



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 8BET / pdb_00008bet
Title : Structure of D188A-fructofuranosidase from *Rhodotorula dairenensis* in complex with sucrose
Authors : Jimenez-Ortega, E.; Sanz-Aparicio, J.
Deposited on : 2022-10-21
Resolution : 2.38 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

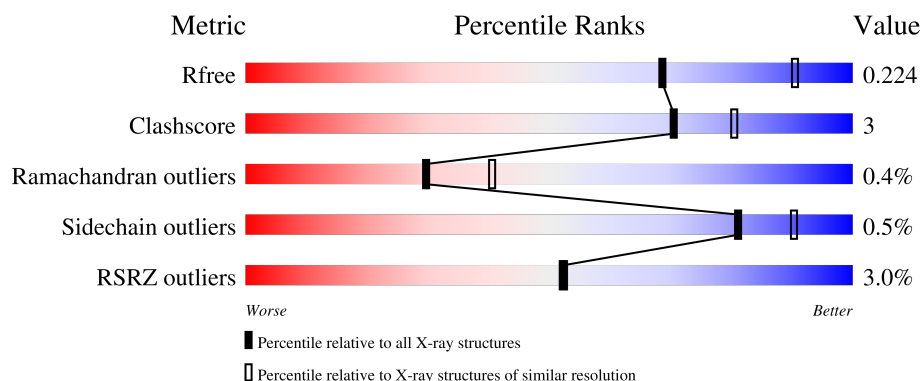
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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.



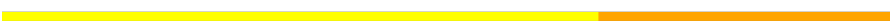
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	675	0% 73% •• 22%
1	B	675	0% 71% 7% 22%
1	C	675	2% 73% 5% 22%
1	D	675	5% 72% 5% 22%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	K	2	 100%
3	F	3	 100%
3	I	3	 67%33%
3	J	3	 33%67%
4	G	6	 33%67%
5	L	2	 100%
5	M	2	 100%
5	N	2	 50%50%
5	O	2	 50%50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17723 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 Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4032	2569	656	796	11			
1	B	526	Total	C	N	O	S	0	0	0
			4038	2572	657	798	11			
1	C	528	Total	C	N	O	S	0	0	0
			4050	2578	659	802	11			
1	D	524	Total	C	N	O	S	0	0	0
			4026	2566	655	794	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
B	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
C	188	ALA	ASP	engineered mutation	UNP A0A856TAI5
D	188	ALA	ASP	engineered mutation	UNP A0A856TAI5

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



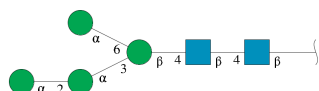
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



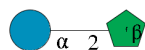
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



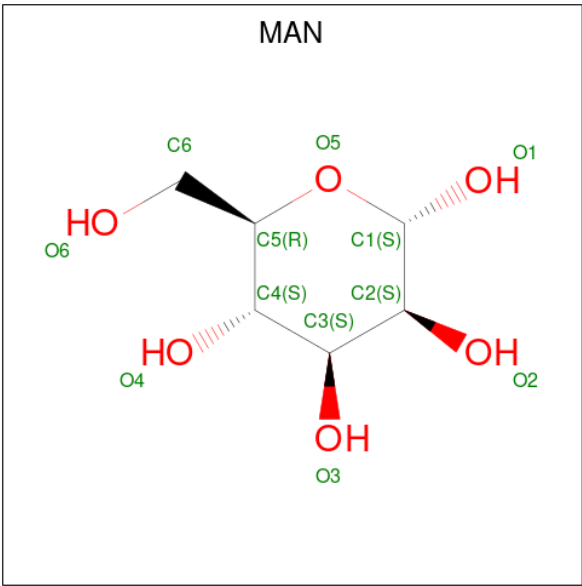
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	L	2	Total	C	O	0	0	0
			23	12	11			
5	M	2	Total	C	O	0	0	0
			23	12	11			
5	N	2	Total	C	O	0	0	0
			23	12	11			
5	O	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		
6	D	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	200	Total O 200 200	0	0
8	B	176	Total O 176 176	0	0
8	C	166	Total O 166 166	0	0

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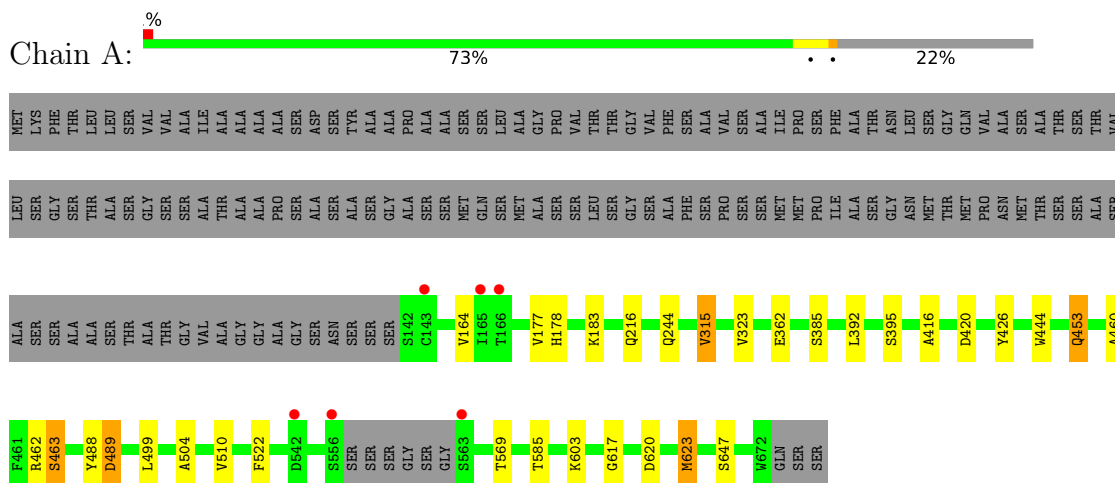
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	152	Total 152	O 152	0	0

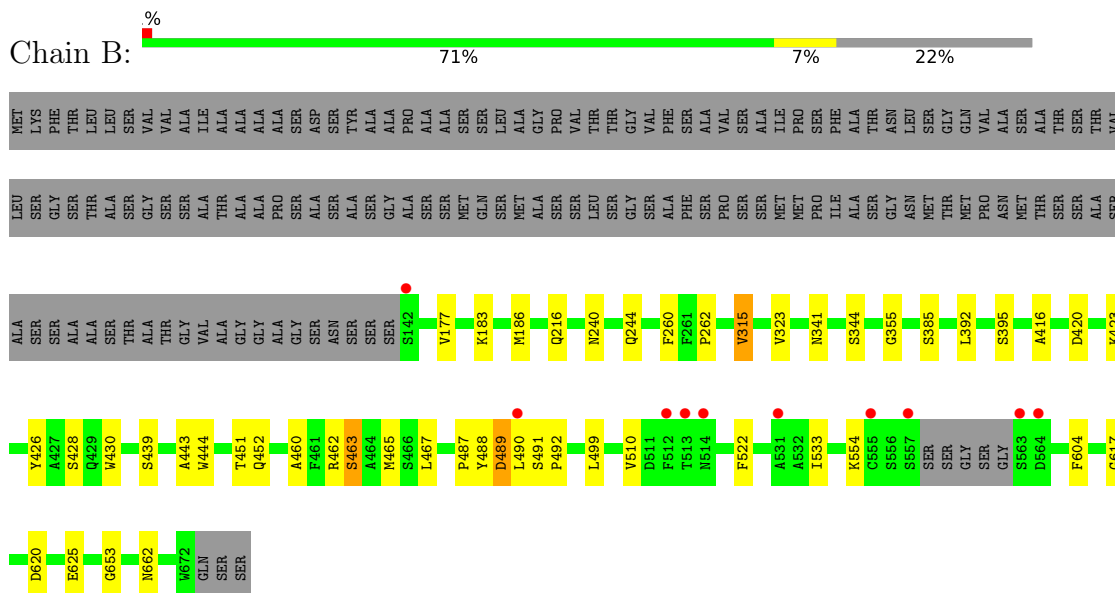
3 Residue-property plots

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.

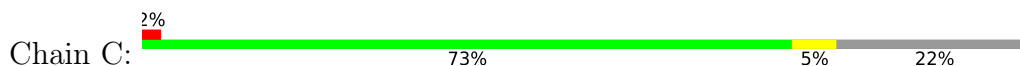
- Molecule 1: Beta-fructofuranosidase

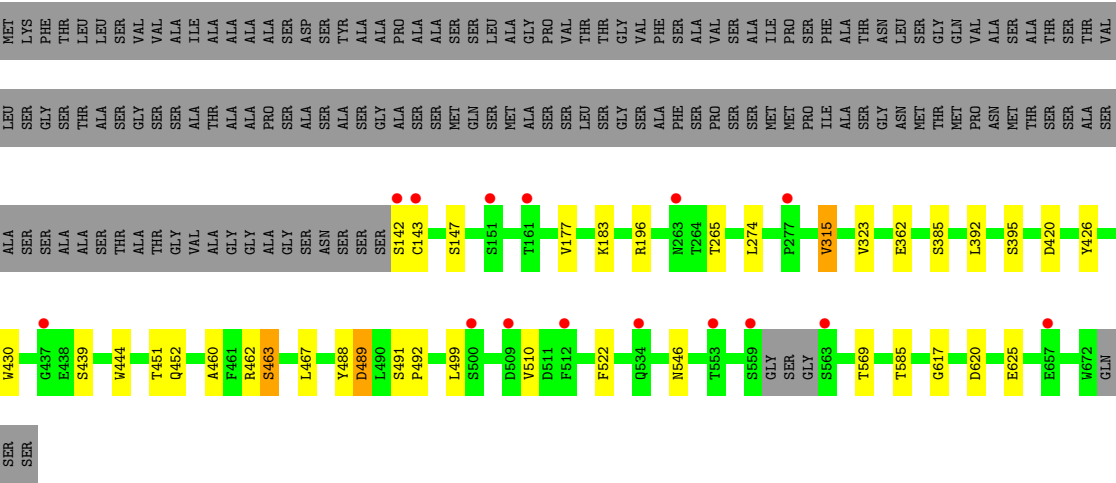


- Molecule 1: Beta-fructofuranosidase

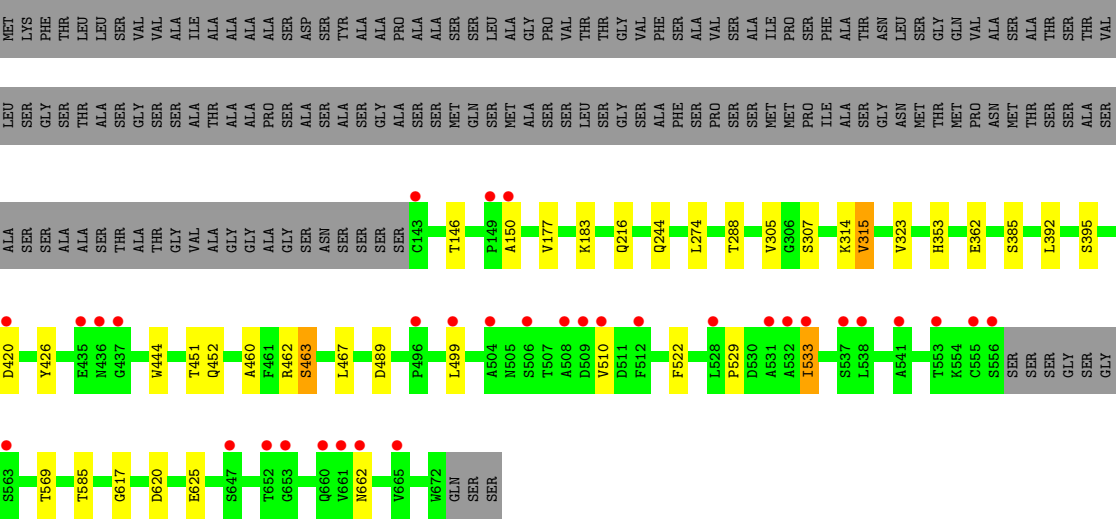


- Molecule 1: Beta-fructofuranosidase

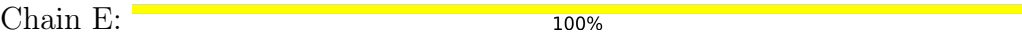




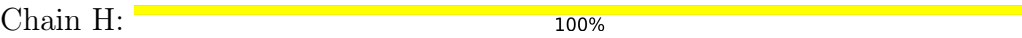
● Molecule 1: Beta-fructofuranosidase



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



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



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

Chain K:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2
BMA3

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

Chain I:  67% 33%

NAG1
NAG2
BMA3

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

Chain J:  33% 67%

NAG1
NAG2
BMA3

- Molecule 4: alpha-D-mannopyranose-(1-2)-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 G:  33% 67%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:  100%

GLC1
FRU2

- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:  100%

GLC1
FRU2

- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:  50% 50%

GLC1
FRU2

- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:  50% 50%

GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.34Å 112.81Å 139.08Å 90.00° 104.74° 90.00°	Depositor
Resolution (Å)	45.69 – 2.38 45.69 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.69-2.38) 99.8 (45.69-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.222 0.186 , 0.224	Depositor DCC
R_{free} test set	4728 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17723	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, FRU, GLC, NAG

