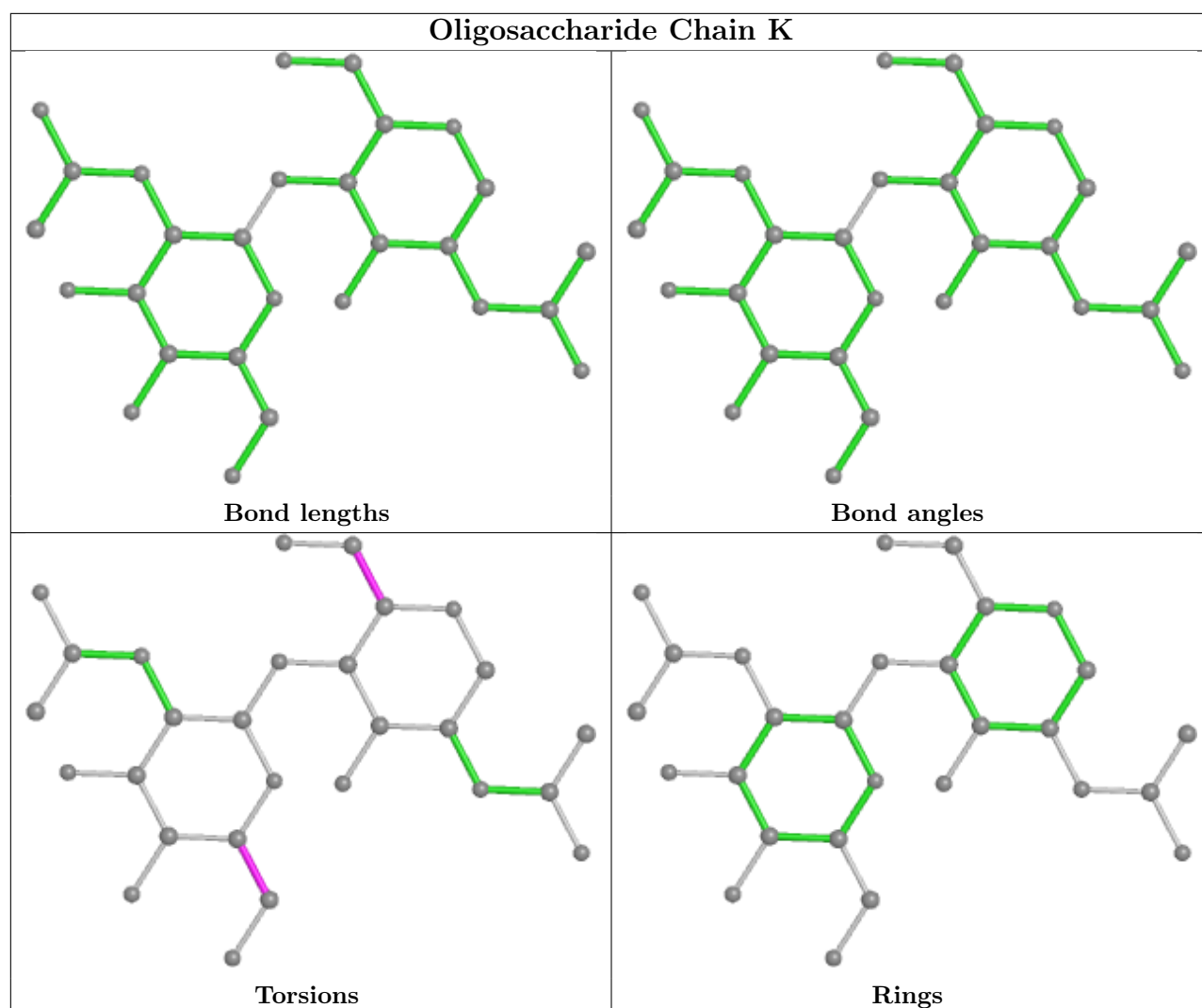




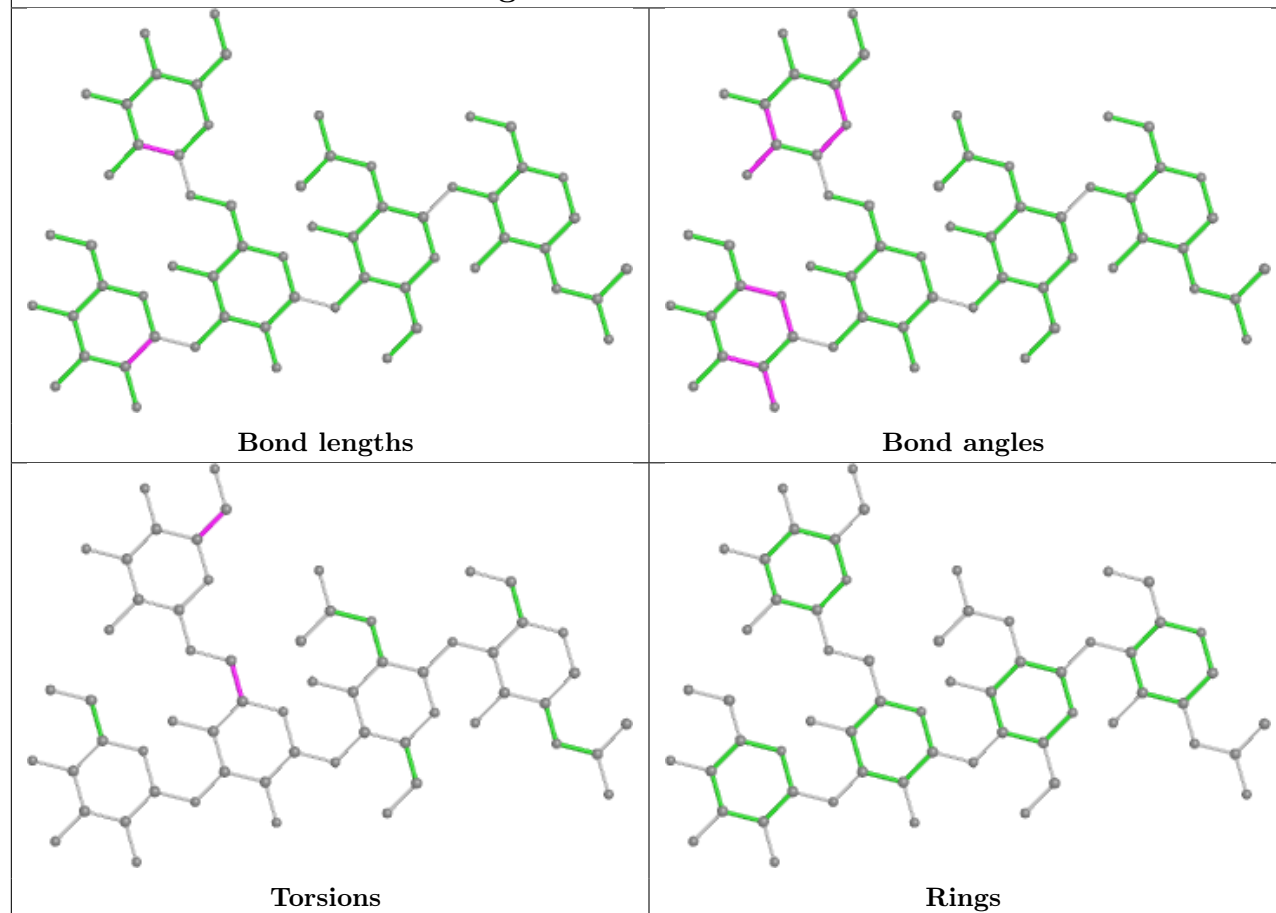




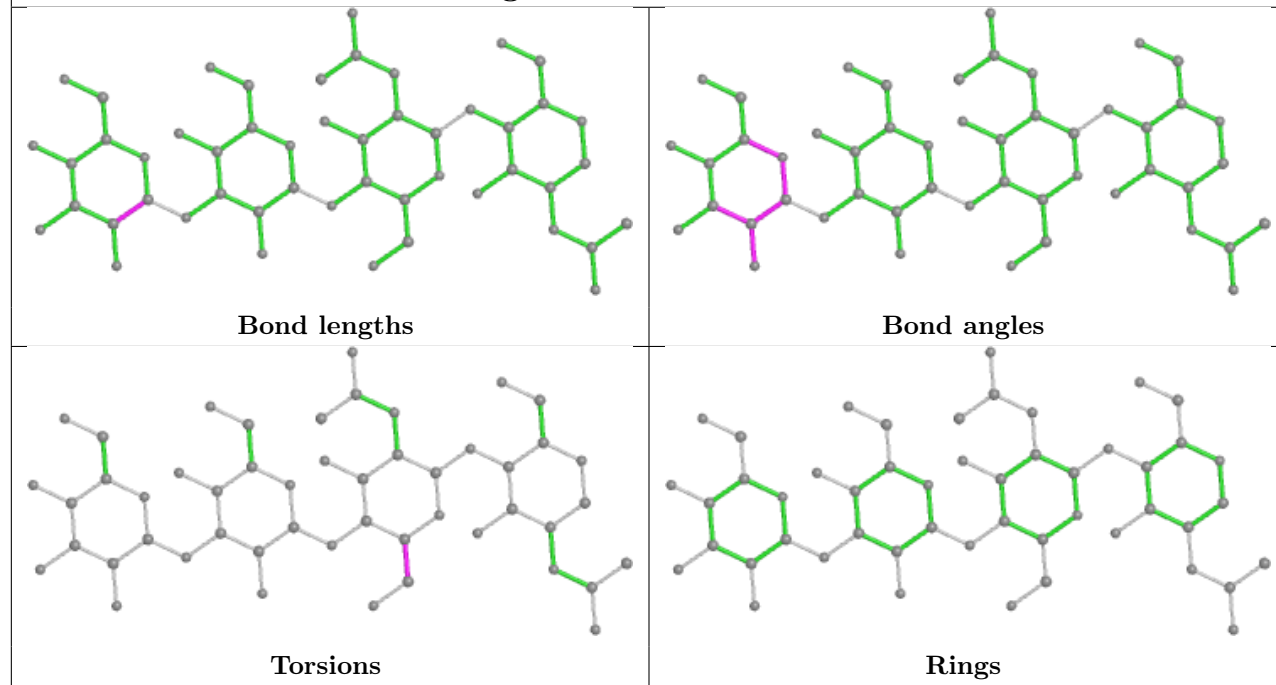


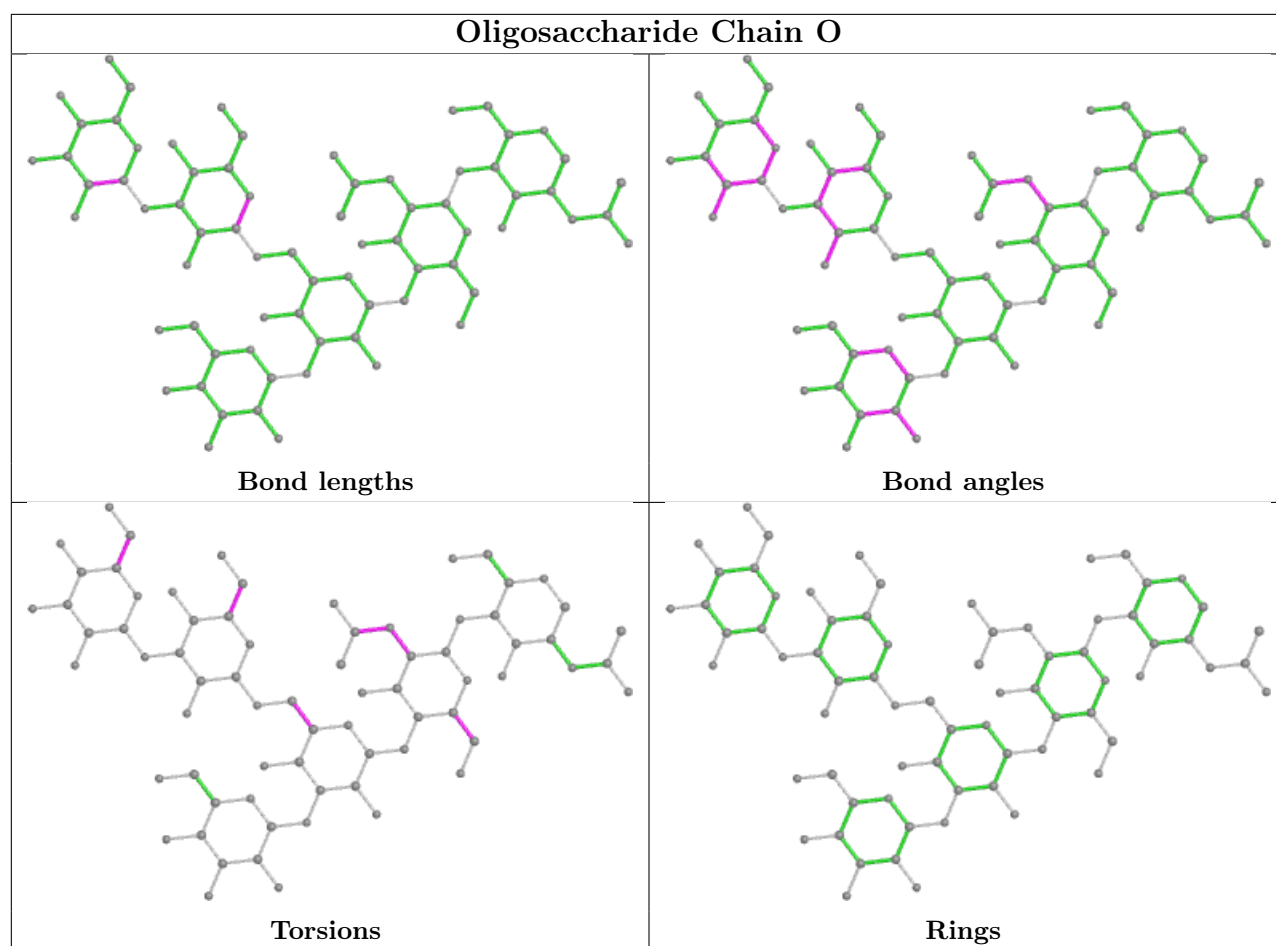


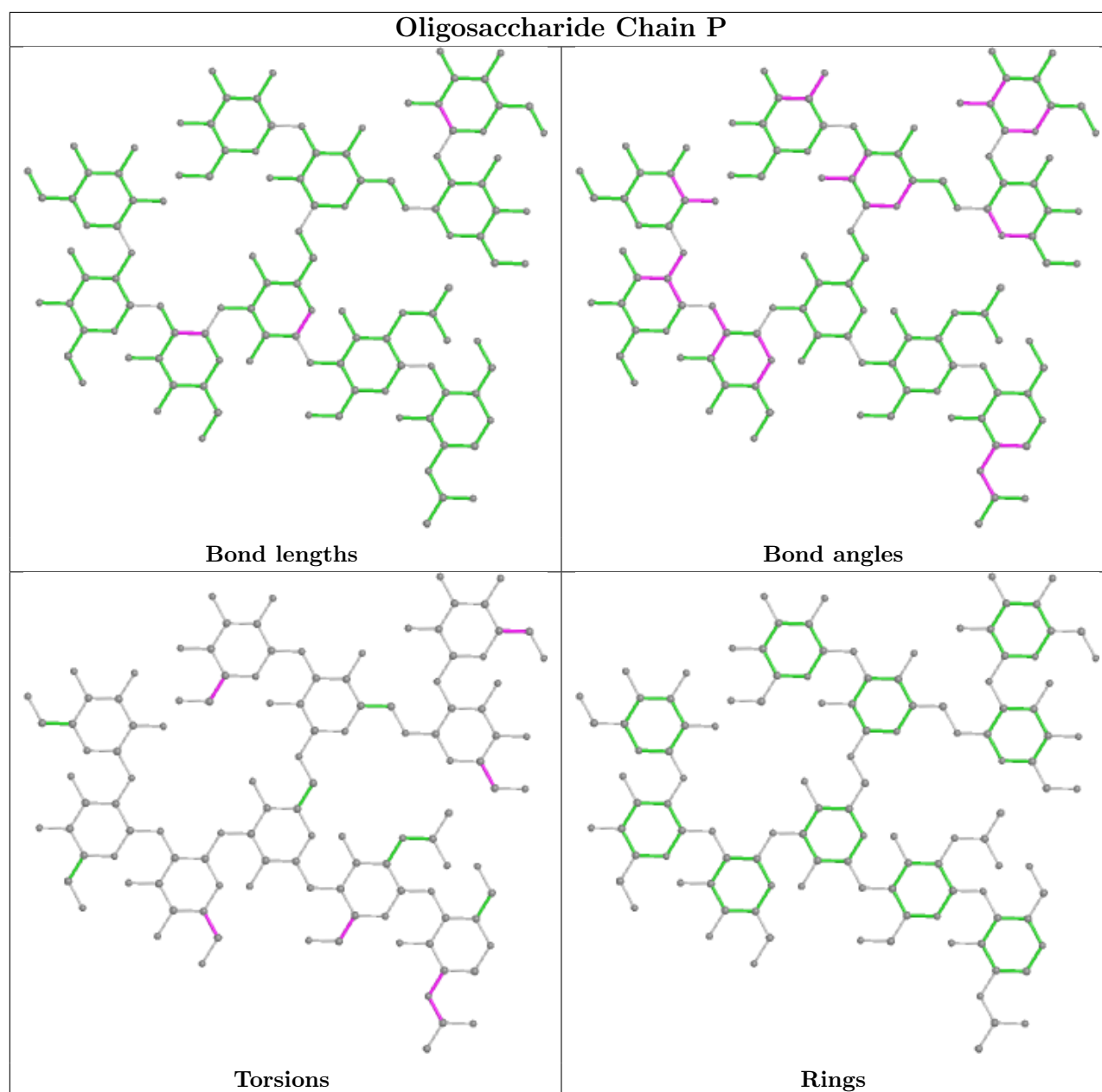
## Oligosaccharide Chain M



## Oligosaccharide Chain N







## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	G	612	4	14,14,15	0.27	0	17,19,21	0.45	0
13	NAG	G	608	4	14,14,15	0.25	0	17,19,21	0.43	0
13	NAG	B	702	1	14,14,15	0.35	0	17,19,21	0.54	0
13	NAG	B	701	1	14,14,15	0.25	0	17,19,21	0.47	0
13	NAG	G	611	4	14,14,15	0.24	0	17,19,21	0.53	0
13	NAG	G	607	4	14,14,15	0.32	0	17,19,21	0.45	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
13	NAG	G	612	4	-	2/6/23/26	0/1/1/1
