



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:53 AM BST

PDB ID : 5ERD
Title : Crystal structure of human Desmoglein-2 ectodomain
Authors : Brasch, J.; Harrison, O.J.; Shapiro, L.
Deposited on : 2015-11-13
Resolution : 2.90 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 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

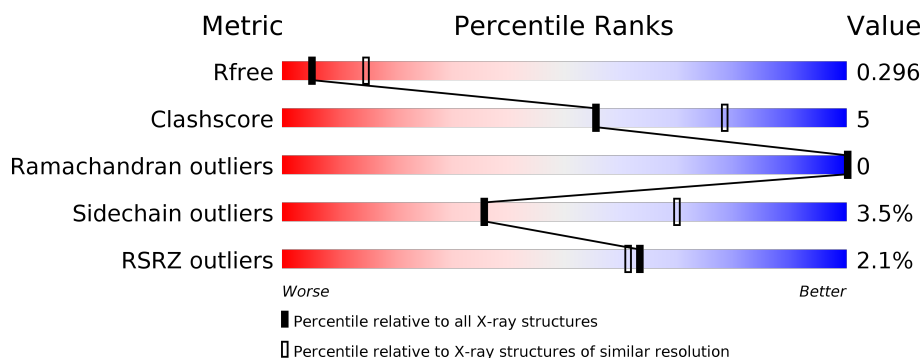
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.




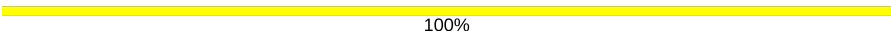

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	559	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 11% .. </div> </div>
1	B	559	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 89% 11% </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 33%, orange 34%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 33% 33% 33% </div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 33%, orange 67%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 33% 67% </div> </div>
2	G	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>
3	E	4	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	 50%50%
4	H	2	 100%
4	I	2	 50%50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18333 atoms, of which 8981 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 Desmoglein-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	554	Total	C	H	N	O	S	0	2	0
			8661	2756	4295	726	873	11			
1	B	559	Total	C	H	N	O	S	0	1	0
			8735	2782	4325	740	877	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	-	expression tag	UNP Q14126
A	555	HIS	-	expression tag	UNP Q14126
A	556	HIS	-	expression tag	UNP Q14126
A	557	HIS	-	expression tag	UNP Q14126
A	558	HIS	-	expression tag	UNP Q14126
A	559	HIS	-	expression tag	UNP Q14126
B	554	HIS	-	expression tag	UNP Q14126
B	555	HIS	-	expression tag	UNP Q14126
B	556	HIS	-	expression tag	UNP Q14126
B	557	HIS	-	expression tag	UNP Q14126
B	558	HIS	-	expression tag	UNP Q14126
B	559	HIS	-	expression tag	UNP Q14126

- Molecule 2 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.



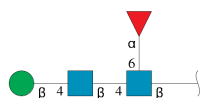
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O		0	0	0
			77	22	38	2	15				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	3	Total	C	H	N	O	0	0	0
			77	22	38	2	15			
2	G	3	Total	C	H	N	O	0	0	0
			77	22	38	2	15			

- Molecule 3 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
3	E	4	Total	C	H	N	O	0	0	0
			98	28	49	2	19			

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



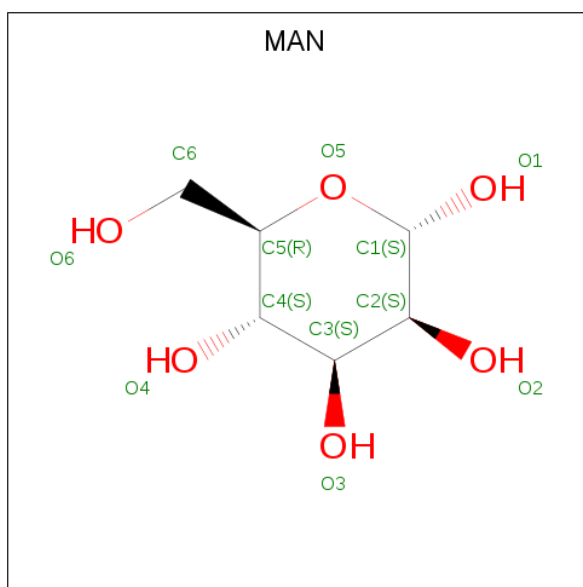
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	2	Total	C	H	N	O	0	0	0
			56	16	28	2	10			
4	H	2	Total	C	H	N	O	0	0	0
			56	16	28	2	10			
4	I	2	Total	C	H	N	O	0	0	0
			56	16	28	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	11	5		

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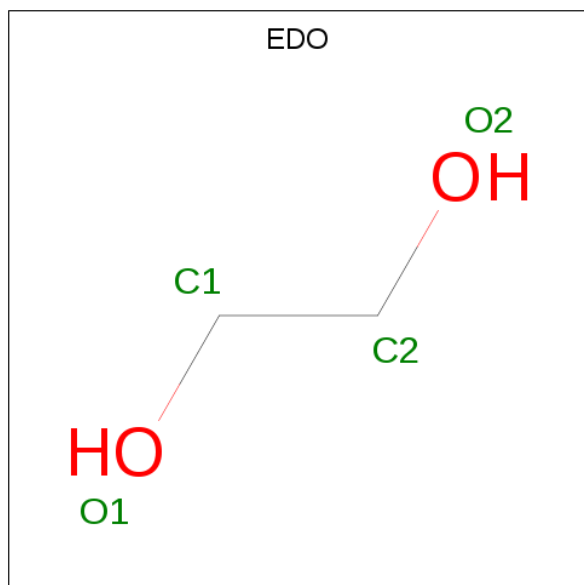
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total	Ca	0	0
			11	11		
7	A	11	Total	Ca	0	0
			11	11		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	98	Total 98	O 98	0	0
9	B	94	Total 94	O 94	0	0

Chain D:  33% 67%

MAG1
MAG2
BGL3

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

Chain G:  100%

MAG1
MAG2
BGL3

- Molecule 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

Chain E:  100%

MAG1
MAG2
BGL3
FUC4

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.97Å 114.48Å 226.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.39 – 2.90 84.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.39-2.90) 86.4 (84.39-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.91Å)	Xtriage
Refinement program	PHENIX dev_1810	Depositor
R, R_{free}	0.241 , 0.287 0.246 , 0.296	Depositor DCC
R_{free} test set	2664 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18333	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, EDO, FUC, 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	0.40	1/4455 (0.0%)	0.55	4/6049 (0.1%)
1	B	0.38	0/4501	0.53	5/6112 (0.1%)
All	All	0.39	1/8956 (0.0%)	0.54	9/12161 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	ASP	CB-CG	5.06	1.62	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	218	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	248	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	525	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	138	ASP	CB-CG-OD1	5.54	123.28	118.30

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	4366	4295	4297	39	2
1	B	4410	4325	4325	30	1
2	C	39	38	34	2	0
2	D	39	38	34	6	0
2	G	39	38	34	7	0
3	E	49	49	43	6	0
4	F	28	28	25	4	0
4	H	28	28	25	0	0
4	I	28	28	25	3	0
5	A	28	28	26	3	0
5	B	14	14	13	1	0
6	A	33	33	30	0	0
6	B	33	33	29	2	1
7	A	11	0	0	0	0
7	B	11	0	0	0	0
8	A	4	6	5	0	0
9	A	98	0	0	5	0
9	B	94	0	0	2	0
All	All	9352	8981	8945	92	3

