



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 05:48 PM EDT

PDB ID : 5WI8  
Title : Crystal structure of murine 4-1BB from HEK293T cells in P21 space group  
Authors : Zajonc, D.M.; Bitra, A.  
Deposited on : 2017-07-18  
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

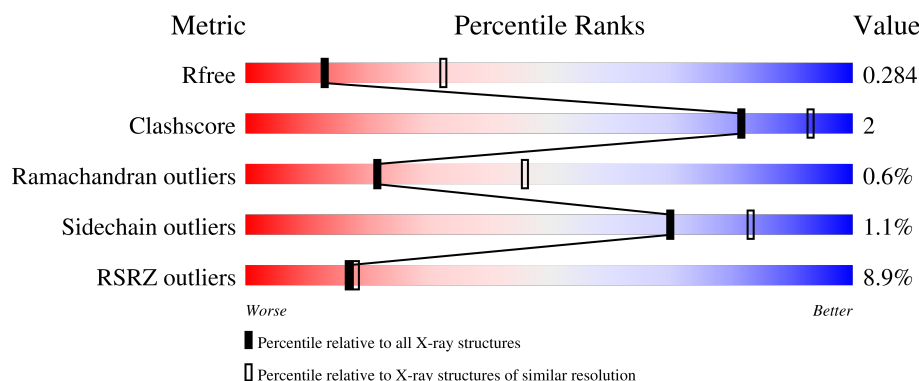
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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.





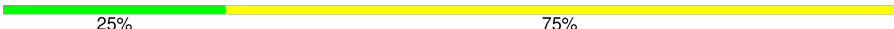
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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  $\geq 3$ , 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	143	<div> <div>8%</div> <div>88%</div> <div>5% • 5%</div> </div>
1	B	143	<div> <div>6%</div> <div>90%</div> <div>5% • 6%</div> </div>
1	C	143	<div> <div>12%</div> <div>91%</div> <div>• 6%</div> </div>
1	D	143	<div> <div>8%</div> <div>92%</div> <div>• 6%</div> </div>
2	E	4	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	5	 40% 60%
3	H	5	 40% 60%
4	G	4	 25% 75%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4333 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 Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			984	594	176	194	20			
1	B	135	Total	C	N	O	S	0	0	0
			969	585	177	187	20			
1	C	134	Total	C	N	O	S	0	0	0
			993	599	181	193	20			
1	D	134	Total	C	N	O	S	0	0	0
			977	586	179	192	20			

There are 24 discrepancies between the modelled and reference sequences:

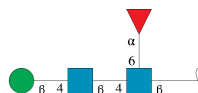
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LEU	-	expression tag	UNP P20334
A	23	GLU	-	expression tag	UNP P20334
A	161	LEU	-	expression tag	UNP P20334
A	162	VAL	-	expression tag	UNP P20334
A	163	PRO	-	expression tag	UNP P20334
A	164	ARG	-	expression tag	UNP P20334
B	22	LEU	-	expression tag	UNP P20334
B	23	GLU	-	expression tag	UNP P20334
B	161	LEU	-	expression tag	UNP P20334
B	162	VAL	-	expression tag	UNP P20334
B	163	PRO	-	expression tag	UNP P20334
B	164	ARG	-	expression tag	UNP P20334
C	22	LEU	-	expression tag	UNP P20334
C	23	GLU	-	expression tag	UNP P20334
C	161	LEU	-	expression tag	UNP P20334
C	162	VAL	-	expression tag	UNP P20334
C	163	PRO	-	expression tag	UNP P20334
C	164	ARG	-	expression tag	UNP P20334
D	22	LEU	-	expression tag	UNP P20334
D	23	GLU	-	expression tag	UNP P20334
D	161	LEU	-	expression tag	UNP P20334

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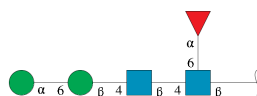
Chain	Residue	Modelled	Actual	Comment	Reference
D	162	VAL	-	expression tag	UNP P20334
D	163	PRO	-	expression tag	UNP P20334
D	164	ARG	-	expression tag	UNP P20334

- 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	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	F	5	Total	C	N	O	0	0	0
			60	34	2	24			
3	H	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 4 is an oligosaccharide called 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
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 8 is water.

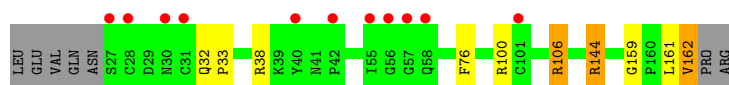
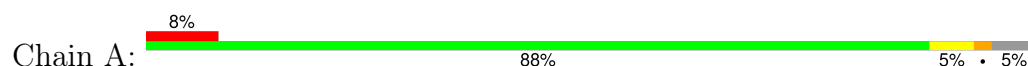
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	25	Total	O	0	0
			25	25		
8	C	18	Total	O	0	0
			18	18		
8	D	21	Total	O	0	0
			21	21		



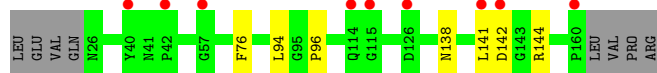
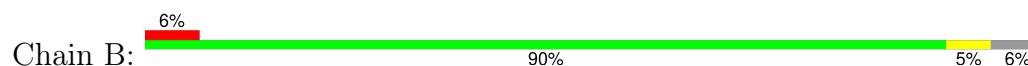
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

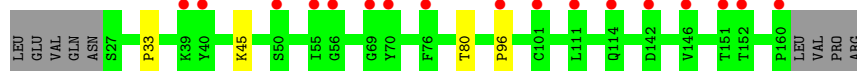
- Molecule 1: Tumor necrosis factor receptor superfamily member 9



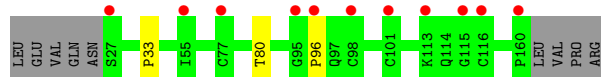
- Molecule 1: Tumor necrosis factor receptor superfamily member 9



