



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:07 PM BST

PDB ID : 6FGO
Title : Fc in complex with engineered calcium binding domain Z
Authors : Venskutonyte, R.; Kanje, S.; Hober, S.; Lindkvist-Petersson, K.
Deposited on : 2018-01-11
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

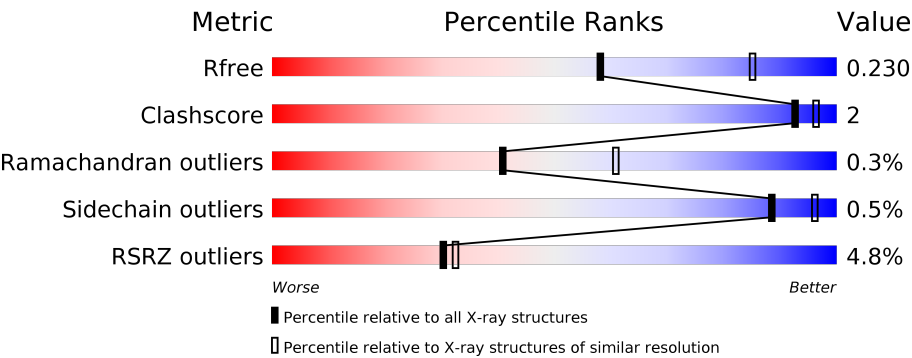
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	210	<div><div></div><div>95%</div><div></div></div>
1	B	210	<div><div>9%</div><div>95%</div><div></div></div>
1	C	210	<div><div>%</div><div>97%</div><div></div></div>
1	D	210	<div><div>9%</div><div>93%</div><div>6%</div></div>
2	E	69	<div><div></div><div>93%</div><div>7%</div></div>
2	F	69	<div><div>%</div><div>91%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	69	<div><div>%</div><div><div></div><div>90%</div><div>6%</div></div></div>
2	H	69	<div><div>14%</div><div><div></div><div>93%</div><div>7%</div></div></div>
3	I	8	<div><div></div><div><div>63%</div><div>38%</div></div></div>
3	K	8	<div><div></div><div><div>75%</div><div>25%</div></div></div>
4	J	7	<div><div></div><div><div>43%</div><div>43%</div><div>14%</div></div></div>
5	L	5	<div><div></div><div><div>60%</div><div>40%</div></div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9382 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1672	1064	281	320	7			
1	B	209	Total	C	N	O	S	0	0	0
			1672	1064	281	320	7			
1	C	208	Total	C	N	O	S	0	0	0
			1665	1059	280	319	7			
1	D	208	Total	C	N	O	S	0	0	0
			1665	1059	280	319	7			

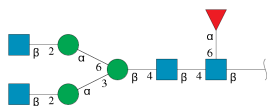
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	GLU	ASP	conflict	UNP P0DOX5
A	358	MET	LEU	conflict	UNP P0DOX5
B	356	GLU	ASP	conflict	UNP P0DOX5
B	358	MET	LEU	conflict	UNP P0DOX5
C	356	GLU	ASP	conflict	UNP P0DOX5
C	358	MET	LEU	conflict	UNP P0DOX5
D	356	GLU	ASP	conflict	UNP P0DOX5
D	358	MET	LEU	conflict	UNP P0DOX5

- Molecule 2 is a protein called Z-Ca.

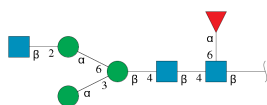
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	64	Total	C	N	O	0	1	0
			511	314	93	104			
2	F	67	Total	C	N	O	0	1	0
			529	325	93	111			
2	G	65	Total	C	N	O	0	0	0
			507	313	90	104			
2	H	64	Total	C	N	O	0	0	0
			498	307	88	103			

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



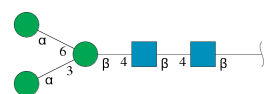
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	K	8	Total	C	N	O	0	0	0
			99	56	4	39			

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



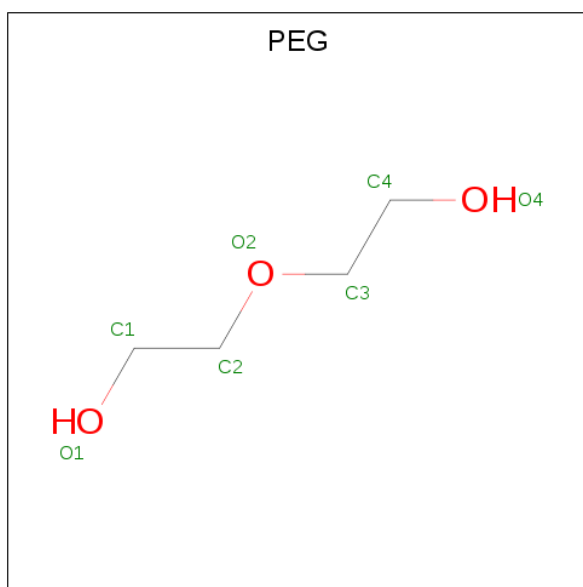
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 5 is an oligosaccharide called 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.



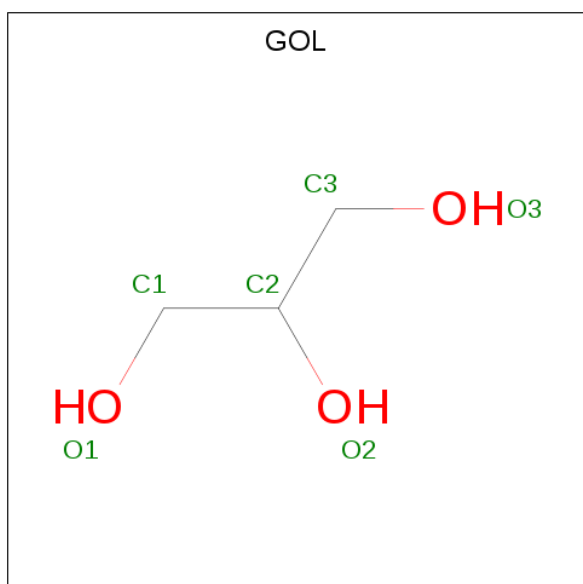
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0
8	F	1	Total Ca 1 1	0	0
8	E	1	Total Ca 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Cl 2 2	0	0
9	D	2	Total Cl 2 2	0	0
9	C	5	Total Cl 5 5	0	0

- Molecule 10 is water.

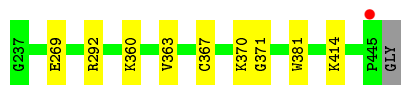
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	76	Total O 77 77	0	1
10	E	18	Total O 18 18	0	0
10	B	28	Total O 29 29	0	1
10	F	26	Total O 26 26	0	0
10	C	23	Total O 23 23	0	0
10	G	1	Total O 1 1	0	0
10	D	5	Total O 5 5	0	0
10	H	2	Total O 2 2	0	0

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.

