



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:31 AM UTC

PDB ID : 5SZR / pdb_00005szr
Title : Protocadherin Gamma B2 extracellular cadherin domains 3-6
Authors : Goodman, K.M.; Mannepalli, S.; Bahna, F.; Rubinstein, R.; Honig, B.;
Shapiro, L.
Deposited on : 2016-08-14
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

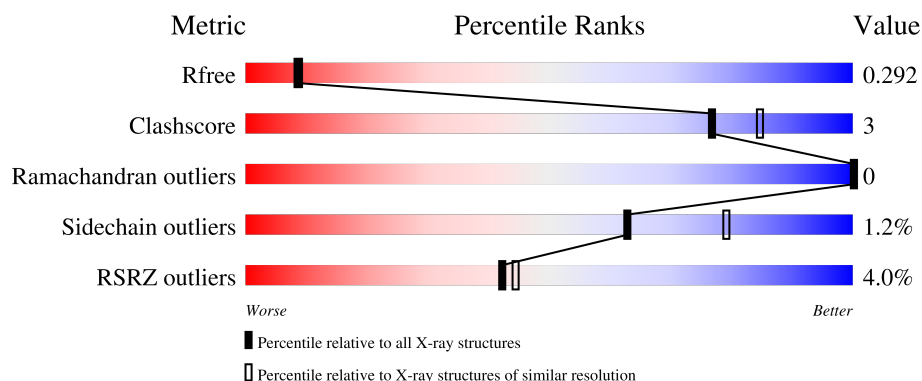
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	441	3% 89% 7% .
1	B	441	5% 86% 9% .
1	C	441	4% 87% 7% 6%
2	D	4	25% 50% 25%
2	F	4	50% 50%

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	G	2	 100%
3	I	2	 50%50%
4	H	3	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10333 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein Pcdhgb2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	2	0
			3222	2017	554	645	6			
1	B	422	Total	C	N	O	S	0	1	0
			3205	2007	550	642	6			
1	C	415	Total	C	N	O	S	0	0	0
			3144	1967	539	632	6			

There are 24 discrepancies between the modelled and reference sequences:

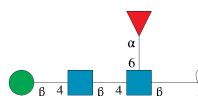
Chain	Residue	Modelled	Actual	Comment	Reference
A	641	HIS	-	expression tag	UNP Q91XX7
A	642	HIS	-	expression tag	UNP Q91XX7
A	643	HIS	-	expression tag	UNP Q91XX7
A	644	HIS	-	expression tag	UNP Q91XX7
A	645	HIS	-	expression tag	UNP Q91XX7
A	646	HIS	-	expression tag	UNP Q91XX7
A	647	HIS	-	expression tag	UNP Q91XX7
A	648	HIS	-	expression tag	UNP Q91XX7
B	641	HIS	-	expression tag	UNP Q91XX7
B	642	HIS	-	expression tag	UNP Q91XX7
B	643	HIS	-	expression tag	UNP Q91XX7
B	644	HIS	-	expression tag	UNP Q91XX7
B	645	HIS	-	expression tag	UNP Q91XX7
B	646	HIS	-	expression tag	UNP Q91XX7
B	647	HIS	-	expression tag	UNP Q91XX7
B	648	HIS	-	expression tag	UNP Q91XX7
C	641	HIS	-	expression tag	UNP Q91XX7
C	642	HIS	-	expression tag	UNP Q91XX7
C	643	HIS	-	expression tag	UNP Q91XX7
C	644	HIS	-	expression tag	UNP Q91XX7
C	645	HIS	-	expression tag	UNP Q91XX7
C	646	HIS	-	expression tag	UNP Q91XX7
C	647	HIS	-	expression tag	UNP Q91XX7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	648	HIS	-	expression tag	UNP Q91XX7

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



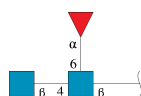
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

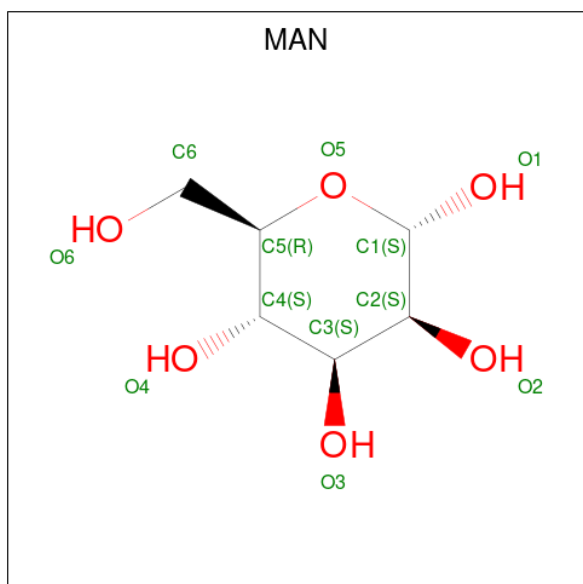


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	Ca	0	0
			9	9		
5	B	9	Total	Ca	0	0
			9	9		
5	C	9	Total	Ca	0	0
			9	9		

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



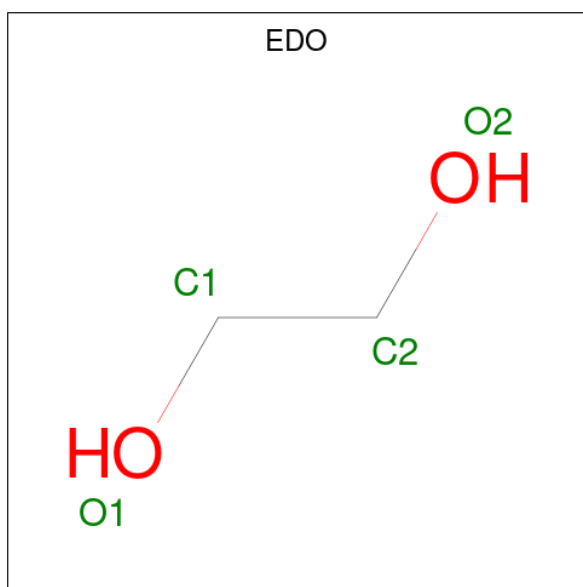
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	114	Total	O	0	0
			114	114		
8	B	82	Total	O	0	0
			82	82		
8	C	80	Total	O	0	0
			80	80		



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

Chain F:



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

Chain E:



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

Chain G:



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

Chain I:



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

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.75Å 104.75Å 352.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.30 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.95-2.30) 83.0 (19.95-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.250 , 0.278 0.256 , 0.292	Depositor DCC
R_{free} test set	4348 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10333	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4198e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MAN, EDO, BMA, NAG, FUC, CA

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	0.17	0/3292	0.35	0/4497
1	B	0.15	0/3272	0.35	0/4470
1	C	0.15	0/3205	0.34	0/4378
All	All	0.16	0/9769	0.35	0/13345

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 [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	3222	0	3112	18	0
1	B	3205	0	3092	20	0
1	C	3144	0	3020	17	0
2	D	49	0	43	1	0
2	F	49	0	43	0	0
3	E	24	0	22	1	0
3	G	24	0	22	1	0
3	I	24	0	22	0	0
4	H	38	0	34	0	0
5	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	9	0	0	0	0
5	C	9	0	0	0	0
6	A	77	0	70	0	0
6	B	77	0	70	1	0
6	C	77	0	70	0	0
7	A	16	0	24	1	0
7	C	4	0	6	0	0
8	A	114	0	0	1	0
8	B	82	0	0	0	0
8	C	80	0	0	0	0
All	All	10333	0	9650	57	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.

