



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:40 AM UTC

PDB ID : 2BF1 / pdb\_00002bf1  
Title : Structure of an unliganded and fully-glycosylated SIV gp120 envelope glycoprotein  
Authors : Chen, B.; Vogan, E.M.; Gong, H.; Skehel, J.J.; Wiley, D.C.; Harrison, S.C.  
Deposited on : 2004-12-02  
Resolution : 4.00 Å (reported)

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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.

The types of validation reports are described at

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

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

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

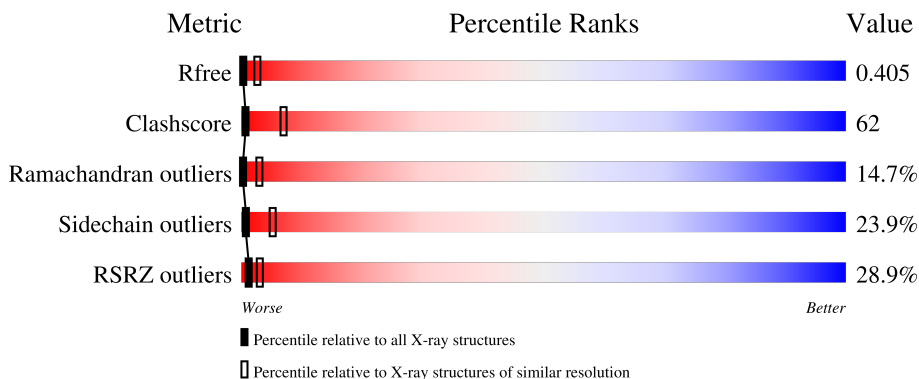
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

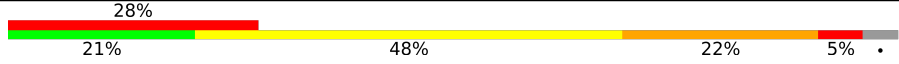

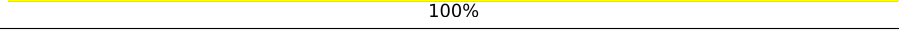
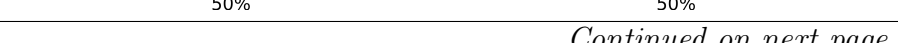
The reported resolution of this entry is 4.00 Å.

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




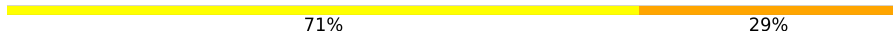
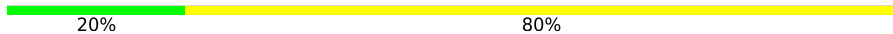
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	316	
2	B	4	
2	F	4	
2	H	4	
3	C	6	

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Mol	Chain	Length	Quality of chain
3	K	6	
4	D	3	
4	E	3	
5	G	2	
6	I	7	
7	J	5	
8	L	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	X	-	-	-
2	FUC	B	4	X	-	-	-
2	FUC	F	4	X	-	-	-
2	NAG	H	1	X	-	-	-
2	FUC	H	4	X	-	-	-
3	NAG	C	2	-	-	-	X
3	FUC	C	6	X	-	-	-
3	NAG	K	1	X	-	-	-
3	FUC	K	6	X	-	-	-
4	NAG	D	1	X	-	-	-
4	FUC	D	3	X	-	-	-
4	NAG	E	1	X	-	-	-
4	FUC	E	3	X	-	-	-
5	NAG	G	1	X	-	-	-
6	NAG	I	1	X	-	-	X
8	NAG	L	1	X	-	-	-

## 2 Entry composition [i](#)

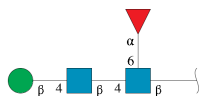
There are 9 unique types of molecules in this entry. The entry contains 3085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EXTERIOR MEMBRANE GLYCOPROTEIN GP120.

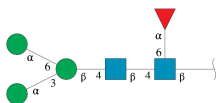
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2470	1556	436	455	23	0	0	0

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



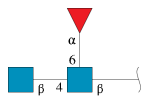
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	49	28	2	19	0	0	0
2	F	4	49	28	2	19	0	0	0
2	H	4	49	28	2	19	0	0	0

- Molecule 3 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	71	40	2	29	0	0	0
3	K	6	71	40	2	29	0	0	0

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



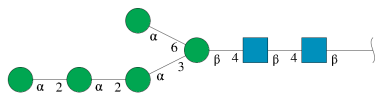
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0
4	E	3	38	22	2	14	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



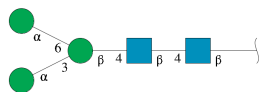
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	2	28	16	2	10	0	0	0

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



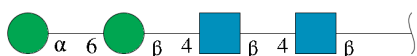
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	I	7	83	46	2	35	0	0	0

- Molecule 7 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.



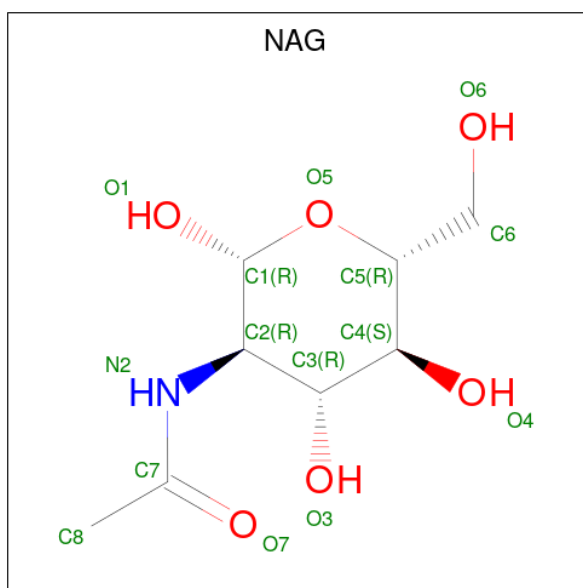
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	J	5	61	34	2	25	0	0	0

- Molecule 8 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
			Total	C	N	O			
8	L	4	50	28	2	20	0	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

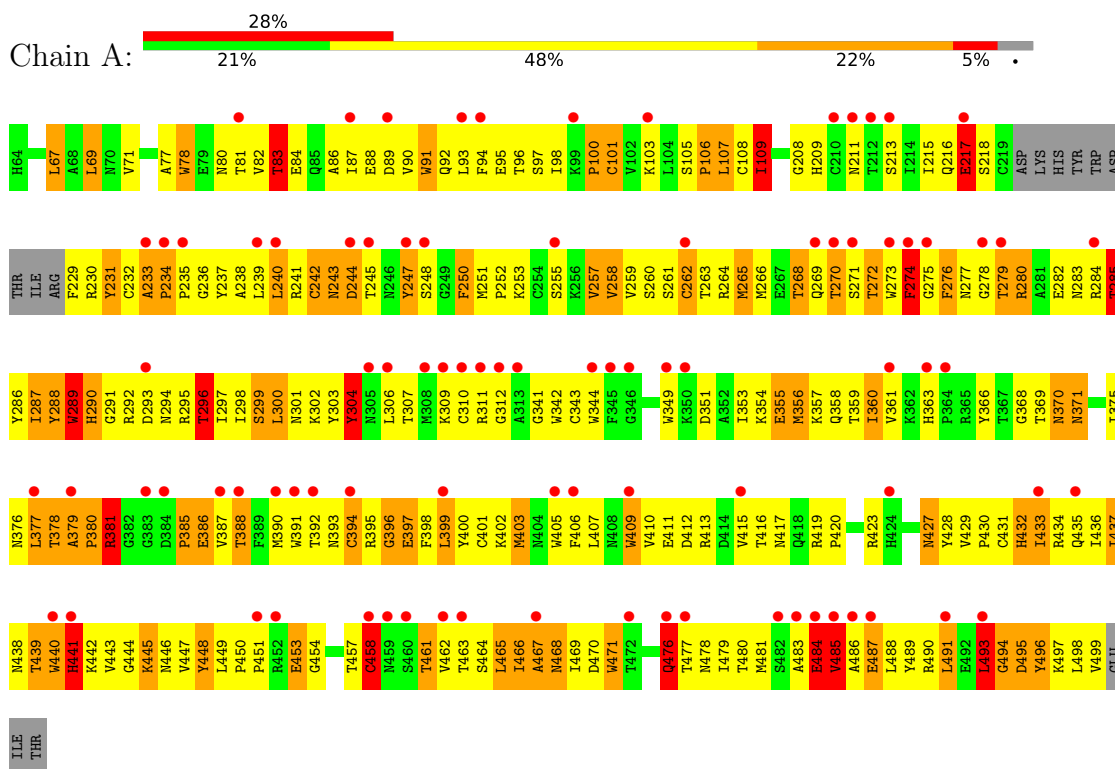


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
9	A	1	14	8	1	5	0	0

### 3 Residue-property plots

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

- Molecule 1: EXTERIOR MEMBRANE GLYCOPROTEIN GP120



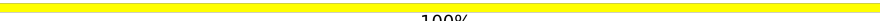
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain H:  100%

MAG1  
MAG2  
BMA3  
FUC4

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

Chain C:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
FUC6

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

Chain K:  33% 33% 33%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
FUC6

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

Chain D:  100%

MAG1  
MAG2  
FUC3

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

Chain E:  67% 33%

MAG1  
MAG2  
FUC3

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

Chain G:  50% 50%

MAG1  
MAG2

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

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

Chain I:  71% 29%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 7: 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:  20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 8: 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 L:  100%

MAG1  
MAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.05Å 108.05Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 4.00 26.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.00-4.00) 97.5 (26.00-4.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.97Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.385 , 0.388 0.388 , 0.405	Depositor DCC
$R_{free}$ test set	280 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	175.1	Xtrriage
Anisotropy	0.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	3085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NAG, FUC, BMA, 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	0.88	0/2534	1.17	16/3441 (0.5%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ASN	N-CA-C	9.14	124.37	108.75
1	A	250	PHE	N-CA-C	7.52	120.85	109.41
1	A	476	GLN	N-CA-C	7.31	120.31	108.32
1	A	289	TRP	N-CA-C	6.05	119.38	108.48
1	A	253	LYS	N-CA-C	-5.79	103.47	110.88
1	A	485	VAL	N-CA-C	5.50	117.92	111.05
1	A	437	ILE	N-CA-C	5.34	116.05	107.98
1	A	467	ALA	N-CA-C	5.31	116.51	108.07
1	A	371	ASN	N-CA-C	5.30	117.32	109.69
1	A	296	THR	N-CA-C	5.27	116.29	108.86
1	A	445	LYS	N-CA-C	5.15	117.08	108.99
1	A	448	TYR	N-CA-C	5.14	116.88	108.76
1	A	396	GLY	N-CA-C	5.10	119.76	113.79
1	A	247	TYR	N-CA-C	5.06	116.12	108.07
1	A	274	PHE	N-CA-C	5.04	117.83	107.69
1	A	403	MET	N-CA-C	5.03	116.84	107.99

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	2470	0	2350	359	0
2	B	49	0	43	1	2
2	F	49	0	43	0	0
2	H	49	0	43	0	0
3	C	71	0	61	2	0
3	K	71	0	61	3	0
4	D	38	0	34	4	0
4	E	38	0	34	4	0
5	G	28	0	25	1	0
6	I	83	0	70	8	0
7	J	61	0	52	0	0
8	L	50	0	43	0	0
9	A	28	0	26	0	0
All	All	3085	0	2885	369	2

