



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:44 PM BST

PDB ID : 5SZL
Title : Protocadherin gamma A1 extracellular cadherin domains 1-4
Authors : Goodman, K.M.; Bahna, F.; Mannepalli, S.; Honig, B.; Shapiro, L.
Deposited on : 2016-08-14
Resolution : 4.20 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

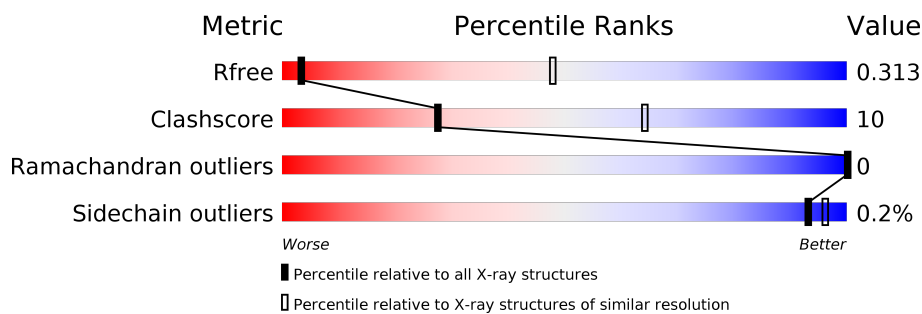
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	427	74% 22% .
1	B	427	75% 22% .
1	C	427	78% 19% .
1	D	427	78% 19% .
2	E	3	100%
3	F	2	100%
4	G	4	75% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12505 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 PROTOCADHERIN GAMMA A1 EXTRACELLULAR CADHERIN DOMAINS 1-4, Protein Pcdhga1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3004	1859	518	618	9			
1	B	412	Total	C	N	O	S	0	0	0
			2974	1840	512	614	8			
1	C	418	Total	C	N	O	S	0	0	0
			3119	1936	535	638	10			
1	D	416	Total	C	N	O	S	0	0	0
			3098	1928	521	640	9			

There are 32 discrepancies between the modelled and reference sequences:

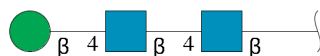
Chain	Residue	Modelled	Actual	Comment	Reference
A	420	HIS	-	expression tag	UNP A0A0A6YW27
A	421	HIS	-	expression tag	UNP A0A0A6YW27
A	422	HIS	-	expression tag	UNP A0A0A6YW27
A	423	HIS	-	expression tag	UNP A0A0A6YW27
A	424	HIS	-	expression tag	UNP A0A0A6YW27
A	425	HIS	-	expression tag	UNP A0A0A6YW27
A	426	HIS	-	expression tag	UNP A0A0A6YW27
A	427	HIS	-	expression tag	UNP A0A0A6YW27
B	420	HIS	-	expression tag	UNP A0A0A6YW27
B	421	HIS	-	expression tag	UNP A0A0A6YW27
B	422	HIS	-	expression tag	UNP A0A0A6YW27
B	423	HIS	-	expression tag	UNP A0A0A6YW27
B	424	HIS	-	expression tag	UNP A0A0A6YW27
B	425	HIS	-	expression tag	UNP A0A0A6YW27
B	426	HIS	-	expression tag	UNP A0A0A6YW27
B	427	HIS	-	expression tag	UNP A0A0A6YW27
C	420	HIS	-	expression tag	UNP A0A0A6YW27
C	421	HIS	-	expression tag	UNP A0A0A6YW27
C	422	HIS	-	expression tag	UNP A0A0A6YW27
C	423	HIS	-	expression tag	UNP A0A0A6YW27

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Chain	Residue	Modelled	Actual	Comment	Reference
C	424	HIS	-	expression tag	UNP A0A0A6YW27
C	425	HIS	-	expression tag	UNP A0A0A6YW27
C	426	HIS	-	expression tag	UNP A0A0A6YW27
C	427	HIS	-	expression tag	UNP A0A0A6YW27
D	420	HIS	-	expression tag	UNP A0A0A6YW27
D	421	HIS	-	expression tag	UNP A0A0A6YW27
D	422	HIS	-	expression tag	UNP A0A0A6YW27
D	423	HIS	-	expression tag	UNP A0A0A6YW27
D	424	HIS	-	expression tag	UNP A0A0A6YW27
D	425	HIS	-	expression tag	UNP A0A0A6YW27
D	426	HIS	-	expression tag	UNP A0A0A6YW27
D	427	HIS	-	expression tag	UNP A0A0A6YW27

- 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.



