Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 05:14 am GMT

PDB ID	:	5MWF
Title	:	Human Jagged2 C2-EGF2
Authors	:	Suckling, R.J.; Handford, P.A.; Lea, S.M.
Deposited on	:	2017-01-18
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

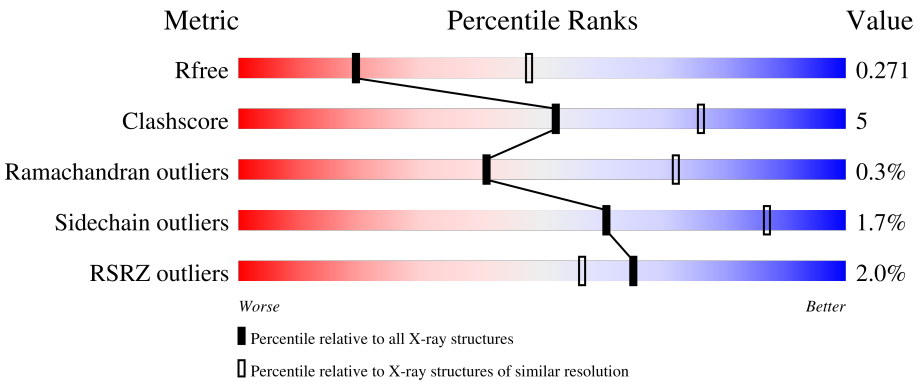
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	293	86% 8% 6%
1	B	293	% 84% 10% 6%
1	C	293	% 82% 7% 11%
1	D	293	2% 80% 10% • 9%
1	E	293	2% 77% 10% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	293	4% 70% 15% • 14%
2	G	4	75% 25%
2	H	4	75% 25%
2	I	4	75% 25%
3	J	3	67% 33%
3	K	3	100%
3	L	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	G	4	X	-	-	-
3	FUC	J	3	X	-	-	-
3	NAG	K	1	X	-	-	-
3	FUC	K	3	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12890 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 Protein jagged-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2136	1326	379	403	28	0	0	0
1	B	275	2133	1325	381	399	28	0	1	0
1	C	262	2038	1272	355	383	28	0	0	0
1	D	266	2068	1290	364	386	28	0	0	0
1	E	260	2024	1265	351	380	28	0	0	0
1	F	253	1979	1238	342	371	28	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q9Y219
A	311	SER	-	expression tag	UNP Q9Y219
A	312	HIS	-	expression tag	UNP Q9Y219
A	313	HIS	-	expression tag	UNP Q9Y219
A	314	HIS	-	expression tag	UNP Q9Y219
A	315	HIS	-	expression tag	UNP Q9Y219
A	316	HIS	-	expression tag	UNP Q9Y219
A	317	HIS	-	expression tag	UNP Q9Y219
A	318	HIS	-	expression tag	UNP Q9Y219
A	319	HIS	-	expression tag	UNP Q9Y219
B	310	GLY	-	expression tag	UNP Q9Y219
B	311	SER	-	expression tag	UNP Q9Y219
B	312	HIS	-	expression tag	UNP Q9Y219
B	313	HIS	-	expression tag	UNP Q9Y219
B	314	HIS	-	expression tag	UNP Q9Y219
B	315	HIS	-	expression tag	UNP Q9Y219
B	316	HIS	-	expression tag	UNP Q9Y219

Continued on next page...

Continued from previous page...

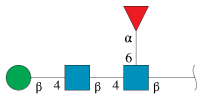
Chain	Residue	Modelled	Actual	Comment	Reference
B	317	HIS	-	expression tag	UNP Q9Y219
B	318	HIS	-	expression tag	UNP Q9Y219
B	319	HIS	-	expression tag	UNP Q9Y219
C	310	GLY	-	expression tag	UNP Q9Y219
C	311	SER	-	expression tag	UNP Q9Y219
C	312	HIS	-	expression tag	UNP Q9Y219
C	313	HIS	-	expression tag	UNP Q9Y219
C	314	HIS	-	expression tag	UNP Q9Y219
C	315	HIS	-	expression tag	UNP Q9Y219
C	316	HIS	-	expression tag	UNP Q9Y219
C	317	HIS	-	expression tag	UNP Q9Y219
C	318	HIS	-	expression tag	UNP Q9Y219
C	319	HIS	-	expression tag	UNP Q9Y219
D	310	GLY	-	expression tag	UNP Q9Y219
D	311	SER	-	expression tag	UNP Q9Y219
D	312	HIS	-	expression tag	UNP Q9Y219
D	313	HIS	-	expression tag	UNP Q9Y219
D	314	HIS	-	expression tag	UNP Q9Y219
D	315	HIS	-	expression tag	UNP Q9Y219
D	316	HIS	-	expression tag	UNP Q9Y219
D	317	HIS	-	expression tag	UNP Q9Y219
D	318	HIS	-	expression tag	UNP Q9Y219
D	319	HIS	-	expression tag	UNP Q9Y219
E	310	GLY	-	expression tag	UNP Q9Y219
E	311	SER	-	expression tag	UNP Q9Y219
E	312	HIS	-	expression tag	UNP Q9Y219
E	313	HIS	-	expression tag	UNP Q9Y219
E	314	HIS	-	expression tag	UNP Q9Y219
E	315	HIS	-	expression tag	UNP Q9Y219
E	316	HIS	-	expression tag	UNP Q9Y219
E	317	HIS	-	expression tag	UNP Q9Y219
E	318	HIS	-	expression tag	UNP Q9Y219
E	319	HIS	-	expression tag	UNP Q9Y219
F	310	GLY	-	expression tag	UNP Q9Y219
F	311	SER	-	expression tag	UNP Q9Y219
F	312	HIS	-	expression tag	UNP Q9Y219
F	313	HIS	-	expression tag	UNP Q9Y219
F	314	HIS	-	expression tag	UNP Q9Y219
F	315	HIS	-	expression tag	UNP Q9Y219
F	316	HIS	-	expression tag	UNP Q9Y219
F	317	HIS	-	expression tag	UNP Q9Y219
F	318	HIS	-	expression tag	UNP Q9Y219

Continued on next page...

Continued from previous page...

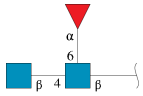
Chain	Residue	Modelled	Actual	Comment	Reference
F	319	HIS	-	expression tag	UNP Q9Y219

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	J	3	38	22	2	14	0	0	0
3	K	3	38	22	2	14	0	0	0
3	L	3	38	22	2	14	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	D	3	3	3	0	0
			Total	Ca		
4	E	3	3	3	0	0
			Total	Ca		
4	F	2	2	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
			Total	Cl		
5	B	1	1	1	0	0

- Molecule 6 is water.

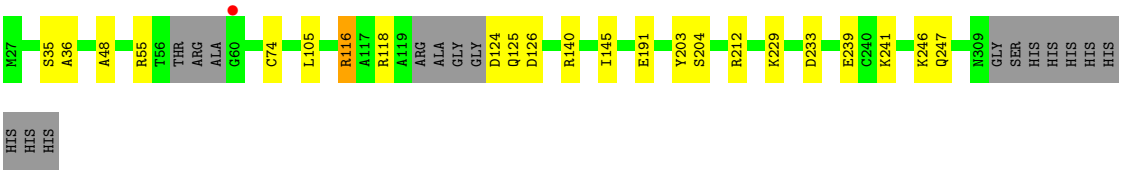
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	61	61	61	0	0
			Total	O		
6	B	34	34	34	0	0
			Total	O		
6	C	33	33	33	0	0
			Total	O		
6	D	32	32	32	0	0
			Total	O		
6	E	35	35	35	0	0
			Total	O		
6	F	37	37	37	0	0

3 Residue-property plots (i)

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

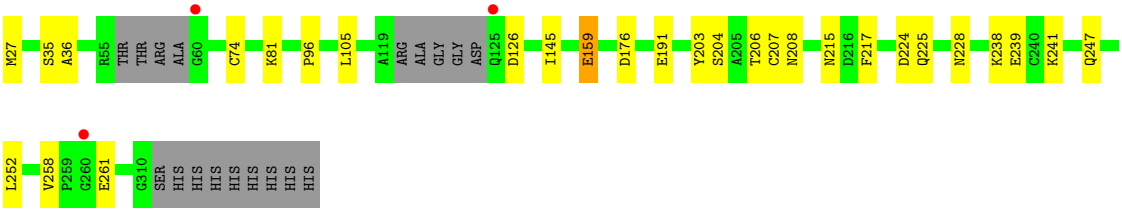
• Molecule 1: Protein jagged-2

Chain A:



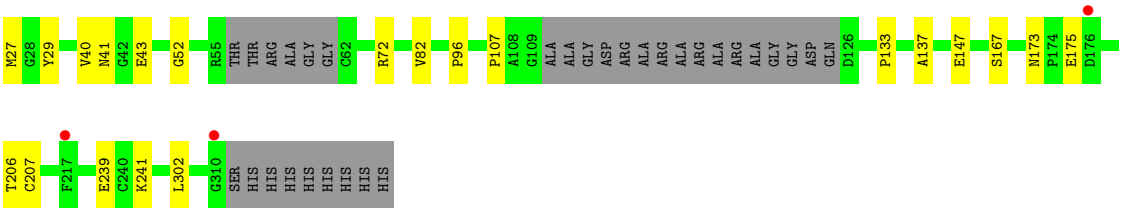
• Molecule 1: Protein jagged-2

Chain B:



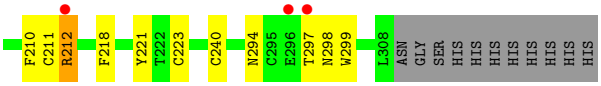
• Molecule 1: Protein jagged-2

Chain C:



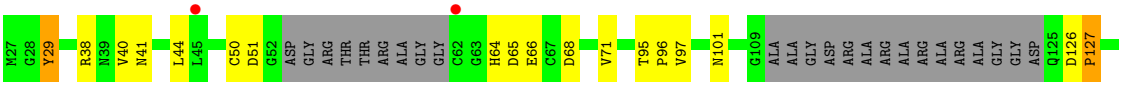
• Molecule 1: Protein jagged-2

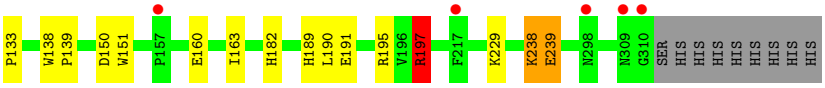
Chain D:



• Molecule 1: Protein jagged-2

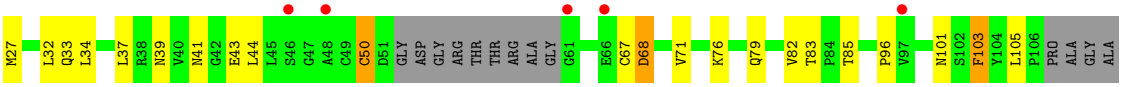
Chain E:

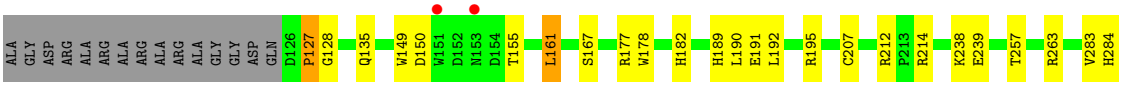


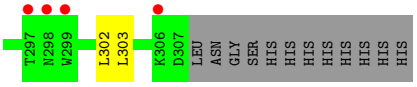


• Molecule 1: Protein jagged-2

Chain F:







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

Chain G:

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

Chain H:

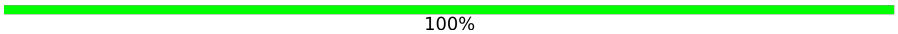
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:

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

Chain K: 

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.63Å 92.93Å 97.00Å 71.68° 83.16° 82.68°	Depositor
Resolution (Å)	38.01 – 2.80 38.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.01-2.80) 97.7 (38.01-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.217 , 0.275 0.213 , 0.271	Depositor DCC
R_{free} test set	2392 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.055 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12890	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, BMA, CA, 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	0.32	0/2194	0.50	0/2975
1	B	0.34	2/2194 (0.1%)	0.51	0/2973
1	C	0.28	0/2096	0.48	0/2844
1	D	0.37	0/2126	0.57	2/2884 (0.1%)
1	E	0.40	3/2082 (0.1%)	0.57	1/2826 (0.0%)
1	F	0.28	0/2036	0.53	0/2763
All	All	0.34	5/12728 (0.0%)	0.53	3/17265 (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	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	GLU	CD-OE1	-6.73	1.18	1.25
1	E	239	GLU	CD-OE1	-5.79	1.19	1.25
1	B	159	GLU	CD-OE2	-5.52	1.19	1.25
1	E	197	ARG	CA-CB	5.29	1.65	1.53
1	E	29	TYR	CB-CG	-5.26	1.43	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	212	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	D	212	ARG	NE-CZ-NH2	8.79	124.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	197	ARG	CA-CB-CG	5.67	125.87	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	64	HIS	Peptide