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	0.99	0/4160	1.18	2/5721 (0.0%)
1	B	0.99	0/4166	1.18	3/5729 (0.1%)
1	C	1.00	0/4178	1.18	1/5745 (0.0%)
1	D	0.98	1/4154 (0.0%)	1.18	1/5713 (0.0%)
All	All	0.99	1/16658 (0.0%)	1.18	7/22908 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	353	HIS	CE1-NE2	5.03	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ASN	CA-CB-CG	5.70	118.30	112.60
1	B	420	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	420	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	420	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	653	GLY	CA-C-O	-5.13	116.45	121.06
1	A	623	MET	O-C-N	-5.08	117.18	123.33
1	D	420	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4032	0	3751	23	0
1	B	4038	0	3757	33	0
1	C	4050	0	3765	27	0
1	D	4026	0	3747	27	0
2	E	28	0	25	0	0
2	H	28	0	25	0	0
2	K	28	0	25	0	0
3	F	39	0	34	0	0
3	I	39	0	34	2	0
3	J	39	0	34	0	0
4	G	72	0	61	0	0
5	L	23	0	21	1	0
5	M	23	0	21	0	0
5	N	23	0	21	1	0
5	O	23	0	21	1	0
6	A	44	0	40	0	0
6	B	33	0	30	0	0
6	C	44	0	40	2	0
6	D	33	0	30	2	0
7	A	98	0	91	2	0
7	B	98	0	91	3	0
7	C	84	0	78	1	0
7	D	84	0	78	4	0
8	A	200	0	0	5	0
8	B	176	0	0	0	0
8	C	166	0	0	0	0
8	D	152	0	0	1	0
All	All	17723	0	15820	110	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 (110) 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:487:PRO:HB2	1:B:490:LEU:HD11	1.14	1.12
1:B:487:PRO:HB2	1:B:490:LEU:CD1	1.96	0.95
1:C:467:LEU:HD12	1:C:625:GLU:OE1	1.80	0.80
1:B:467:LEU:HD12	1:B:625:GLU:OE1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:LEU:HD12	1:D:625:GLU:OE1	1.81	0.79
1:D:467:LEU:CD1	1:D:625:GLU:OE1	2.34	0.76
1:C:467:LEU:CD1	1:C:625:GLU:OE1	2.34	0.75
1:B:467:LEU:CD1	1:B:625:GLU:OE1	2.34	0.75
1:C:467:LEU:CG	1:C:625:GLU:OE1	2.36	0.74
1:B:487:PRO:CB	1:B:490:LEU:HD11	2.06	0.73
1:D:467:LEU:CG	1:D:625:GLU:OE1	2.37	0.73
1:B:467:LEU:CG	1:B:625:GLU:OE1	2.37	0.73
1:B:467:LEU:HG	1:B:625:GLU:OE1	1.89	0.72
1:D:467:LEU:HG	1:D:625:GLU:OE1	1.89	0.72
1:C:467:LEU:HG	1:C:625:GLU:OE1	1.89	0.71
1:D:146:THR:HG21	6:D:701:MAN:H5	1.72	0.70
1:D:662:ASN:ND2	7:D:709:NAG:O7	2.27	0.67
1:A:504:ALA:HB3	7:A:709:NAG:H82	1.79	0.64
1:B:488:TYR:O	1:B:490:LEU:HD12	1.98	0.64
1:A:395:SER:HB2	1:A:426:TYR:CD1	2.34	0.62
1:D:395:SER:HB2	1:D:426:TYR:CD1	2.35	0.62
1:C:395:SER:HB2	1:C:426:TYR:CD1	2.34	0.62
1:B:395:SER:HB2	1:B:426:TYR:CD1	2.35	0.61
1:C:392:LEU:HD23	1:D:392:LEU:HD23	1.83	0.59
1:A:392:LEU:HD23	1:B:392:LEU:HD23	1.85	0.59
1:A:569:THR:OG1	1:A:585:THR:HB	2.03	0.59
1:B:522:PHE:CZ	1:B:617:GLY:HA3	2.39	0.58
1:A:164:VAL:HG23	6:C:704:MAN:O2	2.05	0.57
1:D:314:LYS:HG3	8:D:880:HOH:O	2.04	0.56
1:D:385:SER:HB3	1:D:426:TYR:CE1	2.41	0.55
1:D:150:ALA:HA	6:D:702:MAN:H3	1.89	0.55
1:D:362:GLU:OE1	5:O:1:GLC:H3	2.06	0.55
1:C:385:SER:HB3	1:C:426:TYR:CE1	2.43	0.54
1:D:274:LEU:HD21	7:D:704:NAG:H62	1.89	0.54
1:C:183:LYS:HA	1:C:460:ALA:O	2.08	0.54
1:A:183:LYS:HA	1:A:460:ALA:O	2.08	0.54
1:D:183:LYS:HA	1:D:460:ALA:O	2.09	0.53
1:C:462:ARG:O	1:C:463:SER:HB2	2.08	0.53
1:B:385:SER:HB3	1:B:426:TYR:CE1	2.43	0.53
1:B:662:ASN:ND2	7:B:710:NAG:O7	2.39	0.53
1:B:183:LYS:HA	1:B:460:ALA:O	2.08	0.53
1:C:274:LEU:HD21	7:C:705:NAG:H62	1.91	0.53
1:D:444:TRP:HE1	1:D:463:SER:HB3	1.74	0.53
7:D:705:NAG:H3	7:D:705:NAG:H83	1.91	0.53
1:B:462:ARG:O	1:B:463:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:SER:HB3	1:A:426:TYR:CE1	2.45	0.52
1:D:462:ARG:O	1:D:463:SER:HB2	2.10	0.51
1:D:569:THR:OG1	1:D:585:THR:HB	2.11	0.51
1:A:178:HIS:CD2	1:A:623:MET:HE1	2.46	0.51
1:A:499:LEU:HD22	1:A:510:VAL:HG22	1.92	0.51
1:C:430:TRP:CD1	1:C:439:SER:HG	2.29	0.51
1:A:585:THR:HG21	8:A:985:HOH:O	2.11	0.51
1:B:344:SER:CB	7:B:706:NAG:H5	2.41	0.51
1:B:499:LEU:HD22	1:B:510:VAL:HG22	1.93	0.50
1:D:288:THR:HB	7:D:705:NAG:H81	1.92	0.50
1:A:522:PHE:CE2	1:A:617:GLY:HA3	2.47	0.50
1:A:647:SER:HB3	8:A:852:HOH:O	2.12	0.49
1:C:522:PHE:CE2	1:C:617:GLY:HA3	2.48	0.49
1:B:430:TRP:CD1	1:B:439:SER:HG	2.31	0.48
1:B:491:SER:OG	1:B:492:PRO:HD3	2.13	0.47
1:B:522:PHE:CE2	1:B:617:GLY:HA3	2.50	0.47
1:B:177:VAL:HG22	1:B:620:ASP:OD2	2.15	0.47
1:C:569:THR:OG1	1:C:585:THR:HB	2.14	0.47
1:D:499:LEU:HD13	1:D:510:VAL:HG22	1.97	0.47
1:A:444:TRP:HE1	1:A:463:SER:HB3	1.80	0.46
1:C:315:VAL:HA	1:C:323:VAL:O	2.16	0.46
1:D:522:PHE:CE2	1:D:617:GLY:HA3	2.50	0.46
1:A:416:ALA:O	8:A:801:HOH:O	2.21	0.46
1:B:341:ASN:HD22	7:B:706:NAG:H83	1.81	0.46
1:D:315:VAL:HA	1:D:323:VAL:O	2.17	0.45
1:C:444:TRP:HE1	1:C:463:SER:HB3	1.81	0.45
1:D:305:VAL:HG23	1:D:307:SER:HB3	1.98	0.45
1:D:177:VAL:HG22	1:D:620:ASP:OD2	2.17	0.45
1:D:522:PHE:CZ	1:D:617:GLY:HA3	2.52	0.45
1:A:462:ARG:O	1:A:463:SER:HB2	2.17	0.44
1:C:177:VAL:HG22	1:C:620:ASP:OD2	2.17	0.44
1:B:315:VAL:HA	1:B:323:VAL:O	2.16	0.44
1:C:499:LEU:HD22	1:C:510:VAL:HG22	1.99	0.44
1:A:522:PHE:CZ	1:A:617:GLY:HA3	2.53	0.44
1:C:147:SER:HB3	6:C:701:MAN:H2	1.98	0.44
1:A:315:VAL:HA	1:A:323:VAL:O	2.17	0.43
1:C:522:PHE:CZ	1:C:617:GLY:HA3	2.53	0.43
1:A:362:GLU:OE1	5:L:1:GLC:H3	2.18	0.43
1:B:428:SER:OG	1:B:443:ALA:HB2	2.18	0.43
1:C:546:ASN:HD22	3:I:1:NAG:C7	2.31	0.43
1:C:546:ASN:ND2	3:I:1:NAG:C7	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLU:OE1	5:N:1:GLC:H3	2.17	0.43
1:A:453:GLN:HG3	8:A:989:HOH:O	2.19	0.43
1:B:488:TYR:O	1:B:489:ASP:C	2.61	0.43
1:D:529:PRO:O	1:D:533:ILE:HG13	2.19	0.43
1:A:177:VAL:HG22	1:A:620:ASP:OD2	2.18	0.42
1:D:216:GLN:HB2	1:D:244:GLN:HB3	2.00	0.42
1:C:491:SER:N	1:C:492:PRO:CD	2.82	0.42
1:C:451:THR:HG23	1:C:452:GLN:HG3	2.01	0.42
1:D:451:THR:HG23	1:D:452:GLN:HG3	2.01	0.42
1:B:216:GLN:HB2	1:B:244:GLN:HB3	2.02	0.42
1:C:488:TYR:O	1:C:489:ASP:C	2.63	0.41
1:A:488:TYR:O	1:A:489:ASP:C	2.62	0.41
1:B:451:THR:HG23	1:B:452:GLN:HG3	2.03	0.41
1:B:260:PHE:C	1:B:262:PRO:HD3	2.46	0.41
1:B:423:LYS:HG3	1:B:604:PHE:HE1	1.86	0.41
1:B:385:SER:HB3	1:B:426:TYR:CZ	2.56	0.41
1:B:444:TRP:HE1	1:B:463:SER:HB3	1.85	0.41
1:A:216:GLN:HB2	1:A:244:GLN:HB3	2.03	0.40
1:B:355:GLY:HA2	1:B:416:ALA:HB2	2.03	0.40
1:A:585:THR:HG23	1:A:603:LYS:HG3	2.04	0.40
7:A:706:NAG:H62	8:A:992:HOH:O	2.20	0.40
1:C:142:SER:HB2	1:C:143:CYS:H	1.72	0.40
1:B:186:MET:SD	1:B:465:MET:HE2	2.61	0.40
1:C:196:ARG:NH2	1:C:265:THR:OG1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	521/675 (77%)	501 (96%)	18 (4%)	2 (0%)	30 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	522/675 (77%)	501 (96%)	19 (4%)	2 (0%)	30	40
1	C	524/675 (78%)	502 (96%)	20 (4%)	2 (0%)	30	40
1	D	520/675 (77%)	503 (97%)	15 (3%)	2 (0%)	30	40
All	All	2087/2700 (77%)	2007 (96%)	72 (3%)	8 (0%)	30	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	SER
1	C	463	SER
1	A	463	SER
1	A	489	ASP
1	B	489	ASP
1	C	489	ASP
1	D	463	SER
1	D	489	ASP

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	441/545 (81%)	439 (100%)	2 (0%)	81	90
1	B	442/545 (81%)	439 (99%)	3 (1%)	76	87
1	C	444/545 (82%)	443 (100%)	1 (0%)	87	94
1	D	440/545 (81%)	438 (100%)	2 (0%)	81	90
All	All	1767/2180 (81%)	1759 (100%)	8 (0%)	81	90

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

Mol	Chain	Res	Type
1	A	315	VAL
1	A	453	GLN
1	B	315	VAL

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Mol	Chain	Res	Type
1	B	533	ILE
1	B	554	LYS
1	C	315	VAL
1	D	315	VAL
1	D	533	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	664	GLN
1	A	666	ASN
1	B	354	HIS
1	B	664	GLN
1	B	666	ASN
1	C	387	ASN
1	C	425	ASN
1	D	255	ASN
1	D	354	HIS
1	D	471	ASN
1	D	664	GLN
1	D	666	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](#)

29 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	E	1	1,2	14,14,15	0.79	0	17,19,21	0.94	1 (5%)
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	1.20	2 (11%)
3	NAG	F	1	3,1	14,14,15	0.65	0	17,19,21	1.12	1 (5%)
3	NAG	F	2	3	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
3	BMA	F	3	3	11,11,12	0.70	0	15,15,17	1.03	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
4	NAG	G	2	4	14,14,15	0.36	0	17,19,21	0.92	0
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
4	MAN	G	4	4	11,11,12	0.50	0	15,15,17	0.98	1 (6%)
4	MAN	G	5	4	11,11,12	0.57	0	15,15,17	0.98	0
4	MAN	G	6	4	11,11,12	0.83	0	15,15,17	1.36	2 (13%)
2	NAG	H	1	1,2	14,14,15	0.76	0	17,19,21	1.07	2 (11%)
2	NAG	H	2	2	14,14,15	0.79	0	17,19,21	1.41	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
3	NAG	I	2	3	14,14,15	0.55	0	17,19,21	1.30	2 (11%)
3	BMA	I	3	3	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.48	0	17,19,21	1.29	2 (11%)
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
3	BMA	J	3	3	11,11,12	0.64	0	15,15,17	0.82	0
2	NAG	K	1	1,2	14,14,15	0.57	0	17,19,21	1.23	1 (5%)
2	NAG	K	2	2	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
5	GLC	L	1	5	11,11,12	0.70	0	15,15,17	0.95	0
5	FRU	L	2	5	11,12,12	0.53	0	10,18,18	0.85	1 (10%)
5	GLC	M	1	5	11,11,12	0.66	0	15,15,17	1.41	2 (13%)
5	FRU	M	2	5	11,12,12	0.77	1 (9%)	10,18,18	0.74	0
5	GLC	N	1	5	11,11,12	0.77	0	15,15,17	0.89	1 (6%)
5	FRU	N	2	5	11,12,12	0.73	0	10,18,18	0.73	0
5	GLC	O	1	5	11,11,12	0.53	0	15,15,17	1.77	5 (33%)
5	FRU	O	2	5	11,12,12	0.58	0	10,18,18	0.95	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
5	GLC	L	1	5	-	0/2/19/22	0/1/1/1
5	FRU	L	2	5	-	2/5/24/24	0/1/1/1
5	GLC	M	1	5	-	2/2/19/22	0/1/1/1
5	FRU	M	2	5	-	3/5/24/24	0/1/1/1
5	GLC	N	1	5	-	0/2/19/22	0/1/1/1
5	FRU	N	2	5	-	3/5/24/24	0/1/1/1
5	GLC	O	1	5	-	2/2/19/22	0/1/1/1
5	FRU	O	2	5	-	1/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	2	FRU	O5-C2	-2.14	1.40	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C1-O5-C5	4.38	118.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	GLC	O3-C3-C4	-3.42	102.32	110.38
3	J	1	NAG	O5-C1-C2	-3.41	106.01	111.29
2	K	2	NAG	C1-O5-C5	3.30	116.61	112.19
3	I	2	NAG	C1-O5-C5	3.18	116.44	112.19
2	K	1	NAG	C1-O5-C5	3.11	116.35	112.19
3	F	3	BMA	C1-O5-C5	2.97	116.17	112.19
5	O	1	GLC	O3-C3-C2	2.86	115.90	110.05
5	O	1	GLC	C1-O5-C5	2.72	115.83	112.19
2	E	2	NAG	C1-O5-C5	2.70	115.80	112.19
3	I	1	NAG	C1-C2-N2	-2.66	106.24	110.43
5	O	1	GLC	C6-C5-C4	-2.53	106.80	113.02
3	I	2	NAG	C3-C4-C5	2.53	114.82	110.23
5	M	1	GLC	C1-O5-C5	-2.49	108.85	112.19
2	E	1	NAG	O5-C1-C2	-2.45	107.50	111.29
3	F	1	NAG	O4-C4-C3	-2.40	104.73	110.38
3	F	2	NAG	C4-C3-C2	2.39	114.53	111.02
2	E	2	NAG	O4-C4-C5	2.38	115.18	109.32
5	N	1	GLC	C1-O5-C5	-2.30	109.11	112.19
3	J	1	NAG	C1-O5-C5	2.27	115.22	112.19
2	H	1	NAG	C1-C2-N2	-2.26	106.87	110.43
4	G	3	BMA	C3-C4-C5	2.20	114.22	110.23
5	O	1	GLC	O5-C5-C6	2.18	111.92	107.66
3	J	2	NAG	C1-O5-C5	-2.17	109.27	112.19
4	G	4	MAN	C2-C3-C4	-2.11	107.15	110.86
5	L	2	FRU	O1-C1-C2	-2.10	107.03	111.67
2	H	1	NAG	C1-O5-C5	-2.07	109.41	112.19
4	G	6	MAN	C1-C2-C3	-2.06	106.65	109.64
5	M	1	GLC	O5-C5-C6	2.05	111.65	107.66
3	I	3	BMA	C3-C4-C5	2.04	113.94	110.23
4	G	6	MAN	C1-O5-C5	-2.03	109.46	112.19
4	G	1	NAG	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	2	FRU	O1-C1-C2-O2
5	M	2	FRU	O1-C1-C2-C3
5	M	2	FRU	O1-C1-C2-O2
5	M	2	FRU	O1-C1-C2-O5
5	N	2	FRU	O1-C1-C2-O2
5	N	2	FRU	O1-C1-C2-O5

