



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2026 – 04:51 pm BST

PDB ID : 9S9U / pdb_00009s9u
Title : Structure of the human ADGRG1 GAIN domain with engineered disulfides
Authors : Barth, P.; Dumas, L.; Lau, K.; Pojer, F.
Deposited on : 2025-08-06
Resolution : 1.92 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

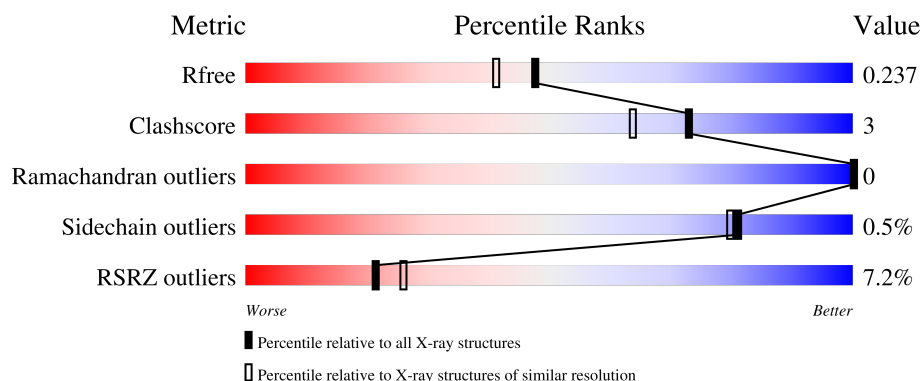
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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.



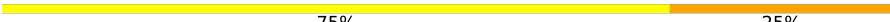
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	255	4% 76% 20%
1	B	255	97%
1	C	255	7% 71% 6% 22%
1	D	255	97%
2	E	6	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	8	 75% 25%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7380 atoms, of which 3565 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 Adhesion G-protein coupled receptor G1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	H	N	O	S	0	7	0
			3271	1024	1638	288	309	12			
1	B	8	Total	C	H	N	O	S	0	0	0
			132	46	67	8	10	1			
1	C	198	Total	C	H	N	O	S	0	5	0
			3192	1001	1598	281	299	13			
1	D	8	Total	C	H	N	O	S	0	0	0
			132	46	67	8	10	1			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9Y653
A	-18	LYS	-	expression tag	UNP Q9Y653
A	-17	LEU	-	expression tag	UNP Q9Y653
A	-16	CYS	-	expression tag	UNP Q9Y653
A	-15	ILE	-	expression tag	UNP Q9Y653
A	-14	LEU	-	expression tag	UNP Q9Y653
A	-13	LEU	-	expression tag	UNP Q9Y653
A	-12	ALA	-	expression tag	UNP Q9Y653
A	-11	VAL	-	expression tag	UNP Q9Y653
A	-10	VAL	-	expression tag	UNP Q9Y653
A	-9	ALA	-	expression tag	UNP Q9Y653
A	-8	PHE	-	expression tag	UNP Q9Y653
A	-7	VAL	-	expression tag	UNP Q9Y653
A	-6	GLY	-	expression tag	UNP Q9Y653
A	-5	LEU	-	expression tag	UNP Q9Y653
A	-4	SER	-	expression tag	UNP Q9Y653
A	-3	LEU	-	expression tag	UNP Q9Y653
A	-2	GLY	-	expression tag	UNP Q9Y653
A	-1	ALA	-	expression tag	UNP Q9Y653
A	0	THR	-	expression tag	UNP Q9Y653
A	1	ASN	-	expression tag	UNP Q9Y653

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q9Y653
A	3	SER	-	expression tag	UNP Q9Y653
A	4	CYS	-	expression tag	UNP Q9Y653
A	5	ASP	-	expression tag	UNP Q9Y653
A	6	MET	-	expression tag	UNP Q9Y653
A	7	SER	-	expression tag	UNP Q9Y653
A	36	CYS	SER	conflict	UNP Q9Y653
A	48	CYS	SER	conflict	UNP Q9Y653
A	181	CYS	GLU	conflict	UNP Q9Y653
A	222	GLY	-	expression tag	UNP Q9Y653
A	223	SER	-	expression tag	UNP Q9Y653
A	224	GLY	-	expression tag	UNP Q9Y653
A	225	SER	-	expression tag	UNP Q9Y653
A	226	HIS	-	expression tag	UNP Q9Y653
A	227	HIS	-	expression tag	UNP Q9Y653
A	228	HIS	-	expression tag	UNP Q9Y653
A	229	HIS	-	expression tag	UNP Q9Y653
A	230	HIS	-	expression tag	UNP Q9Y653
A	231	HIS	-	expression tag	UNP Q9Y653
A	232	HIS	-	expression tag	UNP Q9Y653
A	233	HIS	-	expression tag	UNP Q9Y653
A	234	HIS	-	expression tag	UNP Q9Y653
A	235	HIS	-	expression tag	UNP Q9Y653
B	-19	MET	-	initiating methionine	UNP Q9Y653
B	-18	LYS	-	expression tag	UNP Q9Y653
B	-17	LEU	-	expression tag	UNP Q9Y653
B	-16	CYS	-	expression tag	UNP Q9Y653
B	-15	ILE	-	expression tag	UNP Q9Y653
B	-14	LEU	-	expression tag	UNP Q9Y653
B	-13	LEU	-	expression tag	UNP Q9Y653
B	-12	ALA	-	expression tag	UNP Q9Y653
B	-11	VAL	-	expression tag	UNP Q9Y653
B	-10	VAL	-	expression tag	UNP Q9Y653
B	-9	ALA	-	expression tag	UNP Q9Y653
B	-8	PHE	-	expression tag	UNP Q9Y653
B	-7	VAL	-	expression tag	UNP Q9Y653
B	-6	GLY	-	expression tag	UNP Q9Y653
B	-5	LEU	-	expression tag	UNP Q9Y653
B	-4	SER	-	expression tag	UNP Q9Y653
B	-3	LEU	-	expression tag	UNP Q9Y653
B	-2	GLY	-	expression tag	UNP Q9Y653
B	-1	ALA	-	expression tag	UNP Q9Y653