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	2136	0	1946	15	0
1	B	2133	0	1951	17	1
1	C	2038	0	1853	12	1
1	D	2068	0	1889	24	0
1	E	2024	0	1840	26	0
1	F	1979	0	1798	38	0
2	G	49	0	43	0	0
2	H	49	0	43	1	0
2	I	49	0	43	1	0
3	J	38	0	34	1	0
3	K	38	0	34	0	0
3	L	38	0	34	1	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	61	0	0	1	1
6	B	34	0	0	0	0
6	C	33	0	0	0	0
6	D	32	0	0	0	0
6	E	35	0	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	37	0	0	0	0
All	All	12890	0	11508	132	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (132) 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:E:229:LYS:NZ	1:E:239:GLU:OE2	1.96	0.98
1:D:197:ARG:HG3	1:D:197:ARG:HH11	1.31	0.95
1:E:29:TYR:HB3	1:E:133:PRO:HA	1.60	0.82
1:B:217:PHE:O	1:B:241:LYS:NZ	2.13	0.82
1:F:182:HIS:HD2	1:F:191:GLU:HG2	1.46	0.80
1:D:197:ARG:HG3	1:D:197:ARG:NH1	1.97	0.78
1:F:182:HIS:CD2	1:F:191:GLU:HG2	2.19	0.77
1:F:150:ASP:O	1:F:161:LEU:HD11	1.89	0.72
1:B:247:GLN:OE1	1:B:247:GLN:N	2.19	0.71
1:F:41:ASN:ND2	1:F:43:GLU:OE2	2.24	0.71
1:E:95:THR:HG22	1:E:96:PRO:O	1.93	0.68
1:B:206:THR:HG23	1:B:208:ASN:H	1.59	0.67
1:F:37:LEU:HD13	1:F:190:LEU:HG	1.77	0.66
1:D:212:ARG:HA	1:D:223:CYS:SG	2.38	0.64
1:F:39:ASN:HB3	1:F:101:ASN:HB3	1.79	0.64
1:F:37:LEU:HB3	1:F:103:PHE:CE2	2.34	0.63
1:E:150:ASP:HB2	1:E:163:ILE:HD11	1.81	0.63
1:C:175:GLU:N	1:C:175:GLU:OE1	2.33	0.62
1:E:29:TYR:CB	1:E:133:PRO:HA	2.30	0.62
1:D:201:ASN:OD1	1:D:212:ARG:HG3	2.01	0.61
1:F:302:LEU:HD12	1:F:303:LEU:HD23	1.83	0.61
1:C:173:ASN:HB3	1:C:175:GLU:OE1	2.00	0.61
1:A:229:LYS:NZ	1:A:239:GLU:OE2	2.32	0.61
1:D:96:PRO:HA	3:J:3:FUC:H63	1.83	0.61
1:F:34:LEU:HD22	1:F:71:VAL:HG21	1.83	0.59
1:E:71:VAL:H	1:E:95:THR:HB	1.68	0.59
1:A:35:SER:HA	1:A:105:LEU:HB2	1.85	0.59
1:D:211:CYS:O	1:D:212:ARG:HG2	2.03	0.58
1:D:201:ASN:HB3	1:D:210:PHE:CE1	2.38	0.58
1:E:29:TYR:OH	1:E:197:ARG:HG2	2.04	0.58
1:F:27:MET:N	1:F:207:CYS:O	2.37	0.57
1:F:135:GLN:N	1:F:135:GLN:OE1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:VAL:HG23	1:F:284:HIS:H	1.68	0.57
1:F:257:THR:OG1	1:F:263:ARG:NH1	2.36	0.57
1:F:37:LEU:HD23	1:F:103:PHE:CE2	2.40	0.57
1:F:37:LEU:HD23	1:F:103:PHE:HE2	1.68	0.57
1:F:39:ASN:N	1:F:101:ASN:O	2.38	0.56
1:F:155:THR:O	1:F:155:THR:HG22	2.05	0.56
1:B:74:CYS:HB3	1:B:145:ILE:HB	1.88	0.56
1:F:37:LEU:HA	1:F:189:HIS:O	2.06	0.56
1:E:238:LYS:CE	1:E:239:GLU:HG3	2.36	0.55
1:F:105:LEU:HD22	1:F:127:PRO:HB2	1.88	0.54
1:B:238:LYS:HE2	1:B:239:GLU:CG	2.36	0.54
1:E:38:ARG:HG2	1:E:189:HIS:HB3	1.89	0.54
1:F:82:VAL:HG11	1:F:167:SER:HB2	1.89	0.54
1:E:68:ASP:HB3	1:E:97:VAL:HG11	1.89	0.54
1:F:76:LYS:HE3	1:F:79:GLN:NE2	2.23	0.54
1:C:40:VAL:HG23	1:C:41:ASN:N	2.22	0.54
1:A:116:ARG:HH12	1:A:126:ASP:H	1.56	0.53
1:E:29:TYR:OH	1:E:197:ARG:NE	2.41	0.53
1:B:36:ALA:HB3	1:B:191:GLU:HB2	1.91	0.53
1:D:116:ARG:C	1:D:118:ARG:H	2.10	0.53
1:C:96:PRO:HA	2:I:4:FUC:H63	1.91	0.52
1:A:124:ASP:OD2	1:A:125:GLN:N	2.41	0.52
1:B:238:LYS:HG2	1:B:239:GLU:HG2	1.91	0.52
1:D:182:HIS:ND1	1:D:191:GLU:OE2	2.36	0.52
1:D:106:PRO:CB	1:D:116:ARG:HG3	2.41	0.51
1:D:82:VAL:HG11	1:D:167:SER:HB2	1.91	0.51
1:A:36:ALA:HB3	1:A:191:GLU:HB2	1.92	0.51
1:C:40:VAL:HG23	1:C:41:ASN:H	1.75	0.51
1:B:238:LYS:HE2	1:B:239:GLU:HG3	1.93	0.51
1:E:238:LYS:NZ	1:E:239:GLU:HG3	2.26	0.51
1:C:29:TYR:HA	1:C:133:PRO:HA	1.93	0.50
1:C:72:ARG:NH2	1:C:147:GLU:OE1	2.43	0.50
1:F:212:ARG:HD3	1:F:214:ARG:HH22	1.77	0.50
1:B:35:SER:HA	1:B:105:LEU:HB2	1.94	0.50
1:E:29:TYR:CE2	1:E:197:ARG:NH2	2.80	0.50
1:A:48:ALA:HA	1:A:55:ARG:O	2.12	0.49
1:E:66:GLU:HG2	1:E:101:ASN:ND2	2.27	0.49
1:F:44:LEU:HD11	1:F:50:CYS:HA	1.94	0.49
1:F:178:TRP:CE2	1:F:195:ARG:HD2	2.48	0.49
1:B:96:PRO:HA	2:H:4:FUC:H63	1.94	0.49
1:C:82:VAL:HG11	1:C:167:SER:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:CYS:HB3	1:D:51:ASP:H	1.46	0.48
1:F:238:LYS:HG3	1:F:239:GLU:HG2	1.95	0.48
1:B:27:MET:N	1:B:207:CYS:O	2.47	0.48
1:E:195:ARG:CZ	1:E:197:ARG:HD2	2.43	0.48
1:A:116:ARG:HH11	1:A:125:GLN:HB3	1.79	0.47
1:A:116:ARG:HH22	1:A:126:ASP:HB2	1.79	0.47
1:F:33:GLN:NE2	1:F:128:GLY:O	2.47	0.47
1:E:40:VAL:HG13	1:E:41:ASN:OD1	2.14	0.47
1:F:212:ARG:HB3	1:F:214:ARG:HH12	1.79	0.47
1:F:37:LEU:HB3	1:F:103:PHE:HE2	1.77	0.47
1:E:182:HIS:ND1	1:E:191:GLU:OE1	2.48	0.47
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.09	0.46
1:B:238:LYS:HE2	1:B:239:GLU:HG2	1.98	0.46
1:C:27:MET:N	1:C:207:CYS:O	2.49	0.46
1:F:68:ASP:N	1:F:150:ASP:OD1	2.48	0.46
1:F:76:LYS:HE3	1:F:79:GLN:HE22	1.81	0.46
1:E:44:LEU:HD21	1:E:50:CYS:HA	1.96	0.46
1:E:138:TRP:HA	1:E:139:PRO:HD3	1.83	0.46
1:A:239:GLU:HB2	1:A:241:LYS:HG3	1.98	0.45
1:D:203:TYR:O	1:D:204:SER:HB3	2.16	0.45
1:D:297:THR:O	1:D:298:ASN:HB2	2.16	0.45
1:E:29:TYR:CE2	1:E:197:ARG:CZ	3.00	0.45
1:E:126:ASP:HB3	1:E:127:PRO:HD2	1.98	0.45
1:F:67:CYS:N	1:F:101:ASN:OD1	2.49	0.45
1:E:190:LEU:HA	1:E:190:LEU:HD23	1.61	0.45
1:F:32:LEU:HD11	1:F:192:LEU:HD22	1.99	0.45
1:D:201:ASN:H	1:D:212:ARG:NH2	2.15	0.45
1:F:150:ASP:H	1:F:161:LEU:CD1	2.30	0.45
1:D:204:SER:OG	1:D:205:ALA:N	2.50	0.44
1:A:118:ARG:NH2	6:A:506:HOH:O	2.51	0.43
1:C:41:ASN:ND2	1:C:43:GLU:OE2	2.51	0.43
1:A:203:TYR:O	1:A:204:SER:HB3	2.19	0.43
1:B:225:GLN:HA	1:B:225:GLN:OE1	2.19	0.43
1:C:137:ALA:HB1	1:C:206:THR:HB	2.01	0.43
1:D:197:ARG:NH1	1:D:197:ARG:CG	2.68	0.42
1:E:238:LYS:HD2	1:E:239:GLU:CG	2.50	0.42
1:D:200:GLU:O	1:D:201:ASN:HB2	2.19	0.42
1:F:96:PRO:HB3	3:L:3:FUC:H2	2.01	0.42
1:B:203:TYR:O	1:B:204:SER:HB3	2.20	0.41
1:C:239:GLU:HB2	1:C:241:LYS:HE3	2.01	0.41
1:D:117:ALA:C	1:D:118:ARG:HD2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASN:O	1:B:215:ASN:OD1	2.39	0.41
1:A:116:ARG:HH12	1:A:126:ASP:N	2.17	0.41
1:A:116:ARG:NH1	1:A:126:ASP:H	2.16	0.41
1:A:74:CYS:HB3	1:A:145:ILE:HB	2.01	0.41
1:E:29:TYR:CD2	1:E:29:TYR:C	2.93	0.41
1:E:51:ASP:HB2	1:E:65:ASP:O	2.20	0.41
1:E:150:ASP:OD1	1:E:151:TRP:N	2.54	0.41
1:F:103:PHE:N	1:F:103:PHE:CD2	2.89	0.41
1:F:149:TRP:CE3	1:F:161:LEU:HB3	2.56	0.41
1:D:221:TYR:HB3	1:D:240:CYS:SG	2.61	0.41
1:D:29:TYR:CE1	1:D:133:PRO:HB3	2.56	0.40
1:D:116:ARG:C	1:D:118:ARG:N	2.75	0.40
1:A:116:ARG:HH12	1:A:126:ASP:CB	2.35	0.40
1:B:224:ASP:OD2	1:B:228:ASN:HB2	2.21	0.40
1:B:258:VAL:O	1:B:261:GLU:HG2	2.22	0.40
1:D:27:MET:O	1:D:199:ASP:HB2	2.20	0.40
1:F:83:THR:HG22	1:F:85:THR:H	1.87	0.40
1:F:177:ARG:HD2	1:F:177:ARG:HA	1.90	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LYS:NZ	1:C:52:GLY:O[1_546]	2.17	0.03
6:A:550:HOH:O	6:E:533:HOH:O[1_455]	2.18	0.02

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	270/293 (92%)	253 (94%)	17 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	270/293 (92%)	253 (94%)	17 (6%)	0	100	100
1	C	256/293 (87%)	233 (91%)	22 (9%)	1 (0%)	34	66
1	D	260/293 (89%)	238 (92%)	21 (8%)	1 (0%)	34	66
1	E	254/293 (87%)	230 (91%)	23 (9%)	1 (0%)	34	66
1	F	247/293 (84%)	220 (89%)	25 (10%)	2 (1%)	19	49
All	All	1557/1758 (89%)	1427 (92%)	125 (8%)	5 (0%)	41	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	107	PRO
1	D	50	CYS
1	F	50	CYS
1	F	127	PRO
1	E	127	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/239 (95%)	221 (97%)	6 (3%)	46	79
1	B	226/239 (95%)	222 (98%)	4 (2%)	59	86
1	C	220/239 (92%)	219 (100%)	1 (0%)	88	96
1	D	221/239 (92%)	215 (97%)	6 (3%)	44	78
1	E	219/239 (92%)	216 (99%)	3 (1%)	67	90
1	F	215/239 (90%)	212 (99%)	3 (1%)	67	90
All	All	1328/1434 (93%)	1305 (98%)	23 (2%)	60	87

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	ARG
1	A	212	ARG
1	A	233	ASP
1	A	246	LYS
1	A	247	GLN
1	B	126	ASP
1	B	159	GLU
1	B	176	ASP
1	B	252	LEU
1	C	302	LEU
1	D	50	CYS
1	D	140	ARG
1	D	199	ASP
1	D	218	PHE
1	D	294	ASN
1	D	299	TRP
1	E	160	GLU
1	E	197	ARG
1	E	238	LYS
1	F	68	ASP
1	F	103	PHE
1	F	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	298	ASN
1	C	64	HIS
1	E	101	ASN
1	E	182	HIS
1	E	247	GLN
1	F	79	GLN
1	F	182	HIS
1	F	201	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