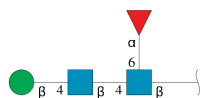
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



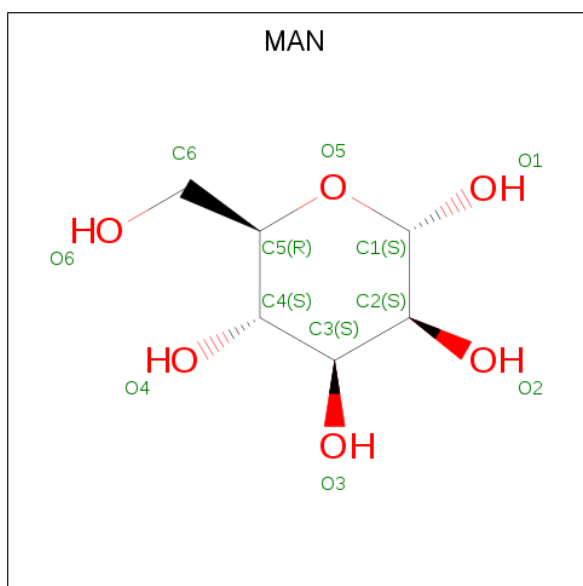
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	G	4	Total	C	N	O	0	0
			49	28	2	19		0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

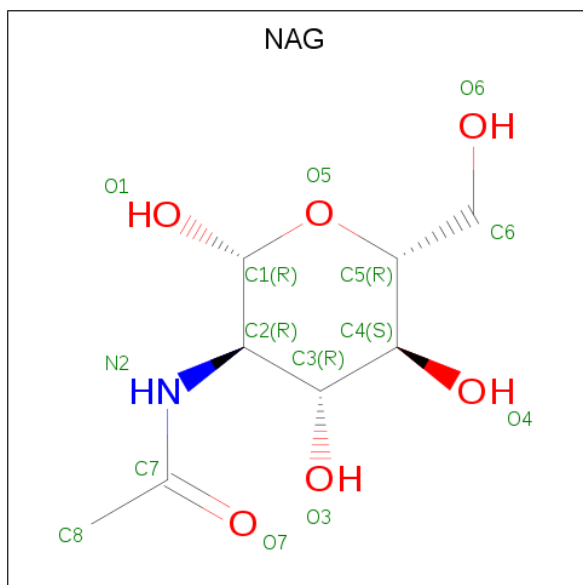


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

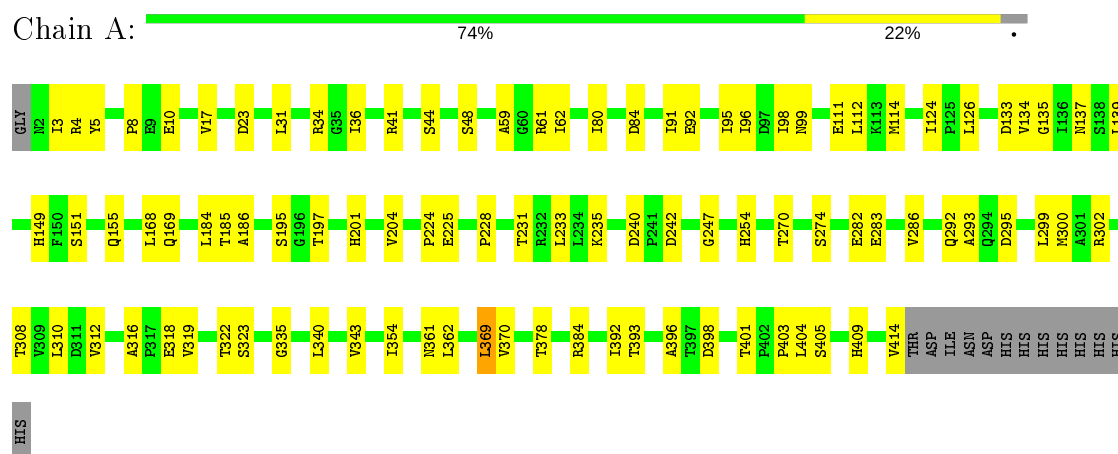


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

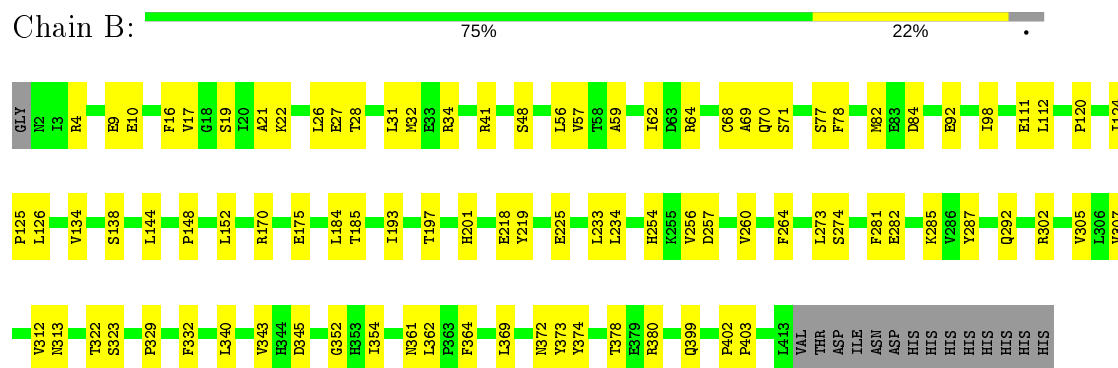
3 Residue-property plots

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. 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. 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.