The worst 5 of 57 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:C:477:VAL:HG12	1:C:484:VAL:HG22	1.77	0.67
1:B:477:VAL:HG12	1:B:484:VAL:HG22	1.77	0.66
1:A:388:TYR:HB2	1:A:410:LEU:HB2	1.78	0.65
1:C:336:ILE:HD11	1:C:376:THR:HG23	1.79	0.64
1:B:388:TYR:HB2	1:B:410:LEU:HB2	1.80	0.63

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	422/441 (96%)	410 (97%)	12 (3%)	0	100	100
1	B	419/441 (95%)	407 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	409/441 (93%)	401 (98%)	8 (2%)	0	100	100
All	All	1250/1323 (94%)	1218 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	357/380 (94%)	354 (99%)	3 (1%)	73	86
1	B	355/380 (93%)	347 (98%)	8 (2%)	44	63
1	C	348/380 (92%)	346 (99%)	2 (1%)	78	89
All	All	1060/1140 (93%)	1047 (99%)	13 (1%)	63	79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	322	VAL
1	B	352	VAL
1	C	363	VAL
1	B	367	SER
1	C	335	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	300	HIS
1	C	370	ASN
1	C	631	HIS
1	C	528	ASN
1	A	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	0.54	0
2	NAG	D	2	2	14,14,15	0.80	1 (7%)	17,19,21	0.93	1 (5%)
2	BMA	D	3	2	11,11,12	0.79	0	15,15,17	1.46	2 (13%)
2	FUC	D	4	2	10,10,11	0.75	0	14,14,16	0.71	0
3	NAG	E	1	1,3	14,14,15	0.55	0	17,19,21	0.42	0
3	FUC	E	2	3	10,10,11	1.20	2 (20%)	14,14,16	1.33	2 (14%)
2	NAG	F	1	1,2	14,14,15	0.22	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.84	1 (7%)	17,19,21	0.79	1 (5%)
2	BMA	F	3	2	11,11,12	0.73	0	15,15,17	1.12	1 (6%)
2	FUC	F	4	2	10,10,11	0.82	0	14,14,16	0.76	0
3	NAG	G	1	1,3	14,14,15	0.50	0	17,19,21	1.19	1 (5%)
3	FUC	G	2	3	10,10,11	2.01	3 (30%)	14,14,16	1.57	3 (21%)
4	NAG	H	1	1,4	14,14,15	0.39	0	17,19,21	0.55	0
4	NAG	H	2	4	14,14,15	0.28	0	17,19,21	0.36	0
4	FUC	H	3	4	10,10,11	0.93	0	14,14,16	0.90	0
3	NAG	I	1	1,3	14,14,15	0.54	0	17,19,21	0.68	0
3	FUC	I	2	3	10,10,11	1.43	1 (10%)	14,14,16	0.99	1 (7%)

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	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	FUC	F	4	2	-	-	0/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	FUC	C1-C2	4.67	1.63	1.52
3	I	2	FUC	O5-C1	-3.14	1.38	1.43
3	G	2	FUC	C2-C3	3.05	1.57	1.52
3	E	2	FUC	O5-C5	2.95	1.49	1.43
2	F	2	NAG	C1-C2	2.67	1.56	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-O5-C5	4.06	117.62	112.19
3	G	2	FUC	C1-C2-C3	3.71	115.04	109.64
3	G	1	NAG	C1-O5-C5	3.60	117.00	112.19
3	E	2	FUC	C1-O5-C5	3.37	120.91	112.97
3	G	2	FUC	C1-O5-C5	3.27	120.68	112.97

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

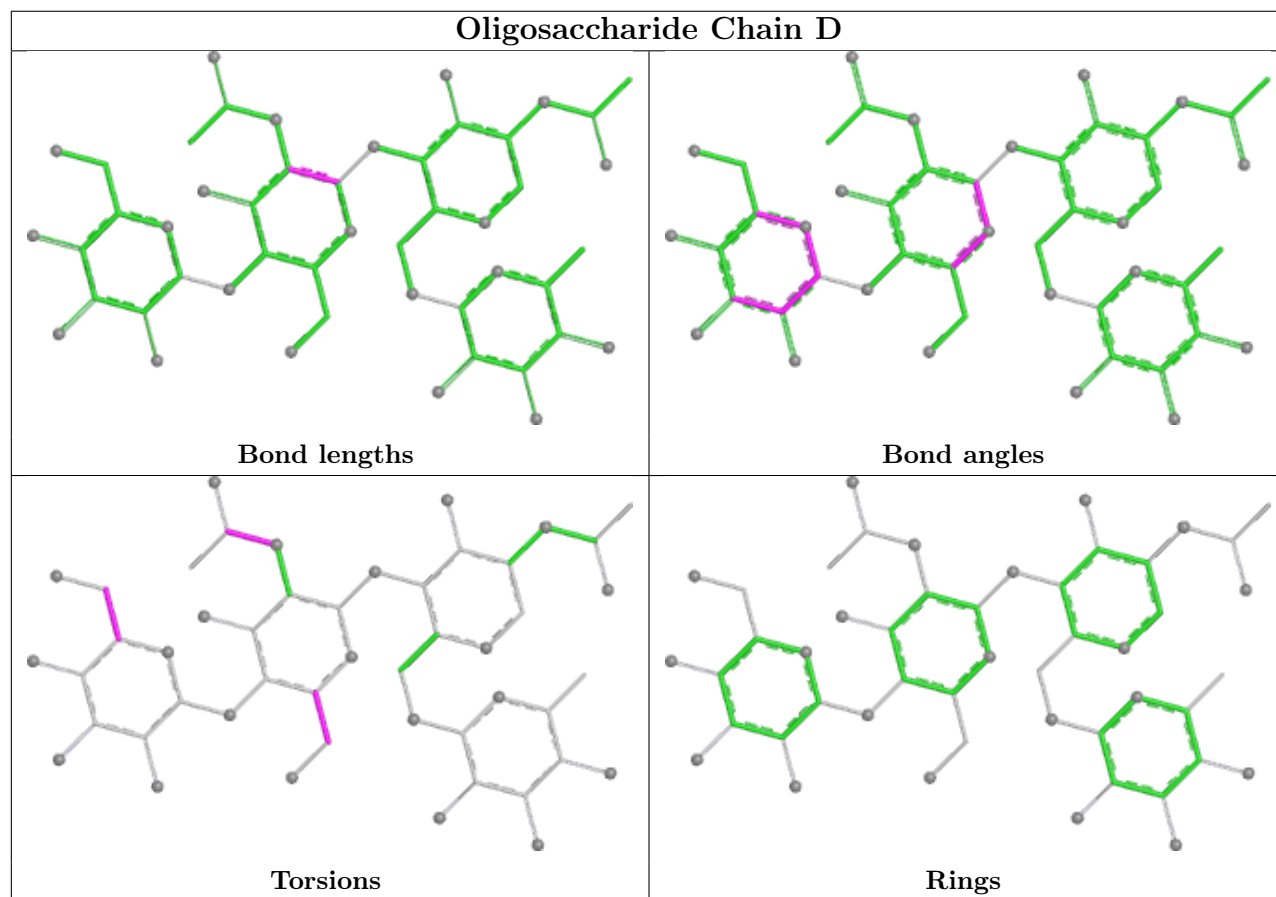
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

