



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 06:01 PM EDT

PDB ID : 4Q6Y  
Title : Crystal structure of a chemoenzymatic glycoengineered disialylated Fc (di-sFc)  
Authors : Ahmed, A.A.; Giddens, J.; Pincetic, A.; Lomino, J.V.; Ravetch, J.V.; Wang, L.X.; Bjorkman, P.J.  
Deposited on : 2014-04-23  
Resolution : 3.00 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.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

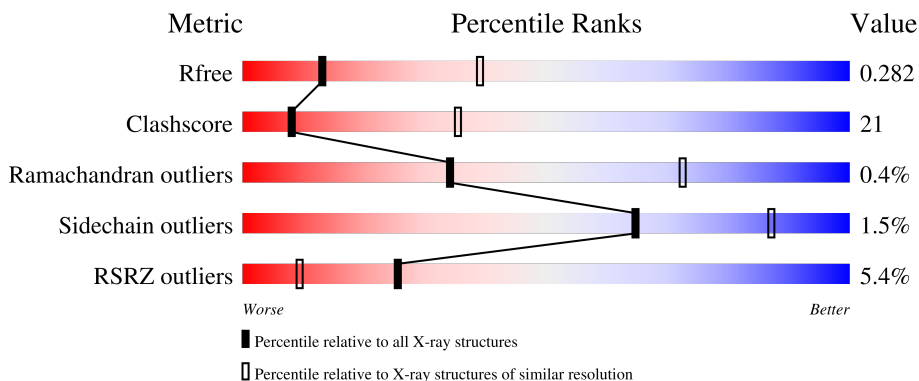
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	221	 3% 68% 25% 6%
1	B	221	 68% 24% 7%
1	C	221	 10% 65% 24% 10%
1	D	221	 6% 64% 22% 12%
2	E	7	 43% 57%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain	
3	F	9		
3	G	9		
4	H	8		

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	E	2	-	-	X	-
3	MAN	F	8	-	-	X	-
3	NAG	G	1	-	-	X	X
3	NAG	G	2	-	-	X	-
3	BMA	G	3	-	-	X	-
3	GAL	G	6	-	-	X	-
3	SIA	G	7	-	-	X	-
3	MAN	G	8	-	-	X	-
4	NAG	H	1	X	-	-	-
4	BMA	H	3	-	-	X	-
4	GAL	H	6	-	-	-	X
4	MAN	H	7	-	-	X	-

## 2 Entry composition [i](#)

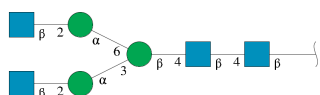
There are 4 unique types of molecules in this entry. The entry contains 6575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ig gamma-1 chain C region.

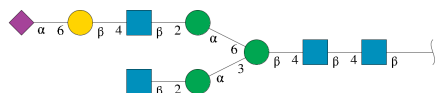
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total 1547	C 985	N 253	O 303	S 6	0	0	0
1	B	206	Total 1610	C 1027	N 269	O 308	S 6	1	0	0
1	C	199	Total 1486	C 946	N 244	O 290	S 6	0	0	0
1	D	195	Total 1503	C 960	N 250	O 287	S 6	1	0	0

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



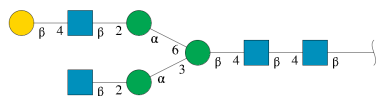
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	7	Total 89	C 50	N 4	O 35	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
			Total	C	N	O			
3	F	9	120	67	5	48	0	0	0
3	G	9	120	67	5	48	0	0	0

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

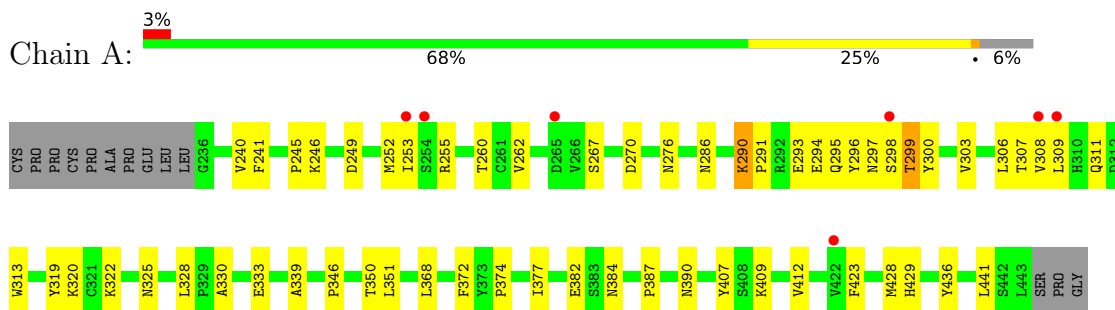


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	8	100	56	4	40	0	0	0

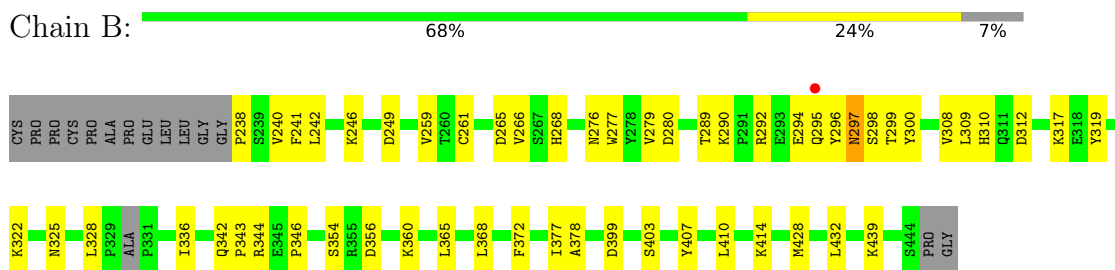
### 3 Residue-property plots [i](#)

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

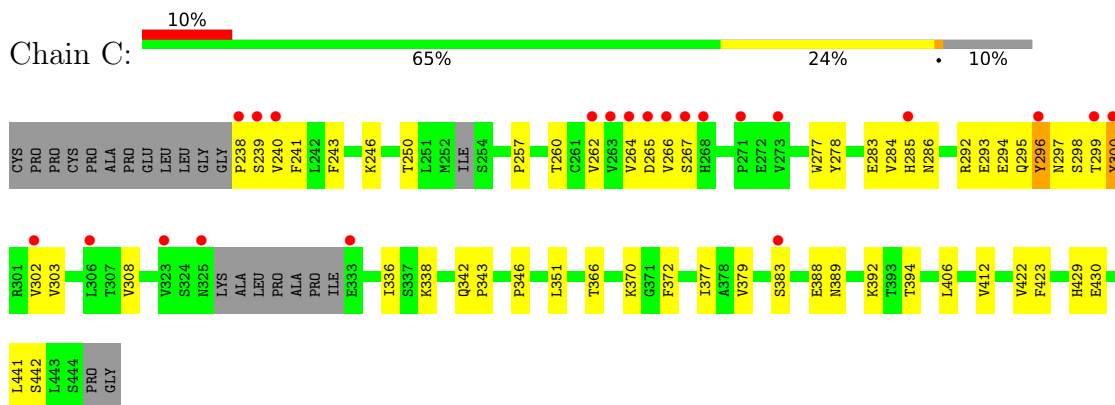
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

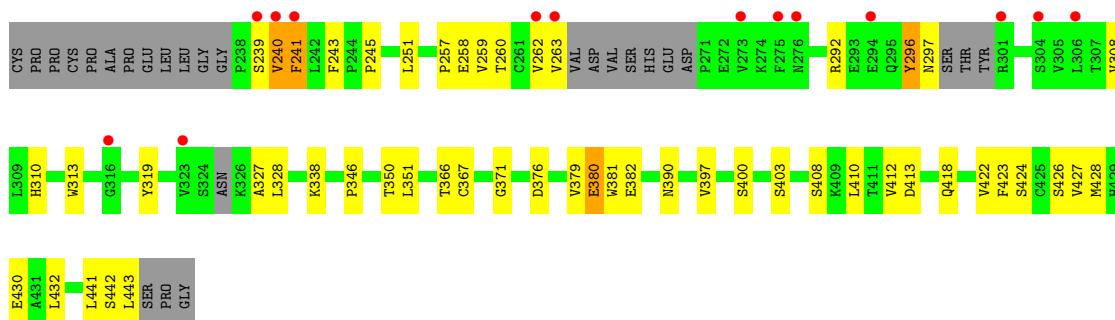


- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 E: 43% 57%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 F: 33% 67%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 G: 11% 89%



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

Chain H: 38% 62%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.73Å 154.22Å 66.12Å 90.00° 110.78° 90.00°	Depositor
Resolution (Å)	48.23 – 3.00 48.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.23-3.00) 97.7 (48.23-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.01Å)	Xtrriage
Refinement program	PHENIX refine	Depositor
R, $R_{free}$	0.260 , 0.280 0.260 , 0.282	Depositor DCC
$R_{free}$ test set	1936 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.566	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 77.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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

### 5.1 Standard geometry

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

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	0.55	0/1590	0.71	2/2186 (0.1%)
1	B	0.58	0/1655	0.74	0/2261
1	C	0.45	0/1524	0.79	4/2089 (0.2%)
1	D	0.58	1/1544 (0.1%)	0.71	1/2107 (0.0%)
All	All	0.54	1/6313 (0.0%)	0.74	7/8643 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	TYR	C-N	5.43	1.46	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	TYR	O-C-N	11.77	141.53	122.70
1	C	300	TYR	C-N-CA	-8.65	100.08	121.70
1	C	300	TYR	CA-C-N	-8.64	98.20	117.20
1	A	246	LYS	C-N-CD	5.98	140.96	128.40
1	A	290	LYS	C-N-CD	5.59	140.13	128.40
1	D	296	TYR	C-N-CA	5.21	134.73	121.70
1	C	441	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	296	TYR	Mainchain

## 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	1547	0	1411	60	14
1	B	1610	0	1535	57	0
1	C	1486	0	1358	61	0
1	D	1503	0	1405	47	0
2	E	89	0	78	14	0
3	F	120	0	102	17	0
3	G	120	0	105	26	14
4	H	100	0	86	13	0
All	All	6575	0	6080	259	14

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 21.