13	NAG	G	608	4	-	0/6/23/26	0/1/1/1
13	NAG	B	702	1	-	0/6/23/26	0/1/1/1
13	NAG	B	701	1	-	1/6/23/26	0/1/1/1
13	NAG	G	611	4	-	2/6/23/26	0/1/1/1
13	NAG	G	607	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	612	NAG	O5-C5-C6-O6
13	G	611	NAG	O5-C5-C6-O6
13	G	612	NAG	C4-C5-C6-O6
13	G	611	NAG	C4-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6
13	G	607	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	607	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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	B	124/153 (81%)	-0.33	3 (2%) 59 57	15, 36, 71, 112	0
2	D	128/134 (95%)	0.20	7 (5%) 25 24	30, 70, 109, 143	0
3	E	112/114 (98%)	0.23	11 (9%) 7 7	28, 59, 104, 129	0
4	G	427/481 (88%)	-0.34	7 (1%) 72 70	13, 32, 80, 113	0
5	H	227/244 (93%)	-0.16	6 (2%) 56 54	18, 48, 88, 115	0
6	L	211/217 (97%)	-0.58	3 (1%) 75 73	13, 33, 57, 98	0
All	All	1229/1343 (91%)	-0.24	37 (3%) 50 49	13, 41, 94, 143	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	106	VAL	9.6
5	H	126	SER	9.6
2	D	41	ALA	8.3
2	D	67	VAL	5.8
2	D	42	GLY	5.3
3	E	106(A)	LEU	5.0
2	D	18	VAL	4.6
4	G	356	ASN	4.3
4	G	135	THR	4.2
3	E	78	LEU	4.1
5	H	187	LEU	4.0
5	H	189	THR	4.0
1	B	517	ALA	3.9
6	L	6	SER	3.5
4	G	66	HIS	3.4
5	H	185	SER	3.4
4	G	80	ASN	3.4
1	B	518	VAL	3.3
4	G	79	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	E	80	PRO	3.1
3	E	79	ARG	3.1
3	E	0	SER	3.1
3	E	105	SER	3.0
5	H	204	LYS	2.9
3	E	7	SER	2.9
2	D	43	ARG	2.8
6	L	67(A)	ILE	2.8
3	E	107	GLY	2.7
6	L	7	TYR	2.7
4	G	465	THR	2.6
4	G	151	ARG	2.6
3	E	76	SER	2.5
5	H	183	PRO	2.5
2	D	59	LEU	2.1
2	D	71	THR	2.0
3	E	1	GLN	2.0
1	B	519	PHE	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
9	BMA	M	3	11/12	0.73	0.30	122,132,140,143	0
10	BMA	N	3	11/12	0.78	0.42	112,153,161,162	0
8	NAG	J	2	14/15	0.83	0.22	56,106,115,119	0
10	MAN	N	4	11/12	0.83	0.42	135,141,153,155	0
8	NAG	J	1	14/15	0.84	0.18	63,91,111,122	0
8	NAG	K	1	14/15	0.84	0.17	77,93,103,108	0
8	NAG	K	2	14/15	0.84	0.43	51,121,147,158	0
7	BMA	A	3	11/12	0.86	0.14	60,80,106,108	0
10	NAG	N	2	14/15	0.86	0.23	53,93,130,139	0
7	MAN	A	4	11/12	0.88	0.18	76,98,109,118	0

