



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 10:14 am BST

PDB ID : 6F39  
Title : C1r homodimer CUB1-EGF-CUB2  
Authors : Almitairi, J.O.M.; Venkatraman Girija, U.; Furze, C.M.; Simpson-Gray, X.;  
Badakshi, F.; Marshall, J.E.; Mitchell, D.A.; Moody, P.C.E.; Wallis, R.  
Deposited on : 2017-11-28  
Resolution : 5.80 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

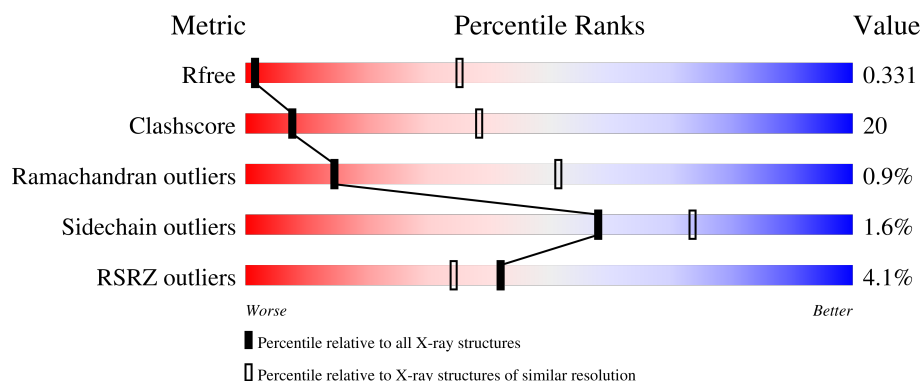
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.80 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	1066 (7.60-4.00)
Clashscore	180529	1107 (7.60-4.00)
Ramachandran outliers	177936	1001 (7.60-3.98)
Sidechain outliers	177891	1006 (7.60-3.96)
RSRZ outliers	164620	1061 (7.60-4.00)

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	285	<div> <div>3%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
1	B	285	<div> <div>5%</div> <div>59%</div> <div>37%</div> <div>..</div> </div>
2	C	6	<div> <div>67%</div> <div>33%</div> </div>
2	D	6	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition [i](#)

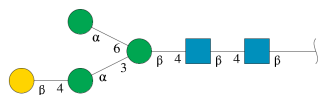
There are 5 unique types of molecules in this entry. The entry contains 4612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Complement C1r subcomponent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2206	1397	362	433	14			
1	B	280	Total	C	N	O	S	0	0	0
			2240	1417	368	440	15			

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



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

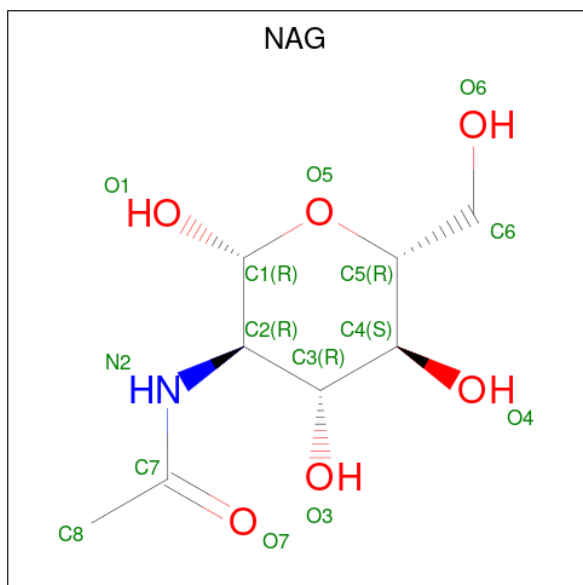
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Na		0	0
			1	1			