21 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	G	1	1,2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	BMA	G	3	2	11,11,12	0.67	0	15,15,17	0.80	0
2	FUC	G	4	2	10,10,11	0.90	1 (10%)	14,14,16	0.75	0
2	NAG	H	1	1,2	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	H	2	2	14,14,15	0.42	0	17,19,21	0.35	0
2	BMA	H	3	2	11,11,12	0.75	0	15,15,17	0.83	0
2	FUC	H	4	2	10,10,11	0.58	0	14,14,16	0.90	0
2	NAG	I	1	1,2	14,14,15	0.56	0	17,19,21	0.44	0
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.47	0
2	BMA	I	3	2	11,11,12	0.67	0	15,15,17	0.93	0
2	FUC	I	4	2	10,10,11	0.76	0	14,14,16	0.84	0
3	NAG	J	1	3	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	J	2	3	14,14,15	0.35	0	17,19,21	0.40	0
3	FUC	J	3	3	10,10,11	0.81	0	14,14,16	0.88	0
3	NAG	K	1	1,3	14,14,15	0.19	0	17,19,21	0.47	0
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	FUC	K	3	3	10,10,11	0.78	0	14,14,16	0.88	0
3	NAG	L	1	1,3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	FUC	L	3	3	10,10,11	0.81	0	14,14,16	0.90	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
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	FUC	G	4	2	1/1/4/5	-	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	2/2/19/22	0/1/1/1
2	FUC	H	4	2	-	-	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	FUC	I	4	2	-	-	0/1/1/1
3	NAG	J	1	3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	FUC	J	3	3	1/1/4/5	-	0/1/1/1
3	NAG	K	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	1/1/4/5	-	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	FUC	L	3	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	FUC	O5-C1	-2.33	1.40	1.43

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	4	FUC	C1
3	J	3	FUC	C1
3	K	1	NAG	C1
3	K	3	FUC	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6

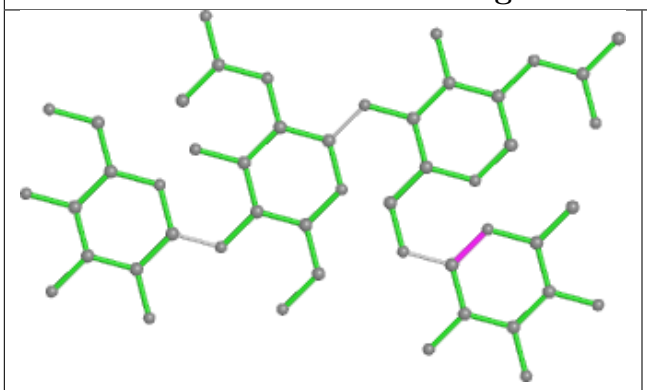
There are no ring outliers.

4 monomers are involved in 4 short contacts:

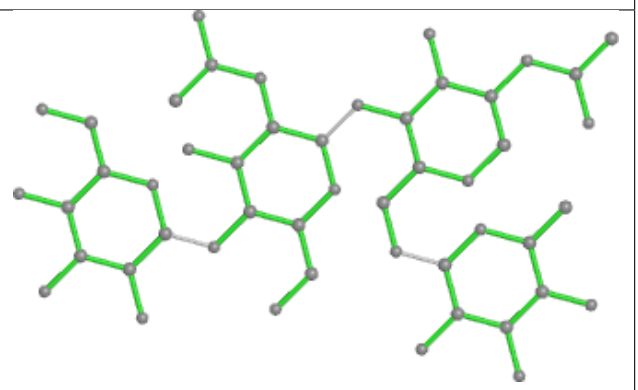
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	FUC	1	0
3	J	3	FUC	1	0
2	H	4	FUC	1	0
3	L	3	FUC	1	0

