



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2025 – 02:12 PM EST

PDB ID : 9MCY / pdb\_00009mcy  
Title : CRYSTAL STRUCTURE OF HUMAN IGG1 FC FRAGMENT-FC-GAMMA  
RECEPTOR IIA COMPLEX R131 VARIANT  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2024-12-05  
Resolution : 2.85 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

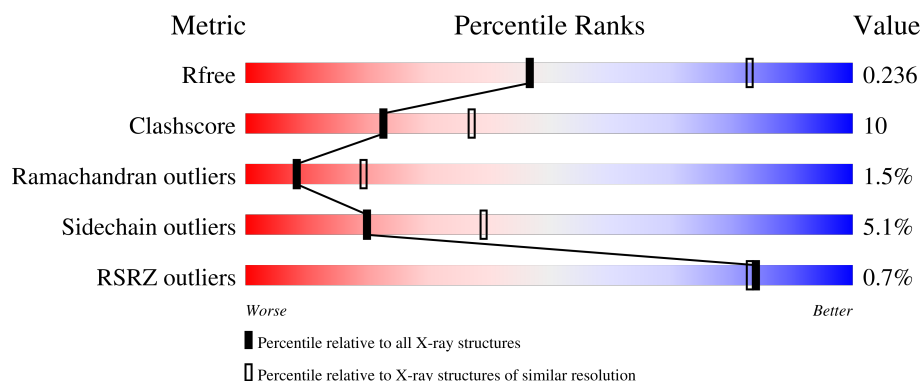
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.85 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))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	223	
1	B	223	
1	C	223	
1	D	223	
2	E	173	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	173	<div><div></div><div>58%31%6%5%</div></div>
3	G	2	<div><div></div><div>50%50%</div></div>
4	H	8	<div><div></div><div>12%88%</div></div>
4	I	8	<div><div></div><div>25%50%25%</div></div>
4	J	8	<div><div></div><div>38%50%12%</div></div>
4	K	8	<div><div></div><div>12%88%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10017 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 Immunoglobulin gamma-1 heavy chain Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1712	1091	287	328	6			
1	B	214	Total	C	N	O	S	0	0	0
			1705	1086	286	327	6			
1	C	215	Total	C	N	O	S	0	1	0
			1720	1095	289	330	6			
1	D	214	Total	C	N	O	S	0	3	0
			1731	1100	292	333	6			

- Molecule 2 is a protein called Fc gamma receptor IIA R131 variant.

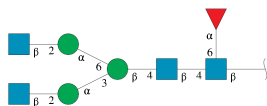
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	172	Total	C	N	O	S	0	0	0
			1363	864	234	260	5			
2	F	164	Total	C	N	O	S	0	0	0
			1307	833	223	246	5			

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



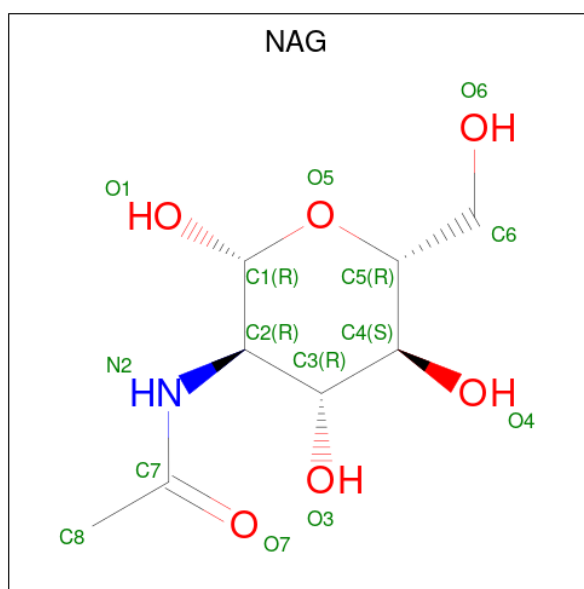
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	8	Total	C	N	O	0	0	0
			99	56	4	39			
4	I	8	Total	C	N	O	0	0	0
			99	56	4	39			
4	J	8	Total	C	N	O	0	0	0
			99	56	4	39			
4	K	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		

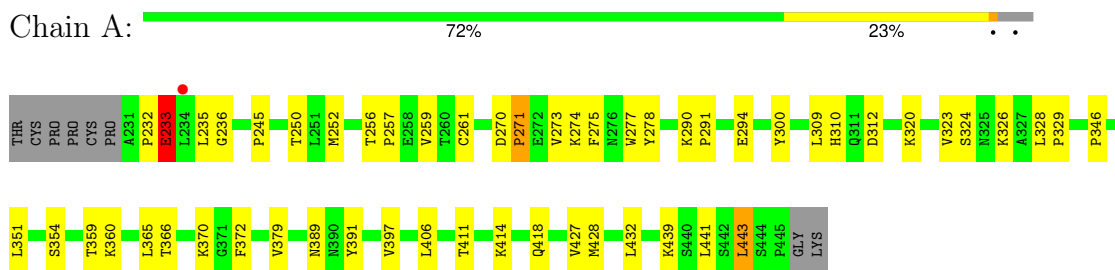
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	3	Total	O	0	0
			3	3		
7	C	1	Total	O	0	0
			1	1		
7	D	1	Total	O	0	0
			1	1		

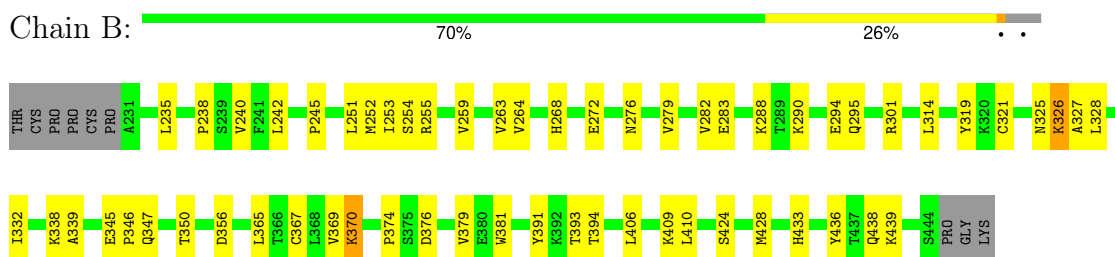
### 3 Residue-property plots

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.

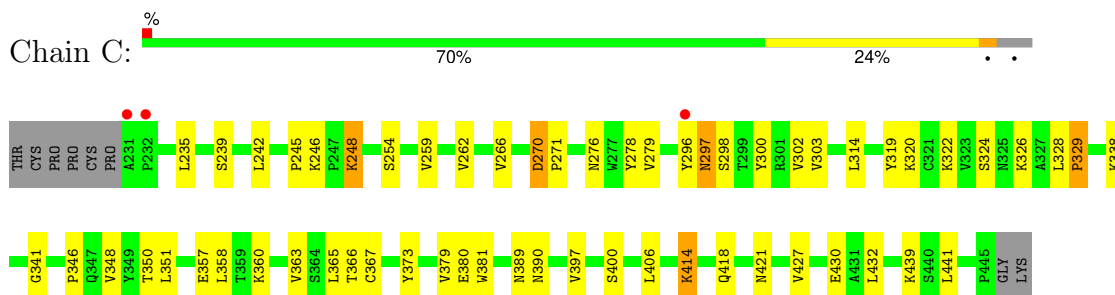
- Molecule 1: Immunoglobulin gamma-1 heavy chain Fc fragment



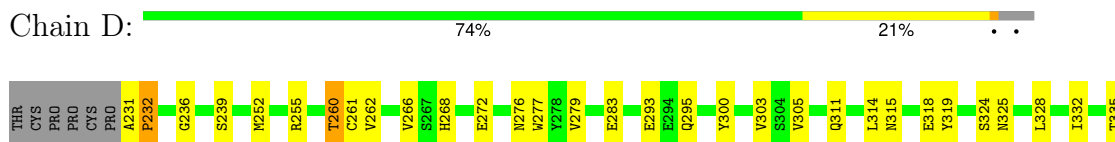
- Molecule 1: Immunoglobulin gamma-1 heavy chain Fc fragment

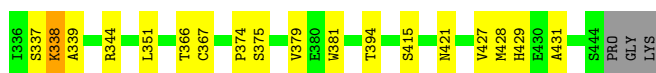


- Molecule 1: Immunoglobulin gamma-1 heavy chain Fc fragment



- Molecule 1: Immunoglobulin gamma-1 heavy chain Fc fragment

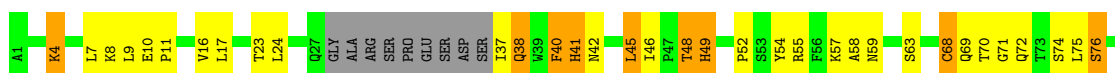




- Molecule 2: Fc gamma receptor IIA R131 variant



- Molecule 2: Fc gamma receptor IIA R131 variant



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



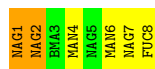
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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







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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.99Å 76.23Å 120.05Å 96.60° 100.24° 90.08°	Depositor
Resolution (Å)	39.89 – 2.85 39.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (39.89-2.85) 95.9 (39.89-2.85)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.177 , 0.236 0.176 , 0.236	Depositor DCC
$R_{free}$ test set	1902 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: MAN, BMA, NAG, MPD, FUC

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	0.45	0/1760	0.63	0/2400
1	B	0.46	0/1752	0.63	0/2388
1	C	0.46	0/1768	0.65	0/2411
1	D	0.43	0/1778	0.60	0/2424
2	E	0.33	0/1404	0.57	0/1918
2	F	0.34	0/1346	0.58	0/1838
All	All	0.42	0/9808	0.61	0/13379