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP Q9Y653
B	1	ASN	-	expression tag	UNP Q9Y653
B	2	ALA	-	expression tag	UNP Q9Y653
B	3	SER	-	expression tag	UNP Q9Y653
B	4	CYS	-	expression tag	UNP Q9Y653
B	5	ASP	-	expression tag	UNP Q9Y653
B	6	MET	-	expression tag	UNP Q9Y653
B	7	SER	-	expression tag	UNP Q9Y653
B	36	CYS	SER	conflict	UNP Q9Y653
B	48	CYS	SER	conflict	UNP Q9Y653
B	181	CYS	GLU	conflict	UNP Q9Y653
B	222	GLY	-	expression tag	UNP Q9Y653
B	223	SER	-	expression tag	UNP Q9Y653
B	224	GLY	-	expression tag	UNP Q9Y653
B	225	SER	-	expression tag	UNP Q9Y653
B	226	HIS	-	expression tag	UNP Q9Y653
B	227	HIS	-	expression tag	UNP Q9Y653
B	228	HIS	-	expression tag	UNP Q9Y653
B	229	HIS	-	expression tag	UNP Q9Y653
B	230	HIS	-	expression tag	UNP Q9Y653
B	231	HIS	-	expression tag	UNP Q9Y653
B	232	HIS	-	expression tag	UNP Q9Y653
B	233	HIS	-	expression tag	UNP Q9Y653
B	234	HIS	-	expression tag	UNP Q9Y653
B	235	HIS	-	expression tag	UNP Q9Y653
C	-19	MET	-	initiating methionine	UNP Q9Y653
C	-18	LYS	-	expression tag	UNP Q9Y653
C	-17	LEU	-	expression tag	UNP Q9Y653
C	-16	CYS	-	expression tag	UNP Q9Y653
C	-15	ILE	-	expression tag	UNP Q9Y653
C	-14	LEU	-	expression tag	UNP Q9Y653
C	-13	LEU	-	expression tag	UNP Q9Y653
C	-12	ALA	-	expression tag	UNP Q9Y653
C	-11	VAL	-	expression tag	UNP Q9Y653
C	-10	VAL	-	expression tag	UNP Q9Y653
C	-9	ALA	-	expression tag	UNP Q9Y653
C	-8	PHE	-	expression tag	UNP Q9Y653
C	-7	VAL	-	expression tag	UNP Q9Y653
C	-6	GLY	-	expression tag	UNP Q9Y653
C	-5	LEU	-	expression tag	UNP Q9Y653
C	-4	SER	-	expression tag	UNP Q9Y653
C	-3	LEU	-	expression tag	UNP Q9Y653