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

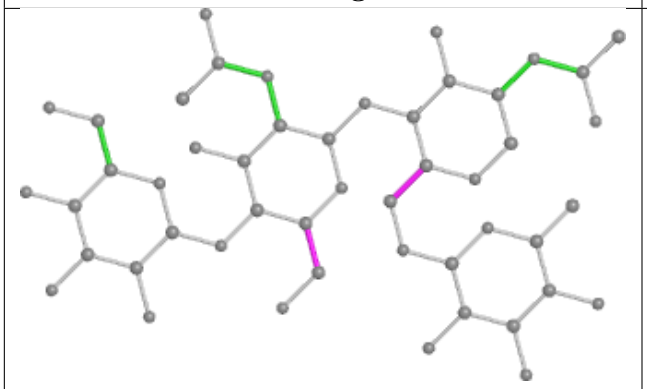
Oligosaccharide Chain G



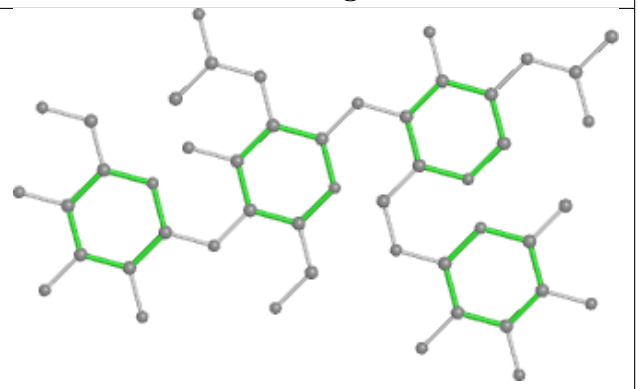
Bond lengths



Bond angles

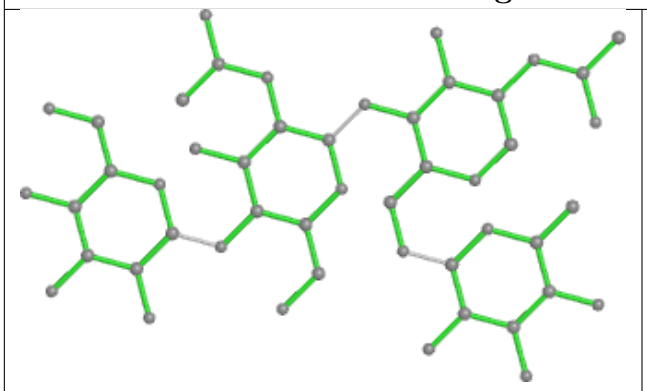


Torsions

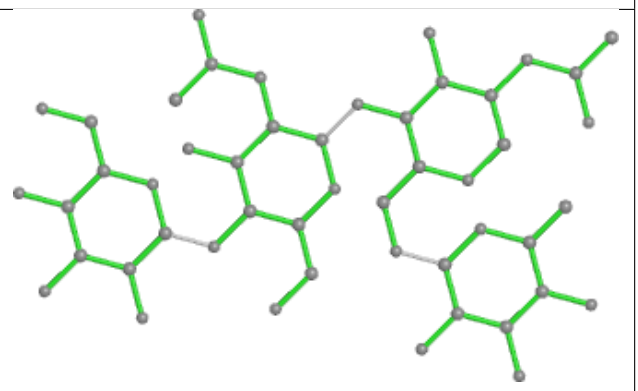


Rings

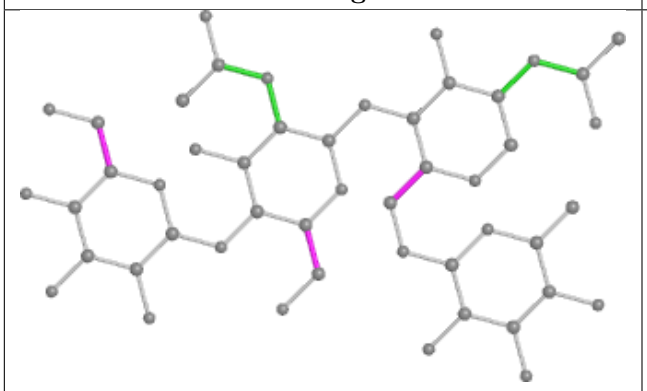
Oligosaccharide Chain H



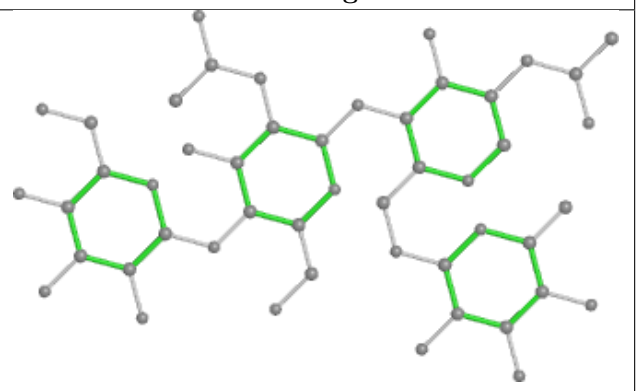
Bond lengths



Bond angles

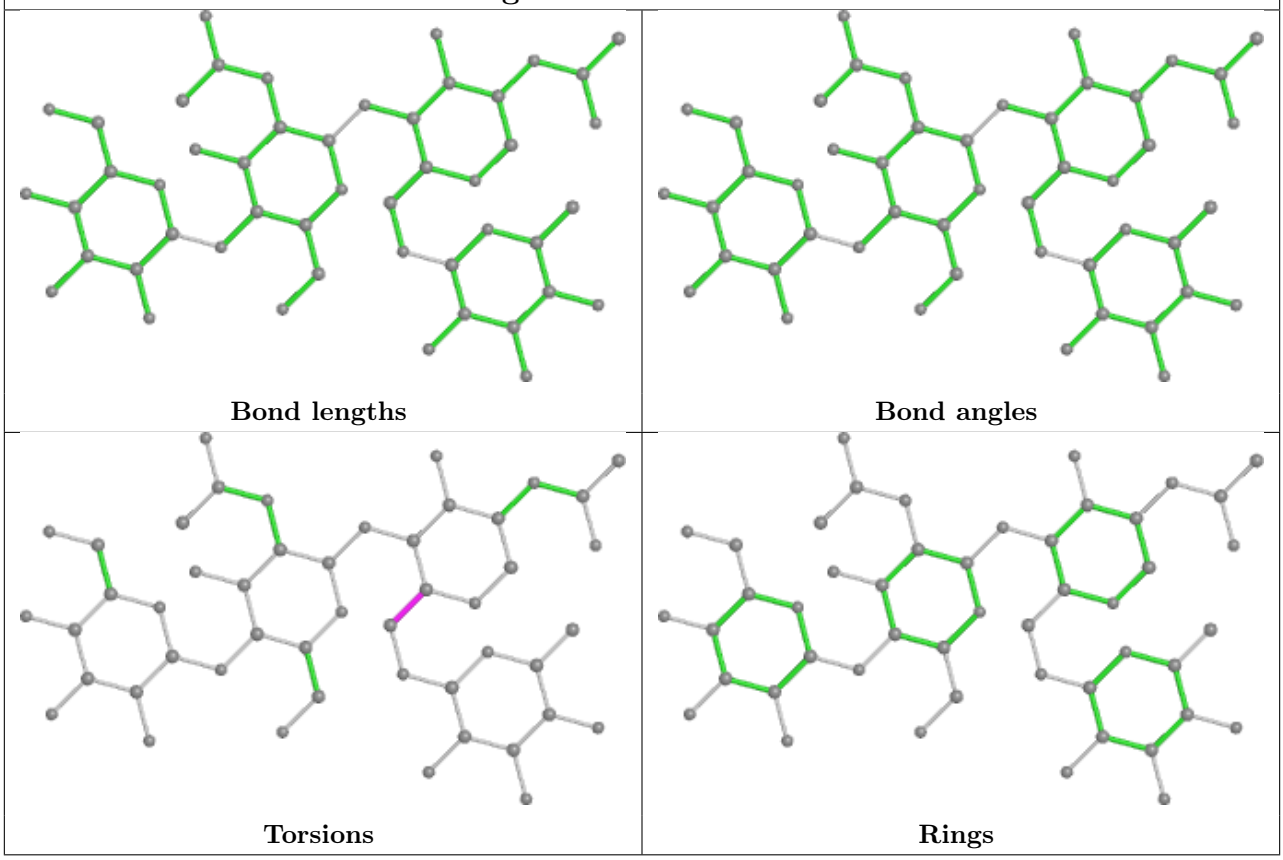


Torsions

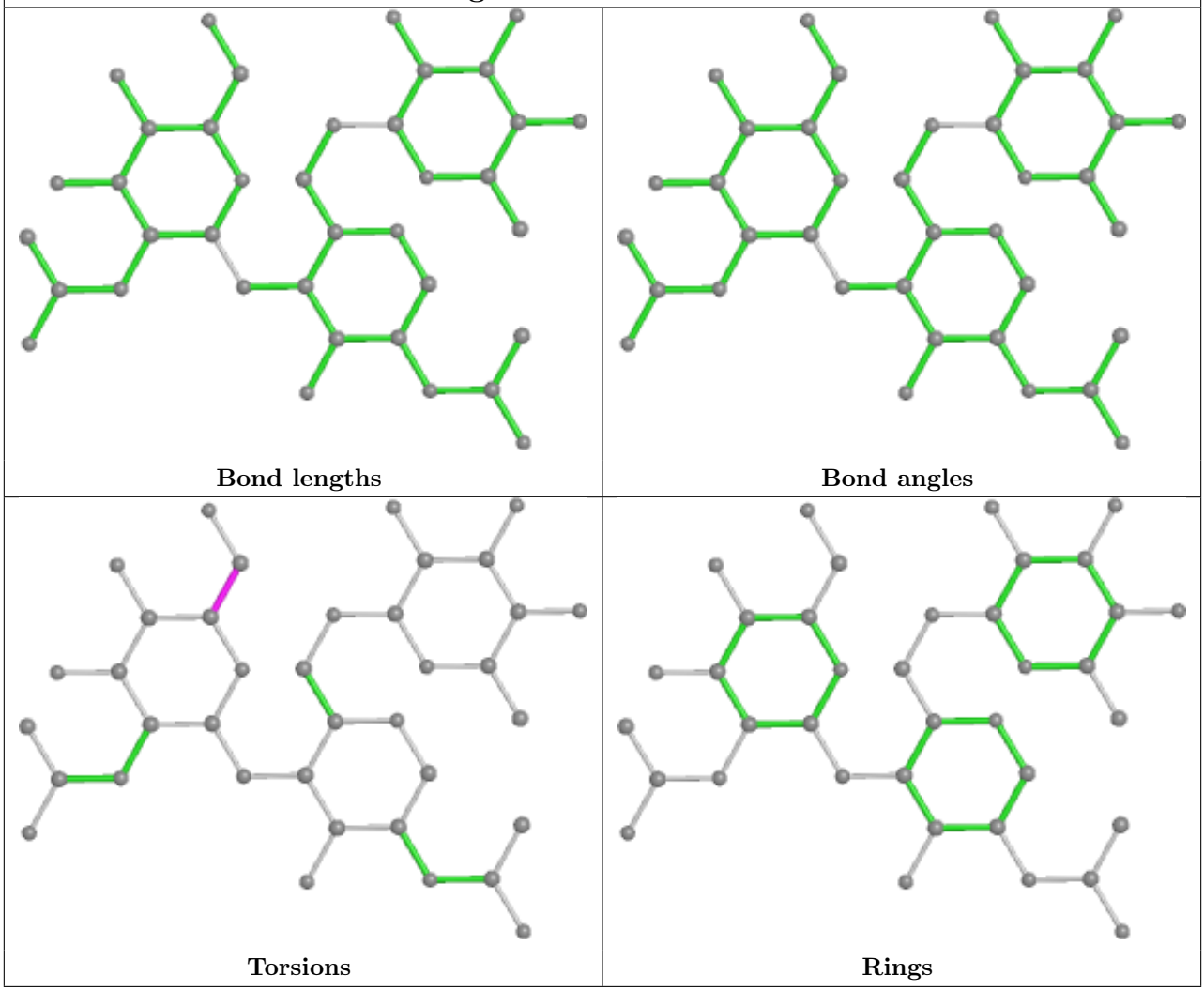


Rings

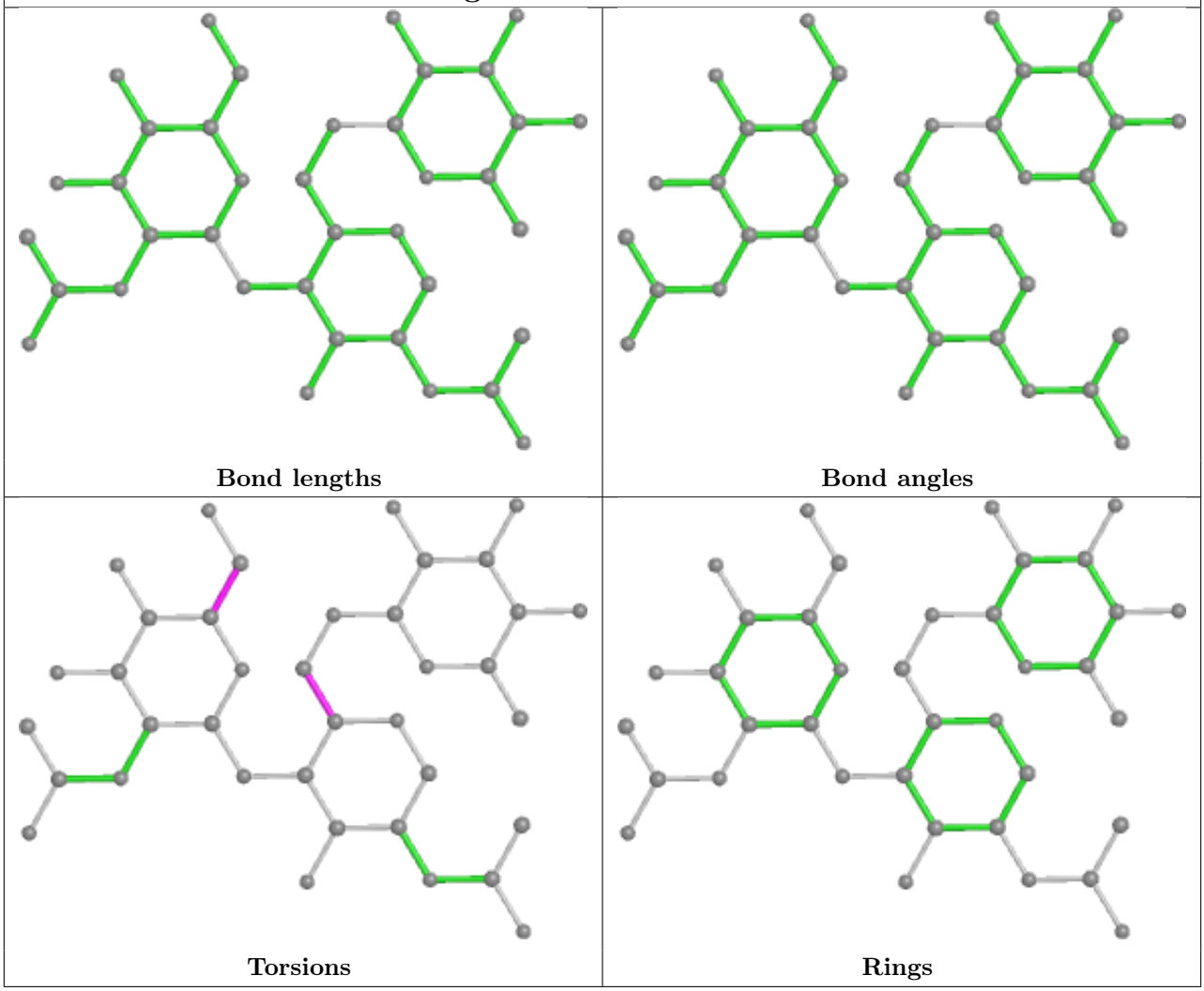
Oligosaccharide Chain I

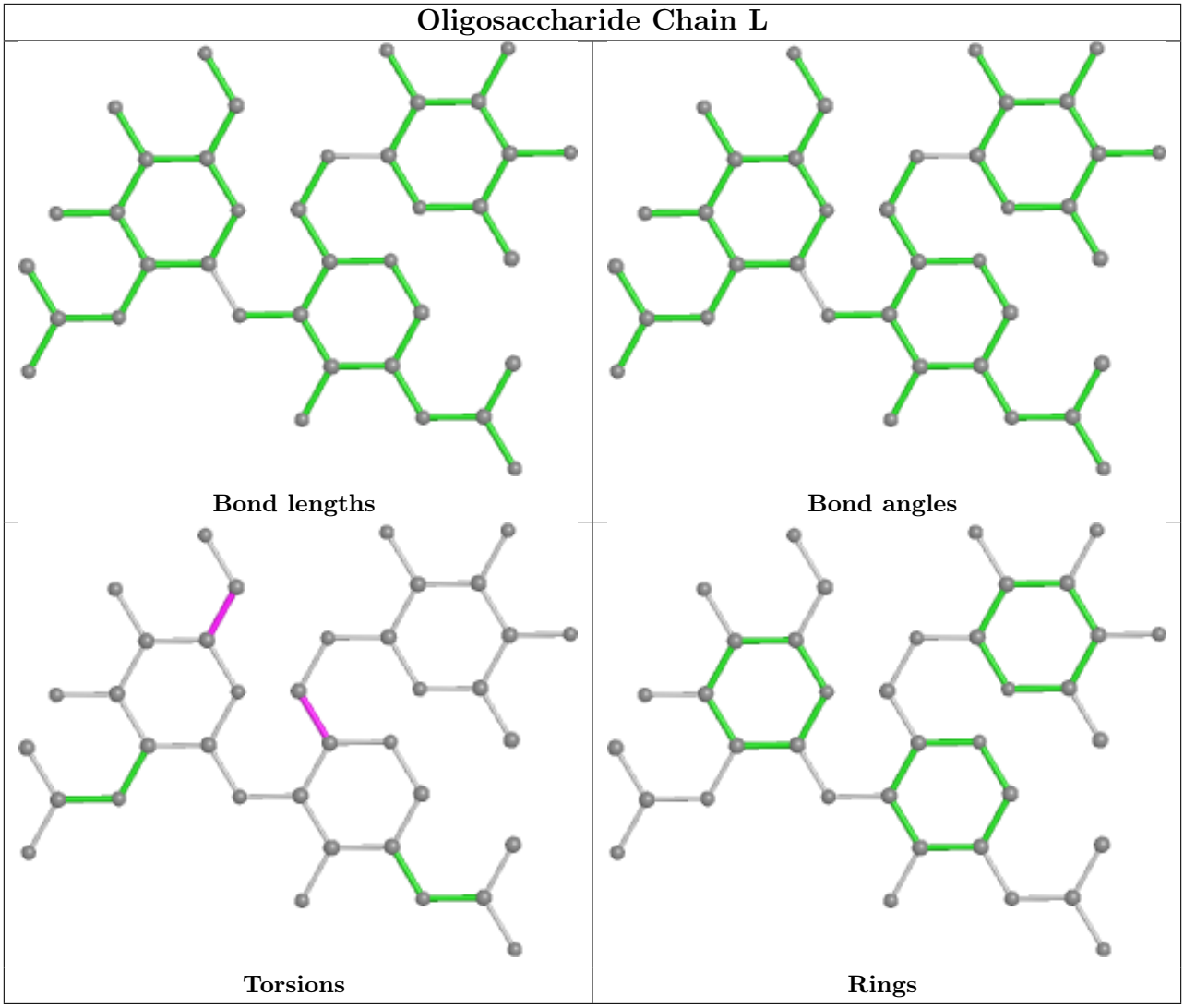


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 (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, 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	276/293 (94%)	-0.12	1 (0%)	92	91	21, 41, 69, 94	0
1	B	275/293 (93%)	-0.05	3 (1%)	80	75	23, 44, 78, 88	0
1	C	262/293 (89%)	-0.07	3 (1%)	80	75	21, 46, 81, 93	0
1	D	266/293 (90%)	0.09	7 (2%)	56	46	25, 52, 92, 108	0
1	E	260/293 (88%)	0.04	7 (2%)	54	44	24, 46, 97, 113	0
1	F	253/293 (86%)	0.17	11 (4%)	35	25	26, 52, 101, 120	0
All	All	1592/1758 (90%)	0.01	32 (2%)	65	56	21, 47, 88, 120	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	310	GLY	8.2