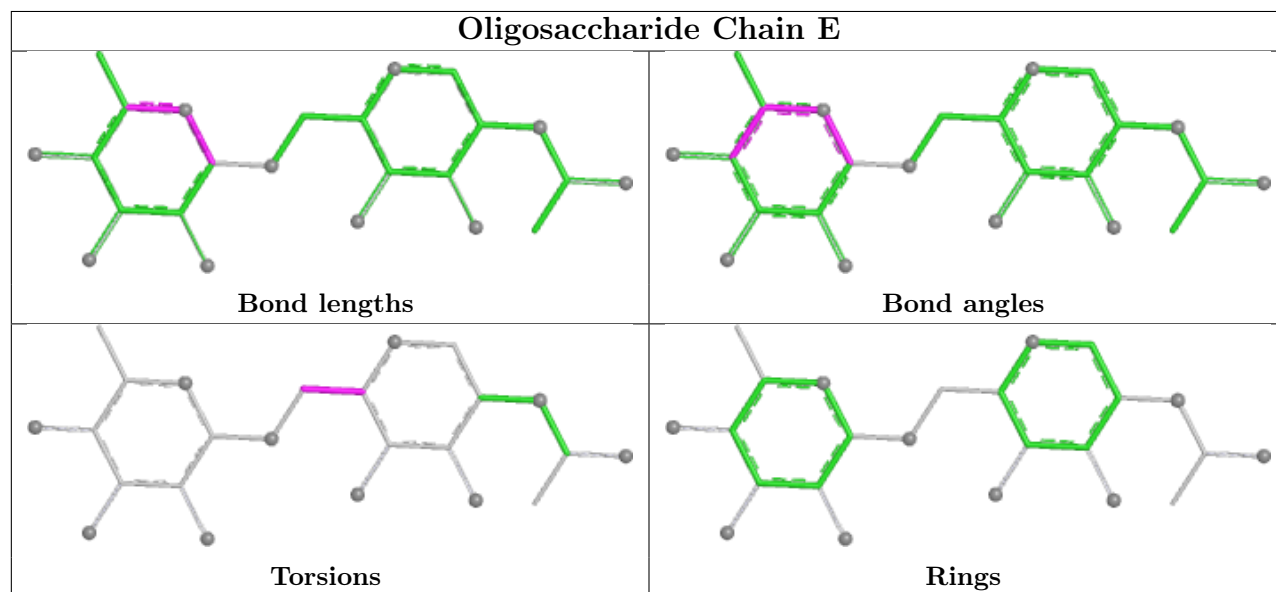
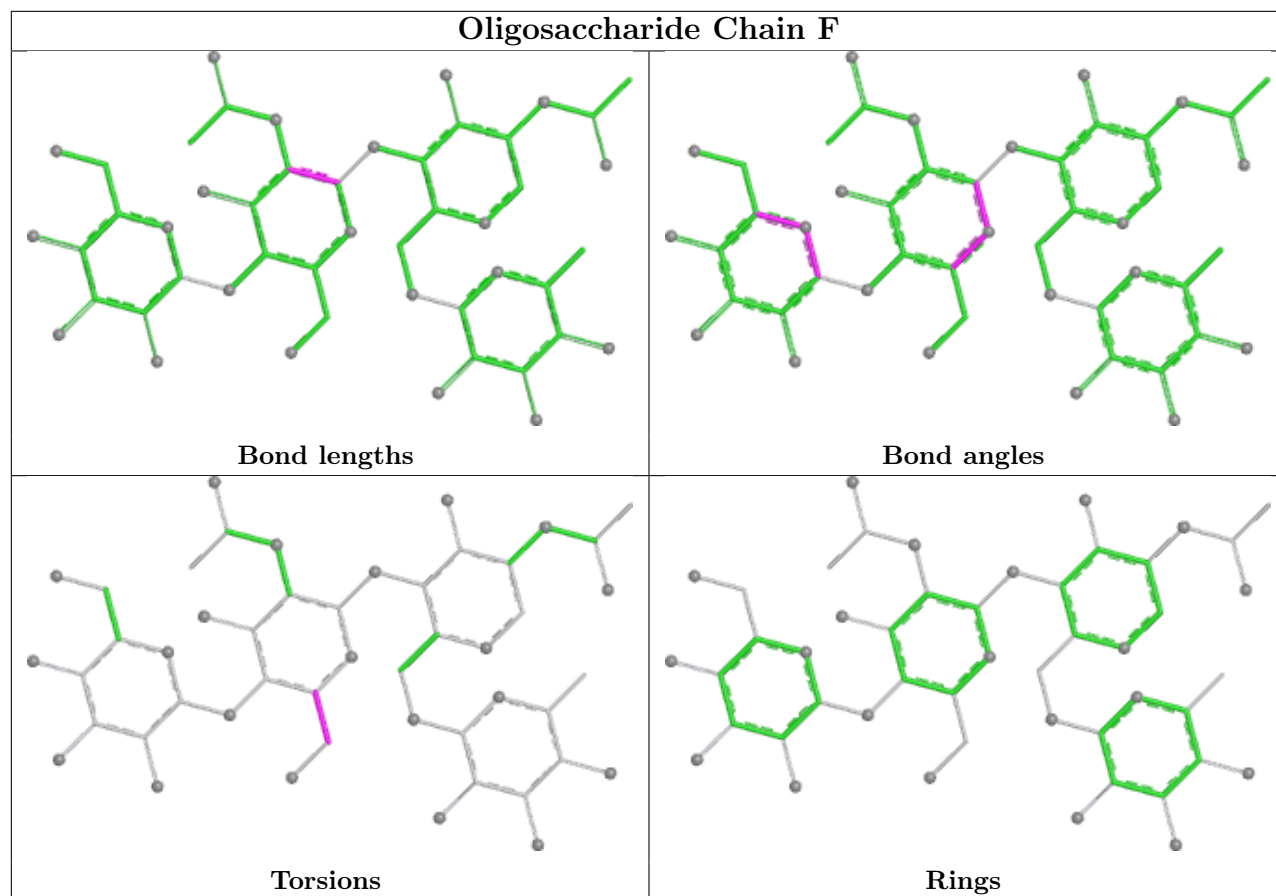
There are no ring outliers.