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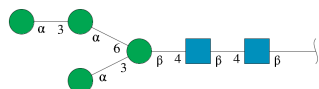
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9Y653
C	-1	ALA	-	expression tag	UNP Q9Y653
C	0	THR	-	expression tag	UNP Q9Y653
C	1	ASN	-	expression tag	UNP Q9Y653
C	2	ALA	-	expression tag	UNP Q9Y653
C	3	SER	-	expression tag	UNP Q9Y653
C	4	CYS	-	expression tag	UNP Q9Y653
C	5	ASP	-	expression tag	UNP Q9Y653
C	6	MET	-	expression tag	UNP Q9Y653
C	7	SER	-	expression tag	UNP Q9Y653
C	36	CYS	SER	conflict	UNP Q9Y653
C	48	CYS	SER	conflict	UNP Q9Y653
C	181	CYS	GLU	conflict	UNP Q9Y653
C	222	GLY	-	expression tag	UNP Q9Y653
C	223	SER	-	expression tag	UNP Q9Y653
C	224	GLY	-	expression tag	UNP Q9Y653
C	225	SER	-	expression tag	UNP Q9Y653
C	226	HIS	-	expression tag	UNP Q9Y653
C	227	HIS	-	expression tag	UNP Q9Y653
C	228	HIS	-	expression tag	UNP Q9Y653
C	229	HIS	-	expression tag	UNP Q9Y653
C	230	HIS	-	expression tag	UNP Q9Y653
C	231	HIS	-	expression tag	UNP Q9Y653
C	232	HIS	-	expression tag	UNP Q9Y653
C	233	HIS	-	expression tag	UNP Q9Y653
C	234	HIS	-	expression tag	UNP Q9Y653
C	235	HIS	-	expression tag	UNP Q9Y653
D	-19	MET	-	initiating methionine	UNP Q9Y653
D	-18	LYS	-	expression tag	UNP Q9Y653
D	-17	LEU	-	expression tag	UNP Q9Y653
D	-16	CYS	-	expression tag	UNP Q9Y653
D	-15	ILE	-	expression tag	UNP Q9Y653
D	-14	LEU	-	expression tag	UNP Q9Y653
D	-13	LEU	-	expression tag	UNP Q9Y653
D	-12	ALA	-	expression tag	UNP Q9Y653
D	-11	VAL	-	expression tag	UNP Q9Y653
D	-10	VAL	-	expression tag	UNP Q9Y653
D	-9	ALA	-	expression tag	UNP Q9Y653
D	-8	PHE	-	expression tag	UNP Q9Y653
D	-7	VAL	-	expression tag	UNP Q9Y653
D	-6	GLY	-	expression tag	UNP Q9Y653
D	-5	LEU	-	expression tag	UNP Q9Y653

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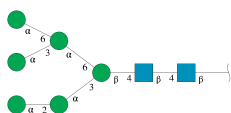
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	SER	-	expression tag	UNP Q9Y653
D	-3	LEU	-	expression tag	UNP Q9Y653
D	-2	GLY	-	expression tag	UNP Q9Y653
D	-1	ALA	-	expression tag	UNP Q9Y653
D	0	THR	-	expression tag	UNP Q9Y653
D	1	ASN	-	expression tag	UNP Q9Y653
D	2	ALA	-	expression tag	UNP Q9Y653
D	3	SER	-	expression tag	UNP Q9Y653
D	4	CYS	-	expression tag	UNP Q9Y653
D	5	ASP	-	expression tag	UNP Q9Y653
D	6	MET	-	expression tag	UNP Q9Y653
D	7	SER	-	expression tag	UNP Q9Y653
D	36	CYS	SER	conflict	UNP Q9Y653
D	48	CYS	SER	conflict	UNP Q9Y653
D	181	CYS	GLU	conflict	UNP Q9Y653
D	222	GLY	-	expression tag	UNP Q9Y653
D	223	SER	-	expression tag	UNP Q9Y653
D	224	GLY	-	expression tag	UNP Q9Y653
D	225	SER	-	expression tag	UNP Q9Y653
D	226	HIS	-	expression tag	UNP Q9Y653
D	227	HIS	-	expression tag	UNP Q9Y653
D	228	HIS	-	expression tag	UNP Q9Y653
D	229	HIS	-	expression tag	UNP Q9Y653
D	230	HIS	-	expression tag	UNP Q9Y653
D	231	HIS	-	expression tag	UNP Q9Y653
D	232	HIS	-	expression tag	UNP Q9Y653
D	233	HIS	-	expression tag	UNP Q9Y653
D	234	HIS	-	expression tag	UNP Q9Y653
D	235	HIS	-	expression tag	UNP Q9Y653

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



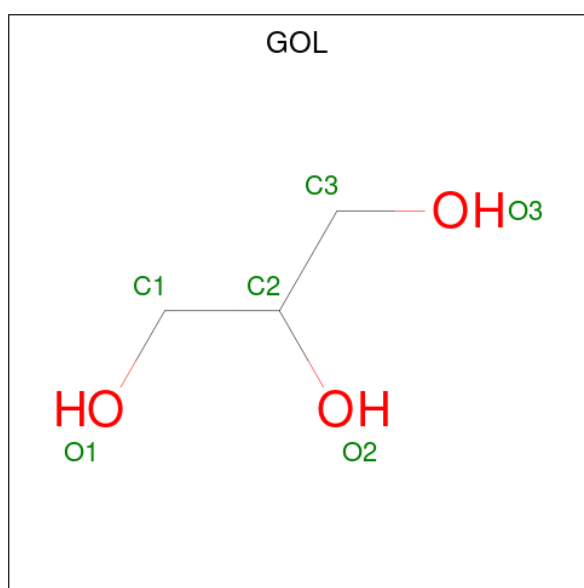
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	H	N	O	0	0	0
			133	40	61	2	30			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