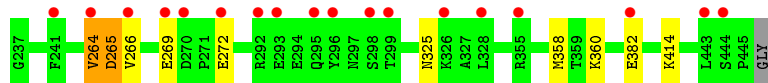
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain A: 



- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain B: 



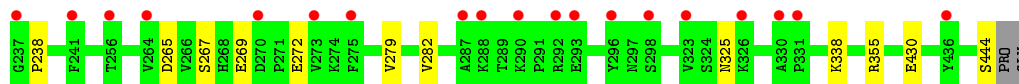
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain C: 



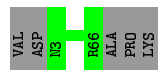
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain D: 



- Molecule 2: Z-Ca

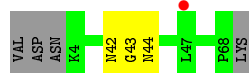
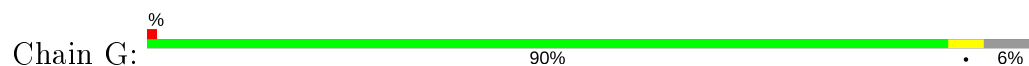
Chain E: 



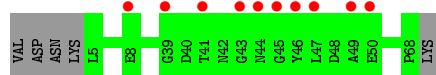
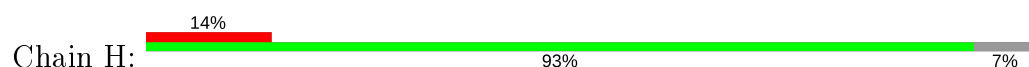
- Molecule 2: Z-Ca



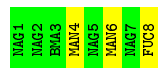
- Molecule 2: Z-Ca



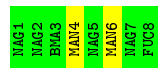
- Molecule 2: Z-Ca



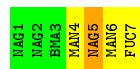
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 5: 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 L:  60% 40%

MAG1	MAG2	MAG3	MAG4	MAG5
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.23 Å 120.30 Å 126.33 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.53 – 2.50 46.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.53-2.50) 97.4 (46.53-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.51 Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.203 , 0.232 0.204 , 0.230	Depositor DCC
R_{free} test set	2256 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9382	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: GOL, BMA, NAG, CL, CA, FUC, PEG, MAN

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	0.26	0/1719	0.44	0/2342
1	B	0.25	0/1719	0.44	0/2342
1	C	0.26	0/1711	0.44	0/2330
1	D	0.25	0/1711	0.43	0/2330
2	E	0.25	0/519	0.40	0/696
2	F	0.27	0/537	0.42	0/722
2	G	0.24	0/513	0.39	0/690
2	H	0.25	0/504	0.39	0/679
All	All	0.25	0/8933	0.43	0/12131

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	1672	0	1637	5	0
1	B	1672	0	1636	8	0
1	C	1665	0	1630	2	0
1	D	1665	0	1629	6	0
2	E	511	0	496	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	529	0	510	2	0
2	G	507	0	489	1	0
2	H	498	0	476	0	0
3	I	99	0	85	0	0
3	K	99	0	85	0	0
4	J	85	0	73	3	0
5	L	61	0	52	0	0
6	A	14	0	20	1	0
6	C	21	0	30	1	0
7	A	18	0	24	0	0
7	B	24	0	32	1	0
7	C	18	0	24	0	0
7	D	12	0	16	0	0
7	E	6	0	8	0	0
7	F	12	0	16	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	B	2	0	0	0	0
9	C	5	0	0	0	0
9	D	2	0	0	0	0
10	A	77	0	0	1	0
10	B	29	0	0	0	0
10	C	23	0	0	1	0
10	D	5	0	0	0	0
10	E	18	0	0	0	0
10	F	26	0	0	0	0
10	G	1	0	0	0	0
10	H	2	0	0	0	0
All	All	9382	0	8968	28	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 2.

All (28) 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:358:MET:O	1:B:414:LYS:NZ	2.19	0.67
2:G:42:ASN:O	2:G:44:ASN:N	2.30	0.64
1:D:272:GLU:O	1:D:325:ASN:ND2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:O	1:B:325:ASN:ND2	2.37	0.57
1:B:360:LYS:O	1:B:414:LYS:HE3	2.06	0.56
4:J:5:NAG:H3	4:J:5:NAG:H83	1.88	0.55
1:B:382:GLU:OE2	7:B:1010:GOL:O2	2.24	0.54
1:D:267:SER:OG	1:D:269:GLU:O	2.26	0.53
1:B:264:VAL:O	1:B:266:VAL:N	2.42	0.52
4:J:5:NAG:C1	4:J:5:NAG:H82	2.41	0.51
2:F:2:ASP:O	2:F:4:LYS:N	2.43	0.50
1:D:338:LYS:HE3	1:D:430:GLU:OE2	2.13	0.49
1:A:292:ARG:NH1	10:A:1106:HOH:O	2.39	0.44
1:B:264:VAL:O	1:B:266:VAL:HG23	2.16	0.44
1:A:269:GLU:N	1:A:269:GLU:OE1	2.46	0.44
1:B:264:VAL:O	1:B:265:ASP:C	2.56	0.43
1:B:269:GLU:N	1:B:269:GLU:OE1	2.47	0.43
1:D:279:VAL:O	1:D:282:VAL:HG22	2.19	0.43
2:F:41:THR:OG1	2:F:51:GLU:HG2	2.17	0.43
1:C:295:GLN:NE2	10:C:1103:HOH:O	2.51	0.43
1:A:360:LYS:O	1:A:414:LYS:HE3	2.19	0.43
1:D:444:SER:O	1:D:444:SER:OG	2.37	0.43
4:J:5:NAG:C1	4:J:5:NAG:C8	2.97	0.42
6:A:1009:PEG:H41	6:A:1009:PEG:H22	1.82	0.42
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.55	0.41
1:D:238:PRO:HA	1:D:265:ASP:HB2	2.03	0.41
1:A:370:LYS:HG2	1:A:371:GLY:N	2.36	0.41
1:C:249:ASP:OD2	6:C:1015:PEG:H41	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/210 (99%)	206 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	207/210 (99%)	203 (98%)	2 (1%)	2 (1%)	15	28
1	C	206/210 (98%)	205 (100%)	1 (0%)	0	100	100
1	D	206/210 (98%)	202 (98%)	4 (2%)	0	100	100
2	E	63/69 (91%)	61 (97%)	2 (3%)	0	100	100
2	F	66/69 (96%)	63 (96%)	3 (4%)	0	100	100
2	G	63/69 (91%)	60 (95%)	2 (3%)	1 (2%)	9	17
2	H	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
All	All	1080/1116 (97%)	1060 (98%)	17 (2%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASP
2	G	43	GLY
1	B	264	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/195 (100%)	194 (100%)	1 (0%)	88	96
1	B	195/195 (100%)	195 (100%)	0	100	100
1	C	194/195 (100%)	192 (99%)	2 (1%)	76	90
1	D	194/195 (100%)	193 (100%)	1 (0%)	88	96
2	E	53/56 (95%)	53 (100%)	0	100	100
2	F	55/56 (98%)	54 (98%)	1 (2%)	59	81
2	G	52/56 (93%)	52 (100%)	0	100	100
2	H	51/56 (91%)	51 (100%)	0	100	100
All	All	989/1004 (98%)	984 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	VAL
2	F	41	THR
1	C	355	ARG
1	C	359	THR
1	D	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	BMA	I	3	3	11,11,12	0.70	0	15,15,17	0.83	0
3	MAN	I	4	3	11,11,12	0.75	1 (9%)	15,15,17	1.08	2 (13%)
3	NAG	I	5	3	14,14,15	0.19	0	17,19,21	0.57	0
3	MAN	I	6	3	11,11,12	0.96	1 (9%)	15,15,17	1.39	1 (6%)
3	NAG	I	7	3	14,14,15	0.25	0	17,19,21	0.41	0
3	FUC	I	8	3	10,10,11	1.23	2 (20%)	14,14,16	1.22	1 (7%)
4	NAG	J	1	1,4	14,14,15	0.17	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.37	0
4	BMA	J	3	4	11,11,12	0.57	0	15,15,17	0.76	0
4	MAN	J	4	4	11,11,12	0.75	0	15,15,17	0.99	1 (6%)
4	NAG	J	5	4	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
4	MAN	J	6	4	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
4	FUC	J	7	4	10,10,11	1.71	2 (20%)	14,14,16	2.14	3 (21%)
3	NAG	K	1	1,3	14,14,15	0.28	0	17,19,21	0.52	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	BMA	K	3	3	11,11,12	0.63	0	15,15,17	0.72	0
3	MAN	K	4	3	11,11,12	0.77	1 (9%)	15,15,17	1.05	2 (13%)
3	NAG	K	5	3	14,14,15	0.24	0	17,19,21	0.47	0
3	MAN	K	6	3	11,11,12	0.74	0	15,15,17	1.10	2 (13%)
3	NAG	K	7	3	14,14,15	0.22	0	17,19,21	0.43	0
3	FUC	K	8	3	10,10,11	0.82	0	14,14,16	0.82	0
5	NAG	L	1	1,5	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	L	2	5	14,14,15	0.20	0	17,19,21	0.41	0
5	BMA	L	3	5	11,11,12	0.57	0	15,15,17	0.82	0
5	MAN	L	4	5	11,11,12	0.66	0	15,15,17	1.24	2 (13%)
5	MAN	L	5	5	11,11,12	0.74	0	15,15,17	1.02	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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	NAG	I	5	3	-	4/6/23/26	0/1/1/1
3	MAN	I	6	3	-	0/2/19/22	1/1/1/1
3	NAG	I	7	3	-	2/6/23/26	0/1/1/1
3	FUC	I	8	3	-	-	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
4	NAG	J	5	4	-	6/6/23/26	0/1/1/1