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 62.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:O	1:A:90:VAL:HG22	1.35	1.25
1:A:92:GLN:NE2	1:A:106:PRO:HG3	1.50	1.24
1:A:88:GLU:HA	1:A:91:TRP:CZ2	1.79	1.16
1:A:285:THR:HG23	1:A:302:LYS:HB2	1.23	1.15
1:A:498:LEU:O	1:A:499:VAL:HG23	1.44	1.14
1:A:391:TRP:CZ2	1:A:393:ASN:HB2	1.85	1.12
1:A:109:ILE:HG12	1:A:499:VAL:HA	1.32	1.07
1:A:470:ASP:HB2	1:A:478:ASN:HB3	1.30	1.06
1:A:311:ARG:HB2	1:A:344:TRP:HE1	1.17	1.05
1:A:342:TRP:HA	1:A:429:VAL:O	1.58	1.03
1:A:354:LYS:O	1:A:358:GLN:N	1.91	1.03
1:A:266:MET:SD	1:A:398:PHE:HZ	1.81	1.02
1:A:92:GLN:NE2	1:A:106:PRO:CG	2.23	1.01
1:A:258:VAL:HG12	1:A:259:VAL:H	1.22	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:HA	1:A:303:TYR:CB	1.92	1.00
1:A:107:LEU:HB3	1:A:211:ASN:HB3	1.45	0.99
1:A:310:CYS:HB2	1:A:458:CYS:CB	1.93	0.98
1:A:266:MET:SD	1:A:398:PHE:CZ	2.57	0.97
1:A:380:PRO:O	1:A:381:ARG:HB2	1.62	0.97
1:A:283:ASN:HA	1:A:303:TYR:HB3	1.47	0.96
1:A:91:TRP:HA	1:A:448:TYR:OH	1.67	0.94
1:A:379:ALA:CB	1:A:480:THR:HG23	1.98	0.93
1:A:437:ILE:HG12	1:A:446:ASN:HB2	1.51	0.92
1:A:92:GLN:HE22	1:A:106:PRO:HG3	1.11	0.92
1:A:237:TYR:OH	1:A:498:LEU:HB3	1.69	0.91
1:A:490:ARG:HA	1:A:493:LEU:HD11	1.53	0.90
1:A:289:TRP:HE1	1:A:291:GLY:HA2	1.34	0.90
1:A:437:ILE:N	1:A:446:ASN:O	2.05	0.89
1:A:86:ALA:O	1:A:90:VAL:HG13	1.74	0.88
1:A:287:ILE:O	1:A:287:ILE:HG13	1.72	0.88
1:A:310:CYS:HB2	1:A:458:CYS:HB2	1.55	0.87
1:A:109:ILE:HD13	1:A:499:VAL:HG13	1.54	0.87
1:A:311:ARG:CB	1:A:344:TRP:HE1	1.87	0.87
1:A:88:GLU:HA	1:A:91:TRP:CE2	2.10	0.85
1:A:355:GLU:O	1:A:359:THR:N	2.09	0.85
1:A:490:ARG:HA	1:A:493:LEU:CD1	2.05	0.85
1:A:496:TYR:CD1	1:A:498:LEU:HG	2.12	0.85
1:A:391:TRP:HZ2	1:A:393:ASN:HB2	1.40	0.84
1:A:376:ASN:OD1	1:A:410:VAL:HG12	1.79	0.83
1:A:310:CYS:HB2	1:A:458:CYS:HB3	1.61	0.82
1:A:278:GLY:HA3	1:A:463:THR:HG21	1.59	0.82
1:A:268:THR:HG22	1:A:269:GLN:H	1.43	0.82
1:A:92:GLN:NE2	1:A:106:PRO:CD	2.44	0.81
1:A:306:LEU:HD23	1:A:462:VAL:HG11	1.63	0.79
1:A:289:TRP:HE1	1:A:291:GLY:CA	1.95	0.79
1:A:437:ILE:HD11	1:A:446:ASN:HD22	1.48	0.78
1:A:91:TRP:CA	1:A:448:TYR:OH	2.30	0.78
1:A:92:GLN:HE21	1:A:106:PRO:CD	1.97	0.78
1:A:92:GLN:HE21	1:A:106:PRO:CG	1.95	0.78
1:A:379:ALA:HB1	1:A:480:THR:HG23	1.64	0.77
1:A:109:ILE:CD1	1:A:499:VAL:HG13	2.13	0.77
1:A:229:PHE:HB3	1:A:231:TYR:OH	1.83	0.77
1:A:296:THR:HG23	1:A:297:ILE:H	1.49	0.77
1:A:488:LEU:HG	1:A:489:TYR:CD2	2.20	0.77
1:A:296:THR:CG2	1:A:297:ILE:N	2.47	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LEU:O	1:A:499:VAL:CG2	2.31	0.76
1:A:269:GLN:HA	1:A:393:ASN:O	1.85	0.76
1:A:436:ILE:HA	1:A:447:VAL:HG22	1.67	0.75
1:A:269:GLN:HG3	1:A:276:PHE:HD1	1.50	0.75
1:A:237:TYR:HE1	1:A:499:VAL:O	1.69	0.75
1:A:283:ASN:HA	1:A:303:TYR:HB2	1.68	0.74
1:A:92:GLN:NE2	1:A:106:PRO:HD3	2.02	0.74
1:A:286:TYR:O	1:A:300:LEU:HD22	1.88	0.74
1:A:351:ASP:O	1:A:354:LYS:HB2	1.88	0.74
1:A:237:TYR:CZ	1:A:498:LEU:HB3	2.23	0.74
1:A:379:ALA:HB2	1:A:480:THR:HG23	1.67	0.74
1:A:106:PRO:O	1:A:107:LEU:HB2	1.88	0.73
1:A:385:PRO:O	1:A:386:GLU:HB2	1.88	0.73
1:A:311:ARG:HB2	1:A:344:TRP:NE1	2.00	0.73
1:A:470:ASP:HB2	1:A:478:ASN:CB	2.13	0.73
1:A:493:LEU:HD13	1:A:495:ASP:N	2.04	0.72
1:A:284:ARG:HD3	4:D:3:FUC:H61	1.70	0.72
1:A:273:TRP:HB2	1:A:390:MET:SD	2.30	0.72
1:A:496:TYR:CD1	1:A:496:TYR:C	2.67	0.72
1:A:233:ALA:HB1	1:A:263:THR:C	2.14	0.72
1:A:486:ALA:O	1:A:490:ARG:HB2	1.89	0.72
1:A:270:THR:O	1:A:392:THR:HG23	1.89	0.72
1:A:435:GLN:O	1:A:447:VAL:HA	1.89	0.72
1:A:303:TYR:O	1:A:304:TYR:O	2.08	0.71
1:A:229:PHE:HB3	1:A:231:TYR:CZ	2.26	0.71
1:A:309:LYS:HG3	1:A:458:CYS:O	1.91	0.71
1:A:354:LYS:HD2	1:A:357:LYS:HE2	1.72	0.71
1:A:270:THR:N	1:A:393:ASN:O	2.24	0.70
1:A:307:THR:CG2	6:I:2:NAG:H83	2.21	0.70
1:A:269:GLN:HG3	1:A:276:PHE:CD1	2.27	0.69
3:K:1:NAG:H4	3:K:6:FUC:O2	1.92	0.69
1:A:237:TYR:OH	1:A:498:LEU:CB	2.38	0.69
1:A:388:THR:HB	1:A:403:MET:O	1.92	0.69
1:A:87:ILE:O	1:A:90:VAL:CG2	2.28	0.69
1:A:268:THR:HG22	1:A:269:GLN:N	2.06	0.69
1:A:341:GLY:O	1:A:431:CYS:N	2.25	0.69
1:A:379:ALA:N	1:A:380:PRO:HD3	2.08	0.69
1:A:285:THR:CG2	1:A:300:LEU:HD11	2.24	0.69
1:A:298:ILE:HG22	1:A:299:SER:N	2.08	0.69
1:A:283:ASN:CA	1:A:303:TYR:HB2	2.23	0.68
1:A:286:TYR:O	1:A:300:LEU:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG12	1:A:416:THR:H	1.57	0.68
1:A:437:ILE:CG1	1:A:446:ASN:HB2	2.23	0.68
1:A:277:ASN:OD1	1:A:461:THR:HG21	1.93	0.67
4:D:1:NAG:H62	4:D:2:NAG:N2	2.09	0.67
1:A:356:MET:O	1:A:360:ILE:HG22	1.94	0.66
1:A:244:ASP:O	3:K:1:NAG:O6	2.13	0.66
1:A:488:LEU:O	1:A:491:LEU:HB2	1.96	0.66
1:A:353:ILE:O	1:A:357:LYS:N	2.22	0.66
1:A:263:THR:HG23	1:A:265:MET:HE3	1.76	0.66
1:A:241:ARG:HG2	1:A:242:CYS:N	2.11	0.66
1:A:92:GLN:HE22	1:A:106:PRO:CG	1.94	0.66
1:A:80:ASN:HB3	1:A:84:GLU:HB2	1.77	0.65
4:E:1:NAG:H62	4:E:3:FUC:O2	1.97	0.65
1:A:289:TRP:NE1	1:A:291:GLY:HA2	2.10	0.65
1:A:283:ASN:O	1:A:302:LYS:HD2	1.97	0.64
1:A:285:THR:HG22	1:A:300:LEU:HD11	1.79	0.64
1:A:283:ASN:N	1:A:303:TYR:HB2	2.12	0.64
3:C:3:BMA:O4	3:C:5:MAN:H2	1.98	0.64
1:A:289:TRP:CD1	1:A:289:TRP:C	2.76	0.64
1:A:484:GLU:H	1:A:484:GLU:CD	2.04	0.64
1:A:285:THR:OG1	1:A:302:LYS:HD3	1.97	0.63
1:A:488:LEU:HG	1:A:489:TYR:CE2	2.33	0.63
1:A:415:VAL:HG12	1:A:416:THR:N	2.14	0.63
4:D:1:NAG:H62	4:D:2:NAG:C7	2.28	0.63
1:A:237:TYR:HH	1:A:498:LEU:HB3	1.63	0.63
1:A:310:CYS:CB	1:A:458:CYS:HB2	2.28	0.62
1:A:290:HIS:ND1	1:A:290:HIS:C	2.57	0.62
1:A:237:TYR:CE1	1:A:499:VAL:O	2.51	0.62
1:A:93:LEU:HD13	1:A:237:TYR:CG	2.35	0.62
1:A:397:GLU:HB3	1:A:399:LEU:HD21	1.80	0.62
1:A:488:LEU:HG	1:A:489:TYR:HD2	1.64	0.62
1:A:91:TRP:O	1:A:448:TYR:OH	2.18	0.61
1:A:263:THR:CG2	1:A:265:MET:HE3	2.30	0.61
1:A:307:THR:HG21	6:I:2:NAG:HN2	1.66	0.60
1:A:343:CYS:O	1:A:429:VAL:HG23	2.01	0.60
1:A:95:GLU:CA	1:A:448:TYR:HE2	2.15	0.60
1:A:311:ARG:HA	1:A:457:THR:HG23	1.82	0.60
1:A:395:ARG:O	1:A:395:ARG:HG3	2.02	0.60
1:A:434:ARG:HD2	1:A:438:ASN:HD22	1.67	0.60
1:A:88:GLU:HG2	1:A:91:TRP:CZ2	2.36	0.60
1:A:269:GLN:CA	1:A:393:ASN:O	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:HA	1:A:91:TRP:CH2	2.36	0.60
1:A:208:GLY:O	1:A:209:HIS:ND1	2.34	0.60
1:A:274:PHE:HB2	1:A:462:VAL:HG13	1.84	0.60
1:A:279:THR:O	1:A:280:ARG:C	2.45	0.59
1:A:247:TYR:HE1	1:A:495:ASP:OD1	1.85	0.59
1:A:270:THR:N	1:A:276:PHE:HE1	2.01	0.59
1:A:402:LYS:HB2	1:A:430:PRO:HG2	1.84	0.59
1:A:268:THR:HG22	1:A:269:GLN:HG2	1.84	0.59
1:A:400:TYR:CD1	1:A:434:ARG:HB2	2.38	0.58
1:A:417:ASN:HA	1:A:420:PRO:HB2	1.85	0.58
1:A:241:ARG:HG2	1:A:242:CYS:H	1.67	0.58
1:A:240:LEU:O	1:A:497:LYS:HB2	2.03	0.58
1:A:100:PRO:O	1:A:101:CYS:SG	2.62	0.58
1:A:258:VAL:HG12	1:A:259:VAL:N	2.04	0.58
1:A:289:TRP:HD1	1:A:290:HIS:C	2.12	0.58
1:A:291:GLY:O	1:A:292:ARG:HG2	2.04	0.58
1:A:342:TRP:NE1	1:A:430:PRO:HA	2.18	0.58
1:A:298:ILE:CD1	1:A:469:ILE:H	2.17	0.58
1:A:234:PRO:CG	1:A:262:CYS:HA	2.34	0.57
1:A:285:THR:HG22	1:A:300:LEU:CD1	2.34	0.57
1:A:378:THR:O	1:A:379:ALA:HB3	2.04	0.57
1:A:96:THR:HG23	1:A:103:LYS:HD2	1.86	0.57
1:A:234:PRO:HG3	1:A:262:CYS:HA	1.86	0.57
1:A:274:PHE:HZ	1:A:406:PHE:CZ	2.22	0.57
1:A:417:ASN:HD22	1:A:420:PRO:HB2	1.69	0.57
1:A:289:TRP:NE1	1:A:291:GLY:CA	2.67	0.57
1:A:302:LYS:HG3	1:A:304:TYR:H	1.69	0.57
1:A:290:HIS:O	1:A:296:THR:HG23	2.04	0.56
1:A:490:ARG:HG3	1:A:495:ASP:HA	1.86	0.56
1:A:379:ALA:H	1:A:380:PRO:HD3	1.68	0.56
1:A:88:GLU:CA	1:A:91:TRP:CZ2	2.72	0.56
1:A:106:PRO:C	1:A:211:ASN:O	2.49	0.56
1:A:93:LEU:HD13	1:A:237:TYR:CD2	2.40	0.56
1:A:266:MET:HE1	1:A:398:PHE:HE2	1.70	0.56
1:A:296:THR:CG2	1:A:297:ILE:H	2.11	0.56
1:A:296:THR:HG22	1:A:297:ILE:N	2.20	0.56
1:A:343:CYS:HB2	1:A:429:VAL:CG2	2.36	0.56
1:A:447:VAL:HG12	1:A:448:TYR:N	2.21	0.55
1:A:91:TRP:HB3	1:A:448:TYR:CE1	2.41	0.55
1:A:485:VAL:O	1:A:488:LEU:HB3	2.06	0.55
1:A:296:THR:O	1:A:468:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PHE:C	1:A:407:LEU:HG	2.31	0.55
1:A:468:ASN:C	1:A:468:ASN:HD22	2.15	0.55
1:A:91:TRP:O	1:A:95:GLU:HB3	2.07	0.55
1:A:269:GLN:C	1:A:270:THR:OG1	2.49	0.55
1:A:437:ILE:CD1	1:A:446:ASN:HD22	2.19	0.55
1:A:229:PHE:HB3	1:A:231:TYR:HH	1.71	0.54
1:A:289:TRP:NE1	1:A:296:THR:HG21	2.22	0.54
1:A:437:ILE:O	1:A:445:LYS:HA	2.07	0.54
1:A:239:LEU:HD13	1:A:489:TYR:HD1	1.71	0.54
1:A:493:LEU:CD1	1:A:494:GLY:H	2.20	0.54
1:A:108:CYS:C	1:A:109:ILE:HG13	2.32	0.54
1:A:490:ARG:CA	1:A:493:LEU:HD11	2.33	0.54
1:A:233:ALA:HB3	1:A:263:THR:H	1.73	0.54
1:A:357:LYS:O	1:A:361:VAL:HG23	2.08	0.54
1:A:360:ILE:HG12	1:A:360:ILE:O	2.07	0.54
1:A:258:VAL:CG1	1:A:259:VAL:H	2.02	0.54
1:A:437:ILE:HG12	1:A:446:ASN:CB	2.34	0.54
1:A:307:THR:HG21	6:I:2:NAG:H83	1.88	0.54
1:A:300:LEU:HD13	1:A:301:ASN:N	2.24	0.53
1:A:388:THR:HG21	1:A:407:LEU:HD13	1.89	0.53
1:A:92:GLN:HE21	1:A:106:PRO:HG3	1.50	0.53
1:A:105:SER:HB3	1:A:213:SER:HB3	1.90	0.53
1:A:296:THR:HG23	1:A:297:ILE:N	2.13	0.53
1:A:298:ILE:HD12	1:A:467:ALA:O	2.08	0.53
1:A:379:ALA:N	1:A:380:PRO:CD	2.70	0.53
1:A:242:CYS:O	1:A:243:ASN:HB2	2.09	0.53
1:A:354:LYS:HA	1:A:357:LYS:HG2	1.91	0.52
1:A:369:THR:HB	1:A:371:ASN:OD1	2.09	0.52
1:A:87:ILE:HG22	1:A:91:TRP:HE1	1.72	0.52
1:A:391:TRP:CD1	1:A:392:THR:N	2.78	0.52
1:A:442:LYS:O	1:A:444:GLY:N	2.42	0.52
1:A:311:ARG:HA	1:A:457:THR:CG2	2.39	0.52
1:A:416:THR:O	1:A:420:PRO:HG2	2.09	0.52
1:A:98:ILE:HD11	1:A:449:LEU:HD12	1.92	0.52
1:A:269:GLN:CD	3:C:1:NAG:H83	2.35	0.52
4:E:1:NAG:C6	4:E:3:FUC:O2	2.58	0.52
1:A:406:PHE:O	1:A:409:TRP:NE1	2.43	0.52
1:A:78:TRP:H	1:A:78:TRP:CD1	2.27	0.51
1:A:269:GLN:HA	1:A:393:ASN:C	2.35	0.51
1:A:289:TRP:CD1	1:A:290:HIS:C	2.88	0.51
1:A:307:THR:HG23	6:I:1:NAG:O6	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TYR:O	1:A:493:LEU:HG	2.11	0.51
1:A:370:ASN:CG	5:G:1:NAG:H5	2.36	0.51
1:A:496:TYR:HE1	1:A:498:LEU:H	1.58	0.51
1:A:88:GLU:HG2	1:A:91:TRP:CH2	2.45	0.51
1:A:286:TYR:HB2	1:A:301:ASN:HB3	1.91	0.51
1:A:351:ASP:O	1:A:355:GLU:OE1	2.29	0.51
1:A:90:VAL:HG23	1:A:91:TRP:CD1	2.46	0.51
1:A:465:LEU:HD23	1:A:465:LEU:C	2.35	0.51
1:A:490:ARG:HA	1:A:493:LEU:HD12	1.93	0.51
1:A:69:LEU:HD11	1:A:250:PHE:HE2	1.76	0.50
1:A:95:GLU:N	1:A:448:TYR:HE2	2.09	0.50
1:A:275:GLY:N	1:A:464:SER:O	2.44	0.50
1:A:311:ARG:HD2	1:A:344:TRP:HZ2	1.76	0.50
1:A:343:CYS:HB2	1:A:429:VAL:HG21	1.92	0.50
1:A:280:ARG:HB2	1:A:280:ARG:CZ	2.42	0.50
1:A:391:TRP:CG	1:A:392:THR:N	2.80	0.50
1:A:487:GLU:O	1:A:491:LEU:N	2.44	0.50
1:A:298:ILE:CG2	1:A:299:SER:N	2.74	0.50
1:A:287:ILE:HD11	1:A:289:TRP:CE3	2.46	0.50
1:A:403:MET:O	1:A:407:LEU:HD12	2.12	0.50
1:A:95:GLU:N	1:A:448:TYR:CE2	2.79	0.50
1:A:355:GLU:HA	1:A:358:GLN:HB2	1.93	0.50
1:A:307:THR:HG21	6:I:2:NAG:N2	2.26	0.50
1:A:369:THR:O	1:A:371:ASN:ND2	2.45	0.50
1:A:91:TRP:C	1:A:448:TYR:OH	2.55	0.49
1:A:243:ASN:O	1:A:244:ASP:HB2	2.11	0.49
1:A:303:TYR:O	1:A:304:TYR:C	2.56	0.49
1:A:216:GLN:O	1:A:217:GLU:HB2	2.11	0.49
1:A:266:MET:HE1	1:A:398:PHE:CE2	2.46	0.49
1:A:471:TRP:HA	1:A:476:GLN:O	2.11	0.49
1:A:489:TYR:HD2	1:A:489:TYR:N	2.10	0.49
1:A:375:ILE:HG12	1:A:477:THR:HB	1.93	0.49
1:A:469:ILE:HG12	1:A:479:ILE:HG12	1.94	0.49
2:B:2:NAG:H61	2:B:3:BMA:H2	1.94	0.49
1:A:294:ASN:OD1	4:E:1:NAG:C7	2.60	0.49
1:A:270:THR:O	1:A:392:THR:CG2	2.57	0.49
1:A:274:PHE:CZ	1:A:406:PHE:CZ	3.01	0.49
1:A:298:ILE:HD11	1:A:469:ILE:H	1.77	0.49
1:A:417:ASN:HD22	1:A:420:PRO:CB	2.25	0.48
1:A:283:ASN:CA	1:A:303:TYR:CB	2.75	0.48
1:A:405:TRP:HB2	1:A:427:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TYR:CD2	1:A:489:TYR:N	2.77	0.48
4:D:1:NAG:O6	4:D:3:FUC:H63	2.13	0.48
1:A:360:ILE:HD12	1:A:469:ILE:HD13	1.95	0.48
1:A:401:CYS:HB3	1:A:429:VAL:HG12	1.96	0.48
1:A:487:GLU:HA	1:A:490:ARG:HB3	1.95	0.48
1:A:78:TRP:CD1	1:A:78:TRP:N	2.81	0.48
1:A:103:LYS:HE3	1:A:215:ILE:HD12	1.95	0.48
1:A:287:ILE:HD11	1:A:289:TRP:HE3	1.78	0.48
1:A:278:GLY:HA3	1:A:463:THR:CG2	2.37	0.48
1:A:354:LYS:C	1:A:358:GLN:HG3	2.38	0.48
1:A:243:ASN:OD1	1:A:244:ASP:N	2.47	0.48
1:A:273:TRP:HD1	1:A:274:PHE:CE2	2.32	0.47
1:A:94:PHE:HB2	1:A:448:TYR:OH	2.14	0.47
1:A:95:GLU:HA	1:A:448:TYR:HE2	1.78	0.47
1:A:242:CYS:HA	1:A:257:VAL:HG12	1.96	0.47
1:A:275:GLY:HA3	1:A:464:SER:HB2	1.96	0.47
1:A:378:THR:O	1:A:379:ALA:CB	2.62	0.47
1:A:419:ARG:N	1:A:420:PRO:CD	2.78	0.47
1:A:105:SER:O	1:A:213:SER:N	2.47	0.47
1:A:234:PRO:O	1:A:236:GLY:N	2.48	0.47
1:A:287:ILE:O	1:A:288:TYR:C	2.57	0.47
1:A:355:GLU:CD	1:A:355:GLU:N	2.72	0.47
1:A:234:PRO:CD	1:A:262:CYS:HA	2.45	0.46
1:A:433:ILE:HG21	1:A:435:GLN:NE2	2.30	0.46
1:A:234:PRO:HD3	1:A:262:CYS:HA	1.98	0.46
1:A:292:ARG:O	1:A:294:ASN:N	2.39	0.46
1:A:466:ILE:O	1:A:481:MET:CE	2.64	0.46
6:I:1:NAG:H62	6:I:2:NAG:C1	2.46	0.46
1:A:354:LYS:O	1:A:355:GLU:C	2.55	0.46
1:A:388:THR:CG2	1:A:407:LEU:HD13	2.45	0.46
1:A:434:ARG:O	1:A:435:GLN:C	2.58	0.46
1:A:496:TYR:CE1	1:A:498:LEU:HG	2.49	0.46
1:A:273:TRP:CZ3	1:A:481:MET:HB3	2.50	0.46
1:A:91:TRP:C	1:A:448:TYR:HH	2.22	0.45
1:A:109:ILE:HG12	1:A:499:VAL:CA	2.24	0.45
1:A:238:ALA:HA	1:A:261:SER:HA	1.99	0.45
1:A:217:GLU:CG	1:A:218:SER:H	2.29	0.45
1:A:229:PHE:CB	1:A:231:TYR:OH	2.60	0.45
1:A:247:TYR:CG	1:A:248:SER:N	2.83	0.45
1:A:269:GLN:HA	1:A:394:CYS:HA	1.97	0.45
1:A:292:ARG:N	1:A:296:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:O	1:A:80:ASN:HB2	2.16	0.45
1:A:107:LEU:N	1:A:211:ASN:O	2.50	0.45
1:A:89:ASP:O	1:A:92:GLN:HB3	2.17	0.45
1:A:401:CYS:HB3	1:A:429:VAL:CG1	2.47	0.45
1:A:396:GLY:O	1:A:398:PHE:CE1	2.70	0.45
1:A:108:CYS:O	1:A:109:ILE:HG13	2.16	0.44
1:A:233:ALA:HB1	1:A:263:THR:O	2.17	0.44
1:A:282:GLU:C	1:A:303:TYR:HB2	2.43	0.44
1:A:109:ILE:HB	1:A:499:VAL:HG22	1.98	0.44
1:A:403:MET:HG2	1:A:406:PHE:HB3	1.99	0.44
1:A:265:MET:O	1:A:266:MET:C	2.60	0.44
1:A:355:GLU:O	1:A:358:GLN:N	2.51	0.44
1:A:270:THR:N	1:A:276:PHE:CE1	2.84	0.43
1:A:493:LEU:HD13	1:A:495:ASP:C	2.43	0.43
1:A:269:GLN:HB3	1:A:394:CYS:HB3	2.00	0.43
1:A:272:THR:HG22	1:A:481:MET:O	2.18	0.43
1:A:400:TYR:O	1:A:431:CYS:HA	2.18	0.43
1:A:466:ILE:HD12	1:A:467:ALA:N	2.34	0.43
1:A:493:LEU:HD13	1:A:495:ASP:H	1.79	0.43
1:A:417:ASN:HA	1:A:420:PRO:CG	2.49	0.43
1:A:233:ALA:HB1	1:A:264:ARG:N	2.34	0.43
1:A:298:ILE:HG22	1:A:299:SER:H	1.82	0.43
1:A:302:LYS:HG3	1:A:304:TYR:N	2.33	0.43
1:A:307:THR:HG22	6:I:2:NAG:H83	1.97	0.43
1:A:449:LEU:HA	1:A:450:PRO:HD3	1.85	0.43
1:A:266:MET:CE	1:A:398:PHE:CE2	3.02	0.43
1:A:270:THR:OG1	1:A:393:ASN:HB3	2.19	0.42
1:A:349:TRP:NE1	1:A:353:ILE:HD11	2.32	0.42
1:A:440:TRP:CE2	1:A:441:HIS:CE1	3.07	0.42
3:K:1:NAG:O5	3:K:6:FUC:C1	2.66	0.42
1:A:81:THR:O	1:A:82:VAL:C	2.61	0.42
1:A:439:THR:HB	1:A:442:LYS:O	2.20	0.42
1:A:287:ILE:O	1:A:287:ILE:CG1	2.51	0.42
1:A:378:THR:HG22	1:A:380:PRO:HD3	2.01	0.42
1:A:266:MET:CE	1:A:398:PHE:CZ	3.03	0.42
1:A:274:PHE:CZ	1:A:406:PHE:HZ	2.38	0.42
1:A:496:TYR:CD1	1:A:497:LYS:CA	3.02	0.42
1:A:380:PRO:HB2	1:A:381:ARG:H	1.68	0.42
1:A:91:TRP:CB	1:A:448:TYR:OH	2.68	0.41
1:A:282:GLU:O	1:A:283:ASN:C	2.63	0.41
1:A:285:THR:HA	1:A:302:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:HA	1:A:420:PRO:CB	2.49	0.41
1:A:80:ASN:OD1	1:A:81:THR:N	2.53	0.41
1:A:417:ASN:HA	1:A:417:ASN:HD22	1.76	0.41
1:A:83:THR:O	1:A:84:GLU:C	2.63	0.41
1:A:378:THR:HB	1:A:379:ALA:H	1.73	0.41
1:A:496:TYR:CD1	1:A:497:LYS:N	2.88	0.41
1:A:107:LEU:CB	1:A:211:ASN:HB3	2.30	0.41
1:A:269:GLN:CB	1:A:394:CYS:HB3	2.51	0.41
1:A:448:TYR:O	1:A:450:PRO:HD3	2.20	0.41
1:A:307:THR:CG2	6:I:1:NAG:O6	2.67	0.41
1:A:432:HIS:O	1:A:434:ARG:HG2	2.19	0.41
1:A:496:TYR:CE1	1:A:498:LEU:N	2.88	0.41
1:A:234:PRO:HG3	1:A:262:CYS:C	2.46	0.41
1:A:276:PHE:HA	1:A:461:THR:O	2.21	0.41
1:A:377:LEU:HD12	1:A:479:ILE:O	2.20	0.41
1:A:490:ARG:CA	1:A:493:LEU:CD1	2.90	0.41
1:A:445:LYS:O	1:A:446:ASN:OD1	2.40	0.40
1:A:96:THR:O	1:A:235:PRO:HG2	2.21	0.40
1:A:109:ILE:CB	1:A:499:VAL:HG22	2.52	0.40
1:A:395:ARG:CZ	1:A:453:GLU:CD	2.94	0.40
1:A:234:PRO:HG3	1:A:262:CYS:CA	2.50	0.40
1:A:251:MET:N	1:A:252:PRO:HD3	2.35	0.40
1:A:303:TYR:C	1:A:304:TYR:O	2.63	0.40
1:A:231:TYR:CD1	1:A:231:TYR:N	2.90	0.40
1:A:239:LEU:O	1:A:260:SER:O	2.38	0.40
1:A:432:HIS:O	1:A:433:ILE:C	2.65	0.40
1:A:471:TRP:NE1	4:E:1:NAG:O7	2.54	0.40