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

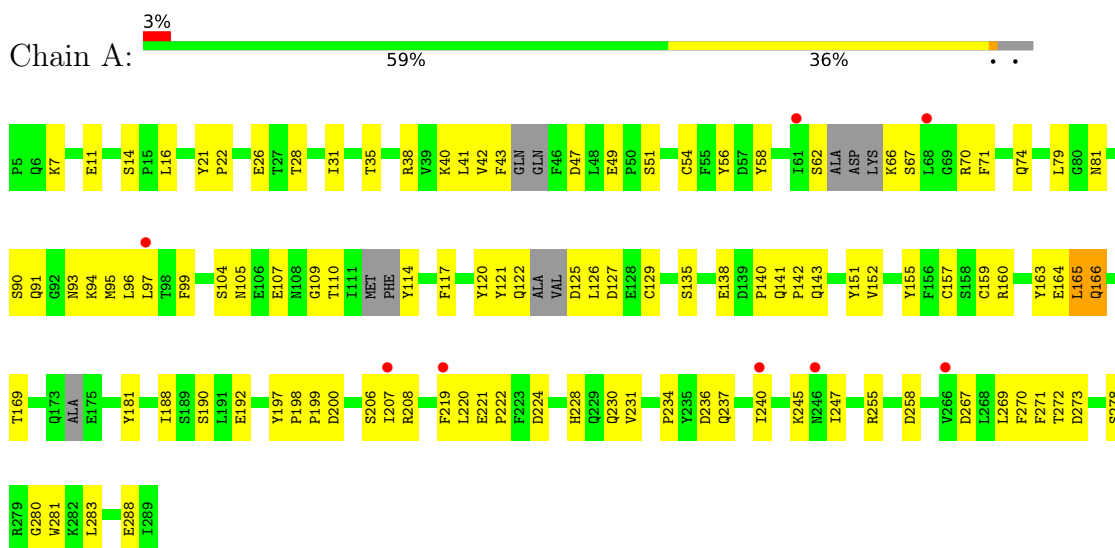


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

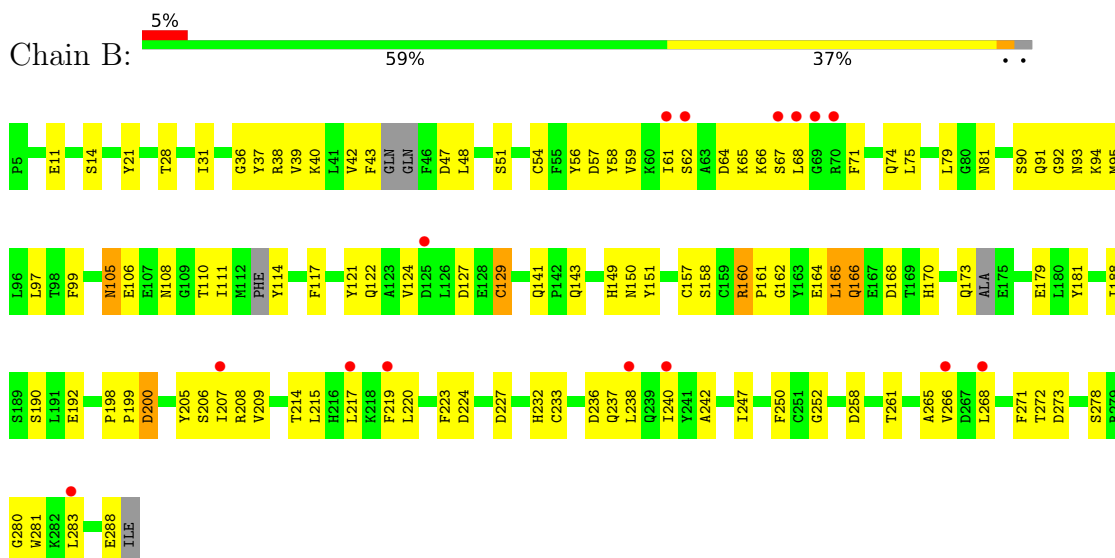
### 3 Residue-property plots [i](#)

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

- Molecule 1: Complement C1r subcomponent



- Molecule 1: Complement C1r subcomponent



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

Chain C:  67% 33%

MAG1
MAG2
BMA3
MAN4
GAL5
MAN6

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

Chain D:  67% 33%

MAG1
MAG2
BMA3
MAN4
GAL5
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.56Å 54.62Å 138.18Å 90.00° 99.90° 90.00°	Depositor
Resolution (Å)	68.06 – 5.80 68.06 – 5.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (68.06-5.80) 98.8 (68.06-5.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.32	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 5.75Å)	Xtriage
Refinement program	PHENIX dev_2722	Depositor
R, $R_{free}$	0.308 , 0.338 0.302 , 0.331	Depositor DCC
$R_{free}$ test set	133 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	140.5	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 449.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	351.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: MAN, NAG, GAL, NA, CA, BMA

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	0.49	0/2264	0.71	0/3060
1	B	0.50	0/2300	0.71	2/3111 (0.1%)
All	All	0.49	0/4564	0.71	2/6171 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	165	LEU	CA-CB-CG	5.30	127.48	115.30
1	B	192	GLU	C-N-CA	5.13	134.52	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	GLN	Peptide
1	B	166	GLN	Peptide



## 5.2 Too-close contacts ⓘ

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	2206	0	2052	90	1
1	B	2240	0	2087	85	0
2	C	72	0	61	6	0
2	D	72	0	61	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	13	0	0
All	All	4612	0	4274	175	1

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 20.

