



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:38 AM UTC

PDB ID : 6XP6 / pdb_00006xp6
Title : 3C11-DQ2-glia-a2 complex
Authors : Petersen, J.; Rossjohn, J.
Deposited on : 2020-07-08
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

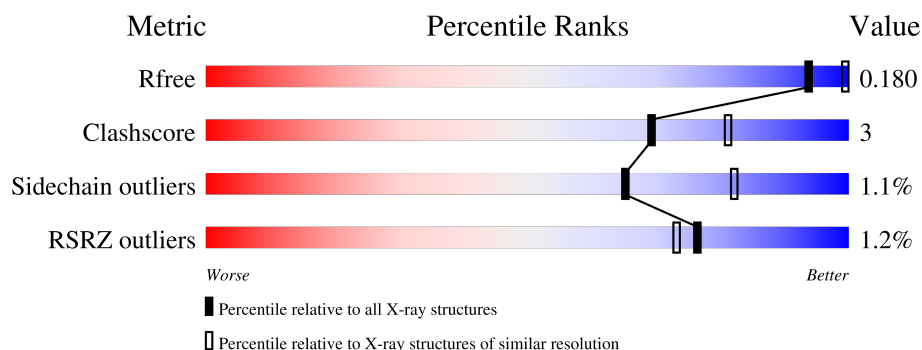
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	191	
1	D	191	
2	B	201	
2	E	201	
3	H	224	
3	J	224	

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Mol	Chain	Length	Quality of chain
4	G	214	% 91% 8% .
4	I	214	3% 89% 9% ..
5	C	26	4% 38% 12% 50%
5	F	26	50% 50%
6	K	2	100%
6	M	2	50% 50%
6	N	2	50% 50%
7	L	7	43% 29% 29%
8	O	4	50% 50%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13695 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	2	0
			1459	940	239	277	3			
1	D	182	Total	C	N	O	S	0	1	0
			1456	938	237	278	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP O19705
A	183	SER	-	expression tag	UNP O19705
A	184	GLY	-	expression tag	UNP O19705
A	185	ASP	-	expression tag	UNP O19705
A	186	ASP	-	expression tag	UNP O19705
A	187	ASP	-	expression tag	UNP O19705
A	188	ASP	-	expression tag	UNP O19705
A	189	LYS	-	expression tag	UNP O19705
D	182	THR	-	expression tag	UNP O19705
D	183	SER	-	expression tag	UNP O19705
D	184	GLY	-	expression tag	UNP O19705
D	185	ASP	-	expression tag	UNP O19705
D	186	ASP	-	expression tag	UNP O19705
D	187	ASP	-	expression tag	UNP O19705
D	188	ASP	-	expression tag	UNP O19705
D	189	LYS	-	expression tag	UNP O19705

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	2	0
			1499	946	266	280	7			
2	E	180	Total	C	N	O	S	0	2	0
			1491	942	265	277	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP O19712
B	193	THR	-	expression tag	UNP O19712
B	194	GLY	-	expression tag	UNP O19712
B	195	GLY	-	expression tag	UNP O19712
B	196	ASP	-	expression tag	UNP O19712
B	197	ASP	-	expression tag	UNP O19712
B	198	ASP	-	expression tag	UNP O19712
B	199	ASP	-	expression tag	UNP O19712
B	200	LYS	-	expression tag	UNP O19712
E	0	SER	-	expression tag	UNP O19712
E	193	THR	-	expression tag	UNP O19712
E	194	GLY	-	expression tag	UNP O19712
E	195	GLY	-	expression tag	UNP O19712
E	196	ASP	-	expression tag	UNP O19712
E	197	ASP	-	expression tag	UNP O19712
E	198	ASP	-	expression tag	UNP O19712
E	199	ASP	-	expression tag	UNP O19712
E	200	LYS	-	expression tag	UNP O19712

- Molecule 3 is a protein called 3.C11 IgH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	2	0
			1638	1024	285	321	8			
3	J	213	Total	C	N	O	S	0	2	0
			1594	1000	277	309	8			

- Molecule 4 is a protein called 3.C11 IgK Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	212	Total	C	N	O	S	0	0	0
			1631	1021	272	333	5			
4	I	212	Total	C	N	O	S	0	2	0
			1639	1026	272	336	5			

- Molecule 5 is a protein called DQ2-glia-a2 peptide.

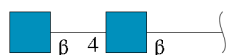
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	13	Total	C	N	O	0	0	0
			96	63	15	18			

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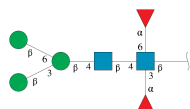
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	13	Total	C	N	O	0	0	0
			96	63	15	18			

- Molecule 6 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
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



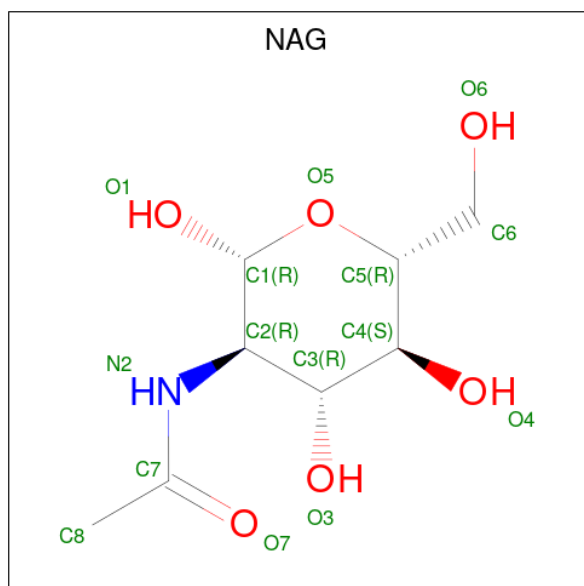
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	L	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 8 is an oligosaccharide called beta-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.



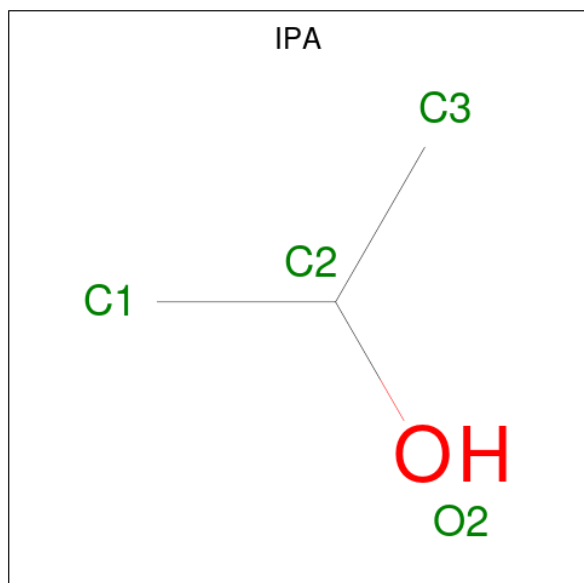
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	O	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 3 1	0	0
10	A	1	Total C O 4 3 1	0	0
10	B	1	Total C O 4 3 1	0	0
10	D	1	Total C O 4 3 1	0	0
10	D	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	G	1	Total C O 4 3 1	0	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	2	Total Cl 2 2	0	0
11	J	1	Total Cl 1 1	0	0
11	G	1	Total Cl 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	113	Total O 113 113	0	0
12	B	94	Total O 94 94	0	0
12	D	106	Total O 106 106	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	121	Total 121	O 121	0	0
12	H	86	Total 86	O 86	0	0
12	J	100	Total 100	O 100	0	0
12	G	109	Total 109	O 109	0	0
12	I	77	Total 77	O 77	0	0
12	C	5	Total 5	O 5	0	0
12	F	4	Total 4	O 4	0	0

3 Residue-property plots

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

- Molecule 1: MHC class II HLA-DQ-alpha chain

Chain A: 



