



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 03:17 PM EDT

PDB ID : 6MKB  
Title : Crystal structure of murine 4-1BB ligand  
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Deposited on : 2018-09-25  
Resolution : 2.50 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)

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<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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

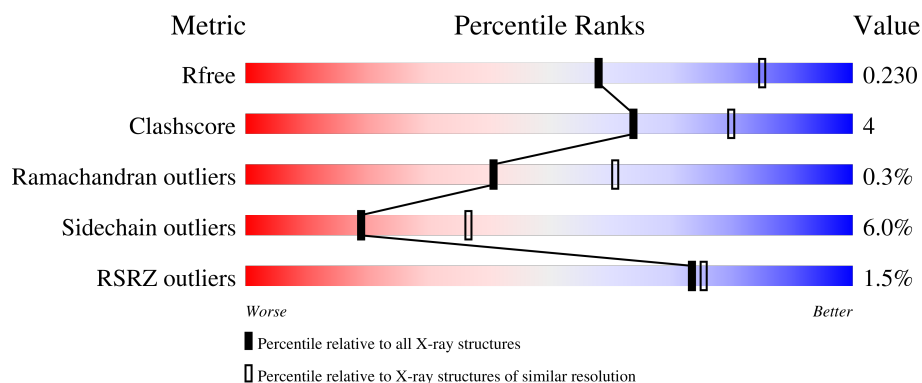
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



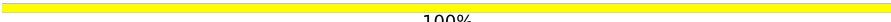


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	171	<div> <div>2%</div> <div>83% 11% 6%</div> </div>
1	B	171	<div> <div>2%</div> <div>80% 16% ..</div> </div>
1	C	171	<div> <div>2%</div> <div>78% 17% ..</div> </div>
1	D	171	<div> <div>2%</div> <div>84% 10% 6%</div> </div>
2	E	4	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	3	 100%
4	G	4	 75% 25%
5	H	5	 20% 80%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5706 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 ligand superfamily member 9.

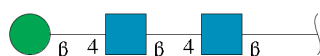
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	1	0
			1273	821	214	236	2			
1	B	165	Total	C	N	O	S	0	0	0
			1313	846	219	245	3			
1	C	165	Total	C	N	O	S	0	2	0
			1324	853	222	246	3			
1	D	160	Total	C	N	O	S	0	0	0
			1265	816	213	234	2			

- Molecule 2 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.



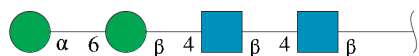
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



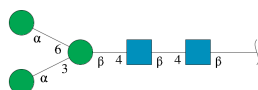
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			4	3	1		
7	D	1	Total	O	S	0	0
			5	4	1		

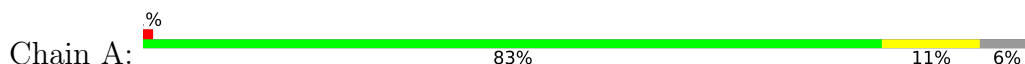
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	58	Total	O	0	0
			58	58		
8	B	89	Total	O	0	0
			89	89		
8	C	78	Total	O	0	0
			78	78		
8	D	61	Total	O	0	0
			61	61		

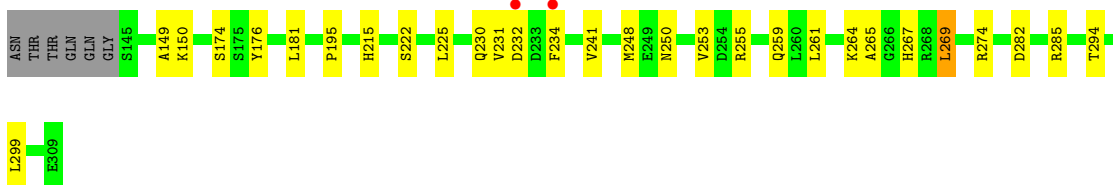
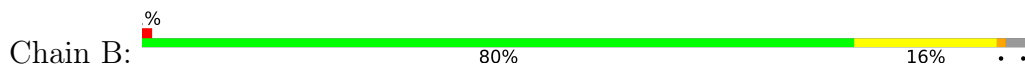
### 3 Residue-property plots [i](#)

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.

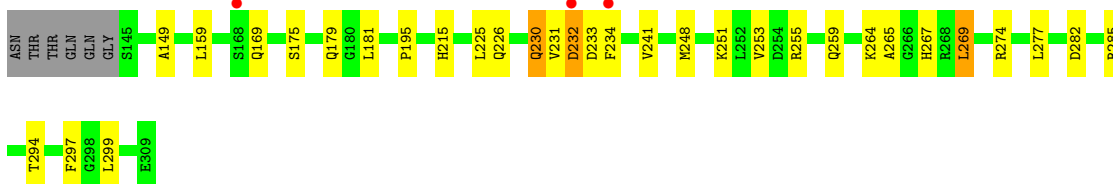
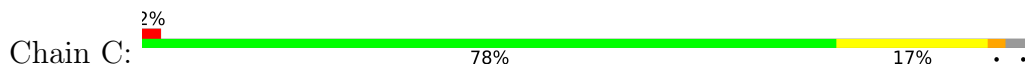
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



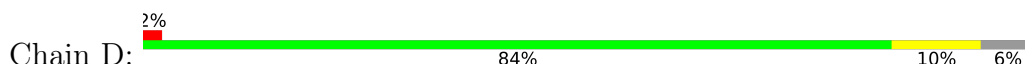
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9