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

The worst 5 of 92 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:NAG:C6	2:D:2:NAG:H2	2.04	0.88
1:A:133:ASN:OD1	1:A:134:ALA:N	2.13	0.82
2:G:2:NAG:O6	2:G:3:BMA:O5	1.98	0.81
2:D:1:NAG:O6	2:D:2:NAG:O7	2.00	0.80
4:I:2:NAG:H82	4:I:2:NAG:H3	1.65	0.79

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:O	6:B:901:MAN:O4[1_554]	1.67	0.53
1:A:158:TYR:OH	1:A:484:VAL:O[2_555]	1.97	0.23
1:B:158:TYR:OH	1:B:484:VAL:O[2_454]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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	554/559 (99%)	527 (95%)	27 (5%)	0	100	100
1	B	558/559 (100%)	527 (94%)	31 (6%)	0	100	100
All	All	1112/1118 (100%)	1054 (95%)	58 (5%)	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	494/497 (99%)	479 (97%)	15 (3%)	41	75
1	B	498/497 (100%)	478 (96%)	20 (4%)	31	65
All	All	992/994 (100%)	957 (96%)	35 (4%)	36	70

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	225	ASN
1	B	544	CYS
1	B	25	HIS
1	B	32	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	ASN

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 ⓘ

19 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	C	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	1.47	3 (17%)
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	2.93	8 (72%)	15,15,17	1.36	1 (6%)
2	NAG	D	1	1,2	14,14,15	2.16	1 (7%)	17,19,21	1.34	2 (11%)
2	NAG	D	2	2	14,14,15	1.92	2 (14%)	17,19,21	2.05	3 (17%)
2	BMA	D	3	2	11,11,12	3.05	8 (72%)	15,15,17	1.90	5 (33%)
3	NAG	E	1	1,3	14,14,15	1.05	1 (7%)	17,19,21	1.65	5 (29%)
3	NAG	E	2	3	14,14,15	0.87	2 (14%)	17,19,21	1.61	4 (23%)
3	BMA	E	3	3	11,11,12	2.44	6 (54%)	15,15,17	1.83	5 (33%)
3	FUC	E	4	3	10,10,11	1.41	2 (20%)	14,14,16	0.90	0
4	NAG	F	1	1,4	14,14,15	0.75	1 (7%)	17,19,21	2.05	3 (17%)
4	NAG	F	2	4	14,14,15	0.85	1 (7%)	17,19,21	0.82	0
2	NAG	G	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	1.95	3 (17%)
2	NAG	G	2	2	14,14,15	0.98	2 (14%)	17,19,21	1.52	3 (17%)
2	BMA	G	3	2	11,11,12	3.27	9 (81%)	15,15,17	1.47	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	1,4	14,14,15	1.05	1 (7%)	17,19,21	1.01	0
4	NAG	H	2	4	14,14,15	1.40	2 (14%)	17,19,21	1.11	1 (5%)
4	NAG	I	1	1,4	14,14,15	1.00	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	I	2	4	14,14,15	0.75	1 (7%)	17,19,21	1.45	1 (5%)

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	-7.83	1.31	1.43
2	D	2	NAG	C1-C2	5.93	1.61	1.52
2	D	3	BMA	O5-C1	5.41	1.52	1.43
2	G	3	BMA	O2-C2	5.09	1.54	1.43
2	C	3	BMA	O2-C2	4.49	1.52	1.43

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C2-N2-C7	6.12	131.61	122.90
2	D	2	NAG	C1-O5-C5	-5.79	104.35	112.19
2	G	1	NAG	C2-N2-C7	5.38	130.57	122.90
4	I	2	NAG	C2-N2-C7	4.86	129.83	122.90
3	E	2	NAG	C1-O5-C5	4.80	118.69	112.19

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

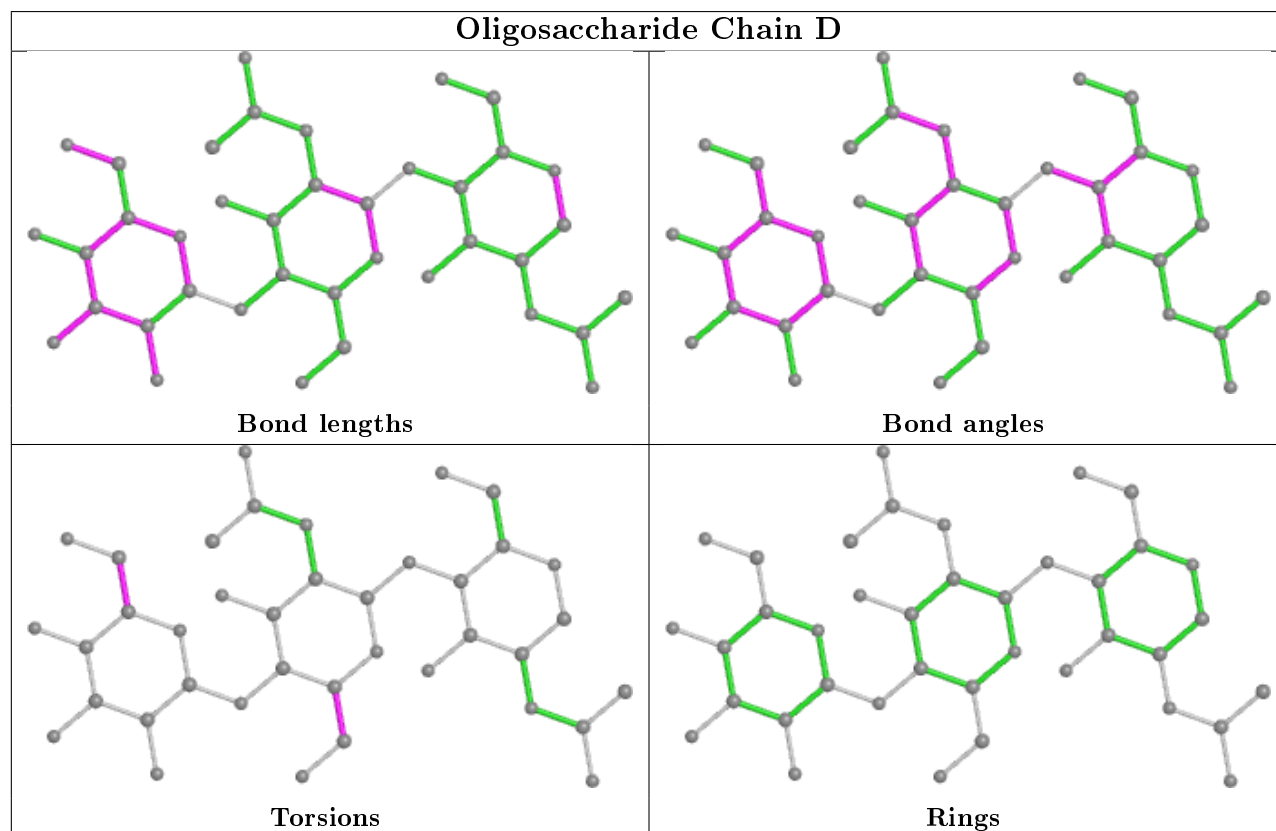
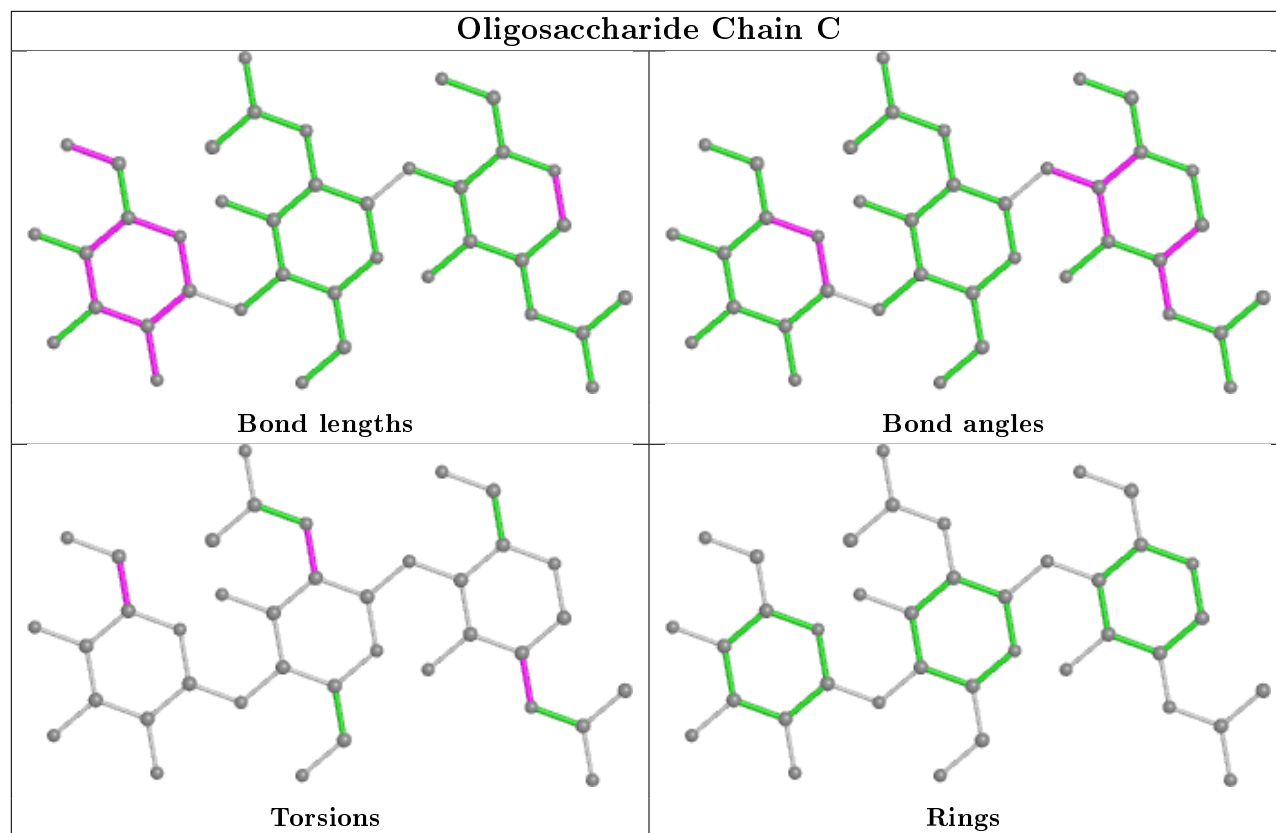
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
4	I	1	NAG	O5-C5-C6-O6