1	F	61	GLY	5.2
1	A	60	GLY	4.2
1	F	297	THR	3.9
1	C	310	GLY	3.8
1	D	64	HIS	3.6
1	D	61	GLY	3.4
1	F	298	ASN	3.3
1	E	45	LEU	3.1
1	D	296	GLU	3.0
1	E	298	ASN	3.0
1	E	157	PRO	2.9
1	B	125	GLN	2.9
1	E	62	CYS	2.8
1	F	48	ALA	2.7
1	D	155	THR	2.7
1	F	46	SER	2.7
1	F	66	GLU	2.7
1	F	97	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	176	ASP	2.4
1	B	60	GLY	2.3
1	F	299	TRP	2.3
1	E	217	PHE	2.3
1	F	153	ASN	2.3
1	F	151	TRP	2.2
1	B	260	GLY	2.2
1	E	309	ASN	2.2
1	D	114	ARG	2.1
1	C	217	PHE	2.1
1	F	306	LYS	2.1
1	D	297	THR	2.0
1	D	212	ARG	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
3	NAG	J	1	14/15	0.69	0.25	88,98,109,112	0
3	NAG	J	2	14/15	0.69	0.28	78,93,101,107	0
3	NAG	K	1	14/15	0.75	0.35	101,113,124,125	0
3	NAG	K	2	14/15	0.76	0.24	91,99,104,105	0
2	BMA	I	3	11/12	0.77	0.31	93,97,100,102	0
3	FUC	L	3	10/11	0.79	0.25	92,94,98,106	0
3	NAG	L	1	14/15	0.82	0.22	84,92,96,96	0
3	NAG	L	2	14/15	0.84	0.21	75,81,87,88	0
3	FUC	J	3	10/11	0.85	0.30	83,91,96,97	0
2	NAG	I	1	14/15	0.87	0.25	70,79,84,87	0
2	BMA	G	3	11/12	0.88	0.14	55,62,67,69	0
2	BMA	H	3	11/12	0.88	0.12	64,71,75,76	0
3	FUC	K	3	10/11	0.89	0.19	83,90,94,94	0
2	FUC	I	4	10/11	0.91	0.21	65,68,75,76	0
2	NAG	I	2	14/15	0.91	0.25	74,84,89,90	0

Continued on next page...