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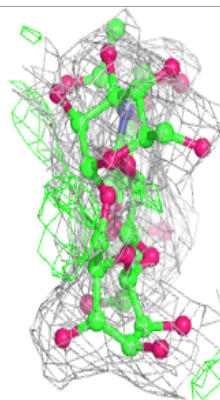
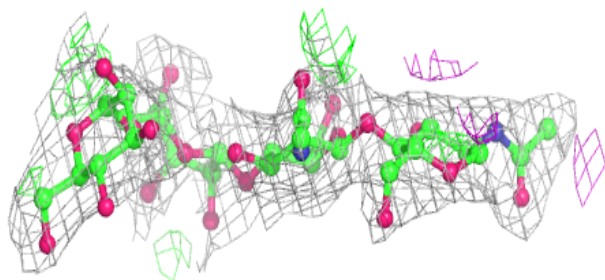
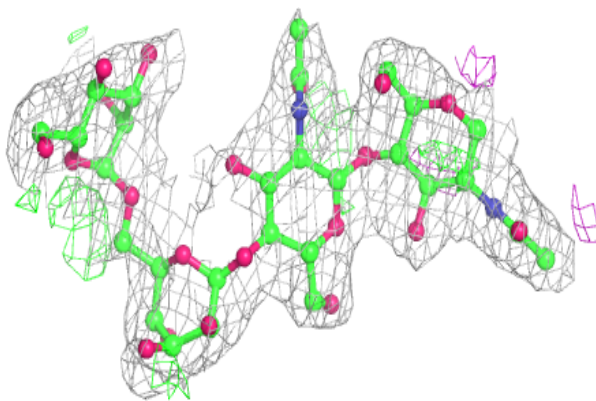
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MAN	M	4	11/12	0.88	0.53	109,134,150,152	0
9	MAN	M	5	11/12	0.88	0.37	70,113,138,140	0
12	MAN	P	9	11/12	0.89	0.31	65,86,98,111	0
12	MAN	P	8	11/12	0.90	0.13	39,54,68,79	0
9	NAG	M	2	14/15	0.91	0.28	70,100,122,129	0
8	NAG	C	2	14/15	0.91	0.20	77,93,112,116	0
8	NAG	I	2	14/15	0.91	0.19	79,102,118,128	0
11	MAN	O	4	11/12	0.92	0.15	58,75,99,112	0
11	MAN	O	5	11/12	0.92	0.16	63,76,97,99	0
12	NAG	P	1	14/15	0.92	0.13	25,35,55,58	0
9	NAG	M	1	14/15	0.92	0.16	19,58,87,95	0
8	NAG	F	2	14/15	0.92	0.16	67,92,115,122	0
12	BMA	P	3	11/12	0.93	0.12	31,42,53,54	0
12	MAN	P	5	11/12	0.93	0.14	24,32,41,43	0
7	NAG	A	2	14/15	0.93	0.12	48,65,82,86	0
12	NAG	P	2	14/15	0.93	0.13	31,47,56,60	0
8	NAG	C	1	14/15	0.94	0.10	34,57,79,98	0
8	NAG	F	1	14/15	0.94	0.11	24,40,67,96	0
12	MAN	P	10	11/12	0.94	0.17	43,61,86,87	0
12	MAN	P	6	11/12	0.95	0.20	30,46,60,61	0
12	MAN	P	7	11/12	0.95	0.11	38,50,59,69	0
8	NAG	I	1	14/15	0.95	0.11	48,69,84,96	0
11	NAG	O	1	14/15	0.95	0.14	20,27,38,46	0
11	BMA	O	3	11/12	0.95	0.10	30,37,49,73	0
11	NAG	O	2	14/15	0.96	0.09	28,32,44,45	0
10	NAG	N	1	14/15	0.96	0.11	29,41,54,72	0
11	MAN	O	6	11/12	0.96	0.10	24,41,54,54	0
7	NAG	A	1	14/15	0.97	0.13	12,28,58,58	0
12	MAN	P	4	11/12	0.97	0.10	10,21,31,47	0

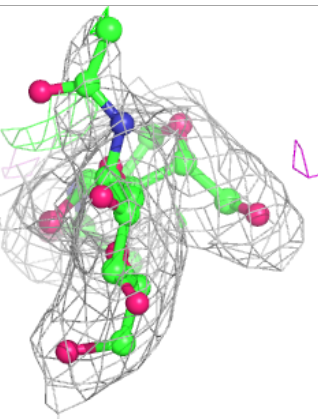
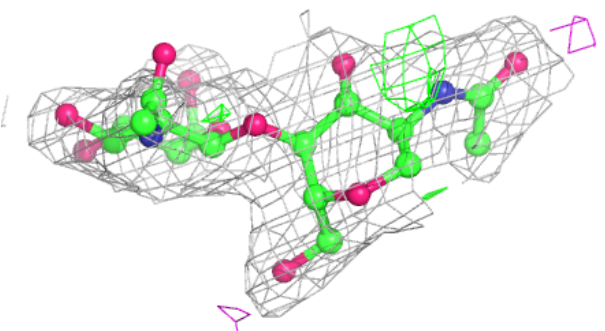
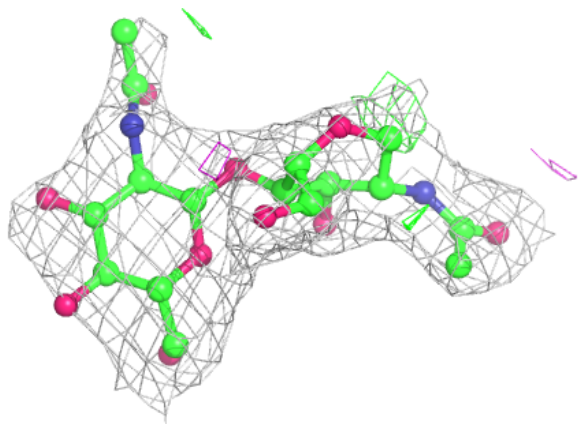
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain A:**