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	7	FUC	O5-C1	-3.42	1.38	1.43
4	J	7	FUC	C2-C3	3.35	1.57	1.52
3	I	8	FUC	O5-C1	-2.78	1.39	1.43
3	I	6	MAN	O5-C1	-2.56	1.39	1.43
3	I	4	MAN	O5-C1	-2.23	1.40	1.43
3	I	8	FUC	C2-C3	2.03	1.55	1.52
3	K	4	MAN	O5-C1	-2.00	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	7	FUC	C1-C2-C3	5.07	115.90	109.67
3	I	6	MAN	C1-O5-C5	4.15	117.82	112.19
4	J	7	FUC	C2-C3-C4	3.73	117.34	110.89
5	L	4	MAN	C1-O5-C5	3.53	116.97	112.19
4	J	7	FUC	C3-C4-C5	3.37	115.02	109.77
3	I	8	FUC	C1-C2-C3	2.95	113.29	109.67
4	J	5	NAG	C2-N2-C7	2.70	126.75	122.90
3	I	4	MAN	C1-O5-C5	2.59	115.71	112.19
3	I	4	MAN	O2-C2-C3	-2.55	105.02	110.14
3	K	6	MAN	O2-C2-C3	-2.43	105.27	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	5	MAN	C1-O5-C5	2.38	115.42	112.19
3	K	4	MAN	O2-C2-C3	-2.38	105.38	110.14
4	J	6	MAN	C1-O5-C5	2.34	115.36	112.19
5	L	5	MAN	O2-C2-C3	-2.25	105.64	110.14
3	K	6	MAN	C1-O5-C5	2.23	115.22	112.19
4	J	6	MAN	O2-C2-C3	-2.20	105.73	110.14
3	K	4	MAN	C1-O5-C5	2.18	115.14	112.19
4	J	4	MAN	O2-C2-C3	-2.17	105.80	110.14
5	L	4	MAN	O2-C2-C3	-2.06	106.00	110.14

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	J	5	NAG	C4-C5-C6-O6
3	I	7	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	J	5	NAG	C1-C2-N2-C7
4	J	4	MAN	O5-C5-C6-O6
3	I	7	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
4	J	5	NAG	C3-C2-N2-C7

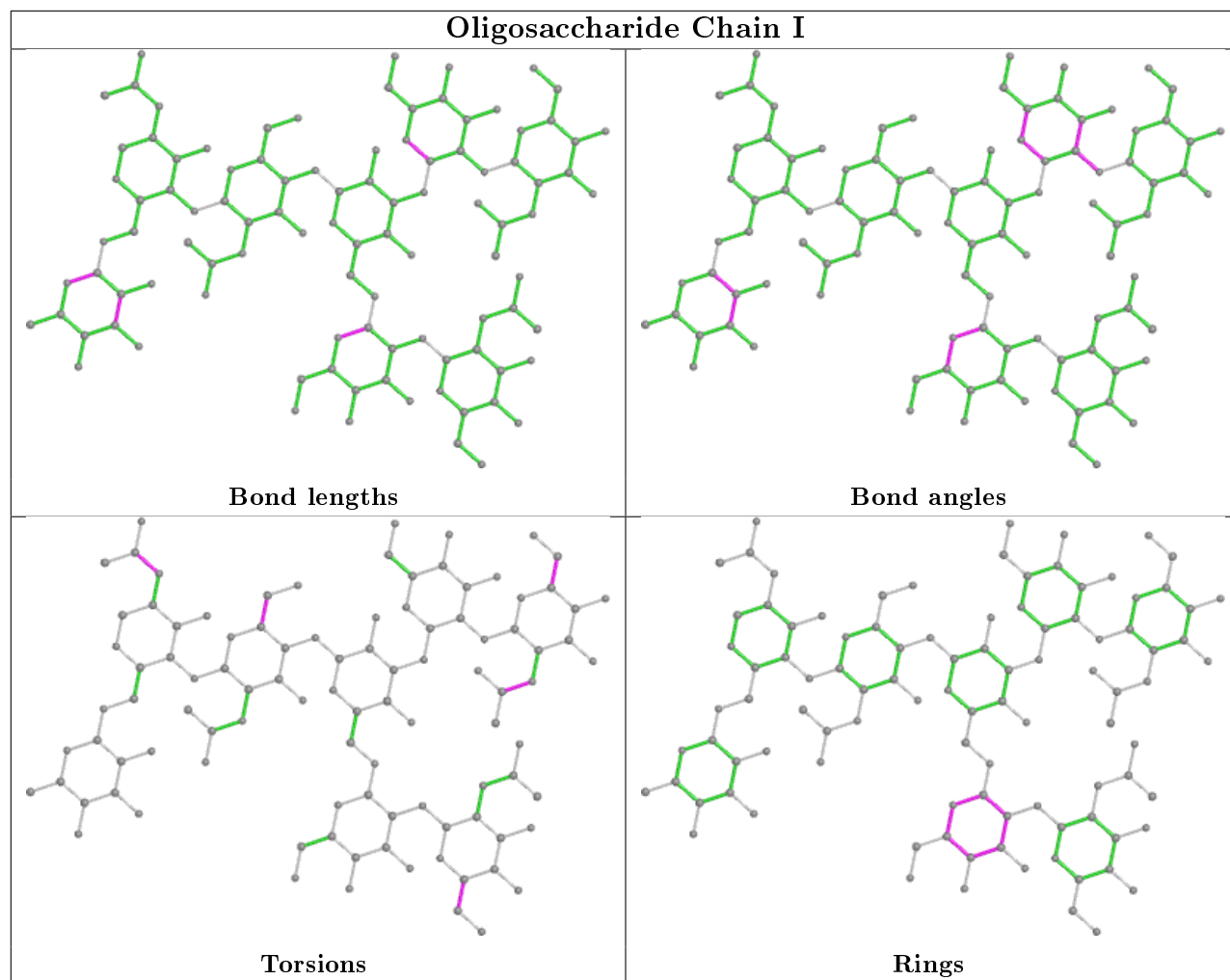
All (2) ring outliers are listed below:

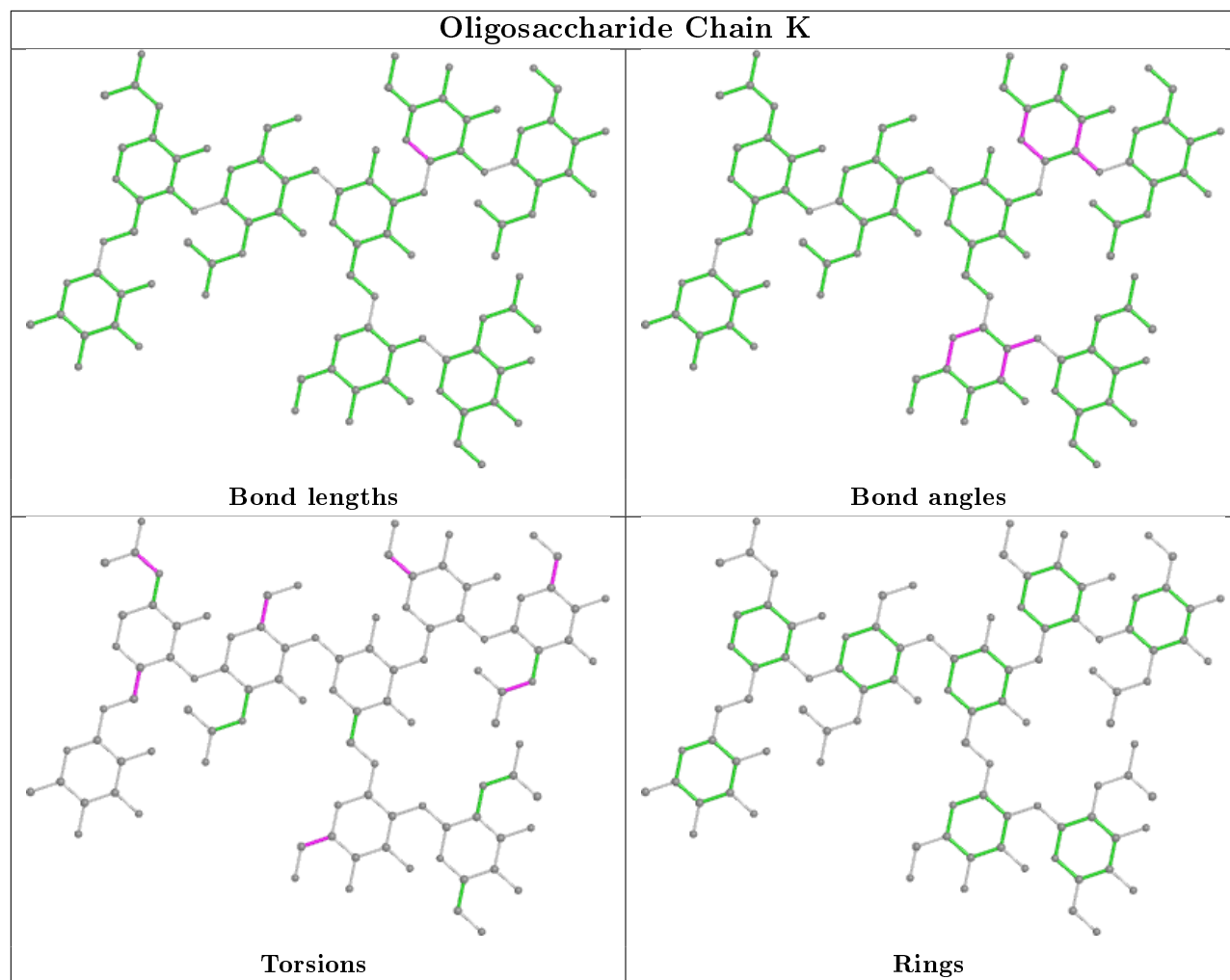
Mol	Chain	Res	Type	Atoms
3	I	6	MAN	C1-C2-C3-C4-C5-O5
5	L	4	MAN	C1-C2-C3-C4-C5-O5