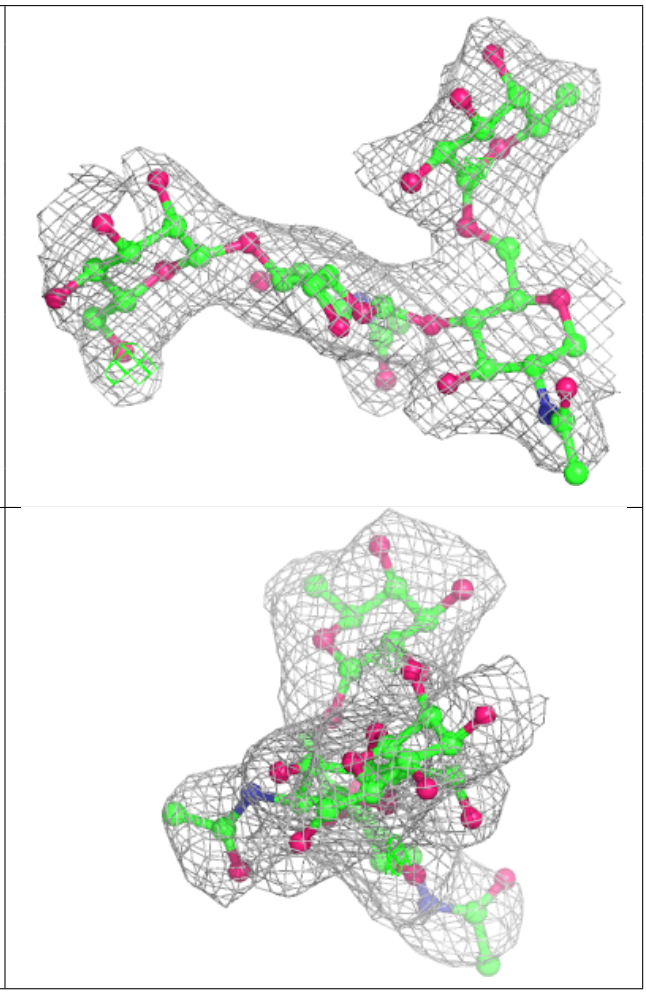
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.93	0.18	36,49,62,62	0
2	FUC	G	4	10/11	0.94	0.15	30,38,43,45	0
2	NAG	H	1	14/15	0.95	0.16	40,51,66,69	0
2	NAG	G	1	14/15	0.95	0.13	42,50,60,65	0
2	FUC	H	4	10/11	0.96	0.19	29,42,53,56	0
2	NAG	G	2	14/15	0.97	0.13	38,42,47,56	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.

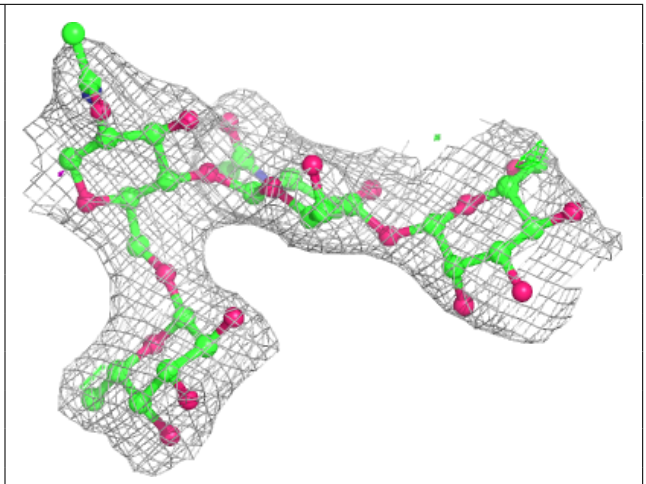
Electron density around Chain G:

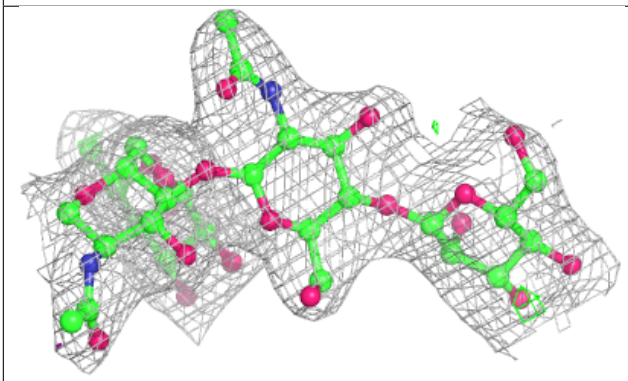
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

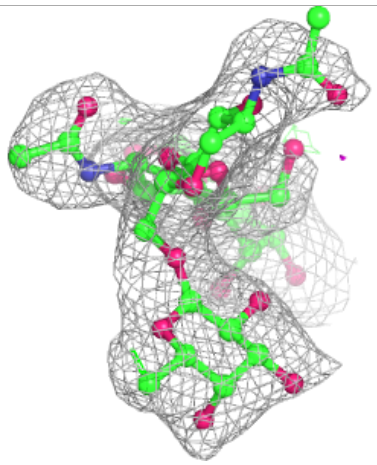


Electron density around Chain H:

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

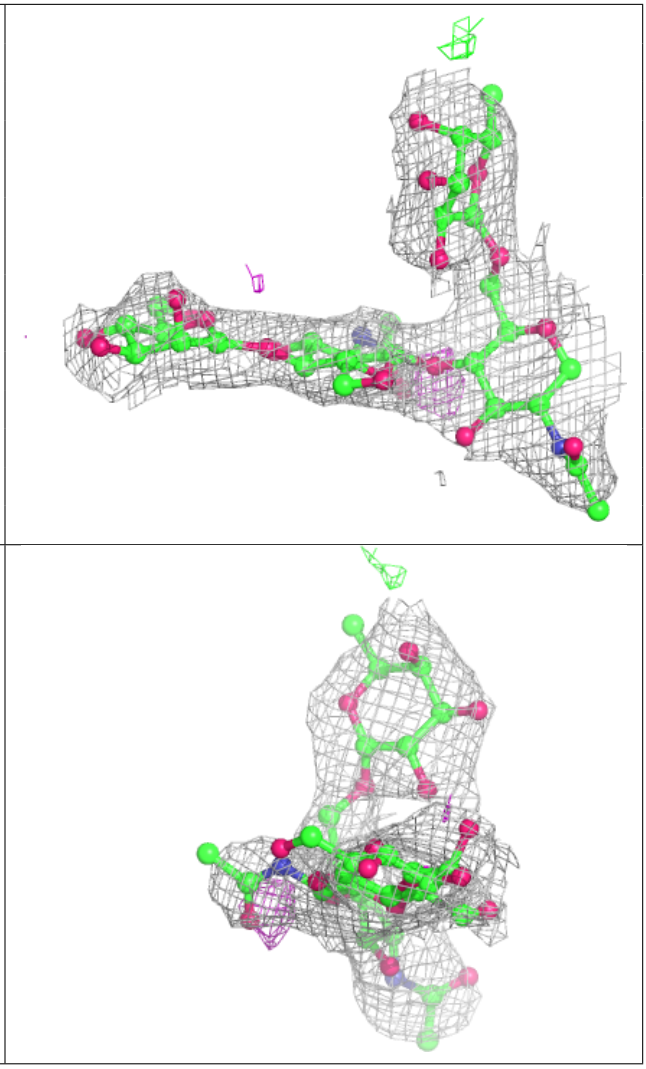


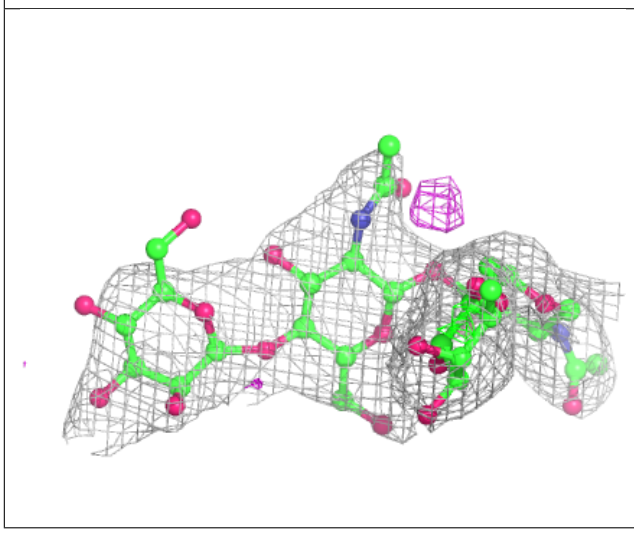




Electron density around Chain I:

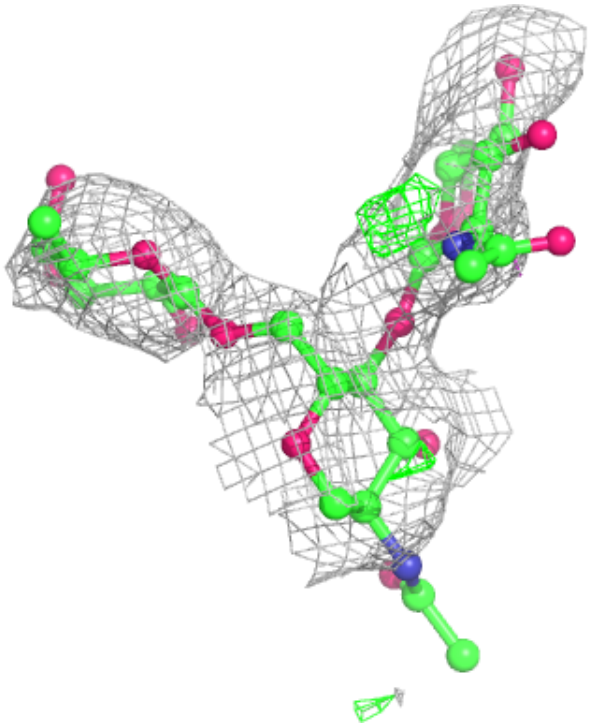
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