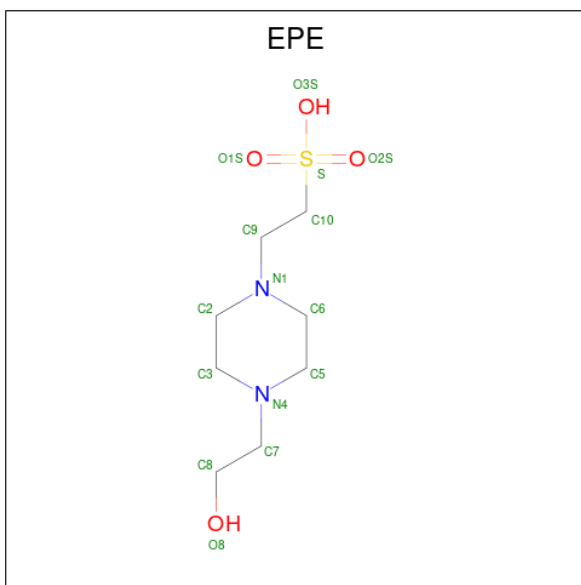
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total	C	H	N	O	0	0	0
			173	52	79	2	40			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	3	7	3		
4	A	1	Total	C	H	O	0	0
			13	3	7	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	1
			135	135		
6	B	3	Total	O	0	0
			3	3		
6	C	108	Total	O	0	0
			108	108		
6	D	1	Total	O	0	0
			1	1		

97%

GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- 33%

NAG1	BMA3
NAG2	MAN4
	MAN5
	MAN6

- 25%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.83Å 68.72Å 66.68Å 90.00° 107.12° 90.00°	Depositor
Resolution (Å)	47.22 – 1.92 47.22 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.22-1.92) 98.5 (47.22-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.92Å)	Xtriage
Refinement program	PHENIX 2.0_5716	Depositor
R, R_{free}	0.190 , 0.237 0.191 , 0.237	Depositor DCC
R_{free} test set	2127 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7380	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: EPE, BMA, GOL, MAN, 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	0.53	0/1680	0.67	0/2269
1	B	0.51	0/66	0.56	0/89
1	C	0.49	0/1637	0.63	0/2211
1	D	0.45	0/66	0.53	0/89
All	All	0.51	0/3449	0.65	0/4658

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	1633	1638	1634	6	0
1	B	65	67	67	0	0
1	C	1594	1598	1598	15	0
1	D	65	67	67	1	0
2	E	72	61	61	2	0
3	F	94	79	79	1	0
4	A	24	30	32	0	0
4	C	6	8	8	0	0
5	C	15	17	18	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	135	0	0	1	0
6	B	3	0	0	0	0
6	C	108	0	0	1	0
6	D	1	0	0	0	0
All	All	3815	3565	3564	23	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 23 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:A:120:LEU:HD11	1:A:143[B]:LEU:HD11	1.67	0.76
3:F:3:BMA:H2	3:F:4:MAN:H5	1.87	0.56
1:A:82:HIS:O	2:E:2:NAG:H83	2.09	0.53
1:C:55[B]:MET:HE2	1:C:66:THR:CG2	2.39	0.53
1:C:80:HIS:CE1	1:C:98:LEU:HD13	2.49	0.47

There are no symmetry-related clashes.

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	203/255 (80%)	202 (100%)	1 (0%)	0	100	100
1	B	6/255 (2%)	6 (100%)	0	0	100	100
1	C	196/255 (77%)	192 (98%)	4 (2%)	0	100	100
1	D	6/255 (2%)	6 (100%)	0	0	100	100
All	All	411/1020 (40%)	406 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	192/228 (84%)	191 (100%)	1 (0%)	81	80
1	B	7/228 (3%)	7 (100%)	0	100	100
1	C	188/228 (82%)	187 (100%)	1 (0%)	81	80
1	D	7/228 (3%)	7 (100%)	0	100	100
All	All	394/912 (43%)	392 (100%)	2 (0%)	81	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	C	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	ASN
1	C	164	GLN
1	C	80	HIS
1	C	105	GLN
1	C	133	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 ⓘ

14 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	2,1	14,14,15	0.92	0	17,19,21	1.54	1 (5%)
2	NAG	E	2	2	14,14,15	1.01	0	17,19,21	2.95	5 (29%)
2	BMA	E	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.69	2 (13%)
2	MAN	E	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.17	1 (6%)
2	MAN	E	5	2	11,11,12	0.80	1 (9%)	15,15,17	1.09	1 (6%)
2	MAN	E	6	2	11,11,12	0.88	1 (9%)	15,15,17	1.34	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.86	0	17,19,21	2.14	3 (17%)
3	NAG	F	2	3	14,14,15	0.74	0	17,19,21	1.55	2 (11%)
3	BMA	F	3	3	11,11,12	1.07	1 (9%)	15,15,17	1.55	5 (33%)
3	MAN	F	4	3	11,11,12	0.77	0	15,15,17	1.97	4 (26%)
3	MAN	F	5	3	11,11,12	0.83	0	15,15,17	1.36	2 (13%)
3	MAN	F	6	3	11,11,12	0.84	1 (9%)	15,15,17	1.22	1 (6%)
3	MAN	F	7	3	11,11,12	0.68	0	15,15,17	1.56	1 (6%)
3	MAN	F	8	3	11,11,12	0.68	0	15,15,17	1.21	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
2	NAG	E	1	2,1	-	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	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BMA	C2-C3	2.59	1.56	1.52
3	F	3	BMA	C2-C3	2.42	1.56	1.52
2	E	6	MAN	O5-C1	-2.33	1.40	1.43
3	F	6	MAN	O5-C1	-2.12	1.40	1.43
2	E	4	MAN	O5-C1	-2.10	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	7.78	133.98	122.90
3	F	1	NAG	O5-C1-C2	-6.39	101.19	111.29
3	F	4	MAN	C1-O5-C5	5.90	120.19	112.19
2	E	2	NAG	C4-C3-C2	-5.81	102.50	111.02
3	F	7	MAN	C1-O5-C5	5.24	119.30	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	E	6	MAN	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