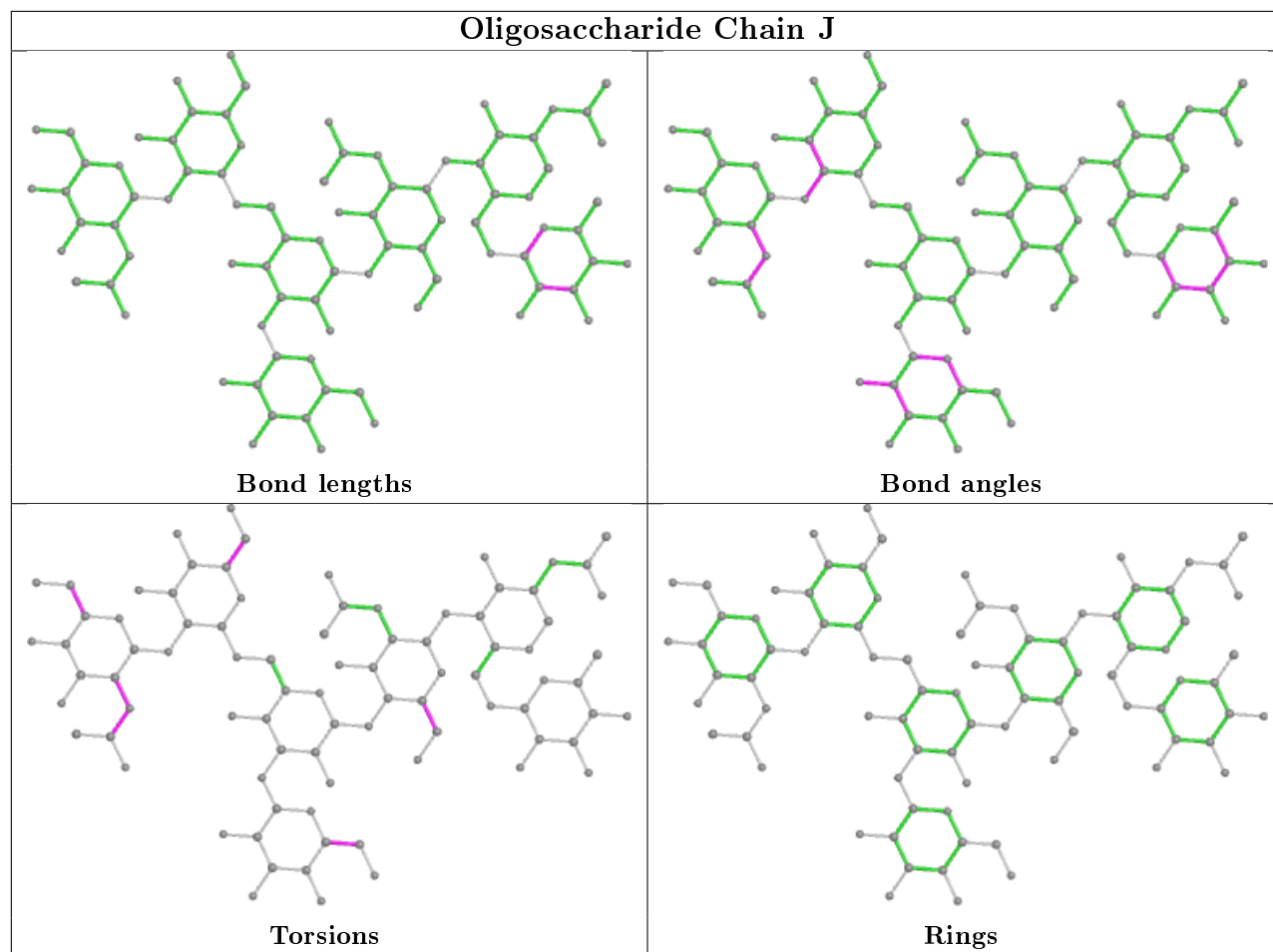
1 monomer is involved in 3 short contacts:

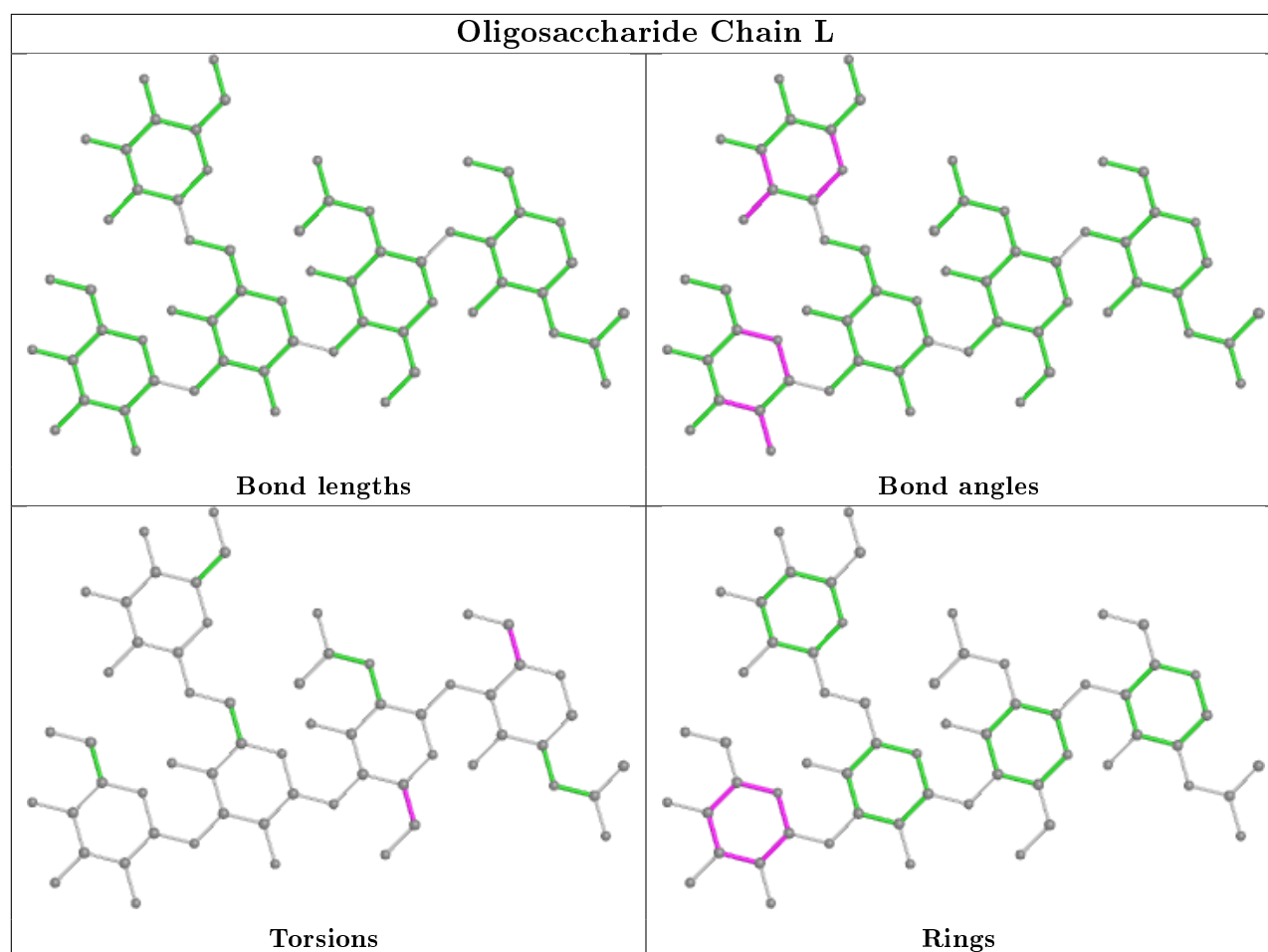
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5	NAG	3	0