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

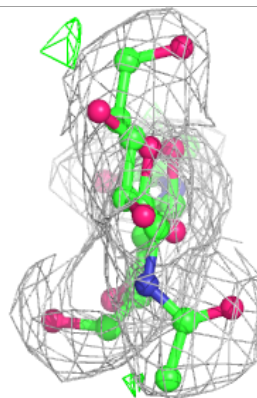
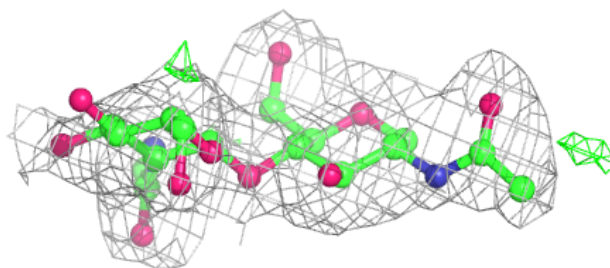
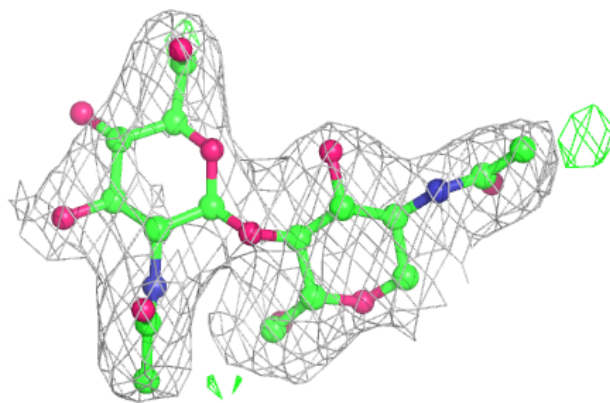
**Electron density around Chain C:**

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



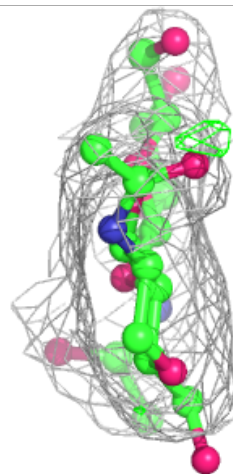
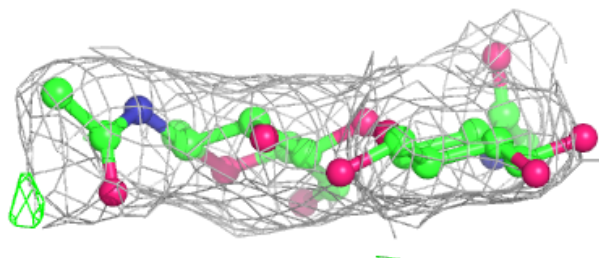
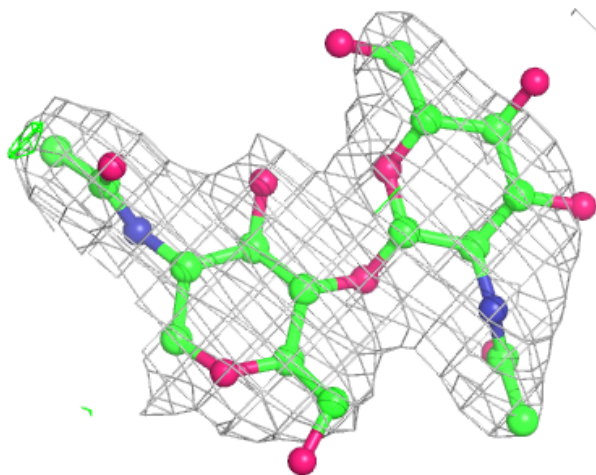
**Electron density around Chain F:**

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



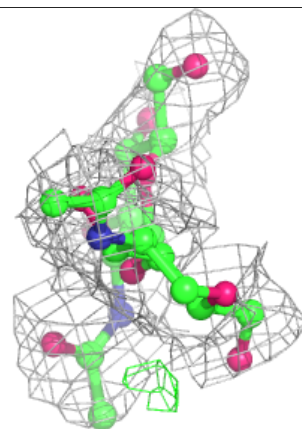
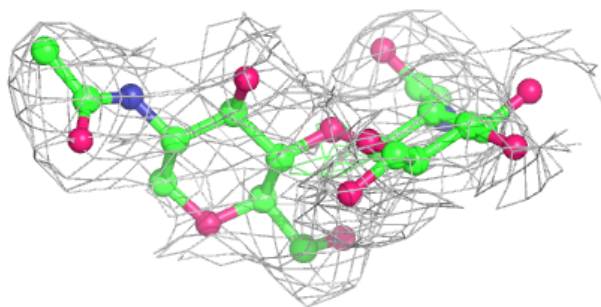
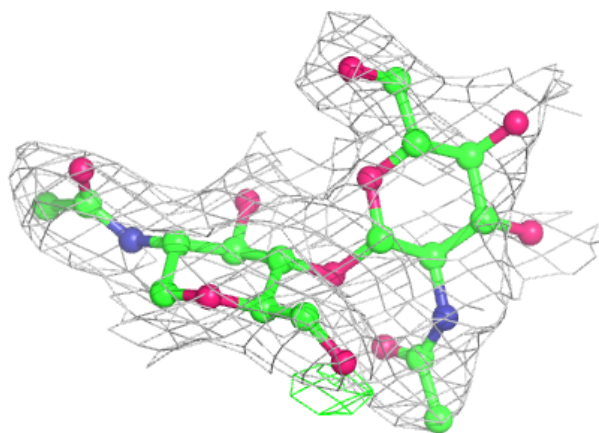
**Electron density around Chain I:**