- Molecule 2: 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 E:  100%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain F:  100%

MAG1  
MAG2  
BMA3

- Molecule 4: 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

Chain G:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-[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

Chain H:  20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.36Å 77.36Å 118.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.14 – 2.50 29.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.14-2.50) 99.7 (29.14-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.188 , 0.241 0.185 , 0.230	Depositor DCC
$R_{free}$ test set	1306 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.488 for h,-h-k,-l 0.011 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: SO4, NA, NAG, BMA, 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	0.45	0/1308	0.70	0/1779
1	B	0.49	0/1348	0.74	0/1835
1	C	0.48	0/1365	0.73	0/1857
1	D	0.47	0/1296	0.69	0/1761
All	All	0.47	0/5317	0.72	0/7232

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	1273	0	1256	7	0
1	B	1313	0	1285	14	0
1	C	1324	0	1303	17	0
1	D	1265	0	1248	7	0
2	E	50	0	43	0	0
3	F	39	0	34	0	0
4	G	50	0	43	0	0
5	H	61	0	52	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
7	B	20	0	0	0	0
7	C	14	0	0	0	0
7	D	5	0	0	0	0
8	A	58	0	0	0	0
8	B	89	0	0	0	0
8	C	78	0	0	0	0
8	D	61	0	0	0	0
All	All	5706	0	5264	45	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 4.

All (45) 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:264:LYS:H	1:A:267:HIS:HD2	1.23	0.87
1:D:264:LYS:H	1:D:267:HIS:HD2	1.24	0.86
1:C:264:LYS:H	1:C:267:HIS:HD2	1.24	0.85
1:B:264:LYS:H	1:B:267:HIS:HD2	1.23	0.85
1:B:231:VAL:HG21	1:B:261:LEU:HD22	1.61	0.81
1:C:230:GLN:HG3	1:C:234:PHE:HB3	1.69	0.74
1:C:226:GLN:HA	1:C:234:PHE:HZ	1.64	0.62
1:B:264:LYS:H	1:B:267:HIS:CD2	2.12	0.62
1:B:230:GLN:HG3	1:B:234:PHE:HB3	1.80	0.62
1:C:226:GLN:HA	1:C:234:PHE:CZ	2.37	0.60
1:C:264:LYS:H	1:C:267:HIS:CD2	2.13	0.58
1:D:264:LYS:H	1:D:267:HIS:CD2	2.13	0.58
1:B:241:VAL:HG22	1:B:255:ARG:HG3	1.88	0.56
1:A:264:LYS:H	1:A:267:HIS:CD2	2.12	0.55
1:D:239:LEU:HD13	1:D:257:TRP:HB2	1.89	0.54
1:B:150:LYS:O	1:B:176:TYR:HB3	2.08	0.54
1:B:241:VAL:HG11	1:B:253:VAL:HG11	1.90	0.52
1:C:215:HIS:HA	1:C:248:MET:HE2	1.92	0.51
1:B:215:HIS:HA	1:B:248:MET:HE2	1.94	0.50
1:C:234:PHE:CD1	1:C:234:PHE:C	2.84	0.50
1:B:231:VAL:HG22	1:B:234:PHE:HB2	1.93	0.50
1:C:159:LEU:HD12	1:C:277:LEU:HD11	1.94	0.50
1:D:241:VAL:HG11	1:D:253:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:O	1:C:234:PHE:CE1	2.65	0.49
1:C:241:VAL:HG11	1:C:253:VAL:HG11	1.95	0.49
1:A:241:VAL:HG11	1:A:253:VAL:HG11	1.95	0.48
1:A:241:VAL:HG22	1:A:255:ARG:HG3	1.94	0.48
1:B:149:ALA:HB2	1:B:181:LEU:HD13	1.95	0.48
1:C:241:VAL:HG22	1:C:255[B]:ARG:HG3	1.96	0.47
1:A:149:ALA:HB2	1:A:181:LEU:HD13	1.98	0.46
1:D:241:VAL:HG22	1:D:255:ARG:HG3	1.96	0.46
1:A:195:PRO:HD3	1:A:265:ALA:HB2	1.99	0.45
1:C:225:LEU:O	1:C:234:PHE:CZ	2.71	0.44
1:B:195:PRO:HD3	1:B:265:ALA:HB2	2.00	0.44
1:C:149:ALA:HB2	1:C:181:LEU:HD13	2.00	0.44
1:D:195:PRO:HD3	1:D:265:ALA:HB2	2.00	0.43
1:C:282:ASP:HB3	1:C:285:ARG:HG3	2.00	0.43
1:B:282:ASP:HB3	1:B:285:ARG:HG3	2.00	0.43
1:C:195:PRO:HD3	1:C:265:ALA:HB2	1.99	0.42
1:A:228:LYS:HB3	1:A:228:LYS:HE2	1.88	0.42
1:B:230:GLN:HA	1:B:234:PHE:HD2	1.84	0.42
1:C:231:VAL:O	1:C:232:ASP:C	2.58	0.41
1:C:225:LEU:HD11	1:C:269:LEU:HG	2.01	0.41
1:D:149:ALA:O	1:D:298:GLY:HA3	2.21	0.41
1:B:225:LEU:HD11	1:B:269:LEU:HG	2.03	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	157/171 (92%)	152 (97%)	5 (3%)	0	100	100
1	B	163/171 (95%)	160 (98%)	2 (1%)	1 (1%)	25	43
1	C	165/171 (96%)	159 (96%)	5 (3%)	1 (1%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	154/171 (90%)	152 (99%)	2 (1%)	0	100	100
All	All	639/684 (93%)	623 (98%)	14 (2%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	232	ASP
1	B	232	ASP