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1712	0	1680	33	0
1	B	1705	0	1673	43	0
1	C	1720	0	1685	32	0
1	D	1731	0	1693	27	0
2	E	1363	0	1311	35	0
2	F	1307	0	1264	40	0
3	G	28	0	25	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	99	0	85	0	0
4	I	99	0	85	4	0
4	J	99	0	85	1	0
4	K	99	0	85	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	C	8	0	14	1	0
6	D	8	0	14	0	0
7	A	6	0	0	0	0
7	B	3	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	10017	0	9725	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:SER:HB2	2:F:83:VAL:HG12	1.51	0.89
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.64	0.79
1:B:288:LYS:O	1:B:288:LYS:NZ	2.15	0.78
1:D:351:LEU:HB2	1:D:366:THR:HB	1.64	0.77
2:F:55:ARG:HH12	2:F:57:LYS:HG3	1.49	0.77
2:E:68:CYS:HB2	2:E:76:SER:HB3	1.68	0.76
1:B:276:ASN:ND2	1:B:283:GLU:OE2	2.20	0.74
1:D:314:LEU:O	1:D:338:LYS:NZ	2.21	0.73
1:C:248:LYS:NZ	1:C:380:GLU:OE2	2.22	0.72
2:E:65:GLU:HG2	2:E:78:PRO:HB2	1.72	0.71
2:E:7:LEU:HD21	2:E:24:LEU:HG	1.72	0.70
1:A:290:LYS:HE2	1:A:291:PRO:HD2	1.73	0.70
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.74	0.69
2:F:68:CYS:HB2	2:F:76:SER:HB3	1.77	0.65
1:D:266:VAL:HB	1:D:300:TYR:HB2	1.79	0.65
1:B:272:GLU:OE1	1:B:272:GLU:N	2.26	0.64
1:B:252:MET:HB2	1:B:255:ARG:HG3	1.80	0.64
1:C:358:LEU:HD23	1:C:363:VAL:HG11	1.80	0.64
2:F:9:LEU:HD12	2:F:24:LEU:HD21	1.80	0.63
1:B:238:PRO:HD2	1:B:328:LEU:HD21	1.81	0.62
2:F:4:LYS:NZ	2:F:75:LEU:O	2.27	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:LEU:HD11	2:F:24:LEU:HD22	1.81	0.62
1:A:250:THR:HG22	1:A:257:PRO:HB3	1.81	0.62
1:A:351:LEU:HB2	1:A:366:THR:HB	1.82	0.62
1:C:328:LEU:HD12	1:C:329:PRO:HD2	1.81	0.61
2:F:59:ASN:O	2:F:83:VAL:HG11	2.00	0.61
1:D:262:VAL:HG22	1:D:303:VAL:HG22	1.82	0.61
1:B:272:GLU:H	1:B:272:GLU:CD	2.08	0.60
1:D:276:ASN:ND2	1:D:283:GLU:OE2	2.33	0.60
1:B:288:LYS:NZ	1:B:290:LYS:HE3	2.16	0.60
1:C:365:LEU:HB3	1:C:441:LEU:HD23	1.84	0.59
1:C:414:LYS:O	1:C:418:GLN:HG3	2.02	0.59
1:C:350:THR:HB	1:C:441:LEU:HD13	1.85	0.59
1:D:260:THR:HG23	1:D:305:VAL:HG22	1.85	0.59
1:C:276:ASN:HB2	1:C:322:LYS:HB3	1.85	0.58
1:B:272:GLU:O	1:B:325:ASN:ND2	2.35	0.58
1:C:271:PRO:HG3	1:C:326:LYS:HB2	1.85	0.57
2:F:70:THR:O	2:F:72:GLN:N	2.37	0.57
2:E:10:GLU:HB3	2:E:11:PRO:HD3	1.85	0.57
1:C:262:VAL:HG22	1:C:303:VAL:HG22	1.86	0.57
2:E:99:GLU:HG3	2:E:171:VAL:HA	1.87	0.57
1:C:246:LYS:NZ	4:J:7:NAG:O4	2.29	0.57
2:E:69:GLN:HG2	2:E:75:LEU:HA	1.86	0.56
2:E:97:PHE:O	2:E:98:GLN:HG2	2.05	0.56
1:A:233:GLU:HB3	2:E:157:TYR:OH	2.04	0.56
1:C:245:PRO:HD3	1:C:259:VAL:HG22	1.87	0.56
2:F:4:LYS:HG2	2:F:75:LEU:O	2.06	0.56
1:D:429:HIS:CD2	1:D:431:ALA:H	2.24	0.55
1:C:270:ASP:OD1	1:C:270:ASP:N	2.39	0.55
1:D:429:HIS:HD2	1:D:431:ALA:H	1.55	0.55
2:F:41:HIS:ND1	2:F:42:ASN:N	2.55	0.55
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.88	0.54
1:B:328:LEU:HD13	1:B:332:ILE:HG13	1.88	0.54
1:A:232:PRO:O	1:A:233:GLU:HB2	2.07	0.54
1:B:288:LYS:HZ1	1:B:290:LYS:HE3	1.73	0.54
2:E:10:GLU:HB2	2:E:23:THR:HB	1.90	0.54
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.89	0.53
1:C:296:TYR:C	1:C:298:SER:H	2.16	0.53
1:D:272:GLU:O	1:D:325:ASN:ND2	2.40	0.53
2:E:18:GLN:NE2	2:E:85:SER:HB3	2.23	0.53
1:D:293:GLU:OE2	1:D:295:GLN:NE2	2.41	0.53
1:D:311:GLN:HE21	1:D:315:ASN:ND2	2.05	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:OE2	1:B:326:LYS:HG3	2.08	0.53
1:C:278:TYR:CD1	1:C:320:LYS:HD2	2.44	0.53
2:E:1:ALA:N	2:F:99:GLU:OE1	2.39	0.53
1:B:252:MET:HG3	1:B:428:MET:HE1	1.90	0.53
1:C:379:VAL:HG21	1:C:406:LEU:HD11	1.90	0.52
2:E:10:GLU:CB	2:E:23:THR:HB	2.39	0.52
2:E:37:ILE:HD13	2:E:52:PRO:HA	1.92	0.52
1:A:294:GLU:HG3	1:A:300:TYR:CZ	2.43	0.52
1:B:436:TYR:OH	1:B:438:GLN:NE2	2.43	0.52
2:F:10:GLU:HB3	2:F:11:PRO:HD3	1.90	0.52
1:C:389:ASN:OD1	1:C:389:ASN:N	2.37	0.51
1:D:252:MET:HB2	1:D:255:ARG:HG3	1.93	0.51
2:F:63:SER:OG	2:F:82:THR:HA	2.10	0.51
1:A:245:PRO:HD3	1:A:259:VAL:HG22	1.92	0.51
1:A:294:GLU:HG3	1:A:300:TYR:CE1	2.45	0.51
1:B:350:THR:HG23	1:B:439:LYS:HB3	1.92	0.51
2:F:96:GLU:OE2	2:F:170:GLN:NE2	2.41	0.51
2:F:99:GLU:HB2	2:F:171:VAL:HA	1.91	0.51
1:C:279:VAL:HG22	1:C:319:TYR:CD1	2.46	0.50
1:A:252:MET:SD	1:A:428:MET:HE1	2.51	0.50
2:F:119:THR:HB	2:F:152:THR:HG22	1.93	0.50
1:B:238:PRO:HD2	1:B:328:LEU:CD2	2.42	0.50
1:B:295:GLN:HG2	4:I:1:NAG:H62	1.92	0.50
1:D:339:ALA:HB3	1:D:374:PRO:HB3	1.94	0.49
1:A:274:LYS:HD3	1:A:275:PHE:N	2.27	0.49
1:B:301:ARG:NH1	4:I:2:NAG:H81	2.26	0.49
1:A:310:HIS:CD2	1:A:310:HIS:H	2.30	0.49
1:B:268:HIS:NE2	1:B:294:GLU:OE1	2.45	0.49
1:D:311:GLN:HE21	1:D:315:ASN:HD21	1.61	0.49
1:D:236:GLY:HA2	2:F:87:TRP:CH2	2.48	0.49
2:F:9:LEU:HD11	2:F:81:LEU:HD13	1.95	0.49
1:A:346:PRO:HG3	1:A:372:PHE:HB3	1.95	0.49
1:A:360:LYS:O	1:A:414:LYS:HE2	2.12	0.49
1:A:365:LEU:HB3	1:A:441:LEU:HD23	1.94	0.49
1:A:418:GLN:HA	1:A:443:LEU:HD12	1.95	0.49
1:A:326:LYS:C	1:A:328:LEU:H	2.20	0.48
1:C:266:VAL:HG12	1:C:300:TYR:HB2	1.95	0.48
1:D:268:HIS:ND1	1:D:300:TYR:HE1	2.11	0.48
2:F:38:GLN:HB3	2:F:40:PHE:CE1	2.48	0.48
1:B:242:LEU:HD21	1:B:321:CYS:HB2	1.95	0.48
2:F:16:VAL:HG22	2:F:17:LEU:O	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:VAL:HG13	2:F:91:GLN:HG2	1.95	0.48
2:E:11:PRO:HG2	2:E:21:SER:O	2.14	0.48
2:F:7:LEU:HD12	2:F:8:LYS:H	1.79	0.48
2:F:99:GLU:HG3	2:F:171:VAL:HG13	1.95	0.48
1:C:351:LEU:HB2	1:C:366:THR:HB	1.96	0.47
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.48	0.47
1:A:389:ASN:O	1:A:391:TYR:N	2.47	0.47
2:F:148:ASP:OD2	2:F:166:THR:OG1	2.22	0.47
1:B:295:GLN:HG2	4:I:1:NAG:C6	2.45	0.47
2:F:99:GLU:HB2	2:F:170:GLN:O	2.15	0.47
1:A:439:LYS:NZ	1:B:356:ASP:OD2	2.42	0.47
1:B:253:ILE:H	1:B:253:ILE:HD12	1.79	0.47
1:B:288:LYS:HZ2	1:B:288:LYS:C	2.12	0.47
1:B:393:THR:CG2	1:B:406:LEU:HD13	2.44	0.47
1:D:279:VAL:HG22	1:D:319:TYR:CD1	2.50	0.47
2:F:87:TRP:HZ3	2:F:113:LYS:HE2	1.80	0.47
1:A:379:VAL:HG22	1:A:427:VAL:HG22	1.98	0.46
2:F:46:ILE:HG22	2:F:48:THR:O	2.15	0.46
1:A:379:VAL:HG21	1:A:406:LEU:HD11	1.98	0.46
1:C:314:LEU:O	1:C:338:LYS:NZ	2.48	0.46
1:B:347:GLN:HB2	1:B:370:LYS:HG3	1.98	0.46
1:D:252:MET:HB2	1:D:255:ARG:CG	2.46	0.46
1:A:235:LEU:HG	1:A:236:GLY:H	1.81	0.46
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.71	0.46
2:E:7:LEU:HD23	2:E:8:LYS:H	1.81	0.46
1:A:271:PRO:HG3	1:A:326:LYS:HB2	1.97	0.46
1:D:328:LEU:HD21	1:D:332:ILE:HG13	1.99	0.45
2:E:89:VAL:HG13	2:E:91:GLN:HG2	1.98	0.45
2:F:97:PHE:CE1	2:F:103:ILE:HG23	2.52	0.45
1:C:397:VAL:HG21	1:D:394:THR:HA	1.99	0.45
1:A:273:VAL:HG13	1:A:323:VAL:HG13	1.98	0.45
2:F:88:LEU:HD21	2:F:115:LEU:HD13	1.99	0.45
1:A:397:VAL:HG21	1:B:394:THR:HA	1.98	0.45
1:A:428:MET:HE2	1:A:428:MET:HB3	1.78	0.45
1:D:428:MET:HB2	1:D:428:MET:HE3	1.87	0.45
1:A:270:ASP:OD1	1:A:270:ASP:N	2.48	0.44
2:E:45:LEU:HD22	2:E:47:PRO:HG3	1.98	0.44
2:E:92:THR:OG1	2:E:97:PHE:HZ	2.00	0.44
2:E:141:ALA:HA	2:E:145:HIS:ND1	2.32	0.44
1:C:297:ASN:N	1:C:297:ASN:OD1	2.50	0.44
1:A:309:LEU:HD12	1:A:312:ASP:OD1	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:ILE:HG21	2:F:52:PRO:HA	1.99	0.44
2:E:84:LEU:HB3	2:E:86:GLU:HG2	2.00	0.44
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.99	0.44
1:A:346:PRO:HD2	1:A:432:LEU:HG	1.99	0.44
2:E:7:LEU:HD23	2:E:8:LYS:N	2.33	0.44
1:C:278:TYR:HD1	1:C:320:LYS:HD2	1.82	0.44
1:D:261:CYS:HB2	1:D:277:TRP:CZ2	2.53	0.44
1:C:346:PRO:HD2	1:C:432:LEU:HG	1.99	0.44
1:B:245:PRO:HD3	1:B:259:VAL:HG22	2.00	0.43
1:B:339:ALA:HB3	1:B:374:PRO:HB3	2.00	0.43
2:E:65:GLU:CG	2:E:78:PRO:HB2	2.46	0.43
1:C:341:GLY:HA3	1:C:373:TYR:CE1	2.52	0.43
1:D:318:GLU:OE1	1:D:335:THR:HG21	2.19	0.43
2:E:97:PHE:CE2	2:E:103:ILE:HG23	2.54	0.43
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.53	0.43
2:F:45:LEU:H	2:F:45:LEU:HG	1.42	0.43
1:B:314:LEU:HA	1:B:338:LYS:HD3	2.01	0.43
1:A:328:LEU:HD23	1:A:329:PRO:HD2	2.01	0.43
1:D:344:ARG:HE	1:D:344:ARG:HB3	1.60	0.43
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.76	0.43
1:C:367:CYS:HB2	1:C:381:TRP:CZ2	2.54	0.43
2:F:163:LYS:HA	2:F:163:LYS:HD3	1.70	0.42
2:E:53:SER:OG	2:E:54:TYR:N	2.52	0.42
1:A:443:LEU:HA	1:A:443:LEU:HD23	1.86	0.42
2:E:111:LYS:HB3	2:E:111:LYS:HE2	1.84	0.42
2:E:125:LYS:HD2	2:E:126:SER:O	2.19	0.42
2:F:96:GLU:OE2	2:F:170:GLN:HB2	2.18	0.42
1:B:295:GLN:CG	4:I:1:NAG:H62	2.50	0.42
1:B:391:TYR:HA	1:B:409:LYS:O	2.18	0.42
2:E:30:ARG:HB3	2:E:34:SER:HB3	2.02	0.42
1:B:288:LYS:HE3	1:B:288:LYS:HB3	1.72	0.42
1:B:347:GLN:O	1:B:369:VAL:HA	2.19	0.42
2:E:84:LEU:HD13	2:E:89:VAL:HG23	2.00	0.42
1:C:348:VAL:HG12	1:C:439:LYS:HG3	2.01	0.42
2:F:49:HIS:CE1	2:F:54:TYR:HB2	2.55	0.42
2:E:97:PHE:O	2:E:101:GLU:HB2	2.20	0.42
2:E:110:TRP:CD2	2:E:111:LYS:HG3	2.54	0.42
1:C:421:ASN:HA	6:C:501:MPD:HM1	2.02	0.42
2:E:4:LYS:HG3	2:F:140:GLN:NE2	2.35	0.42
2:E:26:CYS:O	2:E:27:GLN:HG2	2.20	0.41
1:C:357:GLU:O	1:C:360:LYS:HG2	2.19	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLU:HA	1:B:346:PRO:HD2	1.94	0.41
1:B:379:VAL:HG21	1:B:406:LEU:HD11	2.01	0.41
2:F:98:GLN:O	2:F:101:GLU:HB2	2.20	0.41
1:B:326:LYS:H	1:B:326:LYS:HG2	1.60	0.41
2:E:69:GLN:HE21	2:E:75:LEU:HD12	1.86	0.41
2:E:30:ARG:HD2	2:E:71:GLY:HA3	2.01	0.41
1:B:279:VAL:HG22	1:B:319:TYR:CD2	2.55	0.41
2:E:93:PRO:HB2	2:E:94:HIS:CE1	2.55	0.41
1:D:231:ALA:HA	1:D:232:PRO:HD3	1.94	0.41
1:C:266:VAL:HB	1:C:300:TYR:O	2.20	0.41
1:B:325:ASN:C	1:B:327:ALA:H	2.29	0.41
2:F:90:LEU:HD21	2:F:105:LEU:HD13	2.02	0.41
1:C:242:LEU:HD11	1:C:259:VAL:CG1	2.51	0.40
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.40
1:C:348:VAL:HG22	1:C:427:VAL:HG21	2.03	0.40
2:F:7:LEU:HD12	2:F:8:LYS:N	2.37	0.40
2:F:9:LEU:HD12	2:F:24:LEU:CD2	2.48	0.40
2:F:97:PHE:CZ	2:F:103:ILE:HG23	2.56	0.40