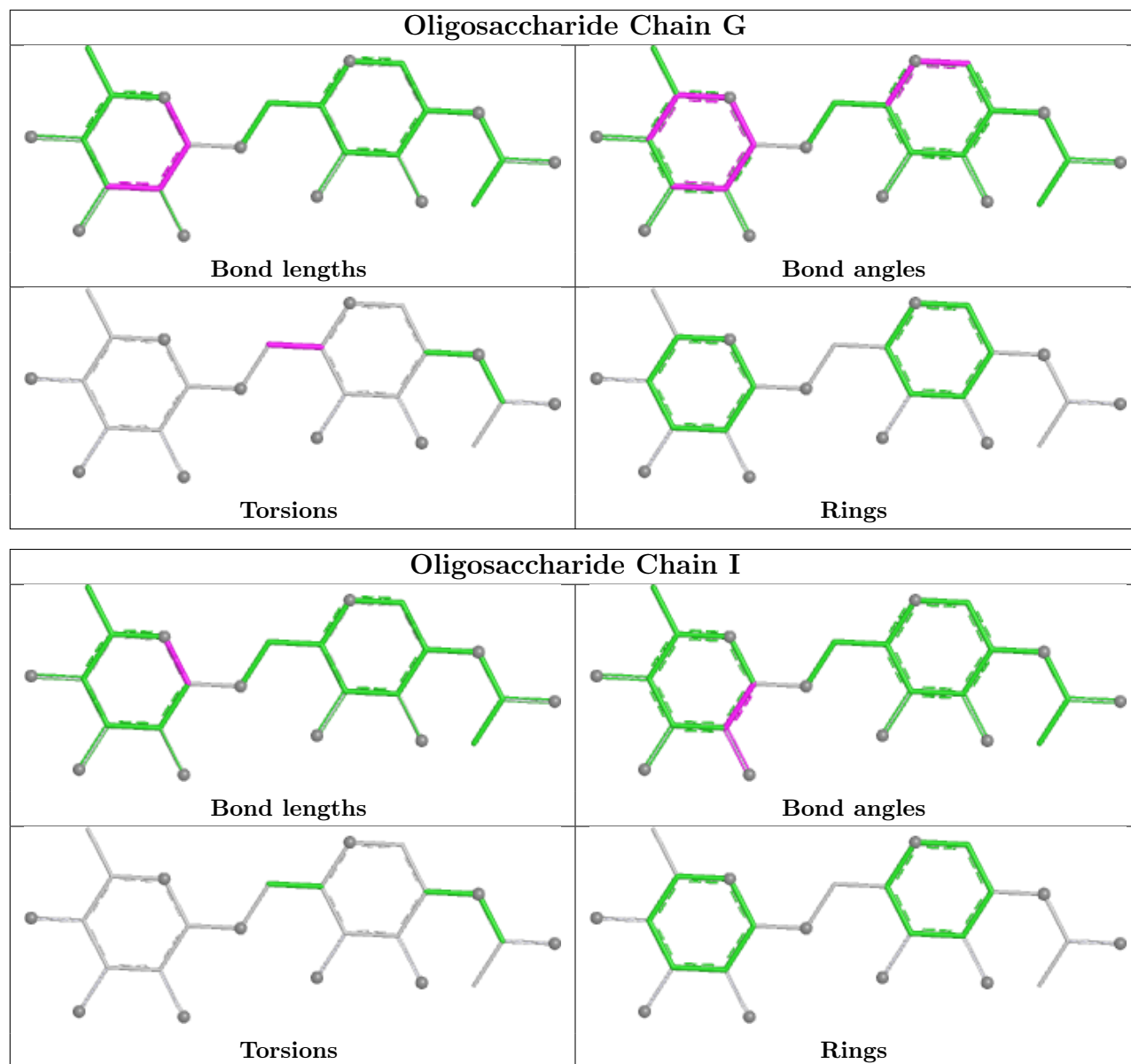
5 monomers are involved in 3 short contacts:

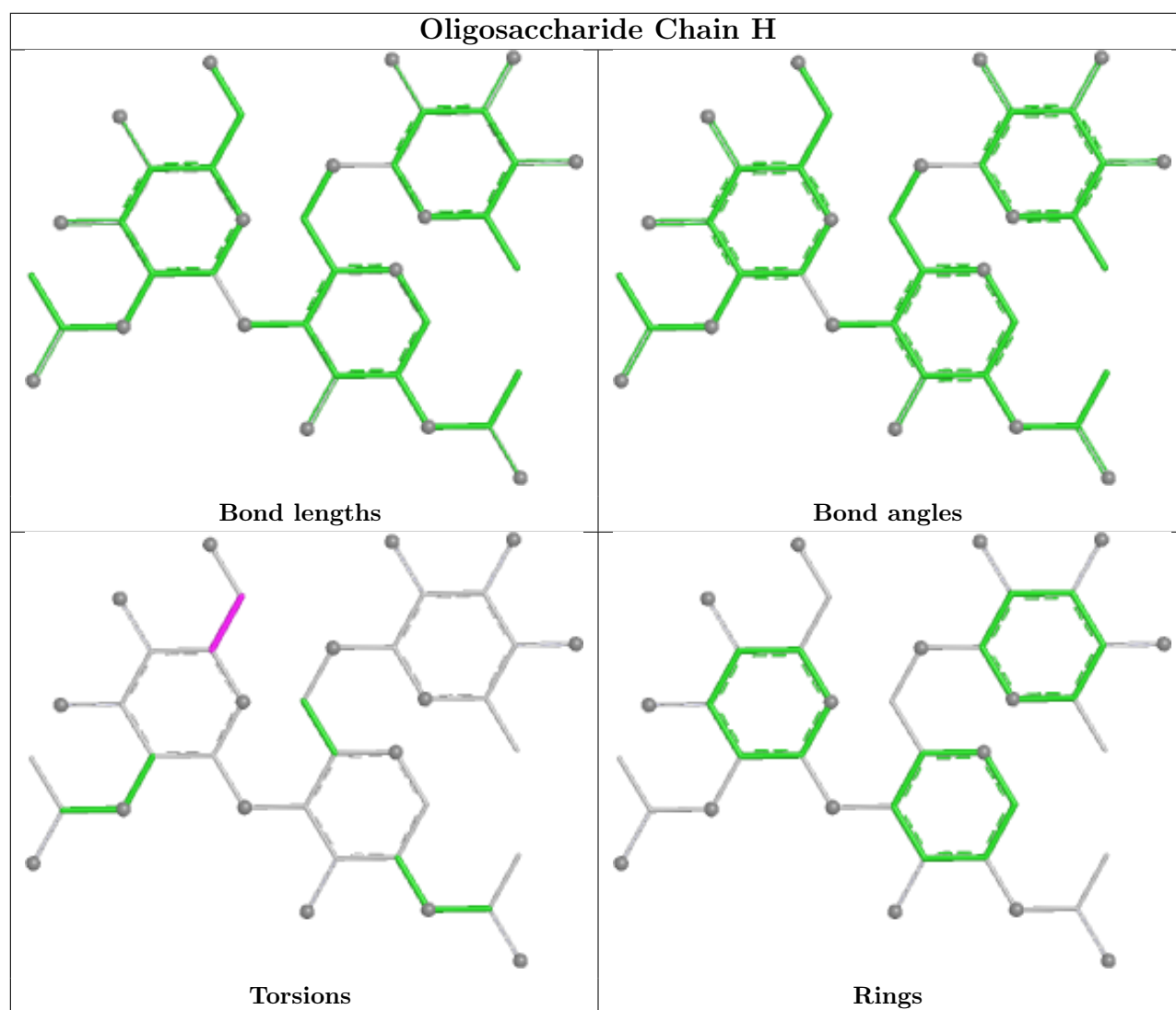
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	G	2	FUC	1	0
2	D	1	NAG	1	0
3	E	1	NAG	1	0
2	D	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 27 are monoatomic - leaving 26 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	$\# Z > 2$
6	MAN	A	720	1	11,11,12	0.74	0	15,15,17	1.19	1 (6%)
6	MAN	C	717	1	11,11,12	0.75	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	721	1	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
6	MAN	B	719	1	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
6	MAN	C	720	1	11,11,12	0.92	0	15,15,17	0.98	1 (6%)
6	MAN	A	719	1	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
6	MAN	C	715	1	11,11,12	0.79	0	15,15,17	1.22	1 (6%)
6	MAN	C	718	1	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
6	MAN	C	719	1	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
6	MAN	C	716	1	11,11,12	0.77	0	15,15,17	1.06	2 (13%)
6	MAN	A	718	1	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
6	MAN	A	722	1	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
7	EDO	A	725	-	3,3,3	0.42	0	2,2,2	0.40	0
7	EDO	A	724	-	3,3,3	0.43	0	2,2,2	0.38	0
6	MAN	B	716	1	11,11,12	0.89	0	15,15,17	0.93	0
6	MAN	B	717	1	11,11,12	0.71	0	15,15,17	1.15	1 (6%)
6	MAN	B	721	1	11,11,12	0.76	0	15,15,17	1.08	2 (13%)
7	EDO	C	722	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	A	723	-	3,3,3	0.44	0	2,2,2	0.36	0
6	MAN	C	721	1	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
6	MAN	B	718	1	11,11,12	0.74	0	15,15,17	1.01	2 (13%)
6	MAN	B	722	1	11,11,12	0.79	0	15,15,17	0.94	2 (13%)
6	MAN	A	716	1	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
6	MAN	A	717	1	11,11,12	0.81	0	15,15,17	1.02	1 (6%)
7	EDO	A	726	-	3,3,3	0.41	0	2,2,2	0.37	0
6	MAN	B	720	1	11,11,12	0.85	0	15,15,17	0.99	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	720	1	-	0/2/19/22	0/1/1/1
6	MAN	C	717	1	-	1/2/19/22	0/1/1/1
6	MAN	A	721	1	-	2/2/19/22	0/1/1/1
6	MAN	B	719	1	-	1/2/19/22	0/1/1/1
6	MAN	C	720	1	-	0/2/19/22	0/1/1/1
6	MAN	A	719	1	-	0/2/19/22	0/1/1/1
6	MAN	C	715	1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	C	718	1	-	0/2/19/22	0/1/1/1
6	MAN	C	719	1	-	0/2/19/22	0/1/1/1
6	MAN	C	716	1	-	1/2/19/22	0/1/1/1
6	MAN	A	718	1	-	1/2/19/22	0/1/1/1
6	MAN	A	722	1	-	0/2/19/22	0/1/1/1
7	EDO	A	725	-	-	0/1/1/1	-
7	EDO	A	724	-	-	0/1/1/1	-
6	MAN	B	716	1	-	1/2/19/22	0/1/1/1
6	MAN	B	717	1	-	0/2/19/22	0/1/1/1
6	MAN	B	721	1	-	1/2/19/22	0/1/1/1
7	EDO	C	722	-	-	0/1/1/1	-
7	EDO	A	723	-	-	1/1/1/1	-
6	MAN	C	721	1	-	2/2/19/22	0/1/1/1
6	MAN	B	718	1	-	0/2/19/22	0/1/1/1
6	MAN	B	722	1	-	0/2/19/22	0/1/1/1
6	MAN	A	716	1	-	1/2/19/22	0/1/1/1
6	MAN	A	717	1	-	0/2/19/22	0/1/1/1
7	EDO	A	726	-	-	0/1/1/1	-
6	MAN	B	720	1	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	719	MAN	C1-O5-C5	3.95	117.48	112.19
6	A	720	MAN	C1-O5-C5	3.79	117.27	112.19
6	C	715	MAN	C1-O5-C5	3.56	116.96	112.19
6	B	717	MAN	C1-O5-C5	3.21	116.48	112.19
6	C	716	MAN	C1-O5-C5	2.89	116.05	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	720	MAN	O5-C5-C6-O6
6	A	721	MAN	O5-C5-C6-O6
6	B	720	MAN	C4-C5-C6-O6
6	C	715	MAN	O5-C5-C6-O6
6	A	721	MAN	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	726	EDO	1	0
6	B	720	MAN	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/441 (96%)	0.22	13 (3%) 51 53	41, 64, 104, 161	2 (0%)
1	B	422/441 (95%)	0.42	21 (4%) 34 35	40, 72, 114, 171	1 (0%)
1	C	415/441 (94%)	0.44	17 (4%) 41 43	46, 67, 131, 169	0
All	All	1261/1323 (95%)	0.36	51 (4%) 42 44	40, 68, 121, 171	3 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	236	ALA	6.2
1	C	210	PRO	5.4
1	B	209	PRO	5.1
1	C	238	ASP	4.8
1	A	209	PRO	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