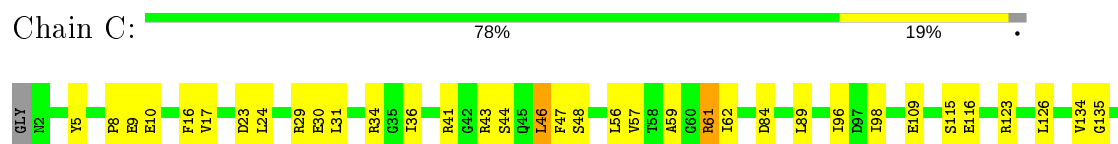
- Molecule 1: PROTOCADHERIN GAMMA A1 EXTRACELLULAR CADHERIN DOMAINS 1-4, Protein Pcdhgal

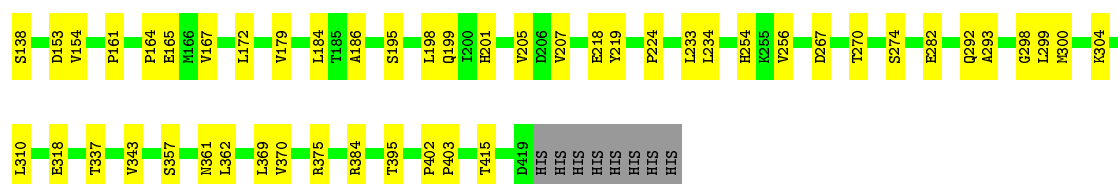


- Molecule 1: PROTOCADHERIN GAMMA A1 EXTRACELLULAR CADHERIN DOMAINS 1-4, Protein Pcdhgal



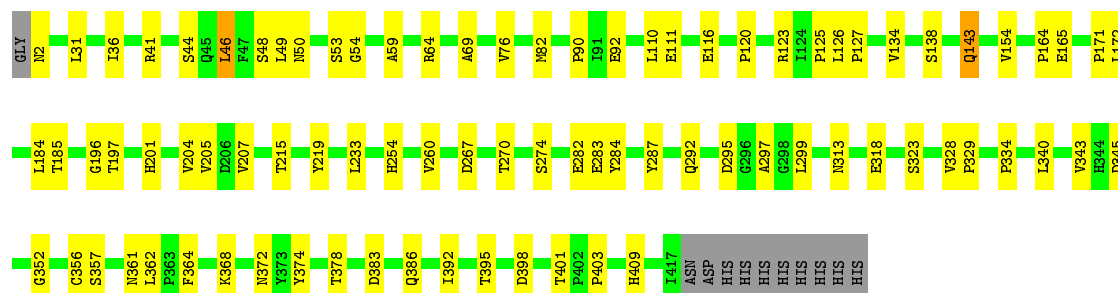
- Molecule 1: PROTOCADHERIN GAMMA A1 EXTRACELLULAR CADHERIN DOMAINS 1-4, Protein Pcdhgal





- Molecule 1: PROTOCADHERIN GAMMA A1 EXTRACELLULAR CADHERIN DOMAINS 1-4, Protein Pcdhga1

Chain D: 78% 19% .



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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.87Å 107.87Å 463.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.96 – 4.20 39.96 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.96-4.20) 80.0 (39.96-4.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.287 , 0.314 0.286 , 0.313	Depositor DCC
R_{free} test set	1192 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	109.7	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12505	wwPDB-VP
Average B, all atoms (Å ²)	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: FUC, CA, BMA, NAG, 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	0.30	0/3061	0.53	0/4195
1	B	0.29	0/3028	0.52	0/4147
1	C	0.27	0/3177	0.50	1/4348 (0.0%)
1	D	0.30	0/3156	0.55	2/4321 (0.0%)
All	All	0.29	0/12422	0.53	3/17011 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	LEU	CB-CG-CD2	-8.06	97.29	111.00
1	D	356	CYS	CA-CB-SG	-6.47	102.35	114.00
1	C	46	LEU	CB-CG-CD1	-5.03	102.45	111.00

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	3004	0	2731	64	0
1	B	2974	0	2688	66	0
1	C	3119	0	2934	57	0
1	D	3098	0	2905	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	39	0	34	2	0
3	F	28	0	25	1	0
4	G	49	0	43	3	0
5	A	22	0	20	1	0
5	B	22	0	20	1	0
5	C	22	0	20	1	0
5	D	22	0	20	0	0
6	A	9	0	0	0	0
6	B	9	0	0	0	0
6	C	9	0	0	0	0
6	D	9	0	0	0	0
7	A	14	0	13	1	0
7	B	28	0	26	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
All	All	12505	0	11505	241	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 10.