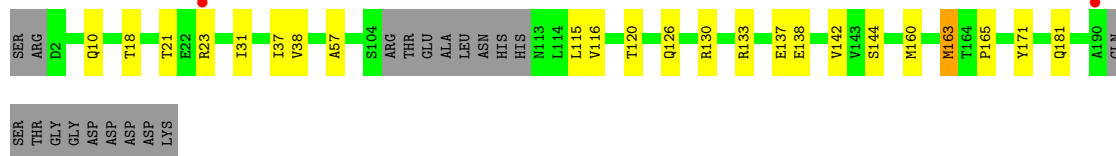
- Molecule 1: MHC class II HLA-DQ-alpha chain

Chain D: 



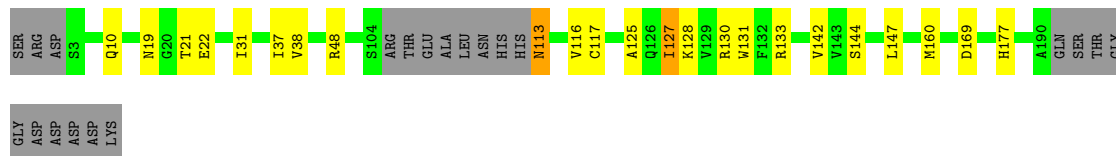
- Molecule 2: MHC class II HLA-DQ-beta-1

Chain B: 



- Molecule 2: MHC class II HLA-DQ-beta-1

Chain E: 

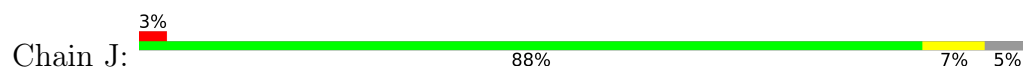


- Molecule 3: 3.C11 IgH Fab

Chain H: 



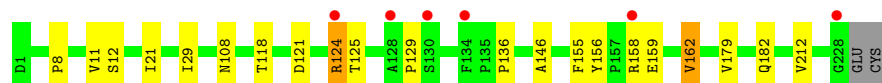
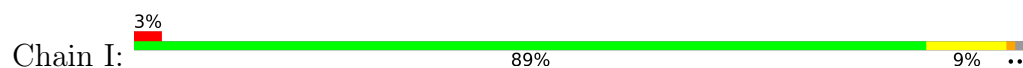
- Molecule 3: 3.C11 IgH Fab



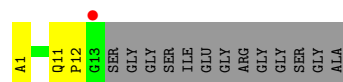
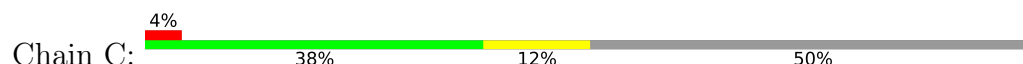
- Molecule 4: 3.C11 IgK Fab



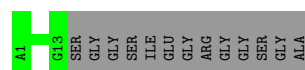
- Molecule 4: 3.C11 IgK Fab



- Molecule 5: DQ2-glia-a2 peptide



- Molecule 5: DQ2-glia-a2 peptide



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%


MAG1
MAG2

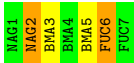
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%


MAG1
MAG2

- Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  43% 29% 29%


MAG1
MAG2
BMA3
BMA4
BMA5
FUC6
FUC7

- Molecule 8: beta-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 O:  50% 50%


MAG1
MAG2
BMA3
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.85Å 143.05Å 170.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 2.40 47.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.03-2.40) 99.9 (47.03-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.176 , 0.212 (Not available) , 0.180	Depositor DCC
R_{free} test set	1831 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13695	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BMA, NAG, IPA, CL, 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	0.27	0/1507	0.44	0/2057
1	D	0.27	0/1501	0.44	0/2050
2	B	0.28	0/1538	0.49	0/2089
2	E	0.29	0/1530	0.49	0/2078
3	H	0.25	0/1678	0.47	0/2282
3	J	0.27	0/1633	0.48	0/2221
4	G	0.26	0/1667	0.50	0/2266
4	I	0.27	0/1681	0.50	0/2286
5	C	0.34	0/101	0.59	0/141
5	F	0.33	0/101	0.60	0/141
All	All	0.27	0/12937	0.48	0/17611

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

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	1459	0	1415	8	0
1	D	1456	0	1404	9	0
2	B	1499	0	1464	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1491	0	1460	13	0
3	H	1638	0	1636	12	0
3	J	1594	0	1592	9	0
4	G	1631	0	1580	10	0
4	I	1639	0	1583	12	0
5	C	96	0	92	3	0
5	F	96	0	92	0	0
6	K	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
7	L	81	0	70	1	0
8	O	50	0	43	0	0
9	A	14	0	13	0	0
10	A	8	0	16	0	0
10	B	4	0	8	1	0
10	D	8	0	16	1	0
10	G	4	0	8	2	0
10	H	12	0	24	4	0
10	J	12	0	24	0	0
11	G	1	0	0	0	0
11	H	2	0	0	0	0
11	J	1	0	0	0	0
12	A	113	0	0	1	0
12	B	94	0	0	2	0
12	C	5	0	0	1	0
12	D	106	0	0	0	0
12	E	121	0	0	0	0
12	F	4	0	0	0	0
12	G	109	0	0	1	0
12	H	86	0	0	0	0
12	I	77	0	0	0	0
12	J	100	0	0	1	0
All	All	13695	0	12615	89	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 3.