### 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	140/150 (93%)	132 (94%)	8 (6%)	20	39
1	B	144/150 (96%)	136 (94%)	8 (6%)	21	40
1	C	146/150 (97%)	133 (91%)	13 (9%)	9	19
1	D	139/150 (93%)	133 (96%)	6 (4%)	29	53
All	All	569/600 (95%)	534 (94%)	35 (6%)	19	35

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	216	LYS
1	A	222	SER
1	A	230	GLN
1	A	233	ASP
1	A	236	ASN
1	A	294	THR
1	A	299	LEU
1	B	174	SER
1	B	222	SER
1	B	250	ASN
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	274	ARG
1	B	294	THR
1	B	299	LEU
1	C	169	GLN
1	C	175[A]	SER
1	C	175[B]	SER
1	C	179	GLN
1	C	230	GLN
1	C	233	ASP
1	C	251	LYS
1	C	259	GLN
1	C	269	LEU
1	C	274	ARG
1	C	294	THR
1	C	297	PHE
1	C	299	LEU
1	D	179	GLN
1	D	236	ASN
1	D	259	GLN
1	D	294	THR
1	D	299	LEU
1	D	303	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	267	HIS
1	B	250	ASN
1	B	267	HIS
1	C	169	GLN
1	C	267	HIS
1	D	179	GLN
1	D	267	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 ⓘ

16 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	0.41	0	17,19,21	1.13	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
2	BMA	E	3	2	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
2	MAN	E	4	2	11,11,12	0.78	0	15,15,17	1.37	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.43	0	17,19,21	1.21	1 (5%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	1.29	1 (5%)
3	BMA	F	3	3	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
4	NAG	G	1	4,1	14,14,15	0.64	0	17,19,21	1.53	3 (17%)
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.75	0
4	BMA	G	3	4	11,11,12	0.24	0	15,15,17	0.93	0
4	MAN	G	4	4	11,11,12	0.24	0	15,15,17	0.88	0
5	NAG	H	1	5,1	14,14,15	0.43	0	17,19,21	1.20	1 (5%)
5	NAG	H	2	5	14,14,15	0.48	0	17,19,21	0.90	0
5	BMA	H	3	5	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
5	MAN	H	4	5	11,11,12	0.68	0	15,15,17	1.19	1 (6%)
5	MAN	H	5	5	11,11,12	0.74	0	15,15,17	1.59	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
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	MAN	C1-O5-C5	4.73	118.60	112.19
3	F	2	NAG	C1-O5-C5	4.66	118.50	112.19
2	E	4	MAN	C1-O5-C5	3.63	117.11	112.19
4	G	1	NAG	C8-C7-N2	3.14	121.42	116.10
5	H	4	MAN	C1-O5-C5	3.04	116.31	112.19
3	F	1	NAG	C2-N2-C7	3.04	127.23	122.90
5	H	3	BMA	O3-C3-C2	3.03	115.79	109.99
2	E	2	NAG	C1-O5-C5	2.73	115.89	112.19
4	G	1	NAG	O7-C7-N2	-2.65	117.08	121.95
2	E	3	BMA	C1-O5-C5	2.64	115.76	112.19
5	H	1	NAG	C2-N2-C7	2.63	126.65	122.90
4	G	1	NAG	O5-C5-C6	2.57	111.24	107.20
5	H	5	MAN	C1-C2-C3	2.53	112.78	109.67
3	F	3	BMA	C1-O5-C5	2.48	115.55	112.19
3	F	3	BMA	C3-C4-C5	2.19	114.15	110.24
2	E	1	NAG	C2-N2-C7	2.07	125.85	122.90
2	E	1	NAG	C8-C7-N2	-2.01	112.69	116.10

There are no chirality outliers.

All (19) torsion outliers are listed below:

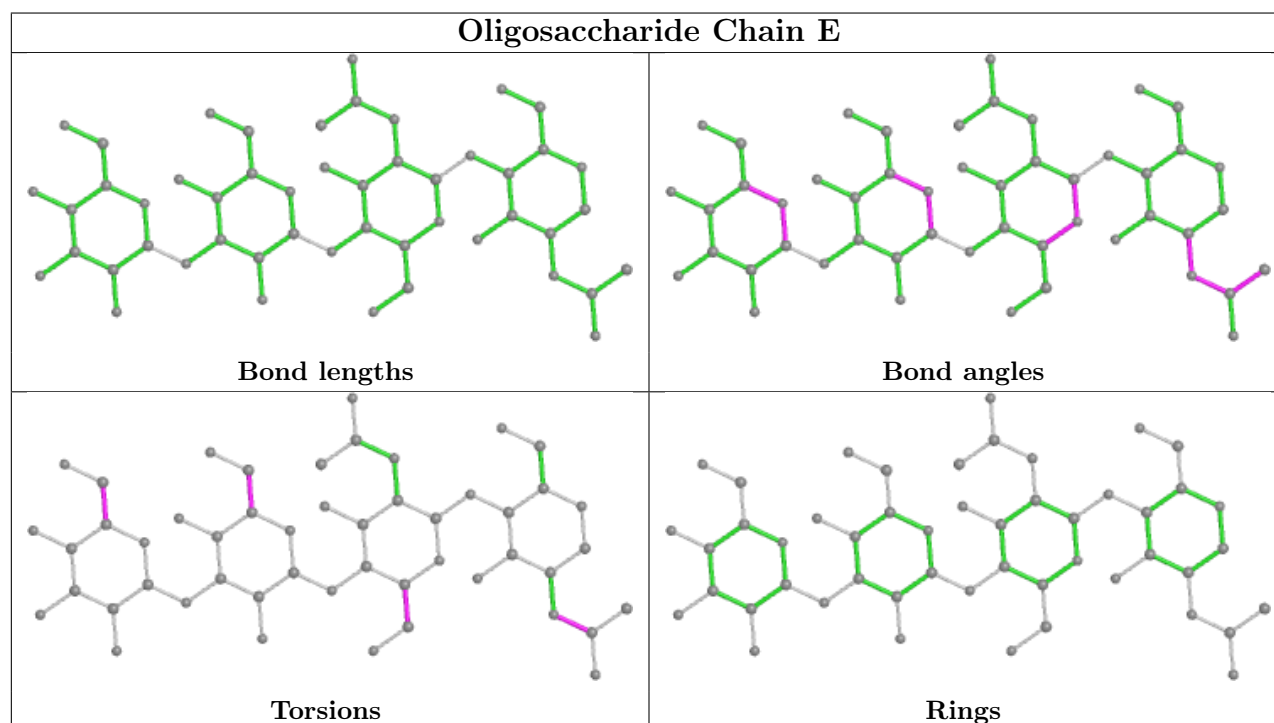


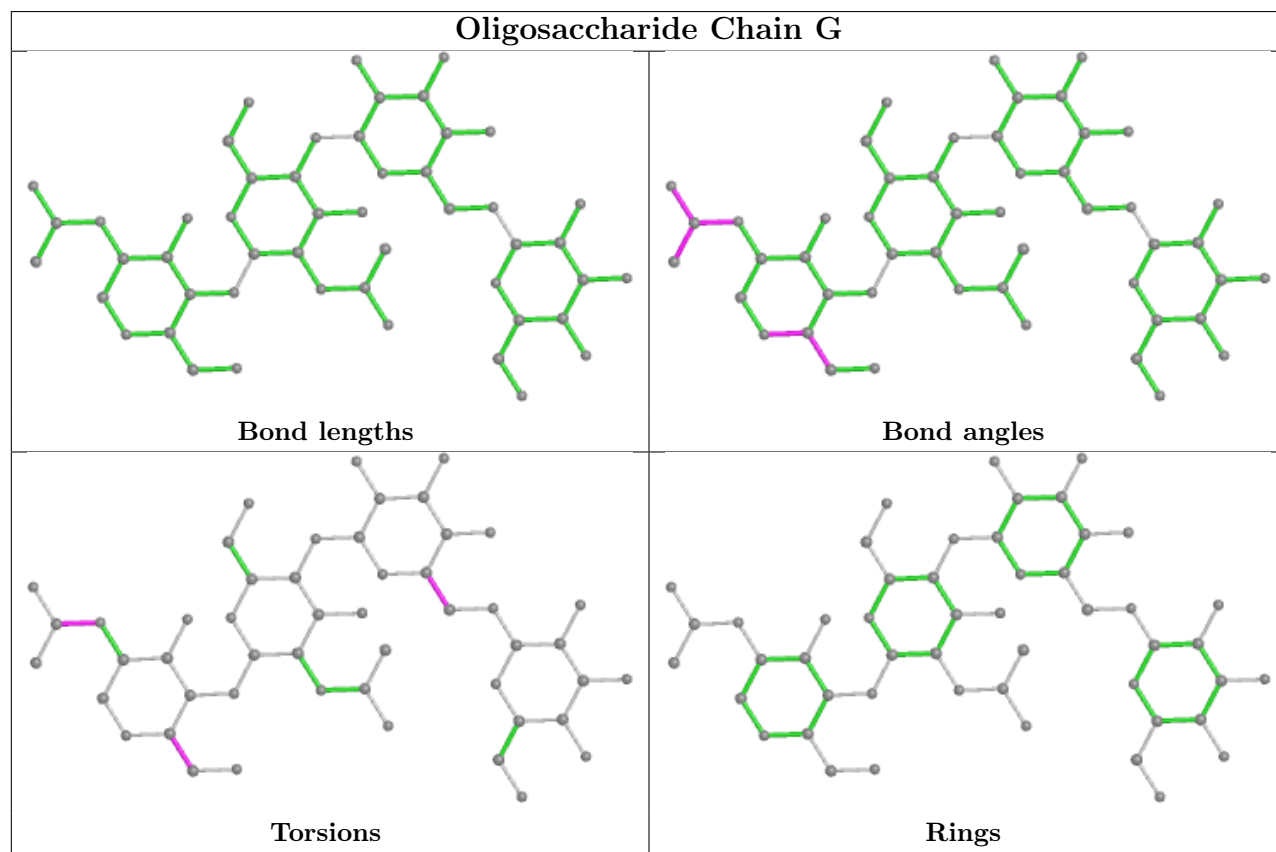