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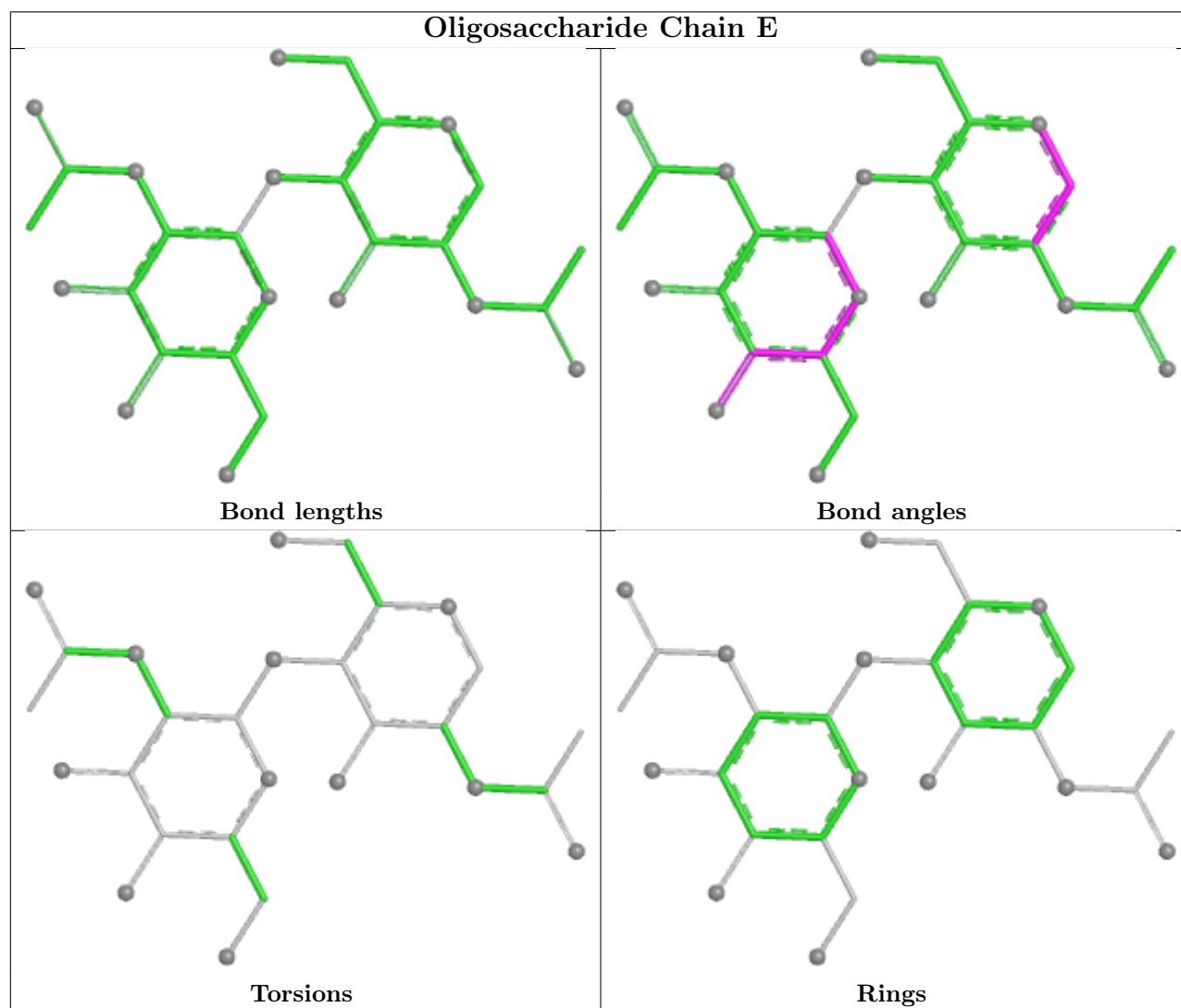
Mol	Chain	Res	Type	Atoms
5	O	1	GLC	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
5	O	1	GLC	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
5	M	1	GLC	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
5	M	1	GLC	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
5	N	2	FRU	O1-C1-C2-C3
4	G	5	MAN	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
4	G	4	MAN	O5-C5-C6-O6
5	O	2	FRU	O1-C1-C2-C3
4	G	2	NAG	C4-C5-C6-O6
5	L	2	FRU	O1-C1-C2-O5
4	G	2	NAG	O5-C5-C6-O6

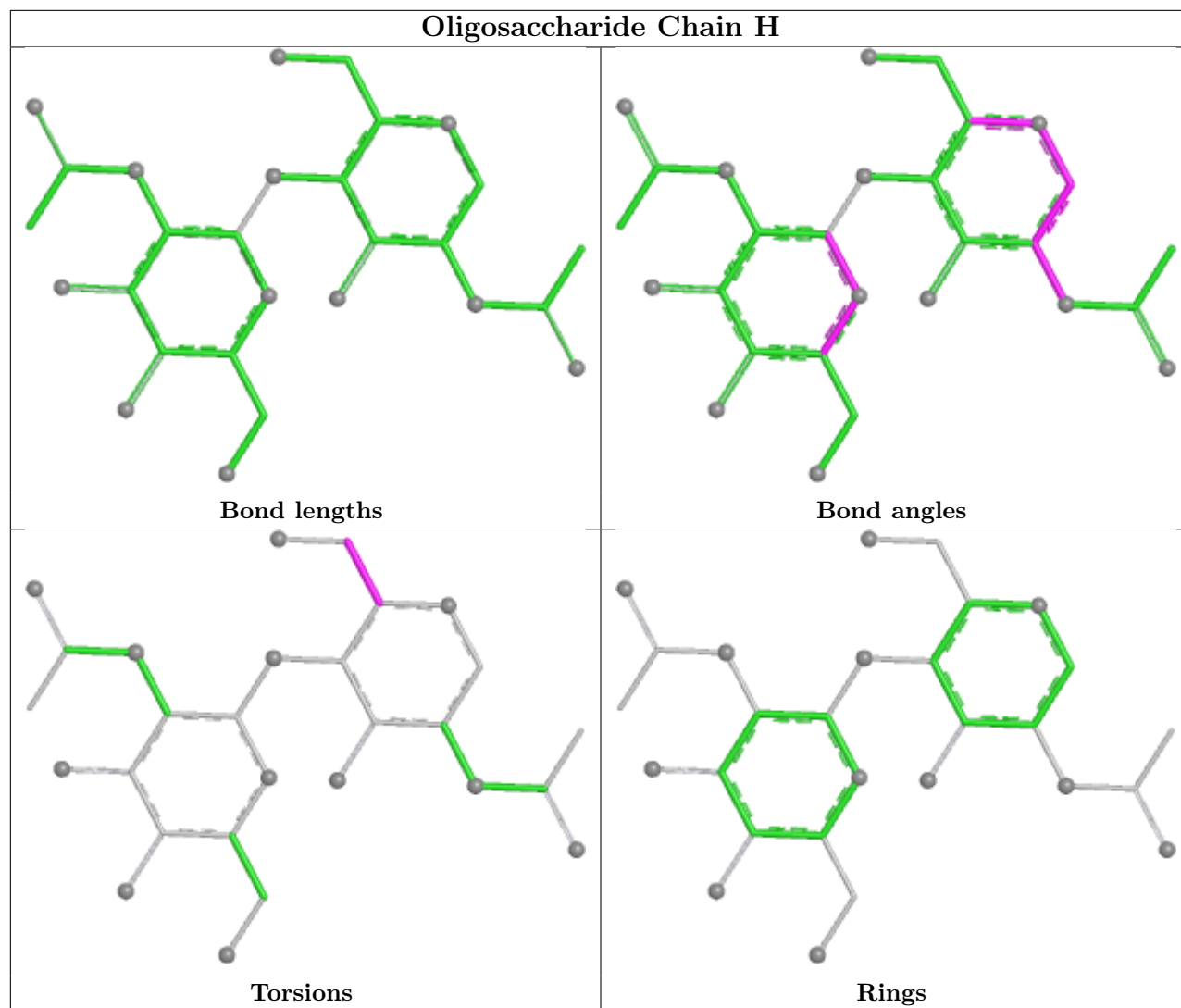
There are no ring outliers.

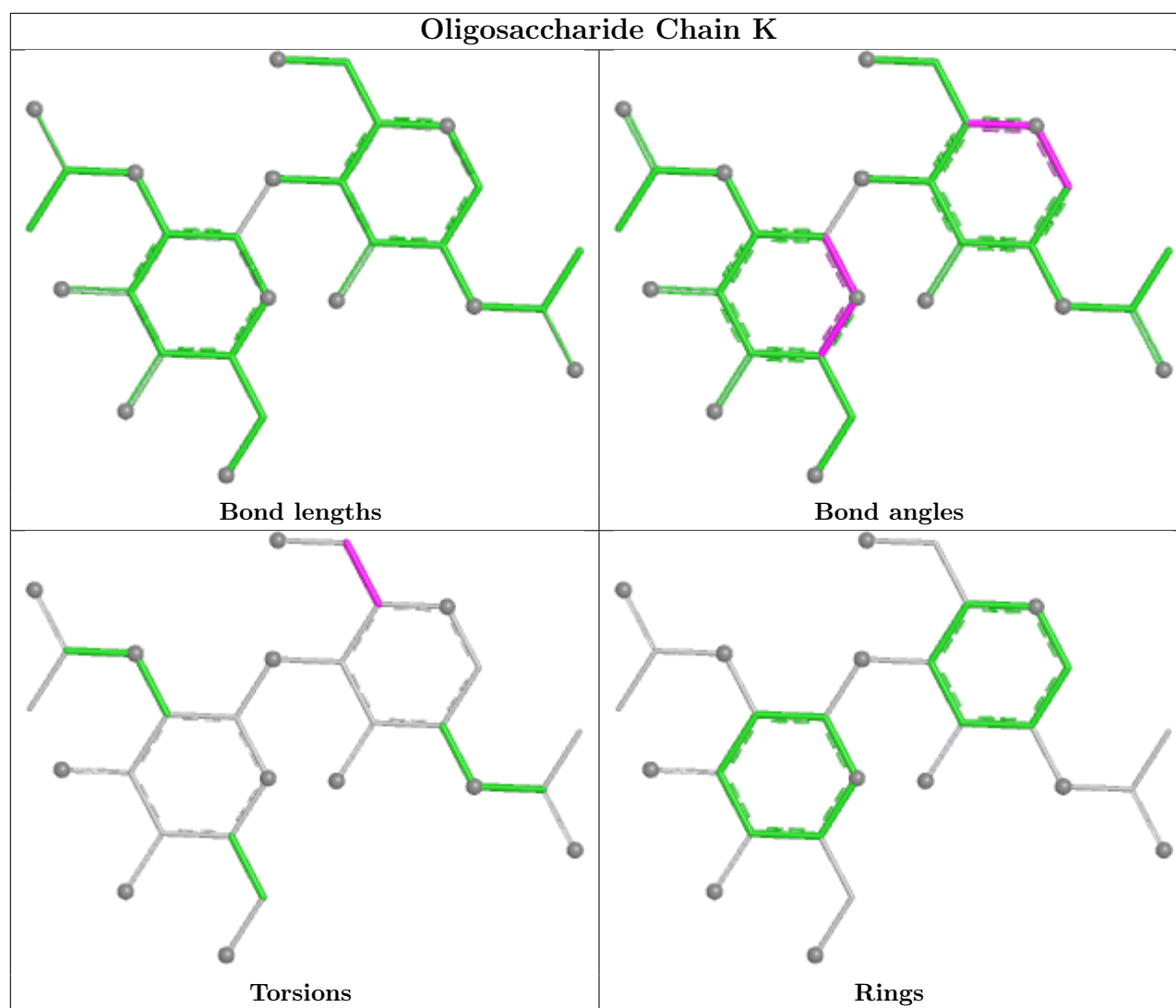
4 monomers are involved in 5 short contacts:

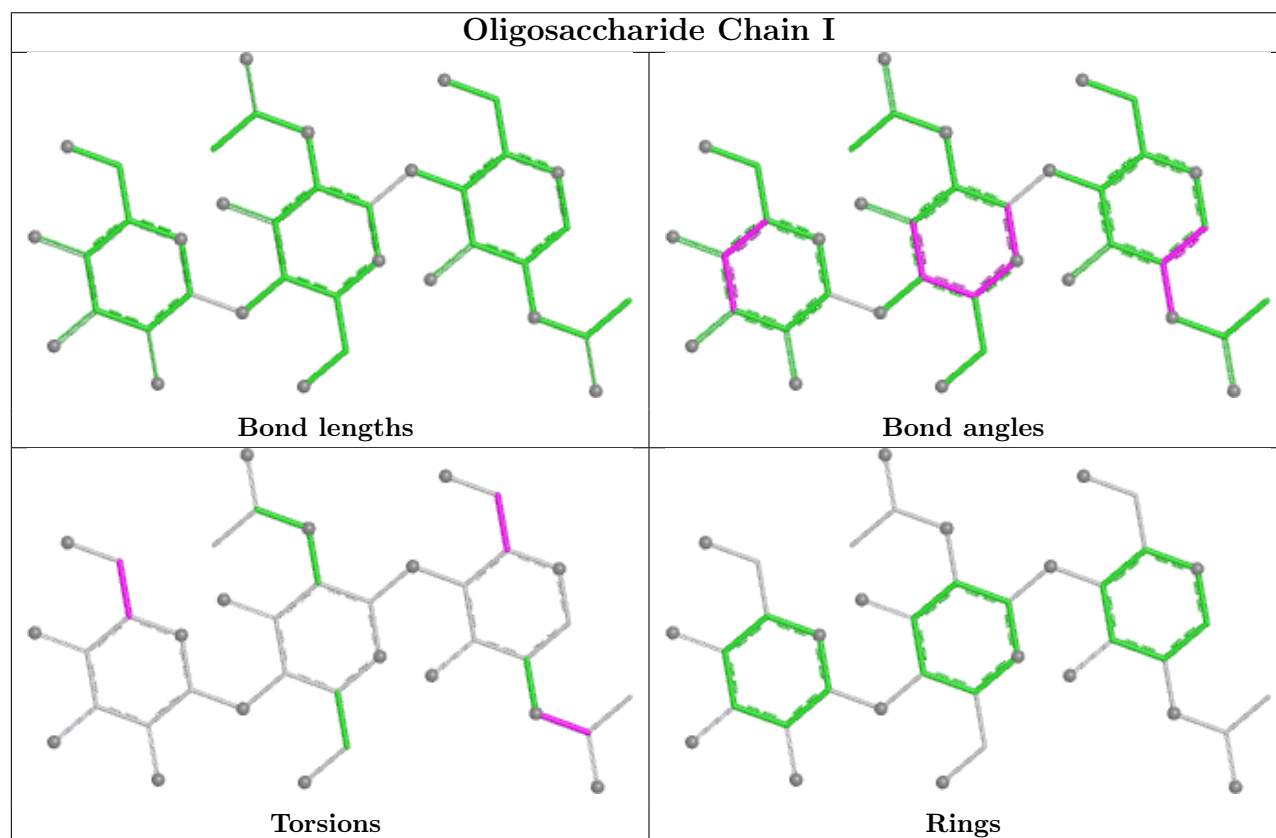
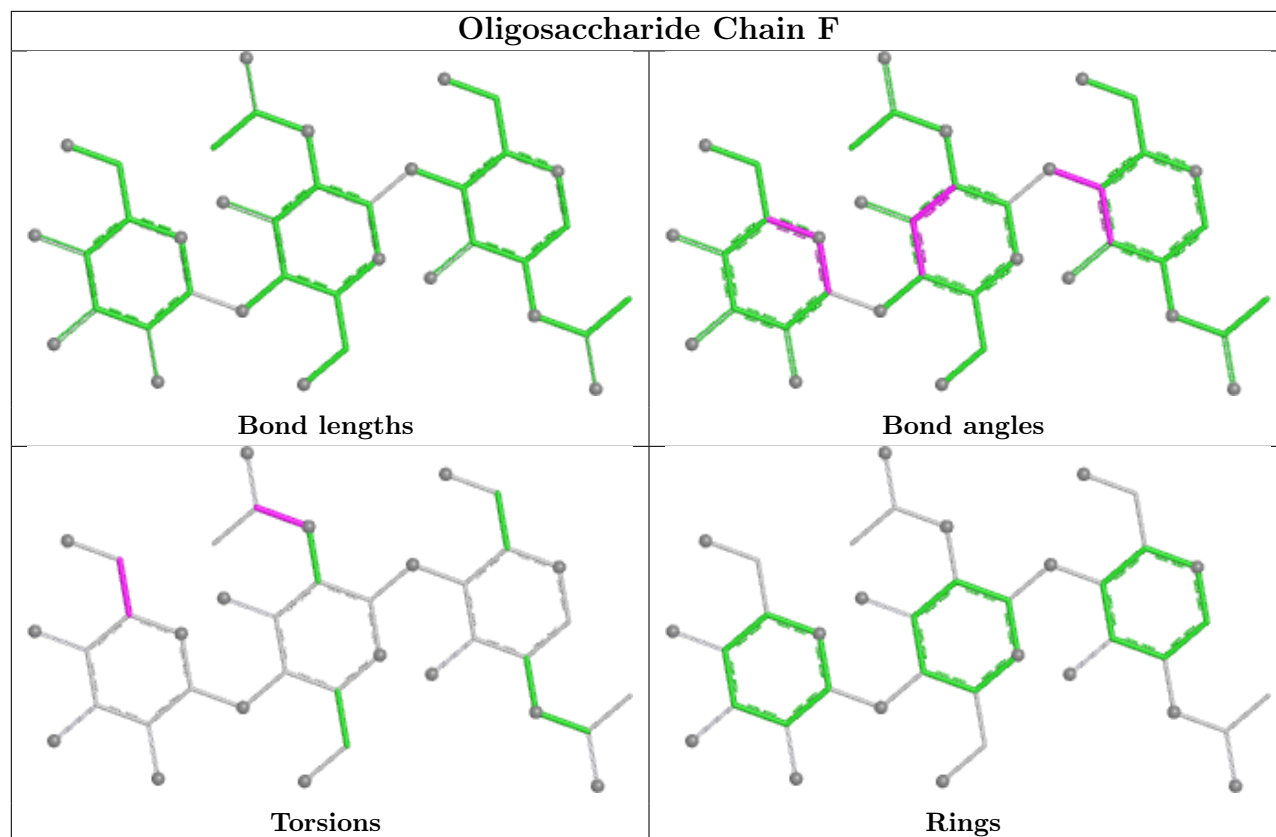
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	2	0
5	O	1	GLC	1	0
5	L	1	GLC	1	0
5	N	1	GLC	1	0

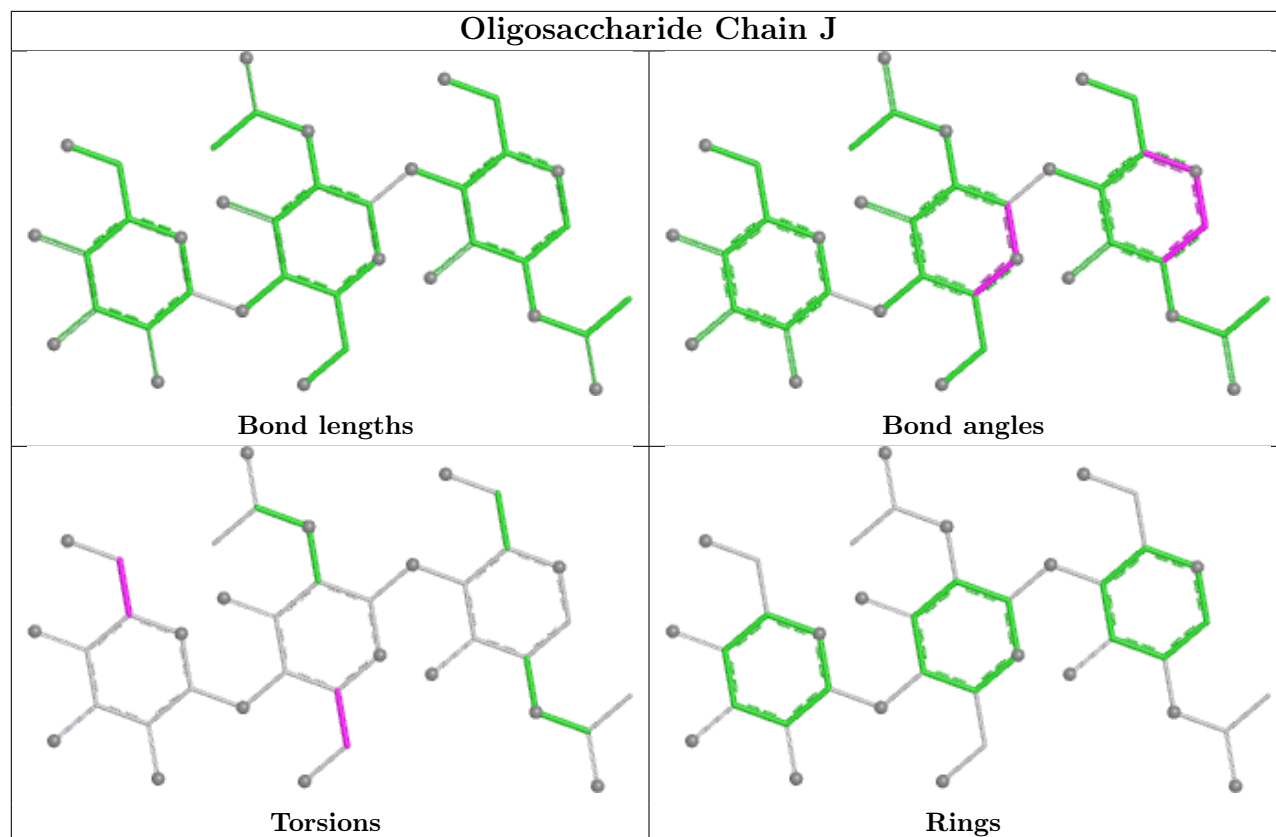
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

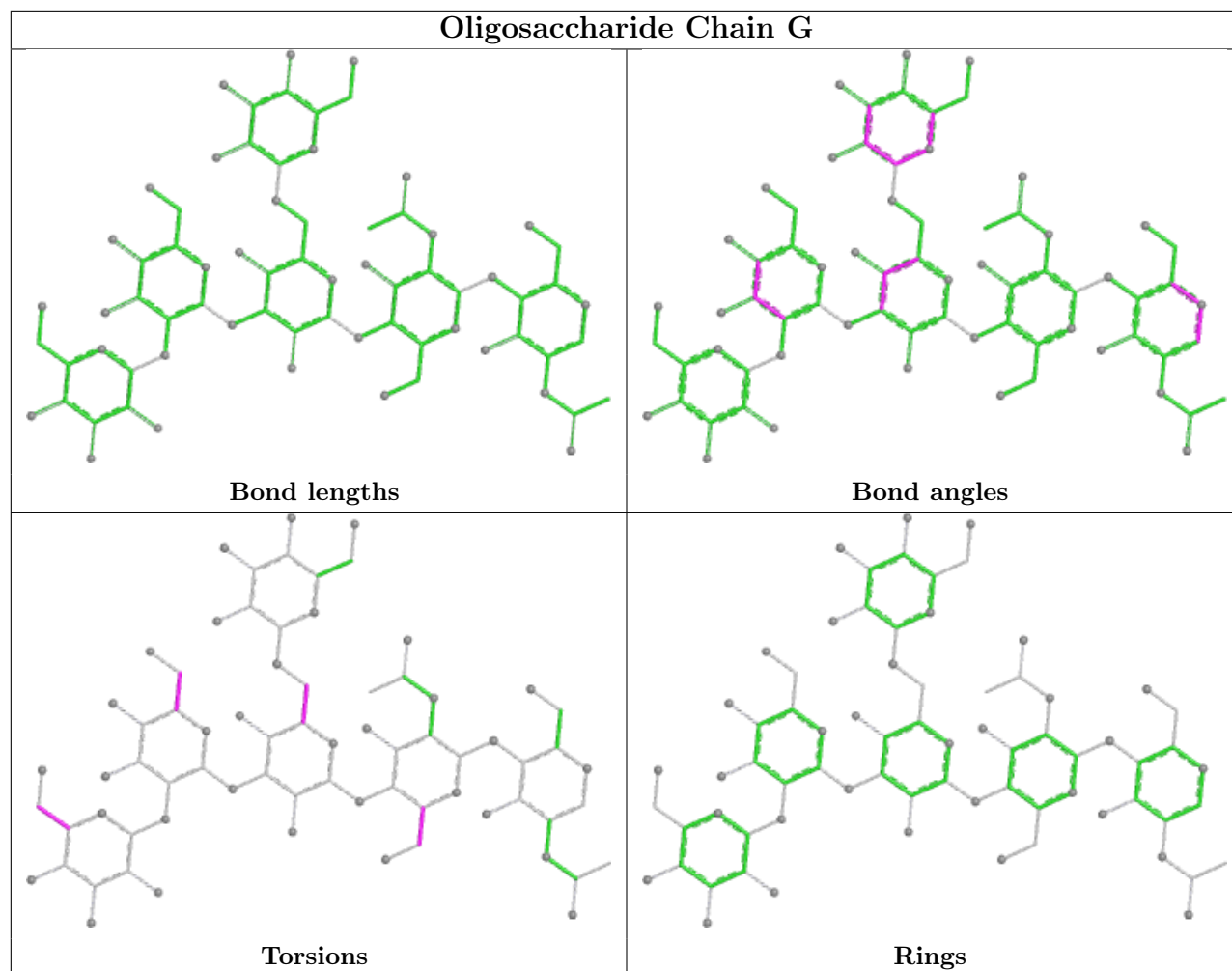


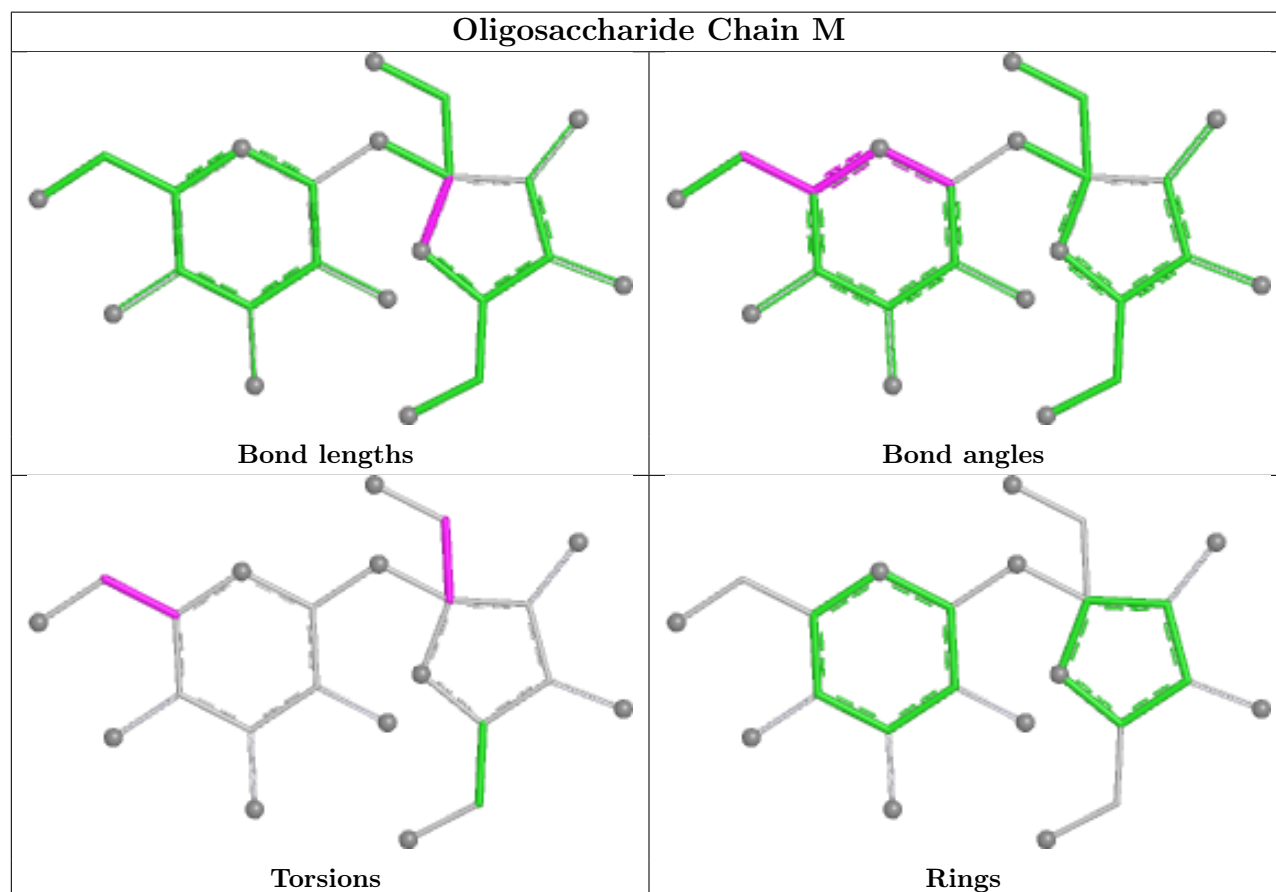
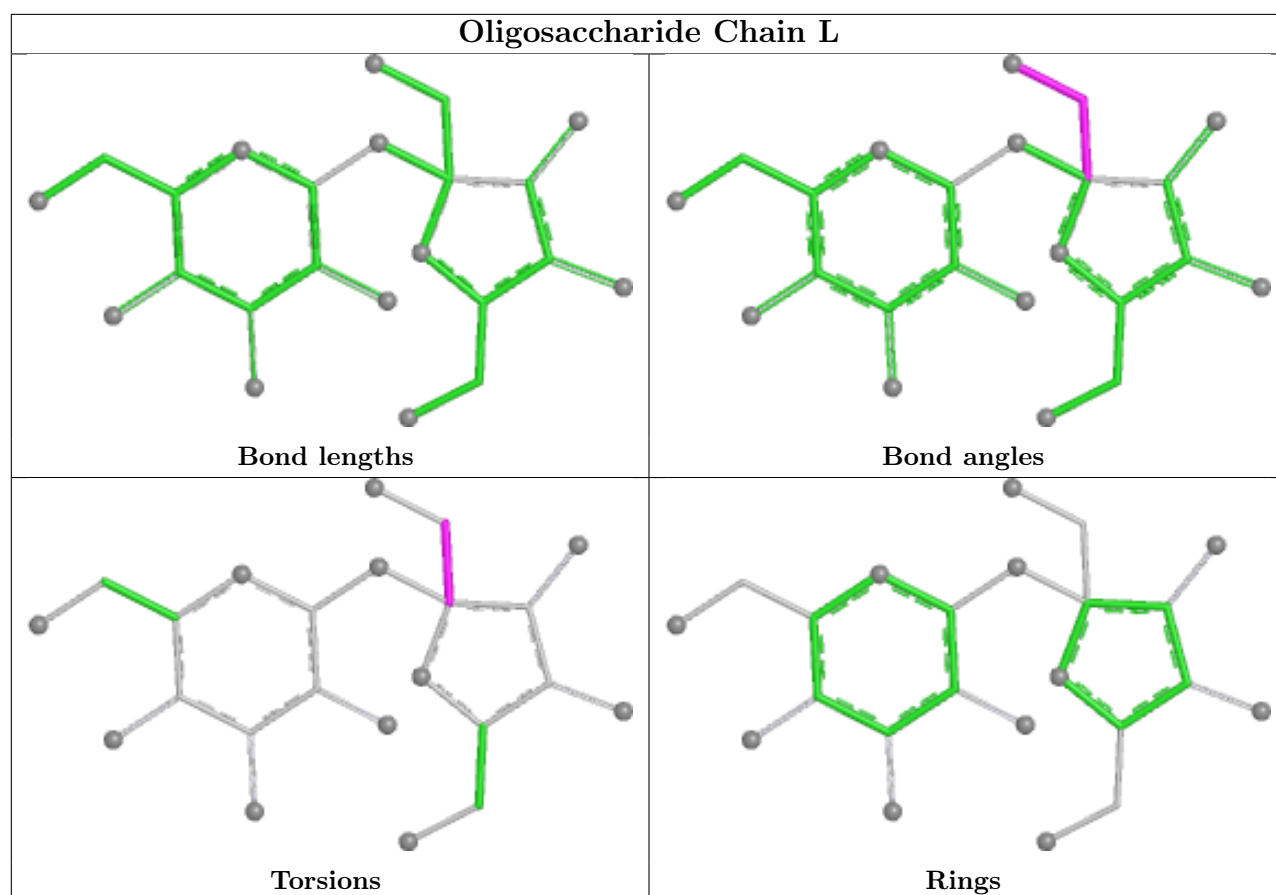