All (89) 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:E:128:LYS:HE3	2:E:130:ARG:HE	1.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:ARG:NH1	2:E:169:ASP:OD2	2.21	0.73
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.71	0.72
3:H:29:THR:HB	10:H:302:IPA:H13	1.73	0.70
4:G:124:ARG:HG3	4:G:125:THR:H	1.57	0.69
7:L:2:NAG:H2	7:L:6:FUC:H61	1.74	0.68
3:J:139:PRO:HD3	3:J:225:LYS:HE2	1.76	0.68
5:C:11:GLN:HG3	5:C:12:PRO:HD2	1.76	0.67
2:E:116:VAL:HG22	2:E:160:MET:HG3	1.75	0.67
5:C:1:ALA:N	12:C:101:HOH:O	2.28	0.65
4:I:124:ARG:HD3	4:I:125:THR:H	1.62	0.62
4:G:51:LYS:NZ	12:G:402:HOH:O	2.29	0.62
3:H:37:HIS:HE2	10:H:303:IPA:H32	1.67	0.59
2:B:163:MET:HG2	2:B:165:PRO:HD3	1.84	0.59
2:B:37:ILE:HG13	2:B:38:VAL:HG12	1.85	0.58
2:E:113:ASN:N	2:E:113:ASN:OD1	2.37	0.57
4:G:158:ARG:NH2	4:G:179:VAL:HG21	2.19	0.57
2:B:57:ALA:HB2	5:C:11:GLN:NE2	2.21	0.55
10:B:1008:IPA:H31	12:B:1190:HOH:O	2.07	0.55
1:A:71:ASN:ND2	12:A:1102:HOH:O	2.39	0.54
2:E:125:ALA:HB1	2:E:147:LEU:HD21	1.91	0.53
2:B:130:ARG:HD2	2:B:137:GLU:OE2	2.08	0.53
4:I:124:ARG:HA	4:I:124:ARG:NH1	2.24	0.53
3:H:66:ASN:ND2	10:H:301:IPA:H2	2.24	0.52
1:D:30:GLU:HB2	1:D:138:LEU:HD21	1.91	0.52
2:E:127:ILE:HD12	2:E:177:HIS:CD2	2.45	0.52
1:D:39:LYS:HG2	1:D:60:LEU:HD11	1.93	0.51
4:I:21:ILE:HD12	4:I:118:THR:HG21	1.93	0.51
3:J:159:LYS:NZ	3:J:187:GLN:OE1	2.43	0.51
2:B:163:MET:HG3	2:B:171:TYR:CZ	2.45	0.51
1:A:39:LYS:HG2	1:A:60:LEU:HD11	1.93	0.50
3:J:41:TRP:CE2	3:J:89:MET:HB2	2.45	0.50
4:G:106:GLN:OE1	4:G:108:ASN:N	2.45	0.50
1:D:97:VAL:HG11	1:D:178:TRP:HZ2	1.76	0.50
4:G:161:LYS:HB3	4:G:213:THR:HB	1.94	0.49
3:H:175:LEU:HD21	3:H:198:VAL:HG21	1.95	0.49
4:G:159:GLU:OE2	10:G:301:IPA:H13	2.13	0.48
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.94	0.48
1:D:118:ASN:HB2	1:D:166:GLU:HB2	1.96	0.47
3:H:159:LYS:HE3	3:H:160:ASP:OD2	2.14	0.47
4:G:4:MET:HE3	4:G:23:CYS:SG	2.54	0.47
3:H:71:PHE:O	3:H:76:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:135:PRO:HB3	3:J:161:TYR:HB3	1.96	0.47
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.97	0.47
1:D:59:ALA:O	1:D:63:ILE:HG12	2.15	0.47
2:E:37:ILE:HG13	2:E:38:VAL:HG12	1.96	0.47
4:G:156:TYR:CD1	4:G:157:PRO:HA	2.50	0.47
1:A:105:LEU:HG	1:A:153:LEU:HD22	1.98	0.46
3:H:139:PRO:HD3	3:H:225:LYS:HE2	1.97	0.46
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.86	0.45
2:B:142:VAL:H	2:E:144:SER:HB3	1.81	0.45
4:G:159:GLU:OE2	10:G:301:IPA:H32	2.15	0.45
3:H:41:TRP:CE2	3:H:89:MET:HB2	2.51	0.45
3:H:184:ALA:HA	3:H:194:LEU:HB3	1.99	0.45
2:B:18:THR:HB	2:B:23:ARG:HB2	1.99	0.45
2:B:144:SER:HB3	2:E:142:VAL:H	1.82	0.45
1:D:160:SER:HB2	1:D:177:HIS:CE1	2.52	0.45
4:I:121:ASP:HB2	4:I:182:GLN:OE1	2.17	0.45
4:I:8:PRO:HD2	4:I:11:VAL:CG1	2.47	0.44
4:I:159:GLU:OE1	4:I:159:GLU:N	2.40	0.44
1:A:96:PRO:HD3	2:B:120:THR:HG21	2.00	0.44
2:B:133:ARG:HD2	2:B:138:GLU:OE2	2.17	0.44
4:I:129:PRO:HB3	4:I:155:PHE:HB3	2.00	0.44
3:J:184:ALA:HA	3:J:194:LEU:HB3	1.99	0.43
2:E:48:ARG:HA	2:E:48:ARG:HD3	1.83	0.43
1:A:122:LEU:HD23	1:A:127:SER:HA	2.01	0.43
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.53	0.43
4:I:158:ARG:NH2	4:I:179:VAL:HG21	2.33	0.43
3:J:170:TRP:CH2	3:J:212:CYS:HB3	2.54	0.42
1:A:8:SER:C	1:A:9(A):GLY:HA2	2.44	0.42
1:D:8:SER:C	1:D:9(A):GLY:HA2	2.44	0.42
2:B:181[A]:GLN:HG2	12:B:1171:HOH:O	2.19	0.42
1:D:36:LEU:N	10:D:205:IPA:H2	2.35	0.42
3:J:35[A]:ARG:NH2	12:J:401:HOH:O	2.21	0.42
4:I:12:SER:CB	4:I:156:TYR:OH	2.68	0.41
1:A:21:GLN:OE1	1:A:136:SER:HB3	2.20	0.41
3:J:205:LEU:HD23	3:J:205:LEU:HA	1.92	0.41
4:I:29:ILE:HB	4:I:108:ASN:HB2	2.02	0.41
3:J:89:MET:HE3	3:J:89:MET:HB3	1.99	0.41
2:E:19:ASN:HD22	2:E:22:GLU:CD	2.27	0.41
4:I:136:PRO:HG3	4:I:146:ALA:HB1	2.01	0.41
2:B:181[A]:GLN:HE21	2:B:181[A]:GLN:HB3	1.67	0.41
3:H:142:PRO:HA	3:H:146:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:HIS:HE2	10:H:303:IPA:C3	2.31	0.41
1:D:35:ASP:CG	1:D:38:ARG:HG3	2.46	0.40
1:A:82:ALA:HB1	1:A:113:PHE:HE2	1.86	0.40
3:H:205:LEU:HD23	3:H:205:LEU:HA	1.91	0.40
4:G:129:PRO:HB3	4:G:155:PHE:HB3	2.03	0.40
4:I:162:VAL:HG22	4:I:212:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	167/174 (96%)	165 (99%)	2 (1%)	63	81
1	D	166/174 (95%)	164 (99%)	2 (1%)	63	81
2	B	168/183 (92%)	165 (98%)	3 (2%)	51	73
2	E	167/183 (91%)	164 (98%)	3 (2%)	51	73
3	H	185/187 (99%)	183 (99%)	2 (1%)	65	82
3	J	179/187 (96%)	178 (99%)	1 (1%)	78	89
4	G	188/190 (99%)	187 (100%)	1 (0%)	81	91
4	I	189/190 (100%)	187 (99%)	2 (1%)	65	82
5	C	10/16 (62%)	10 (100%)	0	100	100
5	F	10/16 (62%)	10 (100%)	0	100	100
All	All	1429/1500 (95%)	1413 (99%)	16 (1%)	65	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	129	THR
2	B	21	THR
2	B	126	GLN
2	B	163	MET
1	D	156	SER
1	D	158	GLU
2	E	21	THR
2	E	113	ASN
2	E	127	ILE
3	H	154	LEU
3	H	217	LYS
3	J	110	ARG
4	G	139	GLU
4	I	124	ARG
4	I	162	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	126	HIS
2	B	150	ASN
2	B	156	GLN
1	D	57	GLN
2	E	113	ASN
2	E	150	ASN
2	E	156	GLN
3	H	48	GLN
3	H	180	HIS
3	J	44	GLN
3	J	48	GLN
4	G	153	ASN
4	I	44	GLN
4	I	140	GLN
4	I	163	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 ⓘ

17 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
6	NAG	K	1	1,6	14,14,15	0.51	0	17,19,21	0.52	0
6	NAG	K	2	6	14,14,15	0.53	0	17,19,21	0.58	0
7	NAG	L	1	2,7	14,14,15	0.35	0	17,19,21	0.60	0
7	NAG	L	2	7	14,14,15	0.25	0	17,19,21	0.65	1 (5%)
7	BMA	L	3	7	11,11,12	0.96	0	15,15,17	1.45	3 (20%)
7	BMA	L	4	7	11,11,12	0.74	0	15,15,17	0.70	0
7	BMA	L	5	7	11,11,12	1.94	2 (18%)	15,15,17	1.56	3 (20%)
7	FUC	L	6	7	10,10,11	1.03	1 (10%)	14,14,16	1.13	1 (7%)
7	FUC	L	7	7	10,10,11	0.97	0	14,14,16	0.93	0
6	NAG	M	1	1,6	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
6	NAG	M	2	6	14,14,15	0.42	0	17,19,21	0.44	0
6	NAG	N	1	1,6	14,14,15	0.50	0	17,19,21	0.57	0
6	NAG	N	2	6	14,14,15	0.67	1 (7%)	17,19,21	0.45	0
8	NAG	O	1	8,2	14,14,15	0.34	0	17,19,21	0.51	0
8	NAG	O	2	8	14,14,15	0.29	0	17,19,21	0.57	0
8	BMA	O	3	8	11,11,12	1.19	1 (9%)	15,15,17	1.16	1 (6%)
8	BMA	O	4	8	11,11,12	1.80	3 (27%)	15,15,17	1.48	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	5	BMA	C1-C2	4.85	1.63	1.52
8	O	4	BMA	C1-C2	4.16	1.62	1.52
7	L	5	BMA	C2-C3	3.39	1.57	1.52
8	O	4	BMA	O5-C1	3.27	1.49	1.43
6	N	2	NAG	C1-C2	2.31	1.55	1.52
8	O	3	BMA	O5-C1	2.10	1.47	1.43
7	L	6	FUC	O5-C5	2.03	1.47	1.43
8	O	4	BMA	C2-C3	2.01	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	3	BMA	O3-C3-C2	3.70	117.60	110.05
8	O	4	BMA	C1-O5-C5	3.49	116.86	112.19
6	M	1	NAG	C1-O5-C5	2.87	116.03	112.19
7	L	5	BMA	C3-C4-C5	-2.86	105.05	110.23
8	O	4	BMA	C1-C2-C3	2.75	113.66	109.64
7	L	5	BMA	O2-C2-C1	2.75	115.51	109.22
7	L	5	BMA	O5-C5-C6	2.73	112.98	107.66
7	L	6	FUC	C1-O5-C5	2.39	118.60	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	3	BMA	C1-C2-C3	-2.11	106.58	109.64
7	L	2	NAG	C1-O5-C5	2.10	115.01	112.19
7	L	3	BMA	C3-C4-C5	-2.01	106.59	110.23
7	L	3	BMA	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