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



**Electron density around Chain J:**

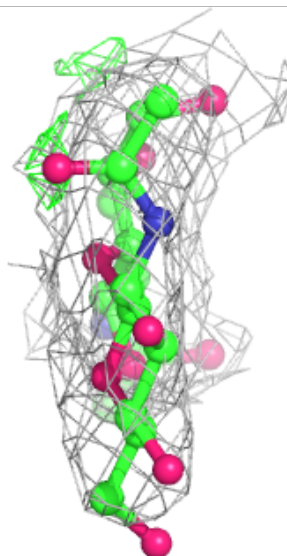
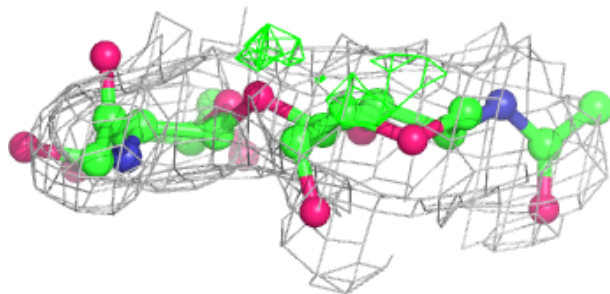
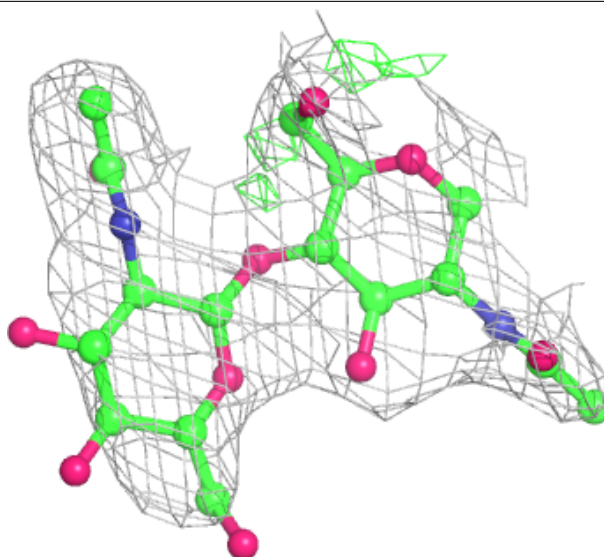
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





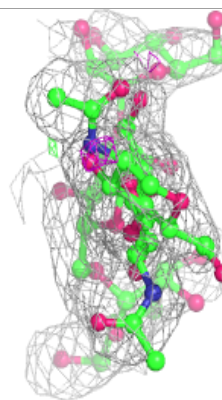
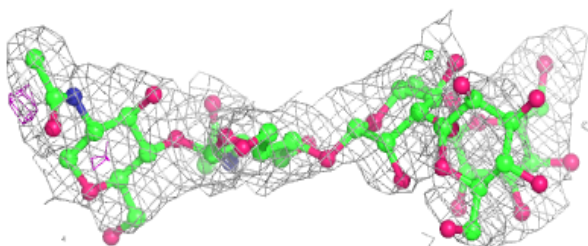
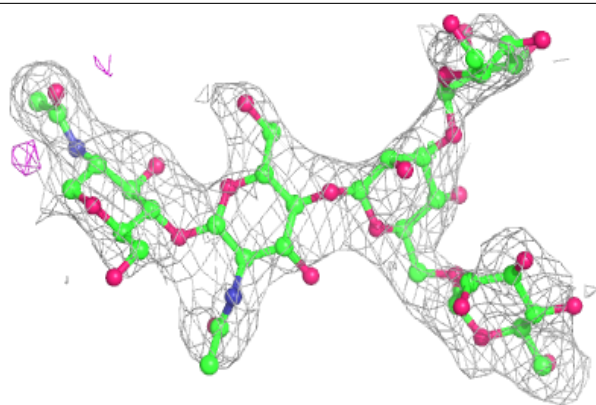
**Electron density around Chain K:**

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

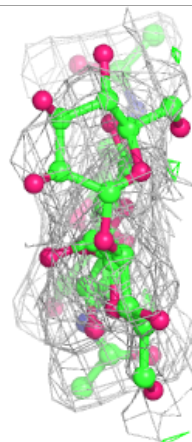
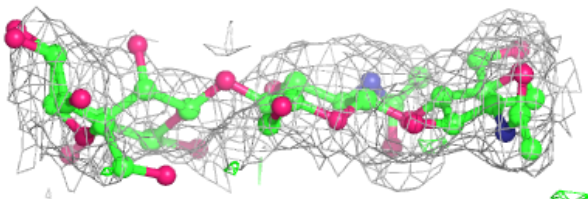
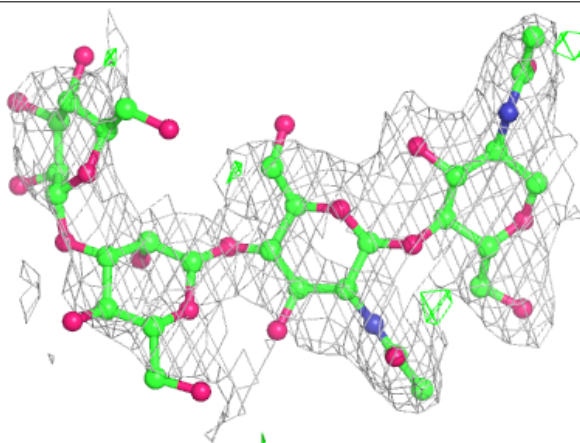