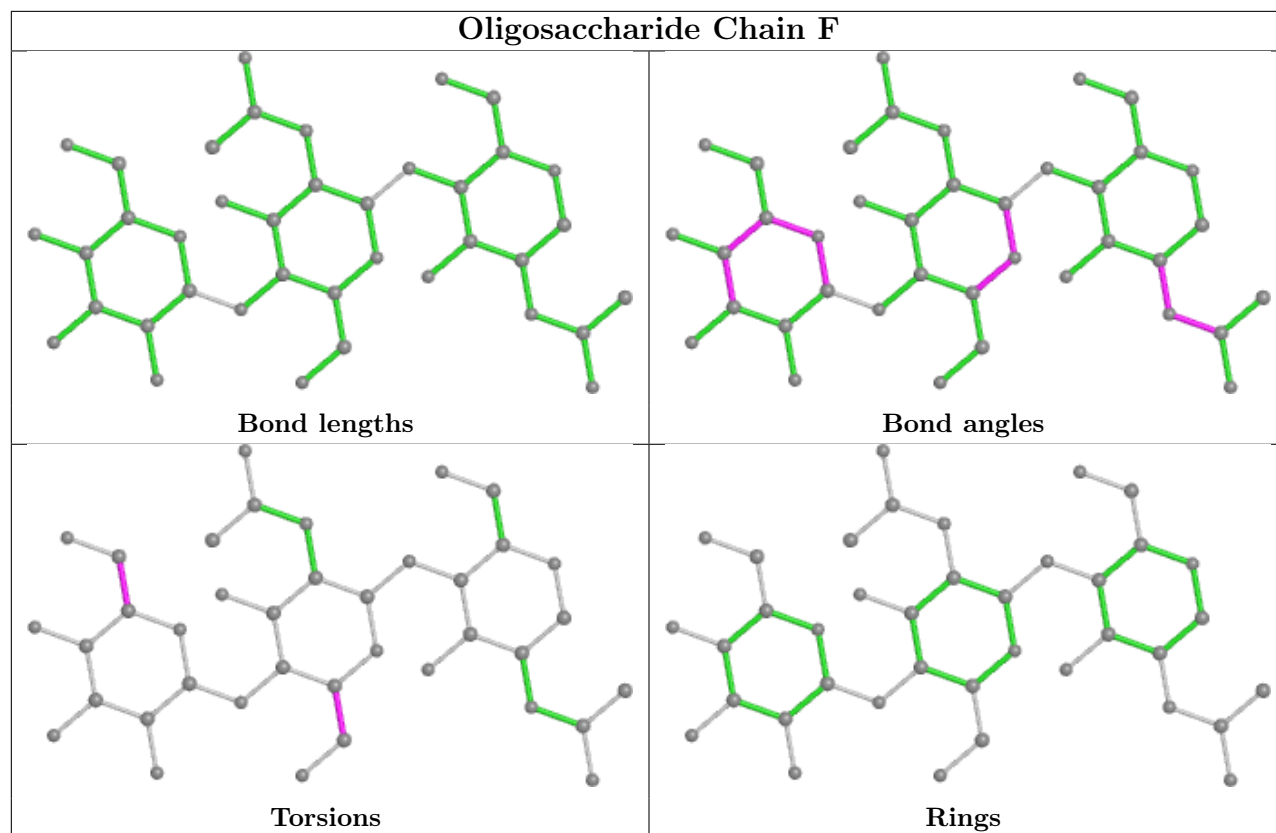
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
4	G	3	BMA	C4-C5-C6-O6