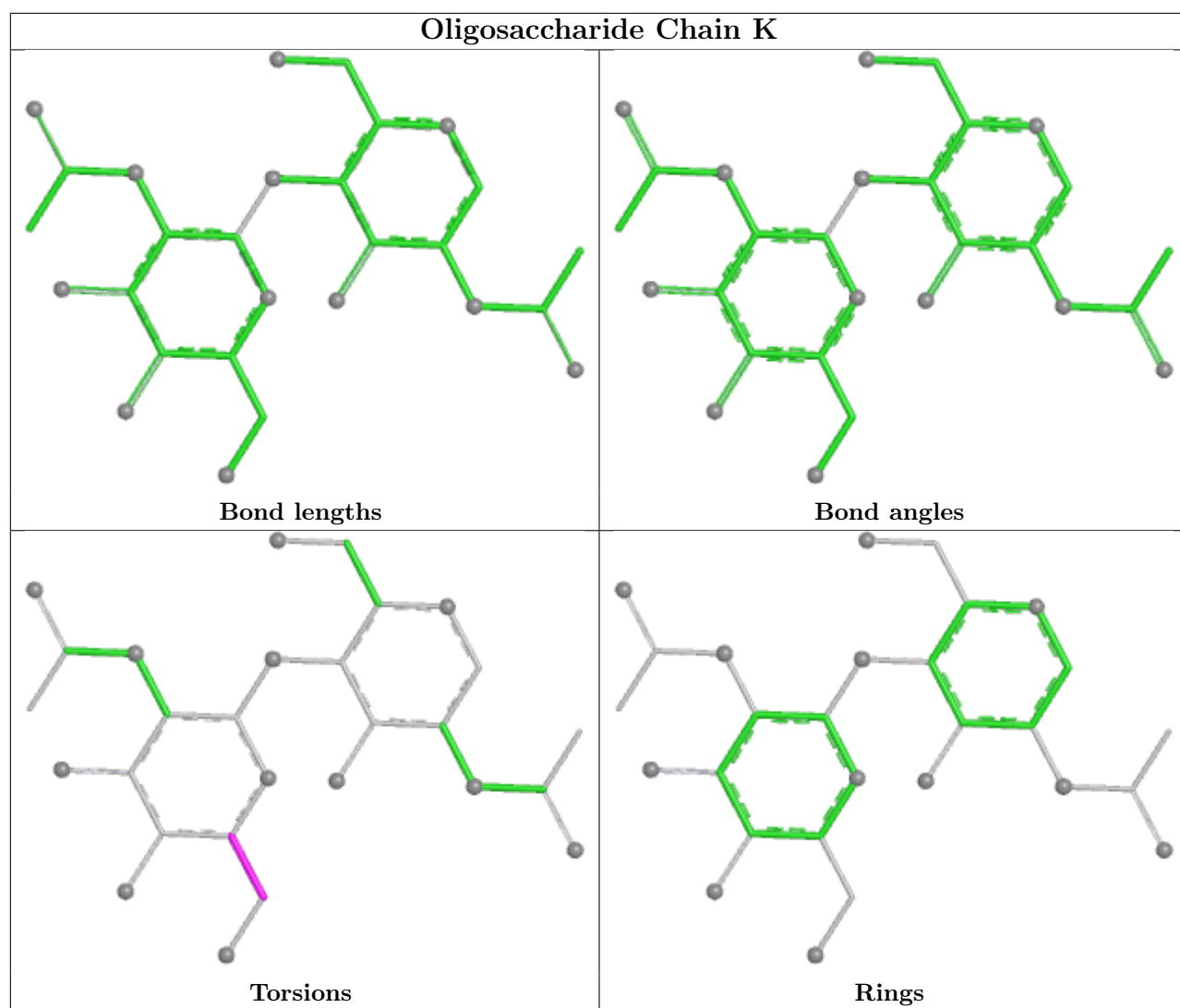
Mol	Chain	Res	Type	Atoms
7	L	3	BMA	O5-C5-C6-O6
8	O	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
7	L	5	BMA	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	L	3	BMA	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
8	O	3	BMA	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	L	5	BMA	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
8	O	4	BMA	C4-C5-C6-O6
6	M	1	NAG	C3-C2-N2-C7
6	M	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
8	O	4	BMA	O5-C5-C6-O6

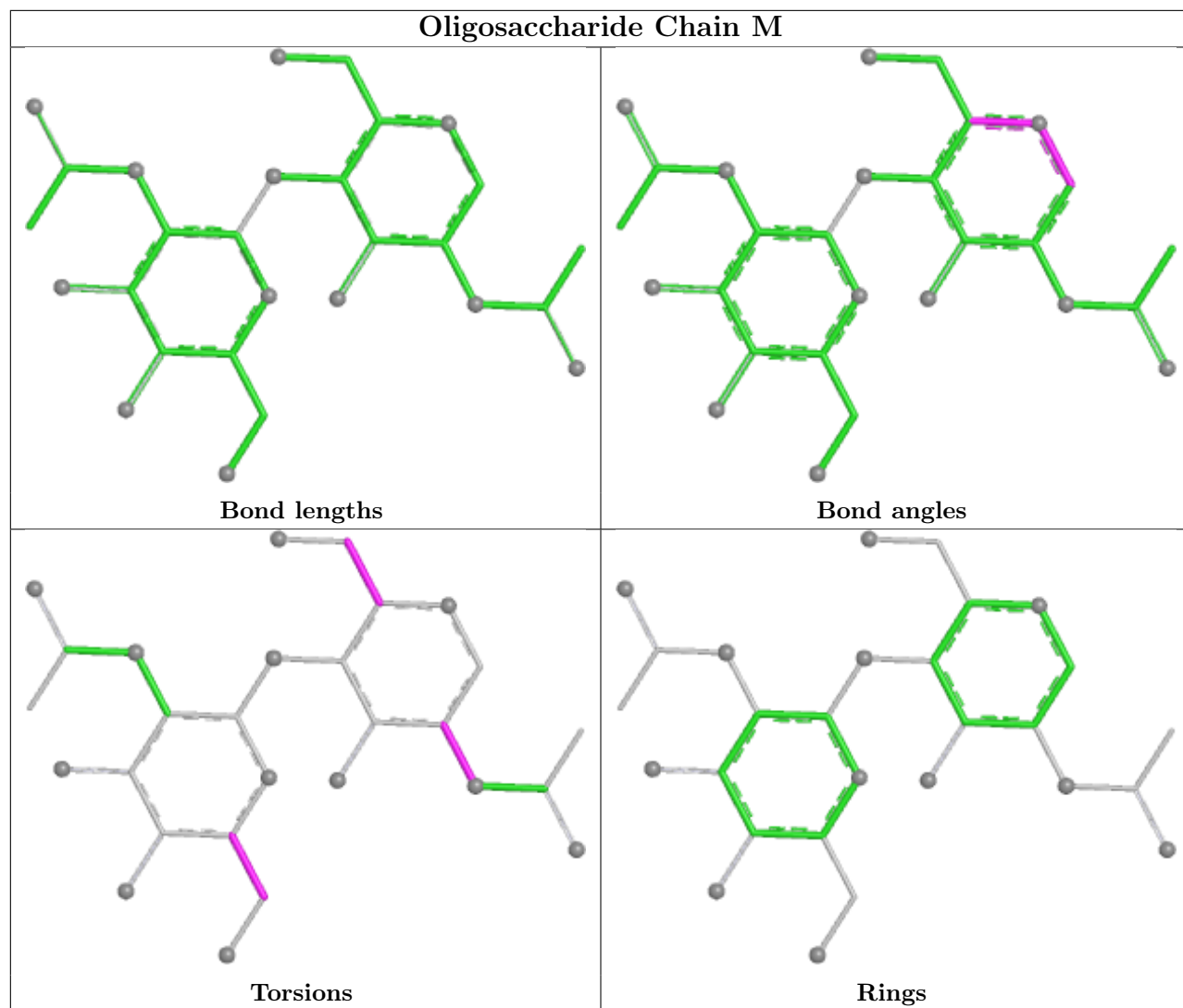
There are no ring outliers.