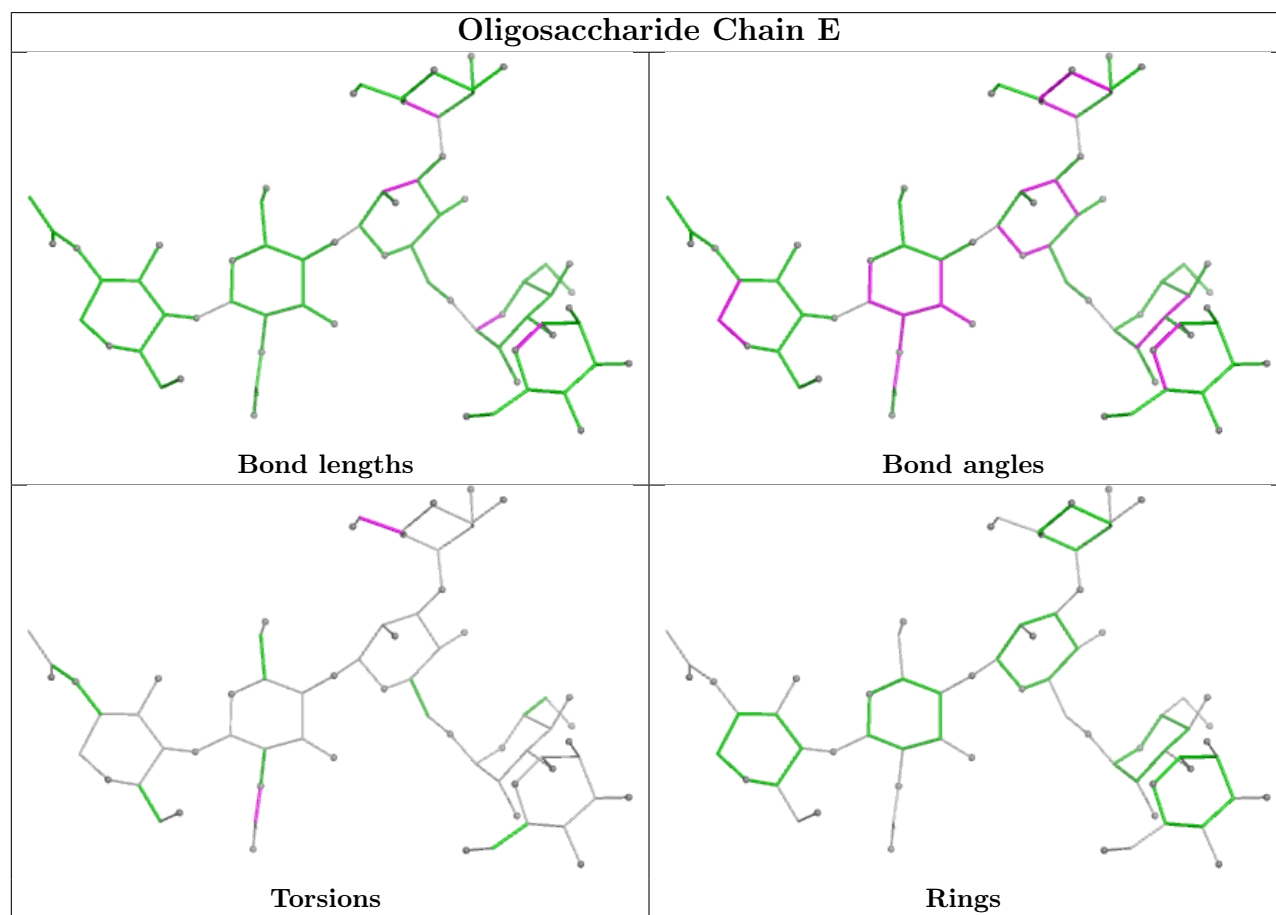
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