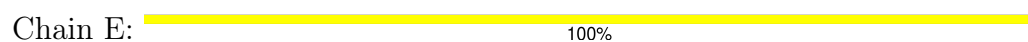
- Molecule 1: Tumor necrosis factor receptor superfamily member 9



- Molecule 1: Tumor necrosis factor receptor superfamily member 9



- 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



- Molecule 3:  $\alpha$ -D-mannopyranose-(1-6)- $\beta$ -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:  40% 60%

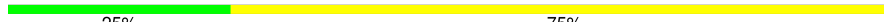


- Molecule 3:  $\alpha$ -D-mannopyranose-(1-6)- $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-[ $\alpha$ -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain H:  40% 60%



- Molecule 4:  $\alpha$ -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

Chain G:  25% 75%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.01Å 61.76Å 110.75Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	40.00 – 2.95 40.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	91.0 (40.00-2.95) 91.0 (40.00-2.95)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.235 , 0.279 0.238 , 0.284	Depositor DCC
$R_{free}$ test set	2553 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, FUC, GOL, NAG, BMA, EDO

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	0.49	0/1005	0.78	2/1363 (0.1%)
1	B	0.49	0/990	0.75	0/1341
1	C	0.45	0/1014	0.70	0/1369
1	D	0.46	0/998	0.72	0/1350
All	All	0.47	0/4007	0.74	2/5423 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	144	ARG	NE-CZ-NH1	5.32	122.96	120.30

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	984	0	871	7	0
1	B	969	0	856	12	0
1	C	993	0	908	3	0
1	D	977	0	863	2	0
2	E	49	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	60	0	52	0	0
3	H	60	0	52	0	0
4	G	50	0	43	0	0
5	A	30	0	40	0	0
5	B	12	0	16	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	4	0	6	0	0
6	B	12	0	18	0	0
6	C	4	0	6	0	0
6	D	12	0	18	0	0
7	B	14	0	13	0	0
8	A	27	0	0	1	0
8	B	25	0	0	0	0
8	C	18	0	0	0	0
8	D	21	0	0	0	0
All	All	4333	0	3821	19	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 2.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:CB	1:B:144:ARG:HH11	1.74	0.98
1:B:142:ASP:HB3	1:B:144:ARG:HH11	1.33	0.93
1:B:142:ASP:CB	1:B:144:ARG:NH1	2.36	0.88
1:B:142:ASP:HB2	1:B:144:ARG:NH1	2.03	0.73
1:B:142:ASP:HB3	1:B:144:ARG:HG3	1.70	0.72
1:B:142:ASP:HB3	1:B:144:ARG:NH1	2.06	0.65
1:A:76:PHE:CD2	1:C:33:PRO:HD2	2.33	0.64
1:A:106:ARG:NH2	8:A:301:HOH:O	2.37	0.57
1:B:142:ASP:HB2	1:B:144:ARG:HH12	1.77	0.49
1:B:76:PHE:CD1	1:D:80:THR:HG21	2.49	0.48
1:A:144:ARG:HD3	1:A:159:GLY:O	2.14	0.47
1:A:76:PHE:CD1	1:C:80:THR:HG21	2.51	0.45
1:B:142:ASP:OD2	1:B:144:ARG:NH1	2.51	0.44
1:A:32:GLN:HB3	1:A:33:PRO:HD2	2.00	0.43
1:B:138:ASN:HB3	1:B:141:LEU:HG	2.02	0.42
1:A:161:LEU:O	1:A:162:VAL:HG22	2.20	0.41
1:A:76:PHE:CE2	1:C:33:PRO:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:CD2	1:D:33:PRO:HD2	2.55	0.41
1:B:142:ASP:CG	1:B:144:ARG:HH11	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	134/143 (94%)	129 (96%)	5 (4%)	0	100	100
1	B	133/143 (93%)	128 (96%)	4 (3%)	1 (1%)	16	39
1	C	132/143 (92%)	127 (96%)	4 (3%)	1 (1%)	16	39
1	D	132/143 (92%)	125 (95%)	6 (4%)	1 (1%)	16	39
All	All	531/572 (93%)	509 (96%)	19 (4%)	3 (1%)	22	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	PRO
1	B	96	PRO
1	C	96	PRO

### 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	111/127 (87%)	108 (97%)	3 (3%)	40	64
1	B	107/127 (84%)	106 (99%)	1 (1%)	75	86
1	C	115/127 (91%)	114 (99%)	1 (1%)	75	86
1	D	110/127 (87%)	110 (100%)	0	100	100
All	All	443/508 (87%)	438 (99%)	5 (1%)	70	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	106	ARG
1	A	162	VAL
1	B	94	LEU
1	C	45	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

18 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	0.47	0	17,19,21	1.29	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	0.99	1 (5%)
2	BMA	E	3	2	11,11,12	0.35	0	15,15,17	0.82	1 (6%)
2	FUC	E	4	2	10,10,11	0.34	0	14,14,16	0.91	1 (7%)
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.89	0
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	1.20	3 (17%)
3	BMA	F	3	3	11,11,12	0.38	0	15,15,17	1.01	1 (6%)
3	MAN	F	4	3	11,11,12	0.47	0	15,15,17	1.81	2 (13%)
3	FUC	F	5	3	10,10,11	0.33	0	14,14,16	0.50	0
4	NAG	G	1	1,4	14,14,15	0.53	0	17,19,21	1.53	3 (17%)
4	NAG	G	2	4	14,14,15	0.46	0	17,19,21	1.00	0
4	BMA	G	3	4	11,11,12	0.60	0	15,15,17	1.17	1 (6%)
4	MAN	G	4	4	11,11,12	0.56	0	15,15,17	1.36	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	1.69	3 (17%)
3	NAG	H	2	3	14,14,15	0.56	0	17,19,21	1.07	2 (11%)
3	BMA	H	3	3	11,11,12	0.45	0	15,15,17	0.82	0
3	MAN	H	4	3	11,11,12	0.39	0	15,15,17	0.74	0
3	FUC	H	5	3	10,10,11	0.56	0	14,14,16	1.26	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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
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	-	2/2/19/22	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1