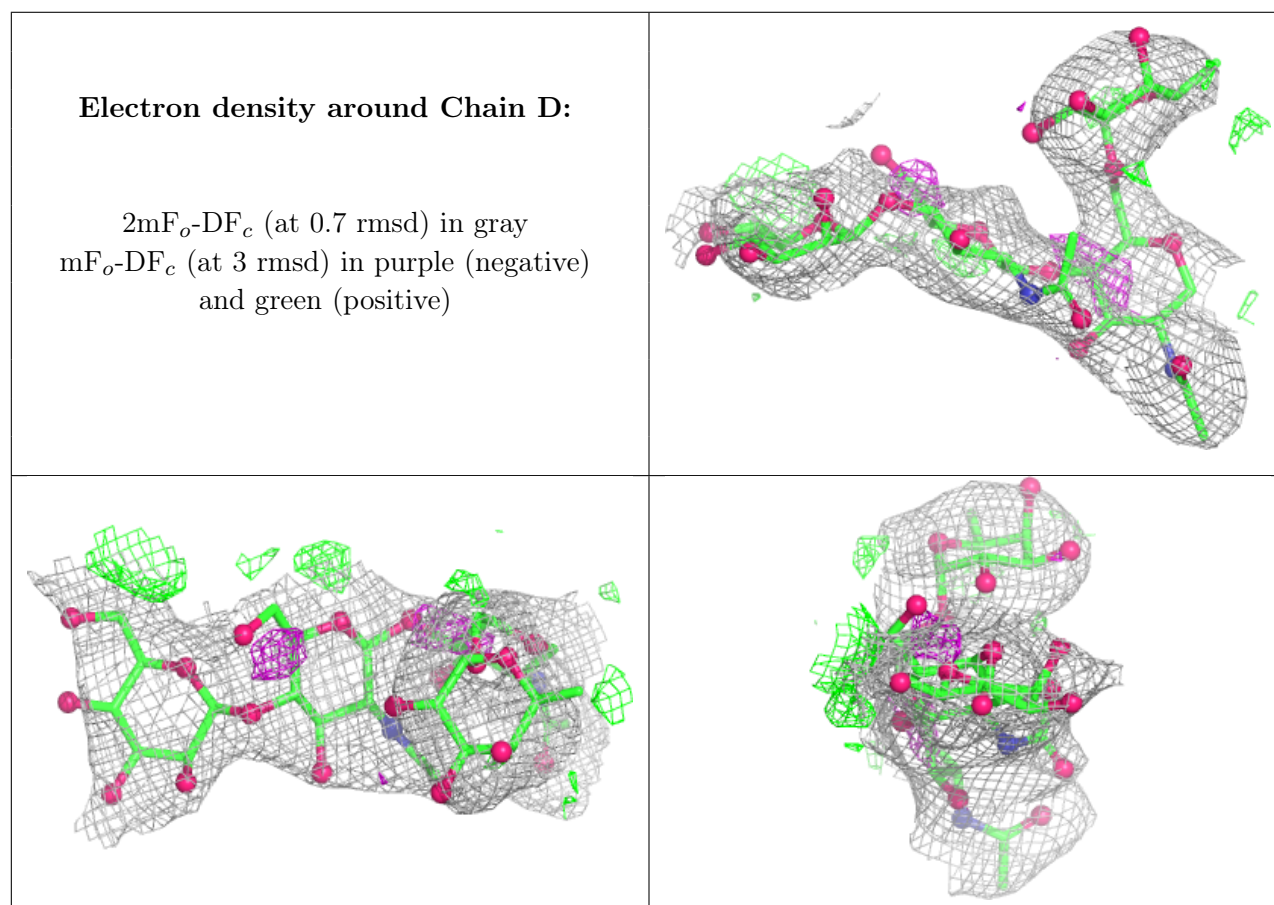
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	E	2	10/11	0.01	0.21	109,112,114,116	0
3	FUC	I	2	10/11	0.15	0.18	109,112,115,115	0
2	BMA	D	3	11/12	0.25	0.14	114,115,116,116	0

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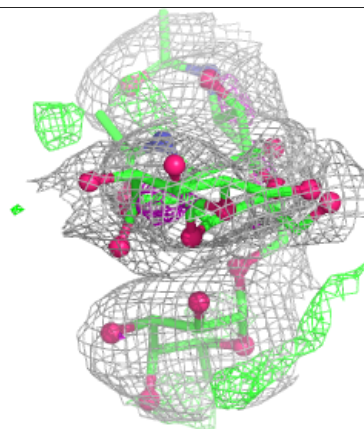
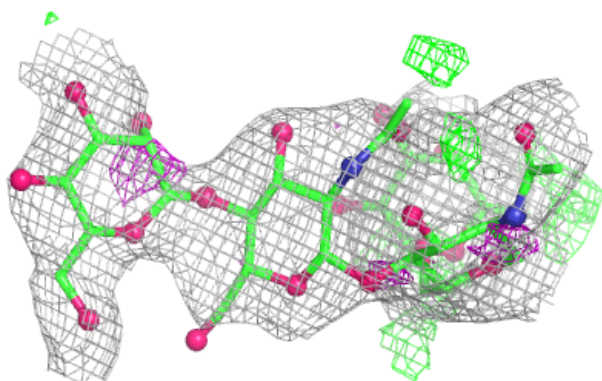
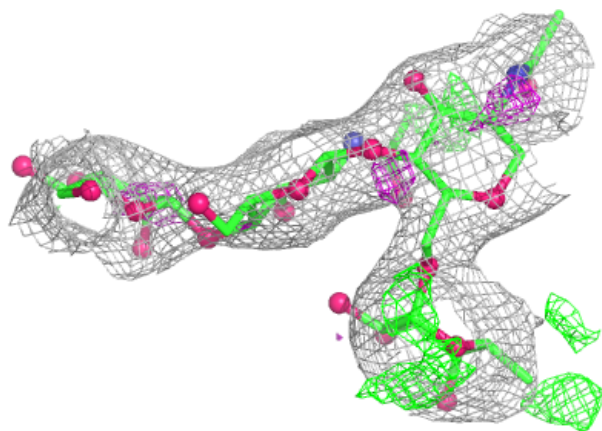
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	F	3	11/12	0.27	0.16	118,119,120,120	0
2	FUC	F	4	10/11	0.44	0.21	105,108,109,110	0
4	FUC	H	3	10/11	0.48	0.19	98,100,100,101	0
2	FUC	D	4	10/11	0.59	0.18	97,100,101,102	0
2	NAG	F	2	14/15	0.60	0.13	105,109,111,115	0
3	FUC	G	2	10/11	0.60	0.14	108,111,113,115	0
2	NAG	D	2	14/15	0.61	0.14	99,106,109,112	0
3	NAG	I	1	14/15	0.66	0.12	76,84,96,103	0
4	NAG	H	2	14/15	0.67	0.13	97,102,105,106	0
3	NAG	G	1	14/15	0.71	0.12	77,84,96,102	0
2	NAG	F	1	14/15	0.72	0.13	78,85,99,100	0
2	NAG	D	1	14/15	0.78	0.12	66,75,92,93	0
4	NAG	H	1	14/15	0.78	0.11	70,77,92,93	0
3	NAG	E	1	14/15	0.79	0.12	72,82,97,104	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.