All (2) 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)
2:B:4:FUC:O3	2:B:4:FUC:O3[8_555]	0.65	1.55
2:B:4:FUC:C3	2:B:4:FUC:O3[8_555]	1.92	0.28

## 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	300/316 (95%)	191 (64%)	65 (22%)	44 (15%)	<b>0</b> <b>3</b>

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	100	PRO
1	A	107	LEU
1	A	217	GLU
1	A	233	ALA
1	A	242	CYS
1	A	244	ASP
1	A	304	TYR
1	A	379	ALA
1	A	381	ARG
1	A	386	GLU
1	A	439	THR
1	A	458	CYS
1	A	493	LEU
1	A	83	THR
1	A	109	ILE
1	A	243	ASN
1	A	265	MET
1	A	380	PRO
1	A	385	PRO
1	A	443	VAL
1	A	454	GLY
1	A	268	THR
1	A	276	PHE
1	A	293	ASP
1	A	494	GLY
1	A	106	PRO
1	A	234	PRO

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Mol	Chain	Res	Type
1	A	285	THR
1	A	288	TYR
1	A	368	GLY
1	A	378	THR
1	A	413	ARG
1	A	483	ALA
1	A	97	SER
1	A	101	CYS
1	A	262	CYS
1	A	280	ARG
1	A	441	HIS
1	A	484	GLU
1	A	232	CYS
1	A	279	THR
1	A	312	GLY
1	A	451	PRO

### 5.3.2 Protein sidechains [i](#)

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	272/284 (96%)	207 (76%)	65 (24%)	<b>1</b> <b>5</b>

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	69	LEU
1	A	71	VAL
1	A	78	TRP
1	A	83	THR
1	A	91	TRP
1	A	109	ILE
1	A	217	GLU
1	A	230	ARG
1	A	231	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	240	LEU
1	A	245	THR
1	A	255	SER
1	A	257	VAL
1	A	258	VAL
1	A	270	THR
1	A	271	SER
1	A	272	THR
1	A	274	PHE
1	A	285	THR
1	A	287	ILE
1	A	289	TRP
1	A	290	HIS
1	A	295	ARG
1	A	296	THR
1	A	299	SER
1	A	300	LEU
1	A	304	TYR
1	A	355	GLU
1	A	356	MET
1	A	360	ILE
1	A	363	HIS
1	A	366	TYR
1	A	370	ASN
1	A	377	LEU
1	A	381	ARG
1	A	387	VAL
1	A	388	THR
1	A	394	CYS
1	A	397	GLU
1	A	399	LEU
1	A	409	TRP
1	A	411	GLU
1	A	412	ASP
1	A	423	ARG
1	A	428	TYR
1	A	432	HIS
1	A	433	ILE
1	A	440	TRP
1	A	441	HIS
1	A	453	GLU
1	A	458	CYS

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Mol	Chain	Res	Type
1	A	461	THR
1	A	465	LEU
1	A	466	ILE
1	A	468	ASN
1	A	471	TRP
1	A	476	GLN
1	A	484	GLU
1	A	485	VAL
1	A	487	GLU
1	A	491	LEU
1	A	493	LEU
1	A	495	ASP
1	A	496	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	363	HIS
1	A	417	ASN
1	A	441	HIS
1	A	446	ASN
1	A	468	ASN