The worst 5 of 241 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:D:154:VAL:HG12	1:D:164:PRO:HA	1.47	0.96
1:D:41:ARG:N	1:D:44:SER:OG	2.04	0.90
1:B:364:PHE:HA	1:B:378:THR:HA	1.51	0.89
1:C:46:LEU:HD11	1:C:62:ILE:HG12	1.62	0.81
1:A:369:LEU:HD23	1:A:370:VAL:H	1.47	0.79

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	411/427 (96%)	388 (94%)	23 (6%)	0	100	100
1	B	410/427 (96%)	388 (95%)	22 (5%)	0	100	100
1	C	416/427 (97%)	393 (94%)	23 (6%)	0	100	100
1	D	414/427 (97%)	392 (95%)	22 (5%)	0	100	100
All	All	1651/1708 (97%)	1561 (94%)	90 (6%)	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	312/380 (82%)	311 (100%)	1 (0%)	92	95
1	B	303/380 (80%)	303 (100%)	0	100	100
1	C	340/380 (90%)	339 (100%)	1 (0%)	92	95
1	D	338/380 (89%)	337 (100%)	1 (0%)	92	95
All	All	1293/1520 (85%)	1290 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	LEU
1	C	61	ARG
1	D	143	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	GLN
1	D	292	GLN
1	C	201	HIS
1	B	147	ASN
1	D	254	HIS

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 ⓘ

9 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	0.35	0	17,19,21	0.47	0
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	BMA	E	3	2	11,11,12	0.91	0	15,15,17	0.93	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.52	0	17,19,21	0.70	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	G	1	1,4	14,14,15	0.88	1 (7%)	17,19,21	1.35	2 (11%)
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.74	0
4	BMA	G	3	4	11,11,12	1.01	1 (9%)	15,15,17	1.47	3 (20%)
4	FUC	G	4	4	10,10,11	0.82	0	14,14,16	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C1-C2	2.93	1.58	1.52
4	G	1	NAG	O5-C1	-2.81	1.39	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C2-N2-C7	4.25	128.96	122.90
4	G	3	BMA	C1-C2-C3	3.41	113.86	109.67
4	G	3	BMA	C1-O5-C5	2.38	115.42	112.19
4	G	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	G	3	BMA	O5-C1-C2	2.17	114.12	110.77

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

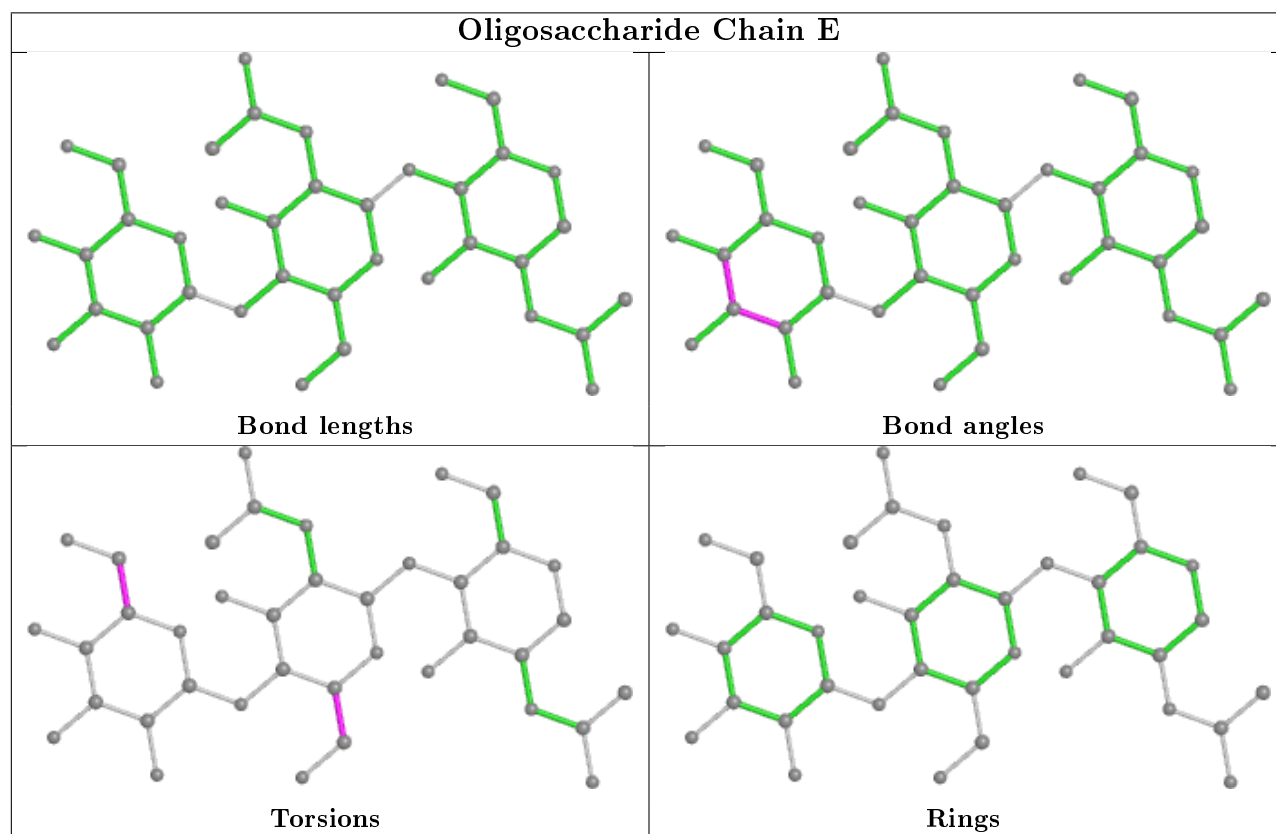
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6