**Electron density around Chain M:**

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

**Electron density around Chain N:**

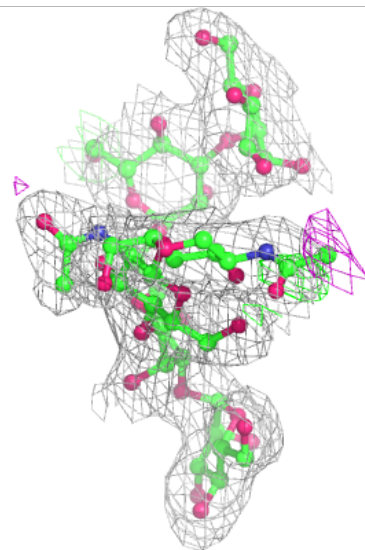
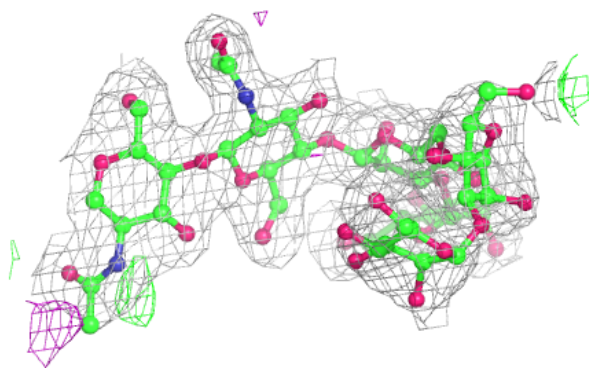
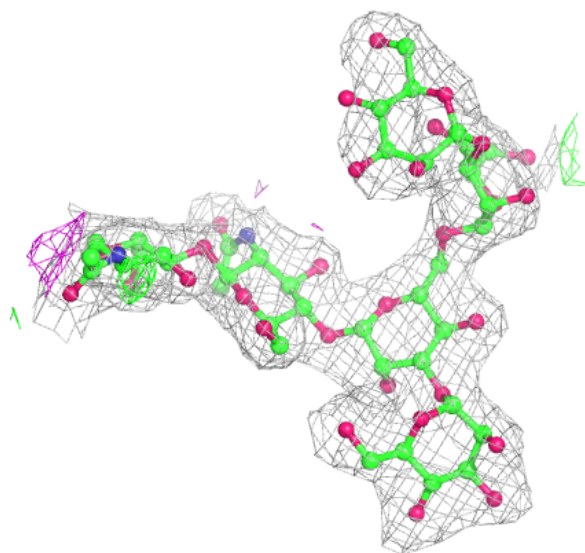
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

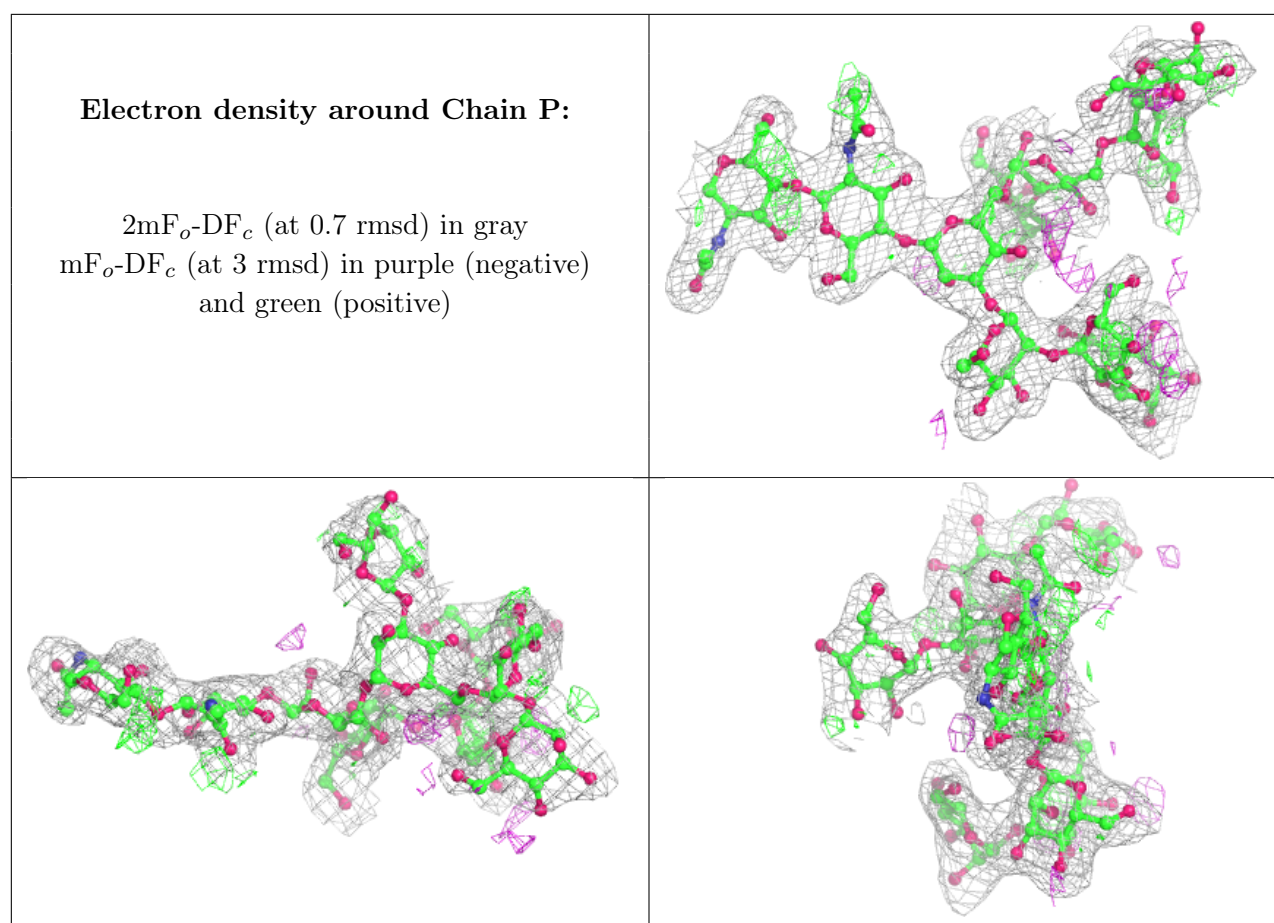




**Electron density around Chain O:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
13	NAG	B	701	14/15	0.89	0.33	90,99,118,128	0
13	NAG	B	702	14/15	0.90	0.33	85,105,120,125	0
13	NAG	G	612	14/15	0.90	0.21	47,76,87,96	0
13	NAG	G	608	14/15	0.91	0.23	48,68,80,81	0
13	NAG	G	611	14/15	0.93	0.13	36,54,69,70	0
13	NAG	G	607	14/15	0.93	0.17	34,63,98,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.