All (175) 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:208:ARG:NH1	1:B:266:VAL:O	2.11	0.82
1:B:190:SER:HB3	1:B:281:TRP:CE2	2.17	0.79
1:B:93:ASN:HD21	1:B:94:LYS:HE3	1.48	0.77
1:A:237:GLN:HB2	1:A:271:PHE:HB3	1.64	0.77
1:B:38:ARG:NE	1:B:90:SER:O	2.14	0.74
1:A:206:SER:OG	1:A:208:ARG:NH1	2.20	0.73
1:B:31:ILE:HB	1:B:95:MET:HB3	1.68	0.73
1:A:38:ARG:HD2	1:A:126:LEU:HB2	1.71	0.72
1:A:31:ILE:HB	1:A:95:MET:HB3	1.72	0.72
1:B:158:SER:HA	1:B:165:LEU:HD21	1.72	0.72
1:A:188:ILE:HB	1:A:283:LEU:HD11	1.71	0.72
1:A:206:SER:OG	1:A:267:ASP:OD1	2.03	0.71
1:B:129:CYS:HB3	1:B:150:ASN:ND2	2.07	0.70
1:A:93:ASN:HD21	1:A:94:LYS:HE3	1.56	0.69
1:A:236:ASP:OD1	1:A:273:ASP:N	2.25	0.69
1:B:71:PHE:CD1	1:B:81:ASN:HB3	2.28	0.68
1:B:143:GLN:HG3	1:B:157:CYS:SG	2.34	0.68
2:C:2:NAG:O3	2:C:3:BMA:O2	2.06	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HB3	1:A:222:PRO:HA	1.76	0.68
1:A:181:TYR:HB2	1:A:207:ILE:HG12	1.76	0.67
2:C:2:NAG:HO3	2:C:3:BMA:HO2	1.38	0.67
1:A:51:SER:HB3	1:A:56:TYR:HD2	1.59	0.66
1:A:208:ARG:NH2	2:C:1:NAG:O6	2.29	0.66
1:A:135:SER:HB2	1:A:138:GLU:HG2	1.76	0.66
1:A:142:PRO:HB2	1:A:155:TYR:CE2	2.31	0.64
1:A:26:GLU:HA	1:A:99:PHE:O	1.98	0.64
1:A:224:ASP:HB3	1:A:280:GLY:H	1.61	0.64
1:B:160:ARG:O	1:B:162:GLY:N	2.30	0.64
1:A:51:SER:HB3	1:A:56:TYR:CD2	2.33	0.64
1:A:54:CYS:HB3	1:A:58:TYR:HB3	1.80	0.63
1:B:62:SER:HA	1:B:68:LEU:HG	1.80	0.63
1:B:129:CYS:HB3	1:B:150:ASN:HD21	1.63	0.63
1:B:47:ASP:O	1:B:114:TYR:HB3	1.99	0.62
1:A:142:PRO:HB2	1:A:155:TYR:HE2	1.65	0.61
1:B:237:GLN:HB2	1:B:271:PHE:HB2	1.83	0.60
1:B:64:ASP:HB3	1:B:65:LYS:HG2	1.82	0.60
1:A:208:ARG:HH21	2:C:2:NAG:C7	2.15	0.59
1:A:51:SER:OG	1:A:54:CYS:HA	2.03	0.59
1:B:208:ARG:HG3	1:B:265:ALA:HB1	1.85	0.58
1:B:214:THR:HG23	1:B:288:GLU:HB3	1.85	0.58
1:A:14:SER:HB3	1:A:117:PHE:CD1	2.39	0.57
1:A:58:TYR:HB2	1:A:70:ARG:HG3	1.86	0.57
1:A:122:GLN:HE22	1:B:150:ASN:N	2.03	0.57
1:A:66:LYS:HE2	1:A:67:SER:H	1.69	0.57
1:B:39:VAL:HG21	1:B:95:MET:HB2	1.88	0.55
1:B:93:ASN:ND2	1:B:94:LYS:HE3	2.18	0.55
1:B:206:SER:HB2	1:B:208:ARG:NH1	2.22	0.55
1:A:109:GLY:O	1:A:110:THR:OG1	2.25	0.54
1:B:108:ASN:O	1:B:110:THR:HG23	2.08	0.54
1:B:215:LEU:HB2	1:B:261:THR:HG21	1.90	0.53
1:B:28:THR:HG23	1:B:97:LEU:O	2.08	0.53
1:A:219:PHE:O	1:A:220:LEU:HD13	2.09	0.53
1:A:71:PHE:CD1	1:A:81:ASN:HB3	2.43	0.53
2:C:1:NAG:O6	2:C:2:NAG:N2	2.39	0.53
1:A:228:HIS:NE2	1:A:230:GLN:OE1	2.40	0.53
1:A:151:TYR:CG	1:A:152:VAL:N	2.78	0.52
1:A:197:TYR:HE2	1:A:278:SER:HB2	1.74	0.52
1:B:51:SER:HB3	1:B:56:TYR:CD2	2.45	0.52
1:B:106:GLU:HG2	1:B:111:ILE:HG23	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:HD1	1:A:81:ASN:HB3	1.74	0.52
1:A:125:ASP:O	1:A:126:LEU:HD12	2.09	0.52
1:B:48:LEU:HD21	1:B:99:PHE:HE1	1.75	0.52
1:A:11:GLU:HG3	1:A:120:TYR:CE1	2.45	0.52
1:A:35:THR:HA	1:A:93:ASN:HB2	1.91	0.52
1:A:221:GLU:HG3	1:A:255:ARG:HD3	1.92	0.52
1:B:14:SER:HB3	1:B:117:PHE:CD1	2.45	0.51
1:B:57:ASP:OD2	1:B:105:ASN:ND2	2.42	0.51
1:A:151:TYR:CE1	1:B:122:GLN:HB3	2.45	0.51
1:B:188:ILE:O	1:B:283:LEU:HG	2.10	0.51
1:A:240:ILE:O	1:A:247:ILE:HG12	2.10	0.51
1:B:143:GLN:OE1	1:B:157:CYS:HB2	2.11	0.51
1:A:197:TYR:HE1	1:A:272:THR:HG1	1.60	0.50
1:B:215:LEU:O	1:B:261:THR:HG23	2.11	0.50
1:A:104:SER:HB2	1:A:107:GLU:OE1	2.10	0.50
1:A:159:CYS:SG	1:A:165:LEU:HD13	2.51	0.50
1:B:59:VAL:HG22	1:B:99:PHE:CD1	2.46	0.50
1:A:127:ASP:OD1	1:A:155:TYR:HB3	2.11	0.50
1:A:40:LYS:O	1:A:121:TYR:HA	2.12	0.49
1:B:62:SER:HB2	1:B:66:LYS:O	2.12	0.49
1:B:188:ILE:HB	1:B:283:LEU:HD11	1.94	0.49
1:A:160:ARG:HH21	1:A:192:GLU:HG3	1.76	0.49
1:A:38:ARG:NE	1:A:90:SER:O	2.44	0.49
1:B:127:ASP:HB3	1:B:150:ASN:OD1	2.11	0.49
1:A:11:GLU:HG3	1:A:120:TYR:CD1	2.48	0.49
1:A:151:TYR:CE1	1:A:152:VAL:HG22	2.48	0.49
1:B:61:ILE:HD12	1:B:68:LEU:HB2	1.94	0.49
1:A:47:ASP:O	1:A:114:TYR:HB3	2.13	0.49