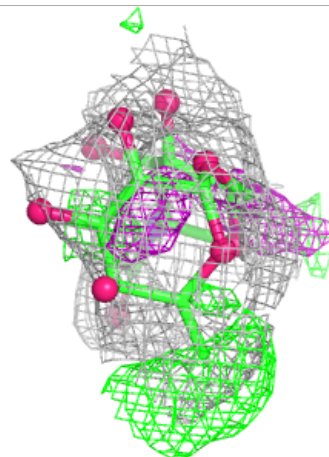
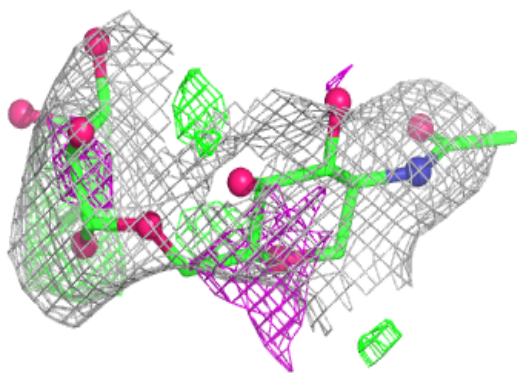
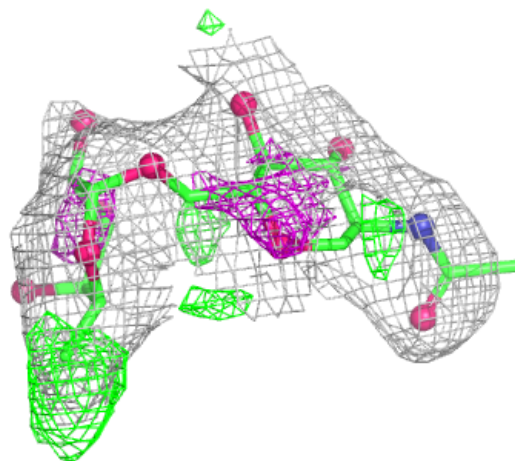
Electron density around Chain F:

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



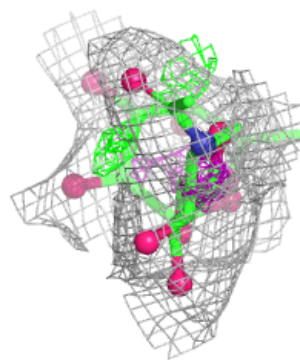
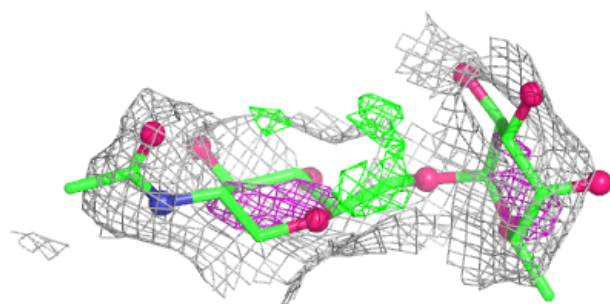
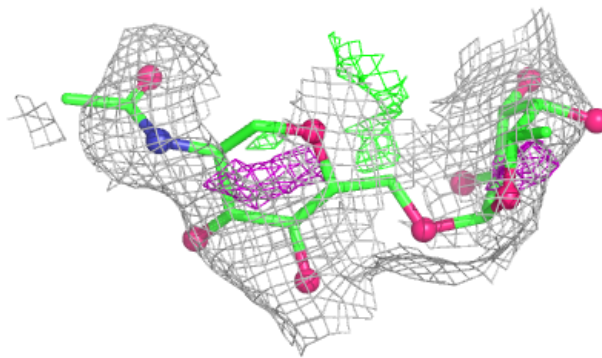
Electron density around Chain E:

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

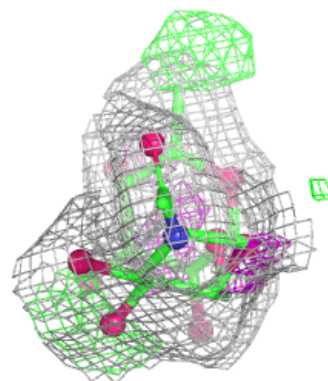
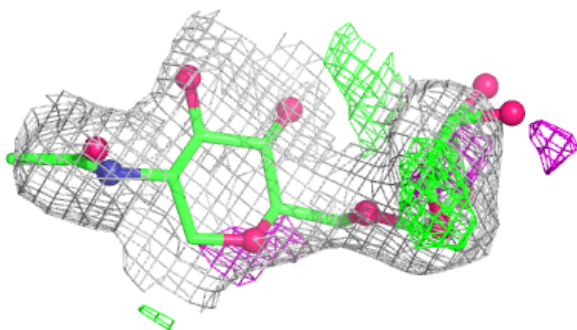
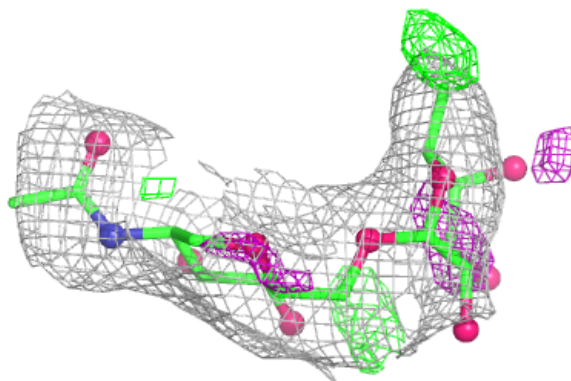