All (259) 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:B:297:ASN:HD21	3:F:1:NAG:C1	1.37	1.37
1:C:297:ASN:HD21	3:G:1:NAG:C1	1.38	1.35
1:B:238:PRO:CG	1:B:328:LEU:HD21	1.80	1.12
1:C:240:VAL:O	1:C:241:PHE:HD1	1.28	1.12
1:B:238:PRO:HG2	1:B:328:LEU:HD21	1.23	1.09
1:D:239:SER:O	1:D:240:VAL:HG22	1.52	1.09
1:B:241:PHE:HE2	3:F:3:BMA:C1	1.65	1.09
1:D:240:VAL:HG11	1:D:263:VAL:HA	1.34	1.03
1:C:297:ASN:OD1	1:C:298:SER:N	1.93	1.02
1:A:328:LEU:HD13	1:A:328:LEU:O	1.64	0.98
1:D:240:VAL:HG11	1:D:263:VAL:CA	1.95	0.97
3:G:3:BMA:C3	3:G:8:MAN:C1	2.42	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:C	1:C:241:PHE:HD1	1.68	0.96
1:B:241:PHE:CE2	3:F:3:BMA:C1	2.48	0.95
1:C:240:VAL:O	1:C:241:PHE:CD1	2.19	0.95
3:G:6:GAL:C6	3:G:7:SIA:C1	2.45	0.94
1:D:241:PHE:CZ	4:H:7:MAN:O6	2.21	0.93
1:A:297:ASN:OD1	1:A:298:SER:N	2.01	0.93
1:C:297:ASN:HD22	3:G:1:NAG:C1	1.80	0.92
1:A:328:LEU:O	1:A:328:LEU:CD1	2.18	0.91
1:C:240:VAL:C	1:C:241:PHE:CD1	2.47	0.88
3:G:6:GAL:O6	3:G:7:SIA:C1	2.21	0.88
1:C:266:VAL:HG12	1:C:267:SER:N	1.87	0.88
3:G:3:BMA:O3	3:G:8:MAN:C2	2.21	0.87
4:H:3:BMA:C3	4:H:7:MAN:C1	2.52	0.87
1:D:239:SER:O	1:D:240:VAL:CG2	2.22	0.87
1:B:268:HIS:NE2	1:B:298:SER:O	2.08	0.87
3:G:2:NAG:HO4	3:G:3:BMA:C1	1.87	0.86
1:C:295:GLN:O	1:C:296:TYR:O	1.93	0.86
1:B:295:GLN:O	1:B:297:ASN:OD1	1.93	0.85
1:A:295:GLN:CB	1:A:296:TYR:C	2.45	0.85
1:C:267:SER:OG	1:C:294:GLU:OE1	1.92	0.85
3:G:6:GAL:H62	3:G:7:SIA:C1	2.06	0.85
1:D:241:PHE:CE1	4:H:7:MAN:O6	2.29	0.84
1:C:267:SER:CB	1:C:294:GLU:OE1	2.25	0.84
1:C:285:HIS:N	1:C:286:ASN:HB2	1.93	0.83
1:D:260:THR:HG21	4:H:5:NAG:H61	1.62	0.82
1:D:240:VAL:HB	1:D:262:VAL:O	1.80	0.81
1:D:240:VAL:HG11	1:D:263:VAL:C	2.00	0.81
3:G:6:GAL:HO6	3:G:7:SIA:C2	1.91	0.81
1:A:290:LYS:HD3	1:A:291:PRO:HD2	1.63	0.80
1:C:266:VAL:CG1	1:C:267:SER:N	2.44	0.80
1:A:295:GLN:CB	1:A:296:TYR:O	2.30	0.79
2:E:2:NAG:H5	3:F:8:MAN:O4	1.83	0.78
1:A:298:SER:O	1:A:299:THR:OG1	2.00	0.78
1:A:308:VAL:HG12	1:A:309:LEU:N	2.00	0.77
1:B:240:VAL:C	1:B:241:PHE:HD1	1.88	0.77
1:D:258:GLU:HB2	4:H:6:GAL:O3	1.85	0.76
3:G:1:NAG:HO4	3:G:2:NAG:C1	1.95	0.76
1:C:297:ASN:OD1	1:C:299:THR:N	2.18	0.76
1:C:296:TYR:O	1:C:297:ASN:OD1	2.04	0.76
1:D:240:VAL:C	1:D:241:PHE:CG	2.59	0.75
1:A:328:LEU:HD13	1:A:328:LEU:C	2.07	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:NAG:C4	3:G:2:NAG:C1	2.64	0.74
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.74
1:A:240:VAL:O	1:A:241:PHE:HD1	1.70	0.74
3:F:2:NAG:H83	3:F:4:MAN:O4	1.88	0.74
1:B:325:ASN:HB3	1:B:328:LEU:CD1	2.18	0.73
1:A:295:GLN:CB	1:A:296:TYR:CA	2.67	0.73
1:D:240:VAL:O	1:D:241:PHE:CG	2.42	0.73
2:E:3:BMA:C3	2:E:4:MAN:C1	2.68	0.71
1:A:298:SER:C	1:A:299:THR:HG23	2.09	0.71
1:C:278:TYR:CE2	1:C:283:GLU:OE1	2.43	0.71
1:C:351:LEU:HB2	1:C:366:THR:HB	1.72	0.71
2:E:2:NAG:C5	3:F:8:MAN:O4	2.38	0.70
3:G:1:NAG:O4	3:G:2:NAG:C2	2.39	0.70
1:D:240:VAL:CG1	1:D:263:VAL:HA	2.16	0.70
3:G:6:GAL:C6	3:G:7:SIA:O1B	2.38	0.70
1:D:260:THR:HG21	4:H:5:NAG:C6	2.21	0.70
1:C:266:VAL:CG1	1:C:267:SER:H	2.04	0.70
1:B:325:ASN:HB3	1:B:328:LEU:HD12	1.75	0.69
1:B:414:LYS:NZ	1:D:413:ASP:OD1	2.26	0.69
1:C:422:VAL:HG22	1:C:442:SER:HB2	1.75	0.69
3:G:3:BMA:H3	3:G:8:MAN:C1	2.23	0.68
1:A:241:PHE:CE2	2:E:2:NAG:H61	2.29	0.68
1:A:308:VAL:CG1	1:A:309:LEU:N	2.57	0.68
1:B:342:GLN:CD	1:B:342:GLN:H	1.97	0.67
1:C:285:HIS:H	1:C:286:ASN:HB2	1.58	0.67
2:E:3:BMA:HO3	2:E:4:MAN:C1	2.01	0.67
1:D:240:VAL:C	1:D:241:PHE:CD2	2.68	0.67
1:D:239:SER:C	1:D:240:VAL:HG22	2.14	0.67
1:A:306:LEU:HD23	1:A:307:THR:O	1.95	0.67
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.77	0.67
1:A:241:PHE:HE2	2:E:2:NAG:H61	1.60	0.67
1:A:290:LYS:HD3	1:A:291:PRO:CD	2.24	0.66
4:H:3:BMA:O6	4:H:4:MAN:O5	2.13	0.66
1:B:297:ASN:OD1	1:B:297:ASN:N	2.27	0.66
1:C:297:ASN:CG	1:C:298:SER:H	1.96	0.66
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.32	0.65
1:B:342:GLN:OE1	1:B:342:GLN:N	2.22	0.64
1:D:327:ALA:C	1:D:328:LEU:HD12	2.17	0.64
2:E:2:NAG:O6	3:F:8:MAN:H5	1.97	0.64
1:C:285:HIS:CB	1:C:286:ASN:HA	2.26	0.64
1:C:278:TYR:CZ	1:C:283:GLU:OE1	2.51	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:SER:HB2	1:C:388:GLU:OE2	1.99	0.63
3:G:3:BMA:H2	3:G:8:MAN:H5	1.81	0.63
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.81	0.62
1:A:295:GLN:CB	1:A:296:TYR:HA	2.28	0.62
1:B:346:PRO:HG2	1:B:432:LEU:HD21	1.82	0.62
1:A:240:VAL:O	1:A:241:PHE:CD1	2.51	0.62
3:F:3:BMA:C3	3:F:8:MAN:C1	2.78	0.61
1:B:342:GLN:O	1:B:342:GLN:HG2	2.01	0.61
1:B:325:ASN:CB	1:B:328:LEU:HD12	2.30	0.60
1:A:299:THR:C	1:A:300:TYR:HD2	2.04	0.60
4:H:3:BMA:O3	4:H:7:MAN:C2	2.50	0.60
1:C:388:GLU:HG3	1:C:389:ASN:H	1.66	0.60
1:A:295:GLN:HA	1:A:299:THR:O	2.02	0.59
1:A:290:LYS:HB2	1:A:303:VAL:O	2.02	0.59
1:C:240:VAL:HG12	1:C:241:PHE:N	2.17	0.59
1:C:239:SER:OG	1:C:264:VAL:CG2	2.50	0.59
3:G:3:BMA:O3	3:G:8:MAN:C3	2.51	0.59
1:C:383:SER:CB	1:C:388:GLU:OE2	2.51	0.59
1:A:328:LEU:HD11	1:A:330:ALA:O	2.02	0.58
1:D:382:GLU:HG2	1:D:424:SER:HB2	1.85	0.58
1:A:298:SER:O	1:A:299:THR:CB	2.49	0.58
1:A:299:THR:O	1:A:300:TYR:HD2	1.86	0.58
1:D:241:PHE:HZ	4:H:7:MAN:O6	1.82	0.58
1:B:297:ASN:HD22	3:F:1:NAG:C1	2.07	0.57
1:D:260:THR:CG2	4:H:5:NAG:H61	2.34	0.57
1:D:241:PHE:CD2	1:D:241:PHE:N	2.72	0.57
1:C:260:THR:HG23	1:C:303:VAL:CG1	2.35	0.57
1:C:377:ILE:HG13	1:C:429:HIS:HB2	1.86	0.57
1:C:257:PRO:HG2	1:C:308:VAL:O	2.04	0.57
1:C:284:VAL:HB	1:C:286:ASN:HB2	1.86	0.57
1:B:265:ASP:HA	1:B:299:THR:HG21	1.87	0.56
1:C:412:VAL:HG11	1:C:423:PHE:CE1	2.41	0.56
1:B:241:PHE:HD1	1:B:241:PHE:N	2.02	0.56
1:C:394:THR:HA	1:D:397:VAL:HG21	1.87	0.56
3:G:6:GAL:H62	3:G:7:SIA:O1B	2.04	0.55
1:A:297:ASN:CG	1:A:298:SER:H	2.10	0.55
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.89	0.55
1:B:241:PHE:N	1:B:241:PHE:CD1	2.73	0.55
1:B:246:LYS:CD	3:F:6:GAL:O4	2.55	0.55
1:A:390:ASN:O	1:A:390:ASN:ND2	2.40	0.55
1:C:292:ARG:HB3	1:C:302:VAL:HG22	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:HD3	3:F:6:GAL:O4	2.08	0.54
1:C:262:VAL:HG22	1:C:303:VAL:HG22	1.90	0.54
1:B:344:ARG:HH11	1:B:403:SER:HB3	1.71	0.54
4:H:3:BMA:H3	4:H:7:MAN:C1	2.36	0.54
4:H:3:BMA:HO3	4:H:7:MAN:C1	2.14	0.54
3:G:3:BMA:O3	3:G:8:MAN:H3	2.07	0.54
1:B:266:VAL:CG2	1:B:300:TYR:HB2	2.38	0.54
2:E:1:NAG:C4	2:E:2:NAG:C1	2.82	0.54
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.89	0.53
3:G:1:NAG:HO3	3:G:2:NAG:C1	2.21	0.53
1:D:251:LEU:HD13	1:D:428:MET:O	2.09	0.53
1:B:238:PRO:CD	1:B:328:LEU:HD21	2.37	0.52
2:E:3:BMA:O3	2:E:4:MAN:C2	2.50	0.52
1:B:280:ASP:OD2	1:B:317:LYS:HD2	2.08	0.52
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.92	0.51
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.45	0.51
1:A:240:VAL:C	1:A:241:PHE:CD1	2.83	0.51
2:E:1:NAG:HO4	2:E:2:NAG:C1	2.16	0.51
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.45	0.51
1:A:325:ASN:HB3	1:A:328:LEU:HB3	1.93	0.51
1:A:241:PHE:HE2	2:E:2:NAG:C6	2.24	0.51
1:A:382:GLU:HA	1:A:387:PRO:HA	1.93	0.50
1:D:308:VAL:HG22	1:D:319:TYR:CE1	2.46	0.50
1:A:328:LEU:O	1:A:328:LEU:HD12	2.07	0.50
1:A:350:THR:HB	1:A:441:LEU:HB2	1.93	0.50
1:D:240:VAL:O	1:D:241:PHE:CD1	2.64	0.49
1:A:377:ILE:HG13	1:A:429:HIS:HB2	1.93	0.49
3:G:1:NAG:O3	3:G:2:NAG:C1	2.61	0.49
1:C:241:PHE:CD1	1:C:241:PHE:N	2.74	0.49
1:D:371:GLY:HA2	1:D:403:SER:OG	2.13	0.49
3:G:2:NAG:O3	3:G:4:MAN:H3	2.12	0.49
1:D:245:PRO:HD3	1:D:259:VAL:HG12	1.94	0.49
1:B:325:ASN:HB3	1:B:328:LEU:HG	1.95	0.48
1:A:298:SER:O	1:A:299:THR:HG23	2.13	0.48
1:A:308:VAL:CG1	1:A:319:TYR:OH	2.61	0.48
1:C:243:PHE:CD2	3:G:5:NAG:H5	2.49	0.48
1:A:328:LEU:CD1	1:A:330:ALA:C	2.82	0.48
1:C:266:VAL:HG13	1:C:267:SER:H	1.79	0.48
1:C:260:THR:CG2	1:C:303:VAL:CG1	2.91	0.48
1:A:328:LEU:CD1	1:A:328:LEU:C	2.75	0.48
2:E:2:NAG:C5	3:F:8:MAN:HO4	2.26	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:LYS:NZ	1:D:400:SER:OG	2.44	0.48
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.96	0.47
1:A:249:ASP:OD1	1:A:255:ARG:NE	2.43	0.47
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.47
1:B:325:ASN:N	1:B:328:LEU:HD12	2.29	0.47
2:E:2:NAG:O6	3:F:8:MAN:O4	2.27	0.47
1:D:346:PRO:HG2	1:D:432:LEU:HD21	1.96	0.47
1:C:238:PRO:HB3	1:C:265:ASP:HB2	1.97	0.47
1:D:422:VAL:HG22	1:D:442:SER:HB2	1.96	0.46
3:F:3:BMA:O3	3:F:8:MAN:C2	2.60	0.46
1:A:293:GLU:HA	1:A:294:GLU:HA	1.67	0.46
1:B:372:PHE:CD1	1:B:377:ILE:HD12	2.51	0.46
1:A:290:LYS:CD	1:A:291:PRO:HD2	2.38	0.46
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.98	0.46
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.16	0.45
1:A:428:MET:HG2	1:A:436:TYR:HD2	1.80	0.45
1:B:241:PHE:CE2	3:F:2:NAG:H4	2.51	0.45
1:B:325:ASN:HB3	1:B:328:LEU:CG	2.46	0.45
1:A:253:ILE:O	1:A:253:ILE:HG22	2.17	0.45
1:A:267:SER:OG	1:A:270:ASP:HB2	2.17	0.45
1:C:277:TRP:HB2	1:C:284:VAL:HG23	1.98	0.45
3:G:7:SIA:H7	3:G:7:SIA:C10	2.47	0.45
1:A:245:PRO:HD2	1:A:313:TRP:CZ2	2.51	0.45
1:B:360:LYS:O	1:B:414:LYS:HE2	2.17	0.45
1:C:338:LYS:HD2	1:C:430:GLU:OE1	2.17	0.45
1:B:325:ASN:CB	1:B:328:LEU:CD1	2.91	0.45
1:C:379:VAL:HG21	1:C:406:LEU:HD11	1.98	0.45
1:A:409:LYS:NZ	1:B:399:ASP:OD2	2.50	0.44
1:D:243:PHE:CZ	4:H:3:BMA:H5	2.52	0.44
1:B:240:VAL:C	1:B:241:PHE:CD1	2.79	0.44
1:B:249:ASP:O	1:B:310:HIS:HE1	2.01	0.44
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.52	0.44
1:A:311:GLN:OE1	1:A:311:GLN:N	2.47	0.44
1:A:339:ALA:HB3	1:A:374:PRO:HB3	2.00	0.44
1:C:336:ILE:HD12	1:C:336:ILE:HA	1.87	0.44
1:B:289:THR:HG22	1:B:290:LYS:O	2.18	0.44
1:D:418:GLN:HA	1:D:443:LEU:HD22	2.00	0.43
1:B:346:PRO:HB3	1:B:372:PHE:HB3	2.01	0.43
1:D:367:CYS:HB3	1:D:408:SER:HB3	1.99	0.43
1:C:243:PHE:CG	3:G:5:NAG:H5	2.52	0.43
1:C:346:PRO:CB	1:C:372:PHE:HB3	2.47	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:PRO:HD3	1:D:310:HIS:CE1	2.54	0.43
1:D:380:GLU:HG2	1:D:426:SER:OG	2.19	0.43
1:B:241:PHE:HE2	3:F:3:BMA:C2	2.25	0.43
1:A:308:VAL:HG11	1:A:319:TYR:OH	2.20	0.42
1:B:344:ARG:NH1	1:B:403:SER:HB3	2.33	0.42
1:C:293:GLU:O	1:C:294:GLU:HB2	2.20	0.42
1:C:342:GLN:HA	1:C:343:PRO:HD3	1.82	0.42
1:B:309:LEU:HD12	1:B:312:ASP:OD2	2.20	0.42
1:C:267:SER:HB3	1:C:294:GLU:OE1	2.14	0.42
1:D:308:VAL:HG11	1:D:313:TRP:HB2	2.01	0.42
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.19	0.42
1:A:412:VAL:HG11	1:A:423:PHE:CE1	2.53	0.42
1:C:239:SER:OG	1:C:264:VAL:HG22	2.19	0.42
1:D:442:SER:OG	1:D:443:LEU:N	2.53	0.42
1:C:383:SER:HB3	1:C:388:GLU:OE2	2.19	0.42
1:A:320:LYS:HD2	1:A:333:GLU:OE1	2.19	0.42
1:D:338:LYS:HD2	1:D:430:GLU:OE1	2.20	0.42
1:D:351:LEU:HB2	1:D:366:THR:HB	2.02	0.42
1:A:299:THR:O	1:A:300:TYR:CD2	2.70	0.42
1:B:296:TYR:O	1:B:296:TYR:CG	2.70	0.42
1:C:370:LYS:HB2	1:C:370:LYS:HE2	1.81	0.42
1:B:279:VAL:HG23	1:B:279:VAL:O	2.19	0.41
1:D:327:ALA:O	1:D:328:LEU:HD12	2.20	0.41
1:D:350:THR:HB	1:D:441:LEU:HD22	2.01	0.41
1:C:266:VAL:HB	1:C:300:TYR:CB	2.50	0.41
1:D:240:VAL:CG1	1:D:263:VAL:C	2.82	0.41
2:E:2:NAG:O6	3:F:8:MAN:C5	2.66	0.41
1:C:240:VAL:CG1	1:C:241:PHE:N	2.83	0.41
1:C:246:LYS:O	1:C:250:THR:HG23	2.20	0.41
1:C:241:PHE:HE2	3:G:3:BMA:C1	2.33	0.41
1:A:260:THR:HG22	1:A:262:VAL:HG23	2.02	0.41
1:A:298:SER:O	1:A:299:THR:CG2	2.69	0.41
1:B:292:ARG:HD2	1:B:300:TYR:CD1	2.56	0.41
1:B:342:GLN:HA	1:B:343:PRO:HD3	1.79	0.41
1:C:241:PHE:CE2	3:G:2:NAG:H4	2.56	0.41
1:C:284:VAL:HB	1:C:286:ASN:CB	2.51	0.41
1:B:294:GLU:HB3	1:B:300:TYR:CD1	2.56	0.41
1:D:390:ASN:O	1:D:410:LEU:HD12	2.21	0.41
1:A:351:LEU:HD23	1:B:354:SER:HB2	2.02	0.40
1:A:328:LEU:CD1	1:A:330:ALA:O	2.67	0.40
1:B:325:ASN:H	1:B:328:LEU:HD12	1.86	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:VAL:HG11	1:D:423:PHE:CE1	2.56	0.40