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 33 ligands modelled in this entry, 13 are monoatomic - leaving 20 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$
7	GOL	B	1011	-	5,5,5	0.94	0	5,5,5	0.97	0
6	PEG	A	1009	-	6,6,6	0.49	0	5,5,5	0.27	0
7	GOL	A	1011	-	5,5,5	0.90	0	5,5,5	0.98	0
6	PEG	C	1016	-	6,6,6	0.49	0	5,5,5	0.26	0
6	PEG	C	1015	-	6,6,6	0.49	0	5,5,5	0.28	0
7	GOL	D	1008	-	5,5,5	0.88	0	5,5,5	1.01	0
7	GOL	C	1019	-	5,5,5	0.90	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	1012	-	5,5,5	0.93	0	5,5,5	0.91	0
6	PEG	C	1014	-	6,6,6	0.49	0	5,5,5	0.31	0
7	GOL	C	1017	-	5,5,5	0.90	0	5,5,5	1.01	0
6	PEG	A	1010	-	6,6,6	0.48	0	5,5,5	0.29	0
7	GOL	A	1013	-	5,5,5	0.89	0	5,5,5	0.97	0
7	GOL	C	1018	-	5,5,5	0.92	0	5,5,5	0.99	0
7	GOL	B	1013	-	5,5,5	0.94	0	5,5,5	0.96	0
7	GOL	A	1012	-	5,5,5	0.92	0	5,5,5	1.01	0
7	GOL	F	102	-	5,5,5	0.93	0	5,5,5	0.95	0
7	GOL	E	102	-	5,5,5	0.97	0	5,5,5	0.97	0
7	GOL	B	1010	-	5,5,5	0.94	0	5,5,5	0.96	0
7	GOL	D	1009	-	5,5,5	0.92	0	5,5,5	0.99	0
7	GOL	F	103	-	5,5,5	0.95	0	5,5,5	0.89	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
7	GOL	B	1011	-	-	2/4/4/4	-
6	PEG	A	1009	-	-	2/4/4/4	-
7	GOL	A	1011	-	-	0/4/4/4	-
6	PEG	C	1016	-	-	2/4/4/4	-
6	PEG	C	1015	-	-	4/4/4/4	-
7	GOL	D	1008	-	-	0/4/4/4	-
7	GOL	C	1019	-	-	1/4/4/4	-
7	GOL	B	1012	-	-	2/4/4/4	-
6	PEG	C	1014	-	-	2/4/4/4	-
7	GOL	C	1017	-	-	1/4/4/4	-
6	PEG	A	1010	-	-	1/4/4/4	-
7	GOL	A	1013	-	-	0/4/4/4	-
7	GOL	C	1018	-	-	2/4/4/4	-
7	GOL	B	1013	-	-	2/4/4/4	-
7	GOL	A	1012	-	-	0/4/4/4	-
7	GOL	F	102	-	-	1/4/4/4	-
7	GOL	E	102	-	-	1/4/4/4	-
7	GOL	B	1010	-	-	2/4/4/4	-
7	GOL	D	1009	-	-	0/4/4/4	-
7	GOL	F	103	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1011	GOL	C1-C2-C3-O3
7	B	1010	GOL	C1-C2-C3-O3
7	F	103	GOL	C1-C2-C3-O3
7	F	103	GOL	O2-C2-C3-O3
7	B	1013	GOL	C1-C2-C3-O3
6	C	1016	PEG	O2-C3-C4-O4
6	C	1015	PEG	O2-C3-C4-O4
6	A	1010	PEG	O1-C1-C2-O2
7	B	1012	GOL	O1-C1-C2-C3
7	C	1019	GOL	O1-C1-C2-C3
7	B	1011	GOL	O2-C2-C3-O3
7	B	1010	GOL	O2-C2-C3-O3
7	B	1013	GOL	O2-C2-C3-O3
6	C	1015	PEG	O1-C1-C2-O2
6	C	1014	PEG	C1-C2-O2-C3
6	C	1015	PEG	C1-C2-O2-C3
7	C	1018	GOL	O1-C1-C2-O2
6	C	1016	PEG	O1-C1-C2-O2
6	C	1015	PEG	C4-C3-O2-C2
7	F	102	GOL	C1-C2-C3-O3
7	B	1012	GOL	O1-C1-C2-O2
6	A	1009	PEG	C4-C3-O2-C2
7	C	1017	GOL	O1-C1-C2-C3
7	C	1018	GOL	O1-C1-C2-C3
7	E	102	GOL	O2-C2-C3-O3
6	C	1014	PEG	O1-C1-C2-O2
6	A	1009	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1009	PEG	1	0
6	C	1015	PEG	1	0
7	B	1010	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	209/210 (99%)	0.07	1 (0%) 91 91	31, 44, 70, 96	0
1	B	209/210 (99%)	0.43	18 (8%) 10 10	34, 60, 108, 136	0
1	C	208/210 (99%)	0.02	3 (1%) 75 77	38, 57, 78, 113	0
1	D	208/210 (99%)	0.57	19 (9%) 9 9	50, 81, 116, 149	0
2	E	64/69 (92%)	0.04	0 100 100	37, 52, 76, 115	0
2	F	67/69 (97%)	0.29	1 (1%) 73 75	33, 44, 77, 110	0
2	G	65/69 (94%)	0.17	1 (1%) 73 75	59, 82, 107, 117	0
2	H	64/69 (92%)	0.86	10 (15%) 2 1	61, 89, 127, 137	0
All	All	1094/1116 (98%)	0.29	53 (4%) 30 32	31, 60, 108, 149	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	43	GLY	7.9
1	D	264	VAL	5.3
1	B	299	THR	5.2
1	B	296	TYR	5.1
2	H	47	LEU	4.5
1	D	296	TYR	4.3
1	B	293	GLU	4.0
1	D	298	SER	4.0
1	D	293	GLU	3.9
1	D	237	GLY	3.5
2	H	45	GLY	3.5
2	H	39	GLY	3.4
1	B	444	SER	3.4
1	B	298	SER	3.4
2	H	41	THR	3.4
1	B	269	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	330	ALA	3.2
1	B	292	ARG	3.0
2	F	67	ALA	2.9
1	D	292	ARG	2.9
2	H	50	GLU	2.9
1	B	270	ASP	2.8
1	D	241	PHE	2.8
1	B	382	GLU	2.7
1	D	331	PRO	2.7
1	B	264	VAL	2.6
1	D	326	LYS	2.6
1	A	445	PRO	2.5
1	B	266	VAL	2.5
2	H	49	ALA	2.5
2	H	46	TYR	2.5
1	B	272	GLU	2.5
1	D	288	LYS	2.4
1	D	323	VAL	2.4
1	D	287	ALA	2.4
1	D	270	ASP	2.4
1	D	256	THR	2.4
2	H	8	GLU	2.3
1	B	326	LYS	2.3
1	B	443	LEU	2.3
1	B	295	GLN	2.3
1	B	355	ARG	2.2
2	G	47	LEU	2.2
1	D	290	LYS	2.2
1	D	273	VAL	2.2
1	B	241	PHE	2.1
2	H	44	ASN	2.1
1	D	436	TYR	2.1
1	C	269	GLU	2.1
1	D	275	PHE	2.1
1	C	382	GLU	2.1
1	C	444	SER	2.1
1	B	328	LEU	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 ⓘ