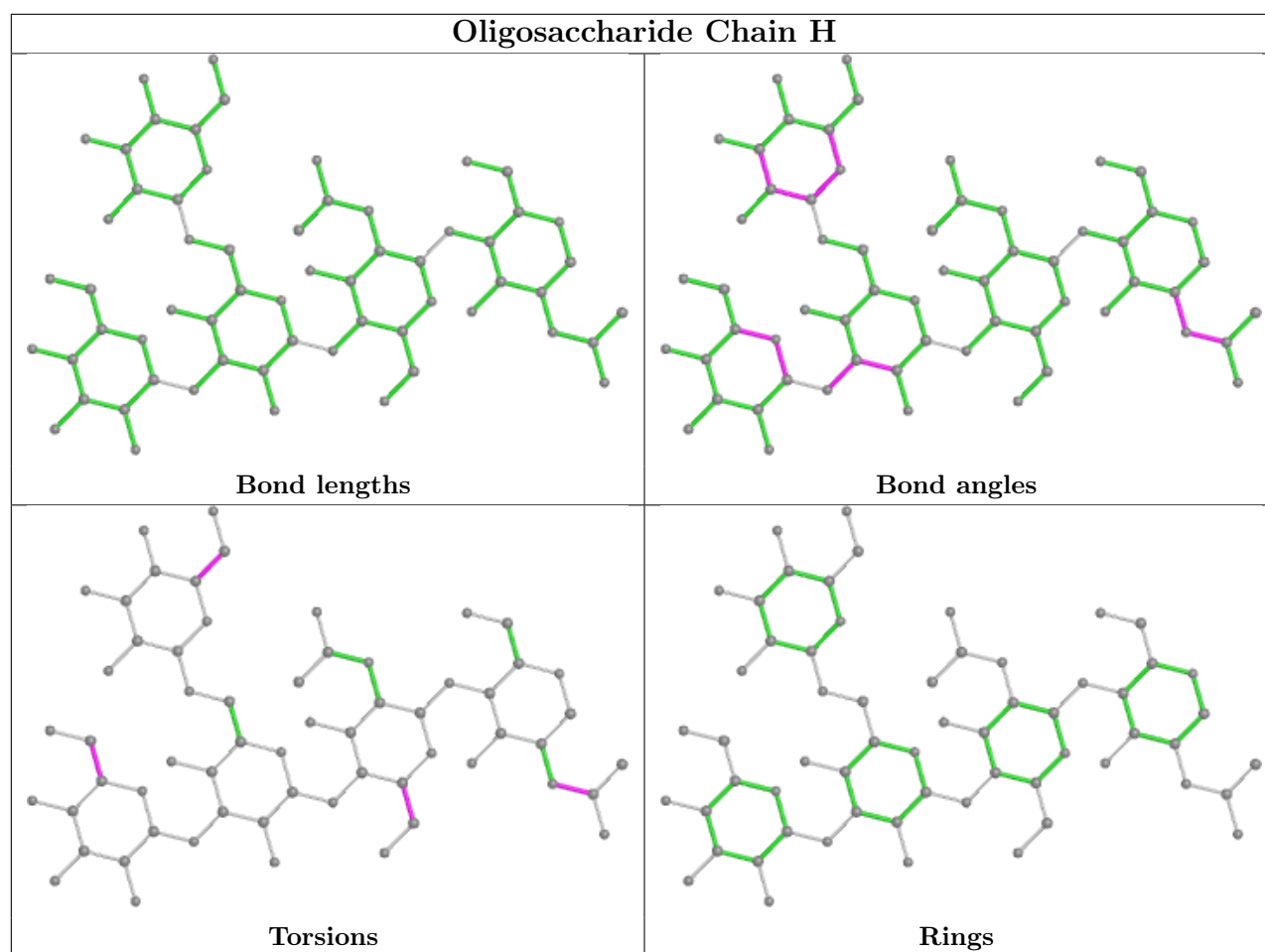
There are no ring outliers.

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](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
7	SO4	D	401	-	4,4,4	0.35	0	6,6,6	0.08	0
7	SO4	C	401	-	4,4,4	0.35	0	6,6,6	0.18	0
7	SO4	C	403	-	1,3,4	1.21	0	0,3,6	-	-
7	SO4	B	403	-	4,4,4	0.44	0	6,6,6	0.21	0
7	SO4	B	402	-	4,4,4	0.30	0	6,6,6	0.18	0
7	SO4	B	401	-	4,4,4	0.34	0	6,6,6	0.24	0
7	SO4	B	404	-	4,4,4	0.36	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	160/171 (93%)	-0.16	2 (1%) 77 79	45, 62, 103, 122	0
1	B	165/171 (96%)	-0.29	2 (1%) 79 80	42, 55, 101, 112	0
1	C	165/171 (96%)	-0.24	3 (1%) 68 71	42, 56, 97, 111	0
1	D	160/171 (93%)	-0.13	3 (1%) 66 69	45, 62, 102, 129	0
All	All	650/684 (95%)	-0.21	10 (1%) 73 75	42, 60, 101, 129	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	PHE	4.4
1	B	234	PHE	3.9
1	A	235	ASP	3.5
1	D	250	ASN	3.3
1	C	168	SER	2.8
1	A	215	HIS	2.4
1	D	235	ASP	2.4
1	B	232	ASP	2.4
1	D	231	VAL	2.3
1	C	232	ASP	2.1