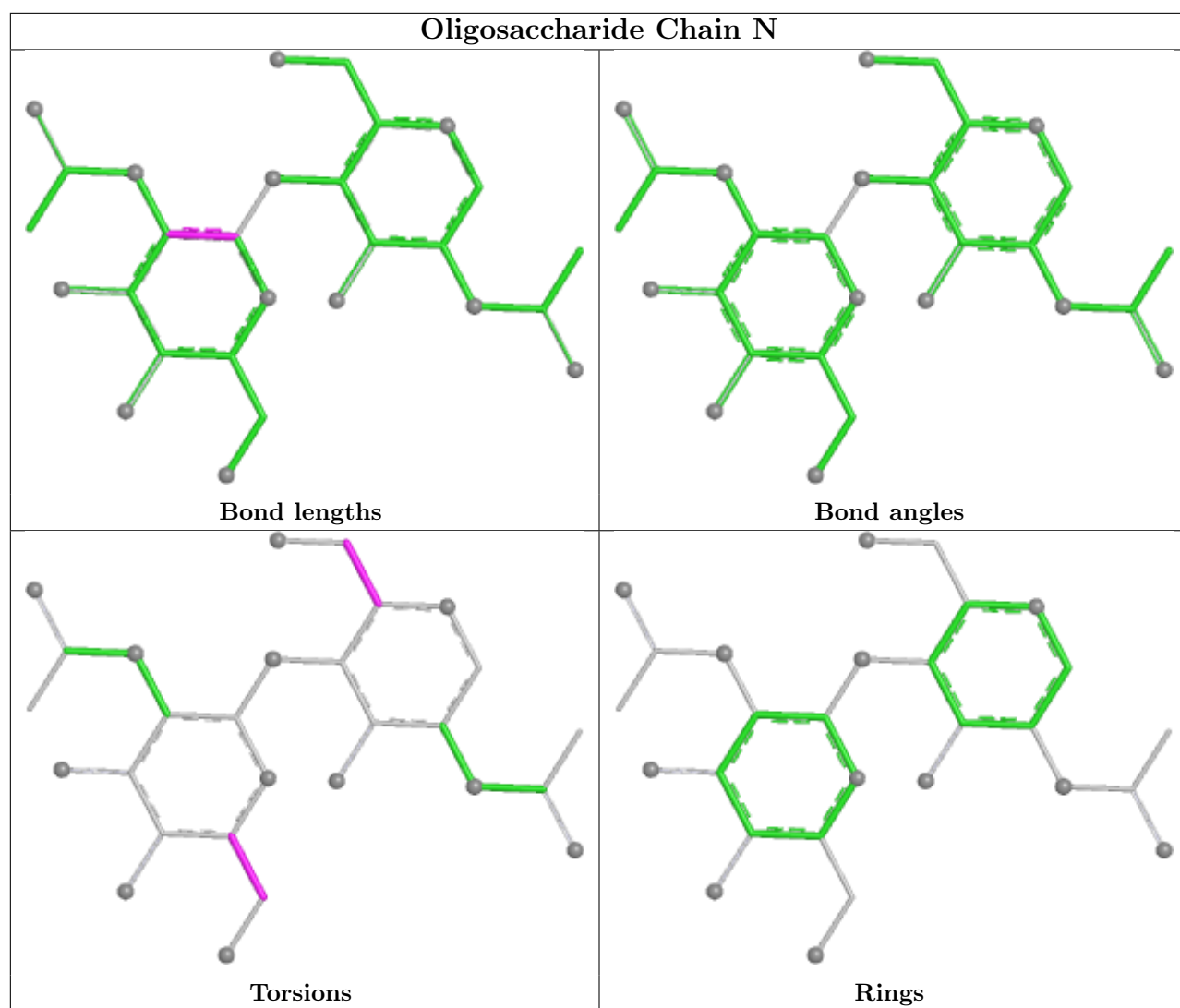
2 monomers are involved in 1 short contact:

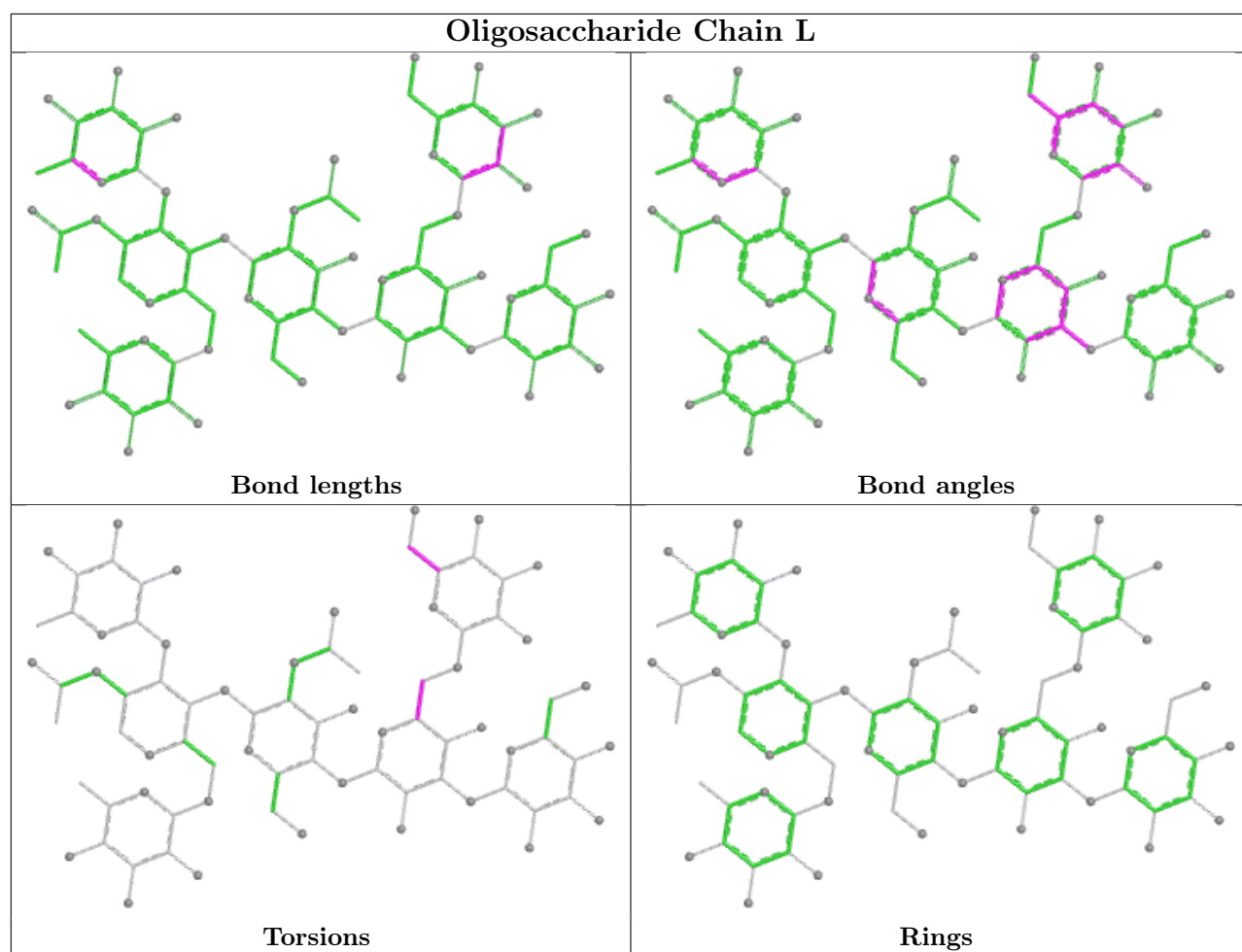
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	6	FUC	1	0
7	L	2	NAG	1	0