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

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	5.33	119.33	112.19
3	H	1	NAG	C1-O5-C5	4.70	118.49	112.19
4	G	1	NAG	C4-C3-C2	4.38	117.43	111.02
3	H	5	FUC	C1-C2-C3	3.78	115.15	109.64
3	H	1	NAG	O5-C1-C2	-3.53	105.83	111.29
4	G	3	BMA	C1-C2-C3	3.44	114.66	109.64
4	G	4	MAN	C1-C2-C3	3.44	114.65	109.64
3	F	4	MAN	C1-C2-C3	3.43	114.63	109.64
4	G	4	MAN	C1-O5-C5	3.08	116.31	112.19
3	F	3	BMA	C1-O5-C5	2.98	116.17	112.19
2	E	1	NAG	C1-O5-C5	2.41	115.42	112.19
2	E	4	FUC	C1-C2-C3	2.40	113.14	109.64
2	E	3	BMA	C1-O5-C5	2.38	115.38	112.19
3	F	2	NAG	C4-C3-C2	2.33	114.43	111.02
4	G	1	NAG	C2-N2-C7	2.26	125.94	122.90
4	G	1	NAG	C3-C4-C5	2.25	114.32	110.23
2	E	2	NAG	C4-C3-C2	2.25	114.31	111.02
3	H	1	NAG	C4-C3-C2	2.24	114.30	111.02
2	E	1	NAG	C2-N2-C7	2.20	125.85	122.90
3	F	2	NAG	C1-O5-C5	2.14	115.05	112.19
3	F	2	NAG	O3-C3-C2	-2.13	104.98	109.40
3	H	2	NAG	O5-C1-C2	-2.11	108.02	111.29
3	H	2	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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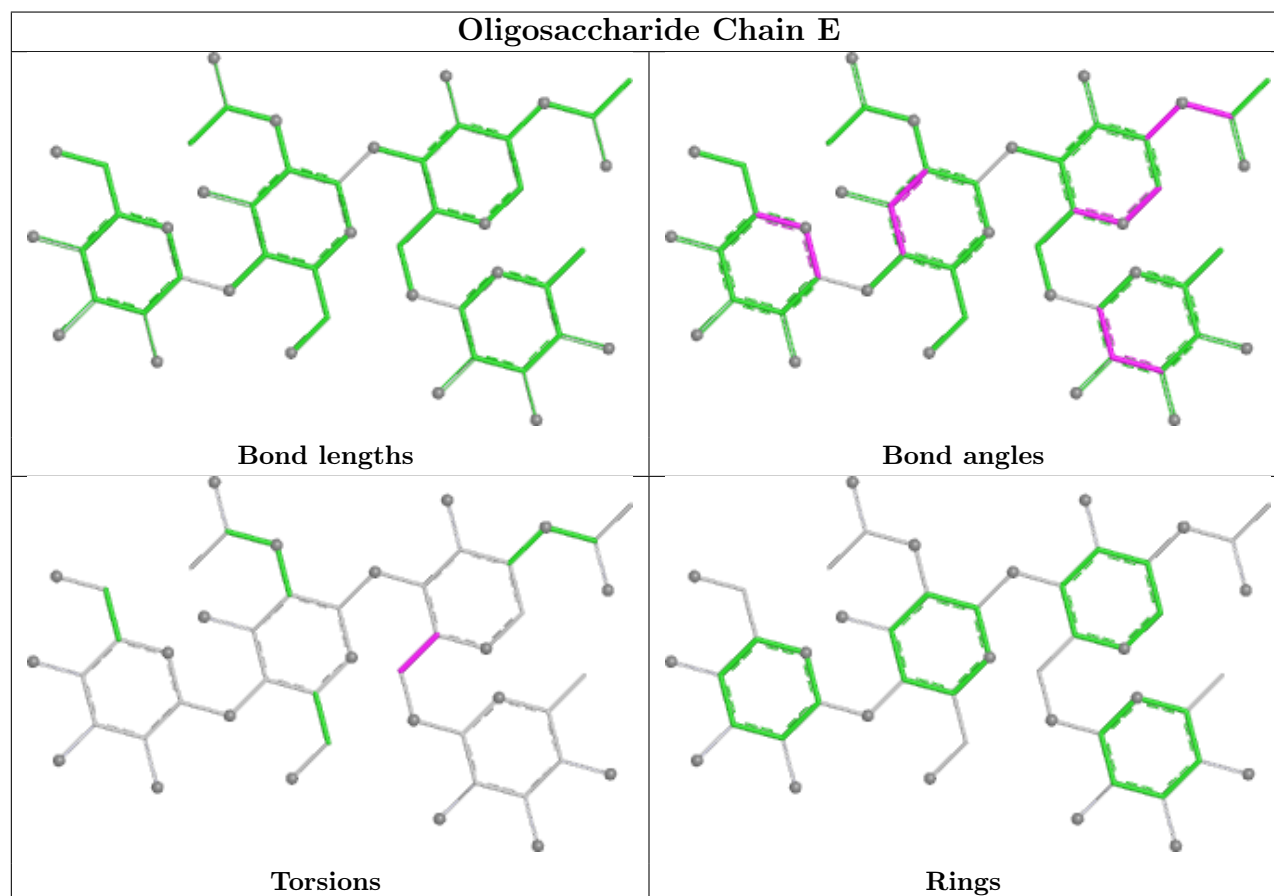
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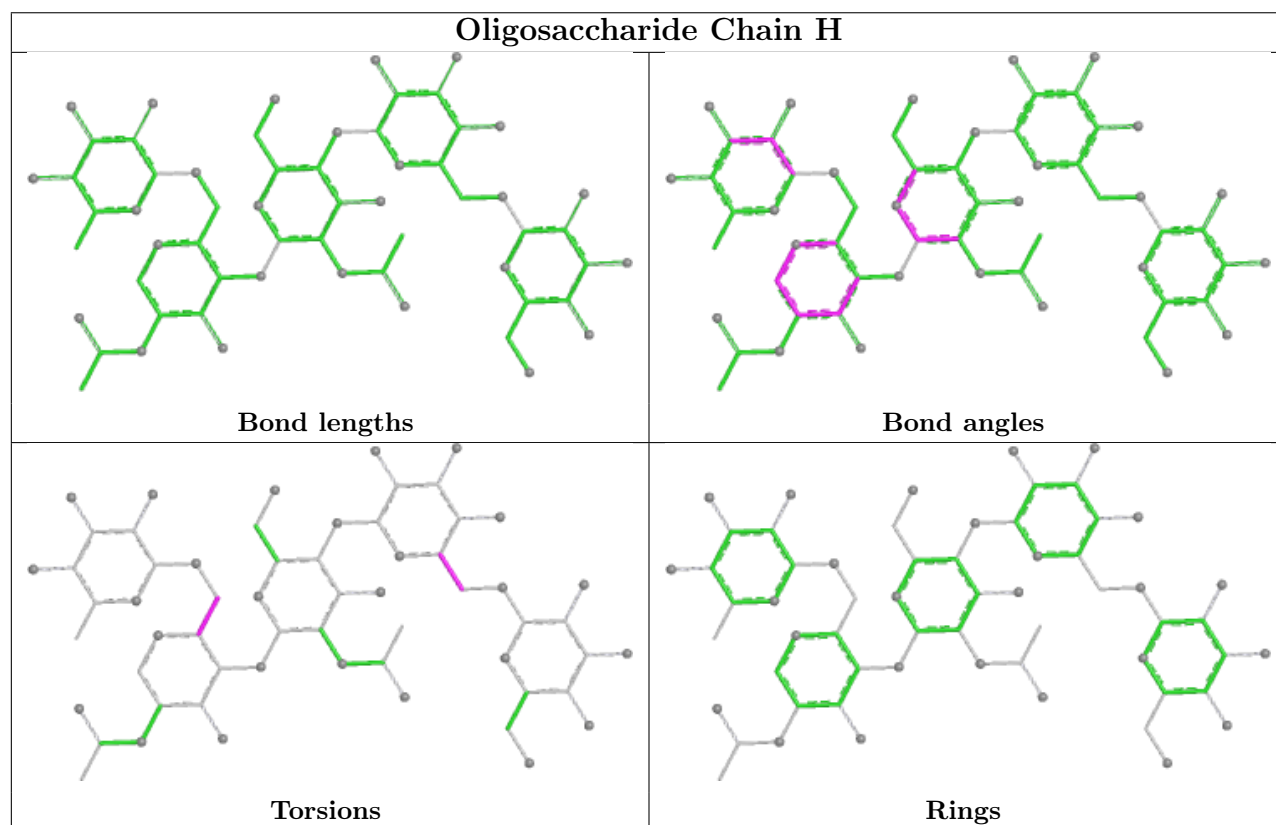
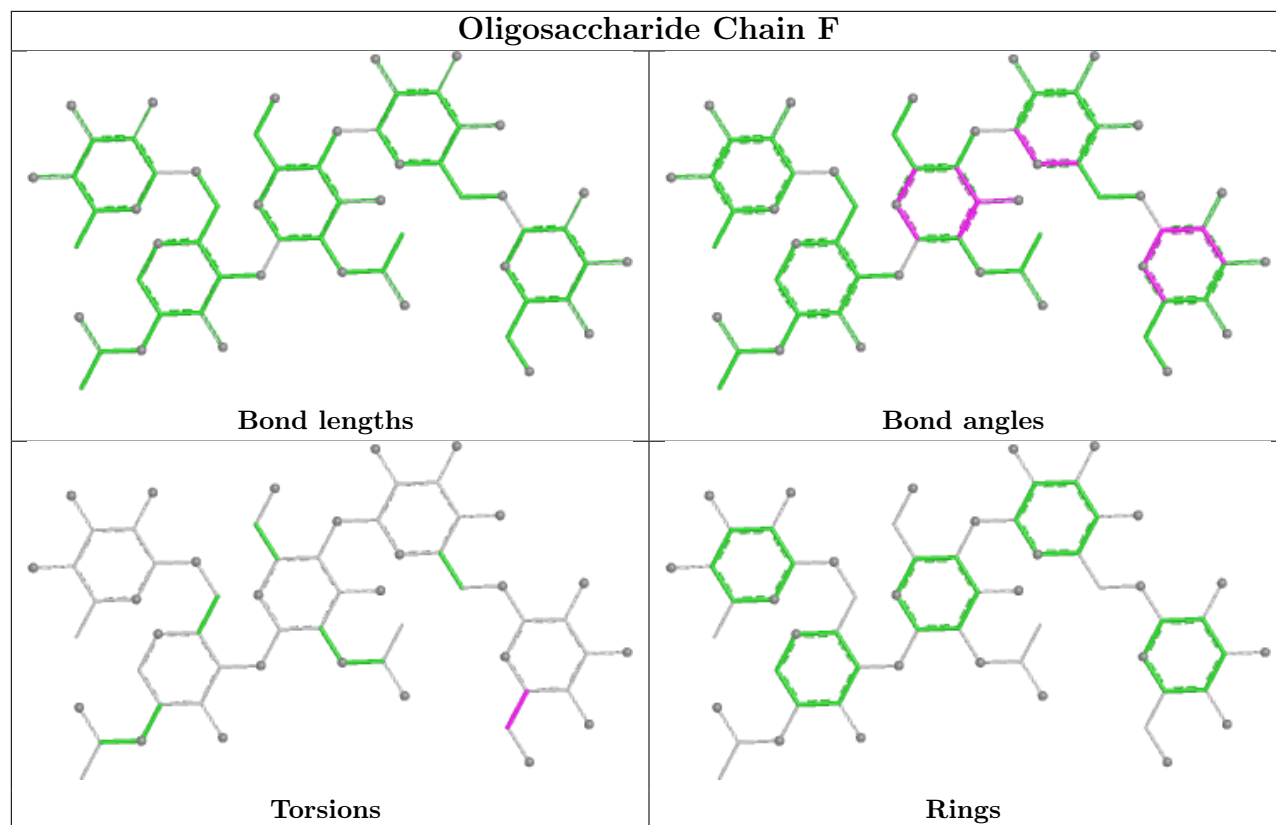
Mol	Chain	Res	Type	Atoms
4	G	4	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7