All (14) 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)
1:A:286:ASN:CG	3:G:7:SIA:N5[2_445]	1.08	1.12
1:A:286:ASN:ND2	3:G:7:SIA:N5[2_445]	1.41	0.79
1:A:286:ASN:OD1	3:G:7:SIA:C6[2_445]	1.46	0.74
1:A:286:ASN:ND2	3:G:7:SIA:C4[2_445]	1.51	0.69
1:A:286:ASN:ND2	3:G:7:SIA:O4[2_445]	1.54	0.66
1:A:286:ASN:ND2	3:G:7:SIA:C5[2_445]	1.60	0.60
1:A:286:ASN:OD1	3:G:7:SIA:C5[2_445]	1.60	0.60
1:A:286:ASN:CG	3:G:7:SIA:C5[2_445]	1.62	0.58
1:A:306:LEU:CD2	3:G:7:SIA:C11[2_445]	1.75	0.45
1:A:286:ASN:CB	3:G:7:SIA:N5[2_445]	1.78	0.42
1:A:286:ASN:OD1	3:G:7:SIA:N5[2_445]	1.91	0.29
1:A:286:ASN:CG	3:G:7:SIA:C4[2_445]	1.97	0.23
1:A:286:ASN:OD1	3:G:7:SIA:C4[2_445]	2.03	0.17
1:A:306:LEU:CG	3:G:7:SIA:C11[2_445]	2.05	0.15