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

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

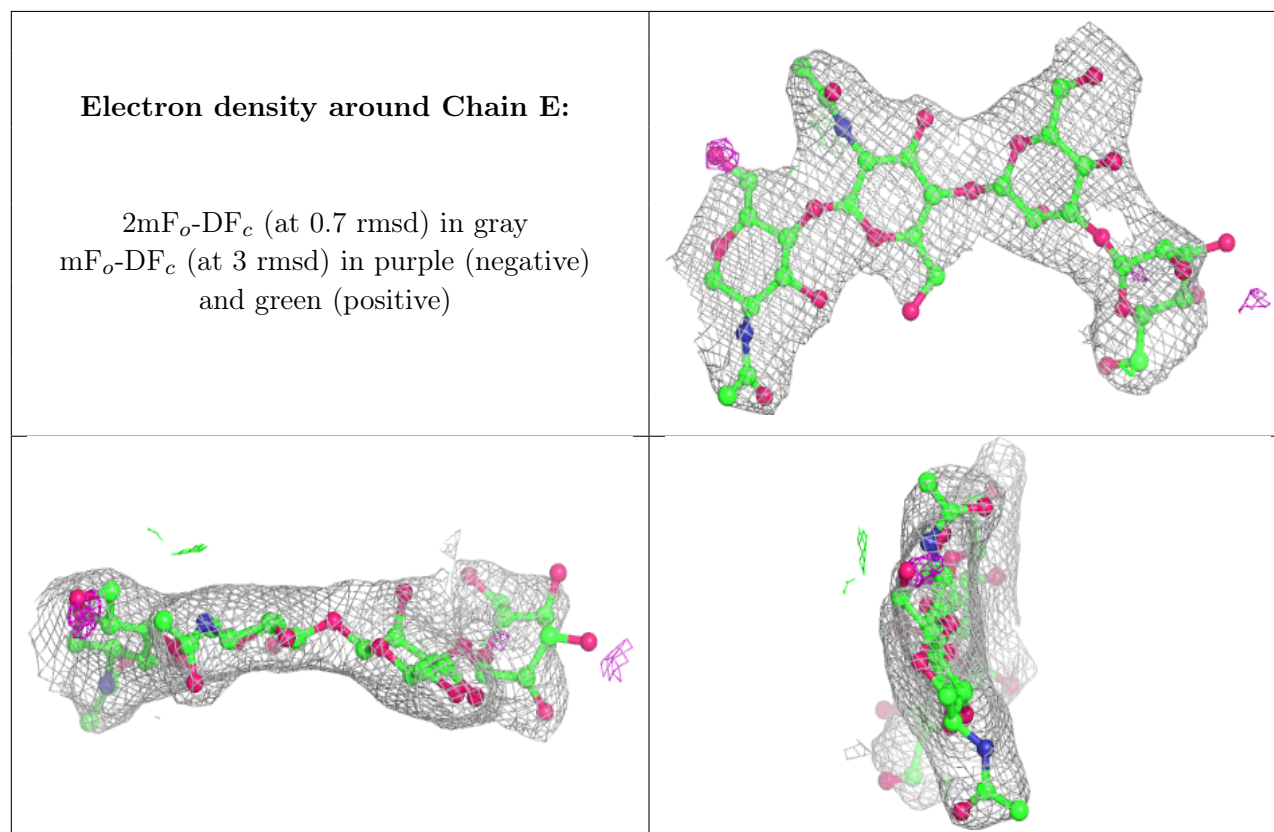
### 6.3 Carbohydrates [i](#)

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.

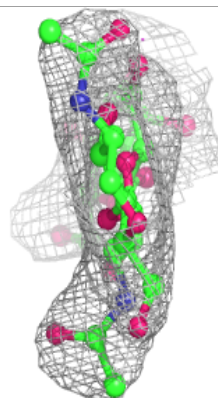
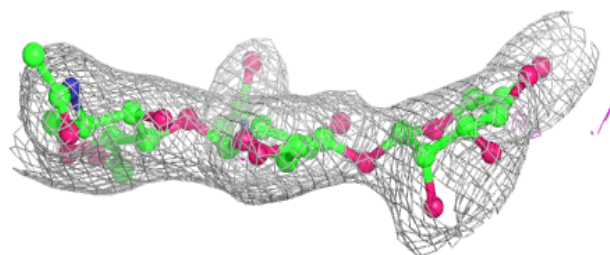
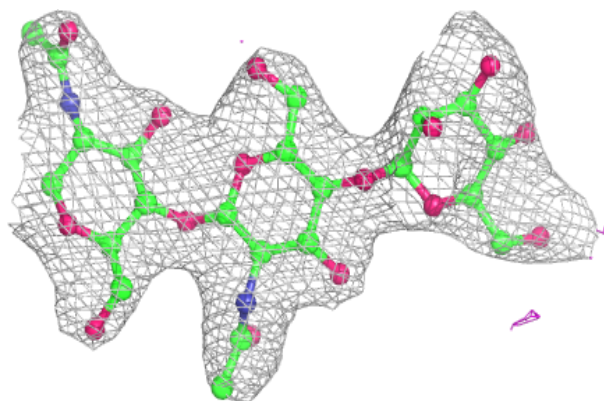
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	E	4	11/12	0.76	0.20	122,127,132,132	0
3	BMA	F	3	11/12	0.77	0.15	103,110,113,113	0
5	MAN	H	5	11/12	0.83	0.13	119,125,130,132	0
5	MAN	H	4	11/12	0.86	0.13	117,119,127,128	0
4	BMA	G	3	11/12	0.87	0.11	105,112,114,115	0
2	BMA	E	3	11/12	0.91	0.12	99,107,110,117	0
5	BMA	H	3	11/12	0.93	0.10	98,104,111,113	0
3	NAG	F	2	14/15	0.94	0.11	63,75,85,97	0
4	NAG	G	2	14/15	0.95	0.13	72,80,89,98	0
2	NAG	E	2	14/15	0.95	0.15	74,81,85,93	0
4	MAN	G	4	11/12	0.95	0.07	30,30,30,30	0
2	NAG	E	1	14/15	0.96	0.19	70,72,79,82	0
5	NAG	H	1	14/15	0.96	0.16	63,65,74,77	0
5	NAG	H	2	14/15	0.96	0.16	72,79,84,94	0
4	NAG	G	1	14/15	0.97	0.14	67,71,78,85	0
3	NAG	F	1	14/15	0.98	0.14	65,68,73,77	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.