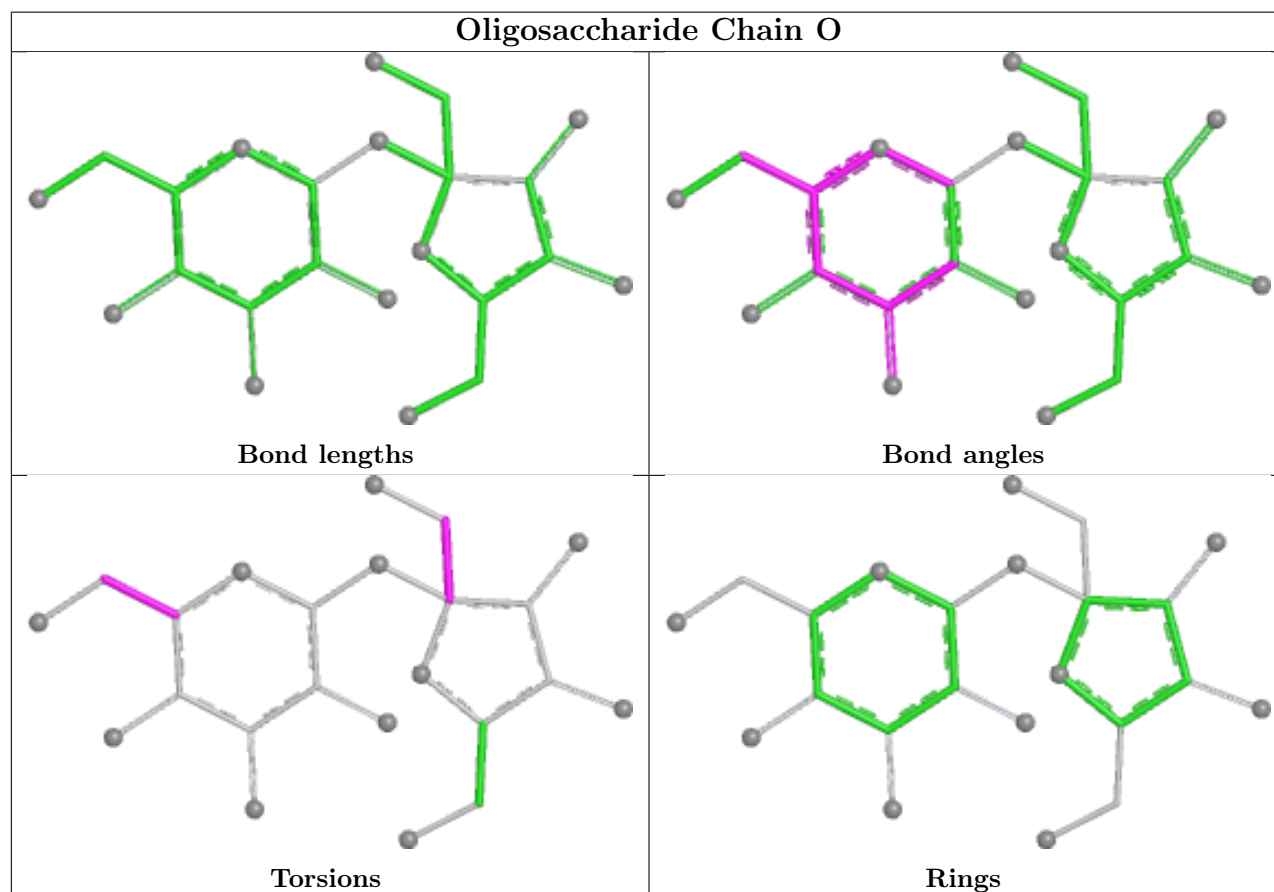
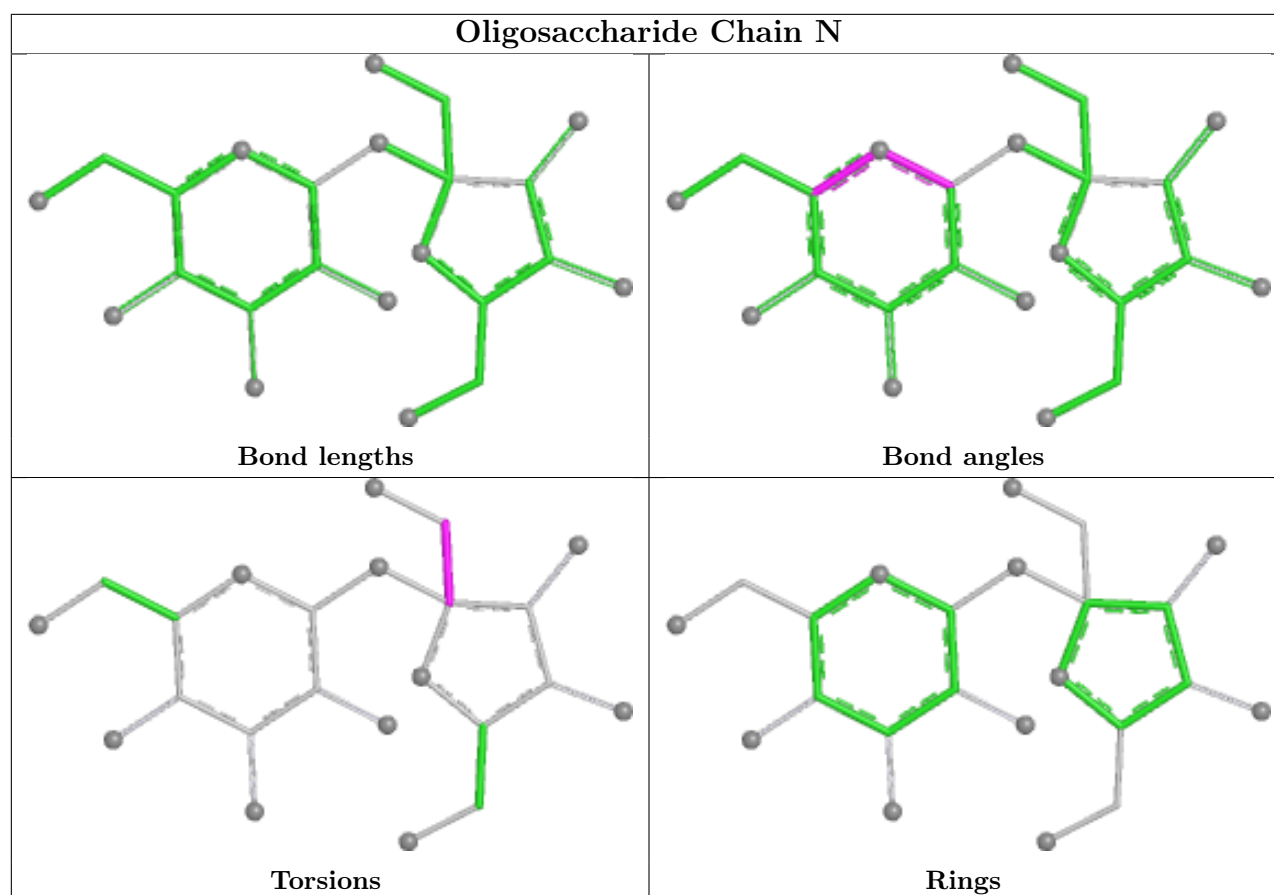