## 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	206/221 (93%)	191 (93%)	14 (7%)	1 (0%)	29	68
1	B	202/221 (91%)	194 (96%)	8 (4%)	0	100	100
1	C	193/221 (87%)	180 (93%)	12 (6%)	1 (0%)	29	68
1	D	187/221 (85%)	179 (96%)	7 (4%)	1 (0%)	29	68
All	All	788/884 (89%)	744 (94%)	41 (5%)	3 (0%)	34	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	296	TYR
1	D	240	VAL
1	A	299	THR

### 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	166/204 (81%)	164 (99%)	2 (1%)	71	90
1	B	182/204 (89%)	179 (98%)	3 (2%)	62	86
1	C	160/204 (78%)	160 (100%)	0	100	100
1	D	164/204 (80%)	159 (97%)	5 (3%)	41	75
All	All	672/816 (82%)	662 (98%)	10 (2%)	65	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	384	ASN
1	B	297	ASN
1	B	356	ASP
1	B	439	LYS
1	D	241	PHE
1	D	292	ARG
1	D	297	ASN
1	D	376	ASP
1	D	380	GLU

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

Mol	Chain	Res	Type
1	A	325	ASN
1	B	419	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	C	325	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](#)

33 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	E	1	1,2	14,14,15	1.66	2 (14%)	17,19,21	1.14	2 (11%)
2	NAG	E	2	2	14,14,15	1.65	2 (14%)	17,19,21	1.13	2 (11%)
2	BMA	E	3	2	11,11,12	0.61	0	15,15,17	1.58	3 (20%)
2	MAN	E	4	2	11,11,12	1.63	2 (18%)	15,15,17	0.98	1 (6%)
2	NAG	E	5	2	14,14,15	0.49	0	17,19,21	1.16	3 (17%)
2	MAN	E	6	2	11,11,12	0.77	0	15,15,17	1.37	1 (6%)
2	NAG	E	7	2	14,14,15	1.66	2 (14%)	17,19,21	1.14	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.68	0	17,19,21	1.50	4 (23%)
3	NAG	F	2	3	14,14,15	0.75	0	17,19,21	1.50	3 (17%)
3	BMA	F	3	3	11,11,12	0.54	0	15,15,17	1.93	6 (40%)
3	MAN	F	4	3	11,11,12	0.92	1 (9%)	15,15,17	2.12	2 (13%)
3	NAG	F	5	3	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
3	GAL	F	6	3	11,11,12	1.47	2 (18%)	15,15,17	0.99	1 (6%)
3	SIA	F	7	3	20,20,21	2.75	9 (45%)	24,28,31	1.31	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	F	8	3	11,11,12	1.63	2 (18%)	15,15,17	0.97	1 (6%)
3	NAG	F	9	3	14,14,15	0.47	0	17,19,21	1.39	2 (11%)
3	NAG	G	1	1,3	14,14,15	1.65	2 (14%)	17,19,21	1.14	2 (11%)
3	NAG	G	2	3	14,14,15	0.74	0	17,19,21	1.50	3 (17%)
3	BMA	G	3	3	11,11,12	0.96	1 (9%)	15,15,17	2.84	5 (33%)
3	MAN	G	4	3	11,11,12	1.63	2 (18%)	15,15,17	0.97	1 (6%)
3	NAG	G	5	3	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
3	GAL	G	6	3	11,11,12	1.46	2 (18%)	15,15,17	0.99	1 (6%)
3	SIA	G	7	3	20,20,21	2.76	8 (40%)	24,28,31	1.30	2 (8%)
3	MAN	G	8	3	11,11,12	1.63	2 (18%)	15,15,17	0.97	1 (6%)
3	NAG	G	9	3	14,14,15	1.64	2 (14%)	17,19,21	1.14	2 (11%)
4	NAG	H	1	1,4	14,14,15	0.67	0	17,19,21	1.50	4 (23%)
4	NAG	H	2	4	14,14,15	1.65	2 (14%)	17,19,21	1.14	2 (11%)
4	BMA	H	3	4	11,11,12	1.00	1 (9%)	15,15,17	1.67	5 (33%)
4	MAN	H	4	4	11,11,12	1.63	2 (18%)	15,15,17	0.98	1 (6%)
4	NAG	H	5	4	14,14,15	0.76	0	17,19,21	0.92	1 (5%)
4	GAL	H	6	4	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
4	MAN	H	7	4	11,11,12	1.64	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	H	8	4	14,14,15	0.46	0	17,19,21	1.38	2 (11%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
2	NAG	E	5	2	-	4/6/23/26	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	NAG	E	7	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	5	3	-	0/6/23/26	0/1/1/1
3	GAL	F	6	3	-	0/2/19/22	0/1/1/1
3	SIA	F	7	3	-	4/18/34/38	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1
3	NAG	F	9	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	NAG	G	5	3	-	0/6/23/26	0/1/1/1
3	GAL	G	6	3	-	2/2/19/22	0/1/1/1
3	SIA	G	7	3	-	6/18/34/38	0/1/1/1
3	MAN	G	8	3	-	2/2/19/22	0/1/1/1
3	NAG	G	9	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
4	NAG	H	5	4	-	0/6/23/26	0/1/1/1
4	GAL	H	6	4	-	1/2/19/22	0/1/1/1
4	MAN	H	7	4	-	2/2/19/22	0/1/1/1
4	NAG	H	8	4	-	2/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7	SIA	O6-C2	7.90	1.54	1.43
3	G	7	SIA	O6-C2	7.88	1.54	1.43
3	G	7	SIA	C4-C5	-5.64	1.48	1.53
3	F	7	SIA	C4-C5	-5.62	1.48	1.53
4	H	2	NAG	O5-C1	3.92	1.50	1.43
2	E	7	NAG	O5-C1	3.92	1.50	1.43
3	G	1	NAG	O5-C1	3.91	1.50	1.43
2	E	1	NAG	O5-C1	3.91	1.50	1.43
2	E	2	NAG	O5-C1	3.88	1.49	1.43
3	G	9	NAG	O5-C1	3.87	1.49	1.43
3	G	7	SIA	C10-N5	3.63	1.46	1.34
3	F	7	SIA	C10-N5	3.61	1.46	1.34
3	F	6	GAL	O5-C1	3.36	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	6	GAL	O5-C1	3.33	1.49	1.43
4	H	2	NAG	C7-N2	3.30	1.45	1.34
2	E	1	NAG	C7-N2	3.30	1.45	1.34
2	E	7	NAG	C7-N2	3.30	1.45	1.34
3	G	9	NAG	C7-N2	3.30	1.45	1.34
3	G	1	NAG	C7-N2	3.27	1.45	1.34
2	E	2	NAG	C7-N2	3.25	1.45	1.34
4	H	4	MAN	O5-C1	3.24	1.48	1.43
4	H	7	MAN	O5-C1	3.24	1.48	1.43
3	F	8	MAN	O5-C1	3.22	1.48	1.43
2	E	4	MAN	O5-C1	3.20	1.48	1.43
3	G	8	MAN	O5-C1	3.20	1.48	1.43
3	G	4	MAN	O5-C1	3.19	1.48	1.43
3	G	4	MAN	C2-C3	-3.06	1.48	1.52
4	H	7	MAN	C2-C3	-3.03	1.48	1.52
2	E	4	MAN	C2-C3	-3.03	1.48	1.52
3	G	8	MAN	C2-C3	-3.03	1.48	1.52
3	F	8	MAN	C2-C3	-3.02	1.48	1.52
4	H	4	MAN	C2-C3	-3.02	1.48	1.52
3	G	7	SIA	C5-N5	2.80	1.50	1.45
3	F	7	SIA	C5-N5	2.77	1.50	1.45
4	H	3	BMA	O6-C6	-2.76	1.30	1.42
3	F	4	MAN	O5-C1	2.71	1.48	1.43
3	F	6	GAL	C2-C3	-2.55	1.48	1.52
3	G	6	GAL	C2-C3	-2.54	1.48	1.52
3	G	7	SIA	C6-C5	-2.39	1.49	1.53
3	F	7	SIA	C3-C4	-2.38	1.48	1.52
3	G	7	SIA	C3-C4	-2.34	1.48	1.52
3	F	7	SIA	C6-C5	-2.34	1.49	1.53
3	G	7	SIA	O8-C8	-2.12	1.38	1.43
3	F	7	SIA	O8-C8	-2.10	1.38	1.43
3	G	7	SIA	C2-C1	-2.08	1.50	1.52
3	G	3	BMA	O6-C6	2.08	1.51	1.42
3	F	7	SIA	C2-C1	-2.05	1.50	1.52
3	F	7	SIA	C11-C10	2.01	1.54	1.50