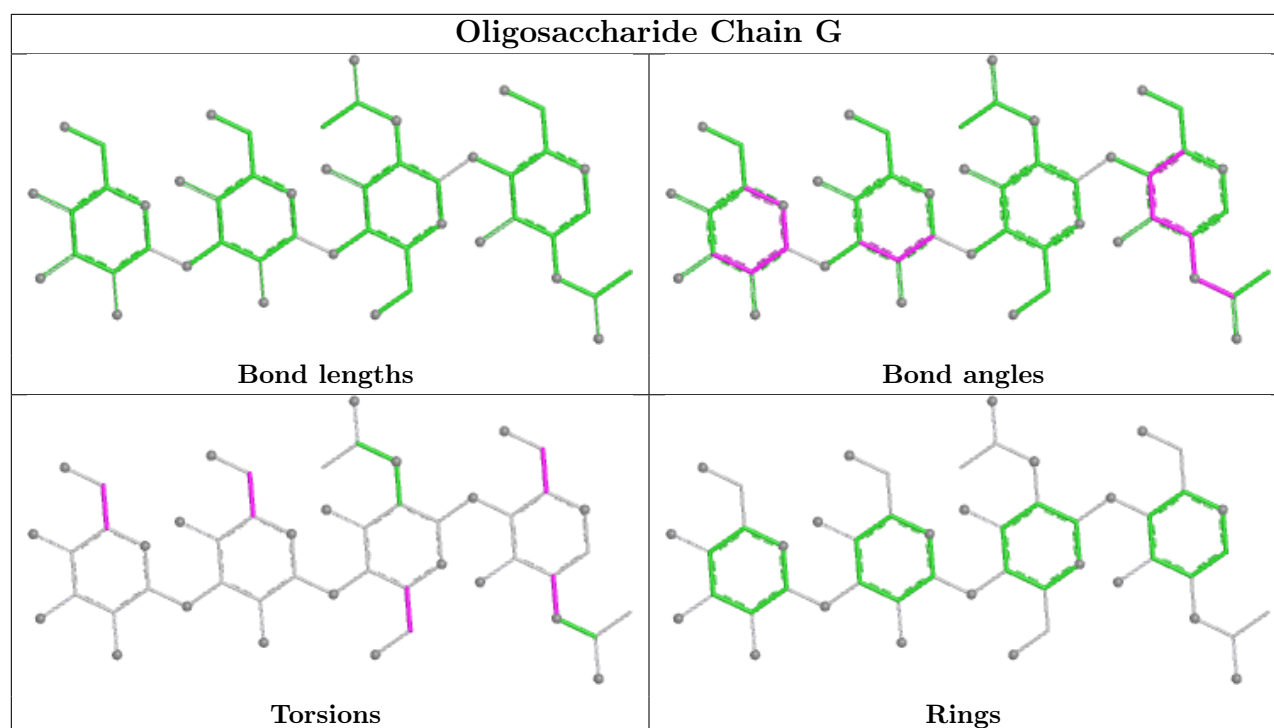
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

18 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	$\# Z  > 2$
5	GOL	A	209	-	5,5,5	0.37	0	5,5,5	0.29	0
6	EDO	D	401	-	3,3,3	0.42	0	2,2,2	0.35	0
6	EDO	C	401	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	D	402	-	3,3,3	0.45	0	2,2,2	0.14	0
5	GOL	A	208	-	5,5,5	0.42	0	5,5,5	0.35	0
5	GOL	B	211	-	5,5,5	0.39	0	5,5,5	0.36	0
6	EDO	B	204	-	3,3,3	0.48	0	2,2,2	0.29	0
6	EDO	B	203	-	3,3,3	0.42	0	2,2,2	0.46	0
5	GOL	B	201	-	5,5,5	0.30	0	5,5,5	0.19	0
5	GOL	D	409	-	5,5,5	0.39	0	5,5,5	0.29	0
6	EDO	A	210	-	3,3,3	0.46	0	2,2,2	0.17	0
6	EDO	D	403	-	3,3,3	0.50	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	210	1	14,14,15	0.49	0	17,19,21	0.93	1 (5%)
5	GOL	A	205	-	5,5,5	0.39	0	5,5,5	0.61	0
6	EDO	B	202	-	3,3,3	0.42	0	2,2,2	0.25	0
5	GOL	A	206	-	5,5,5	0.43	0	5,5,5	0.43	0
5	GOL	C	406	-	5,5,5	0.29	0	5,5,5	0.28	0
5	GOL	A	207	-	5,5,5	0.38	0	5,5,5	0.25	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
5	GOL	A	209	-	-	3/4/4/4	-
6	EDO	D	401	-	-	0/1/1/1	-
6	EDO	C	401	-	-	0/1/1/1	-
6	EDO	D	402	-	-	1/1/1/1	-
5	GOL	A	208	-	-	2/4/4/4	-
5	GOL	B	211	-	-	2/4/4/4	-
6	EDO	B	204	-	-	0/1/1/1	-
6	EDO	B	203	-	-	0/1/1/1	-
5	GOL	B	201	-	-	0/4/4/4	-
5	GOL	D	409	-	-	2/4/4/4	-
6	EDO	A	210	-	-	1/1/1/1	-
6	EDO	D	403	-	-	1/1/1/1	-
7	NAG	B	210	1	-	2/6/23/26	0/1/1/1
5	GOL	A	205	-	-	2/4/4/4	-
6	EDO	B	202	-	-	0/1/1/1	-
5	GOL	A	206	-	-	2/4/4/4	-
5	GOL	C	406	-	-	0/4/4/4	-
5	GOL	A	207	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	210	NAG	O5-C5-C6	2.15	111.85	107.66