There are no symmetry-related clashes.

## 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	213/223 (96%)	201 (94%)	9 (4%)	3 (1%)	9	20
1	B	212/223 (95%)	199 (94%)	12 (6%)	1 (0%)	25	43
1	C	214/223 (96%)	199 (93%)	12 (6%)	3 (1%)	9	20
1	D	215/223 (96%)	205 (95%)	9 (4%)	1 (0%)	25	43
2	E	170/173 (98%)	146 (86%)	20 (12%)	4 (2%)	5	11
2	F	160/173 (92%)	133 (83%)	21 (13%)	6 (4%)	2	5

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1184/1238 (96%)	1083 (92%)	83 (7%)	18 (2%)	8 19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
2	E	27	GLN
2	F	71	GLY
1	A	443	LEU
2	E	98	GLN
2	F	41	HIS
1	B	433	HIS
1	C	329	PRO
2	F	38	GLN
2	F	49	HIS
2	F	69	GLN
1	A	271	PRO
2	E	39	TRP
2	E	49	HIS
2	F	58	ALA
1	C	297	ASN
1	C	390	ASN
1	D	232	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	199/206 (97%)	193 (97%)	6 (3%)	36 62
1	B	198/206 (96%)	191 (96%)	7 (4%)	31 57
1	C	200/206 (97%)	190 (95%)	10 (5%)	20 40
1	D	201/206 (98%)	193 (96%)	8 (4%)	27 51
2	E	158/159 (99%)	146 (92%)	12 (8%)	11 23
2	F	152/159 (96%)	139 (91%)	13 (9%)	8 18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1108/1142 (97%)	1052 (95%)	56 (5%)	20	39