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C6-C5-C4	-7.90	94.50	113.00
3	F	4	MAN	O5-C1-C2	-6.12	101.33	110.77
3	G	3	BMA	O5-C5-C6	5.20	115.35	107.20

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	MAN	C1-O5-C5	4.55	118.36	112.19
3	F	3	BMA	O6-C6-C5	3.78	124.25	111.29
3	G	3	BMA	C1-O5-C5	3.33	116.70	112.19
2	E	3	BMA	O3-C3-C4	-3.33	102.66	110.35
4	H	3	BMA	C1-O5-C5	3.31	116.68	112.19
3	F	3	BMA	C1-O5-C5	3.31	116.68	112.19
3	F	4	MAN	O5-C5-C4	-3.26	102.88	110.83
3	G	2	NAG	O5-C5-C6	3.17	112.18	107.20
3	F	2	NAG	O5-C5-C6	3.14	112.13	107.20
2	E	5	NAG	C1-O5-C5	3.12	116.42	112.19
3	F	2	NAG	C4-C3-C2	2.99	115.41	111.02
3	G	2	NAG	C4-C3-C2	2.96	115.35	111.02
2	E	3	BMA	C1-O5-C5	2.95	116.19	112.19
3	F	3	BMA	O5-C5-C6	2.76	111.52	107.20
4	H	3	BMA	O5-C5-C6	2.73	111.49	107.20
2	E	3	BMA	O6-C6-C5	-2.68	102.10	111.29
3	F	9	NAG	C8-C7-N2	2.65	120.58	116.10
4	H	8	NAG	C8-C7-N2	2.63	120.56	116.10
3	G	3	BMA	C3-C4-C5	2.62	114.91	110.24
3	F	3	BMA	C3-C4-C5	2.58	114.84	110.24
4	H	3	BMA	C3-C4-C5	2.57	114.83	110.24
3	F	2	NAG	O7-C7-C8	-2.55	117.32	122.06
4	H	5	NAG	O5-C1-C2	-2.54	107.27	111.29
3	G	2	NAG	O7-C7-C8	-2.54	117.33	122.06
3	G	5	NAG	O5-C1-C2	-2.52	107.31	111.29
3	F	5	NAG	O5-C1-C2	-2.49	107.35	111.29
3	F	7	SIA	O1B-C1-C2	2.46	120.04	113.03
4	H	1	NAG	C1-O5-C5	2.44	115.50	112.19
3	G	7	SIA	O1B-C1-C2	2.44	119.99	113.03
3	F	1	NAG	C1-O5-C5	2.43	115.48	112.19
3	F	9	NAG	O5-C1-C2	-2.42	107.47	111.29
4	H	1	NAG	O6-C6-C5	-2.40	103.06	111.29
3	F	1	NAG	O6-C6-C5	-2.39	103.08	111.29
4	H	8	NAG	O5-C1-C2	-2.38	107.53	111.29
3	G	1	NAG	C8-C7-N2	2.31	120.01	116.10
3	F	7	SIA	C11-C10-N5	2.30	120.00	116.10
3	G	7	SIA	C11-C10-N5	2.30	120.00	116.10
3	G	9	NAG	C8-C7-N2	2.30	120.00	116.10
3	F	1	NAG	C8-C7-N2	2.29	119.97	116.10
2	E	2	NAG	C8-C7-N2	2.29	119.97	116.10
2	E	1	NAG	C8-C7-N2	2.28	119.96	116.10
2	E	7	NAG	C8-C7-N2	2.28	119.95	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C8-C7-N2	2.27	119.95	116.10
4	H	1	NAG	C8-C7-N2	2.25	119.92	116.10
4	H	3	BMA	O3-C3-C4	-2.22	105.23	110.35
4	H	1	NAG	O5-C1-C2	-2.21	107.80	111.29
3	F	3	BMA	O3-C3-C4	-2.20	105.27	110.35
3	G	3	BMA	O3-C3-C4	-2.18	105.30	110.35
3	F	1	NAG	O5-C1-C2	-2.18	107.85	111.29
3	G	6	GAL	C1-C2-C3	2.17	112.33	109.67
3	F	6	GAL	C1-C2-C3	2.15	112.31	109.67
2	E	7	NAG	C2-N2-C7	-2.14	119.85	122.90
3	G	9	NAG	C2-N2-C7	-2.14	119.86	122.90
3	G	1	NAG	C2-N2-C7	-2.13	119.87	122.90
2	E	1	NAG	C2-N2-C7	-2.13	119.88	122.90
4	H	2	NAG	C2-N2-C7	-2.13	119.88	122.90
2	E	2	NAG	C2-N2-C7	-2.11	119.90	122.90
2	E	5	NAG	O5-C1-C2	2.09	114.58	111.29
4	H	4	MAN	C1-C2-C3	2.08	112.23	109.67
3	F	3	BMA	C6-C5-C4	-2.08	108.14	113.00
2	E	4	MAN	C1-C2-C3	2.06	112.20	109.67
3	G	4	MAN	C1-C2-C3	2.06	112.20	109.67
4	H	7	MAN	C1-C2-C3	2.06	112.19	109.67
4	H	3	BMA	C6-C5-C4	-2.06	108.19	113.00
4	H	6	GAL	C1-O5-C5	2.05	114.97	112.19
3	F	8	MAN	C1-C2-C3	2.03	112.16	109.67
3	G	8	MAN	C1-C2-C3	2.03	112.16	109.67
2	E	5	NAG	O5-C5-C6	2.02	110.37	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	1	NAG	C1

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	NAG	C8-C7-N2-C2
2	E	5	NAG	O7-C7-N2-C2
3	F	7	SIA	C5-C6-C7-O7
3	F	7	SIA	O6-C6-C7-O7
3	F	7	SIA	C7-C8-C9-O9
3	G	7	SIA	C5-C6-C7-C8
3	G	7	SIA	C5-C6-C7-O7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	G	7	SIA	O6-C6-C7-O7
3	G	7	SIA	O8-C8-C9-O9
3	G	4	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
3	F	7	SIA	O8-C8-C9-O9
3	G	7	SIA	C7-C8-C9-O9
3	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
3	G	6	GAL	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	9	NAG	C8-C7-N2-C2
3	F	9	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	9	NAG	C8-C7-N2-C2
3	G	9	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	8	NAG	C8-C7-N2-C2
4	H	8	NAG	O7-C7-N2-C2
4	H	3	BMA	O5-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
3	G	8	MAN	O5-C5-C6-O6
4	H	7	MAN	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	E	5	NAG	C4-C5-C6-O6
2	E	5	NAG	O5-C5-C6-O6
2	E	7	NAG	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
4	H	6	GAL	O5-C5-C6-O6
2	E	7	NAG	O5-C5-C6-O6
3	G	6	GAL	C4-C5-C6-O6
3	G	7	SIA	O6-C6-C7-C8
4	H	3	BMA	C4-C5-C6-O6
3	F	8	MAN	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