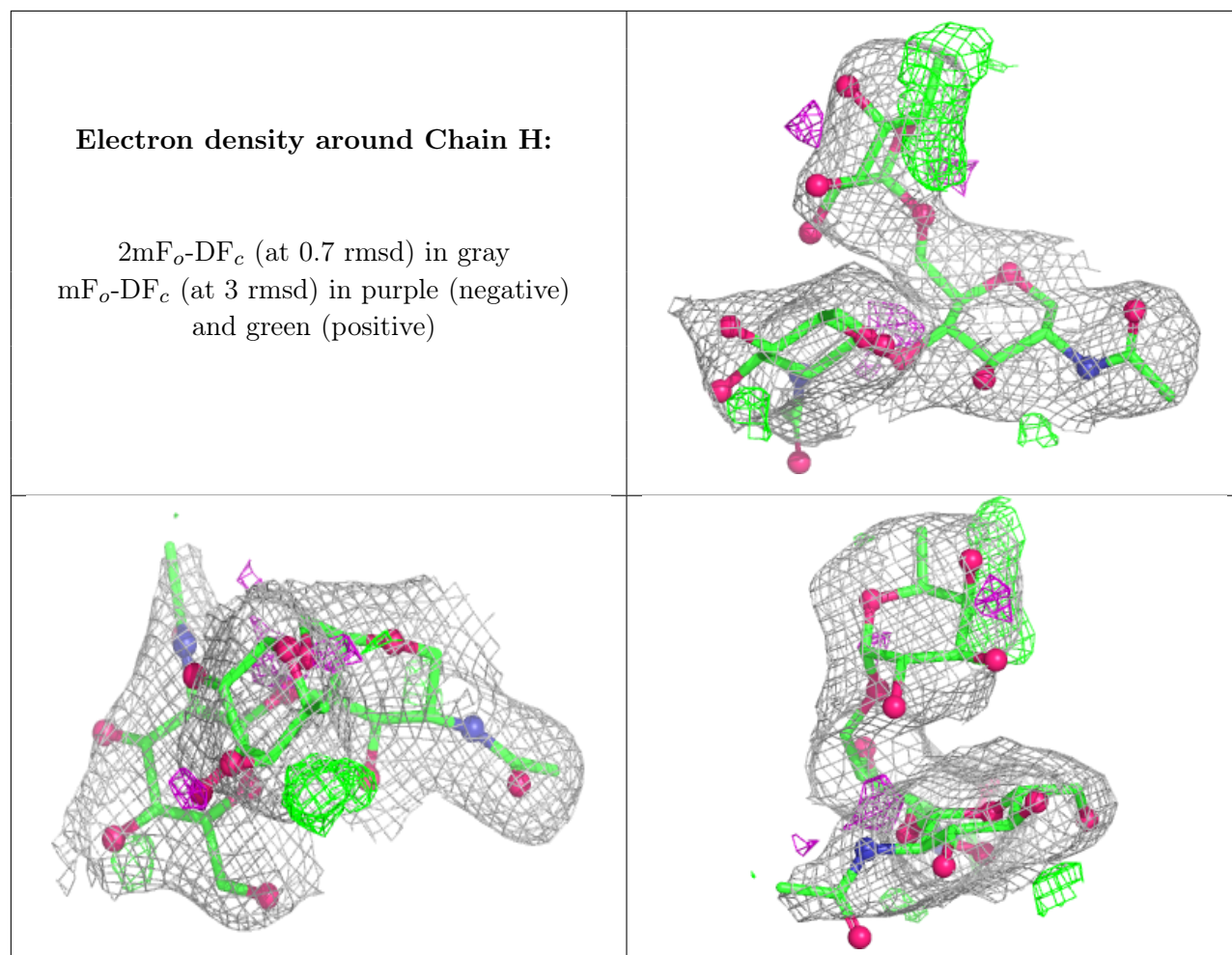
Electron density around Chain G:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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	A	721	11/12	0.60	0.14	71,81,87,93	0
6	MAN	C	715	11/12	0.63	0.11	72,79,82,83	0
6	MAN	B	721	11/12	0.67	0.13	76,85,89,91	0
6	MAN	C	720	11/12	0.67	0.13	73,80,83,83	0
6	MAN	C	721	11/12	0.70	0.13	68,76,80,82	0
6	MAN	B	722	11/12	0.71	0.13	69,78,82,86	0
6	MAN	C	719	11/12	0.71	0.11	65,73,76,77	0
6	MAN	A	716	11/12	0.75	0.11	70,78,82,84	0
7	EDO	A	725	4/4	0.76	0.18	73,73,75,77	0
6	MAN	B	716	11/12	0.78	0.10	70,74,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	723	4/4	0.80	0.17	62,64,66,67	0
6	MAN	A	720	11/12	0.80	0.10	55,63,70,75	0
6	MAN	A	722	11/12	0.81	0.11	61,70,74,77	0
6	MAN	B	719	11/12	0.82	0.10	65,71,78,81	0
6	MAN	B	720	11/12	0.82	0.10	58,68,75,77	0
7	EDO	A	726	4/4	0.82	0.14	76,78,82,84	0
6	MAN	C	718	11/12	0.86	0.08	65,69,74,74	0
6	MAN	A	717	11/12	0.87	0.10	60,70,75,77	0
6	MAN	A	719	11/12	0.89	0.08	59,68,71,72	0
6	MAN	C	716	11/12	0.91	0.07	53,61,64,68	0
6	MAN	C	717	11/12	0.91	0.07	52,59,61,62	0
6	MAN	B	718	11/12	0.91	0.07	50,59,62,63	0
7	EDO	C	722	4/4	0.92	0.15	76,76,78,80	0
6	MAN	A	718	11/12	0.93	0.06	47,53,58,58	0
6	MAN	B	717	11/12	0.93	0.07	66,73,76,77	0
7	EDO	A	724	4/4	0.94	0.12	72,73,73,73	4
5	CA	B	713	1/1	0.94	0.07	68,68,68,68	0
5	CA	B	711	1/1	0.96	0.06	63,63,63,63	0
5	CA	A	714	1/1	0.97	0.04	52,52,52,52	0
5	CA	C	706	1/1	0.97	0.06	81,81,81,81	0
5	CA	C	707	1/1	0.97	0.04	74,74,74,74	0
5	CA	C	712	1/1	0.97	0.04	55,55,55,55	0
5	CA	B	708	1/1	0.97	0.04	68,68,68,68	0
5	CA	A	713	1/1	0.97	0.04	50,50,50,50	0
5	CA	C	708	1/1	0.98	0.04	75,75,75,75	0
5	CA	B	714	1/1	0.98	0.03	55,55,55,55	0
5	CA	B	707	1/1	0.98	0.04	64,64,64,64	0
5	CA	A	712	1/1	0.98	0.02	47,47,47,47	0
5	CA	C	713	1/1	0.99	0.02	52,52,52,52	0
5	CA	C	714	1/1	0.99	0.02	51,51,51,51	0
5	CA	B	710	1/1	0.99	0.02	61,61,61,61	0
5	CA	A	707	1/1	0.99	0.03	61,61,61,61	0
5	CA	B	712	1/1	0.99	0.03	60,60,60,60	0
5	CA	A	708	1/1	0.99	0.04	62,62,62,62	0
5	CA	A	709	1/1	0.99	0.03	63,63,63,63	0
5	CA	B	715	1/1	0.99	0.07	66,66,66,66	0
5	CA	A	715	1/1	0.99	0.02	43,43,43,43	0
5	CA	A	710	1/1	0.99	0.04	54,54,54,54	0
5	CA	A	711	1/1	0.99	0.07	56,56,56,56	0
5	CA	C	710	1/1	0.99	0.03	55,55,55,55	0
5	CA	C	711	1/1	0.99	0.03	54,54,54,54	0
5	CA	B	709	1/1	0.99	0.03	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	C	709	1/1	1.00	0.02	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.