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	A	256	THR
1	A	324	SER
1	A	354	SER
1	A	359	THR
1	A	411	THR
1	B	235	LEU
1	B	254	SER
1	B	282	VAL
1	B	326	LYS
1	B	370	LYS
1	B	376	ASP
1	B	424	SER
2	E	21	SER
2	E	35	ASP
2	E	37	ILE
2	E	48	THR
2	E	65	GLU
2	E	67	THR
2	E	68	CYS
2	E	70	THR
2	E	74	SER
2	E	76	SER
2	E	92	THR
2	E	158	THR
1	C	235	LEU
1	C	239	SER
1	C	248	LYS
1	C	254	SER
1	C	270	ASP
1	C	302	VAL
1	C	324	SER
1	C	400	SER
1	C	414	LYS
1	C	430	GLU
1	D	239	SER
1	D	260	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	324	SER
1	D	337	SER
1	D	338	LYS
1	D	375	SER
1	D	415	SER
1	D	421	ASN
2	F	4	LYS
2	F	23	THR
2	F	40	PHE
2	F	45	LEU
2	F	48	THR
2	F	68	CYS
2	F	74	SER
2	F	76	SER
2	F	86	GLU
2	F	126	SER
2	F	158	THR
2	F	168	THR
2	F	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	310	HIS
1	A	419	GLN
1	B	311	GLN
1	B	390	ASN
1	B	438	GLN
2	E	27	GLN
2	E	41	HIS
2	E	69	GLN
2	E	80	HIS
2	E	98	GLN
1	C	362	GLN
1	C	418	GLN
1	D	311	GLN
1	D	315	ASN
1	D	325	ASN
1	D	429	HIS
2	F	27	GLN
2	F	150	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	G	1	2,3	14,14,15	0.65	0	17,19,21	1.38	2 (11%)
3	NAG	G	2	3	14,14,15	0.49	0	17,19,21	0.58	0
4	NAG	H	1	4,1	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
4	NAG	H	2	4	14,14,15	0.50	0	17,19,21	0.77	0
4	BMA	H	3	4	11,11,12	0.50	0	15,15,17	0.89	1 (6%)
4	MAN	H	4	4	11,11,12	0.95	0	15,15,17	1.38	2 (13%)
4	NAG	H	5	4	14,14,15	0.73	1 (7%)	17,19,21	0.53	0
4	MAN	H	6	4	11,11,12	1.84	4 (36%)	15,15,17	1.27	3 (20%)
4	NAG	H	7	4	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	FUC	H	8	4	10,10,11	1.34	2 (20%)	14,14,16	1.36	2 (14%)
4	NAG	I	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	0.50	0
4	NAG	I	2	4	14,14,15	0.69	0	17,19,21	0.82	1 (5%)
4	BMA	I	3	4	11,11,12	0.64	0	15,15,17	1.04	0
4	MAN	I	4	4	11,11,12	1.08	1 (9%)	15,15,17	1.36	1 (6%)
4	NAG	I	5	4	14,14,15	0.57	0	17,19,21	0.46	0
4	MAN	I	6	4	11,11,12	1.08	1 (9%)	15,15,17	1.07	1 (6%)
4	NAG	I	7	4	14,14,15	0.49	0	17,19,21	0.66	1 (5%)
4	FUC	I	8	4	10,10,11	1.34	2 (20%)	14,14,16	1.18	1 (7%)
4	NAG	J	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	J	2	4	14,14,15	0.37	0	17,19,21	0.72	0
4	BMA	J	3	4	11,11,12	0.63	0	15,15,17	1.06	1 (6%)
4	MAN	J	4	4	11,11,12	1.01	1 (9%)	15,15,17	1.04	2 (13%)
4	NAG	J	5	4	14,14,15	0.42	0	17,19,21	0.51	0
4	MAN	J	6	4	11,11,12	2.07	3 (27%)	15,15,17	1.37	2 (13%)
4	NAG	J	7	4	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
4	FUC	J	8	4	10,10,11	1.38	2 (20%)	14,14,16	1.14	2 (14%)
4	NAG	K	1	4,1	14,14,15	0.56	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.47	0	17,19,21	0.79	1 (5%)
4	BMA	K	3	4	11,11,12	1.03	1 (9%)	15,15,17	1.15	1 (6%)
4	MAN	K	4	4	11,11,12	1.24	0	15,15,17	1.27	2 (13%)
4	NAG	K	5	4	14,14,15	0.64	1 (7%)	17,19,21	0.45	0
4	MAN	K	6	4	11,11,12	1.18	1 (9%)	15,15,17	1.04	2 (13%)
4	NAG	K	7	4	14,14,15	0.56	0	17,19,21	0.80	1 (5%)
4	FUC	K	8	4	10,10,11	1.66	3 (30%)	14,14,16	1.29	2 (14%)

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

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

Continued on next page...

*Continued from previous page...*

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	6	MAN	C2-C3	3.74	1.58	1.52
4	H	6	MAN	C2-C3	3.71	1.58	1.52
4	J	6	MAN	O5-C1	-3.57	1.37	1.43
4	H	6	MAN	O5-C1	-3.29	1.38	1.43
4	K	8	FUC	C4-C5	3.27	1.60	1.52
4	J	4	MAN	O5-C1	-2.99	1.38	1.43
4	J	6	MAN	O2-C2	-2.87	1.37	1.43
4	H	8	FUC	C1-C2	2.82	1.58	1.52
4	J	8	FUC	C1-C2	2.62	1.58	1.52
4	K	8	FUC	C1-C2	2.58	1.58	1.52
4	I	4	MAN	O5-C1	-2.58	1.39	1.43
4	H	6	MAN	O5-C5	2.43	1.48	1.43
4	I	1	NAG	O5-C1	2.43	1.47	1.43
4	H	5	NAG	C1-C2	2.41	1.55	1.52
4	K	6	MAN	C2-C3	2.37	1.56	1.52
4	I	8	FUC	C4-C5	2.34	1.58	1.52
4	I	8	FUC	C1-C2	2.32	1.57	1.52
4	H	8	FUC	C2-C3	2.31	1.56	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	6	MAN	C2-C3	2.30	1.56	1.52
4	K	8	FUC	O5-C5	2.29	1.48	1.43
4	K	5	NAG	C1-C2	2.23	1.55	1.52
4	H	6	MAN	C4-C3	2.20	1.58	1.52
4	K	3	BMA	C1-C2	2.15	1.57	1.52
4	H	1	NAG	C1-C2	2.10	1.55	1.52
4	J	8	FUC	O5-C1	2.08	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	4	MAN	O2-C2-C3	-3.97	101.94	110.15
4	K	4	MAN	O2-C2-C3	-3.80	102.29	110.15
3	G	1	NAG	C2-N2-C7	3.58	127.69	122.90
4	H	4	MAN	O2-C2-C3	-3.34	103.23	110.15
4	J	6	MAN	O2-C2-C3	-3.23	103.47	110.15
4	H	4	MAN	C1-O5-C5	3.13	116.38	112.19
4	I	2	NAG	C1-O5-C5	2.86	116.02	112.19
4	K	2	NAG	C1-O5-C5	2.83	115.98	112.19
4	K	7	NAG	C1-O5-C5	2.74	115.86	112.19
4	J	7	NAG	C1-O5-C5	2.74	115.85	112.19
4	K	3	BMA	C1-O5-C5	2.71	115.82	112.19
4	J	6	MAN	C1-O5-C5	-2.67	108.61	112.19
4	K	8	FUC	O5-C5-C4	2.50	114.06	109.55
4	J	3	BMA	C1-O5-C5	2.48	115.51	112.19
4	H	6	MAN	O2-C2-C3	-2.44	105.10	110.15
4	I	8	FUC	C6-C5-C4	2.43	117.53	113.08
4	J	8	FUC	O2-C2-C1	2.43	114.78	109.22
4	H	8	FUC	O2-C2-C1	2.42	114.76	109.22
4	J	4	MAN	O2-C2-C3	-2.29	105.42	110.15
3	G	1	NAG	C1-C2-N2	2.28	114.02	110.43
4	I	6	MAN	O3-C3-C2	2.28	114.70	110.05
4	H	8	FUC	C1-O5-C5	2.27	118.33	112.97
4	J	8	FUC	C1-O5-C5	2.25	118.27	112.97
4	I	7	NAG	C1-O5-C5	2.24	115.18	112.19
4	K	4	MAN	C1-O5-C5	2.22	115.16	112.19
4	H	7	NAG	C1-O5-C5	2.20	115.13	112.19
4	H	6	MAN	C1-O5-C5	-2.20	109.24	112.19
4	K	8	FUC	O2-C2-C1	2.17	114.20	109.22
4	J	4	MAN	C3-C4-C5	-2.11	106.40	110.23
4	H	3	BMA	C1-O5-C5	2.11	115.01	112.19
4	K	6	MAN	C1-O5-C5	2.10	115.01	112.19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6	MAN	C2-C3-C4	2.04	114.44	110.86
4	K	6	MAN	O3-C3-C2	2.04	114.21	110.05

There are no chirality outliers.