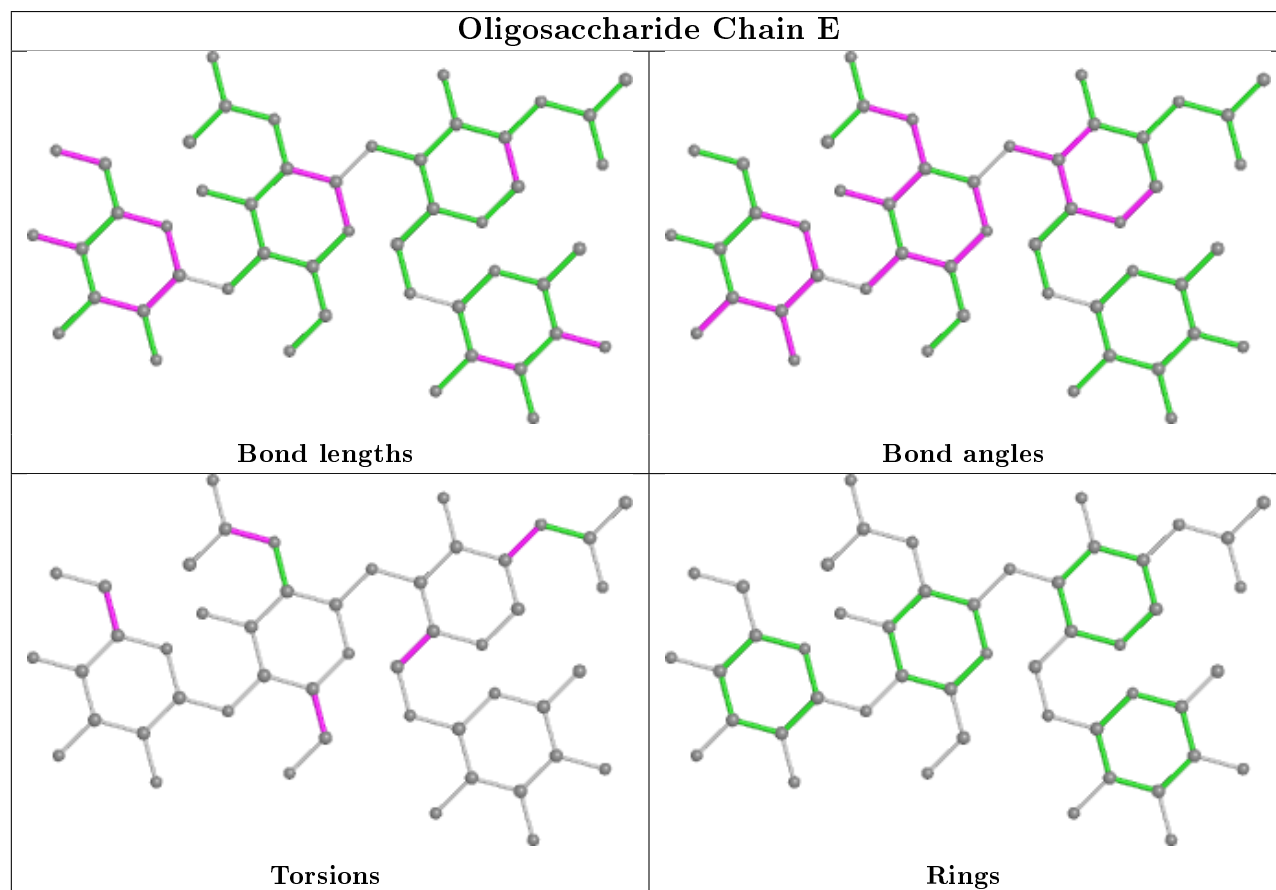
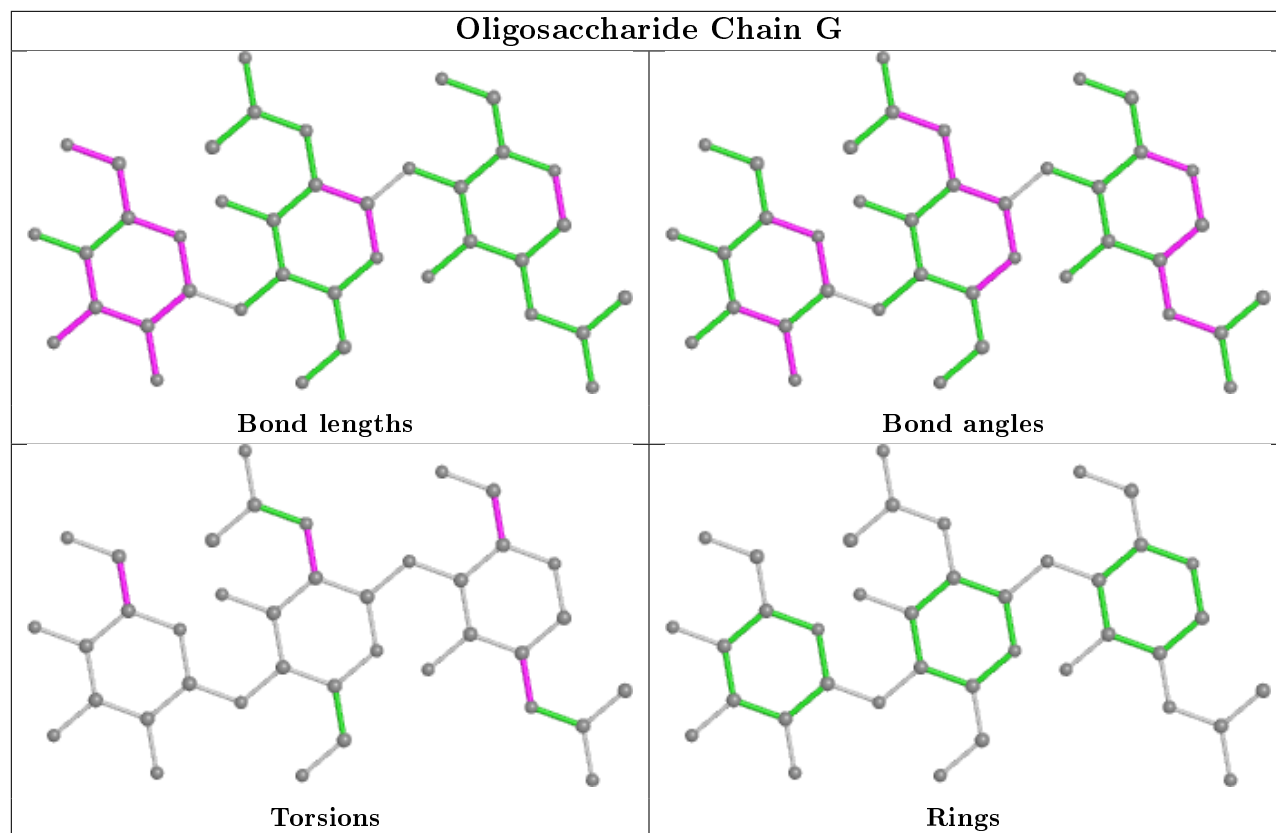
There are no ring outliers.