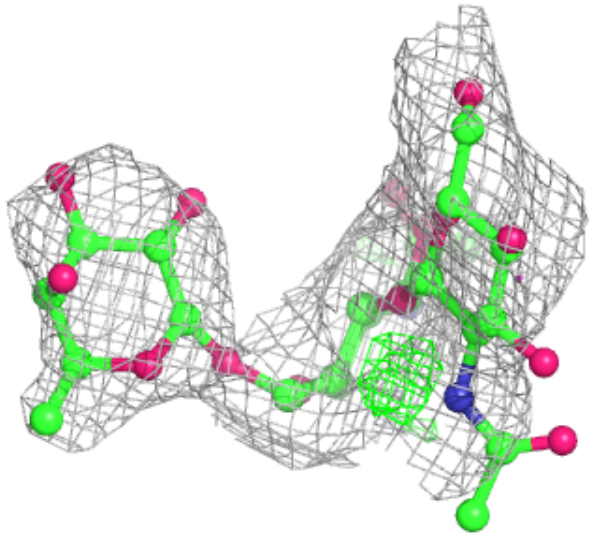


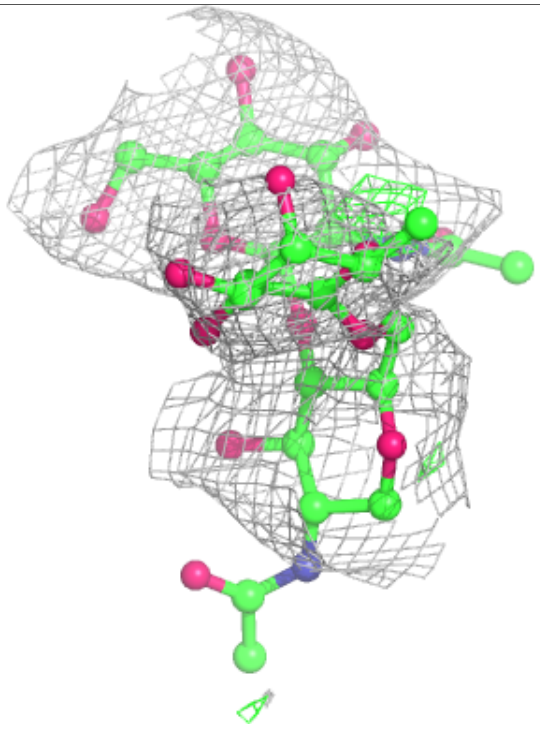


Electron density around Chain J:

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

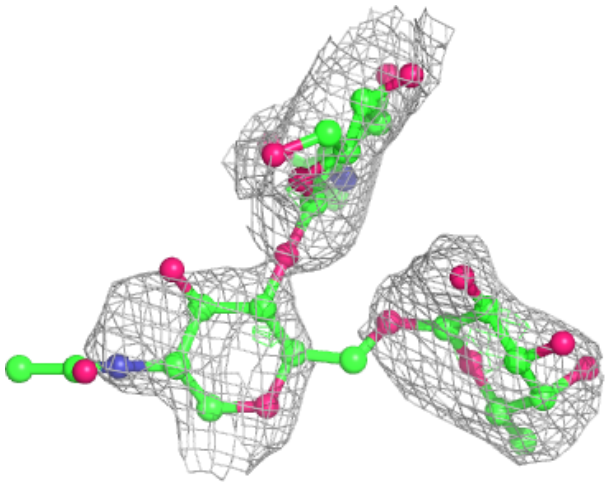


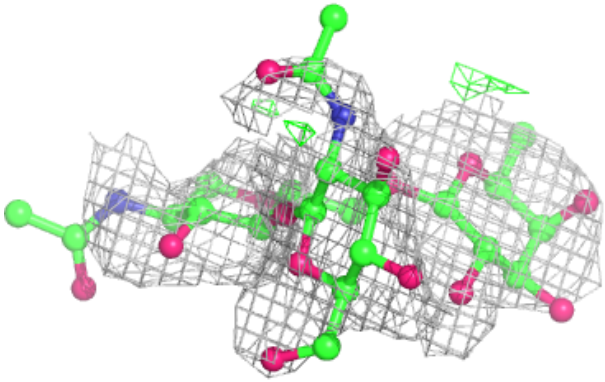


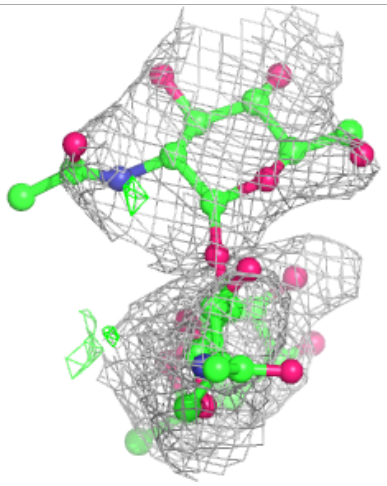


Electron density around Chain K:

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

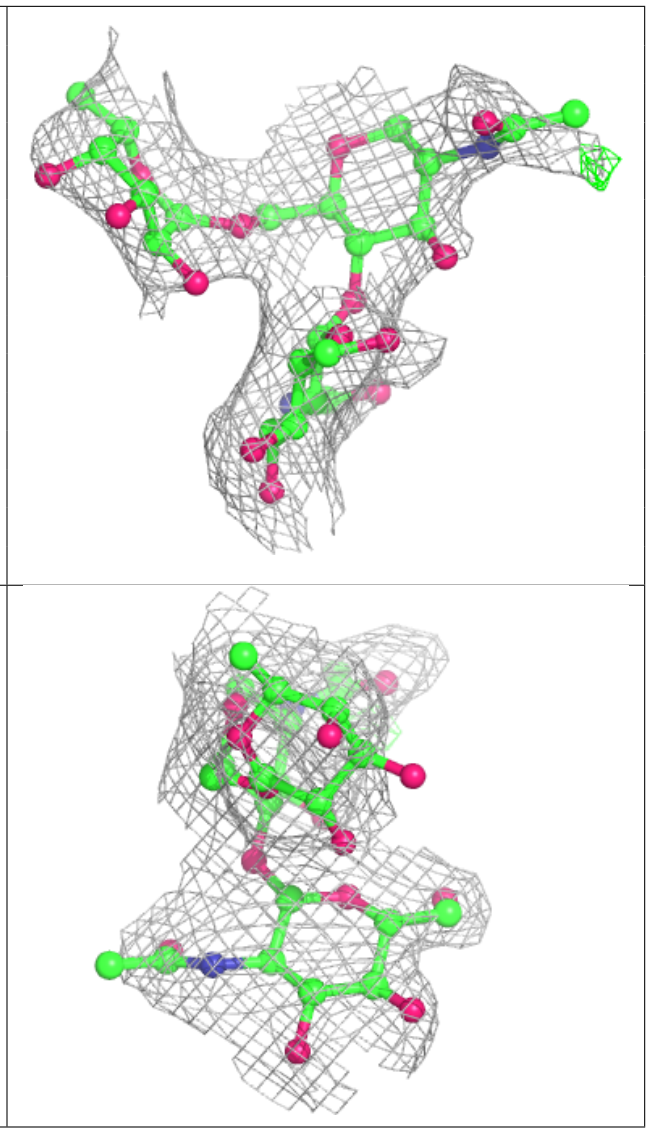






Electron density around Chain L:

$2mF_o$-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(Å^2)	Q<0.9
4	CA	D	404	1/1	0.59	0.21	106,106,106,106	0
4	CA	E	406	1/1	0.69	0.08	96,96,96,96	0
4	CA	F	404	1/1	0.71	0.08	108,108,108,108	0
4	CA	E	405	1/1	0.73	0.09	110,110,110,110	0
4	CA	C	405	1/1	0.74	0.18	70,70,70,70	0
4	CA	E	404	1/1	0.75	0.14	89,89,89,89	0
4	CA	D	405	1/1	0.78	0.05	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	C	406	1/1	0.80	0.06	69,69,69,69	0
4	CA	A	407	1/1	0.81	0.12	60,60,60,60	0
4	CA	F	405	1/1	0.81	0.09	97,97,97,97	0
4	CA	B	407	1/1	0.83	0.20	70,70,70,70	0
4	CA	A	406	1/1	0.90	0.10	34,34,34,34	0
4	CA	D	406	1/1	0.91	0.06	100,100,100,100	0
4	CA	B	405	1/1	0.91	0.13	42,42,42,42	0
5	CL	A	408	1/1	0.94	0.16	46,46,46,46	0
5	CL	B	408	1/1	0.94	0.18	57,57,57,57	0
4	CA	C	407	1/1	0.95	0.07	68,68,68,68	0
4	CA	A	405	1/1	0.97	0.10	36,36,36,36	0
4	CA	B	406	1/1	0.97	0.07	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.