All (44) torsion outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

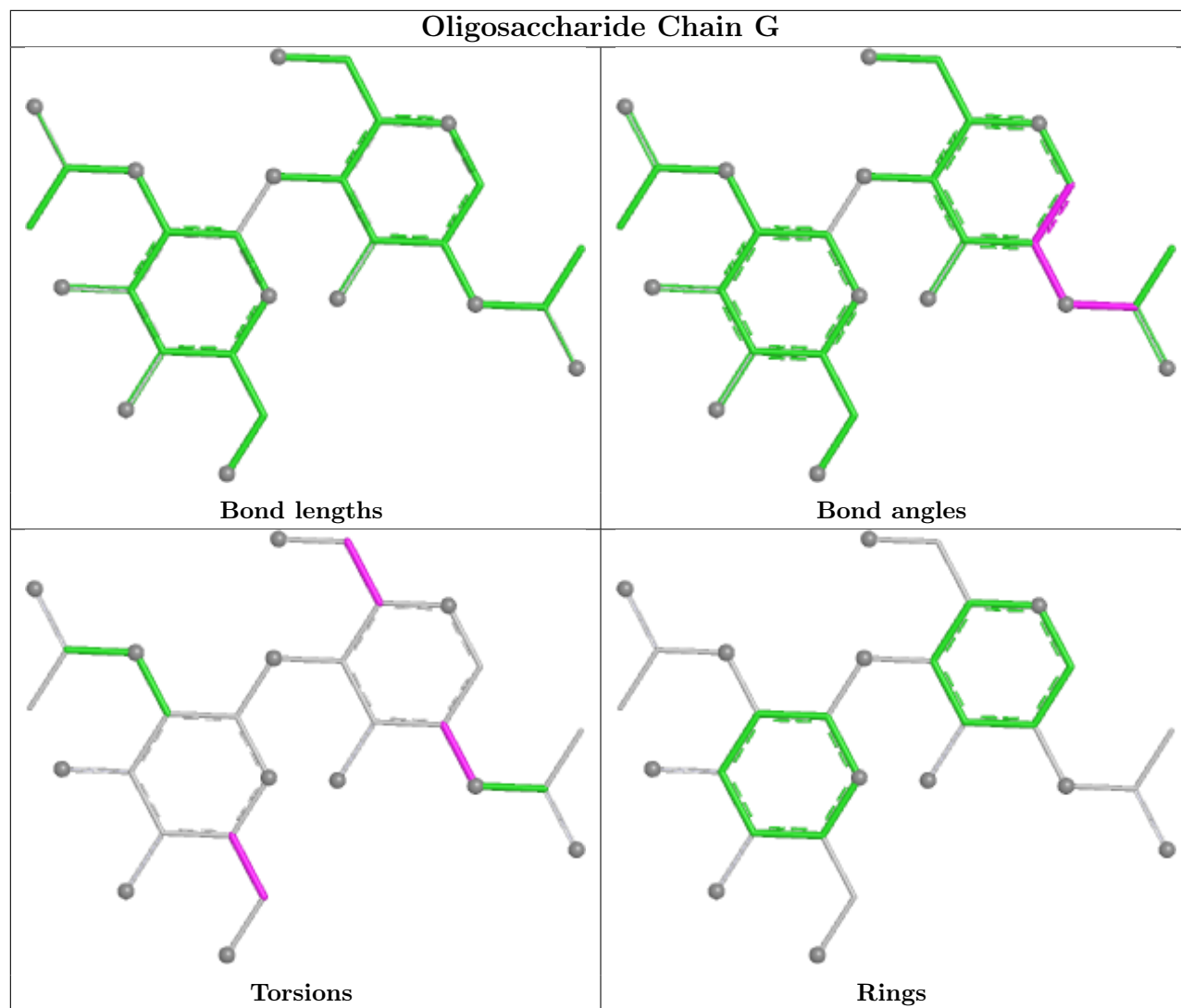
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	H	6	MAN	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	7	NAG	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	J	7	NAG	O5-C5-C6-O6
4	J	5	NAG	C1-C2-N2-C7
4	K	3	BMA	O5-C5-C6-O6

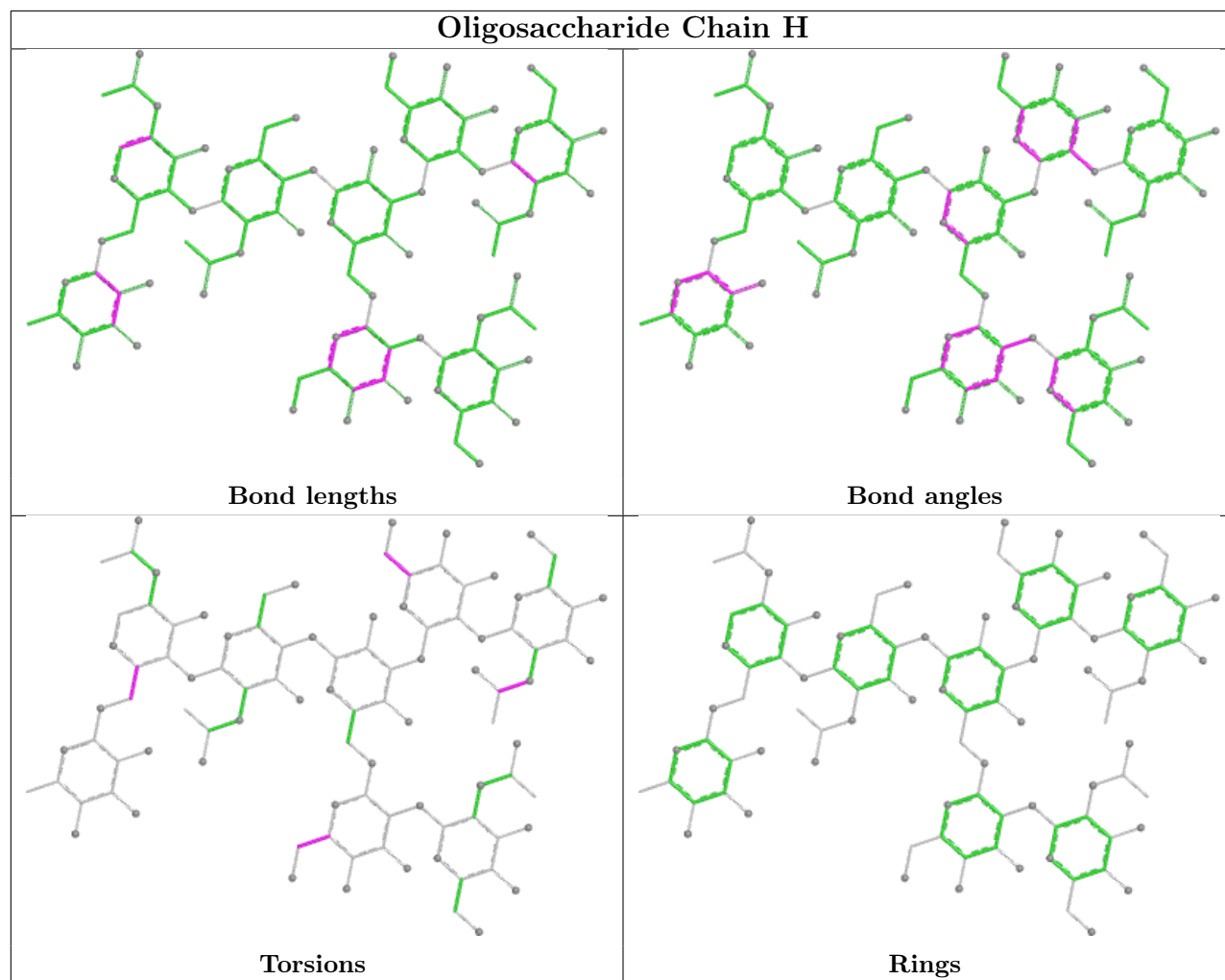
There are no ring outliers.

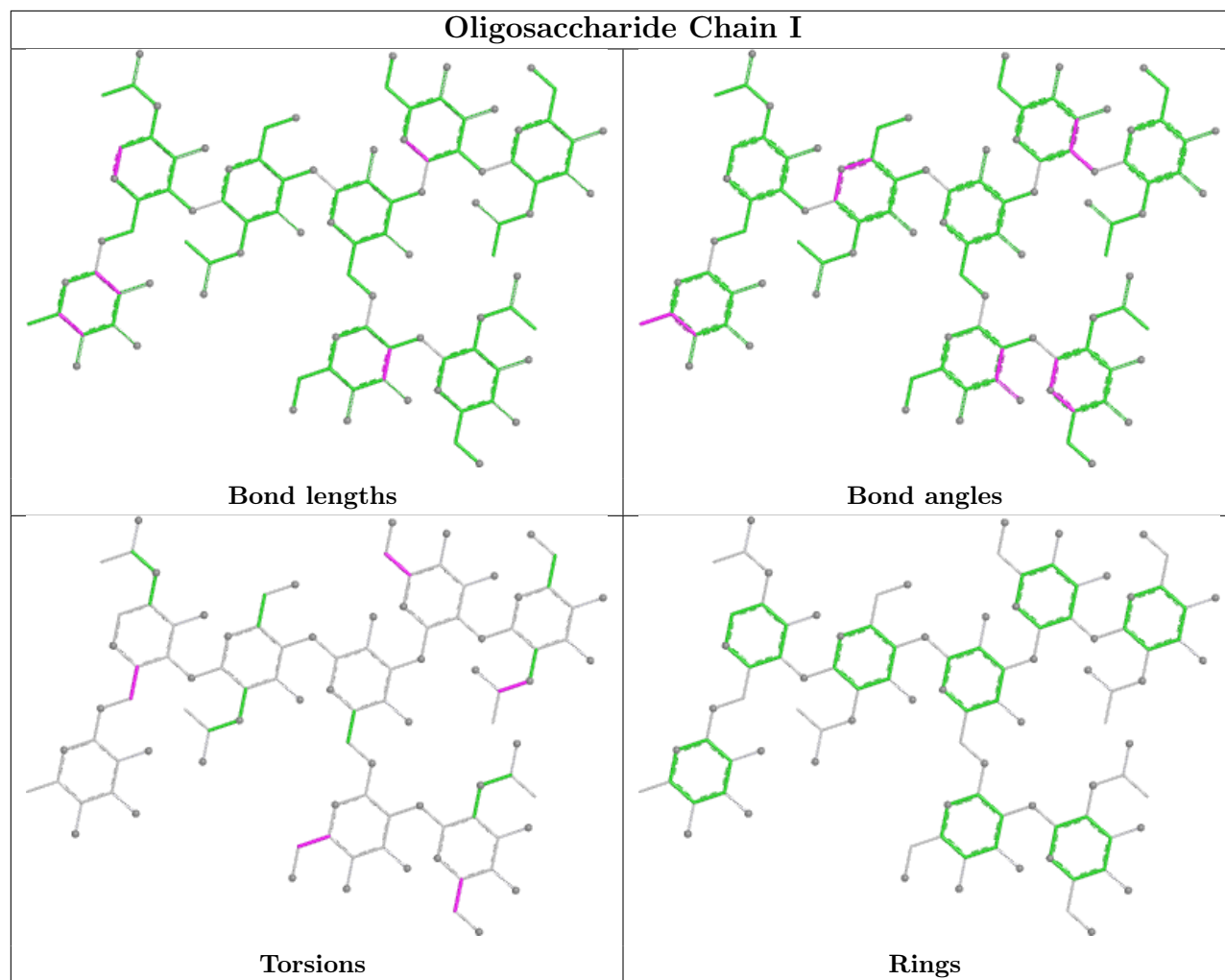
3 monomers are involved in 5 short contacts:

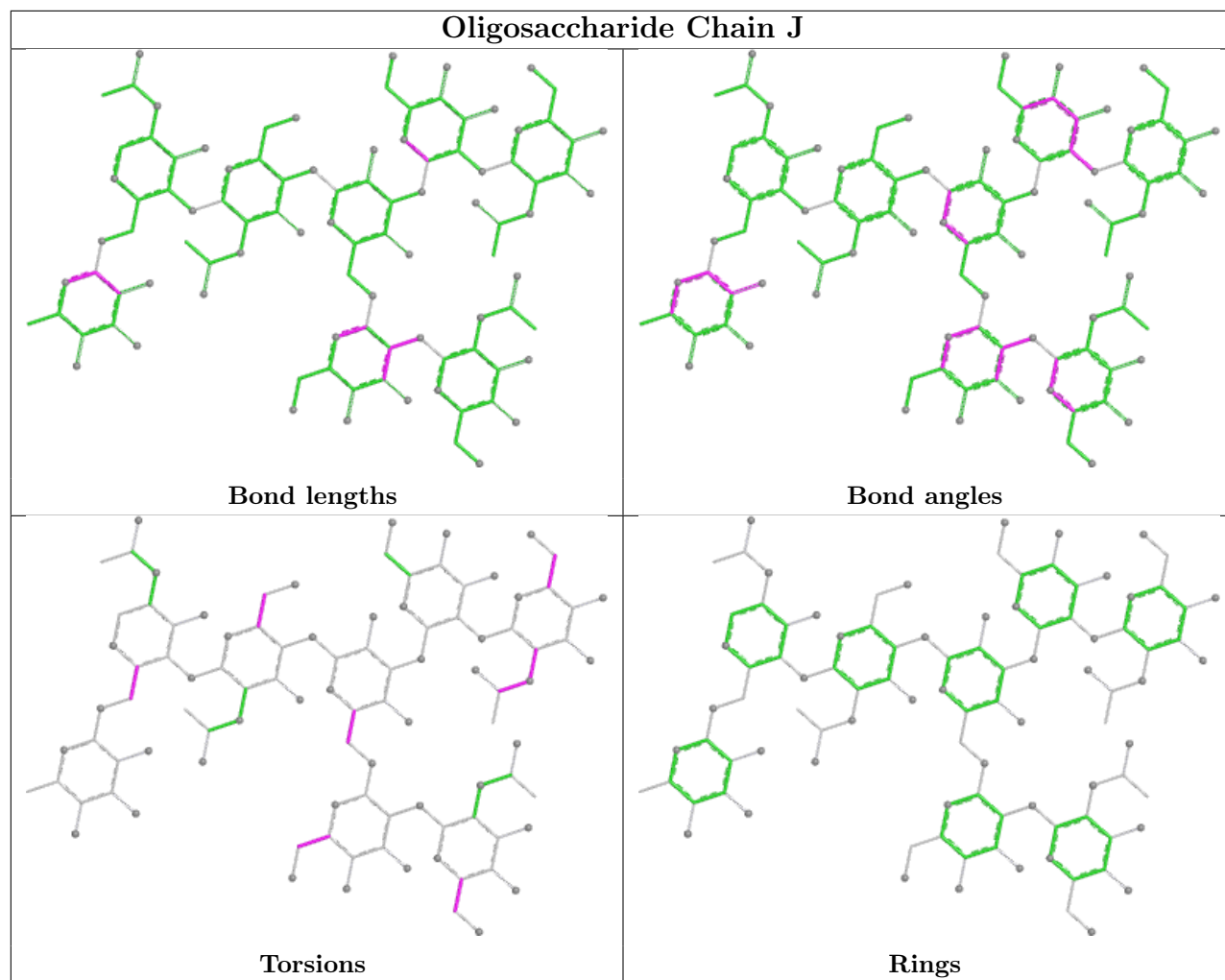
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	7	NAG	1	0
4	I	2	NAG	1	0
4	I	1	NAG	3	0

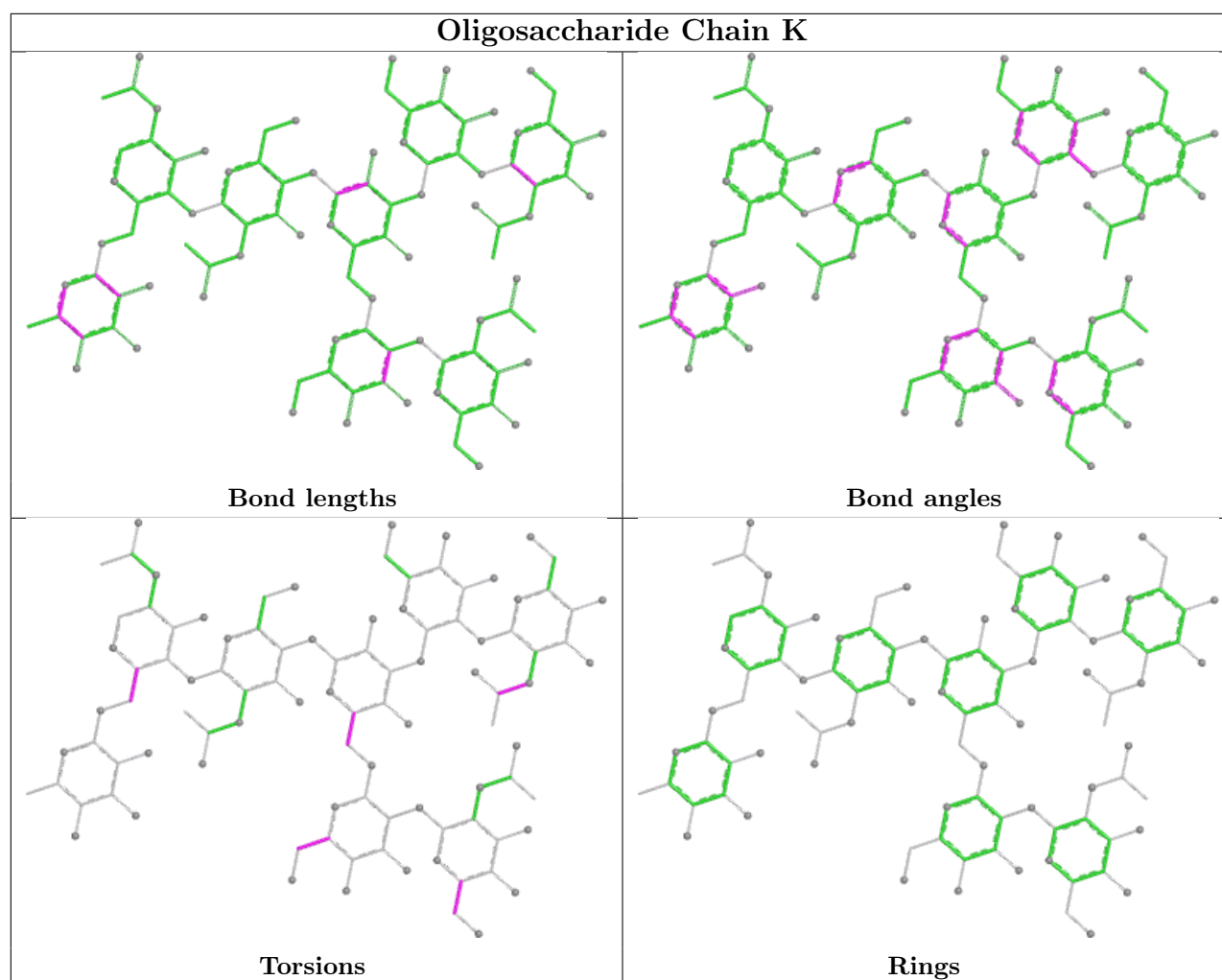
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
5	NAG	E	201	2	14,14,15	0.40	0	17,19,21	0.79	0
6	MPD	C	501	-	7,7,7	0.53	0	9,10,10	1.66	1 (11%)
6	MPD	D	501	-	7,7,7	0.75	0	9,10,10	1.51	1 (11%)
5	NAG	F	201	2	14,14,15	0.68	1 (7%)	17,19,21	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	201	2	-	4/6/23/26	0/1/1/1
6	MPD	C	501	-	-	4/5/5/5	-
6	MPD	D	501	-	-	3/5/5/5	-
5	NAG	F	201	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	201	NAG	C1-C2	2.10	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	501	MPD	O2-C2-CM	-4.05	95.36	107.99
6	C	501	MPD	CM-C2-C1	-3.44	102.92	110.63