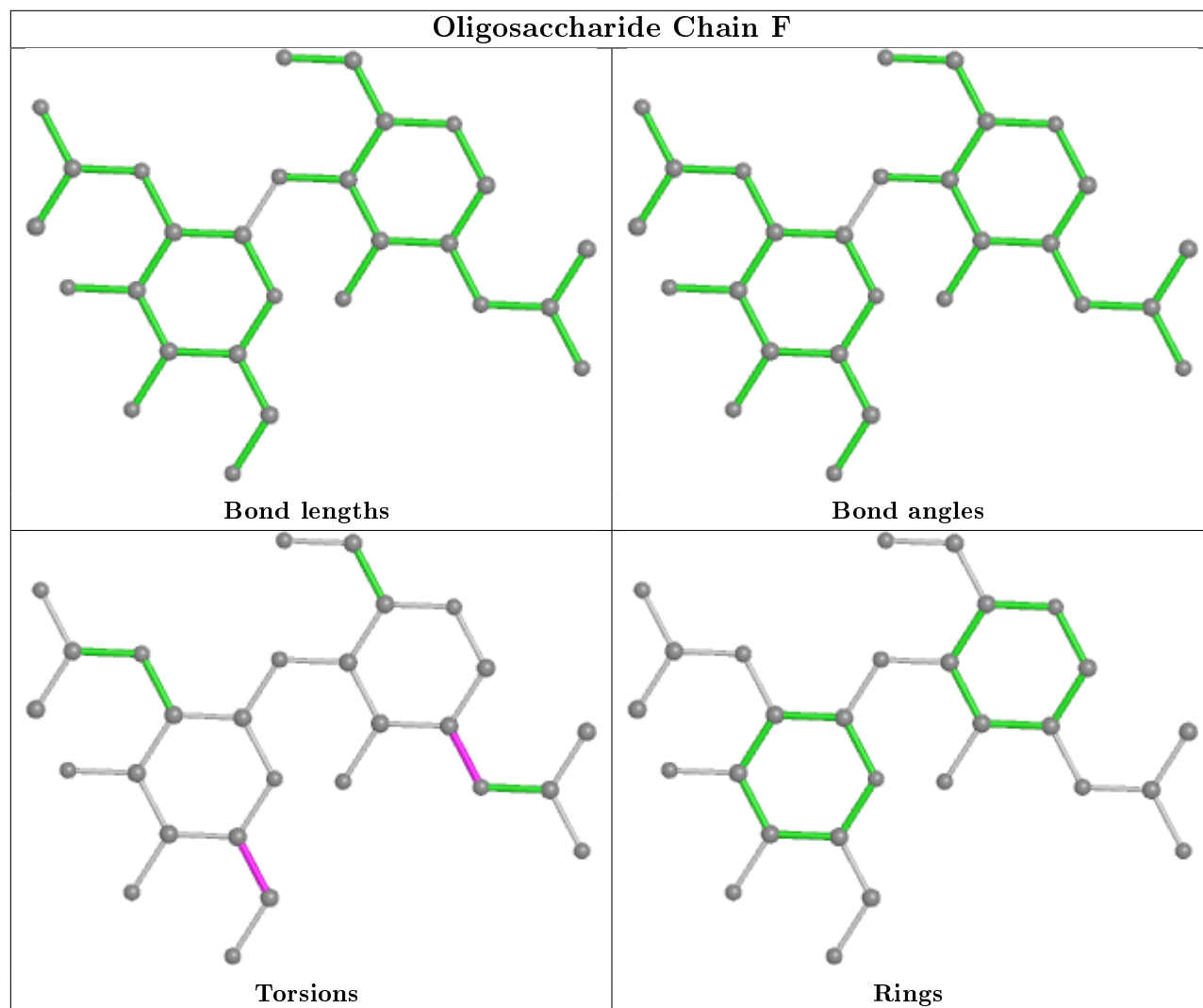
There are no ring outliers.