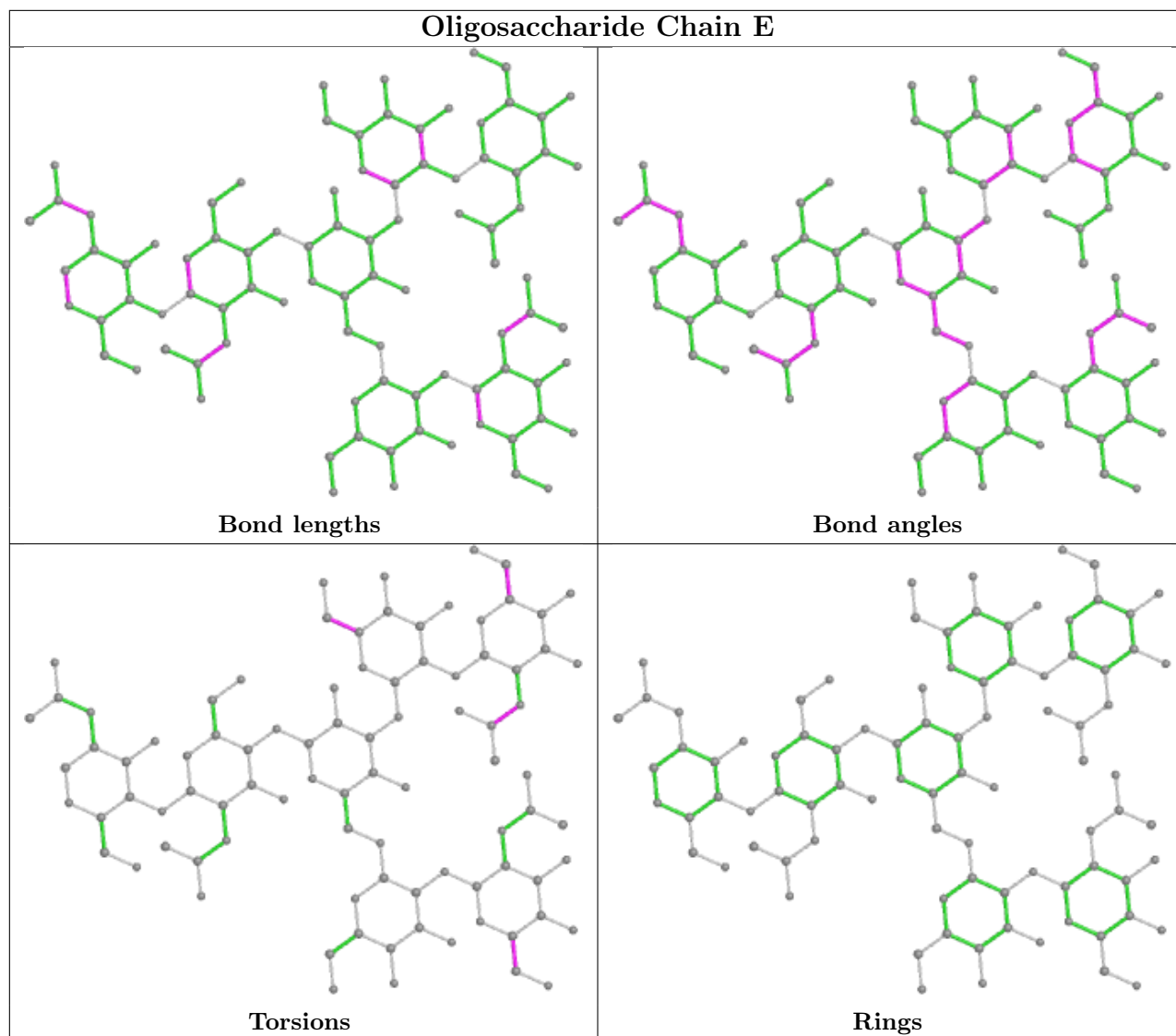
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C4-C5-C6-O6
4	H	7	MAN	C4-C5-C6-O6
3	G	8	MAN	C4-C5-C6-O6

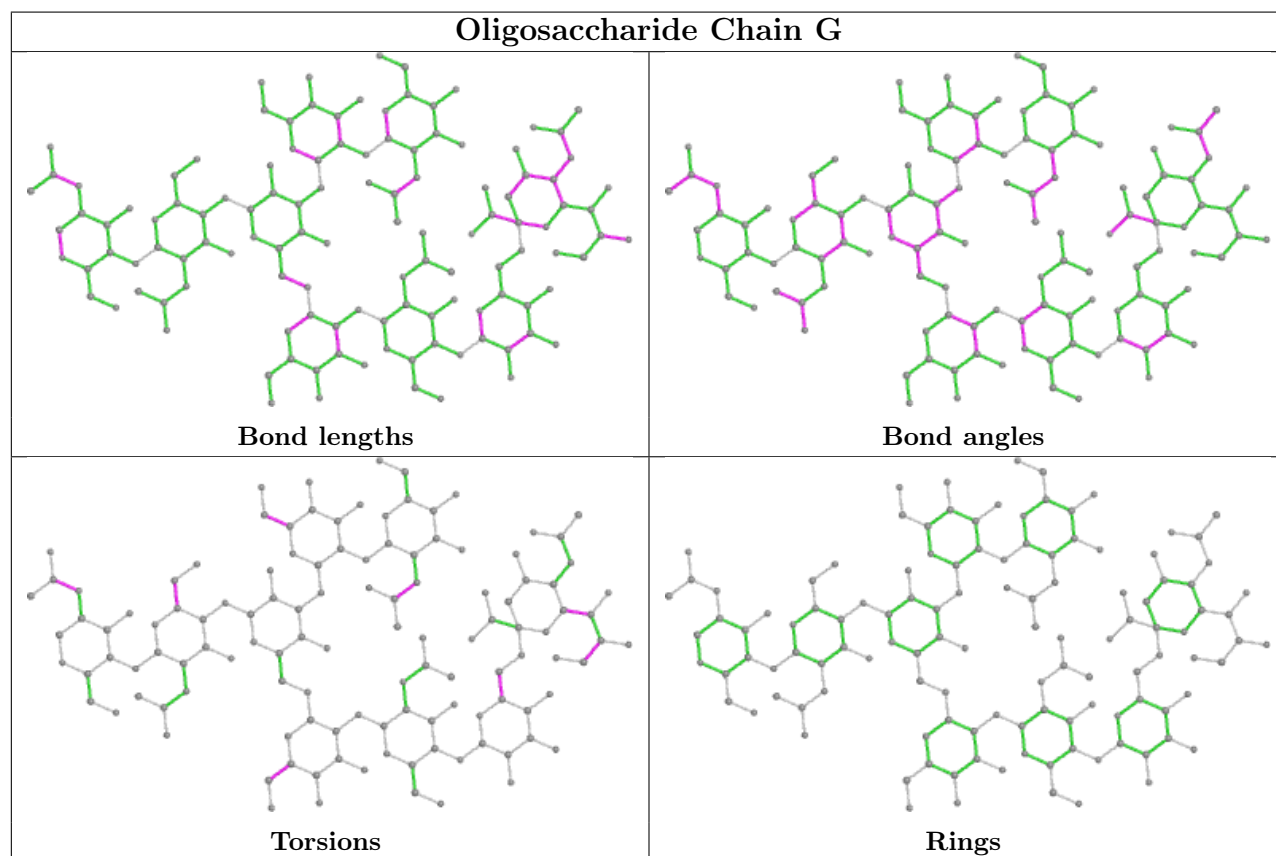
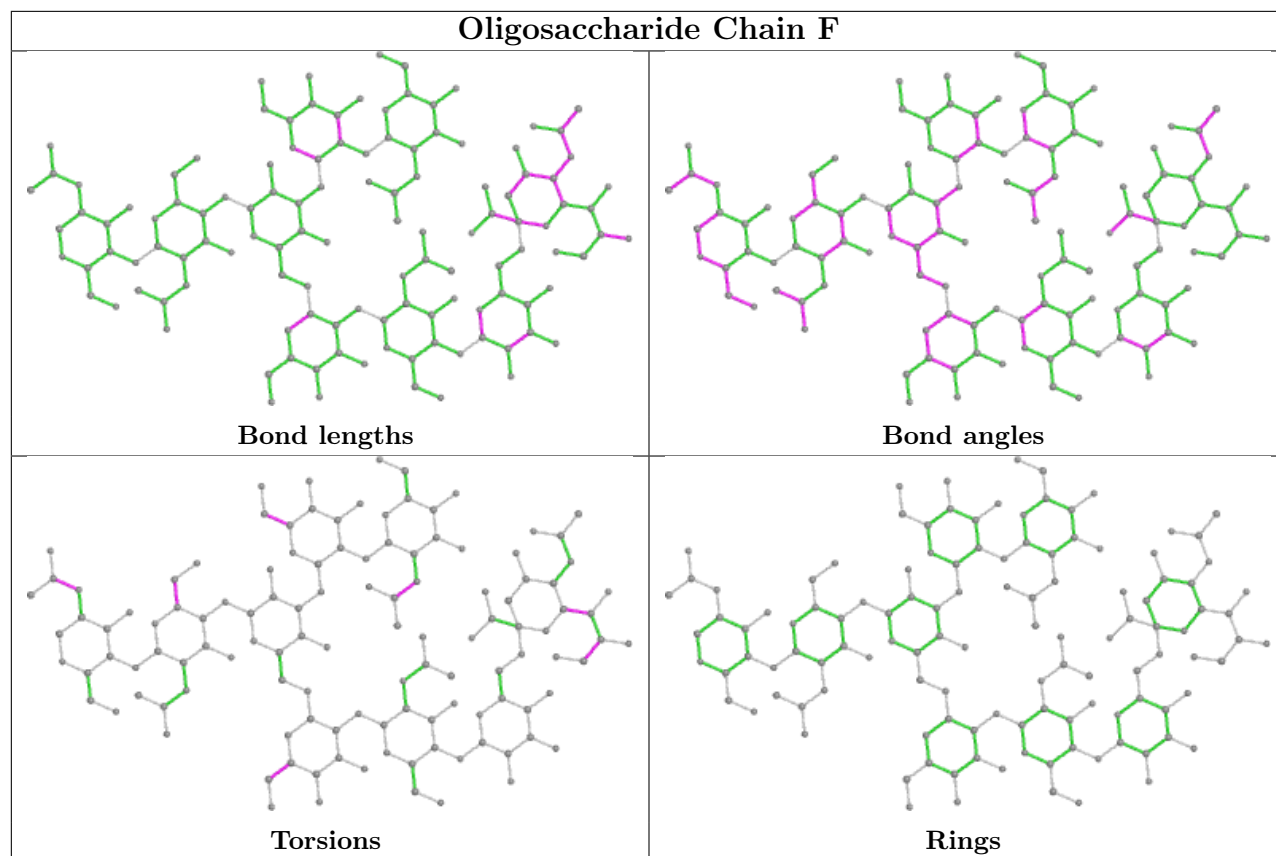
There are no ring outliers.