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	205	GOL	O1-C1-C2-C3
5	A	206	GOL	C1-C2-C3-O3
5	A	206	GOL	O2-C2-C3-O3
5	B	211	GOL	C1-C2-C3-O3
7	B	210	NAG	O5-C5-C6-O6
5	A	205	GOL	O1-C1-C2-O2
5	B	211	GOL	O2-C2-C3-O3
7	B	210	NAG	C4-C5-C6-O6
5	A	207	GOL	O1-C1-C2-C3
5	A	208	GOL	C1-C2-C3-O3
5	A	209	GOL	O1-C1-C2-C3
5	D	409	GOL	O1-C1-C2-C3
6	A	210	EDO	O1-C1-C2-O2
6	D	402	EDO	O1-C1-C2-O2
5	A	208	GOL	O2-C2-C3-O3
5	A	209	GOL	O1-C1-C2-O2
6	D	403	EDO	O1-C1-C2-O2
5	D	409	GOL	O1-C1-C2-O2
5	A	209	GOL	O2-C2-C3-O3
5	A	207	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	136/143 (95%)	0.49	11 (8%) 19 20	44, 62, 112, 132	0
1	B	135/143 (94%)	0.65	9 (6%) 25 24	44, 67, 106, 119	0
1	C	134/143 (93%)	0.81	17 (12%) 9 12	54, 75, 105, 119	0
1	D	134/143 (93%)	0.82	11 (8%) 19 20	56, 75, 102, 111	0
All	All	539/572 (94%)	0.69	48 (8%) 17 18	44, 71, 108, 132	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	4.2
1	D	96	PRO	4.0
1	B	126	ASP	3.8
1	D	115	GLY	3.7
1	A	57	GLY	3.4
1	B	142	ASP	3.2
1	A	27	SER	3.1
1	C	55	ILE	3.1
1	A	101	CYS	3.0
1	A	55	ILE	2.9
1	C	40	TYR	2.9
1	B	57	GLY	2.9
1	C	39	LYS	2.8
1	B	115	GLY	2.8
1	D	95	GLY	2.7
1	C	70	TYR	2.7
1	B	160	PRO	2.7
1	C	146	VAL	2.7
1	C	111	LEU	2.7
1	C	142	ASP	2.6
1	A	28	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	2.6
1	B	40	TYR	2.6
1	B	141	LEU	2.6
1	A	31	CYS	2.5
1	D	116	CYS	2.5
1	B	114	GLN	2.5
1	C	114	GLN	2.5
1	C	96	PRO	2.5
1	C	50	SER	2.5
1	A	58	GLN	2.5
1	D	77	CYS	2.5
1	C	160	PRO	2.4
1	B	42	PRO	2.3
1	A	30	ASN	2.3
1	C	151	THR	2.3
1	C	101	CYS	2.2
1	A	40	TYR	2.2
1	C	76	PHE	2.2
1	D	98	CYS	2.2
1	D	160	PRO	2.2
1	A	42	PRO	2.1
1	D	113	LYS	2.1
1	C	152	THR	2.1
1	D	101	CYS	2.1
1	D	55	ILE	2.1
1	D	27	SER	2.0
1	C	69	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
4	MAN	G	4	11/12	0.35	0.20	123,134,137,139	0