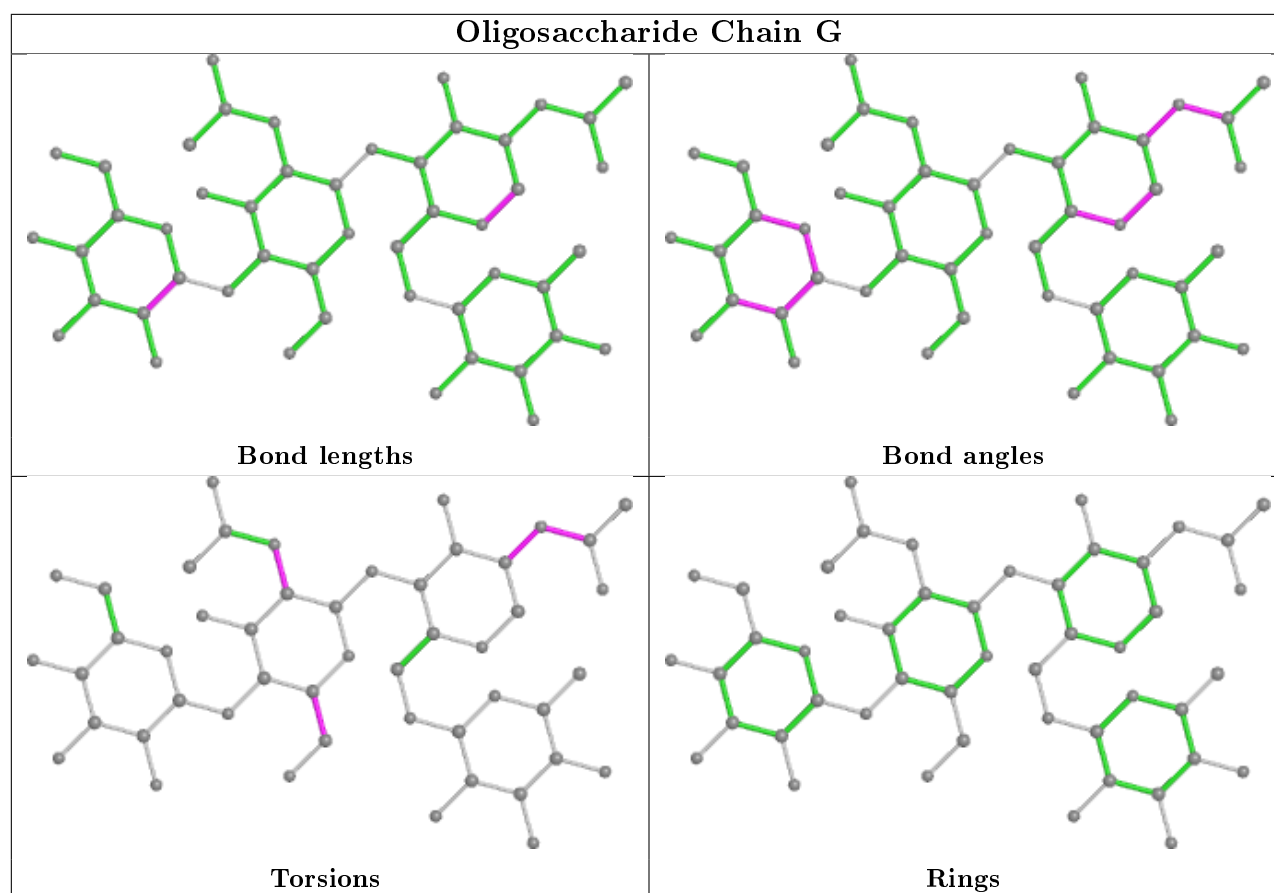
7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	F	1	NAG	1	0
4	G	1	NAG	2	0
2	E	2	NAG	2	0
4	G	2	NAG	1	0
4	G	4	FUC	1	0
2	E	1	NAG	2	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 49 ligands modelled in this entry, 36 are monoatomic - leaving 13 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	MAN	D	501	1	11,11,12	0.72	0	15,15,17	0.99	1 (6%)
5	MAN	A	502	1	11,11,12	0.99	1 (9%)	15,15,17	0.88	1 (6%)
7	NAG	C	514	1	14,14,15	0.30	0	17,19,21	0.43	0
5	MAN	C	502	1	11,11,12	0.90	1 (9%)	15,15,17	0.89	1 (6%)
5	MAN	B	502	1	11,11,12	0.89	1 (9%)	15,15,17	0.82	1 (6%)
5	MAN	D	502	1	11,11,12	0.84	1 (9%)	15,15,17	0.90	1 (6%)
5	MAN	C	501	1	11,11,12	0.85	1 (9%)	15,15,17	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	516	1	14,14,15	0.29	0	17,19,21	0.43	0
5	MAN	A	501	1	11,11,12	0.81	0	15,15,17	0.96	1 (6%)
7	NAG	B	513	1	14,14,15	0.56	0	17,19,21	0.46	0
7	NAG	B	512	1	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	A	515	1	14,14,15	0.30	0	17,19,21	0.48	0
5	MAN	B	501	1	11,11,12	0.71	0	15,15,17	0.99	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
5	MAN	D	501	1	-	0/2/19/22	0/1/1/1
5	MAN	A	502	1	-	0/2/19/22	0/1/1/1
7	NAG	C	514	1	-	3/6/23/26	0/1/1/1
5	MAN	C	502	1	-	0/2/19/22	0/1/1/1
5	MAN	B	502	1	-	0/2/19/22	0/1/1/1
5	MAN	D	502	1	-	0/2/19/22	0/1/1/1
5	MAN	C	501	1	-	0/2/19/22	0/1/1/1
7	NAG	D	516	1	-	2/6/23/26	0/1/1/1
5	MAN	A	501	1	-	0/2/19/22	0/1/1/1
7	NAG	B	513	1	-	4/6/23/26	0/1/1/1
7	NAG	B	512	1	-	2/6/23/26	0/1/1/1
7	NAG	A	515	1	-	4/6/23/26	0/1/1/1
5	MAN	B	501	1	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	MAN	O5-C1	-2.59	1.39	1.43
5	C	501	MAN	O5-C1	-2.34	1.40	1.43
5	C	502	MAN	O5-C1	-2.29	1.40	1.43
5	B	502	MAN	O5-C1	-2.02	1.40	1.43
5	D	502	MAN	O5-C1	-2.01	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	MAN	O2-C2-C3	-2.50	105.13	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	MAN	O2-C2-C3	-2.34	105.45	110.14
5	C	501	MAN	O2-C2-C3	-2.30	105.53	110.14
5	D	502	MAN	O2-C2-C3	-2.25	105.63	110.14
5	A	501	MAN	O2-C2-C3	-2.22	105.70	110.14