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	501	MPD	C2-C3-C4-O4
5	E	201	NAG	C8-C7-N2-C2
5	E	201	NAG	O7-C7-N2-C2
5	E	201	NAG	C4-C5-C6-O6
5	E	201	NAG	O5-C5-C6-O6
6	D	501	MPD	O2-C2-C3-C4
6	C	501	MPD	C1-C2-C3-C4
6	C	501	MPD	C2-C3-C4-C5
6	D	501	MPD	C2-C3-C4-C5
5	F	201	NAG	C3-C2-N2-C7
6	D	501	MPD	C2-C3-C4-O4
6	C	501	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	501	MPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	215/223 (96%)	-0.53	1 (0%) 87 86	29, 55, 97, 180	0
1	B	214/223 (95%)	-0.47	0 100 100	32, 59, 107, 137	0
1	C	215/223 (96%)	-0.46	3 (1%) 73 70	28, 56, 99, 184	1 (0%)
1	D	214/223 (95%)	-0.49	0 100 100	23, 58, 106, 128	3 (1%)
2	E	172/173 (99%)	0.07	4 (2%) 61 58	67, 91, 141, 186	0
2	F	164/173 (94%)	0.07	0 100 100	67, 97, 150, 163	0
All	All	1194/1238 (96%)	-0.33	8 (0%) 84 83	23, 67, 130, 186	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	54	TYR	3.1
2	E	1	ALA	2.7
2	E	31	SER	2.7
1	C	231	ALA	2.5
1	A	234	LEU	2.4
1	C	296	TYR	2.1
1	C	232	PRO	2.1
2	E	35	ASP	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,

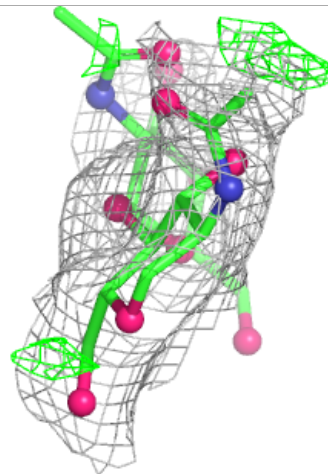
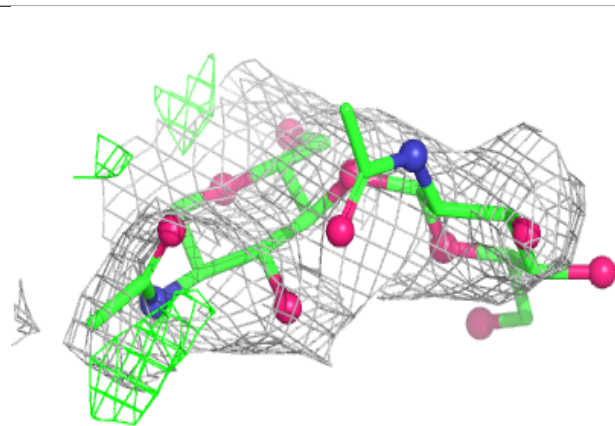
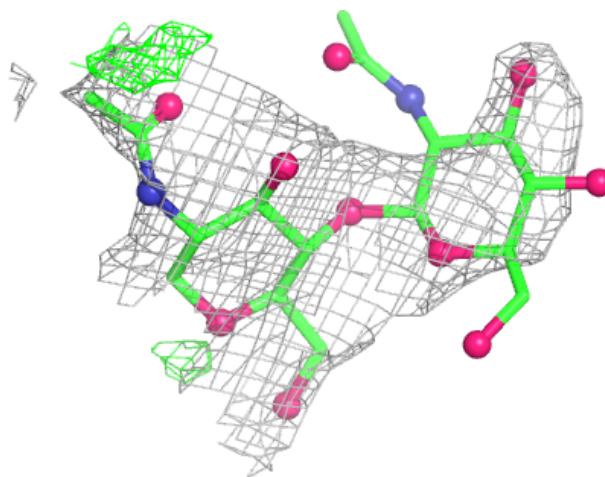
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	G	1	14/15	0.45	0.14	95,125,135,140	0
3	NAG	G	2	14/15	0.68	0.13	119,147,155,161	0
4	NAG	I	5	14/15	0.71	0.12	80,99,114,116	0
4	FUC	K	8	10/11	0.78	0.13	85,102,110,113	0
4	NAG	K	5	14/15	0.79	0.12	81,95,114,118	0
4	NAG	H	5	14/15	0.80	0.11	69,95,102,106	0
4	FUC	I	8	10/11	0.80	0.15	90,101,116,119	0
4	NAG	J	5	14/15	0.84	0.09	90,102,120,120	0
4	MAN	H	4	11/12	0.84	0.10	73,76,93,96	0
4	MAN	I	4	11/12	0.84	0.12	83,89,98,99	0
4	MAN	K	6	11/12	0.89	0.10	78,82,89,93	0
4	MAN	J	4	11/12	0.89	0.10	75,84,93,106	0
4	MAN	K	4	11/12	0.90	0.09	66,88,95,99	0
4	MAN	I	6	11/12	0.90	0.09	66,70,81,82	0
4	FUC	J	8	10/11	0.91	0.10	63,82,87,91	0
4	MAN	J	6	11/12	0.92	0.08	46,60,72,75	0
4	FUC	H	8	10/11	0.92	0.10	70,73,86,97	0
4	NAG	K	1	14/15	0.93	0.09	73,89,96,104	0
4	NAG	I	1	14/15	0.93	0.09	76,93,105,105	0
4	NAG	I	7	14/15	0.93	0.07	41,67,79,95	0
4	NAG	I	2	14/15	0.93	0.08	61,75,87,88	0
4	BMA	J	3	11/12	0.93	0.08	55,62,75,79	0
4	NAG	J	1	14/15	0.94	0.10	62,73,83,85	0
4	NAG	J	2	14/15	0.94	0.08	53,60,73,74	0
4	MAN	H	6	11/12	0.94	0.07	47,59,68,72	0
4	NAG	H	7	14/15	0.94	0.08	46,53,79,81	0
4	BMA	I	3	11/12	0.94	0.07	63,66,82,84	0
4	NAG	K	7	14/15	0.94	0.07	55,74,88,105	0
4	NAG	H	2	14/15	0.94	0.08	52,60,66,68	0
4	NAG	H	1	14/15	0.95	0.10	59,72,78,81	0
4	NAG	J	7	14/15	0.95	0.08	41,64,73,75	0
4	BMA	H	3	11/12	0.95	0.06	40,60,67,75	0
4	NAG	K	2	14/15	0.96	0.07	62,76,86,97	0
4	BMA	K	3	11/12	0.97	0.05	60,66,76,81	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.

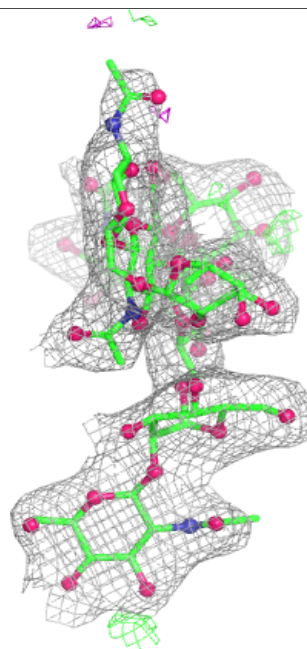
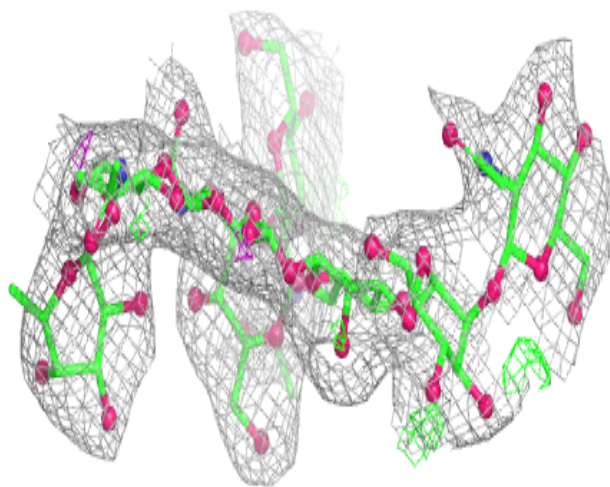
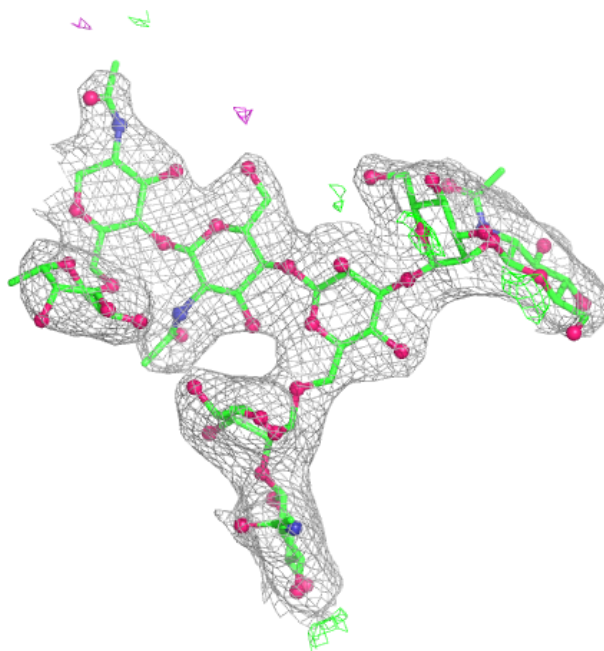
**Electron density around Chain G:**