### 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](#)

48 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1	1,2	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
2	NAG	B	2	2	14,14,15	0.92	1 (7%)	17,19,21	1.05	1 (5%)
2	BMA	B	3	2	11,11,12	0.79	0	15,15,17	1.04	0
2	FUC	B	4	2	10,10,11	0.78	0	14,14,16	1.36	3 (21%)
3	NAG	C	1	1,3	14,14,15	0.77	0	17,19,21	1.64	5 (29%)
3	NAG	C	2	3	14,14,15	1.09	2 (14%)	17,19,21	1.79	2 (11%)
3	BMA	C	3	3	11,11,12	0.94	1 (9%)	15,15,17	1.80	3 (20%)
3	MAN	C	4	3	11,11,12	0.52	0	15,15,17	1.45	1 (6%)
3	MAN	C	5	3	11,11,12	0.60	0	15,15,17	1.29	2 (13%)
3	FUC	C	6	3	10,10,11	0.74	0	14,14,16	1.04	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.67	0	17,19,21	1.73	5 (29%)
4	NAG	D	2	4	14,14,15	0.73	0	17,19,21	1.46	2 (11%)
4	FUC	D	3	4	10,10,11	0.74	0	14,14,16	0.93	1 (7%)
4	NAG	E	1	1,4	14,14,15	0.53	0	17,19,21	1.58	3 (17%)
4	NAG	E	2	4	14,14,15	0.54	0	17,19,21	1.63	3 (17%)
4	FUC	E	3	4	10,10,11	0.70	0	14,14,16	0.84	0
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	1.97	5 (29%)
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	1.19	1 (5%)
2	BMA	F	3	2	11,11,12	0.54	0	15,15,17	0.87	0
2	FUC	F	4	2	10,10,11	0.59	0	14,14,16	0.94	0
5	NAG	G	1	1,5	14,14,15	0.63	0	17,19,21	1.96	4 (23%)
5	NAG	G	2	5	14,14,15	0.77	0	17,19,21	1.15	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.71	0	17,19,21	1.27	3 (17%)
2	NAG	H	2	2	14,14,15	0.75	0	17,19,21	1.65	1 (5%)
2	BMA	H	3	2	11,11,12	0.83	1 (9%)	15,15,17	1.53	2 (13%)
2	FUC	H	4	2	10,10,11	0.67	0	14,14,16	1.07	1 (7%)
6	NAG	I	1	1,6	14,14,15	0.83	1 (7%)	17,19,21	1.45	3 (17%)
6	NAG	I	2	6	14,14,15	0.45	0	17,19,21	3.03	3 (17%)
6	BMA	I	3	6	11,11,12	0.98	0	15,15,17	1.75	4 (26%)
6	MAN	I	4	6	11,11,12	0.51	0	15,15,17	1.87	2 (13%)
6	MAN	I	5	6	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
6	MAN	I	6	6	11,11,12	0.67	0	15,15,17	1.67	3 (20%)
6	MAN	I	7	6	11,11,12	0.57	0	15,15,17	1.86	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	J	1	1,7	14,14,15	0.58	0	17,19,21	1.44	2 (11%)
7	NAG	J	2	7	14,14,15	1.06	1 (7%)	17,19,21	1.74	5 (29%)
7	BMA	J	3	7	11,11,12	0.70	0	15,15,17	1.10	0
7	MAN	J	4	7	11,11,12	0.81	0	15,15,17	1.68	2 (13%)
7	MAN	J	5	7	11,11,12	0.58	0	15,15,17	1.23	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	1.81	4 (23%)
3	NAG	K	2	3	14,14,15	0.65	0	17,19,21	0.86	0
3	BMA	K	3	3	11,11,12	0.57	0	15,15,17	2.65	4 (26%)
3	MAN	K	4	3	11,11,12	0.53	0	15,15,17	1.52	2 (13%)
3	MAN	K	5	3	11,11,12	0.71	0	15,15,17	0.95	0
3	FUC	K	6	3	10,10,11	1.08	0	14,14,16	1.61	2 (14%)
8	NAG	L	1	1,8	14,14,15	0.60	0	17,19,21	1.96	4 (23%)
8	NAG	L	2	8	14,14,15	0.64	0	17,19,21	1.40	2 (11%)
8	BMA	L	3	8	11,11,12	0.73	0	15,15,17	1.15	1 (6%)
8	MAN	L	4	8	11,11,12	0.57	0	15,15,17	1.46	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	5/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	FUC	B	4	2	1/1/4/5	-	0/1/1/1
3	NAG	C	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	FUC	C	6	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	FUC	D	3	4	1/1/4/5	-	0/1/1/1
4	NAG	E	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	E	3	4	1/1/4/5	-	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
2	FUC	F	4	2	1/1/4/5	-	0/1/1/1
5	NAG	G	1	1,5	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	FUC	H	4	2	1/1/4/5	-	0/1/1/1
6	NAG	I	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	2/2/19/22	0/1/1/1
6	MAN	I	6	6	-	0/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	2/2/19/22	0/1/1/1
3	NAG	K	1	1,3	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	MAN	K	5	3	-	2/2/19/22	0/1/1/1
3	FUC	K	6	3	1/1/4/5	-	0/1/1/1
8	NAG	L	1	1,8	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	L	2	8	-	4/6/23/26	0/1/1/1
8	BMA	L	3	8	-	2/2/19/22	0/1/1/1
8	MAN	L	4	8	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	2	NAG	C1-C2	2.92	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	C1-C2	2.68	1.56	1.52
3	C	2	NAG	C1-C2	2.64	1.55	1.52
6	I	1	NAG	C1-C2	2.39	1.55	1.52
2	B	2	NAG	C1-C2	2.32	1.55	1.52
2	H	3	BMA	C2-C3	2.26	1.55	1.52
3	C	3	BMA	C2-C3	2.14	1.55	1.52
3	C	2	NAG	C3-C2	2.10	1.56	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2	NAG	C4-C3-C2	-9.19	97.55	111.02
3	K	3	BMA	C1-O5-C5	8.21	123.19	112.19
6	I	2	NAG	C1-O5-C5	6.61	121.04	112.19
6	I	4	MAN	C1-O5-C5	6.12	120.39	112.19
8	L	1	NAG	C2-N2-C7	6.06	131.02	122.90
7	J	4	MAN	C1-C2-C3	5.18	117.19	109.64
6	I	7	MAN	C1-O5-C5	5.03	118.93	112.19
3	C	2	NAG	C4-C3-C2	5.01	118.36	111.02
2	H	2	NAG	C4-C3-C2	4.89	118.18	111.02
3	K	4	MAN	C1-O5-C5	4.81	118.63	112.19
3	C	3	BMA	C1-C2-C3	4.73	116.53	109.64
5	G	1	NAG	O5-C1-C2	-4.66	104.08	111.29
8	L	4	MAN	C1-O5-C5	4.64	118.41	112.19
2	F	1	NAG	C3-C4-C5	4.56	118.50	110.23
3	C	4	MAN	C1-O5-C5	4.46	118.17	112.19
4	D	2	NAG	C4-C3-C2	4.36	117.41	111.02
8	L	2	NAG	C4-C3-C2	4.34	117.38	111.02
3	K	6	FUC	O2-C2-C3	-4.26	101.33	110.15
7	J	5	MAN	C1-O5-C5	4.19	117.81	112.19
2	F	1	NAG	O5-C1-C2	-4.08	104.97	111.29
4	D	1	NAG	C4-C3-C2	-4.04	105.09	111.02
2	H	3	BMA	C1-O5-C5	4.00	117.55	112.19
4	E	1	NAG	C3-C4-C5	-3.98	103.02	110.23
5	G	1	NAG	C4-C3-C2	3.95	116.80	111.02
3	K	1	NAG	C1-O5-C5	3.91	117.43	112.19
4	E	2	NAG	C4-C3-C2	3.88	116.71	111.02
7	J	2	NAG	C2-N2-C7	3.87	128.09	122.90
3	K	3	BMA	O5-C1-C2	3.68	119.58	110.79
7	J	1	NAG	C1-O5-C5	3.64	117.06	112.19
6	I	3	BMA	C1-C2-C3	3.62	114.91	109.64
6	I	1	NAG	C2-N2-C7	-3.55	118.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	3.54	116.21	111.02
6	I	6	MAN	C3-C4-C5	3.53	116.63	110.23
3	K	1	NAG	C4-C3-C2	-3.47	105.94	111.02
6	I	7	MAN	C3-C4-C5	3.39	116.37	110.23
3	K	1	NAG	O4-C4-C5	3.39	117.66	109.32
3	K	3	BMA	C1-C2-C3	3.38	114.57	109.64
4	E	2	NAG	O5-C1-C2	-3.33	106.13	111.29
4	E	2	NAG	C3-C4-C5	3.27	116.15	110.23
7	J	1	NAG	O5-C1-C2	-3.25	106.26	111.29
6	I	6	MAN	C1-O5-C5	3.21	116.49	112.19
6	I	3	BMA	C3-C4-C5	3.19	116.02	110.23
2	H	1	NAG	C2-N2-C7	3.11	127.07	122.90
3	C	5	MAN	C1-O5-C5	3.11	116.35	112.19
4	E	1	NAG	O5-C5-C6	3.10	113.70	107.66
2	F	2	NAG	C2-N2-C7	2.98	126.90	122.90
8	L	1	NAG	C4-C3-C2	2.85	115.19	111.02
3	C	1	NAG	O5-C1-C2	-2.80	106.95	111.29
6	I	3	BMA	C1-O5-C5	2.78	115.91	112.19
7	J	2	NAG	C4-C3-C2	2.76	115.06	111.02
3	C	6	FUC	C3-C4-C5	2.75	113.99	109.81
5	G	2	NAG	C4-C3-C2	2.71	115.00	111.02
3	C	3	BMA	C1-O5-C5	2.71	115.82	112.19
2	F	1	NAG	C4-C3-C2	2.69	114.96	111.02
7	J	2	NAG	O7-C7-C8	-2.68	117.27	122.05
6	I	1	NAG	O5-C1-C2	-2.68	107.14	111.29
8	L	1	NAG	C1-O5-C5	2.66	115.75	112.19
2	F	1	NAG	O4-C4-C3	-2.66	104.12	110.38
6	I	1	NAG	C1-C2-N2	2.65	114.60	110.43
3	K	4	MAN	C1-C2-C3	2.62	113.45	109.64
2	B	4	FUC	C1-O5-C5	2.62	119.14	112.97
7	J	2	NAG	O7-C7-N2	2.61	126.59	121.98
4	D	1	NAG	O5-C1-C2	-2.61	107.26	111.29
7	J	2	NAG	C1-O5-C5	2.59	115.66	112.19
4	E	1	NAG	C1-O5-C5	2.59	115.65	112.19
2	B	4	FUC	C3-C4-C5	2.57	113.71	109.81
3	C	1	NAG	C3-C4-C5	2.51	114.78	110.23
3	C	2	NAG	C2-N2-C7	2.49	126.24	122.90
2	H	4	FUC	C1-O5-C5	2.44	118.73	112.97
5	G	2	NAG	O5-C5-C4	-2.43	104.91	110.83
6	I	5	MAN	O2-C2-C3	-2.40	105.18	110.15
3	K	6	FUC	C3-C4-C5	2.40	113.46	109.81
2	F	1	NAG	C2-N2-C7	-2.38	119.71	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	FUC	O5-C5-C4	2.37	113.81	109.55
3	C	5	MAN	O5-C1-C2	2.36	116.43	110.79
3	C	1	NAG	C1-O5-C5	-2.35	109.03	112.19
3	C	3	BMA	C2-C3-C4	2.29	114.89	110.86
6	I	4	MAN	O2-C2-C3	2.24	114.79	110.15
6	I	6	MAN	O4-C4-C3	-2.23	105.11	110.38
2	H	1	NAG	C1-O5-C5	2.20	115.13	112.19
8	L	3	BMA	O5-C5-C6	2.19	111.92	107.66
6	I	7	MAN	C2-C3-C4	2.18	114.70	110.86
4	D	1	NAG	O4-C4-C5	2.17	114.67	109.32
5	G	1	NAG	C3-C4-C5	2.16	114.14	110.23
4	D	2	NAG	C3-C4-C5	2.13	114.09	110.23
3	K	1	NAG	O5-C5-C6	-2.12	103.54	107.66
6	I	3	BMA	O3-C3-C4	2.11	115.34	110.38
2	H	1	NAG	O5-C1-C2	-2.10	108.04	111.29
8	L	2	NAG	C3-C4-C5	2.10	114.04	110.23
2	B	2	NAG	C1-O5-C5	2.10	114.99	112.19
3	C	1	NAG	O6-C6-C5	-2.09	104.20	111.33
5	G	1	NAG	O5-C5-C6	2.08	111.71	107.66
3	K	3	BMA	O5-C5-C4	2.08	115.88	110.83
2	H	3	BMA	C1-C2-C3	2.07	112.66	109.64
4	D	1	NAG	O3-C3-C2	2.07	113.70	109.40
6	I	2	NAG	C3-C4-C5	-2.06	106.49	110.23
4	D	3	FUC	C3-C4-C5	2.06	112.94	109.81
4	D	1	NAG	O7-C7-C8	-2.06	118.39	122.05
7	J	4	MAN	C2-C3-C4	2.02	114.42	110.86
8	L	1	NAG	O7-C7-N2	2.01	125.54	121.98
2	B	1	NAG	O5-C1-C2	-2.01	108.19	111.29

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
2	B	4	FUC	C1
2	F	4	FUC	C1
2	H	1	NAG	C1
2	H	4	FUC	C1
3	C	6	FUC	C1
3	K	1	NAG	C1
3	K	6	FUC	C1
4	D	1	NAG	C1
4	D	3	FUC	C1

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Mol	Chain	Res	Type	Atom
4	E	1	NAG	C1
4	E	3	FUC	C1
5	G	1	NAG	C1
6	I	1	NAG	C1
8	L	1	NAG	C1

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
8	L	1	NAG	C1-C2-N2-C7
8	L	1	NAG	C8-C7-N2-C2
8	L	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	L	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
8	L	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
3	C	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	K	5	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	I	5	MAN	C4-C5-C6-O6
7	J	5	MAN	C4-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	K	5	MAN	O5-C5-C6-O6
7	J	5	MAN	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	4	MAN	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
8	L	3	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
8	L	3	BMA	C4-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
3	C	4	MAN	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
4	D	2	NAG	C3-C2-N2-C7
2	B	3	BMA	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7
2	B	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
8	L	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
8	L	2	NAG	C4-C5-C6-O6
8	L	2	NAG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 25 short contacts:

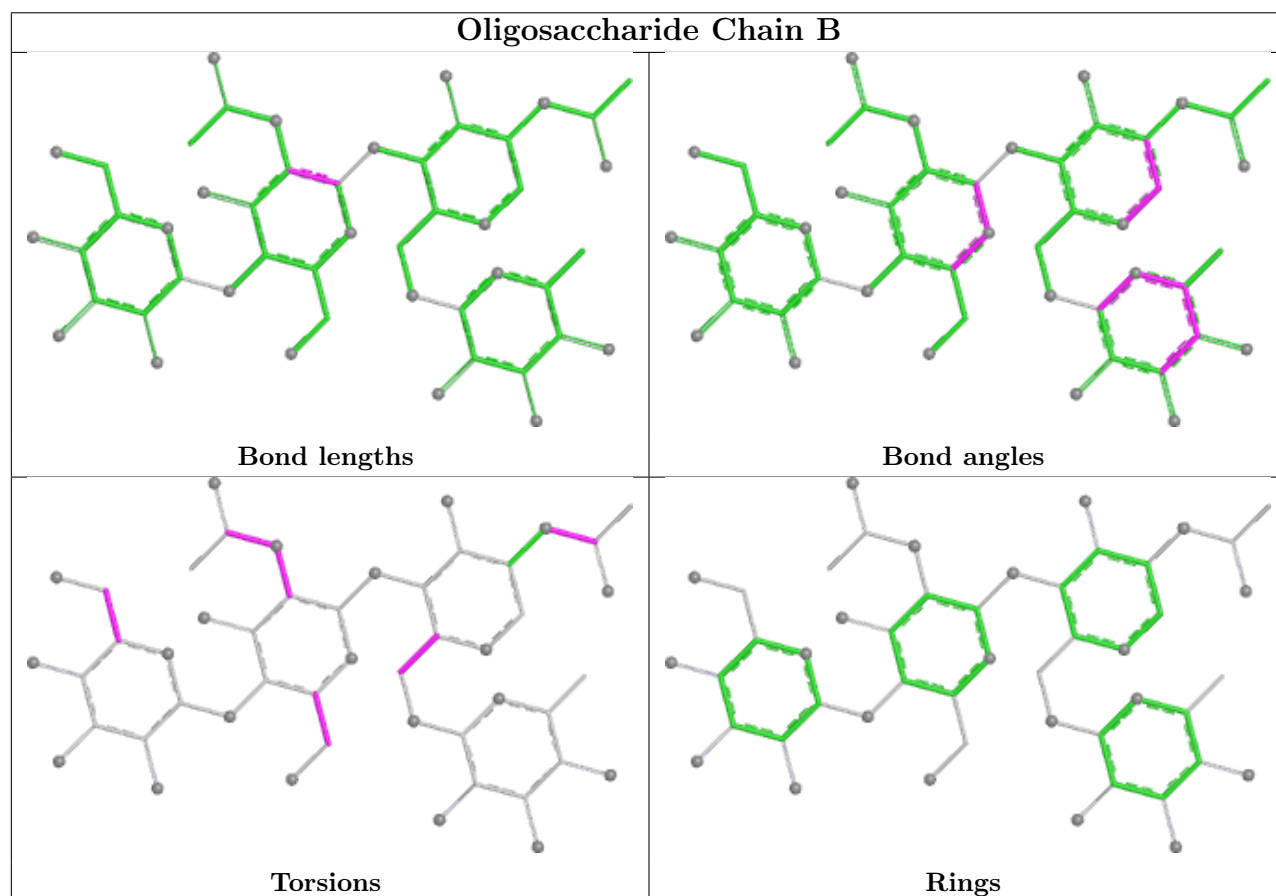
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	3	0
2	B	4	FUC	0	2
3	C	5	MAN	1	0
4	D	3	FUC	2	0
3	K	6	FUC	2	0
5	G	1	NAG	1	0
3	C	3	BMA	1	0
4	E	1	NAG	4	0
4	D	2	NAG	2	0
4	E	3	FUC	2	0
2	B	3	BMA	1	0