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	515	NAG	C1-C2-N2-C7
7	B	513	NAG	C4-C5-C6-O6
7	A	515	NAG	C4-C5-C6-O6
7	C	514	NAG	O5-C5-C6-O6
7	B	512	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	MAN	1	0
5	C	501	MAN	1	0
5	A	501	MAN	1	0
7	A	515	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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

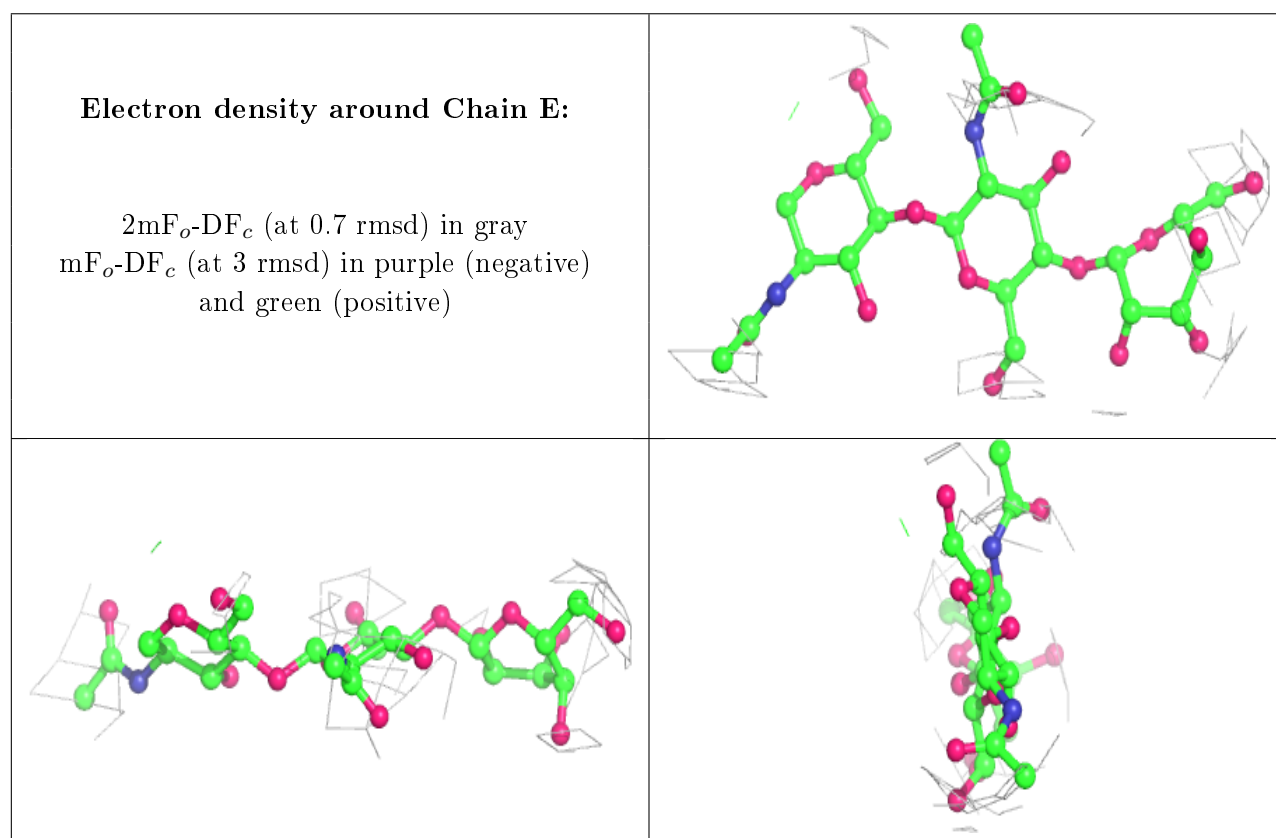
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