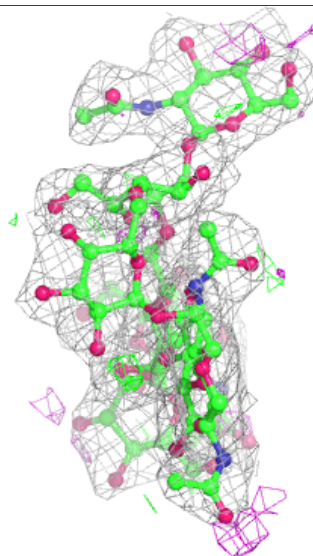
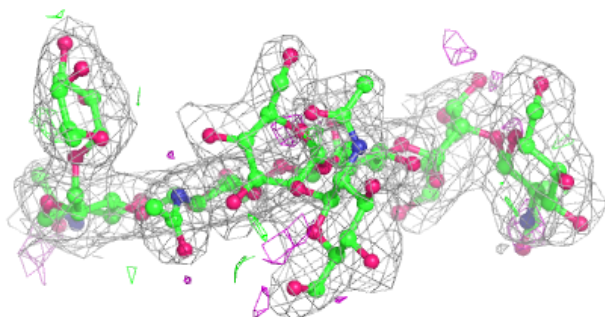
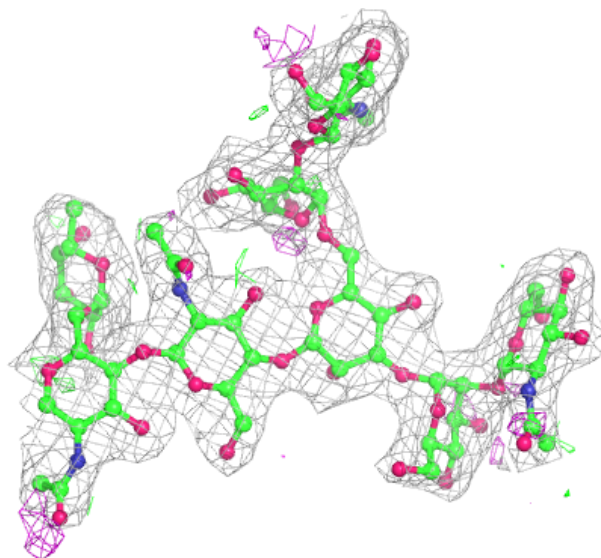
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	L	5	11/12	0.75	0.18	93,94,95,96	0
5	NAG	L	1	14/15	0.77	0.16	67,77,83,84	0
4	NAG	J	5	14/15	0.80	0.29	92,93,94,95	0
3	NAG	K	5	14/15	0.83	0.16	86,87,88,89	0
5	MAN	L	4	11/12	0.84	0.14	95,95,97,97	0
5	NAG	L	2	14/15	0.85	0.22	87,90,92,93	0
3	NAG	I	5	14/15	0.87	0.18	60,62,67,69	0
4	NAG	J	2	14/15	0.88	0.16	79,80,83,84	0
4	BMA	J	3	11/12	0.88	0.13	85,87,87,88	0
4	NAG	J	1	14/15	0.88	0.32	68,77,80,85	0
4	MAN	J	6	11/12	0.89	0.14	90,92,93,94	0
3	NAG	K	7	14/15	0.89	0.16	66,69,71,71	0
3	MAN	K	6	11/12	0.90	0.15	63,65,67,69	0
4	FUC	J	7	10/11	0.91	0.37	85,86,87,89	0
3	NAG	K	1	14/15	0.92	0.11	42,52,58,63	0
3	MAN	K	4	11/12	0.92	0.12	72,74,78,84	0
4	MAN	J	4	11/12	0.92	0.19	87,87,89,91	0
5	BMA	L	3	11/12	0.93	0.12	91,91,91,92	0
3	FUC	I	8	10/11	0.93	0.13	48,49,51,52	0
3	MAN	I	6	11/12	0.94	0.15	41,42,48,49	0
3	BMA	K	3	11/12	0.94	0.13	58,61,63,65	0
3	FUC	K	8	10/11	0.94	0.13	61,62,63,63	0
3	NAG	I	7	14/15	0.95	0.15	37,41,45,46	0
3	MAN	I	4	11/12	0.96	0.16	51,55,58,60	0
3	NAG	K	2	14/15	0.96	0.13	52,53,56,56	0
3	NAG	I	2	14/15	0.97	0.15	40,42,45,45	0
3	NAG	I	1	14/15	0.97	0.12	34,41,46,48	0
3	BMA	I	3	11/12	0.97	0.16	40,41,43,47	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.

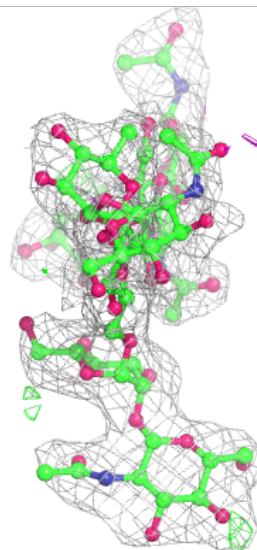
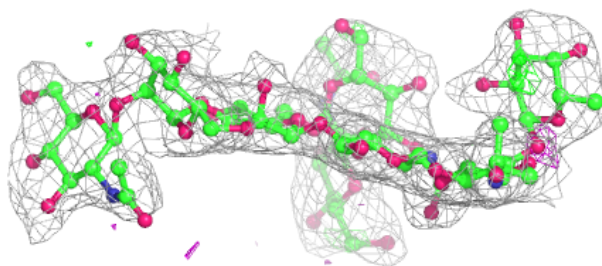
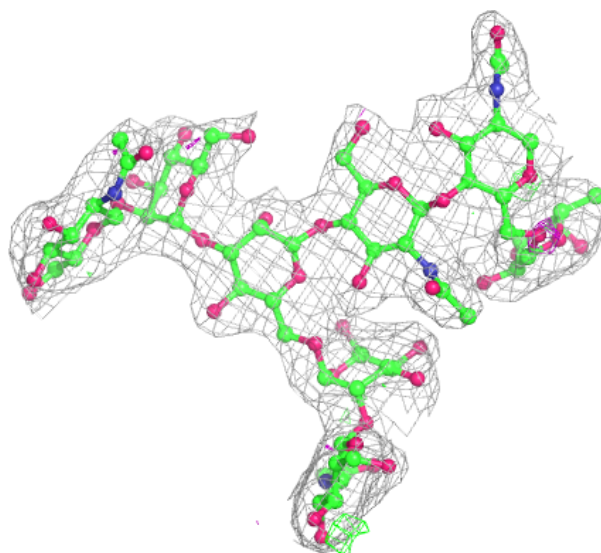
Electron density around Chain I:

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



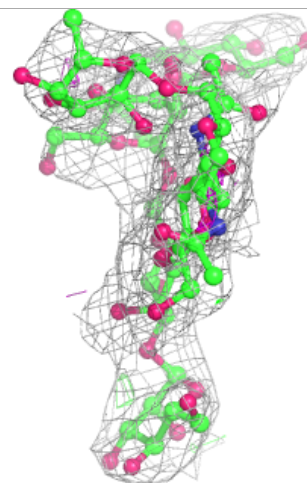
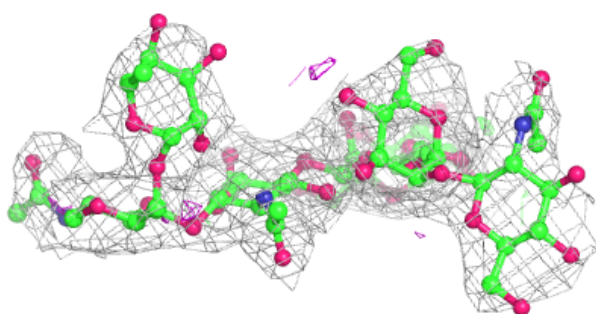
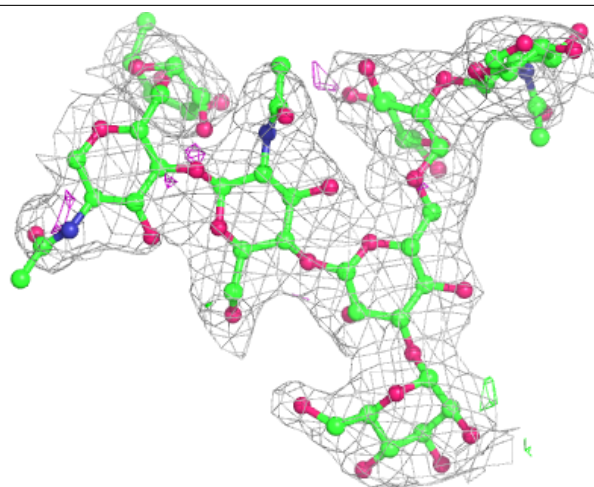
Electron density around Chain K:

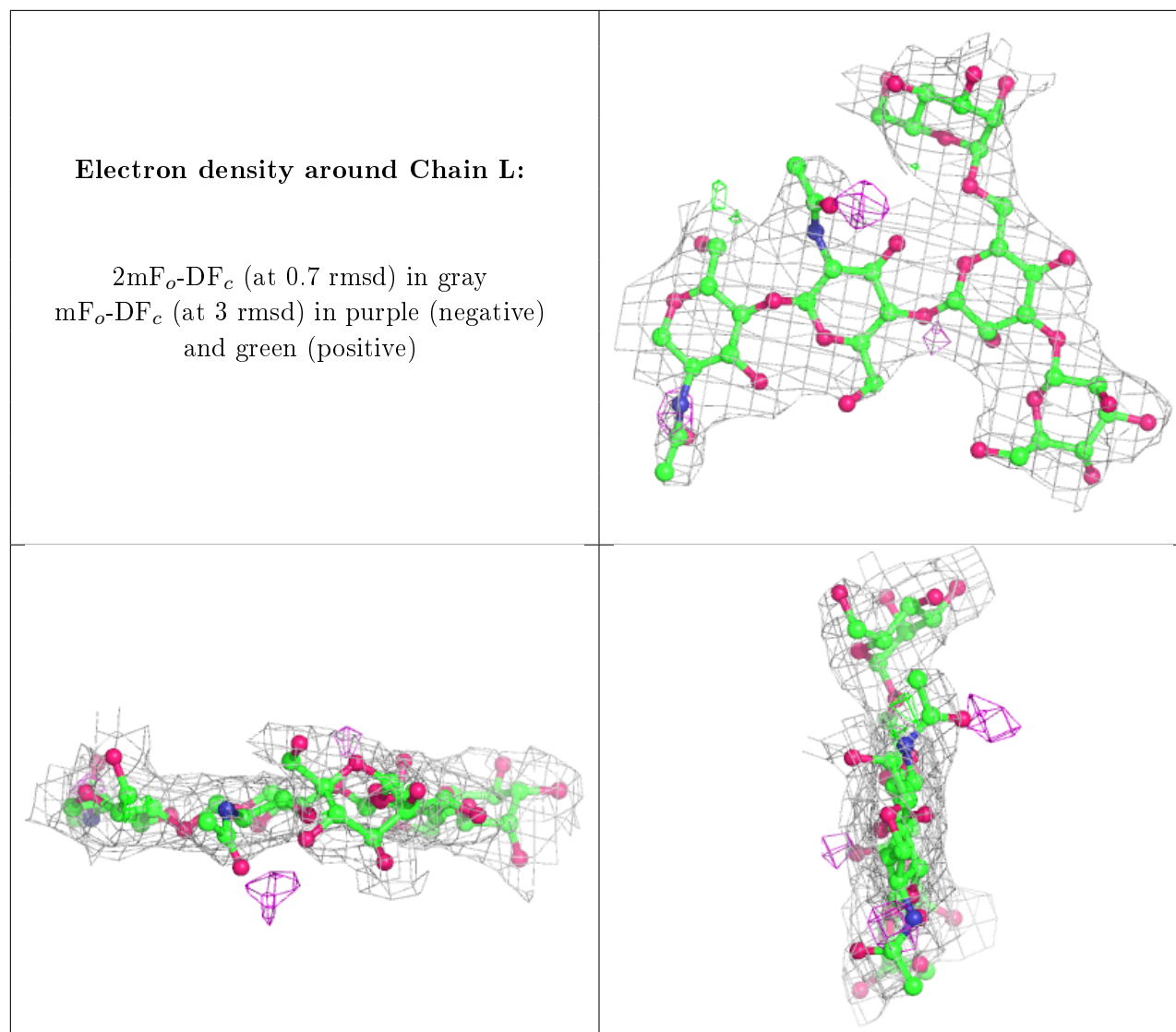
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands ⓘ

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
8	CA	H	101	1/1	0.12	0.07	143,143,143,143	0
6	PEG	C	1015	7/7	0.69	0.23	81,81,82,82	0
7	GOL	C	1019	6/6	0.71	0.27	91,92,92,92	0
6	PEG	C	1016	7/7	0.72	0.32	81,82,84,84	0
7	GOL	B	1011	6/6	0.72	0.35	86,87,87,87	0
7	GOL	B	1012	6/6	0.73	0.28	80,81,82,83	0
7	GOL	F	103	6/6	0.75	0.31	78,78,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	F	102	6/6	0.76	0.30	80,81,83,83	0
7	GOL	A	1013	6/6	0.76	0.18	89,90,90,90	0
9	CL	D	1006	1/1	0.76	0.12	84,84,84,84	0
7	GOL	E	102	6/6	0.79	0.29	79,82,83,83	0
7	GOL	A	1012	6/6	0.79	0.31	83,84,85,85	0
7	GOL	D	1009	6/6	0.80	0.51	105,106,106,106	0
9	CL	B	1008	1/1	0.81	0.10	72,72,72,72	0
9	CL	D	1007	1/1	0.84	0.19	81,81,81,81	0
9	CL	B	1009	1/1	0.84	0.08	84,84,84,84	0
7	GOL	B	1013	6/6	0.84	0.25	93,94,95,95	0
6	PEG	C	1014	7/7	0.84	0.18	70,72,74,74	0
7	GOL	B	1010	6/6	0.85	0.21	82,83,84,84	0
9	CL	C	1013	1/1	0.85	0.11	83,83,83,83	0
7	GOL	C	1018	6/6	0.86	0.16	94,94,95,95	0
6	PEG	A	1009	7/7	0.86	0.19	61,61,63,64	0
7	GOL	C	1017	6/6	0.86	0.41	93,93,94,95	0
7	GOL	D	1008	6/6	0.88	0.14	74,75,76,77	0
8	CA	G	101	1/1	0.89	0.05	80,80,80,80	0
7	GOL	A	1011	6/6	0.90	0.17	64,68,69,70	0
6	PEG	A	1010	7/7	0.91	0.19	70,70,73,73	0
9	CL	C	1010	1/1	0.92	0.08	74,74,74,74	0
9	CL	C	1011	1/1	0.93	0.14	75,75,75,75	0
9	CL	C	1009	1/1	0.93	0.09	66,66,66,66	0
9	CL	C	1012	1/1	0.95	0.16	72,72,72,72	0
8	CA	F	101	1/1	0.98	0.14	40,40,40,40	0
8	CA	E	101	1/1	0.99	0.11	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.