5.6 Ligand geometry

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	C	706	1	14,14,15	0.38	0	17,19,21	1.21	1 (5%)
7	NAG	C	707	1	14,14,15	0.77	1 (7%)	17,19,21	0.81	0
7	NAG	B	706	1	14,14,15	0.60	0	17,19,21	1.62	3 (17%)
7	NAG	B	705	1	14,14,15	0.99	1 (7%)	17,19,21	1.45	3 (17%)
6	MAN	D	703	1	11,11,12	0.94	0	15,15,17	1.15	1 (6%)
7	NAG	A	710	1	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
7	NAG	A	707	1	14,14,15	0.71	1 (7%)	17,19,21	0.77	0
7	NAG	D	707	1	14,14,15	0.40	0	17,19,21	1.41	3 (17%)
7	NAG	D	705	1	14,14,15	0.74	0	17,19,21	2.47	6 (35%)
6	MAN	C	704	1	11,11,12	0.59	0	15,15,17	0.71	0
7	NAG	A	709	1	14,14,15	0.75	0	17,19,21	1.21	2 (11%)
7	NAG	B	707	1	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
7	NAG	D	704	1	14,14,15	0.62	0	17,19,21	1.39	1 (5%)
6	MAN	B	703	1	11,11,12	0.55	0	15,15,17	1.04	1 (6%)
7	NAG	C	710	1	14,14,15	0.47	0	17,19,21	1.55	3 (17%)
6	MAN	A	701	1	11,11,12	0.62	0	15,15,17	0.86	0
7	NAG	A	708	1	14,14,15	0.89	1 (7%)	17,19,21	0.96	1 (5%)
6	MAN	A	703	1	11,11,12	0.85	0	15,15,17	1.45	1 (6%)
6	MAN	B	701	1	11,11,12	0.62	0	15,15,17	1.41	2 (13%)
6	MAN	A	702	1	11,11,12	0.74	0	15,15,17	1.11	1 (6%)
7	NAG	A	706	1	14,14,15	0.42	0	17,19,21	1.71	2 (11%)
6	MAN	D	701	1	11,11,12	0.74	0	15,15,17	1.35	1 (6%)
6	MAN	C	702	1	11,11,12	0.51	0	15,15,17	1.50	2 (13%)
7	NAG	C	708	1	14,14,15	0.49	0	17,19,21	0.95	0
6	MAN	C	701	1	11,11,12	0.67	0	15,15,17	1.31	3 (20%)
7	NAG	A	711	1	14,14,15	0.78	0	17,19,21	1.51	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	709	1	14,14,15	0.66	0	17,19,21	1.29	1 (5%)
7	NAG	B	709	1	14,14,15	0.35	0	17,19,21	0.73	0
6	MAN	D	702	1	11,11,12	0.50	0	15,15,17	0.95	1 (6%)
7	NAG	D	706	1	14,14,15	0.48	0	17,19,21	1.06	2 (11%)
6	MAN	C	703	1	11,11,12	2.53	6 (54%)	15,15,17	1.51	3 (20%)
7	NAG	D	709	1	14,14,15	0.53	0	17,19,21	0.84	0
7	NAG	B	708	1	14,14,15	0.84	0	17,19,21	0.98	0
7	NAG	B	710	1	14,14,15	0.65	0	17,19,21	1.35	2 (11%)
7	NAG	B	704	1	14,14,15	0.72	0	17,19,21	1.49	1 (5%)
7	NAG	C	705	1	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
7	NAG	A	705	1	14,14,15	0.51	0	17,19,21	1.09	2 (11%)
6	MAN	B	702	1	11,11,12	2.20	4 (36%)	15,15,17	1.49	3 (20%)
7	NAG	D	708	1	14,14,15	0.65	0	17,19,21	1.39	2 (11%)
6	MAN	A	704	1	11,11,12	0.63	0	15,15,17	1.27	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
7	NAG	C	706	1	-	2/6/23/26	0/1/1/1
7	NAG	C	707	1	-	2/6/23/26	0/1/1/1
7	NAG	B	706	1	-	4/6/23/26	0/1/1/1
7	NAG	B	705	1	-	4/6/23/26	0/1/1/1
6	MAN	D	703	1	-	2/2/19/22	0/1/1/1
7	NAG	A	710	1	-	1/6/23/26	0/1/1/1
7	NAG	A	707	1	-	1/6/23/26	0/1/1/1
7	NAG	D	707	1	-	2/6/23/26	0/1/1/1
7	NAG	D	705	1	-	5/6/23/26	0/1/1/1
6	MAN	C	704	1	-	0/2/19/22	0/1/1/1
7	NAG	A	709	1	-	2/6/23/26	0/1/1/1
7	NAG	B	707	1	-	2/6/23/26	0/1/1/1
7	NAG	D	704	1	-	2/6/23/26	0/1/1/1
6	MAN	B	703	1	-	2/2/19/22	0/1/1/1
7	NAG	C	710	1	-	2/6/23/26	0/1/1/1
6	MAN	A	701	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	708	1	-	0/6/23/26	0/1/1/1
6	MAN	A	703	1	-	1/2/19/22	0/1/1/1
6	MAN	B	701	1	-	0/2/19/22	0/1/1/1
6	MAN	A	702	1	-	2/2/19/22	0/1/1/1
7	NAG	A	706	1	-	2/6/23/26	0/1/1/1
6	MAN	D	701	1	-	0/2/19/22	0/1/1/1
6	MAN	C	702	1	-	2/2/19/22	0/1/1/1
7	NAG	C	708	1	-	2/6/23/26	0/1/1/1
6	MAN	C	701	1	-	2/2/19/22	0/1/1/1
7	NAG	A	711	1	-	2/6/23/26	0/1/1/1
7	NAG	C	709	1	-	3/6/23/26	0/1/1/1
7	NAG	B	709	1	-	0/6/23/26	0/1/1/1
6	MAN	D	702	1	-	1/2/19/22	0/1/1/1
7	NAG	D	706	1	-	2/6/23/26	0/1/1/1
6	MAN	C	703	1	-	1/2/19/22	0/1/1/1
7	NAG	D	709	1	-	2/6/23/26	0/1/1/1
7	NAG	B	708	1	-	0/6/23/26	0/1/1/1
7	NAG	B	710	1	-	2/6/23/26	0/1/1/1
7	NAG	B	704	1	-	5/6/23/26	0/1/1/1
7	NAG	C	705	1	-	4/6/23/26	0/1/1/1
7	NAG	A	705	1	-	2/6/23/26	0/1/1/1
6	MAN	B	702	1	-	2/2/19/22	0/1/1/1
7	NAG	D	708	1	-	3/6/23/26	0/1/1/1
6	MAN	A	704	1	-	2/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	703	MAN	O3-C3	4.24	1.53	1.43
6	B	702	MAN	O4-C4	4.20	1.53	1.43
6	C	703	MAN	O2-C2	3.95	1.51	1.43
6	B	702	MAN	O5-C1	3.63	1.49	1.43
6	C	703	MAN	O5-C1	3.44	1.49	1.43
6	C	703	MAN	O4-C4	2.67	1.49	1.43
6	C	703	MAN	C2-C3	-2.62	1.48	1.52
7	B	705	NAG	C1-C2	2.47	1.55	1.52
6	B	702	MAN	O3-C3	2.29	1.48	1.43
6	B	702	MAN	O2-C2	2.27	1.48	1.43
7	A	707	NAG	C1-C2	2.26	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	707	NAG	C1-C2	2.21	1.55	1.52
6	C	703	MAN	O6-C6	2.04	1.51	1.42
7	A	708	NAG	O5-C1	-2.01	1.40	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	705	NAG	C2-N2-C7	7.08	132.39	122.90
7	A	706	NAG	O5-C1-C2	-5.44	102.87	111.29
7	B	704	NAG	C2-N2-C7	-5.20	115.93	122.90
6	D	701	MAN	C1-O5-C5	4.61	118.36	112.19
6	A	703	MAN	C1-O5-C5	4.54	118.28	112.19
7	B	706	NAG	O5-C1-C2	-4.49	104.34	111.29
7	D	708	NAG	C1-C2-N2	4.14	116.96	110.43
7	C	710	NAG	C1-C2-N2	-3.94	104.22	110.43
7	D	704	NAG	C1-C2-N2	3.90	116.58	110.43
7	D	705	NAG	O5-C1-C2	-3.90	105.26	111.29
7	B	710	NAG	C2-N2-C7	-3.65	118.01	122.90
7	C	710	NAG	C2-N2-C7	-3.64	118.02	122.90
7	B	705	NAG	C2-N2-C7	-3.47	118.25	122.90
6	C	701	MAN	C1-O5-C5	-3.37	107.68	112.19
6	C	702	MAN	O5-C1-C2	-3.36	102.77	110.79
7	A	711	NAG	C1-C2-N2	-3.24	105.33	110.43
7	C	709	NAG	C1-C2-N2	-3.21	105.38	110.43
6	B	702	MAN	O3-C3-C4	-3.13	102.99	110.38
6	B	701	MAN	C3-C4-C5	3.12	115.89	110.23
7	A	711	NAG	C2-N2-C7	-3.08	118.77	122.90
6	A	704	MAN	O5-C1-C2	-3.06	103.49	110.79
7	D	707	NAG	C1-C2-N2	3.04	115.23	110.43
6	C	703	MAN	O5-C1-C2	-2.99	103.66	110.79
7	A	709	NAG	C2-N2-C7	-2.96	118.93	122.90
6	B	702	MAN	O5-C5-C4	-2.96	103.63	110.83
7	D	705	NAG	C1-C2-N2	2.86	114.94	110.43
6	A	704	MAN	C2-C3-C4	-2.85	105.84	110.86
7	B	710	NAG	C4-C3-C2	-2.84	106.86	111.02
7	D	706	NAG	O5-C1-C2	-2.78	106.99	111.29
7	B	706	NAG	C1-O5-C5	-2.76	108.48	112.19
7	A	706	NAG	C1-C2-N2	2.63	114.58	110.43
7	A	708	NAG	C1-C2-N2	-2.60	106.34	110.43
7	D	707	NAG	C3-C4-C5	-2.57	105.56	110.23
7	C	705	NAG	C1-O5-C5	-2.54	108.78	112.19
7	D	705	NAG	C8-C7-N2	2.50	120.27	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	703	MAN	C1-O5-C5	-2.50	108.84	112.19
6	B	702	MAN	O5-C1-C2	-2.48	104.87	110.79
7	B	705	NAG	O7-C7-C8	-2.47	117.66	122.05
7	D	707	NAG	C4-C3-C2	-2.47	107.40	111.02
7	B	705	NAG	C4-C3-C2	2.46	114.62	111.02
7	B	706	NAG	O4-C4-C3	-2.46	104.58	110.38
6	B	701	MAN	O5-C1-C2	-2.45	104.94	110.79
7	D	705	NAG	O5-C5-C6	2.45	112.43	107.66
7	A	709	NAG	C1-C2-N2	-2.44	106.58	110.43
6	D	702	MAN	O5-C5-C6	2.42	112.37	107.66
7	D	705	NAG	O5-C5-C4	-2.42	104.94	110.83
6	A	702	MAN	C1-C2-C3	2.31	113.01	109.64
6	C	702	MAN	C1-O5-C5	-2.30	109.11	112.19
6	B	703	MAN	O5-C1-C2	-2.28	105.36	110.79
7	A	711	NAG	O5-C1-C2	-2.20	107.89	111.29
7	D	708	NAG	C2-N2-C7	2.16	125.79	122.90
7	A	705	NAG	C8-C7-N2	-2.12	112.60	116.12
6	C	703	MAN	O6-C6-C5	-2.09	104.21	111.33
7	B	707	NAG	O6-C6-C5	-2.08	104.24	111.33
7	A	710	NAG	C1-C2-N2	-2.08	107.16	110.43
7	C	706	NAG	O7-C7-N2	2.07	125.64	121.98
7	A	711	NAG	C3-C4-C5	-2.06	106.49	110.23
7	D	706	NAG	O5-C5-C4	-2.06	105.81	110.83
6	C	701	MAN	O5-C1-C2	-2.06	105.88	110.79
6	D	703	MAN	O5-C1-C2	-2.06	105.89	110.79
6	C	701	MAN	O2-C2-C1	2.03	113.86	109.22
7	A	705	NAG	O5-C1-C2	-2.01	108.18	111.29
7	C	710	NAG	O5-C5-C4	-2.00	105.95	110.83

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	704	NAG	C3-C2-N2-C7
7	B	704	NAG	C8-C7-N2-C2
7	B	704	NAG	O7-C7-N2-C2
7	B	705	NAG	C3-C2-N2-C7
7	B	705	NAG	C8-C7-N2-C2
7	B	705	NAG	O7-C7-N2-C2
7	C	709	NAG	C8-C7-N2-C2
7	C	709	NAG	O7-C7-N2-C2
7	C	710	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	705	NAG	O5-C5-C6-O6
7	C	707	NAG	O5-C5-C6-O6
7	A	709	NAG	O5-C5-C6-O6
7	B	704	NAG	C4-C5-C6-O6
7	B	704	NAG	O5-C5-C6-O6
7	D	705	NAG	O5-C5-C6-O6
7	C	708	NAG	O5-C5-C6-O6
7	B	706	NAG	O5-C5-C6-O6
6	A	704	MAN	O5-C5-C6-O6
7	A	706	NAG	O5-C5-C6-O6
7	B	706	NAG	C4-C5-C6-O6
7	A	705	NAG	C4-C5-C6-O6
6	C	702	MAN	O5-C5-C6-O6
6	D	703	MAN	O5-C5-C6-O6
6	A	704	MAN	C4-C5-C6-O6
7	C	707	NAG	C4-C5-C6-O6
6	B	702	MAN	O5-C5-C6-O6
6	C	701	MAN	O5-C5-C6-O6
7	C	708	NAG	C4-C5-C6-O6
7	D	706	NAG	C4-C5-C6-O6
7	A	706	NAG	C4-C5-C6-O6
7	A	709	NAG	C4-C5-C6-O6
6	B	702	MAN	C4-C5-C6-O6
7	C	705	NAG	C8-C7-N2-C2
7	D	705	NAG	C4-C5-C6-O6
7	D	706	NAG	O5-C5-C6-O6
7	B	710	NAG	O5-C5-C6-O6
7	C	706	NAG	C4-C5-C6-O6
7	A	711	NAG	C8-C7-N2-C2
7	B	706	NAG	C8-C7-N2-C2
7	B	706	NAG	O7-C7-N2-C2
7	C	710	NAG	O7-C7-N2-C2
7	D	705	NAG	C8-C7-N2-C2
7	D	705	NAG	O7-C7-N2-C2
7	C	706	NAG	O5-C5-C6-O6
7	B	710	NAG	C4-C5-C6-O6
7	D	704	NAG	O5-C5-C6-O6
6	D	703	MAN	C4-C5-C6-O6
7	D	708	NAG	O5-C5-C6-O6
7	D	707	NAG	O5-C5-C6-O6
7	D	704	NAG	C4-C5-C6-O6
6	A	702	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	703	MAN	C4-C5-C6-O6
6	A	703	MAN	O5-C5-C6-O6
7	A	707	NAG	O5-C5-C6-O6
6	C	702	MAN	C4-C5-C6-O6
7	C	709	NAG	O5-C5-C6-O6
7	C	705	NAG	C4-C5-C6-O6
6	C	703	MAN	O5-C5-C6-O6
7	D	709	NAG	C4-C5-C6-O6
7	C	705	NAG	O7-C7-N2-C2
7	A	710	NAG	C8-C7-N2-C2
6	C	701	MAN	C4-C5-C6-O6
6	B	703	MAN	O5-C5-C6-O6
6	A	702	MAN	O5-C5-C6-O6
7	B	707	NAG	C4-C5-C6-O6
7	D	705	NAG	C3-C2-N2-C7
6	D	702	MAN	O5-C5-C6-O6
7	B	707	NAG	O5-C5-C6-O6
7	D	709	NAG	O5-C5-C6-O6
7	A	711	NAG	O7-C7-N2-C2
7	C	705	NAG	O5-C5-C6-O6
7	D	708	NAG	C1-C2-N2-C7
7	B	705	NAG	O5-C5-C6-O6
7	D	707	NAG	C4-C5-C6-O6
7	D	708	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	706	NAG	2	0
7	D	705	NAG	2	0
6	C	704	MAN	1	0
7	A	709	NAG	1	0
7	D	704	NAG	1	0
7	A	706	NAG	1	0
6	D	701	MAN	1	0
6	C	701	MAN	1	0
6	D	702	MAN	1	0
7	D	709	NAG	1	0
7	B	710	NAG	1	0
7	C	705	NAG	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	525/675 (77%)	0.04	6 (1%) 78 77	22, 32, 56, 87	0
1	B	526/675 (77%)	0.16	10 (1%) 66 65	22, 35, 72, 105	0
1	C	528/675 (78%)	0.20	15 (2%) 55 54	22, 36, 62, 109	0
1	D	524/675 (77%)	0.42	33 (6%) 26 25	22, 38, 78, 103	0
All	All	2103/2700 (77%)	0.21	64 (3%) 52 52	22, 35, 68, 109	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	661	VAL	3.8
1	B	564	ASP	3.4
1	C	559	SER	3.3
1	C	437	GLY	3.3
1	A	165	ILE	3.0
1	A	563	SER	2.9
1	C	657	GLU	2.9
1	C	563	SER	2.9
1	D	437	GLY	2.8
1	B	512	PHE	2.8
1	D	555	CYS	2.8
1	A	556	SER	2.8
1	D	563	SER	2.8
1	A	542	ASP	2.8
1	B	563	SER	2.8
1	D	556	SER	2.8
1	D	499	LEU	2.7
1	D	420	ASP	2.7
1	D	653	GLY	2.7
1	B	490	LEU	2.6
1	D	496	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	143	CYS	2.6
1	D	509	ASP	2.6
1	D	531	ALA	2.5
1	D	662	ASN	2.5
1	D	506	SER	2.5
1	D	537	SER	2.5
1	D	512	PHE	2.5
1	D	436	ASN	2.5
1	A	143	CYS	2.4
1	C	534	GLN	2.4
1	B	557	SER	2.4
1	D	510	VAL	2.4
1	D	660	GLN	2.4
1	D	435	GLU	2.4
1	C	143	CYS	2.4
1	D	508	ALA	2.4
1	C	263	ASN	2.3
1	D	652	THR	2.3
1	D	665	VAL	2.3
1	D	150	ALA	2.3
1	B	513	THR	2.3
1	D	504	ALA	2.3
1	A	166	THR	2.3
1	D	533	ILE	2.3
1	D	149	PRO	2.2
1	C	509	ASP	2.2
1	C	277	PRO	2.2
1	C	553	THR	2.2
1	B	555	CYS	2.2
1	B	142	SER	2.2
1	D	647	SER	2.2
1	D	528	LEU	2.1
1	B	531	ALA	2.1
1	C	151	SER	2.1
1	D	553	THR	2.1
1	D	538	LEU	2.1
1	B	514	ASN	2.1
1	C	512	PHE	2.1
1	D	532	ALA	2.1
1	D	541	ALA	2.1
1	C	142	SER	2.0
1	C	500	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	161	THR	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.