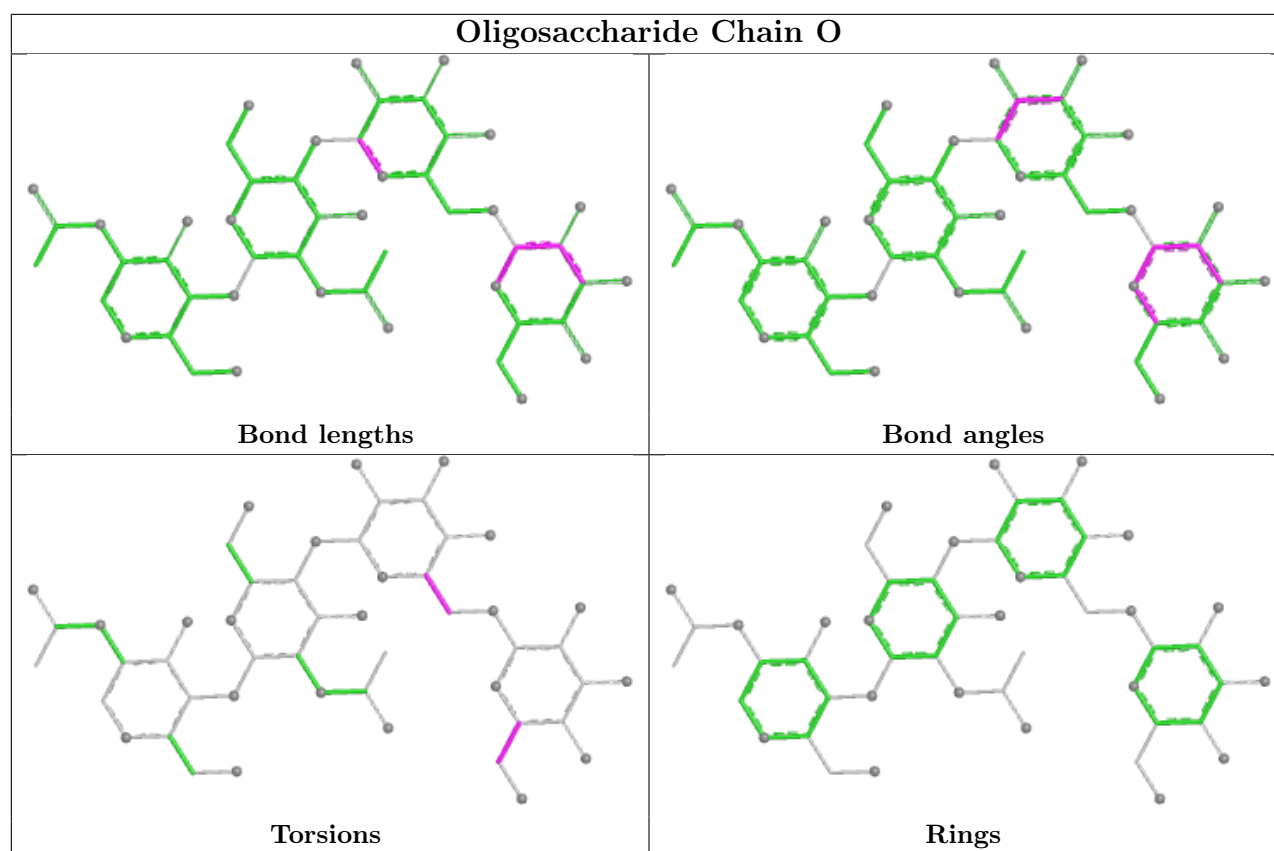
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
10	IPA	J	301	-	3,3,3	0.61	0	3,3,3	0.37	0
10	IPA	J	302	-	3,3,3	0.59	0	3,3,3	0.31	0
10	IPA	H	301	-	3,3,3	0.57	0	3,3,3	0.11	0
10	IPA	B	1008	-	3,3,3	0.60	0	3,3,3	0.35	0
10	IPA	H	302	-	3,3,3	0.60	0	3,3,3	0.27	0
10	IPA	A	1005	-	3,3,3	0.58	0	3,3,3	0.29	0
10	IPA	A	1004	-	3,3,3	0.59	0	3,3,3	0.32	0
10	IPA	D	206	-	3,3,3	0.66	0	3,3,3	0.29	0
9	NAG	A	1003	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	IPA	G	301	-	3,3,3	0.59	0	3,3,3	0.32	0
10	IPA	J	303	-	3,3,3	0.64	0	3,3,3	0.29	0
10	IPA	H	303	-	3,3,3	0.60	0	3,3,3	0.22	0
10	IPA	D	205	-	3,3,3	0.61	0	3,3,3	0.24	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
9	NAG	A	1003	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	301	IPA	1	0
10	B	1008	IPA	1	0
10	H	302	IPA	1	0
10	G	301	IPA	2	0
10	H	303	IPA	2	0
10	D	205	IPA	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	181/191 (94%)	-0.50	0 100 100	27, 40, 58, 93	2 (1%)
1	D	182/191 (95%)	-0.44	1 (0%) 87 85	25, 38, 69, 99	1 (0%)
2	B	181/201 (90%)	-0.43	2 (1%) 78 74	27, 41, 69, 101	2 (1%)
2	E	180/201 (89%)	-0.44	0 100 100	24, 38, 71, 105	2 (1%)
3	H	220/224 (98%)	-0.19	1 (0%) 87 85	22, 48, 77, 98	2 (0%)
3	J	213/224 (95%)	0.04	7 (3%) 49 45	24, 48, 98, 115	2 (0%)
4	G	212/214 (99%)	-0.33	2 (0%) 81 78	27, 44, 70, 82	0
4	I	212/214 (99%)	0.20	6 (2%) 55 51	23, 56, 104, 114	2 (0%)
5	C	13/26 (50%)	-0.21	1 (7%) 19 16	34, 39, 60, 62	0
5	F	13/26 (50%)	-0.18	0 100 100	29, 33, 53, 58	0
All	All	1607/1712 (93%)	-0.24	20 (1%) 76 73	22, 43, 88, 115	13 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	141	ALA	3.5
4	I	124	ARG	3.2
3	J	150	GLY	3.0
1	D	0	ASP	3.0
4	G	228	GLY	2.6
3	J	151	THR	2.4
3	J	211	ILE	2.2
2	B	23	ARG	2.2
4	I	158	ARG	2.2
4	I	228	GLY	2.2
5	C	13	GLY	2.1
3	J	229	PRO	2.1
2	B	190	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	I	128	ALA	2.1
3	H	35[A]	ARG	2.1
3	J	207	THR	2.1
3	J	215	ASN	2.0
4	I	130	SER	2.0
4	I	134	PHE	2.0
4	G	170	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](#)