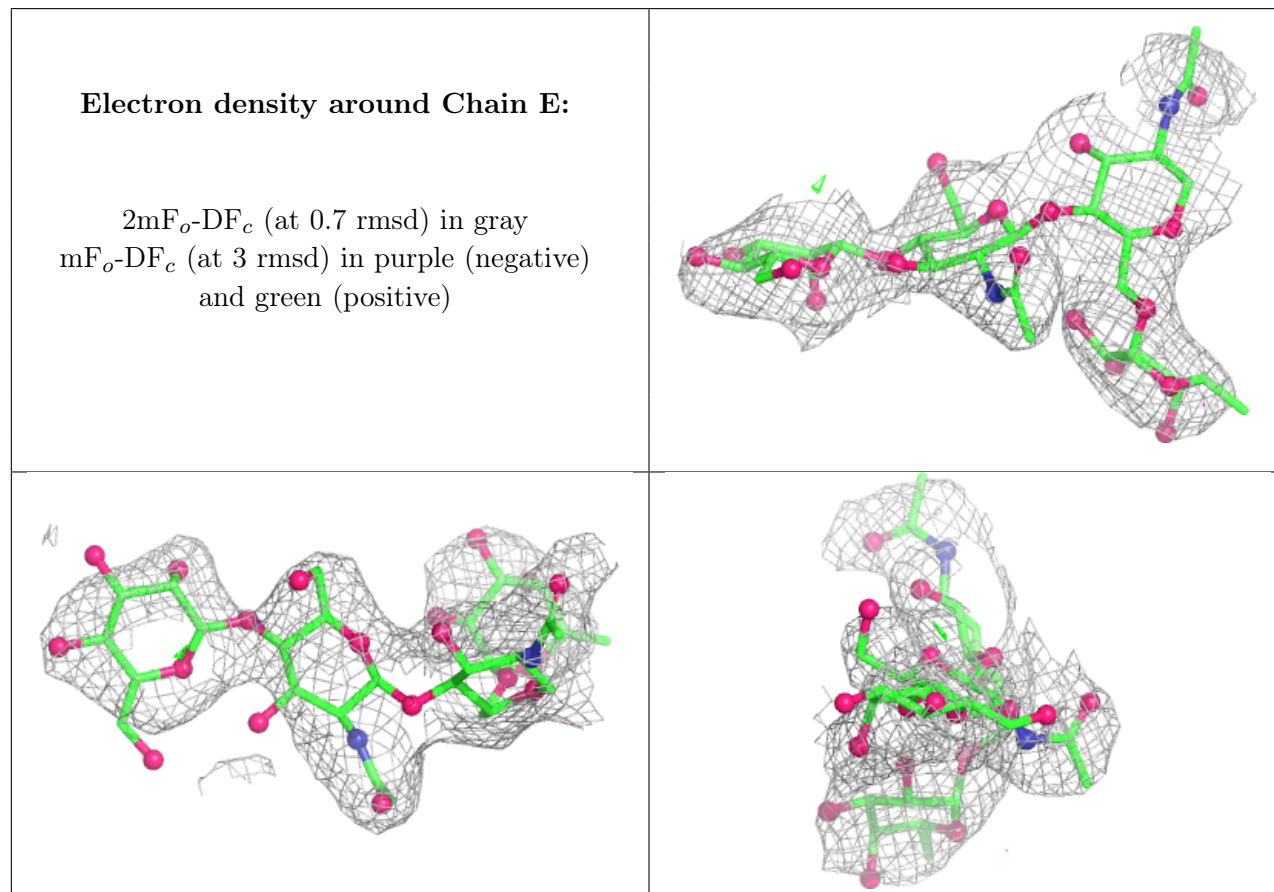
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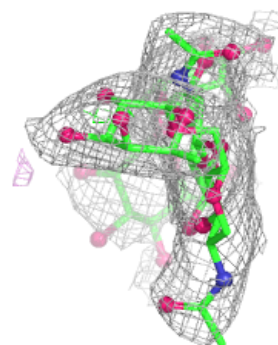
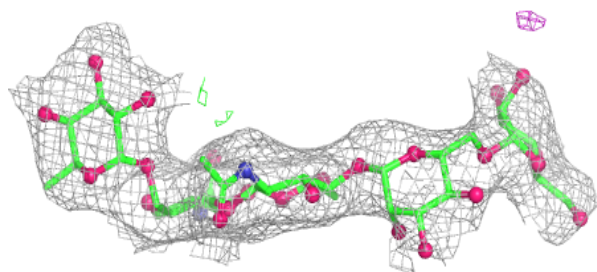
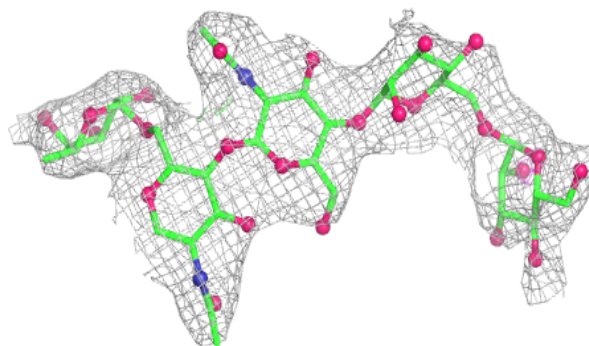
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	G	3	11/12	0.48	0.12	136,138,142,143	0
3	FUC	H	5	10/11	0.53	0.17	92,99,101,103	0
3	MAN	H	4	11/12	0.57	0.14	115,123,124,124	0
2	BMA	E	3	11/12	0.70	0.11	110,115,117,118	0
4	NAG	G	2	14/15	0.70	0.13	106,120,122,131	0
3	BMA	H	3	11/12	0.71	0.11	100,106,116,118	0
3	MAN	F	4	11/12	0.74	0.17	99,110,115,118	0
3	BMA	F	3	11/12	0.78	0.13	82,91,100,102	0
4	NAG	G	1	14/15	0.79	0.12	103,109,111,114	0
2	NAG	E	2	14/15	0.81	0.12	85,95,105,113	0
3	NAG	H	2	14/15	0.89	0.11	88,90,94,99	0
2	NAG	E	1	14/15	0.89	0.10	66,73,77,86	0
2	FUC	E	4	10/11	0.91	0.14	76,77,80,82	0
3	NAG	F	2	14/15	0.92	0.08	54,58,61,72	0
3	NAG	H	1	14/15	0.93	0.09	80,83,89,97	0
3	FUC	F	5	10/11	0.94	0.08	61,64,65,65	0
3	NAG	F	1	14/15	0.94	0.09	52,55,61,62	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.



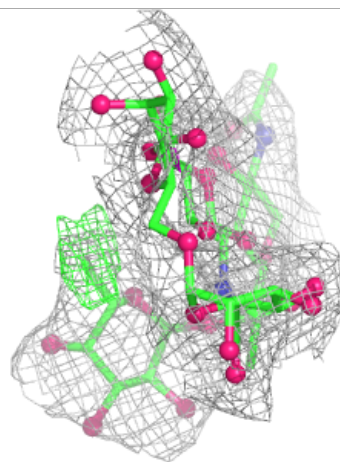
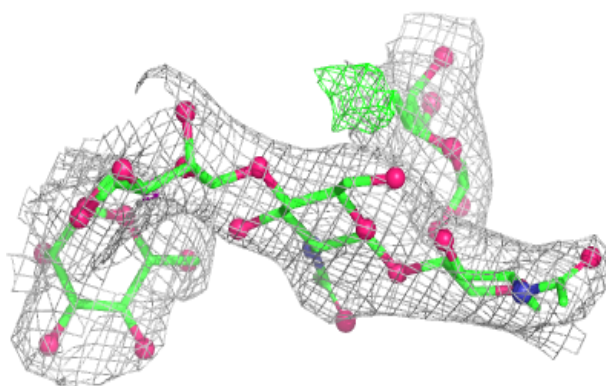
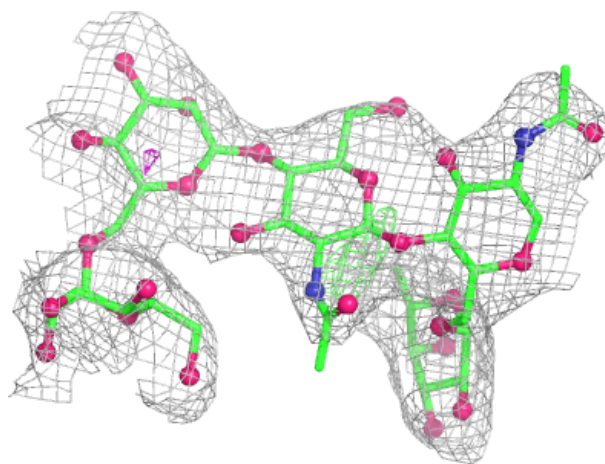
**Electron density around Chain F:**