1:A:56:TYR:HB3	1:A:107:GLU:OE2	2.13	0.48
1:B:208:ARG:NH2	2:D:1:NAG:O6	2.45	0.48
1:B:215:LEU:HB2	1:B:261:THR:CG2	2.43	0.48
1:A:14:SER:HB3	1:A:117:PHE:CE1	2.48	0.48
1:B:224:ASP:CG	1:B:278:SER:HB3	2.34	0.48
1:A:7:LYS:HD3	1:A:121:TYR:OH	2.13	0.48
1:A:270:PHE:CE2	1:A:272:THR:HB	2.49	0.48
1:B:21:TYR:CE2	1:B:114:TYR:HB2	2.48	0.48
1:B:224:ASP:HB3	1:B:280:GLY:H	1.79	0.48
1:A:38:ARG:NH1	1:A:126:LEU:HD22	2.29	0.48
1:B:36:GLY:C	1:B:37:TYR:CD1	2.87	0.48
1:B:190:SER:HB3	1:B:281:TRP:NE1	2.28	0.47
1:A:157:CYS:HB2	1:A:169:THR:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:OG	1:A:96:LEU:HB2	2.13	0.47
1:A:224:ASP:N	1:A:280:GLY:O	2.47	0.47
1:B:59:VAL:HG22	1:B:99:PHE:HD1	1.80	0.47
1:A:221:GLU:CB	1:A:222:PRO:HA	2.45	0.47
1:B:227:ASP:CG	1:B:252:GLY:HA2	2.35	0.47
1:B:141:GLN:HB2	1:B:170:HIS:NE2	2.30	0.46
1:B:205:TYR:O	1:B:268:LEU:HB2	2.15	0.46
1:A:190:SER:HB3	1:A:281:TRP:CE2	2.49	0.46
1:B:66:LYS:HE2	1:B:67:SER:H	1.81	0.46
1:A:127:ASP:OD2	1:A:151:TYR:N	2.48	0.46
1:A:160:ARG:HE	1:A:192:GLU:HG3	1.80	0.46
1:A:41:LEU:HD11	1:A:95:MET:HG2	1.98	0.46
1:B:223:PHE:CE1	1:B:281:TRP:HB3	2.51	0.46
1:A:164:GLU:O	1:A:164:GLU:HG2	2.16	0.45
2:D:2:NAG:O3	2:D:3:BMA:O2	2.15	0.45
1:A:21:TYR:CE2	1:A:114:TYR:HB2	2.51	0.45
1:B:209:VAL:HG11	1:B:215:LEU:HD21	1.98	0.45
1:A:198:PRO:HA	1:A:199:PRO:HD3	1.77	0.45
1:B:236:ASP:OD1	1:B:273:ASP:N	2.42	0.45
1:A:152:VAL:HG13	1:B:124:VAL:HG13	1.99	0.45
1:A:228:HIS:CD2	1:A:230:GLN:HB2	2.52	0.45
1:B:242:ALA:HB2	1:B:247:ILE:HD13	1.99	0.45
1:B:232:HIS:HB3	1:B:233:CYS:SG	2.57	0.45
1:B:179:GLU:HB2	1:B:205:TYR:CE1	2.52	0.44
1:A:38:ARG:HD3	1:A:126:LEU:HD13	2.00	0.44
1:A:122:GLN:NE2	1:B:149:HIS:HB3	2.32	0.44
1:B:160:ARG:O	1:B:160:ARG:HG3	2.17	0.44
1:B:42:VAL:HG23	1:B:43:PHE:O	2.18	0.44
1:A:62:SER:OG	1:A:62:SER:O	2.36	0.43
1:B:238:LEU:HB3	1:B:250:PHE:O	2.18	0.43
1:A:16:LEU:HD13	1:A:22:PRO:HD3	2.00	0.43
1:A:31:ILE:HD12	1:A:95:MET:HB3	2.00	0.43
1:B:90:SER:OG	1:B:92:GLY:O	2.28	0.43
1:A:28:THR:HG23	1:A:97:LEU:O	2.19	0.43
1:A:197:TYR:OH	1:A:236:ASP:OD2	2.28	0.43
1:B:160:ARG:NH2	1:B:173:GLN:HB2	2.34	0.43
1:B:198:PRO:HA	1:B:199:PRO:HD3	1.80	0.43
1:A:105:ASN:HD21	1:A:114:TYR:N	2.17	0.43
1:A:231:VAL:O	1:A:234:PRO:HD3	2.19	0.42
1:A:140:PRO:O	1:A:142:PRO:HD3	2.19	0.42
1:A:269:LEU:HD21	2:C:1:NAG:O7	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:PHE:HD1	1:B:81:ASN:HB3	1.82	0.42
1:B:181:TYR:O	1:B:207:ILE:HG12	2.20	0.42
1:A:142:PRO:HD2	1:A:143:GLN:HG2	2.00	0.42
1:B:240:ILE:O	1:B:247:ILE:HG12	2.19	0.42
1:A:49:GLU:OE2	1:A:107:GLU:HB2	2.19	0.42
1:B:66:LYS:HE2	1:B:67:SER:N	2.34	0.42
1:A:35:THR:HA	1:A:93:ASN:CB	2.48	0.42
1:A:38:ARG:HH21	1:A:91:GLN:HA	1.85	0.42
1:A:42:VAL:HG23	1:A:43:PHE:O	2.19	0.42
1:B:40:LYS:O	1:B:121:TYR:HA	2.20	0.42
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.85	0.42
1:A:47:ASP:OD1	1:A:74:GLN:HG3	2.19	0.42
1:A:258:ASP:N	1:A:258:ASP:OD1	2.53	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.95	0.41
1:A:219:PHE:C	1:A:220:LEU:HD22	2.41	0.41
1:A:165:LEU:HD12	1:A:169:THR:HA	2.02	0.41
1:B:91:GLN:OE1	1:B:91:GLN:N	2.53	0.41
1:B:160:ARG:C	1:B:162:GLY:H	2.23	0.41
1:B:31:ILE:HD12	1:B:95:MET:HG2	2.03	0.41
1:B:219:PHE:O	1:B:220:LEU:HD13	2.20	0.41
1:A:163:TYR:HD2	1:A:165:LEU:H	1.69	0.41
1:B:168:ASP:HB2	1:B:170:HIS:ND1	2.36	0.41
1:B:199:PRO:HA	1:B:272:THR:HB	2.01	0.41
1:B:217:LEU:HD11	1:B:261:THR:HG22	2.02	0.41
1:A:38:ARG:HH11	1:A:126:LEU:HD22	1.84	0.41
1:B:164:GLU:C	1:B:165:LEU:HD23	2.41	0.41
1:B:200:ASP:N	1:B:273:ASP:O	2.45	0.40
1:A:41:LEU:HD23	1:A:120:TYR:O	2.20	0.40
1:B:64:ASP:OD2	1:B:92:GLY:HA3	2.21	0.40
1:B:74:GLN:HG2	1:B:75:LEU:H	1.86	0.40
1:B:208:ARG:HH21	2:D:2:NAG:C7	2.34	0.40
1:B:54:CYS:HB3	1:B:58:TYR:HB3	2.02	0.40
1:B:179:GLU:HB2	1:B:205:TYR:CD1	2.55	0.40
1:B:258:ASP:OD1	1:B:258:ASP:N	2.54	0.40