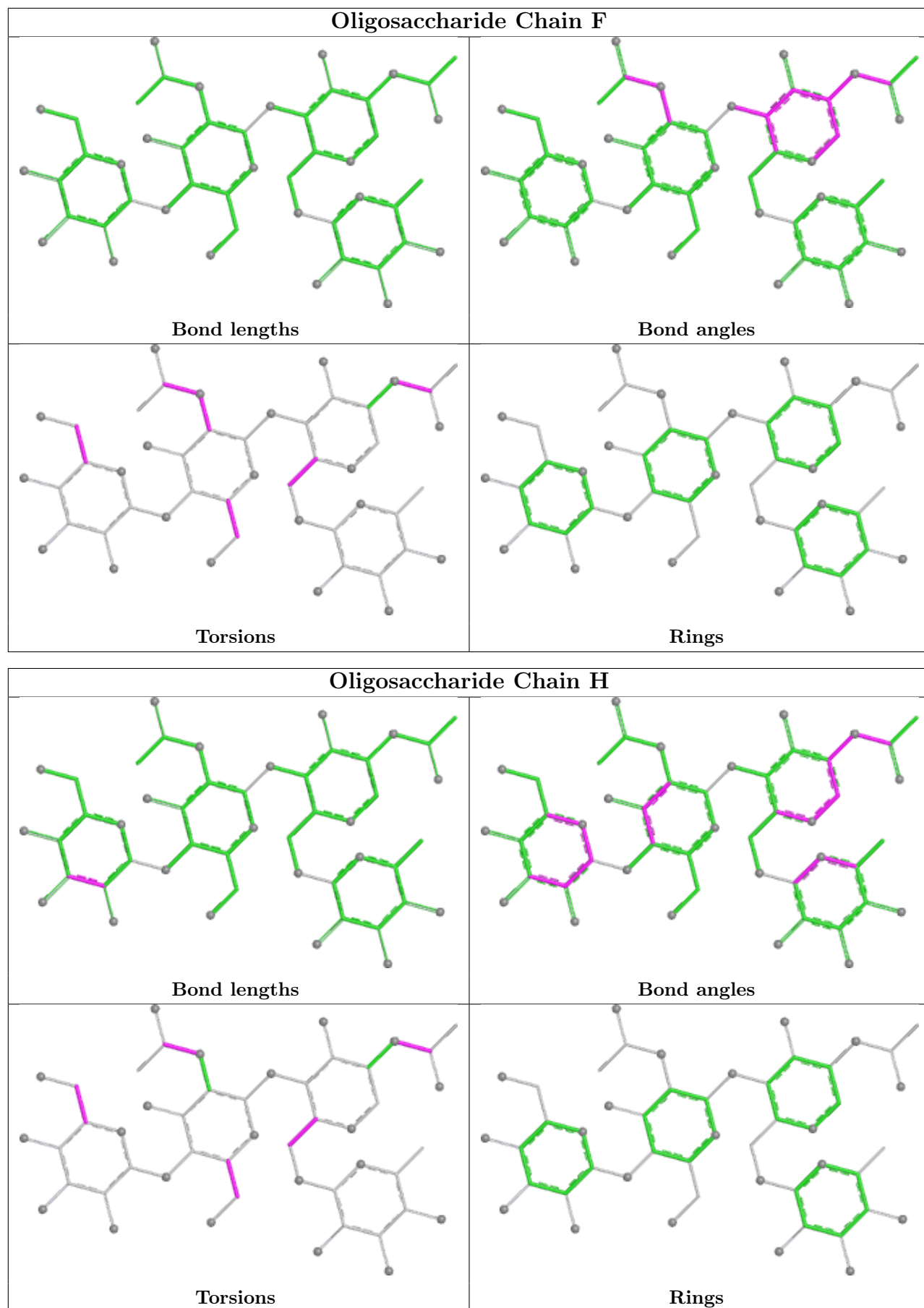
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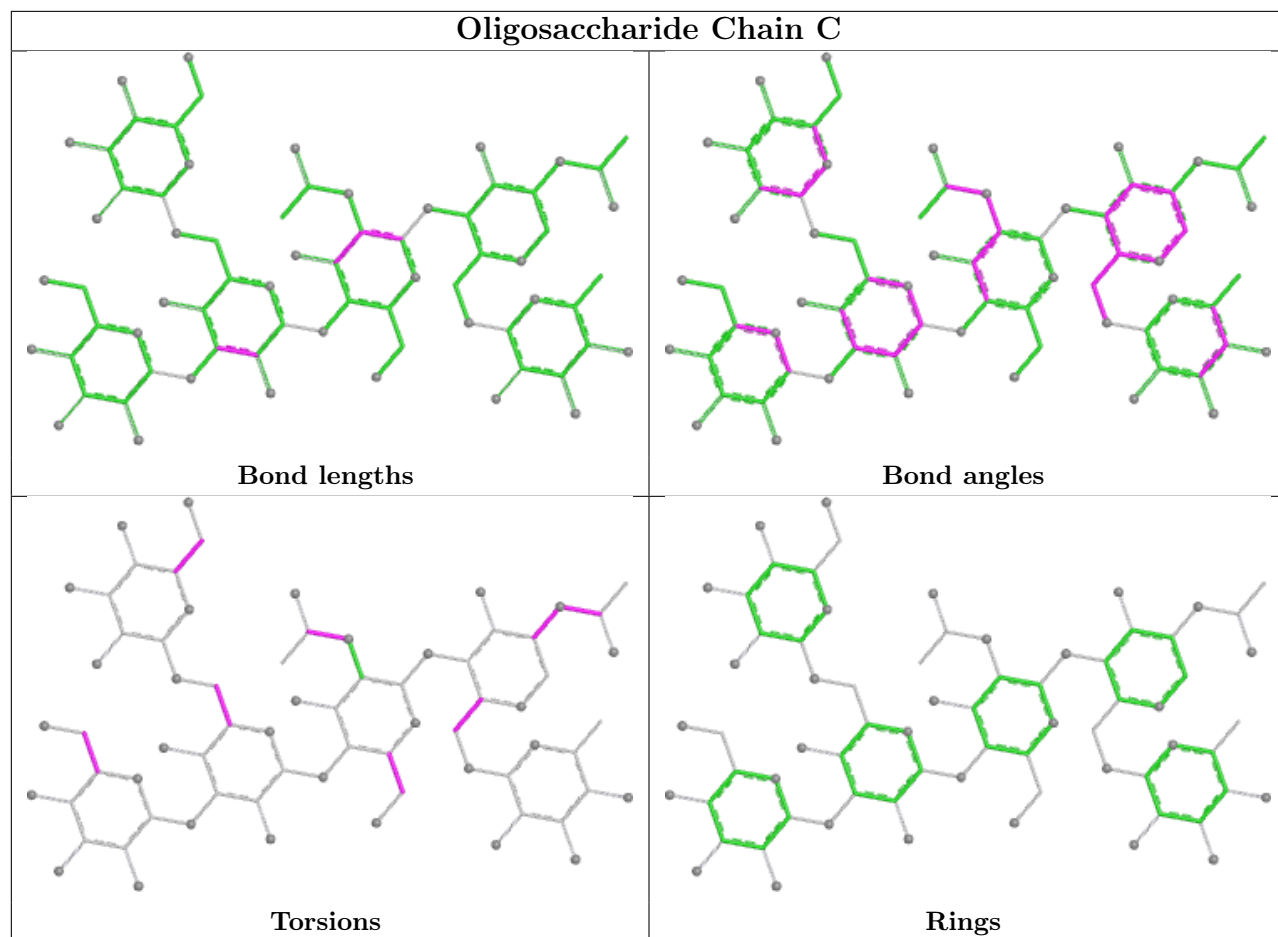
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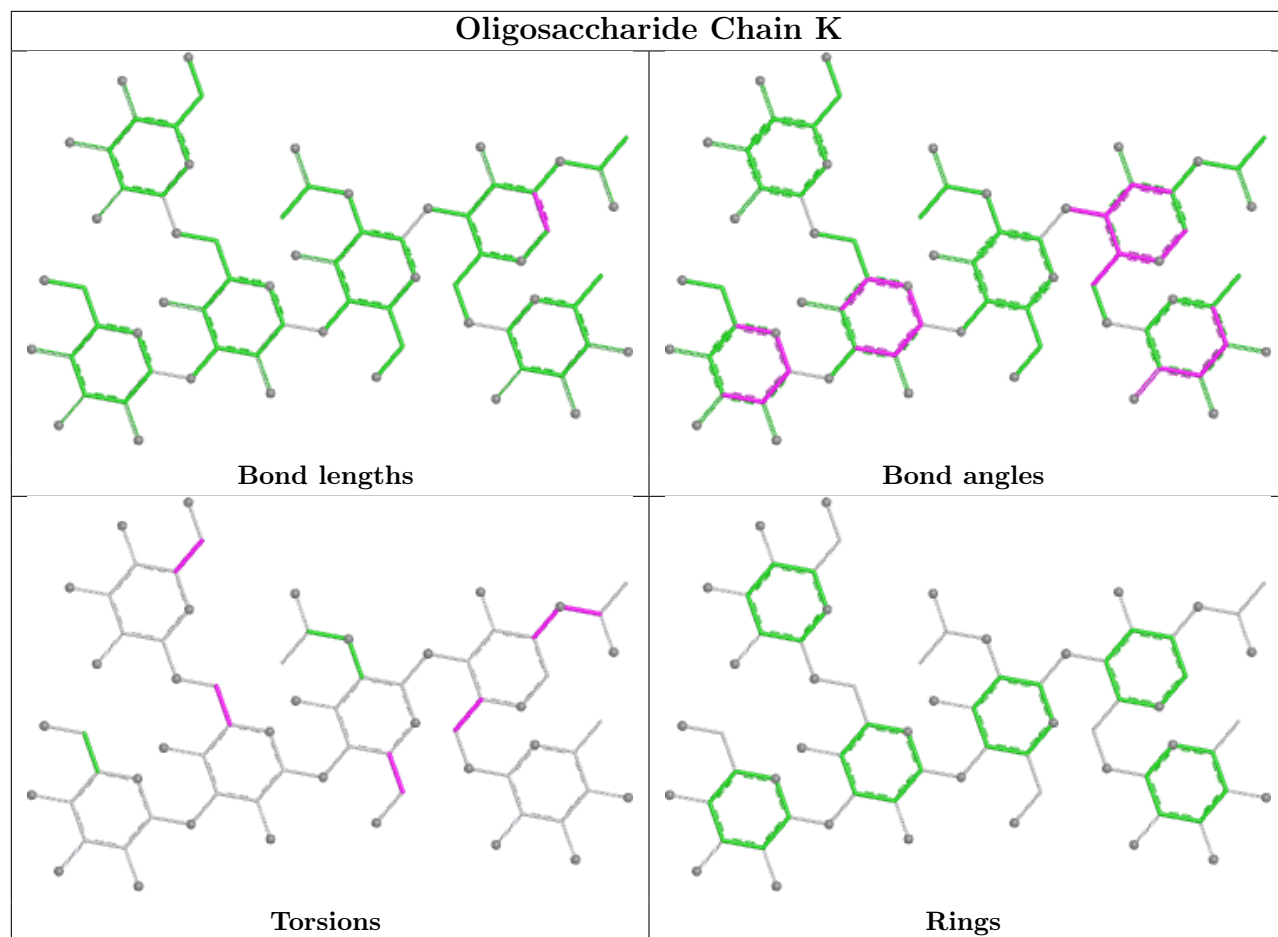
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
3	C	1	NAG	1	0
6	I	2	NAG	6	0
6	I	1	NAG	3	0
3	K	1	NAG	3	0

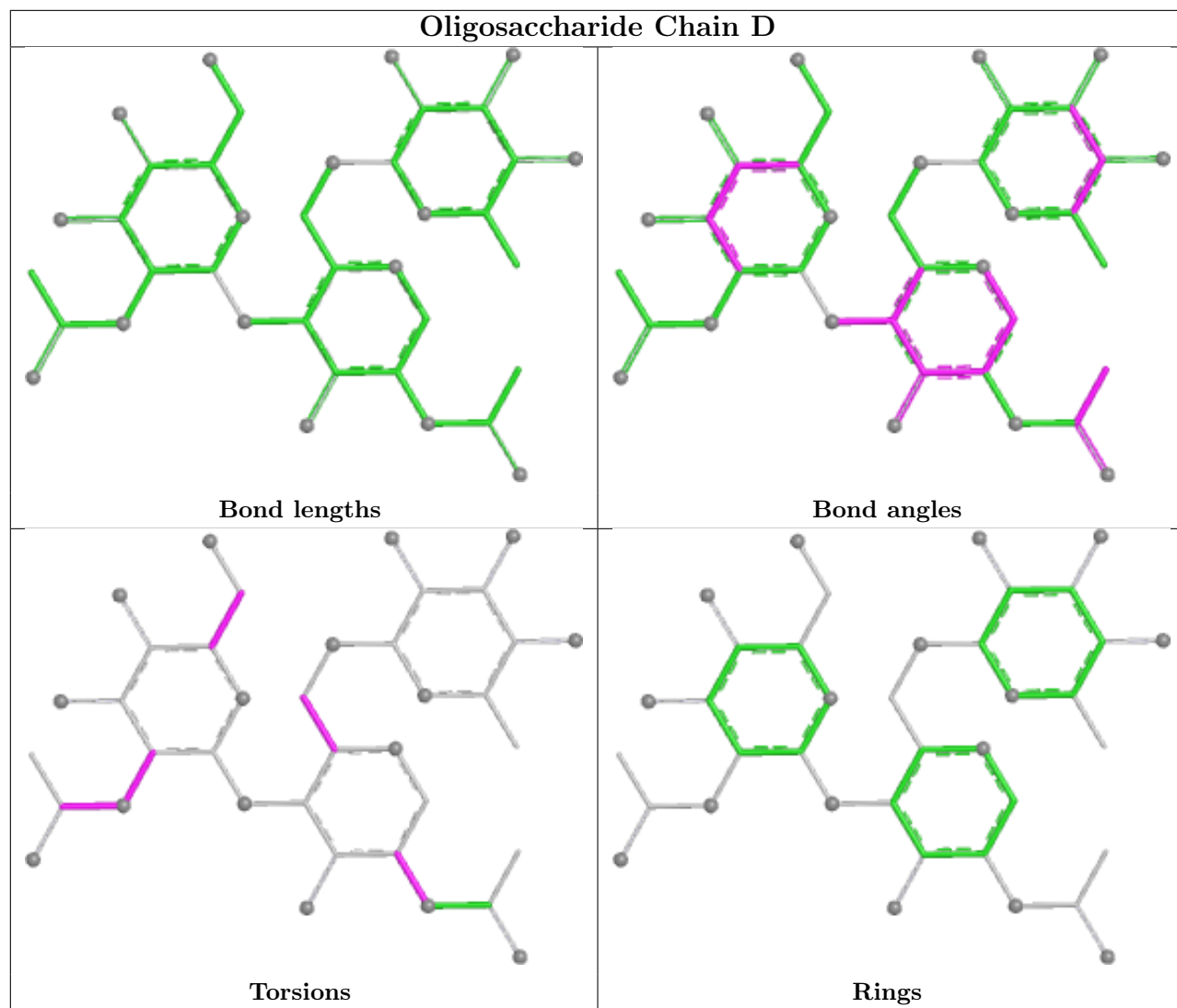
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