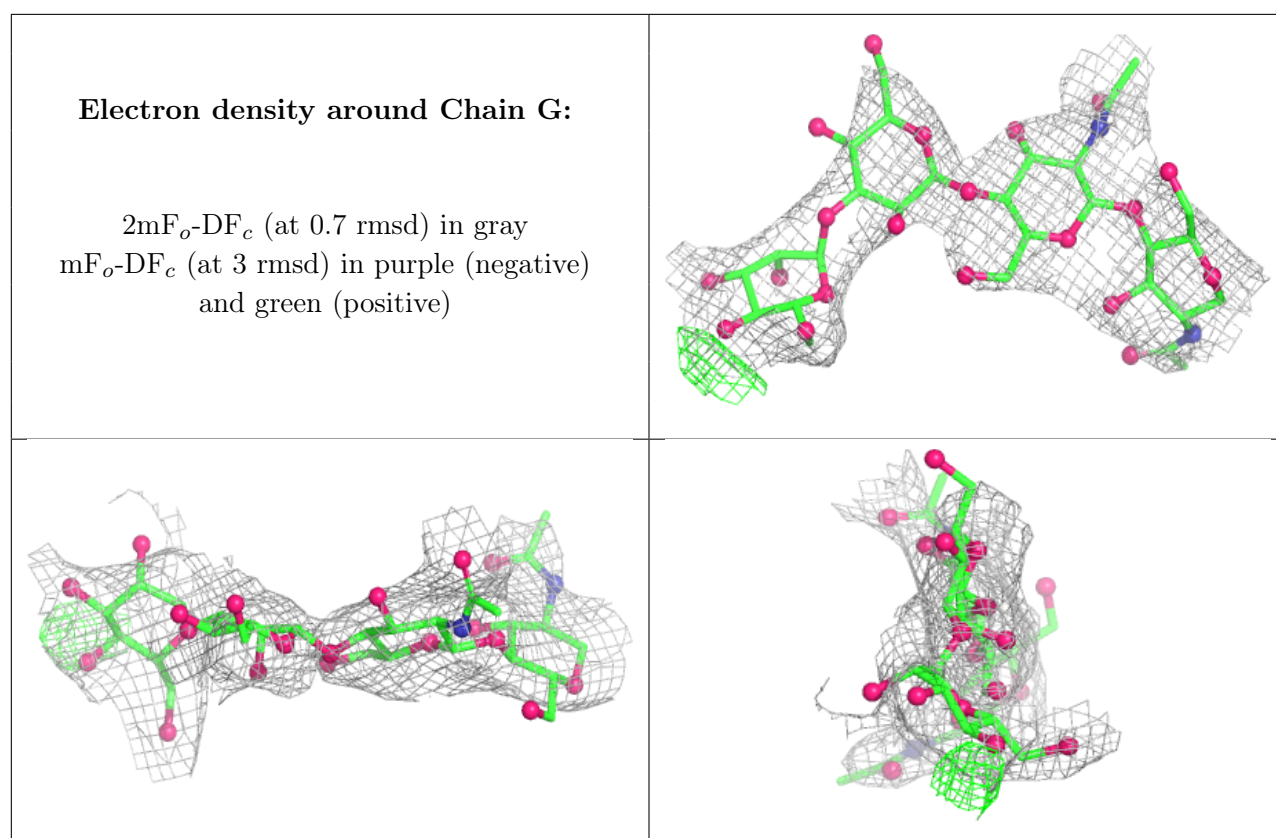
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	D	402	4/4	0.62	0.29	81,81,81,83	0
5	GOL	A	206	6/6	0.64	0.15	111,115,117,118	0
7	NAG	B	210	14/15	0.68	0.16	102,109,113,113	0
5	GOL	C	406	6/6	0.70	0.20	112,115,116,117	0
6	EDO	B	203	4/4	0.72	0.23	57,58,58,60	0
6	EDO	B	202	4/4	0.76	0.24	66,69,71,74	0
5	GOL	B	201	6/6	0.78	0.20	90,98,99,100	0
6	EDO	D	401	4/4	0.79	0.24	69,71,72,75	0
5	GOL	D	409	6/6	0.82	0.12	80,87,89,90	0
6	EDO	D	403	4/4	0.85	0.21	93,95,95,96	0
5	GOL	A	209	6/6	0.86	0.12	90,92,93,93	0
5	GOL	A	205	6/6	0.86	0.13	57,59,61,62	0
6	EDO	B	204	4/4	0.87	0.14	73,77,80,83	0
5	GOL	A	208	6/6	0.88	0.18	85,88,88,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	211	6/6	0.91	0.07	93,95,96,96	0
6	EDO	C	401	4/4	0.91	0.14	66,66,68,69	0
5	GOL	A	207	6/6	0.94	0.09	74,78,79,79	0
6	EDO	A	210	4/4	0.95	0.12	54,55,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.