All (1) 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:245:LYS:NZ	1:A:288:GLU:OE1[4_646]	2.19	0.01

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/285 (92%)	227 (86%)	34 (13%)	2 (1%)	16	55
1	B	272/285 (95%)	233 (86%)	36 (13%)	3 (1%)	12	46
All	All	535/570 (94%)	460 (86%)	70 (13%)	5 (1%)	14	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	B	166	GLN
1	B	161	PRO
1	B	160	ARG
1	A	141	GLN

### 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	248/255 (97%)	245 (99%)	3 (1%)	67	78
1	B	251/255 (98%)	246 (98%)	5 (2%)	50	68
All	All	499/510 (98%)	491 (98%)	8 (2%)	58	73

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	LEU
1	A	200	ASP
1	B	11	GLU
1	B	105	ASN
1	B	129	CYS
1	B	151	TYR
1	B	200	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN

### 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 ⓘ

12 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	C	1	2,1	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.52	0
2	BMA	C	3	2	11,11,12	1.63	3 (27%)	15,15,17	1.07	2 (13%)
2	MAN	C	4	2	11,11,12	1.56	3 (27%)	15,15,17	1.87	1 (6%)
2	GAL	C	5	2	11,11,12	1.15	2 (18%)	15,15,17	1.23	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	C	6	2	11,11,12	0.84	1 (9%)	15,15,17	0.97	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.20	0	17,19,21	0.84	1 (5%)
2	NAG	D	2	2	14,14,15	0.48	0	17,19,21	0.65	0
2	BMA	D	3	2	11,11,12	1.30	2 (18%)	15,15,17	0.99	0
2	MAN	D	4	2	11,11,12	1.78	4 (36%)	15,15,17	1.74	1 (6%)
2	GAL	D	5	2	11,11,12	1.31	2 (18%)	15,15,17	1.41	3 (20%)
2	MAN	D	6	2	11,11,12	0.74	0	15,15,17	1.19	1 (6%)

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

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	O4-C4	3.99	1.52	1.43
2	C	3	BMA	C4-C3	2.91	1.59	1.52
2	C	4	MAN	O5-C5	2.83	1.49	1.43
2	D	5	GAL	C1-C2	2.59	1.58	1.52
2	C	3	BMA	O3-C3	2.53	1.48	1.43
2	D	3	BMA	C1-C2	2.48	1.57	1.52
2	C	3	BMA	C4-C5	2.43	1.58	1.53
2	C	4	MAN	O4-C4	2.41	1.48	1.43
2	D	3	BMA	C4-C5	2.30	1.57	1.53
2	D	4	MAN	C2-C3	2.21	1.55	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	O5-C5	2.21	1.47	1.43
2	C	4	MAN	C2-C3	2.18	1.55	1.52
2	C	5	GAL	C1-C2	2.13	1.57	1.52
2	D	5	GAL	O5-C5	2.11	1.47	1.43
2	D	4	MAN	C4-C3	2.10	1.57	1.52
2	C	6	MAN	O5-C1	-2.08	1.40	1.43
2	C	5	GAL	C2-C3	2.03	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	6.01	120.34	112.19
2	D	4	MAN	C1-O5-C5	5.19	119.22	112.19
2	D	6	MAN	C1-O5-C5	3.31	116.68	112.19
2	C	1	NAG	C1-O5-C5	3.28	116.64	112.19
2	C	3	BMA	O2-C2-C3	-2.79	104.54	110.14
2	D	1	NAG	C1-O5-C5	2.61	115.72	112.19
2	D	5	GAL	C1-O5-C5	2.56	115.66	112.19
2	C	6	MAN	O2-C2-C3	-2.47	105.19	110.14
2	D	5	GAL	O5-C1-C2	-2.46	106.98	110.77
2	D	5	GAL	O2-C2-C1	2.22	113.68	109.15
2	C	3	BMA	C3-C4-C5	2.09	113.97	110.24
2	C	5	GAL	O5-C1-C2	-2.07	107.58	110.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6