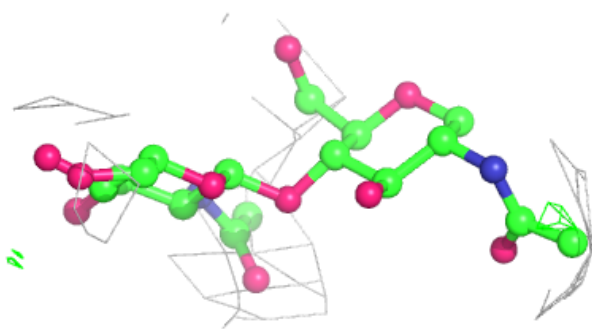
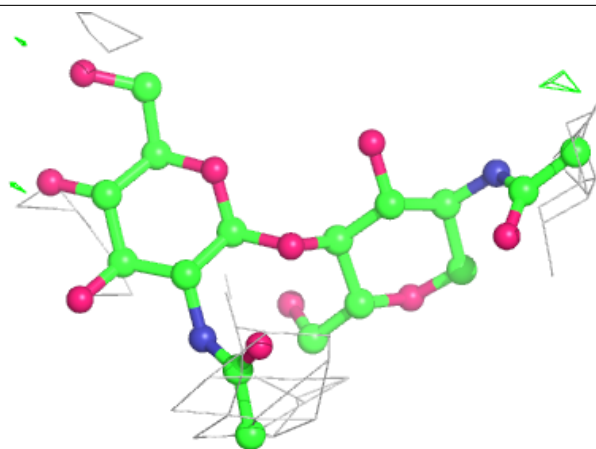
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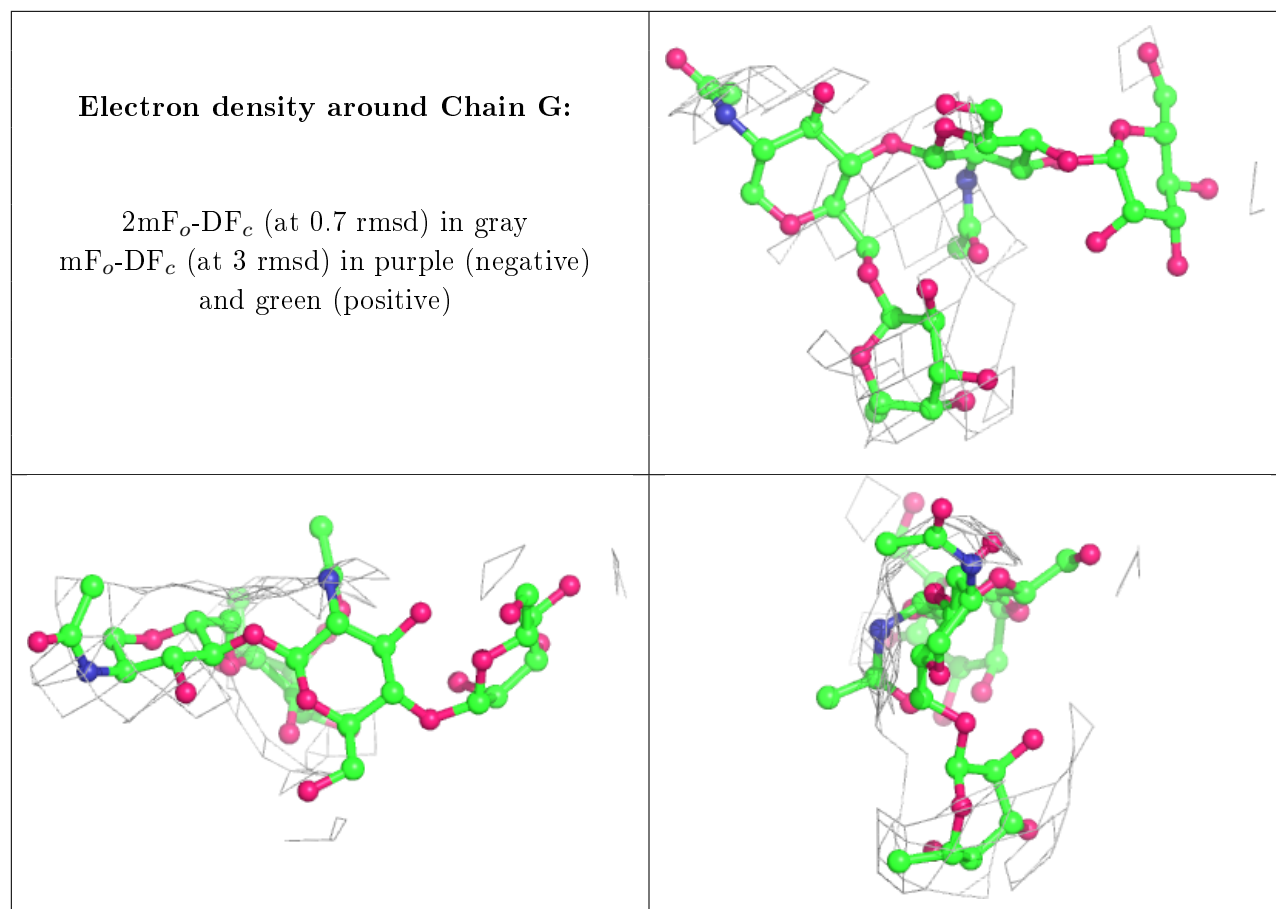
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.