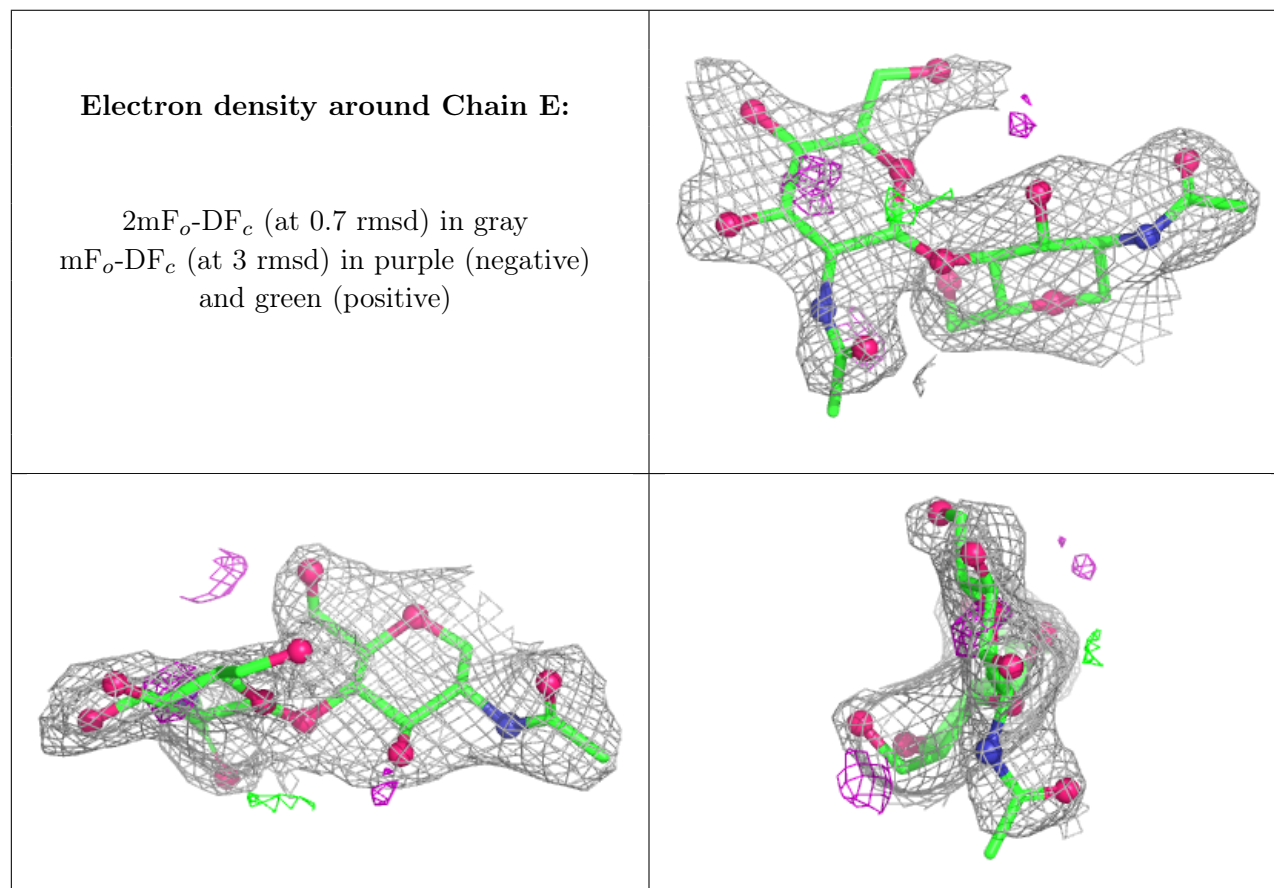
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	G	5	11/12	0.37	0.17	92,102,108,109	0
3	BMA	I	3	11/12	0.50	0.16	89,103,108,111	0
3	BMA	J	3	11/12	0.52	0.14	85,95,101,101	0
3	BMA	F	3	11/12	0.56	0.15	70,74,80,81	0
4	MAN	G	6	11/12	0.57	0.20	27,28,29,31	11
2	NAG	H	2	14/15	0.64	0.17	71,78,91,91	0
4	BMA	G	3	11/12	0.65	0.13	66,78,82,84	0
3	NAG	J	2	14/15	0.71	0.15	59,72,80,85	0
3	NAG	F	2	14/15	0.72	0.15	54,67,79,80	0
4	MAN	G	4	11/12	0.72	0.13	84,86,90,96	0
3	NAG	I	2	14/15	0.77	0.14	69,89,95,97	0
2	NAG	K	2	14/15	0.78	0.13	79,92,102,103	0
2	NAG	E	2	14/15	0.80	0.13	60,67,72,73	0
3	NAG	I	1	14/15	0.86	0.12	56,68,72,77	0
4	NAG	G	2	14/15	0.86	0.12	51,61,72,75	0
5	GLC	N	1	11/12	0.87	0.10	44,48,52,53	0
2	NAG	E	1	14/15	0.91	0.09	42,47,50,57	0
3	NAG	J	1	14/15	0.91	0.08	34,38,41,51	0
2	NAG	H	1	14/15	0.93	0.07	37,42,46,57	0
4	NAG	G	1	14/15	0.93	0.08	46,51,55,56	0
3	NAG	F	1	14/15	0.93	0.08	35,40,45,47	0
5	GLC	M	1	11/12	0.93	0.08	35,37,41,43	0
2	NAG	K	1	14/15	0.93	0.07	44,48,60,66	0
5	GLC	O	1	11/12	0.93	0.08	34,37,41,43	0
5	FRU	M	2	12/12	0.94	0.08	27,30,34,44	0
5	GLC	L	1	11/12	0.95	0.06	37,39,41,44	0
5	FRU	N	2	12/12	0.95	0.07	29,35,40,44	0

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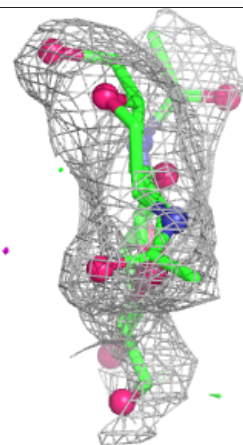
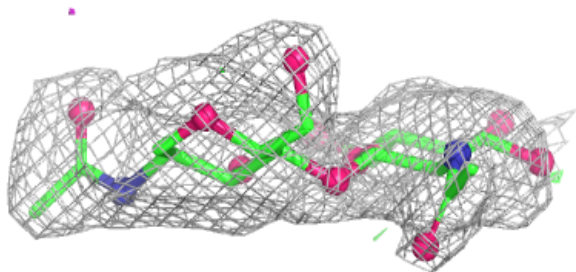
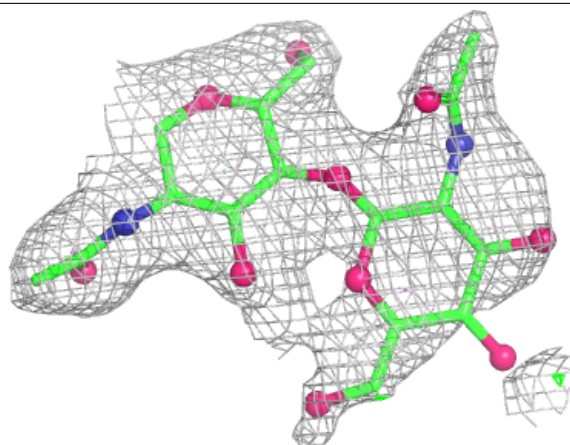
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FRU	L	2	12/12	0.95	0.07	28,32,34,37	0
5	FRU	O	2	12/12	0.96	0.06	26,29,33,38	0

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.



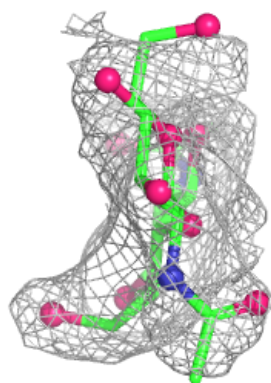
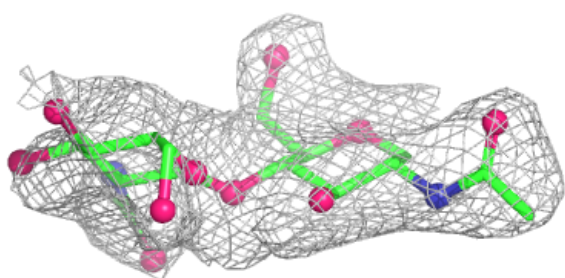
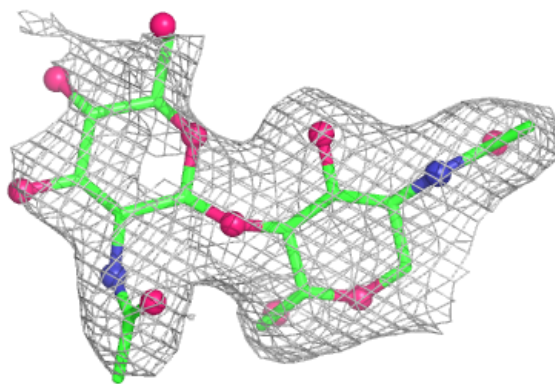
Electron density around Chain H:

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

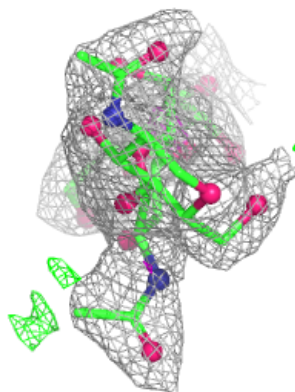
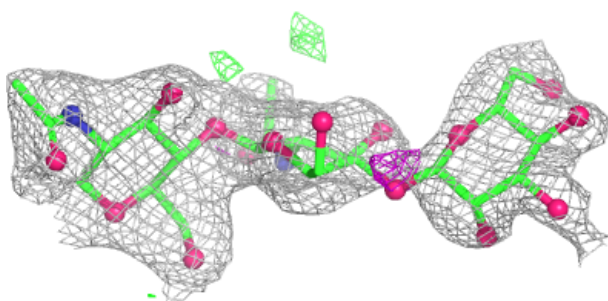
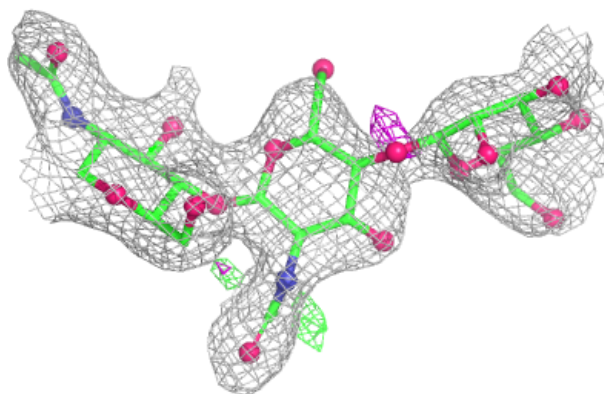


Electron density around Chain K:

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

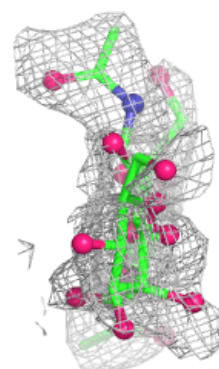
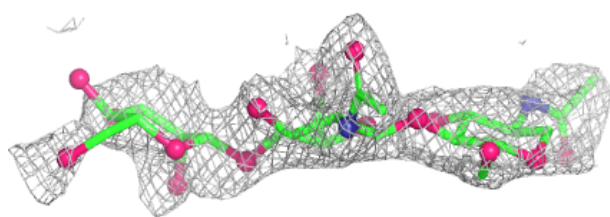
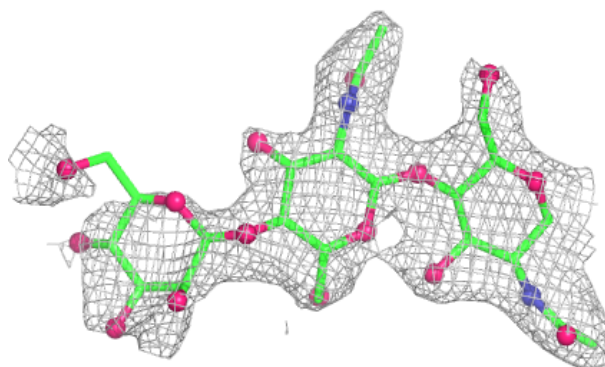
**Electron density around Chain F:**

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

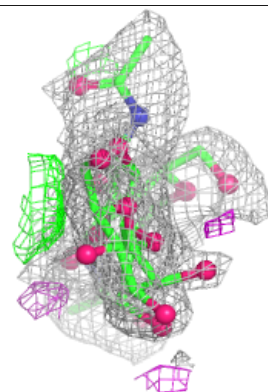
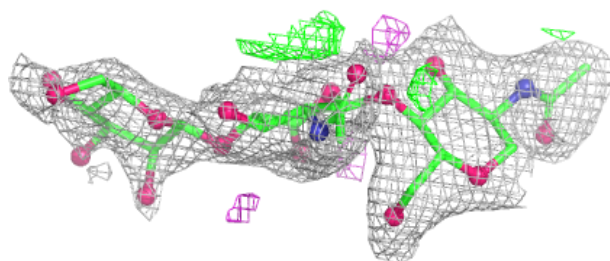
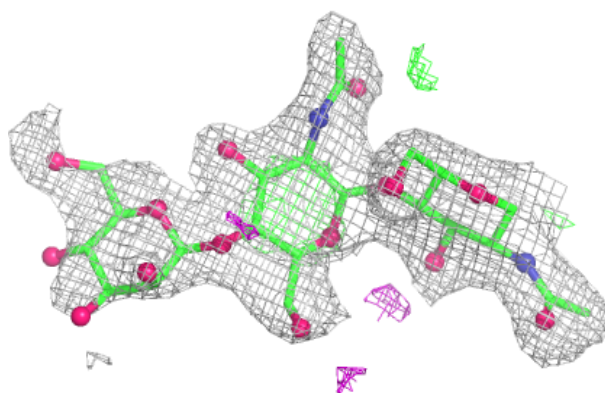


Electron density around Chain I:

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

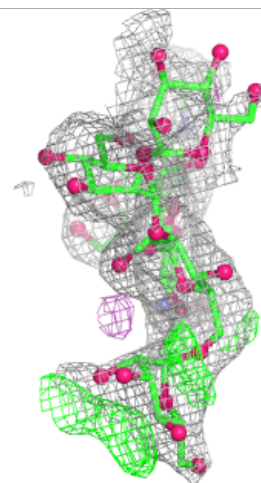
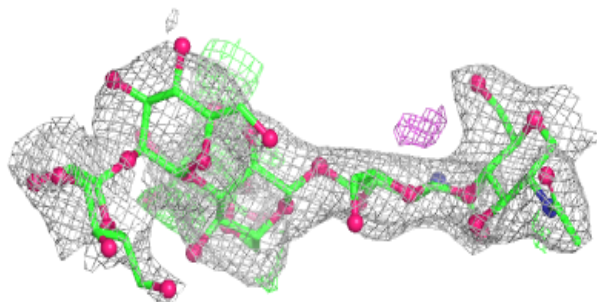
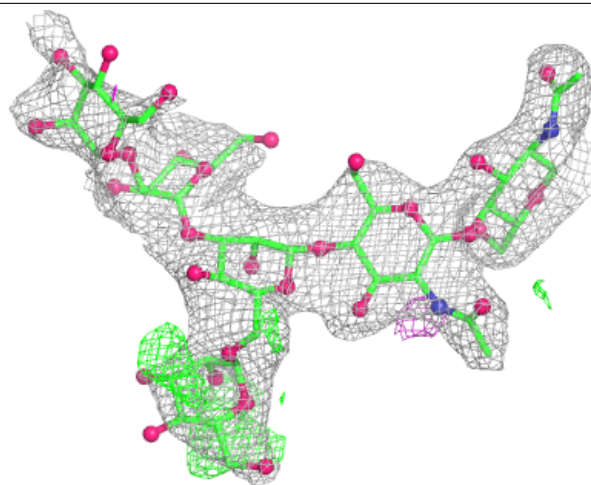
**Electron density around Chain J:**