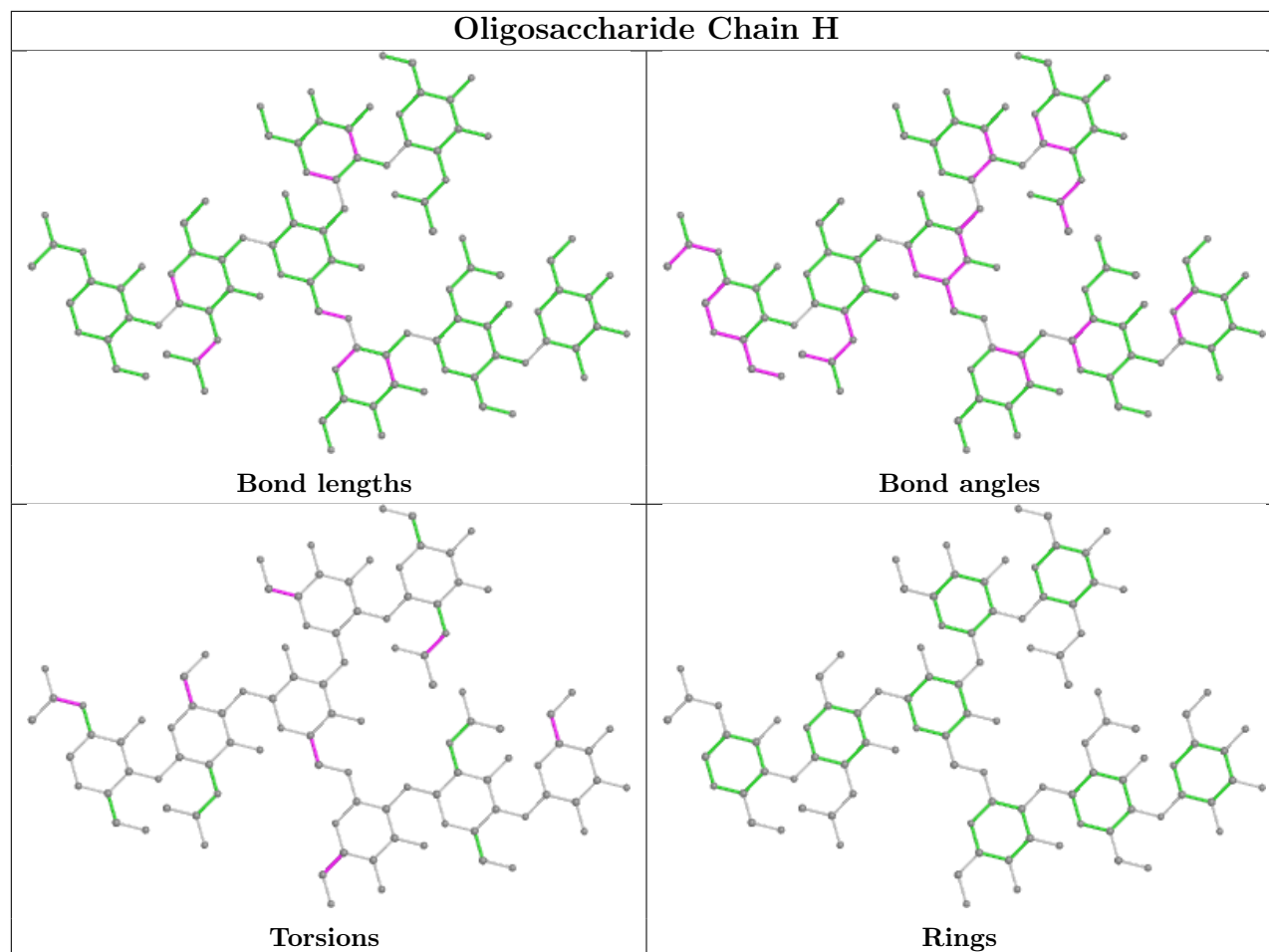
23 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	8	MAN	6	0
3	F	1	NAG	2	0
4	H	7	MAN	7	0
3	G	2	NAG	8	0
4	H	6	GAL	1	0
2	E	4	MAN	3	0
3	F	6	GAL	2	0
3	F	4	MAN	1	0
2	E	2	NAG	11	0
4	H	3	BMA	6	0
3	G	3	BMA	8	0
3	G	1	NAG	7	0
3	G	6	GAL	6	0
3	G	4	MAN	1	0
3	F	8	MAN	8	0
2	E	1	NAG	2	0
2	E	3	BMA	3	0
3	F	2	NAG	2	0
3	G	5	NAG	2	0
4	H	5	NAG	3	0
4	H	4	MAN	1	0
3	G	7	SIA	7	14
3	F	3	BMA	5	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](#)

There are no ligands in this entry.

## 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	208/221 (94%)	0.26	7 (3%) 45 19	22, 70, 149, 268	0
1	B	206/221 (93%)	0.01	1 (0%) 91 75	15, 54, 111, 169	1 (0%)
1	C	199/221 (90%)	0.39	22 (11%) 5 1	14, 70, 174, 262	0
1	D	195/221 (88%)	0.28	14 (7%) 15 4	16, 53, 156, 215	0
All	All	808/884 (91%)	0.23	44 (5%) 25 9	14, 62, 151, 268	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	SER	6.8
1	C	271	PRO	6.4
1	C	285	HIS	5.6
1	C	266	VAL	5.3
1	D	262	VAL	5.2
1	D	263	VAL	4.5
1	C	273	VAL	4.4
1	D	239	SER	4.3
1	C	302	VAL	4.1
1	D	276	ASN	3.6
1	B	295	GLN	3.5
1	D	240	VAL	3.5
1	D	241	PHE	3.3
1	C	264	VAL	3.3
1	C	300	TYR	3.3
1	C	240	VAL	3.2
1	D	275	PHE	3.2
1	C	265	ASP	3.2
1	D	304	SER	3.1
1	A	298	SER	3.1
1	D	323	VAL	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	254	SER	2.8
1	D	316	GLY	2.8
1	A	265	ASP	2.8
1	C	268	HIS	2.6
1	C	299	THR	2.6
1	A	253	ILE	2.5
1	D	273	VAL	2.5
1	C	323	VAL	2.5
1	A	309	LEU	2.5
1	C	333	GLU	2.4
1	D	301	ARG	2.2
1	C	296	TYR	2.2
1	A	308	VAL	2.2
1	C	267	SER	2.2
1	A	422	VAL	2.2
1	C	262	VAL	2.1
1	C	325	ASN	2.1
1	C	306	LEU	2.1
1	C	238	PRO	2.1
1	C	383	SER	2.1
1	D	294	GLU	2.0
1	C	263	VAL	2.0
1	D	306	LEU	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
4	GAL	H	6	11/12	0.38	0.54	85,85,85,85	0
4	BMA	H	3	11/12	0.55	0.39	74,79,83,84	0
3	MAN	G	4	11/12	0.55	0.27	88,91,98,108	0
4	NAG	H	8	14/15	0.56	0.35	108,118,131,132	0
4	NAG	H	1	14/15	0.57	0.35	174,180,186,188	0

*Continued on next page...*

Continued from previous page...