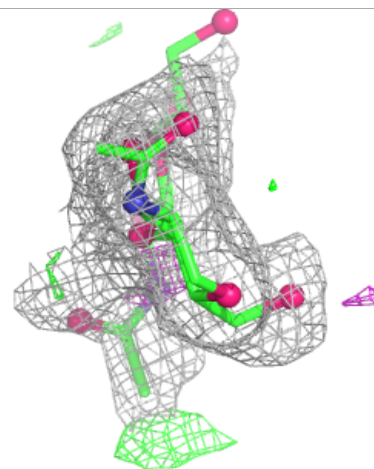
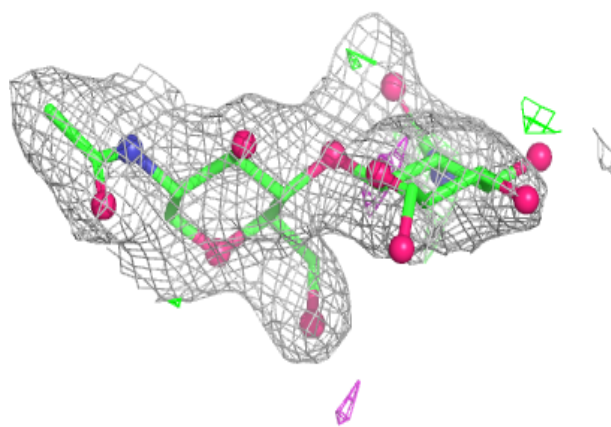
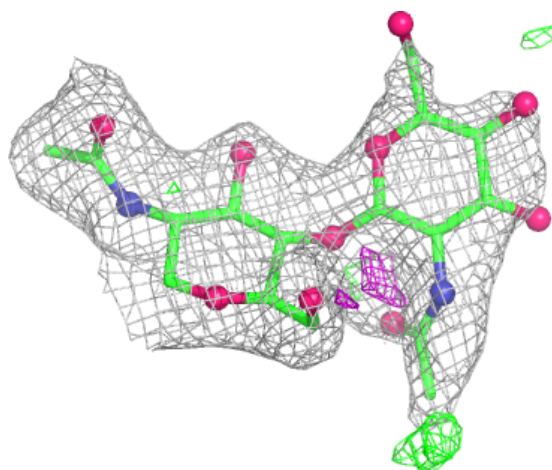
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	FUC	L	7	10/11	0.32	0.22	95,103,106,113	0
6	NAG	N	2	14/15	0.40	0.20	89,116,122,122	0
7	FUC	L	6	10/11	0.47	0.21	89,103,110,114	0
6	NAG	M	2	14/15	0.50	0.17	104,121,124,128	0
6	NAG	K	2	14/15	0.54	0.16	74,91,97,100	0
6	NAG	M	1	14/15	0.59	0.15	92,101,111,112	0
7	NAG	L	2	14/15	0.70	0.16	76,90,96,97	0
8	NAG	O	2	14/15	0.71	0.14	84,90,96,97	0
8	NAG	O	1	14/15	0.72	0.13	64,77,84,89	0
7	NAG	L	1	14/15	0.72	0.14	68,80,93,100	0
7	BMA	L	4	11/12	0.76	0.14	73,81,88,88	0
8	BMA	O	3	11/12	0.79	0.12	78,87,94,97	0
8	BMA	O	4	11/12	0.79	0.16	68,72,84,90	0
6	NAG	N	1	14/15	0.83	0.12	48,87,100,113	0
7	BMA	L	5	11/12	0.84	0.17	46,64,82,83	0
6	NAG	K	1	14/15	0.85	0.11	40,61,79,84	0
7	BMA	L	3	11/12	0.87	0.11	59,69,80,80	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.

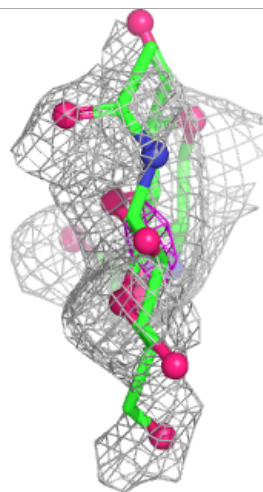
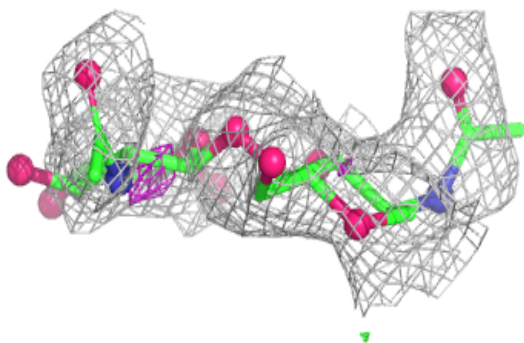
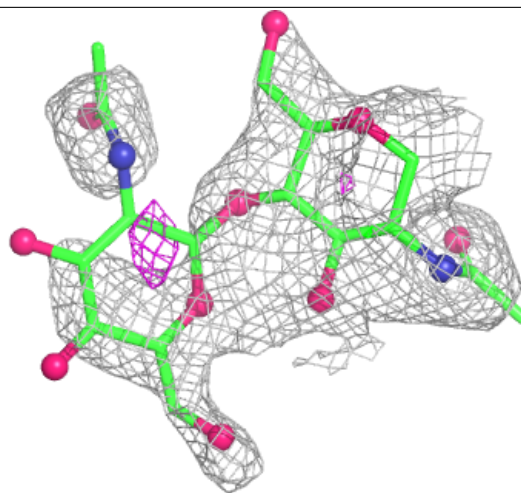
Electron density around Chain K:

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



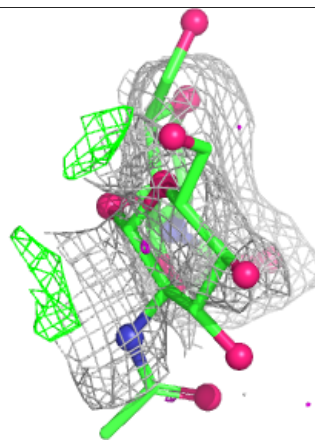
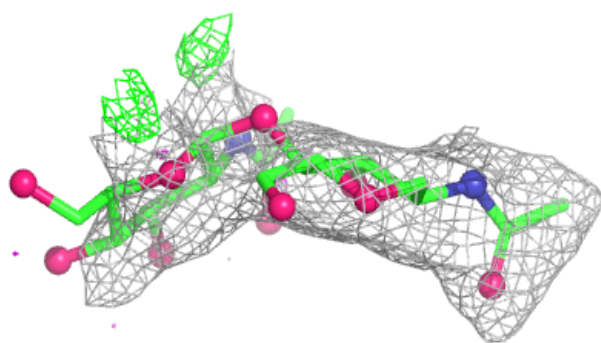
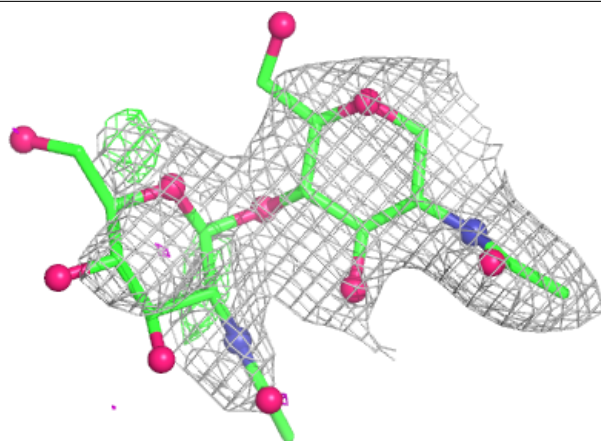
Electron density around Chain M:

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



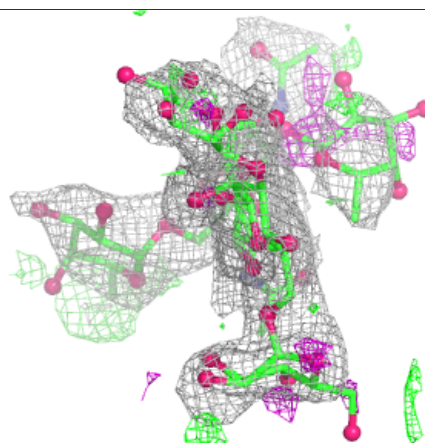
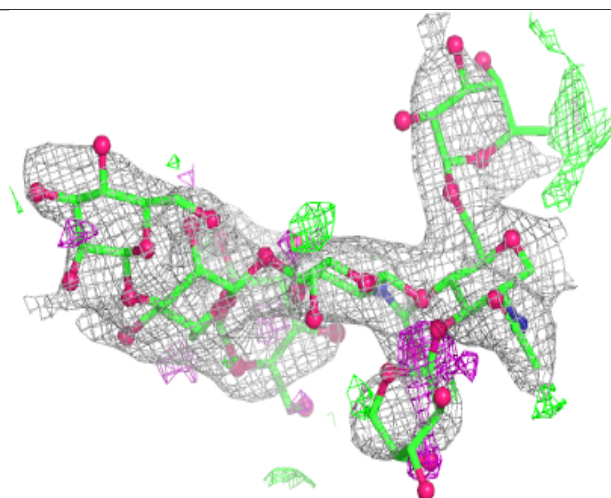
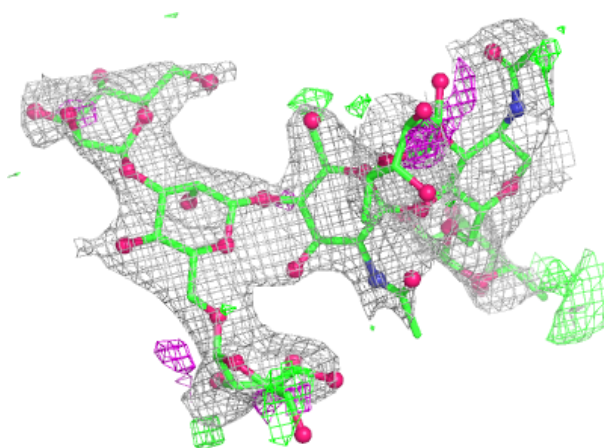
Electron density around Chain N:

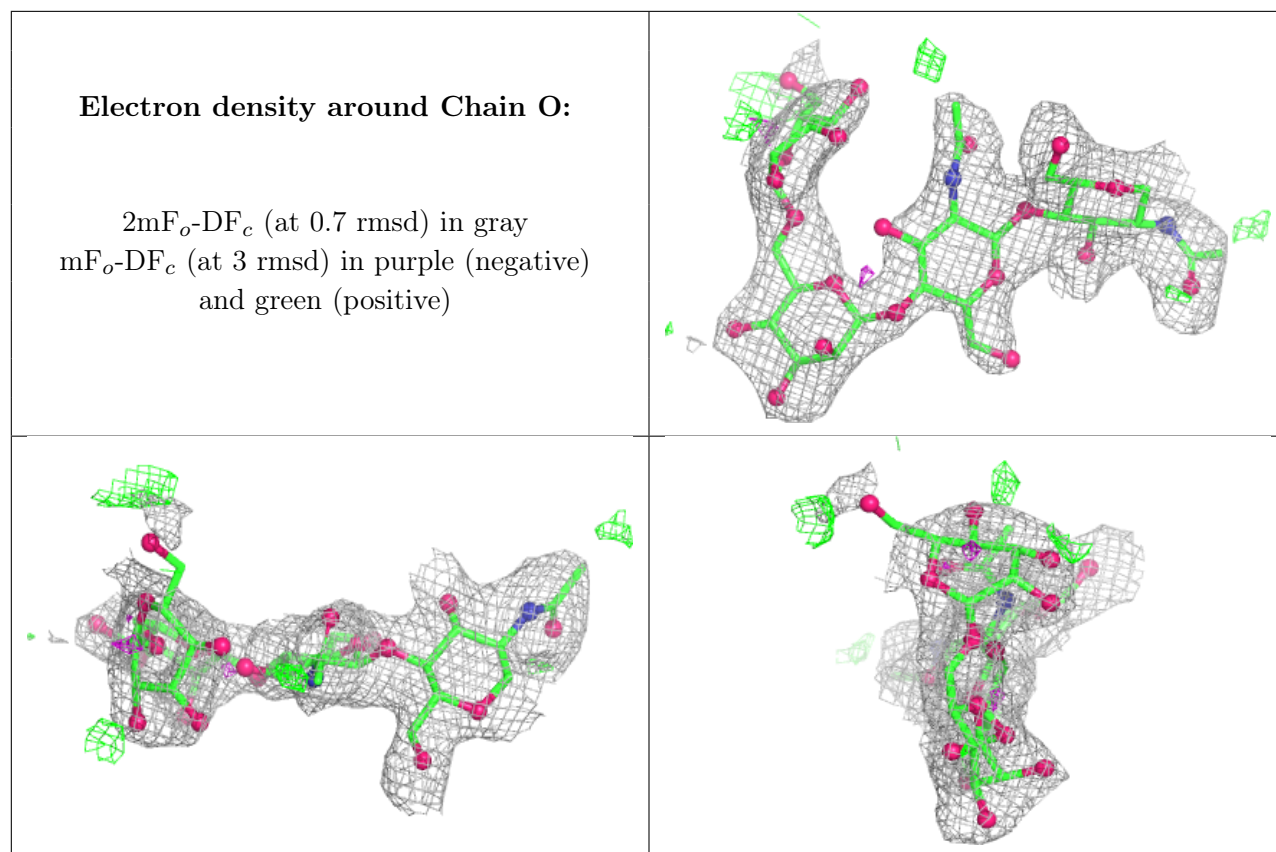
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o-DF_c$ (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, 95th 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
9	NAG	A	1003	14/15	0.73	0.14	82,92,97,98	0
10	IPA	H	302	4/4	0.74	0.21	49,57,61,66	0
10	IPA	B	1008	4/4	0.78	0.23	55,57,59,64	0
10	IPA	G	301	4/4	0.79	0.17	49,54,60,64	0
10	IPA	J	303	4/4	0.85	0.17	36,38,51,53	0
10	IPA	A	1004	4/4	0.87	0.16	31,42,44,45	0
10	IPA	D	205	4/4	0.88	0.16	38,42,43,60	0
10	IPA	D	206	4/4	0.89	0.14	33,38,49,54	0
10	IPA	H	303	4/4	0.92	0.26	43,52,59,65	0
11	CL	H	305	1/1	0.93	0.09	76,76,76,76	0
10	IPA	A	1005	4/4	0.94	0.14	36,45,50,50	0
10	IPA	H	301	4/4	0.95	0.12	42,42,45,52	0
11	CL	G	302	1/1	0.95	0.08	65,65,65,65	0
10	IPA	J	302	4/4	0.96	0.09	39,42,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	CL	J	304	1/1	0.98	0.04	36,36,36,36	0
10	IPA	J	301	4/4	0.98	0.06	29,33,37,38	0
11	CL	H	304	1/1	0.99	0.03	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.