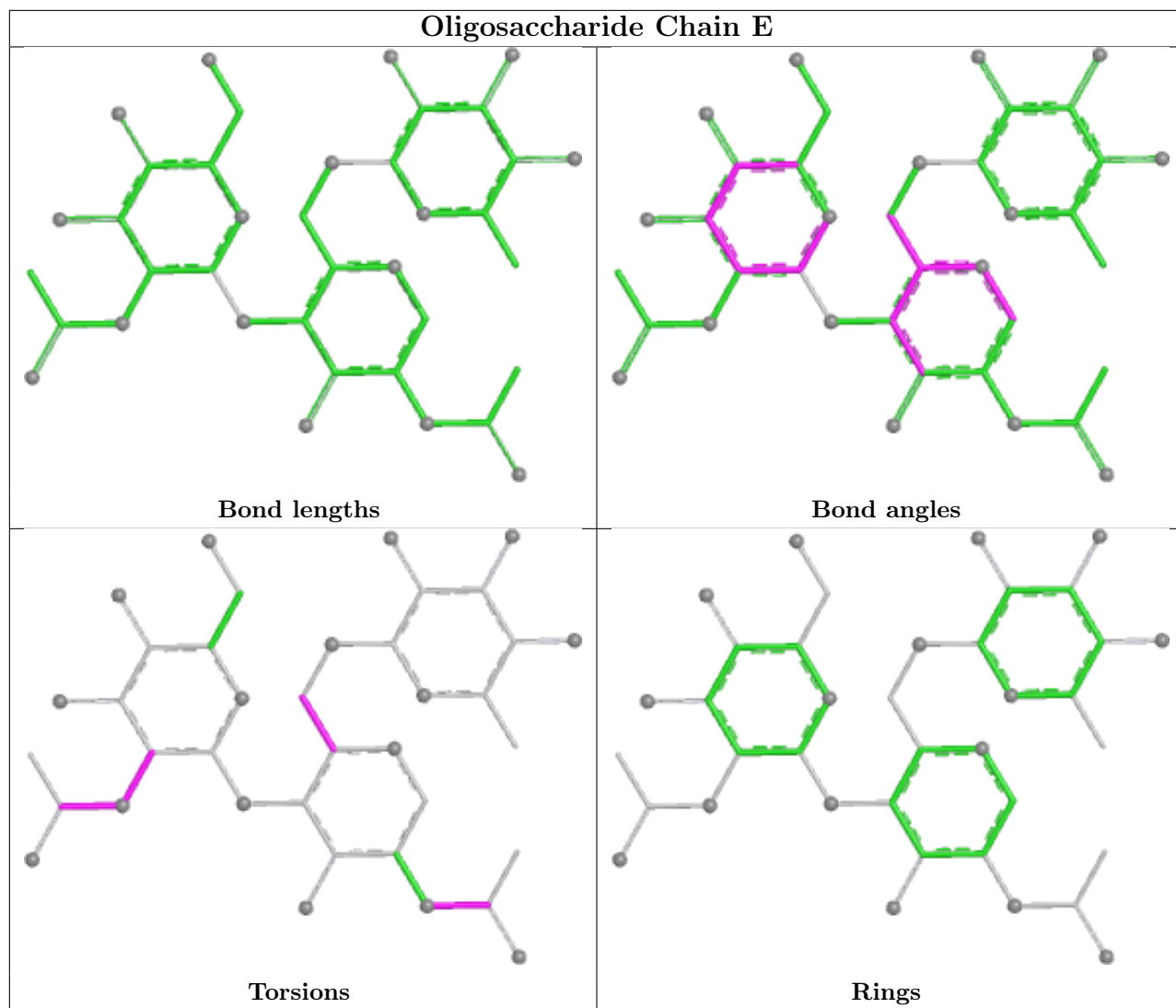


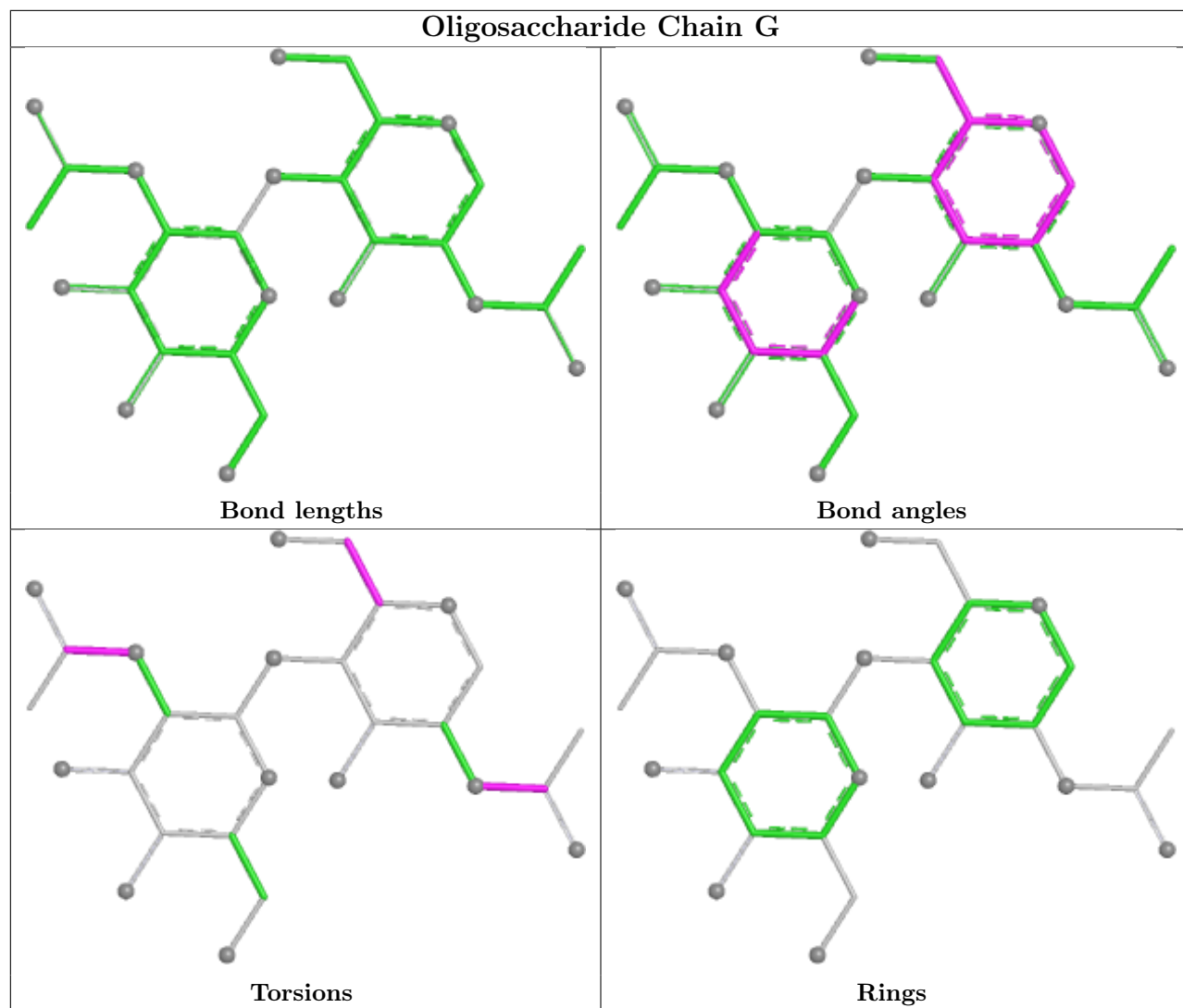


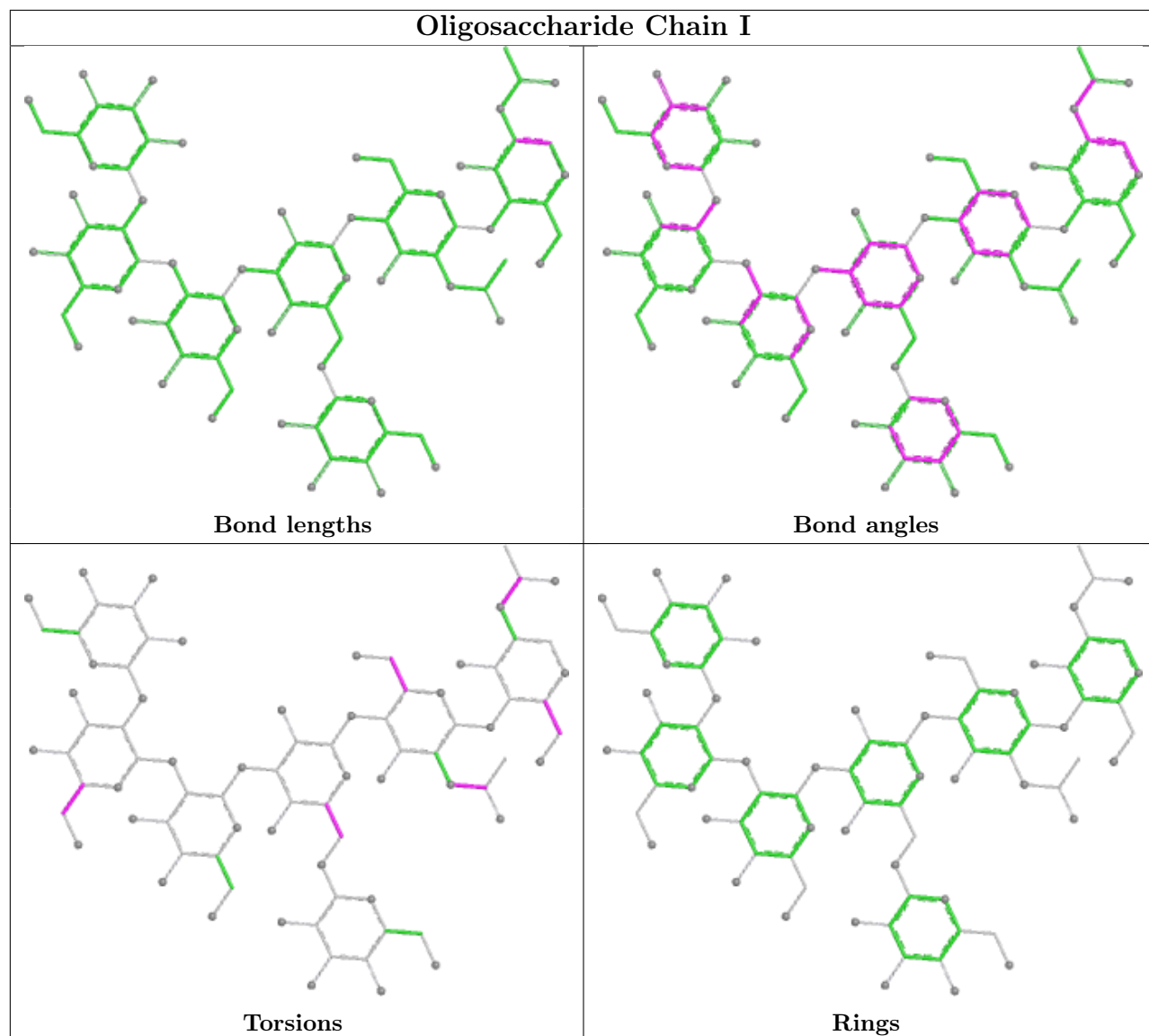


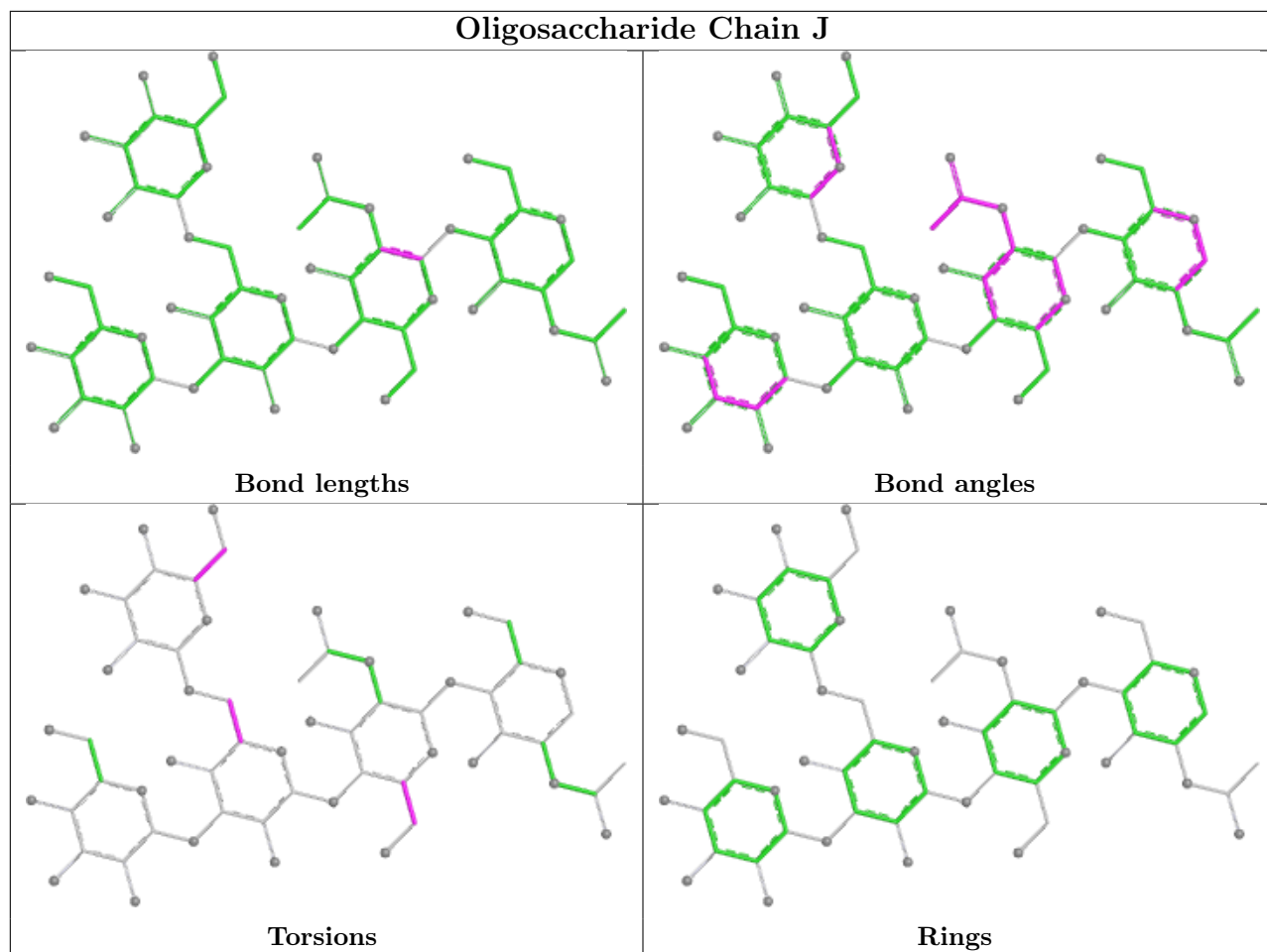


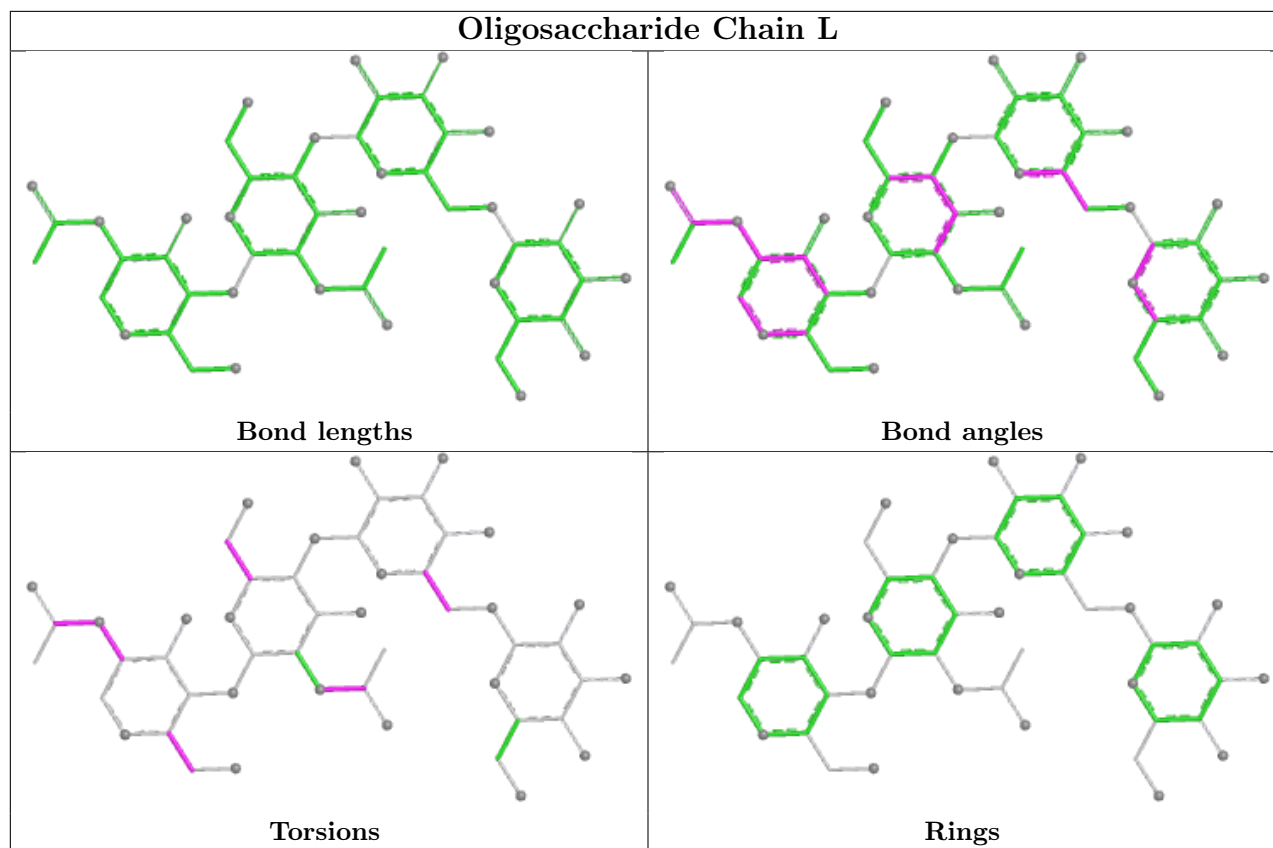












## 5.6 Ligand geometry [i](#)

2 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$
9	NAG	A	1501	1	14,14,15	0.92	1 (7%)	17,19,21	1.00	0
9	NAG	A	1500	1	14,14,15	0.70	0	17,19,21	1.32	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
9	NAG	A	1500	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1501	NAG	O6-C6	2.48	1.52	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1500	NAG	C2-N2-C7	-3.61	118.07	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1500	NAG	C8-C7-N2-C2
9	A	1500	NAG	O7-C7-N2-C2
9	A	1501	NAG	C8-C7-N2-C2
9	A	1501	NAG	O7-C7-N2-C2
9	A	1501	NAG	C4-C5-C6-O6
9	A	1501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	304/316 (96%)	1.60	88 (28%) <b>1</b> <b>3</b>	96, 124, 157, 183	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	GLU	11.6
1	A	311	ARG	8.1
1	A	210	CYS	8.1
1	A	255	SER	7.9
1	A	89	ASP	7.7
1	A	459	ASN	7.7
1	A	306	LEU	6.8
1	A	476	GLN	5.9
1	A	405	TRP	5.7
1	A	391	TRP	5.6
1	A	483	ALA	5.3
1	A	233	ALA	5.1
1	A	467	ALA	5.1
1	A	99	LYS	5.0
1	A	383	GLY	5.0
1	A	93	LEU	4.9
1	A	485	VAL	4.8
1	A	279	THR	4.8
1	A	435	GLN	4.7
1	A	433	ILE	4.7
1	A	313	ALA	4.7
1	A	245	THR	4.3
1	A	274	PHE	4.2
1	A	363	HIS	4.1
1	A	312	GLY	3.9
1	A	271	SER	3.8
1	A	293	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	462	VAL	3.7
1	A	211	ASN	3.6
1	A	482	SER	3.4
1	A	440	TRP	3.4
1	A	284	ARG	3.4
1	A	305	ASN	3.3
1	A	452	ARG	3.3
1	A	217	GLU	3.2
1	A	270	THR	3.2
1	A	278	GLY	3.0
1	A	394	CYS	3.0
1	A	103	LYS	3.0
1	A	349	TRP	3.0
1	A	364	PRO	2.9
1	A	458	CYS	2.9
1	A	309	LYS	2.9
1	A	244	ASP	2.8
1	A	460	SER	2.8
1	A	308	MET	2.8
1	A	424	HIS	2.8
1	A	310	CYS	2.7
1	A	415	VAL	2.7
1	A	350	LYS	2.6
1	A	486	ALA	2.5
1	A	273	TRP	2.5
1	A	346	GLY	2.5
1	A	87	ILE	2.5
1	A	409	TRP	2.5
1	A	441	HIS	2.5
1	A	487	GLU	2.4
1	A	94	PHE	2.4
1	A	399	LEU	2.4
1	A	212	THR	2.3
1	A	344	TRP	2.3
1	A	235	PRO	2.3
1	A	472	THR	2.3
1	A	477	THR	2.3
1	A	361	VAL	2.3
1	A	213	SER	2.3
1	A	387	VAL	2.3
1	A	248	SER	2.2
1	A	377	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	463	THR	2.2
1	A	234	PRO	2.2
1	A	81	THR	2.2
1	A	262	CYS	2.2
1	A	247	TYR	2.2
1	A	491	LEU	2.2
1	A	388	THR	2.2
1	A	240	LEU	2.1
1	A	493	LEU	2.1
1	A	390	MET	2.1
1	A	275	GLY	2.1
1	A	392	THR	2.1
1	A	384	ASP	2.0
1	A	379	ALA	2.0
1	A	451	PRO	2.0
1	A	239	LEU	2.0
1	A	406	PHE	2.0
1	A	269	GLN	2.0
1	A	345	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
2	NAG	H	2	14/15	0.20	0.25	151,156,162,163	0
2	NAG	B	2	14/15	0.24	0.20	114,121,126,130	0
7	NAG	J	2	14/15	0.34	0.21	168,172,184,186	0
2	BMA	H	3	11/12	0.36	0.26	165,174,183,185	0
3	MAN	C	5	11/12	0.46	0.17	132,137,143,145	0