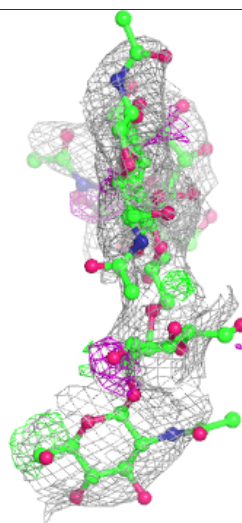
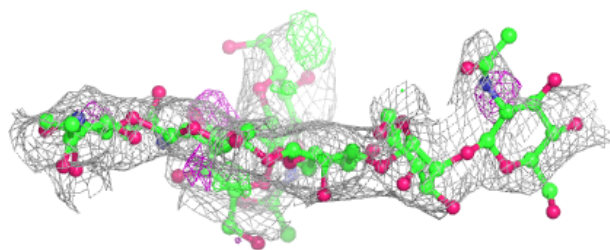
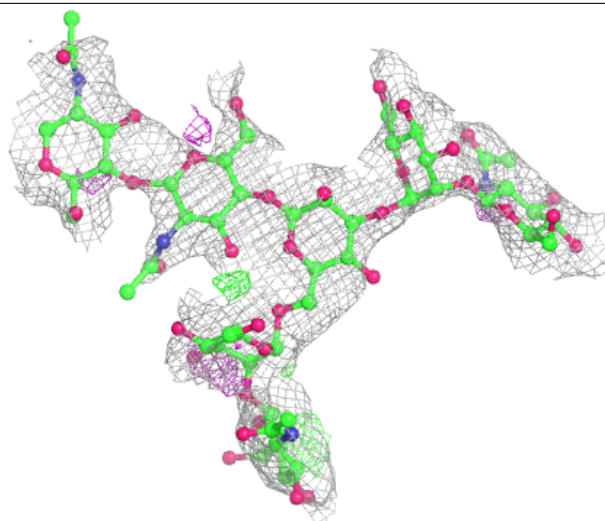
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	9	14/15	0.58	0.38	80,90,102,104	0
2	NAG	E	5	14/15	0.59	0.40	99,105,109,110	0
3	GAL	G	6	11/12	0.60	0.30	64,69,78,95	0
3	BMA	F	3	11/12	0.66	0.34	67,71,75,77	0
2	MAN	E	4	11/12	0.66	0.27	133,137,143,151	0
3	NAG	G	1	14/15	0.67	0.41	101,107,113,115	0
2	MAN	E	6	11/12	0.67	0.35	88,89,94,99	0
3	NAG	F	9	14/15	0.68	0.28	88,98,110,112	0
4	NAG	H	5	14/15	0.69	0.39	59,65,70,71	0
2	NAG	E	1	14/15	0.70	0.34	78,79,81,83	0
2	NAG	E	7	14/15	0.71	0.33	105,111,118,120	0
3	SIA	F	7	20/21	0.71	0.37	122,131,136,136	0
3	SIA	G	7	20/21	0.71	0.35	80,89,93,93	0
3	NAG	G	2	14/15	0.72	0.38	96,106,113,113	0
3	MAN	G	8	11/12	0.72	0.30	97,106,109,125	0
4	MAN	H	7	11/12	0.74	0.31	127,136,139,155	0
3	BMA	G	3	11/12	0.76	0.27	101,105,110,111	0
3	MAN	F	8	11/12	0.77	0.35	87,97,100,115	0
3	NAG	G	5	14/15	0.77	0.27	47,53,58,59	0
3	GAL	F	6	11/12	0.78	0.31	27,32,41,58	0
4	MAN	H	4	11/12	0.78	0.38	114,114,114,114	0
3	MAN	F	4	11/12	0.79	0.20	41,44,51,61	0
3	NAG	F	1	14/15	0.80	0.29	46,52,58,60	0
4	NAG	H	2	14/15	0.80	0.25	96,106,112,113	0
2	NAG	E	2	14/15	0.82	0.38	81,85,89,91	0
2	BMA	E	3	11/12	0.82	0.16	74,76,78,80	0
3	NAG	F	5	14/15	0.84	0.32	72,78,83,84	0
3	NAG	F	2	14/15	0.87	0.25	26,36,43,43	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.



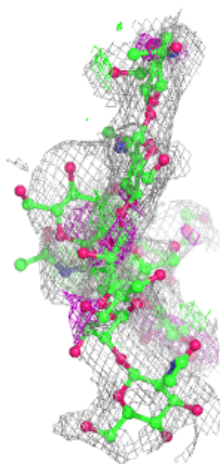
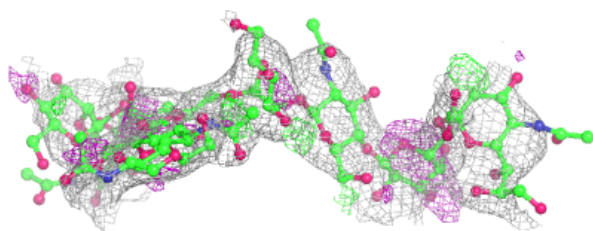
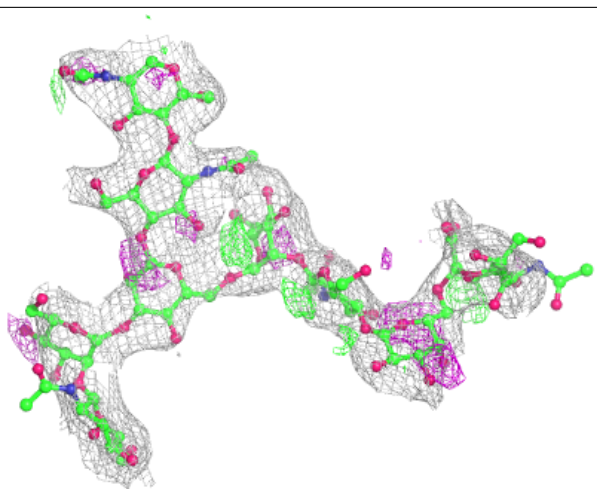
**Electron density around Chain E:**

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



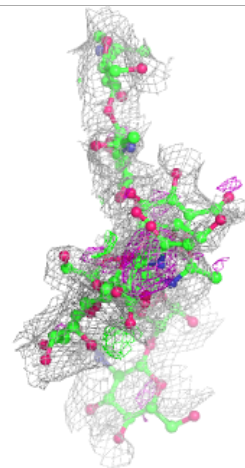
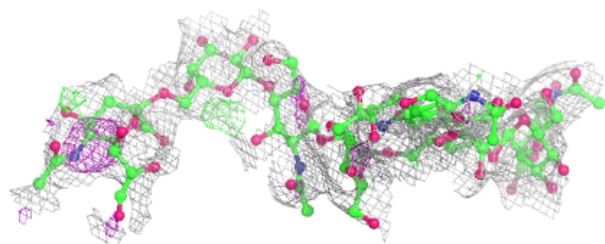
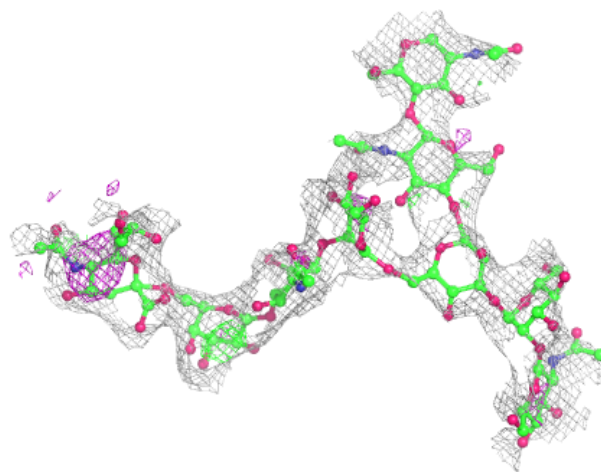
**Electron density around Chain F:**

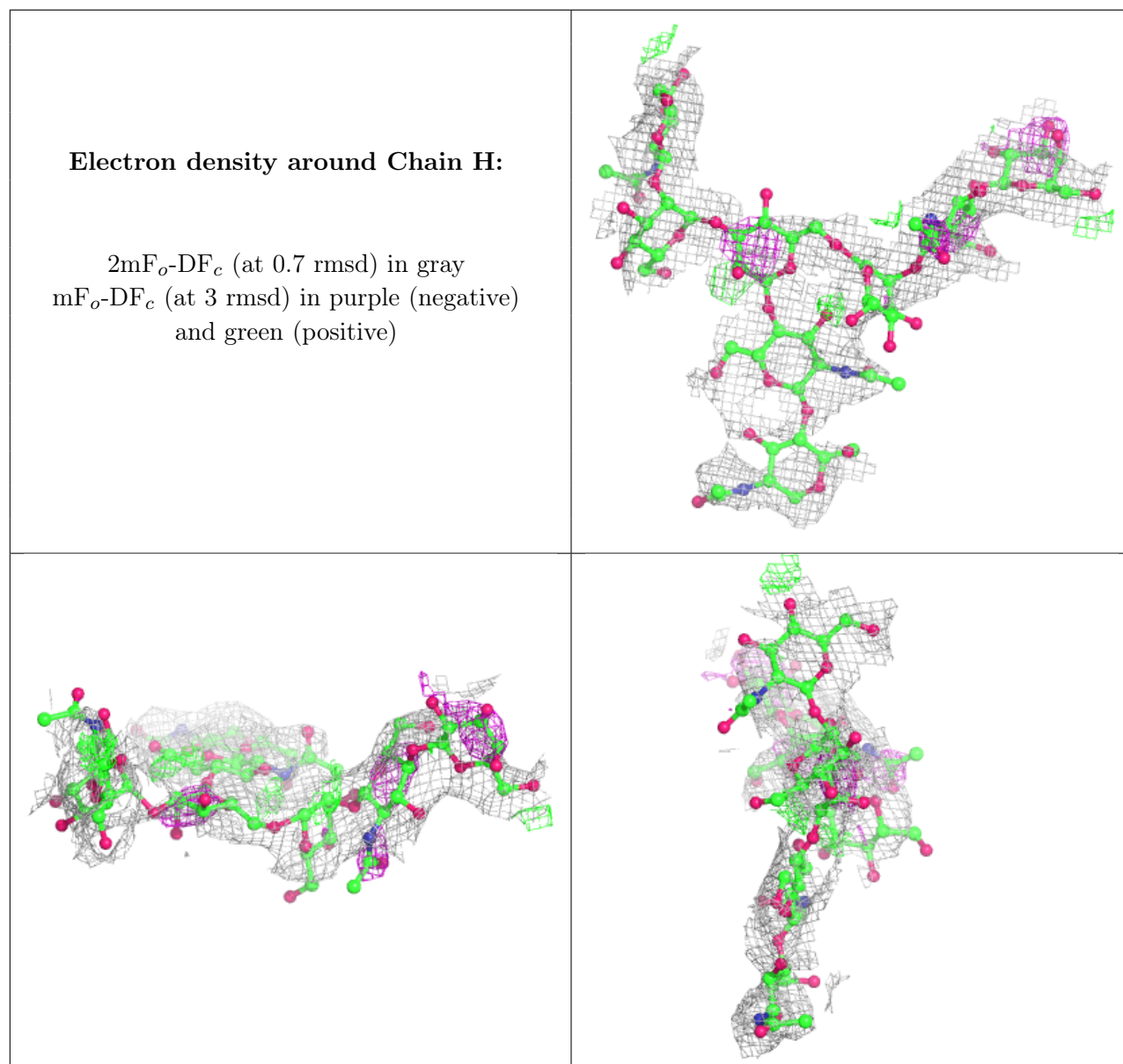
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.