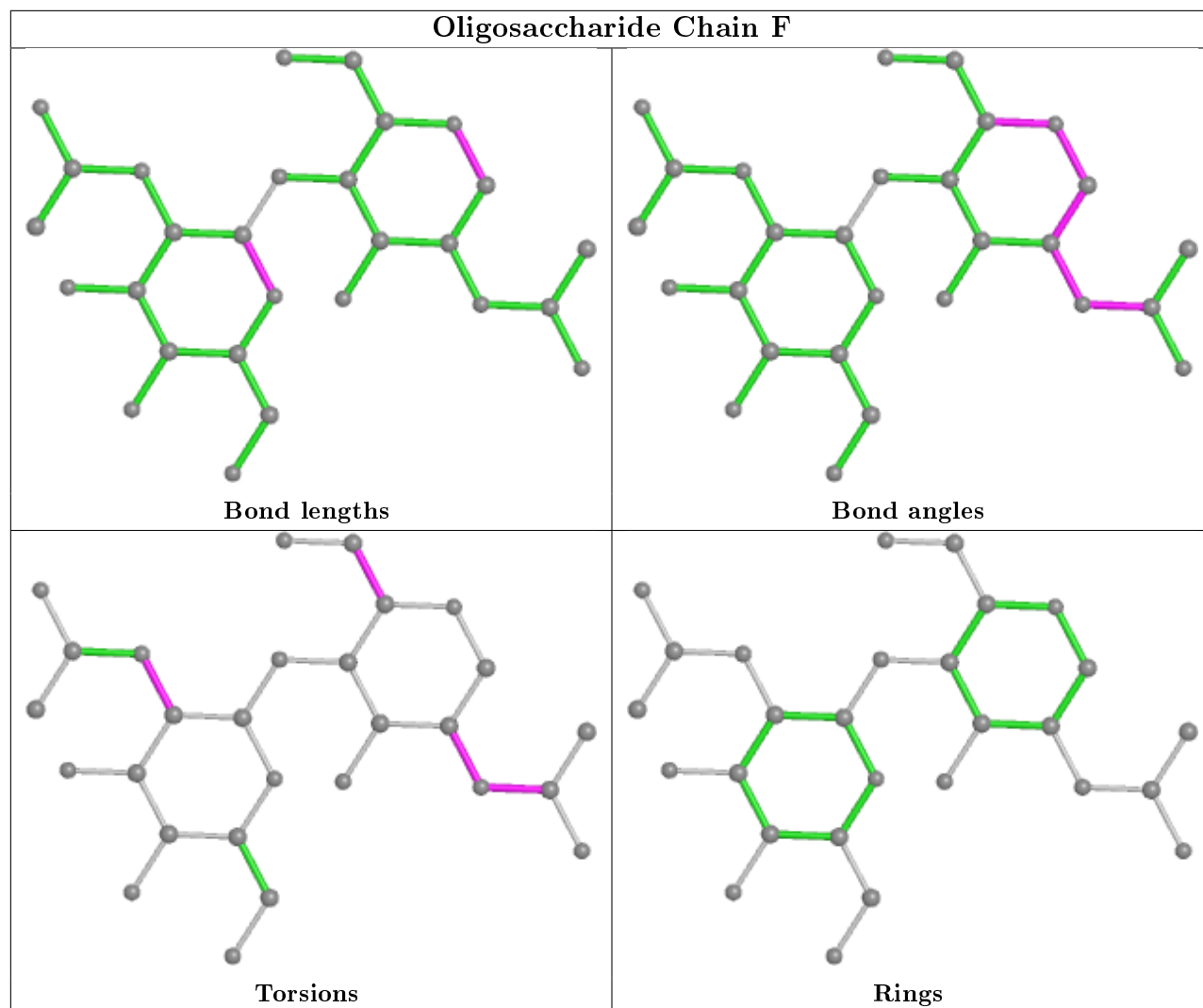
12 monomers are involved in 28 short contacts:

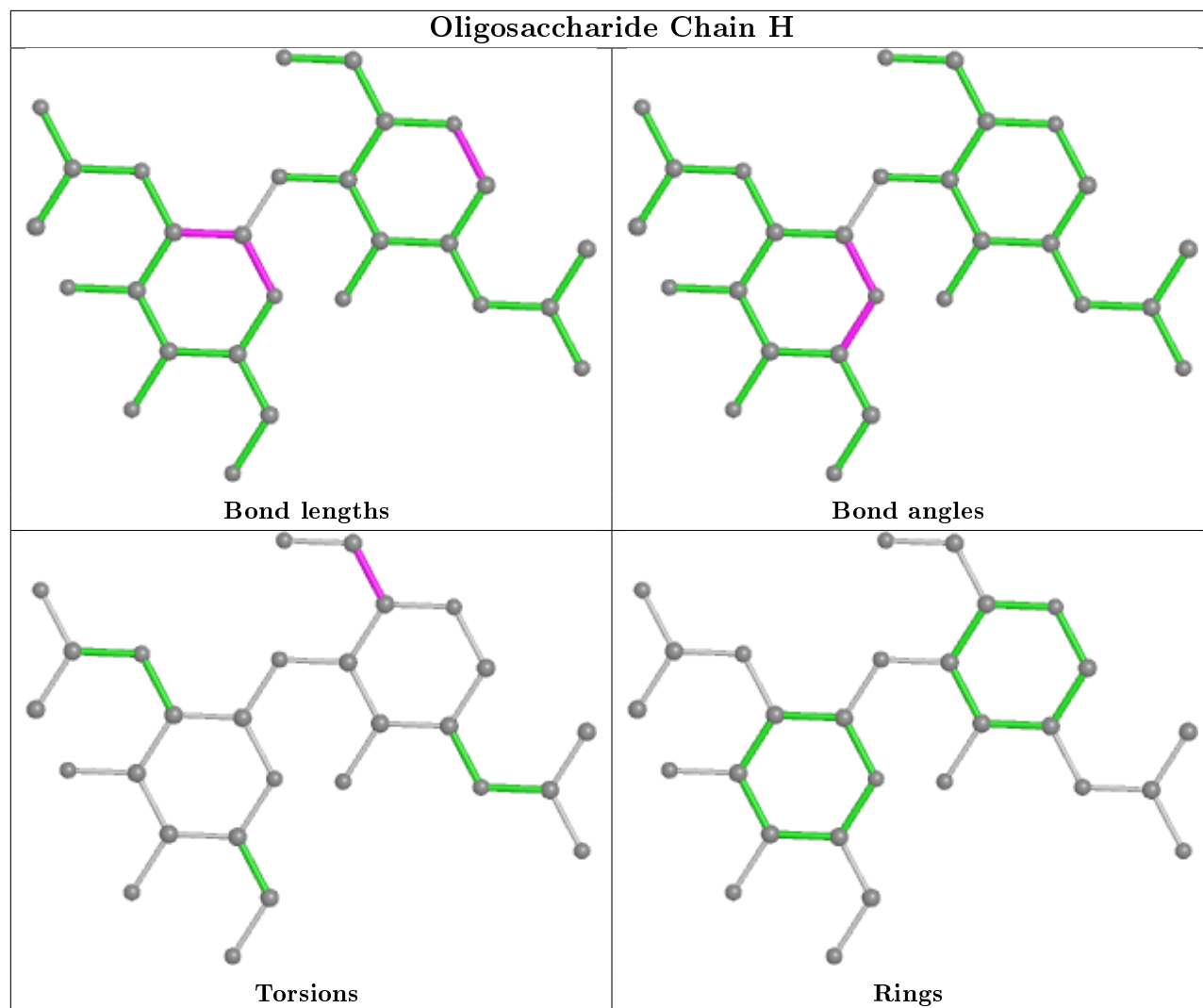
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	BMA	1	0
3	E	4	FUC	2	0
2	D	2	NAG	6	0
2	G	1	NAG	4	0
4	I	2	NAG	3	0
2	D	1	NAG	6	0
4	F	1	NAG	4	0
3	E	3	BMA	1	0
2	G	2	NAG	3	0
2	C	1	NAG	2	0
3	E	2	NAG	4	0
3	E	1	NAG	4	0

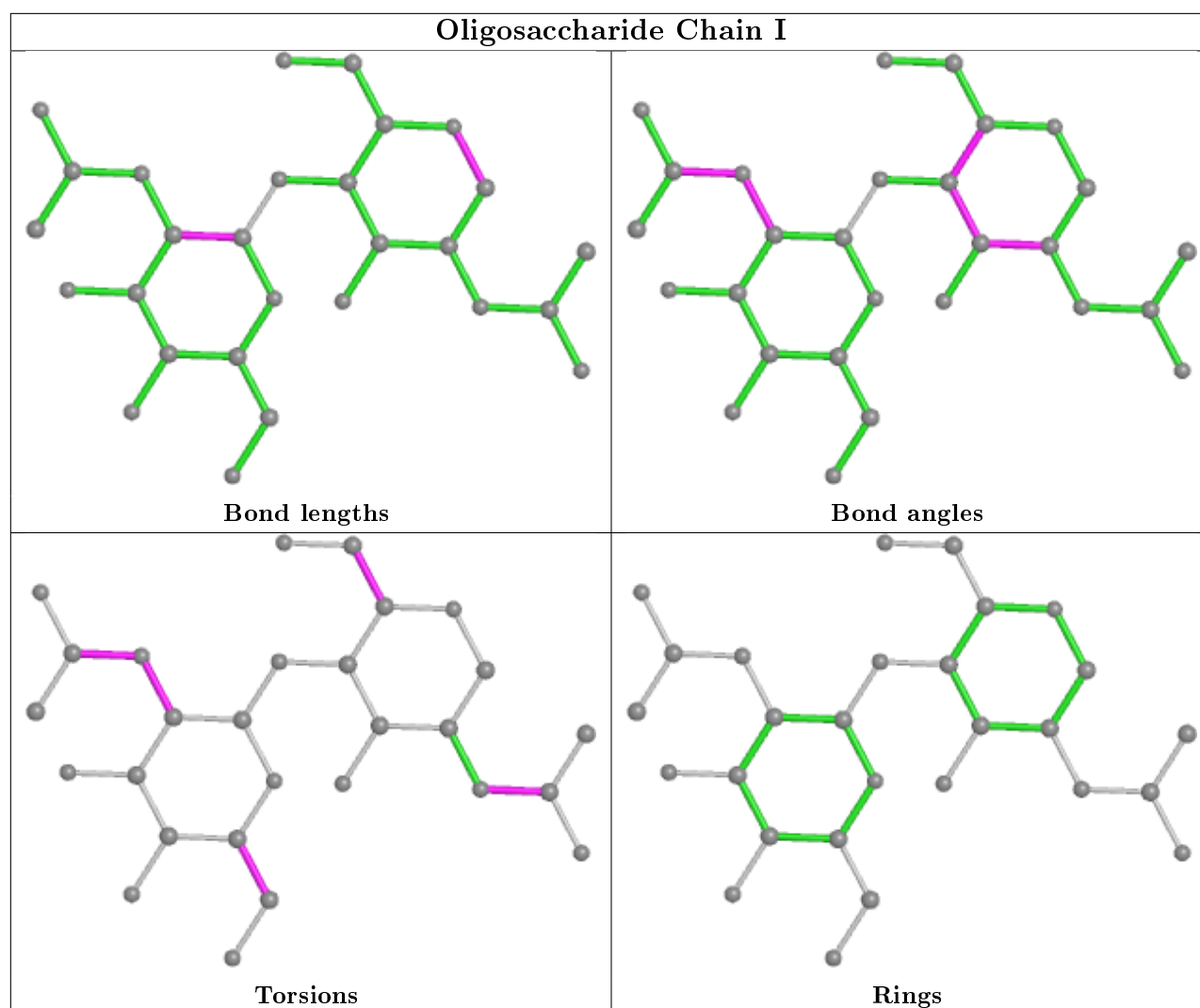
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 22 are monoatomic - leaving 10 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	$\# Z > 2$
5	NAG	A	601	1	14,14,15	1.02	1 (7%)	17,19,21	2.49	5 (29%)
6	MAN	B	902	1	11,11,12	1.30	2 (18%)	15,15,17	2.17	4 (26%)
6	MAN	A	615	1	11,11,12	0.92	1 (9%)	15,15,17	1.51	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	B	903	1	11,11,12	1.35	2 (18%)	15,15,17	2.09	4 (26%)
6	MAN	A	614	1	11,11,12	1.10	1 (9%)	15,15,17	2.51	3 (20%)
5	NAG	A	608	1	14,14,15	0.92	1 (7%)	17,19,21	1.50	3 (17%)
6	MAN	A	613	1	11,11,12	0.86	0	15,15,17	2.03	3 (20%)
5	NAG	B	911	1	14,14,15	0.37	0	17,19,21	0.47	0
8	EDO	A	627	-	3,3,3	0.66	0	2,2,2	0.65	0
6	MAN	B	901	1	11,11,12	1.86	3 (27%)	15,15,17	2.53	6 (40%)