7	MAN	J	5	11/12	0.49	0.16	164,169,173,173	0
2	BMA	B	3	11/12	0.50	0.15	132,135,141,141	0
2	NAG	F	2	14/15	0.52	0.13	125,135,142,145	0
6	MAN	I	4	11/12	0.52	0.15	143,149,156,158	0

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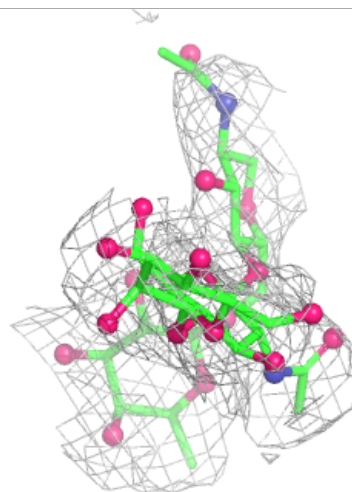
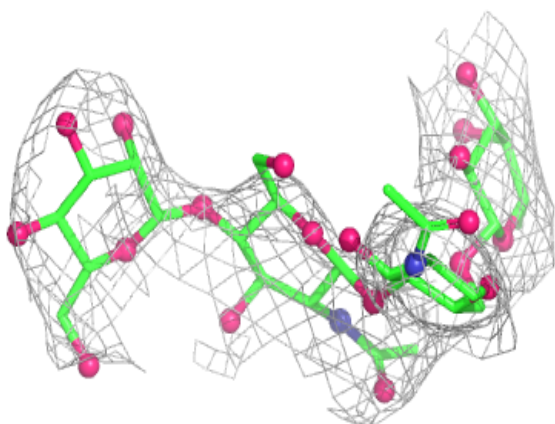
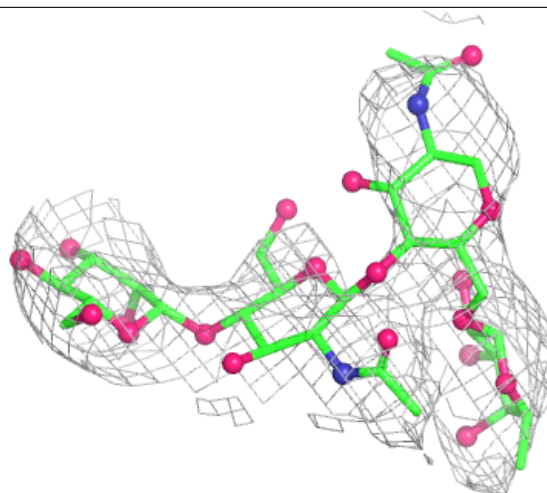
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	L	4	11/12	0.52	0.14	176,184,190,194	0
2	FUC	F	4	10/11	0.54	0.13	121,126,130,132	0
5	NAG	G	2	14/15	0.54	0.20	185,198,212,214	0
3	NAG	C	2	14/15	0.54	0.43	112,115,119,123	0
7	BMA	J	3	11/12	0.56	0.12	177,185,195,199	0
3	MAN	K	5	11/12	0.57	0.14	117,121,125,126	0
3	FUC	K	6	10/11	0.57	0.16	112,117,121,122	0
8	BMA	L	3	11/12	0.58	0.13	163,171,177,180	0
6	MAN	I	6	11/12	0.61	0.19	160,163,168,170	0
7	MAN	J	4	11/12	0.63	0.16	195,203,214,216	0
5	NAG	G	1	14/15	0.66	0.21	182,192,205,210	0
4	NAG	D	1	14/15	0.67	0.16	122,125,128,129	0
4	NAG	D	2	14/15	0.68	0.15	133,138,145,146	0
4	FUC	E	3	10/11	0.69	0.27	154,158,162,163	0
8	NAG	L	2	14/15	0.70	0.15	145,149,157,158	0
3	BMA	C	3	11/12	0.71	0.11	125,129,136,136	0
2	NAG	B	1	14/15	0.72	0.13	110,113,117,117	0
4	NAG	E	2	14/15	0.72	0.14	162,170,178,178	0
3	FUC	C	6	10/11	0.73	0.13	109,111,113,114	0
6	MAN	I	5	11/12	0.73	0.33	140,146,153,155	0
8	NAG	L	1	14/15	0.74	0.12	123,131,138,141	0
7	NAG	J	1	14/15	0.74	0.29	159,163,167,168	0
2	BMA	F	3	11/12	0.75	0.09	149,153,162,164	0
6	MAN	I	7	11/12	0.76	0.17	123,129,133,136	0
2	NAG	H	1	14/15	0.76	0.20	136,140,147,148	0
6	NAG	I	1	14/15	0.77	0.55	114,122,128,131	0
3	MAN	K	4	11/12	0.77	0.07	117,119,124,126	0
6	BMA	I	3	11/12	0.79	0.14	129,133,140,141	0
4	FUC	D	3	10/11	0.79	0.13	121,127,129,132	0
4	NAG	E	1	14/15	0.81	0.17	137,146,154,159	0
3	NAG	C	1	14/15	0.81	0.12	101,106,109,110	0
3	BMA	K	3	11/12	0.82	0.08	111,114,117,118	0
2	FUC	B	4	10/11	0.83	0.10	114,117,121,121	0
2	FUC	H	4	10/11	0.83	0.14	136,141,143,145	0
3	MAN	C	4	11/12	0.84	0.09	136,140,144,147	0
2	NAG	F	1	14/15	0.86	0.15	120,123,128,130	0
6	NAG	I	2	14/15	0.87	0.12	118,125,134,134	0
3	NAG	K	2	14/15	0.87	0.12	107,110,112,112	0
3	NAG	K	1	14/15	0.87	0.16	105,108,110,112	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.

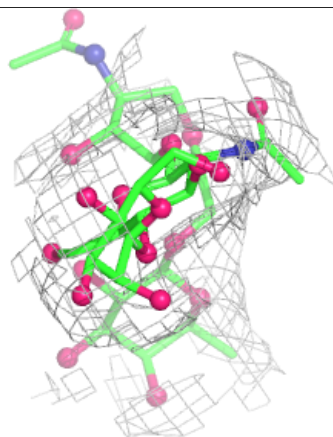
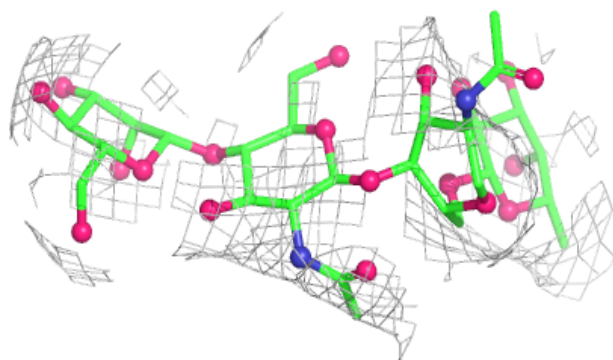
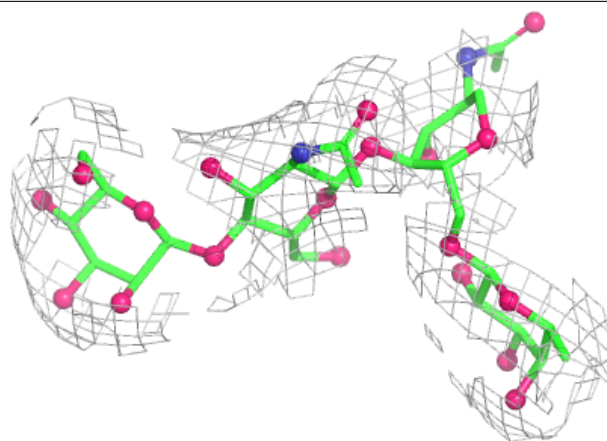
**Electron density around Chain B:**

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

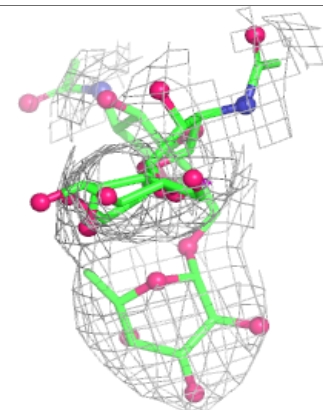
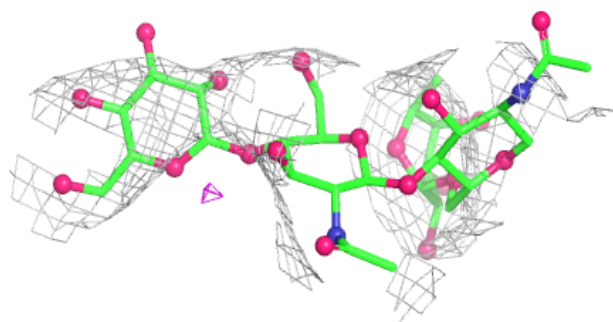
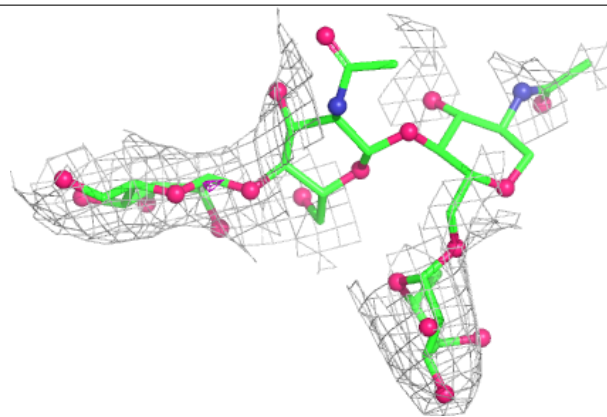


**Electron density around Chain F:**

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

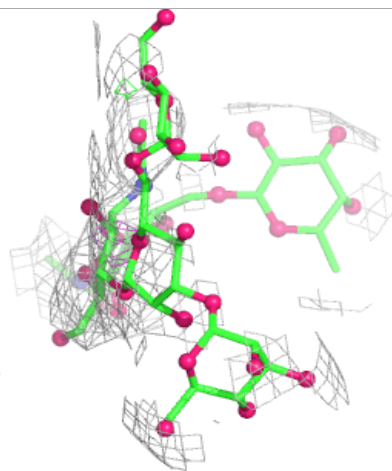
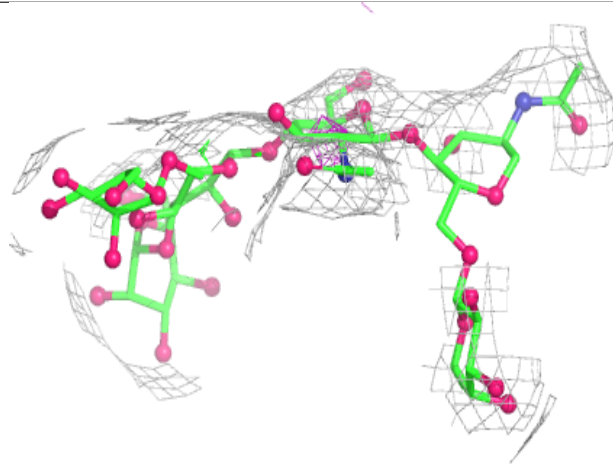
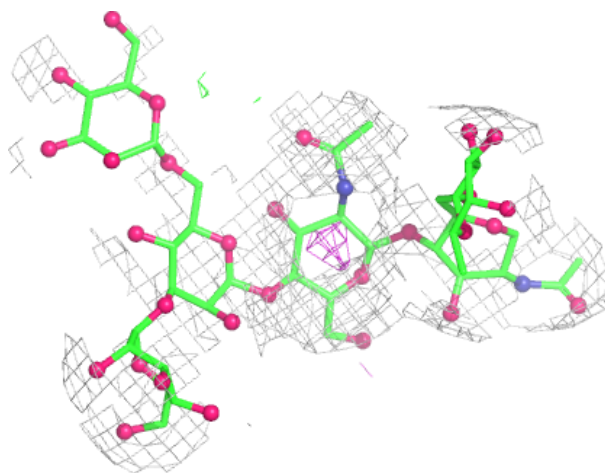
**Electron density around Chain H:**