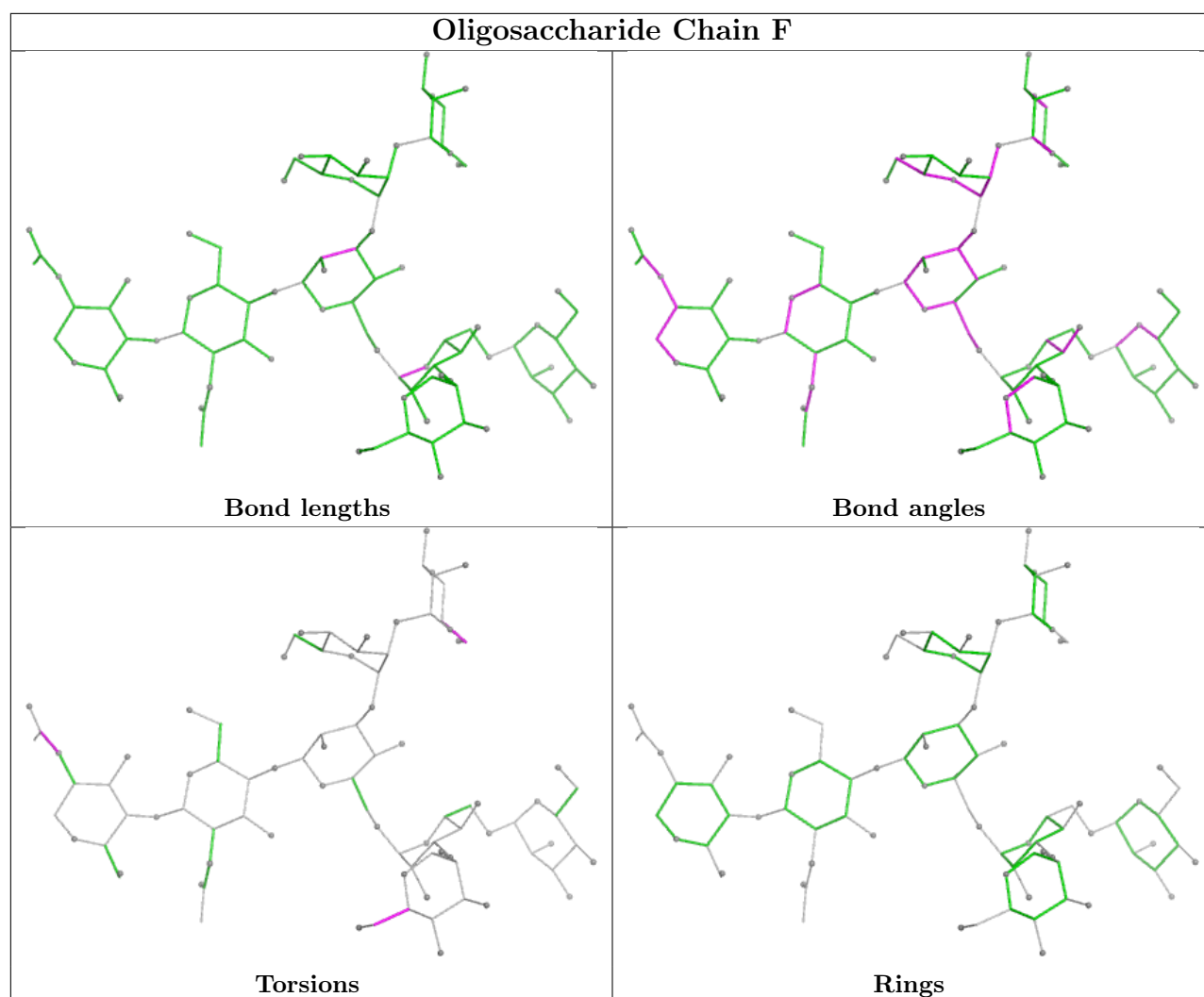
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	F	3	BMA	1	0
3	F	4	MAN	1	0

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](#)

6 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	$\# Z > 2$
4	GOL	A	303	-	5,5,5	0.47	0	5,5,5	1.27	1 (20%)
4	GOL	A	301	-	5,5,5	0.56	0	5,5,5	0.67	0
4	GOL	A	304	-	5,5,5	0.29	0	5,5,5	0.17	0
4	GOL	A	302	-	5,5,5	0.26	0	5,5,5	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EPE	C	301	-	15,15,15	0.73	0	18,20,20	1.86	4 (22%)
4	GOL	C	302	-	5,5,5	0.29	0	5,5,5	0.33	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
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	A	301	-	-	3/4/4/4	-
4	GOL	A	304	-	-	4/4/4/4	-
4	GOL	A	302	-	-	0/4/4/4	-
5	EPE	C	301	-	-	4/9/19/19	0/1/1/1
4	GOL	C	302	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	EPE	C7-N4-C3	5.17	124.44	111.23
5	C	301	EPE	C3-C2-N1	3.34	117.49	110.64
5	C	301	EPE	O1S-S-C10	-2.58	103.81	106.92
4	A	303	GOL	O2-C2-C3	2.38	119.62	109.12
5	C	301	EPE	C9-N1-C6	2.05	116.49	111.23

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	GOL	C1-C2-C3-O3
5	C	301	EPE	C8-C7-N4-C3
4	A	301	GOL	C1-C2-C3-O3
4	A	304	GOL	O1-C1-C2-C3
4	A	304	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	EPE	5	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	203/255 (79%)	-0.12	9 (4%) 39 43	9, 24, 56, 71	6 (2%)
1	B	8/255 (3%)	-0.12	1 (12%) 8 10	18, 19, 33, 51	0
1	C	198/255 (77%)	0.14	19 (9%) 13 17	9, 29, 65, 117	5 (2%)
1	D	8/255 (3%)	0.34	1 (12%) 8 10	23, 27, 40, 57	0
All	All	417/1020 (40%)	0.01	30 (7%) 21 26	9, 26, 64, 117	11 (2%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	VAL	4.0
1	C	170	LYS	3.9
1	C	171	ASN	3.7
1	A	114	ALA	3.4
1	C	105	GLN	3.4

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.