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
5	NAG	A	601	1	-	3/6/23/26	0/1/1/1
6	MAN	B	902	1	-	2/2/19/22	0/1/1/1
6	MAN	A	615	1	-	0/2/19/22	0/1/1/1
6	MAN	B	903	1	-	2/2/19/22	0/1/1/1
6	MAN	A	614	1	-	0/2/19/22	0/1/1/1
5	NAG	A	608	1	-	1/6/23/26	0/1/1/1
6	MAN	A	613	1	-	2/2/19/22	0/1/1/1
5	NAG	B	911	1	-	2/6/23/26	0/1/1/1
8	EDO	A	627	-	-	0/1/1/1	-
6	MAN	B	901	1	-	1/2/19/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	MAN	O4-C4	-4.51	1.32	1.43
6	B	903	MAN	C1-C2	3.67	1.60	1.52
6	B	902	MAN	C1-C2	3.44	1.60	1.52
6	A	614	MAN	C1-C2	3.30	1.59	1.52
5	A	601	NAG	C1-C2	2.80	1.56	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C1-O5-C5	7.48	122.33	112.19
6	A	614	MAN	C1-O5-C5	6.58	121.11	112.19
6	A	613	MAN	C1-O5-C5	5.74	119.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	MAN	O5-C1-C2	5.50	119.27	110.77
6	A	614	MAN	O5-C1-C2	5.28	118.92	110.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	NAG	C3-C2-N2-C7
6	A	613	MAN	O5-C5-C6-O6
6	B	902	MAN	O5-C5-C6-O6
6	A	613	MAN	C4-C5-C6-O6
6	B	902	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	MAN	1	0
5	A	608	NAG	3	0
5	B	911	NAG	1	0
6	B	901	MAN	1	1

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	554/559 (99%)	0.43	7 (1%) 77 77	47, 70, 98, 189	0
1	B	559/559 (100%)	0.44	16 (2%) 51 47	42, 72, 107, 135	0
All	All	1113/1118 (99%)	0.43	23 (2%) 63 61	42, 71, 104, 189	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	HIS	6.8
1	A	554	HIS	6.7
1	B	31	GLU	3.7
1	B	451	ILE	3.7
1	B	30	GLU	3.3

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.

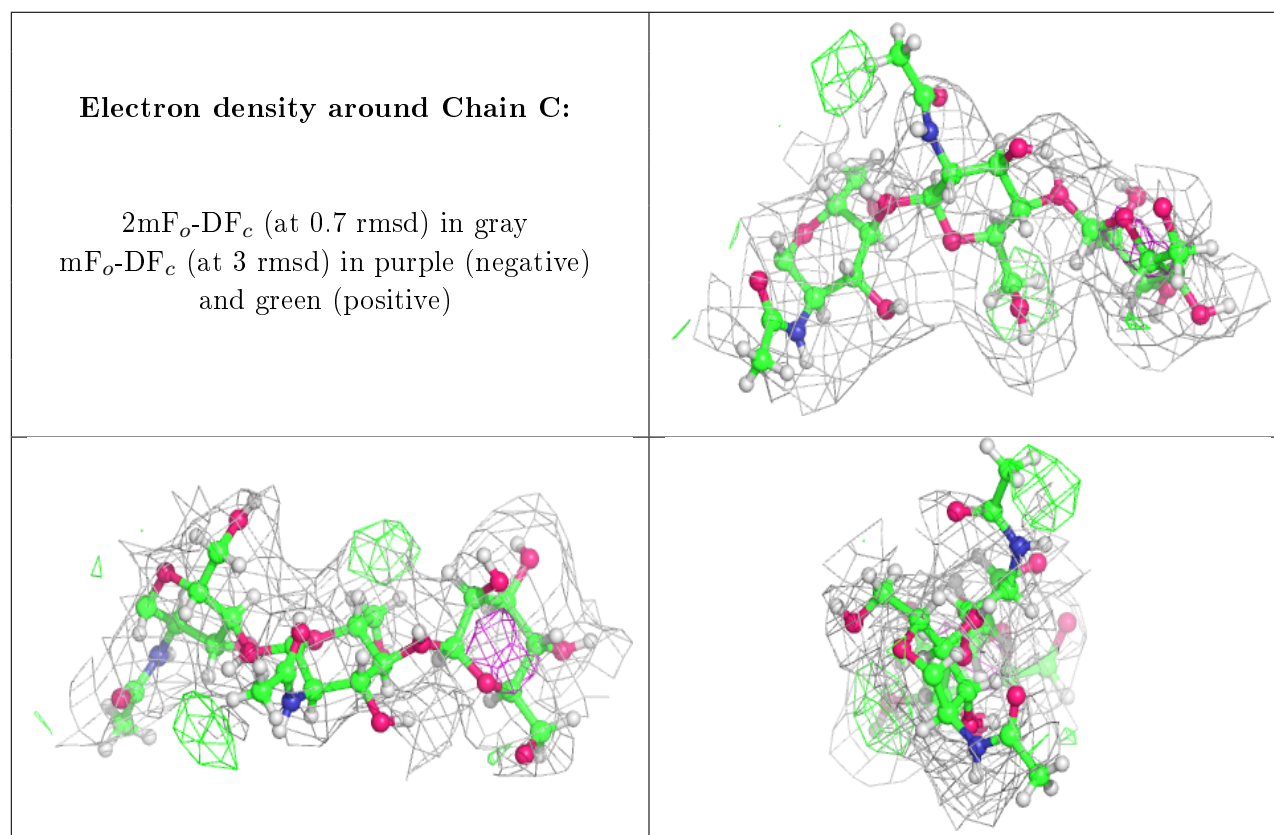
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	G	3	11/12	0.53	0.28	70,87,104,109	0
2	BMA	D	3	11/12	0.61	0.28	65,84,101,111	0
2	NAG	G	1	14/15	0.66	0.33	118,141,167,175	0
2	NAG	C	2	14/15	0.67	0.24	89,117,145,153	0
4	NAG	H	2	14/15	0.70	0.29	65,82,98,102	0

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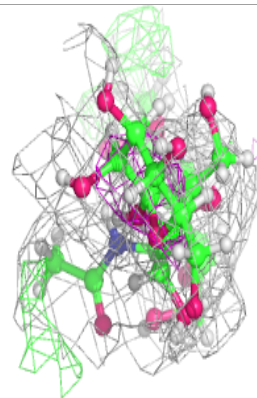
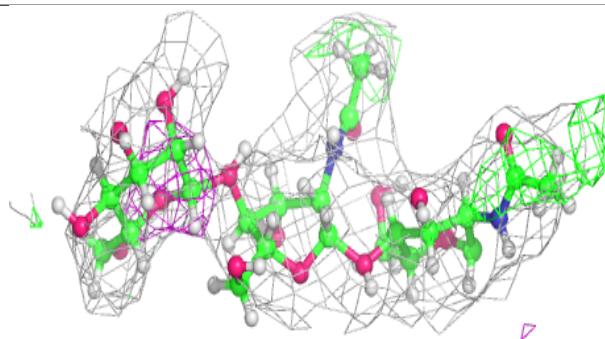
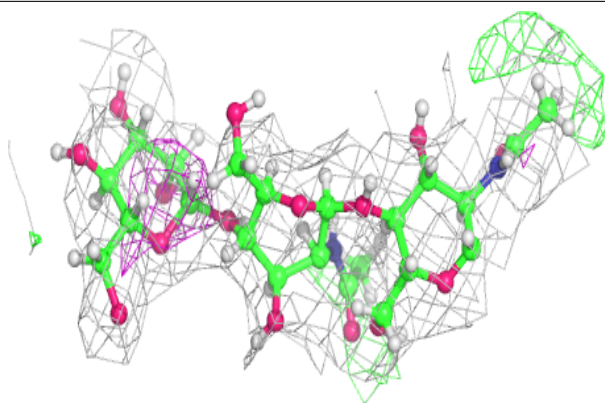
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.75	0.17	68,126,154,161	0
2	BMA	C	3	11/12	0.76	0.18	71,84,95,111	0
4	NAG	I	2	14/15	0.77	0.20	93,128,157,162	0
2	NAG	G	2	14/15	0.78	0.26	90,130,157,162	0
4	NAG	H	1	14/15	0.81	0.24	68,83,97,102	0
3	NAG	E	1	14/15	0.81	0.24	84,115,141,162	0
3	NAG	E	2	14/15	0.83	0.19	112,129,149,154	0
3	FUC	E	4	10/11	0.83	0.36	116,140,167,174	0
3	BMA	E	3	11/12	0.84	0.17	60,77,94,99	0
2	NAG	D	1	14/15	0.84	0.17	84,115,138,143	0
4	NAG	I	1	14/15	0.86	0.21	87,120,146,162	0
2	NAG	C	1	14/15	0.87	0.19	78,99,119,148	0
4	NAG	F	2	14/15	0.87	0.16	91,116,139,144	0
4	NAG	F	1	14/15	0.89	0.24	86,110,129,138	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.