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



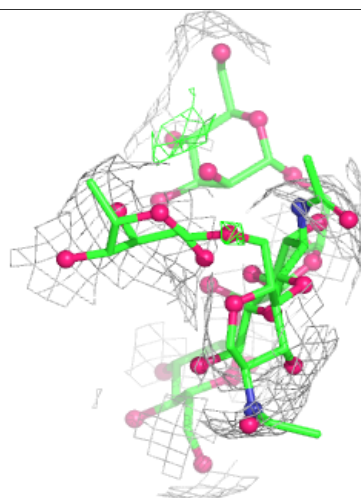
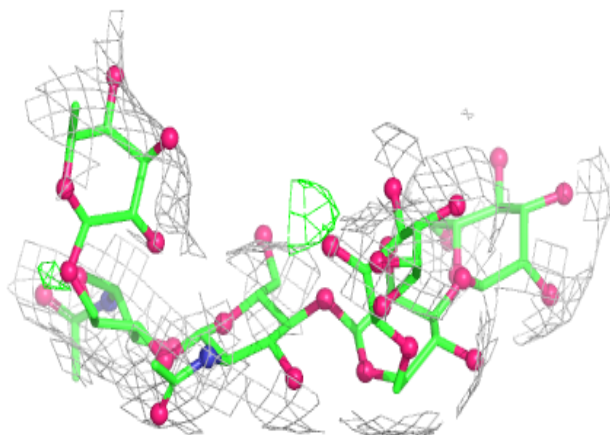
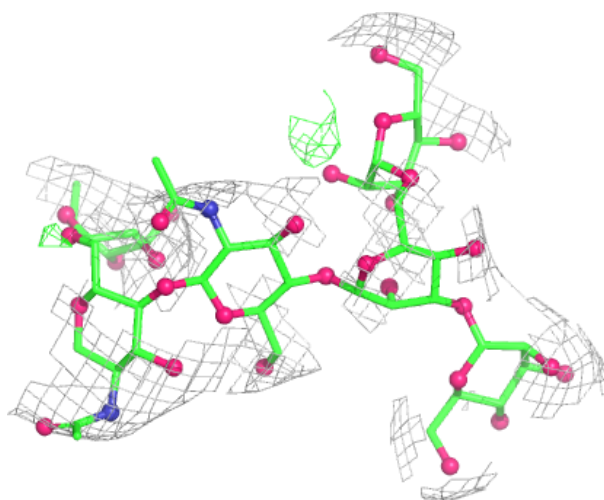
**Electron density around Chain C:**

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



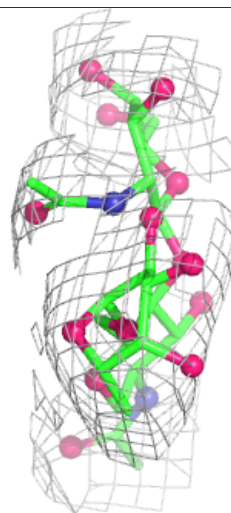
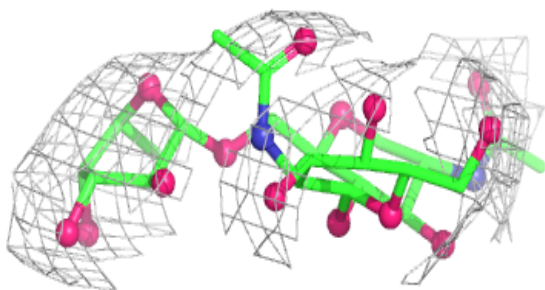
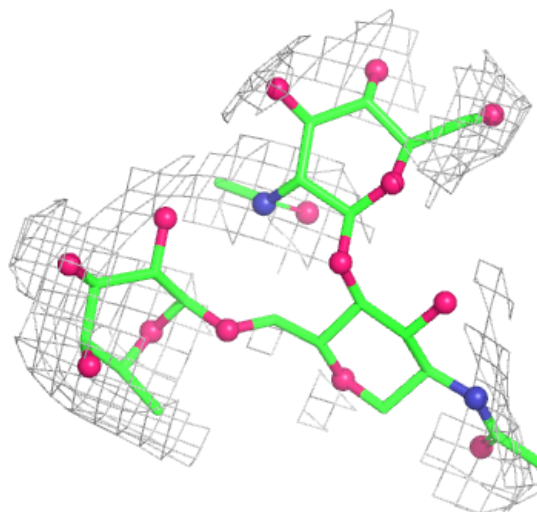
**Electron density around Chain K:**

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



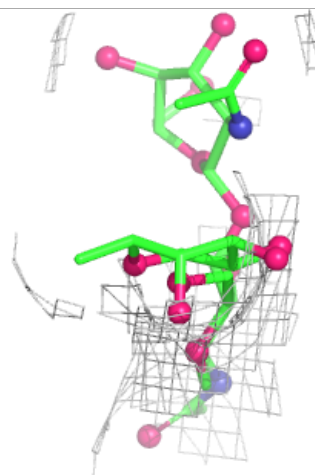
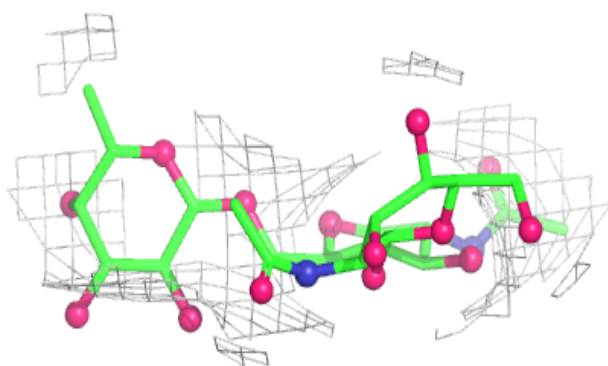
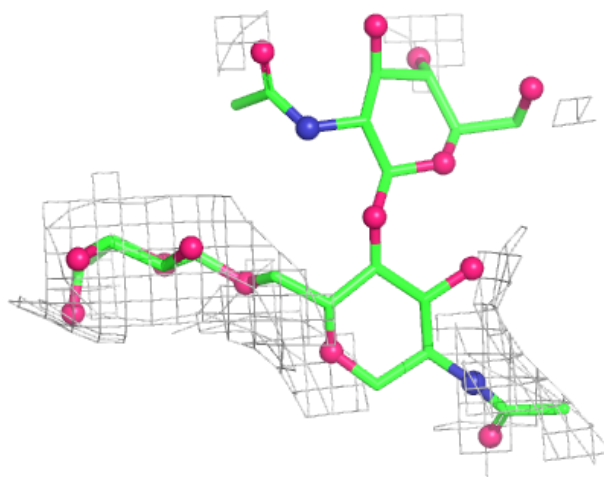
**Electron density around Chain D:**

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



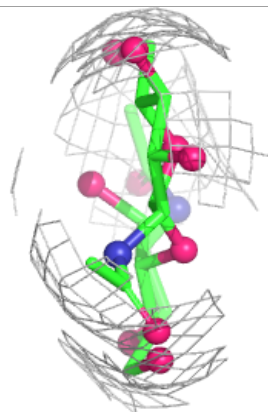
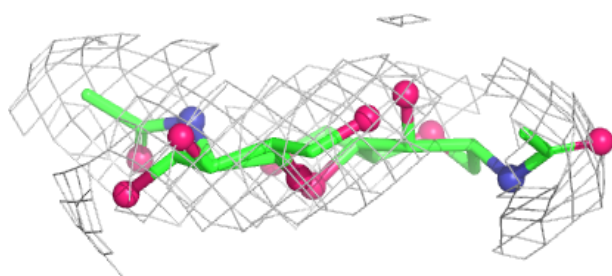
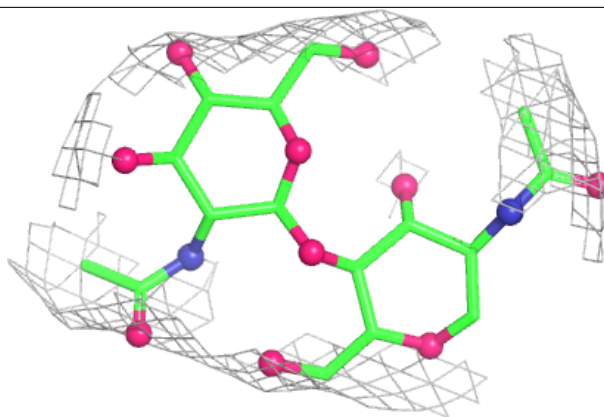
**Electron density around Chain E:**

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

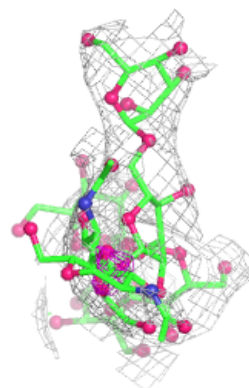
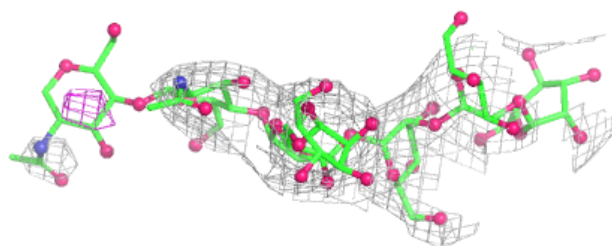
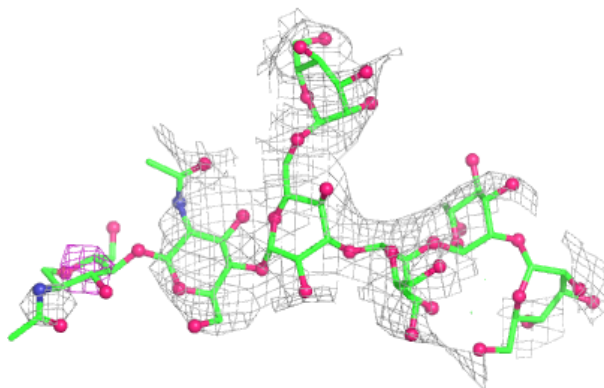


**Electron density around Chain G:**

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

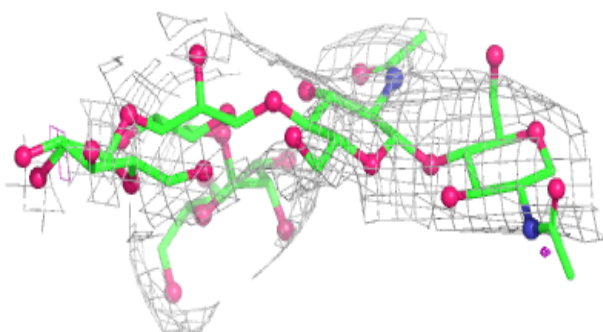
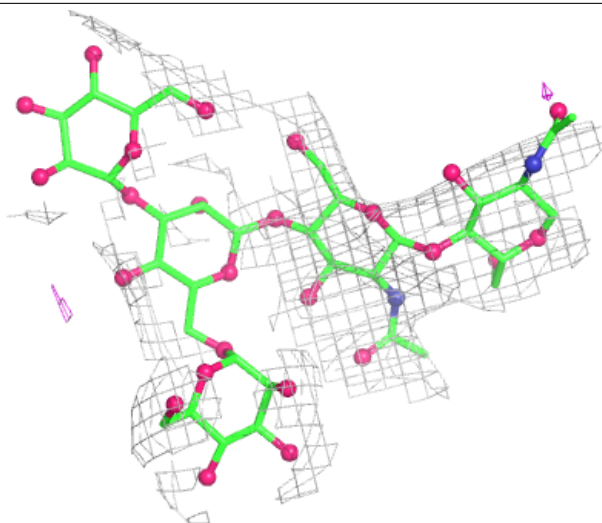
**Electron density around Chain I:**

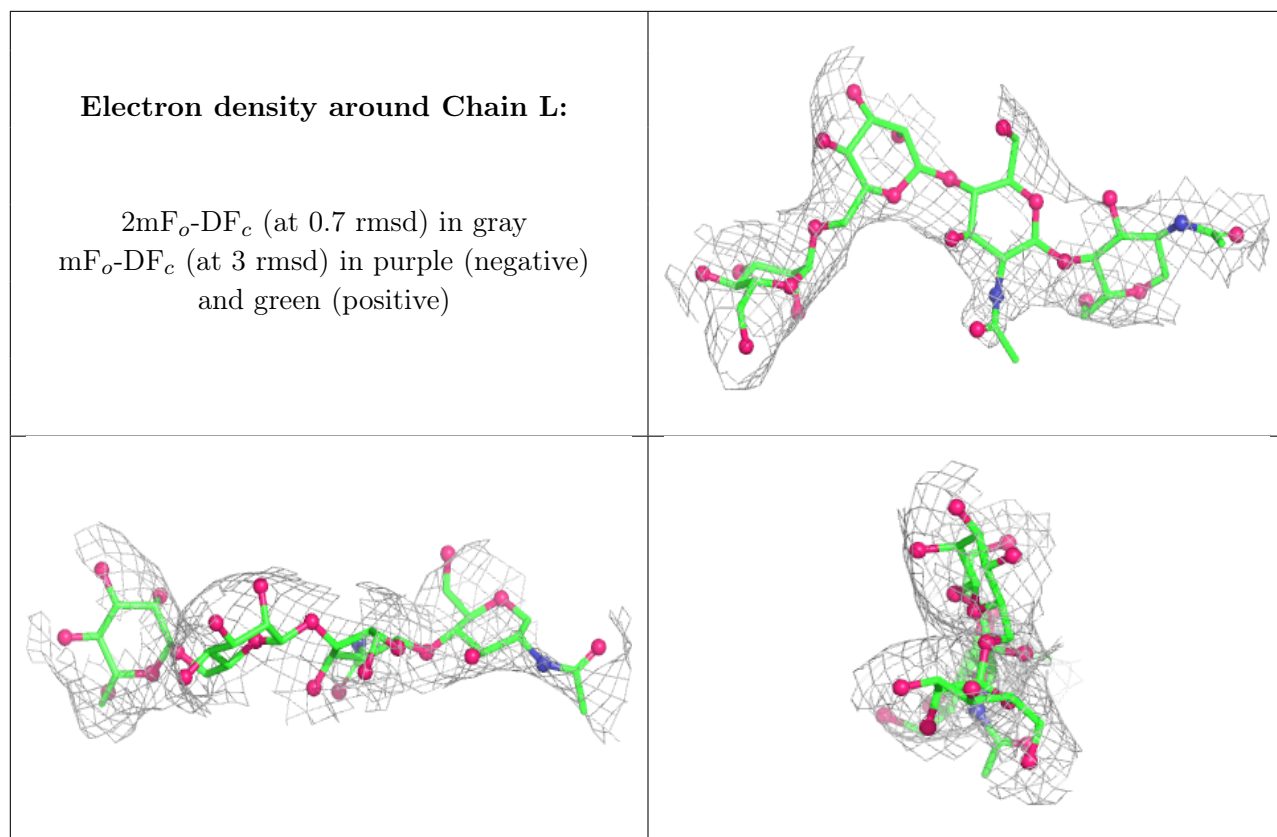
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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
9	NAG	A	1500	14/15	0.71	0.12	147,151,157,160	0
9	NAG	A	1501	14/15	0.84	0.12	140,145,150,155	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.