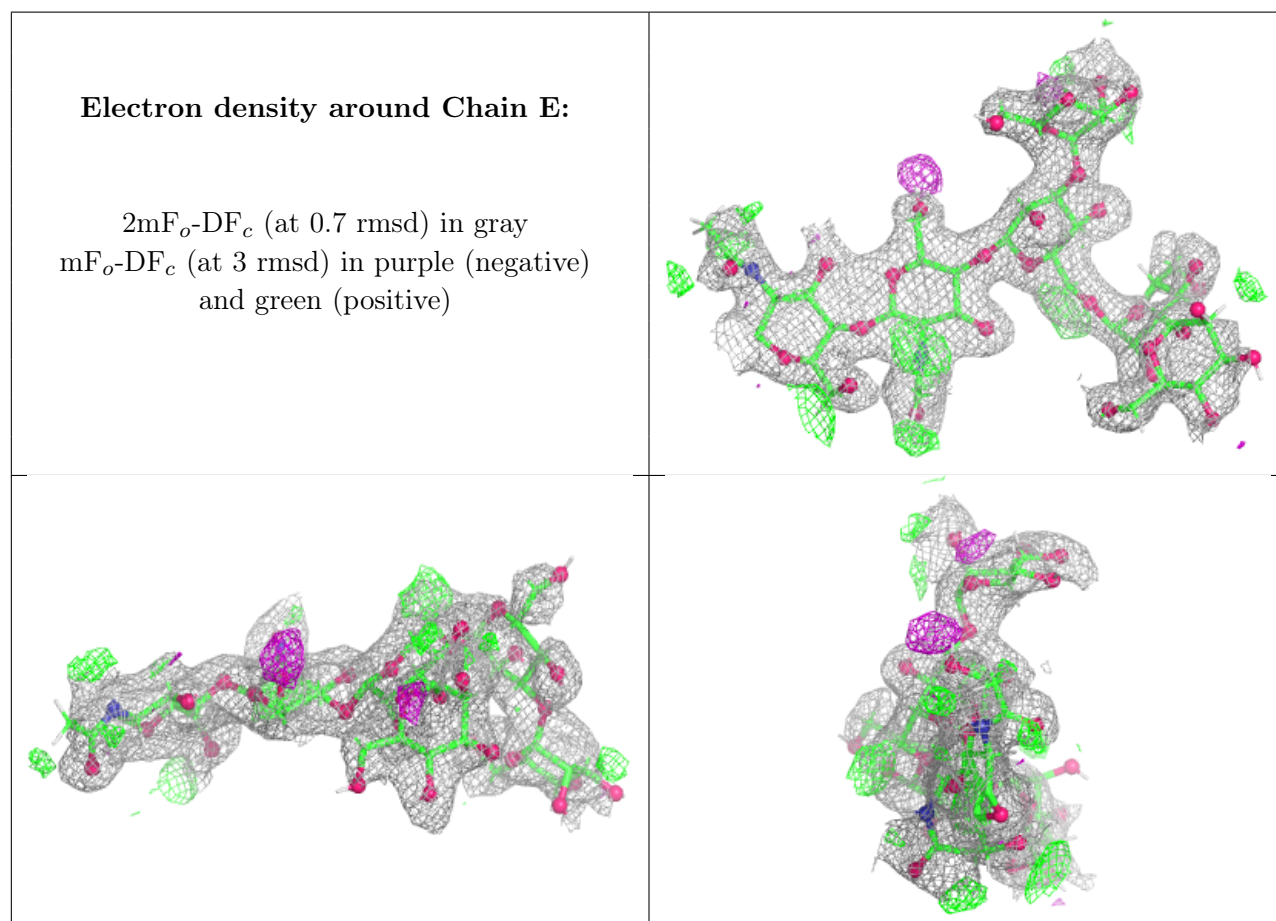
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	5	11/12	0.34	0.26	75,99,117,139	0
3	MAN	F	8	11/12	0.62	0.19	63,96,114,120	0