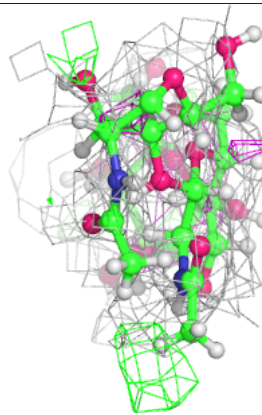
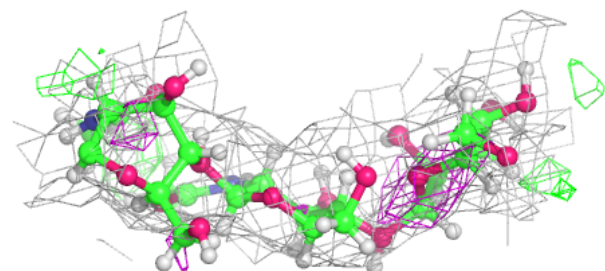
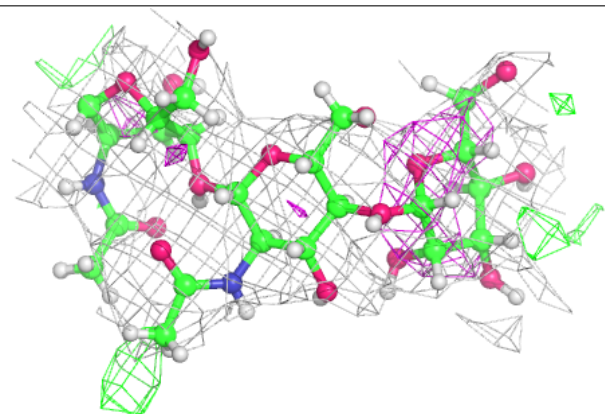


Electron density around Chain D:

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

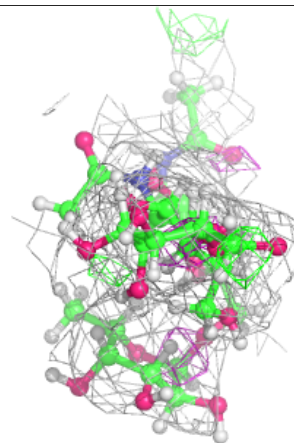
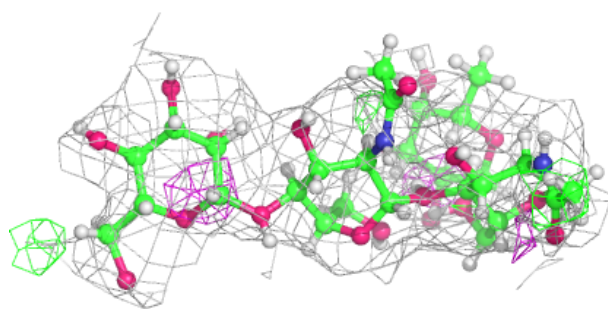
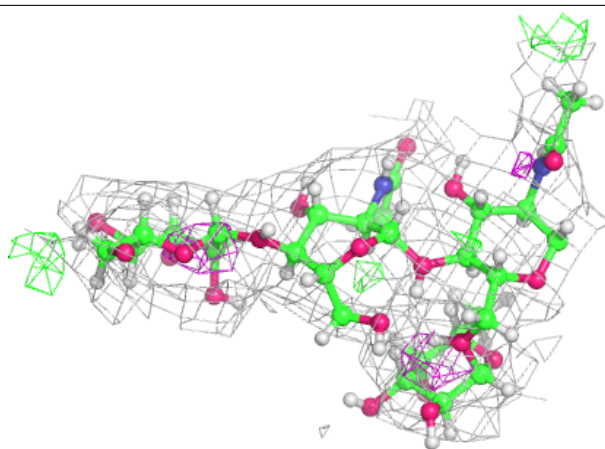
**Electron density around Chain G:**

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



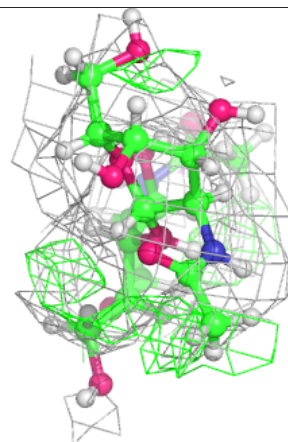
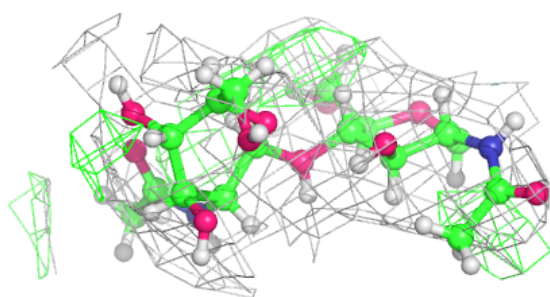
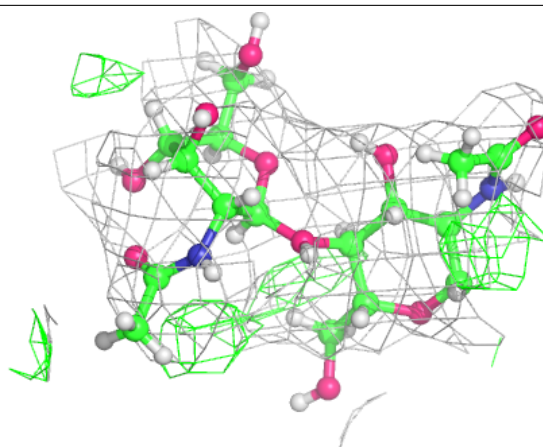
Electron density around Chain E:

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

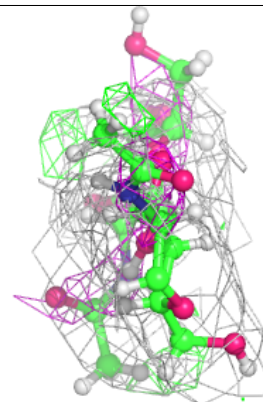
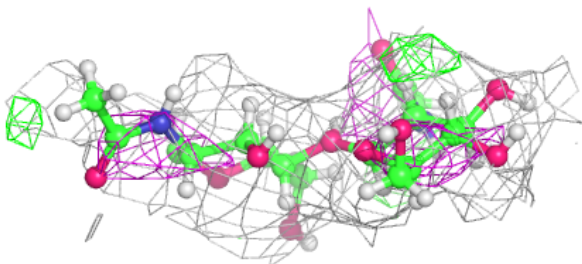
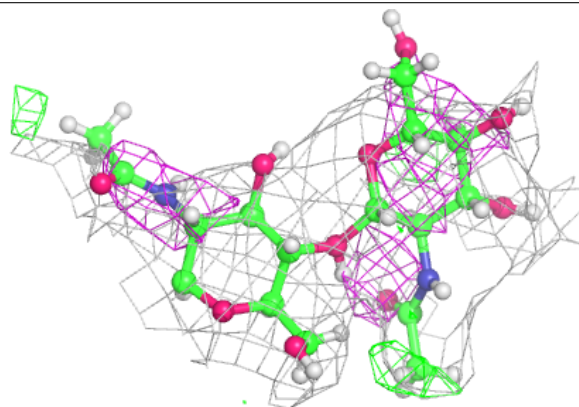


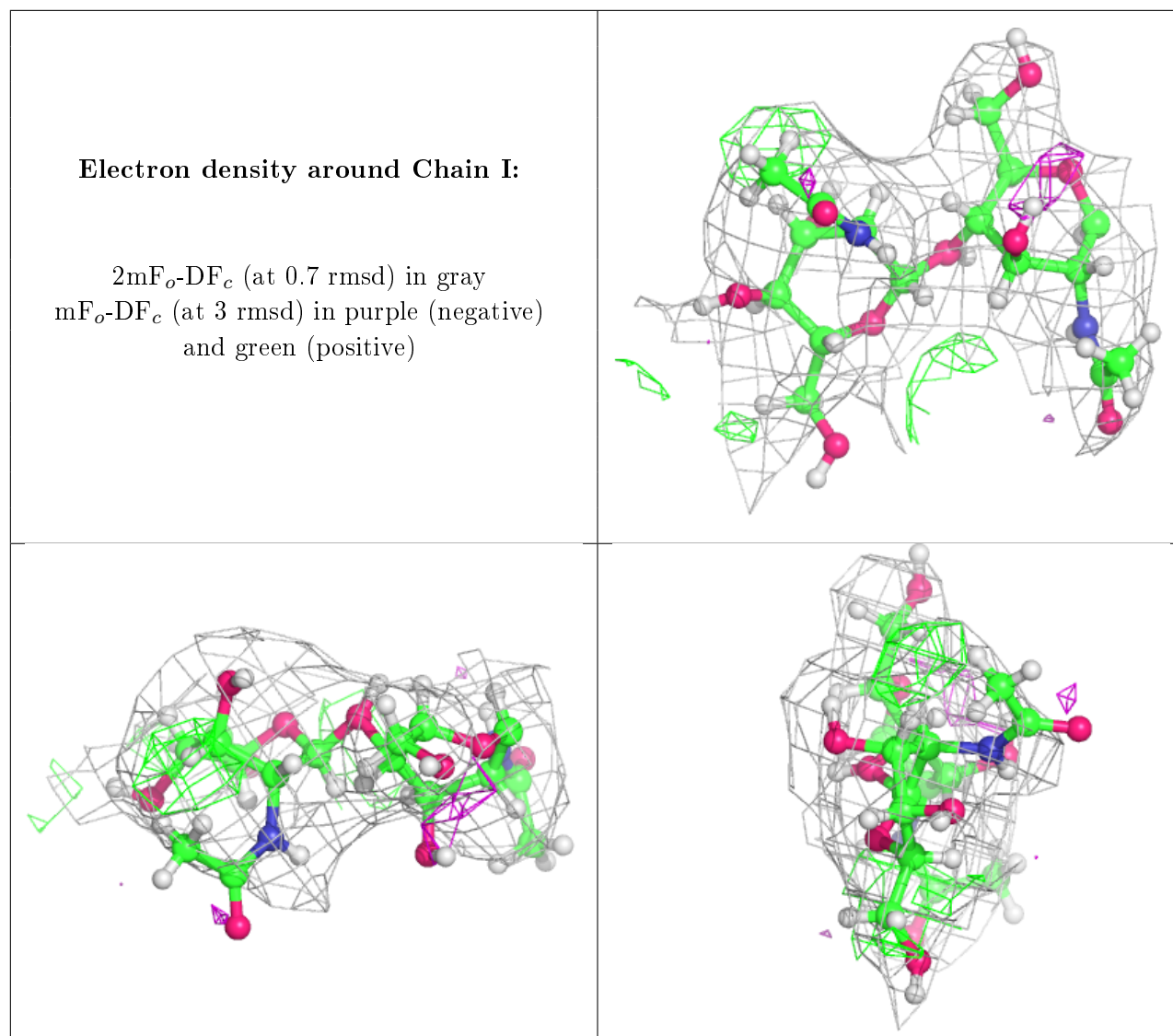
Electron density around Chain F:

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

**Electron density around Chain H:**

$2mF_o - DF_c$ (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
7	CA	A	623	1/1	0.55	0.17	79,79,79,79	0
5	NAG	A	601	14/15	0.71	0.21	113,165,199,201	0
7	CA	A	624	1/1	0.72	0.25	65,65,65,65	0
7	CA	B	915	1/1	0.73	0.20	79,79,79,79	0
7	CA	B	918	1/1	0.76	0.23	70,70,70,70	0
7	CA	B	917	1/1	0.77	0.16	71,71,71,71	0
5	NAG	B	911	14/15	0.79	0.21	97,138,173,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EDO	A	627	4/4	0.82	0.22	63,77,99,119	0
5	NAG	A	608	14/15	0.82	0.17	80,114,137,146	0
6	MAN	B	901	11/12	0.83	0.29	92,116,139,157	0
6	MAN	A	615	11/12	0.84	0.38	98,118,134,158	0
7	CA	A	626	1/1	0.84	0.20	78,78,78,78	0
7	CA	A	620	1/1	0.86	0.17	78,78,78,78	0
6	MAN	B	903	11/12	0.87	0.29	93,111,129,133	0
6	MAN	A	614	11/12	0.87	0.30	109,129,150,155	0
7	CA	B	919	1/1	0.87	0.21	63,63,63,63	0
7	CA	B	920	1/1	0.89	0.21	69,69,69,69	0
7	CA	A	621	1/1	0.89	0.13	58,58,58,58	0
6	MAN	A	613	11/12	0.90	0.30	98,123,141,148	0
6	MAN	B	902	11/12	0.90	0.22	77,99,115,134	0
7	CA	A	616	1/1	0.91	0.18	66,66,66,66	0
7	CA	B	924	1/1	0.91	0.17	71,71,71,71	0
7	CA	B	921	1/1	0.92	0.23	51,51,51,51	0
7	CA	B	923	1/1	0.93	0.23	77,77,77,77	0
7	CA	B	922	1/1	0.94	0.20	59,59,59,59	0
7	CA	A	625	1/1	0.94	0.16	58,58,58,58	0
7	CA	A	618	1/1	0.94	0.20	71,71,71,71	0
7	CA	B	914	1/1	0.95	0.23	64,64,64,64	0
7	CA	A	617	1/1	0.95	0.22	71,71,71,71	0
7	CA	A	622	1/1	0.97	0.22	64,64,64,64	0
7	CA	B	916	1/1	0.97	0.24	46,46,46,46	0
7	CA	A	619	1/1	0.98	0.23	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.