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



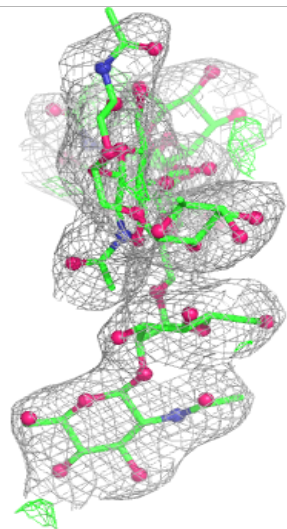
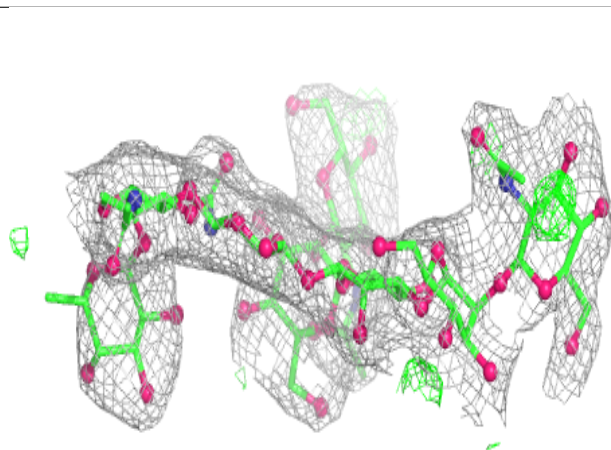
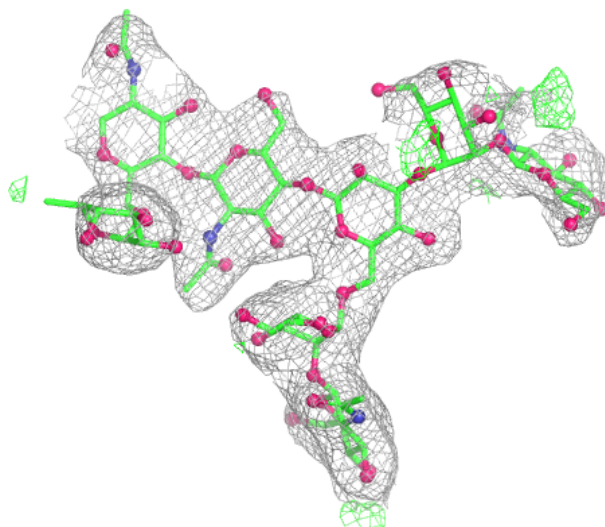
**Electron density around Chain H:**

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



**Electron density around Chain I:**

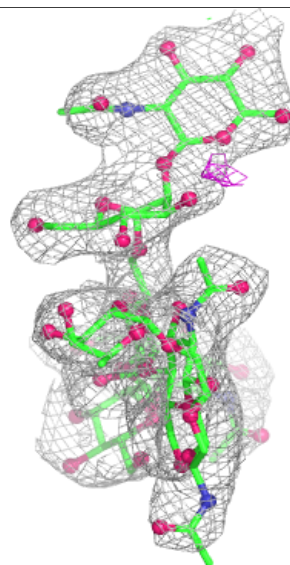
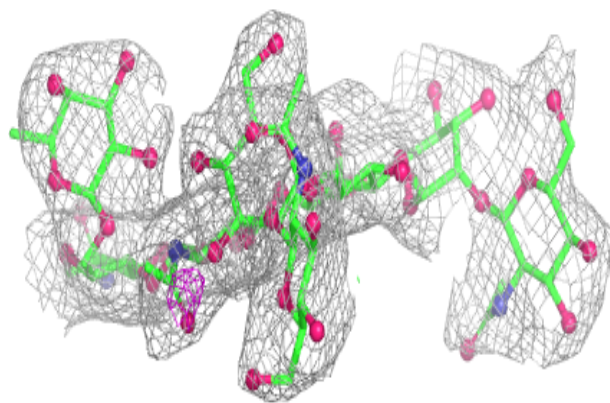
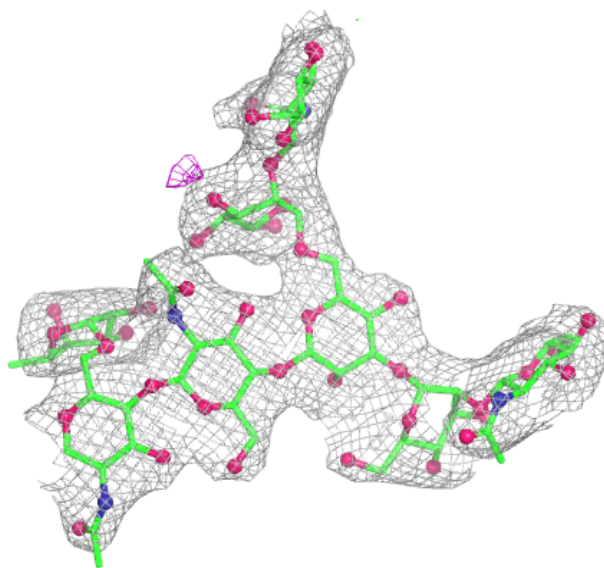
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

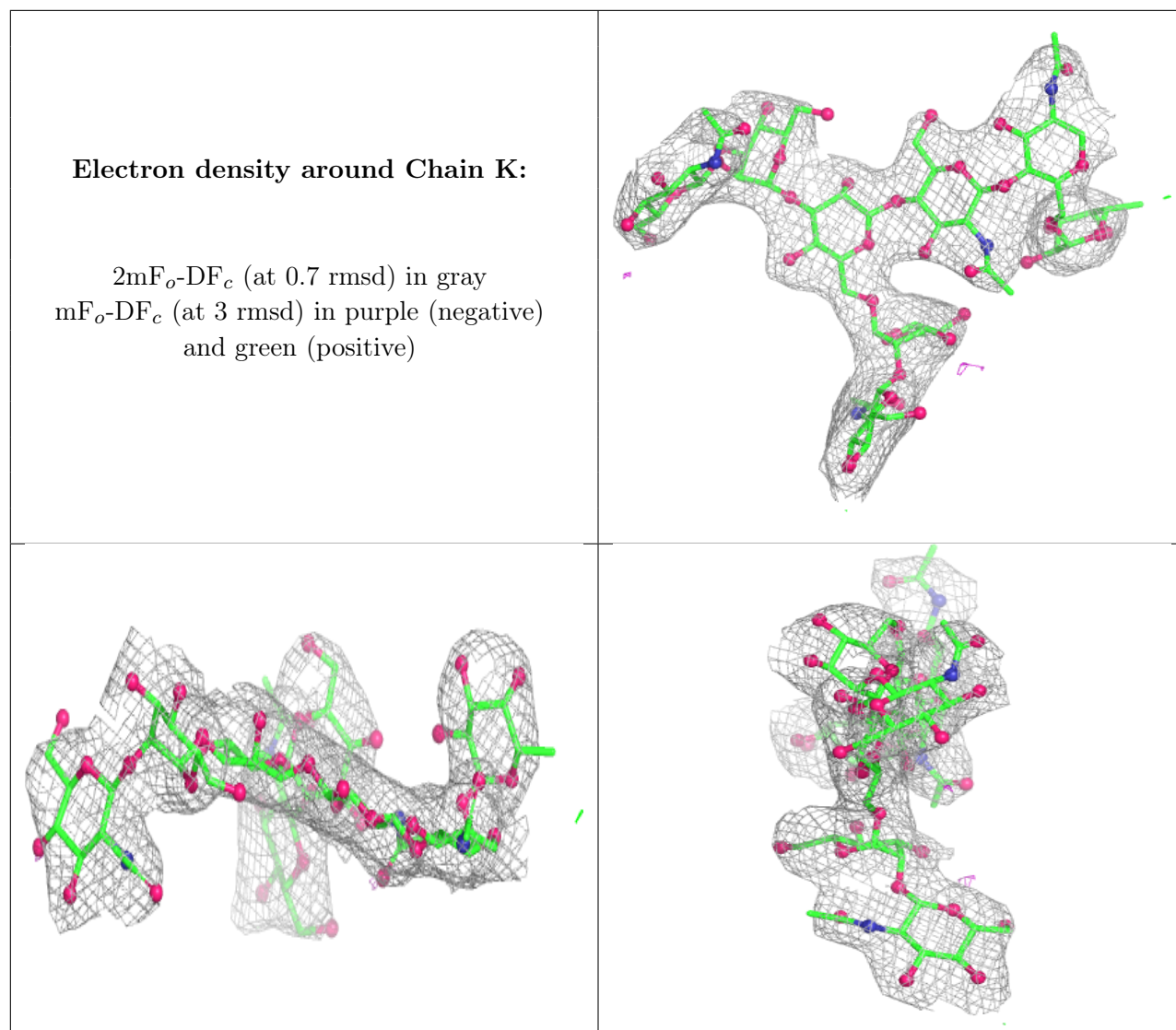




**Electron density around Chain J:**

$2mF_o-DF_c$  (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
5	NAG	E	201	14/15	0.21	0.15	98,136,143,146	0
5	NAG	F	201	14/15	0.63	0.14	87,113,122,126	0
6	MPD	C	501	8/8	0.83	0.16	57,73,92,97	0
6	MPD	D	501	8/8	0.86	0.20	48,72,100,112	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.