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



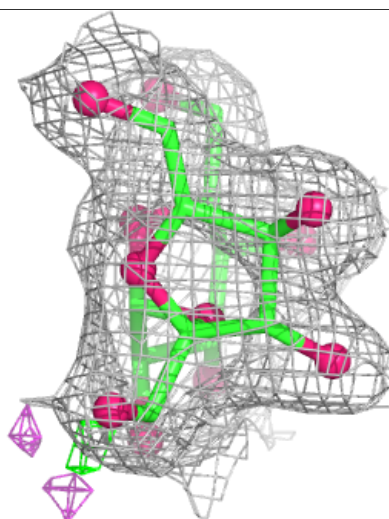
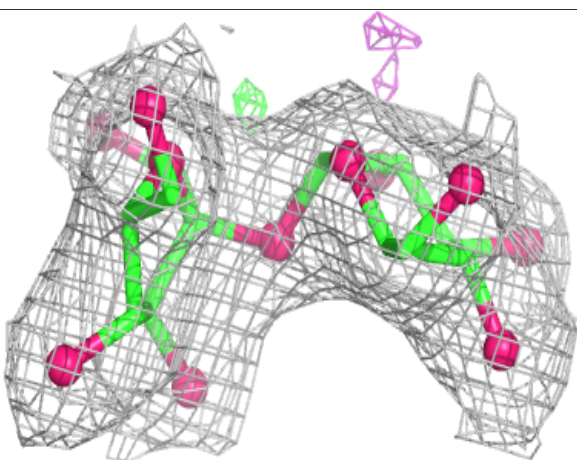
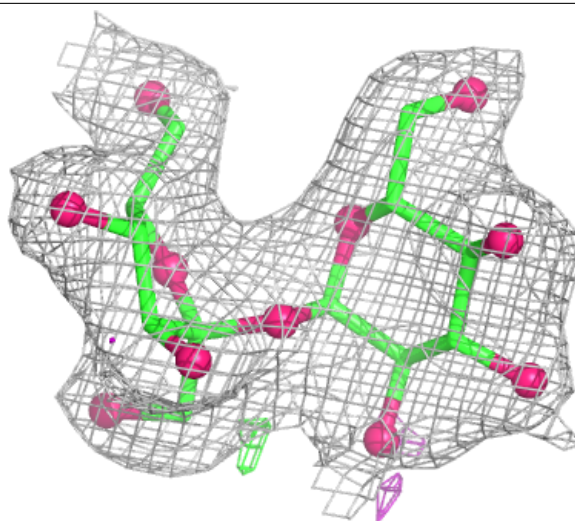
Electron density around Chain G:

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



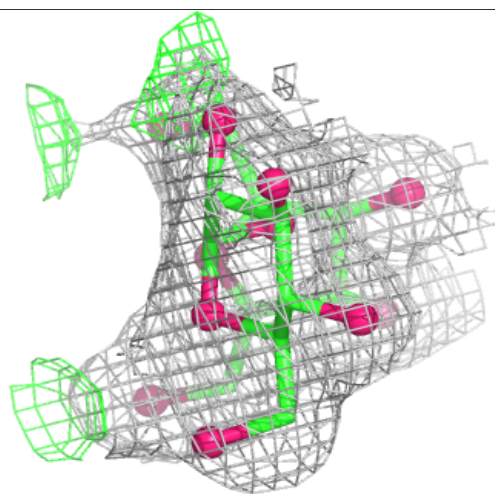
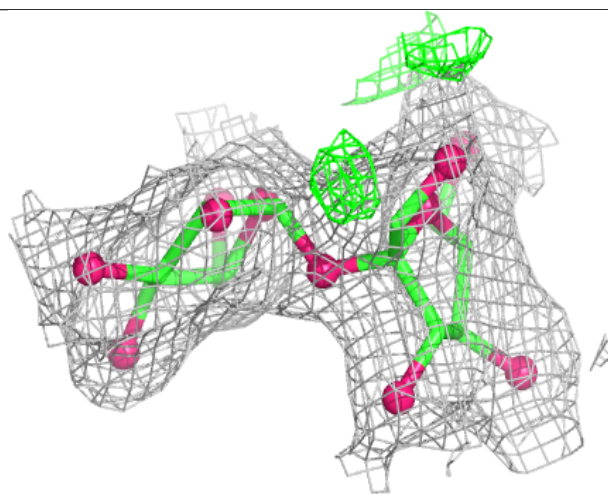
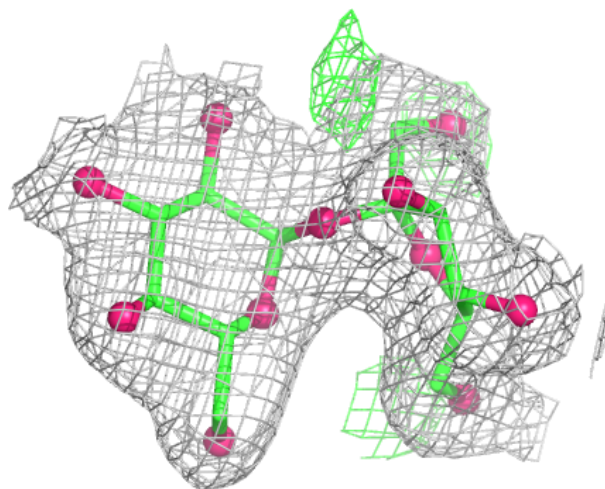
Electron density around Chain L:

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



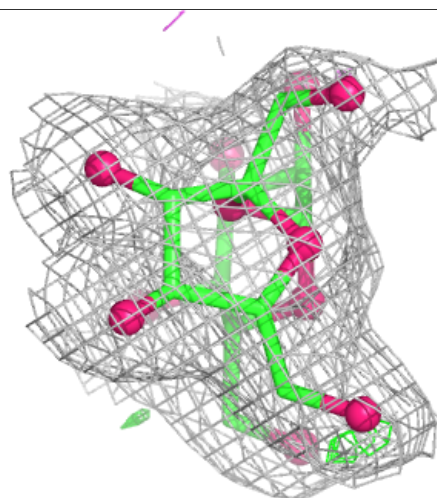
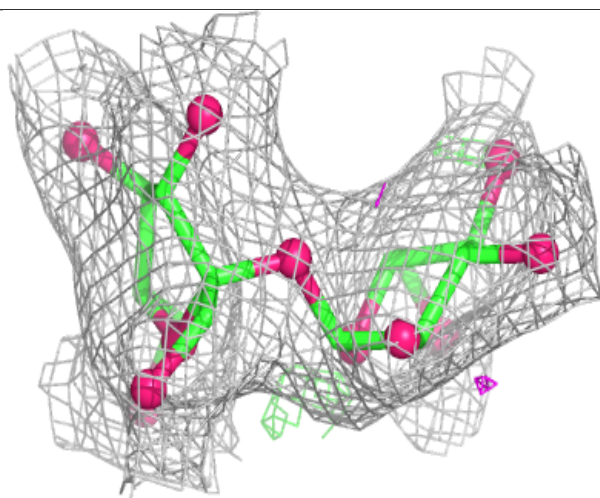
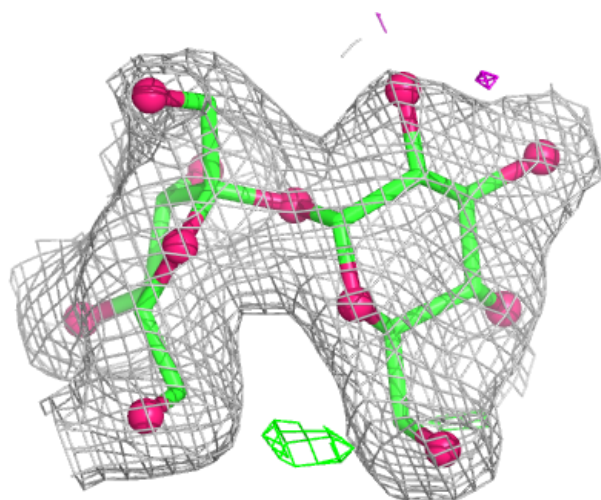
Electron density around Chain M:

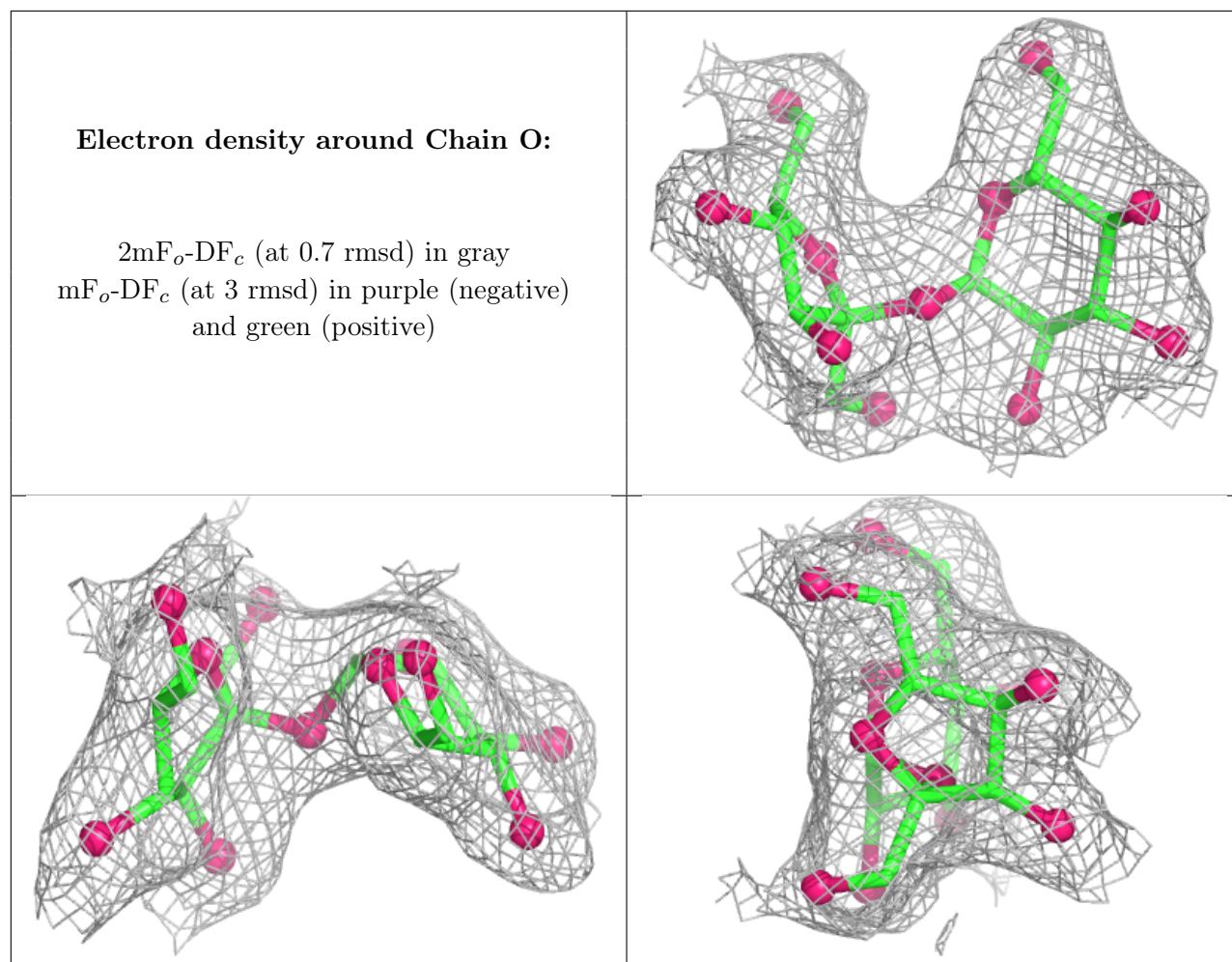
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
6	MAN	D	701	11/12	0.36	0.19	88,106,121,121	0
7	NAG	B	705	14/15	0.55	0.17	72,80,83,84	0
7	NAG	D	708	14/15	0.58	0.18	96,112,121,129	0
7	NAG	A	706	14/15	0.59	0.16	66,74,77,78	0
6	MAN	C	702	11/12	0.63	0.16	76,85,88,89	0
6	MAN	C	703	11/12	0.63	0.28	27,29,31,32	0
6	MAN	D	703	11/12	0.64	0.14	74,79,84,86	0
6	MAN	A	702	11/12	0.65	0.13	82,90,95,96	0
6	MAN	A	701	11/12	0.65	0.13	72,79,82,83	0
7	NAG	D	706	14/15	0.67	0.17	59,70,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	706	14/15	0.67	0.16	63,74,84,85	0
6	MAN	D	702	11/12	0.70	0.15	81,92,99,110	0
6	MAN	B	702	11/12	0.71	0.22	27,29,31,31	0
6	MAN	B	701	11/12	0.73	0.13	79,86,89,89	0
7	NAG	B	704	14/15	0.73	0.16	59,67,82,84	0
6	MAN	C	701	11/12	0.74	0.11	71,79,84,85	0
7	NAG	B	710	14/15	0.74	0.12	66,75,80,80	0
6	MAN	A	704	11/12	0.74	0.16	64,71,78,78	0
6	MAN	B	703	11/12	0.74	0.13	77,80,89,90	0
6	MAN	C	704	11/12	0.76	0.17	56,64,69,71	0
7	NAG	D	709	14/15	0.76	0.13	69,72,78,85	0
7	NAG	C	709	14/15	0.78	0.13	54,63,71,76	0
6	MAN	A	703	11/12	0.79	0.14	63,68,75,76	0
7	NAG	A	705	14/15	0.80	0.14	58,65,79,80	0
7	NAG	C	705	14/15	0.80	0.13	62,71,81,84	0
7	NAG	B	709	14/15	0.80	0.09	64,71,80,82	0
7	NAG	C	710	14/15	0.81	0.13	50,52,62,68	0
7	NAG	D	705	14/15	0.82	0.13	57,63,69,69	0
7	NAG	A	710	14/15	0.85	0.12	51,65,70,75	0
7	NAG	D	704	14/15	0.85	0.11	55,59,66,67	0
7	NAG	C	707	14/15	0.87	0.10	51,58,61,65	0
7	NAG	C	706	14/15	0.87	0.11	55,63,72,72	0
7	NAG	A	709	14/15	0.88	0.10	46,53,56,60	0
7	NAG	A	711	14/15	0.89	0.11	46,56,64,67	0
7	NAG	A	707	14/15	0.89	0.10	46,51,55,56	0
7	NAG	A	708	14/15	0.91	0.08	37,40,46,47	0
7	NAG	C	708	14/15	0.91	0.08	48,52,57,58	0
7	NAG	B	708	14/15	0.91	0.08	40,43,49,50	0
7	NAG	B	707	14/15	0.93	0.07	30,33,41,42	0
7	NAG	D	707	14/15	0.93	0.08	43,48,56,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.