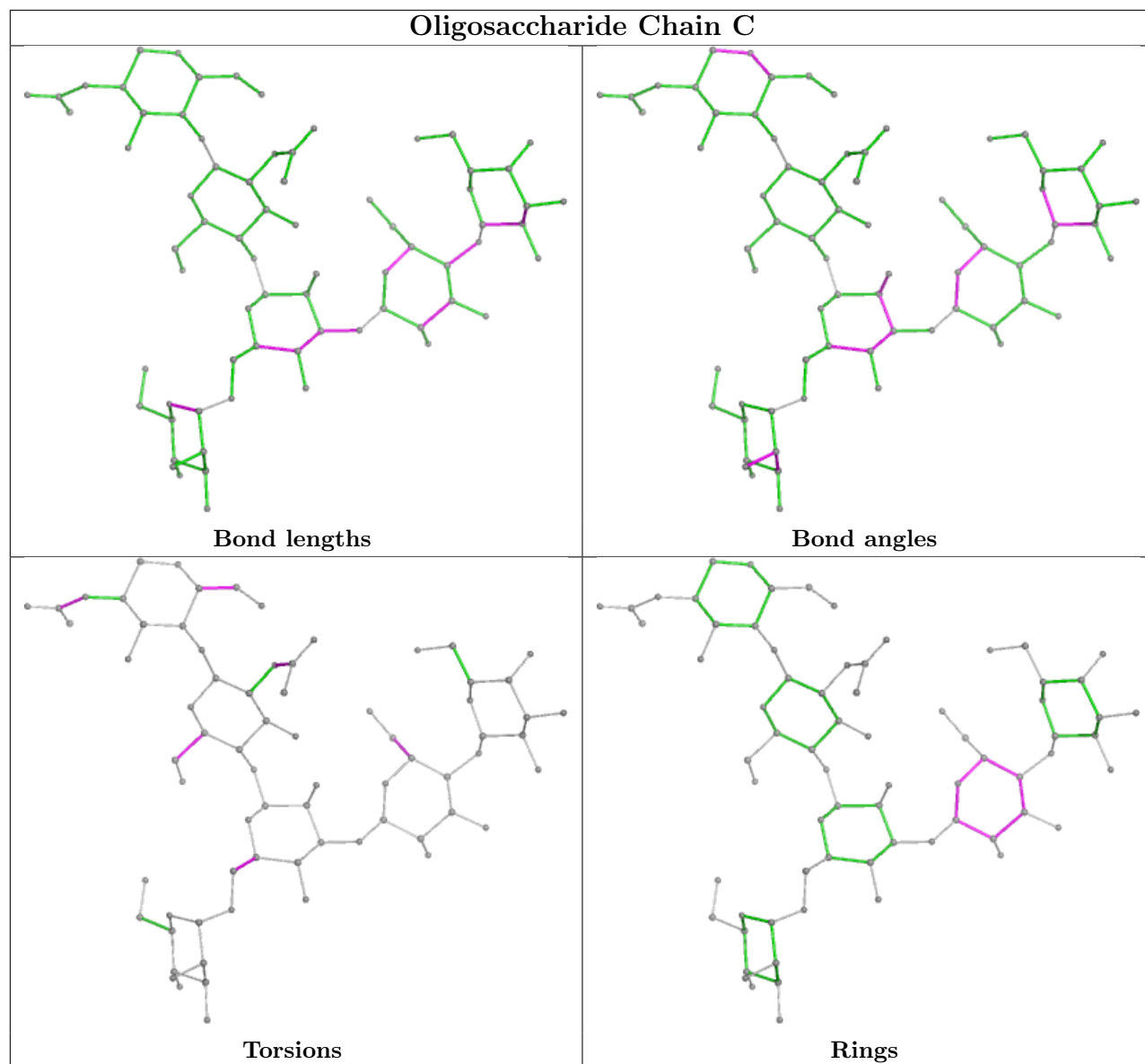
All (1) ring outliers are listed below:

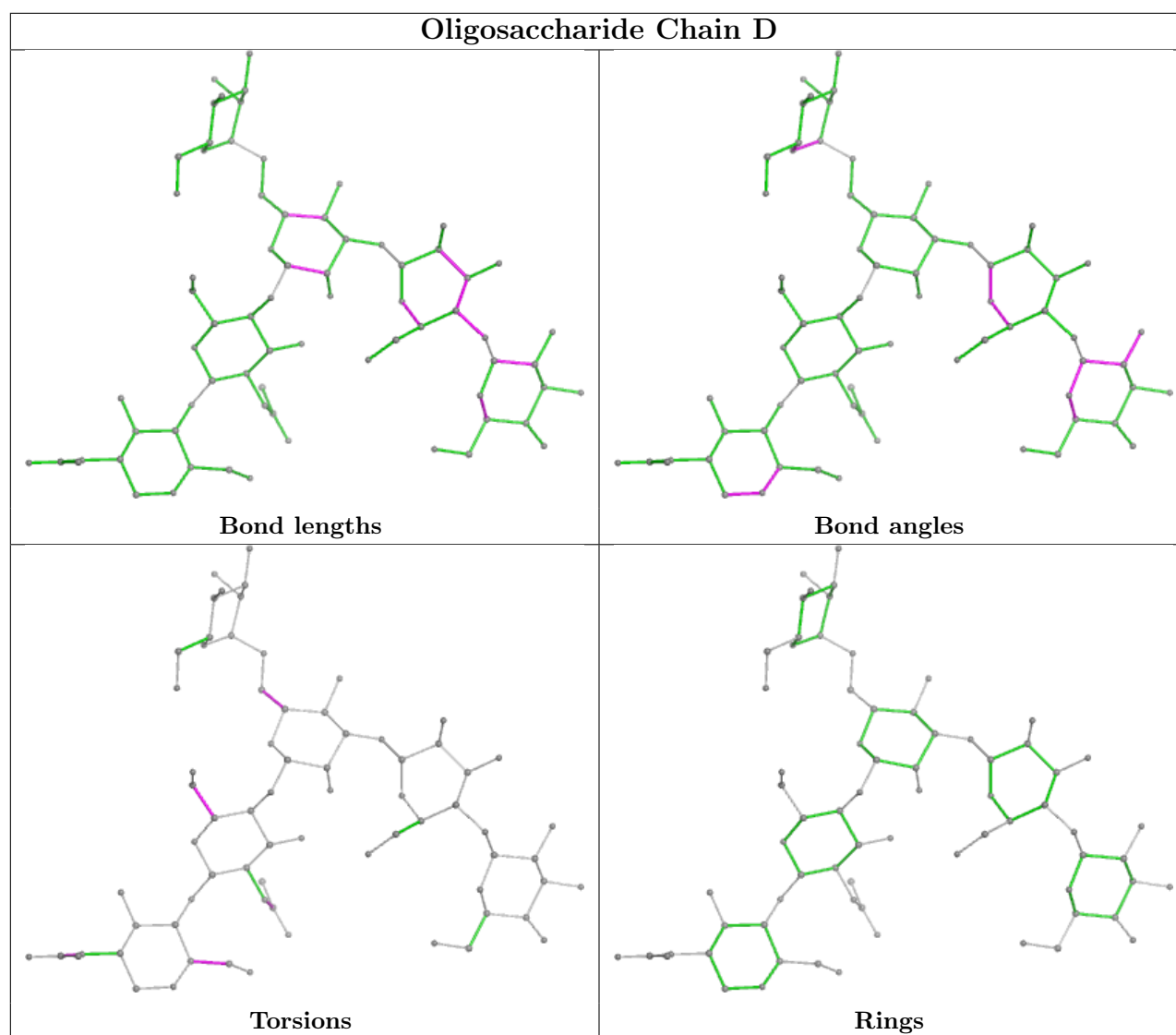
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	2	0
2	C	2	NAG	4	0
2	D	3	BMA	1	0
2	D	2	NAG	2	0
2	D	1	NAG	1	0
2	C	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](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	305	1	14,14,15	1.31	2 (14%)	17,19,21	1.33	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	305	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	NAG	O5-C1	4.09	1.50	1.43
5	A	305	NAG	C1-C2	2.57	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	NAG	C1-O5-C5	5.14	119.16	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	NAG	O5-C5-C6-O6
5	A	305	NAG	C4-C5-C6-O6
5	A	305	NAG	C8-C7-N2-C2
5	A	305	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	275/285 (96%)	-0.41	8 (2%) 54 41	289, 347, 395, 429	0
1	B	280/285 (98%)	-0.13	15 (5%) 32 28	316, 354, 400, 430	0
All	All	555/570 (97%)	-0.27	23 (4%) 42 34	289, 352, 399, 430	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	VAL	7.1
1	B	266	VAL	6.7
1	B	268	LEU	6.2
1	B	61	ILE	5.1
1	A	207	ILE	5.0
1	B	240	ILE	4.4
1	B	207	ILE	4.3
1	B	69	GLY	3.9
1	B	68	LEU	3.9
1	B	67	SER	3.6
1	A	240	ILE	2.9
1	B	217	LEU	2.7
1	B	219	PHE	2.7
1	B	125	ASP	2.7
1	A	68	LEU	2.5
1	A	61	ILE	2.4
1	B	238	LEU	2.4
1	B	62	SER	2.4
1	A	97	LEU	2.3
1	B	283	LEU	2.3
1	B	70	ARG	2.1
1	A	246	ASN	2.1
1	A	219	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

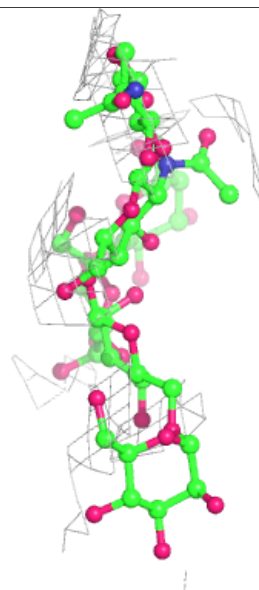
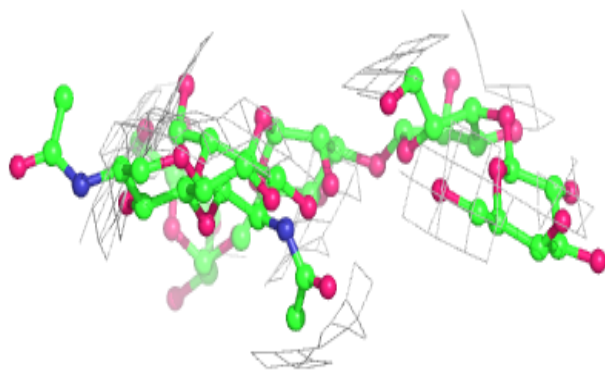
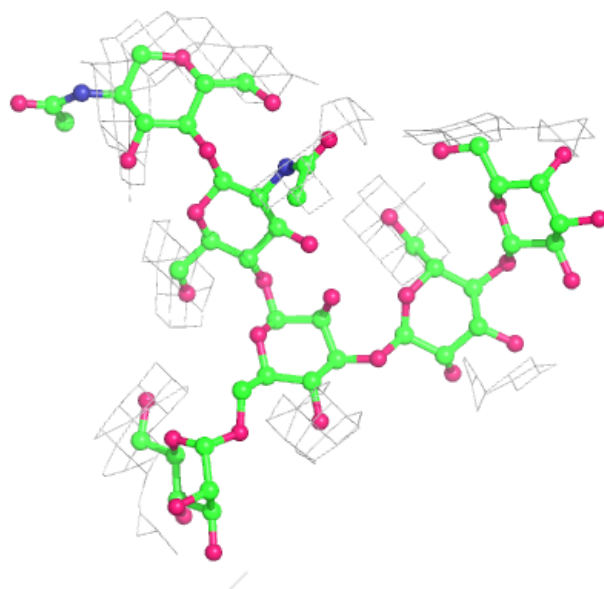
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.36	0.09	383,383,383,383	0
2	BMA	D	3	11/12	0.36	0.05	406,406,406,406	0
2	MAN	D	6	11/12	0.38	0.07	376,376,376,376	0
2	BMA	C	3	11/12	0.48	0.04	427,427,427,427	0
2	MAN	D	4	11/12	0.51	0.07	398,398,398,398	0
2	GAL	C	5	11/12	0.60	0.08	422,422,422,422	0
2	GAL	D	5	11/12	0.68	0.06	421,421,421,421	0
2	MAN	C	6	11/12	0.68	0.07	403,403,403,403	0
2	NAG	C	2	14/15	0.70	0.07	393,393,393,393	0
2	MAN	C	4	11/12	0.76	0.04	431,431,431,431	0
2	NAG	D	1	14/15	0.79	0.14	362,362,362,362	0
2	NAG	C	1	14/15	0.88	0.24	383,383,383,383	0