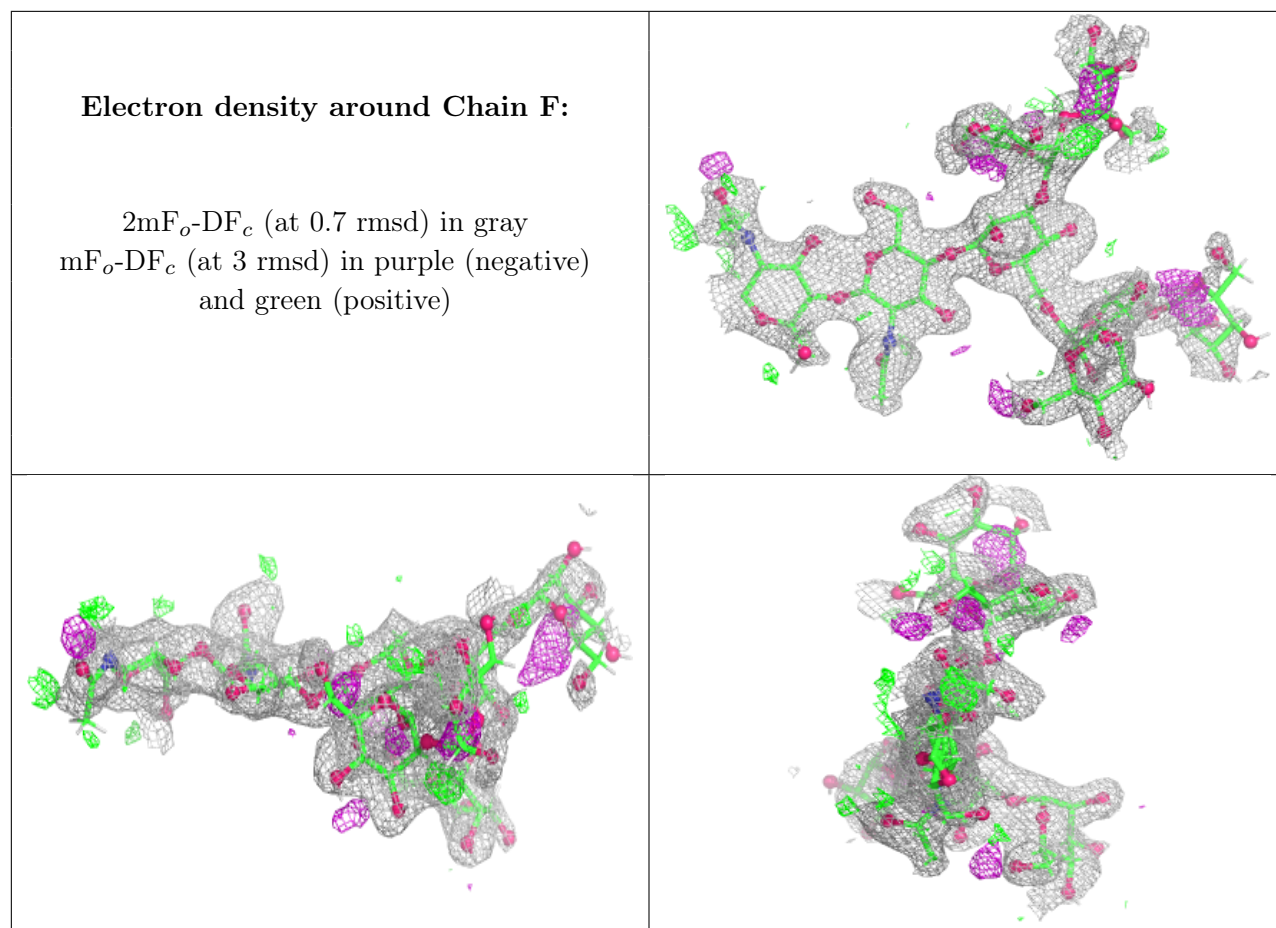
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	E	4	11/12	0.66	0.17	63,78,96,96	0
2	MAN	E	5	11/12	0.70	0.17	47,79,99,107	0
3	MAN	F	4	11/12	0.70	0.20	52,66,90,90	0
3	MAN	F	7	11/12	0.79	0.17	46,61,84,90	0
2	MAN	E	6	11/12	0.82	0.13	36,46,58,70	0
3	MAN	F	6	11/12	0.86	0.12	50,62,77,77	0
2	BMA	E	3	11/12	0.86	0.11	27,44,56,60	0
2	NAG	E	2	14/15	0.86	0.14	25,39,56,67	0
3	NAG	F	1	14/15	0.87	0.14	27,49,61,61	0
2	NAG	E	1	14/15	0.91	0.12	19,43,65,65	0
3	BMA	F	3	11/12	0.93	0.09	28,45,57,62	0
3	NAG	F	2	14/15	0.93	0.08	22,32,48,48	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.





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(Å ²)	Q<0.9
4	GOL	A	303	6/6	0.75	0.17	30,47,58,62	0
4	GOL	A	304	6/6	0.76	0.17	48,69,80,83	0
5	EPE	C	301	15/15	0.79	0.16	33,45,57,69	0
4	GOL	A	302	6/6	0.86	0.12	33,40,48,48	0
4	GOL	C	302	6/6	0.91	0.13	29,36,43,49	0
4	GOL	A	301	6/6	0.92	0.22	14,25,41,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.