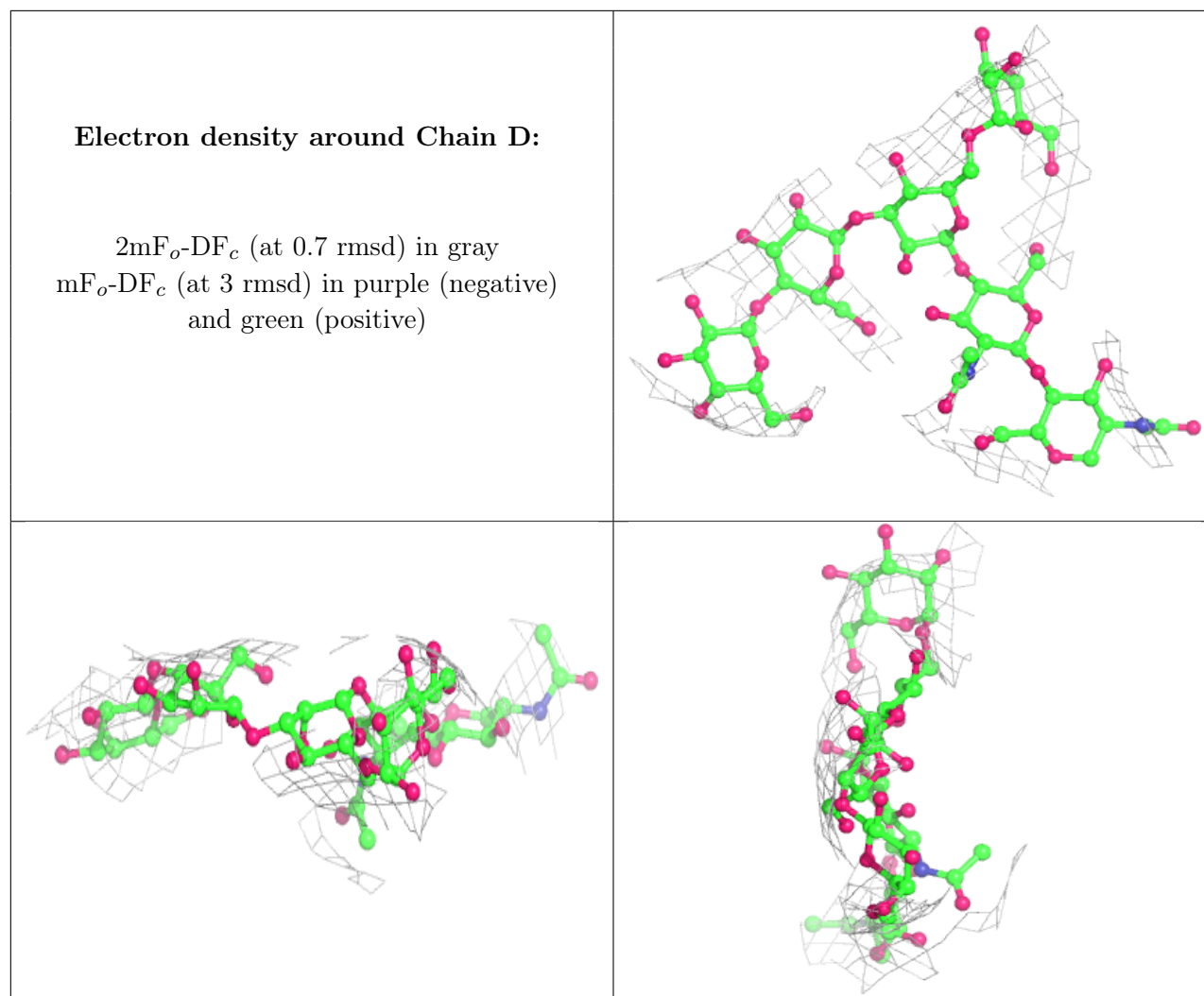
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	305	14/15	0.79	0.06	320,320,320,320	0
3	CA	A	303	1/1	0.83	0.10	376,376,376,376	0
4	NA	B	304	1/1	0.96	0.05	315,315,315,315	0
3	CA	B	303	1/1	0.96	0.08	350,350,350,350	0
3	CA	B	302	1/1	0.97	0.17	254,254,254,254	0
3	CA	A	302	1/1	0.97	0.14	276,276,276,276	0
4	NA	A	304	1/1	0.98	0.06	374,374,374,374	0
3	CA	B	301	1/1	0.99	0.07	359,359,359,359	0
3	CA	A	301	1/1	0.99	0.08	303,303,303,303	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.