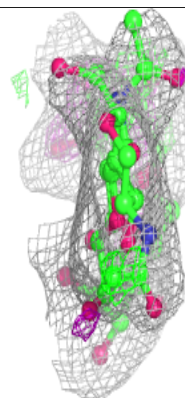
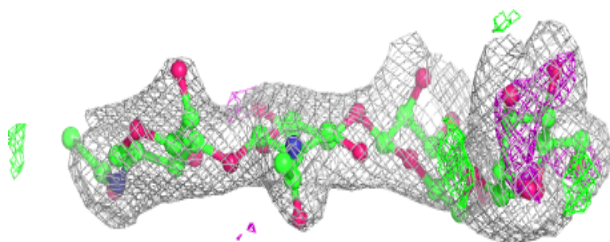
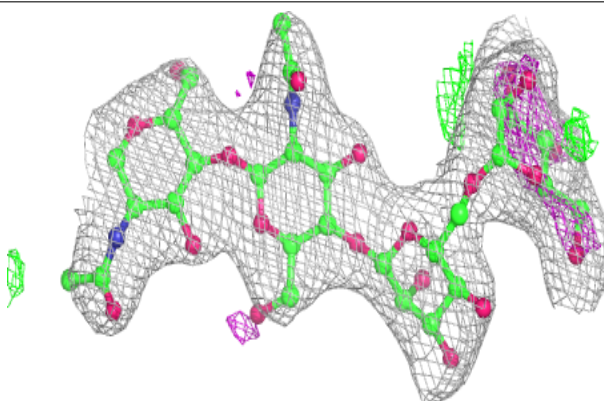


**Electron density around Chain F:**

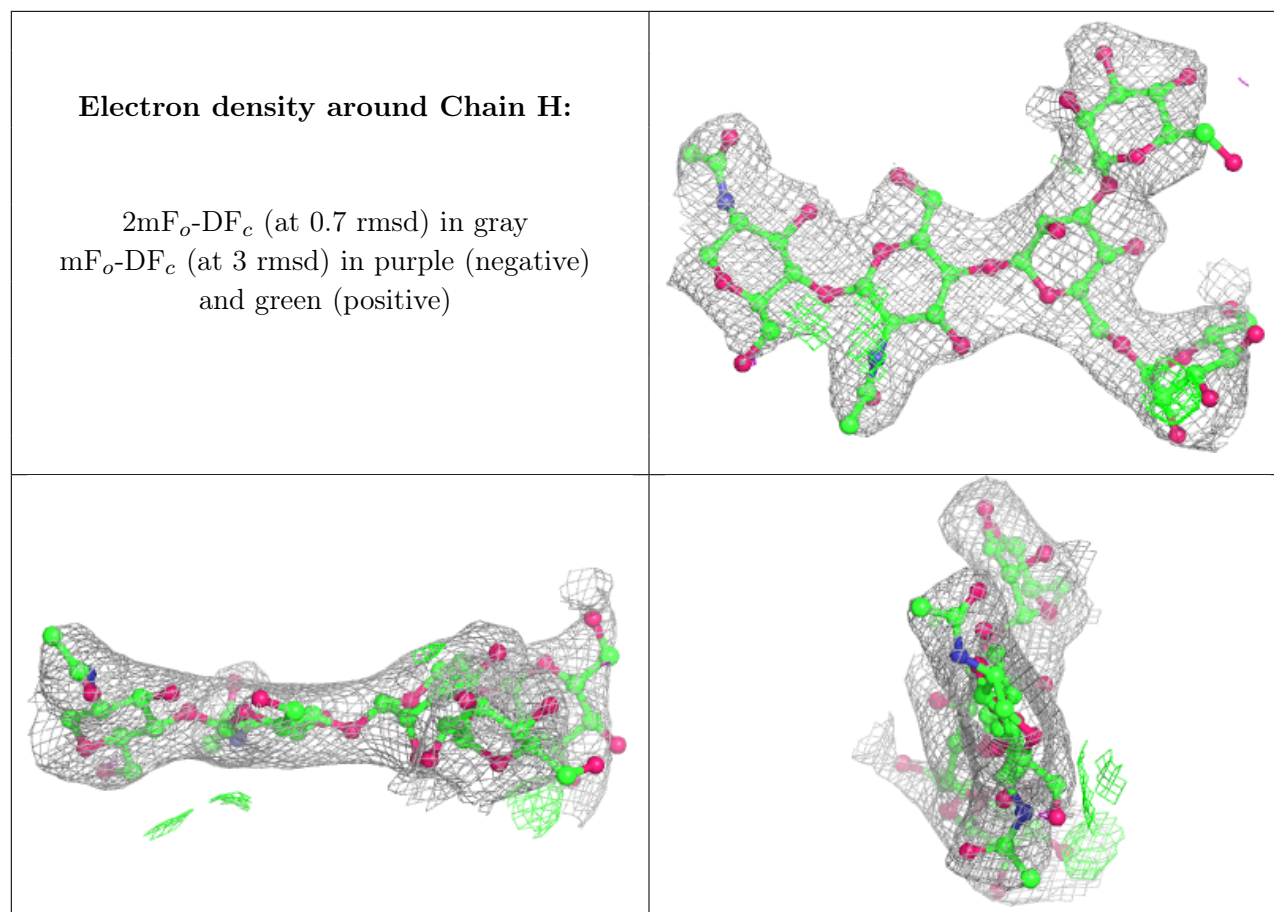
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain G:**

$2mF_o - DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
7	SO4	C	401	5/5	0.89	0.17	153,154,155,155	0
7	SO4	D	401	5/5	0.89	0.15	147,150,151,152	0
7	SO4	C	403	4/5	0.93	0.15	83,88,89,90	0
7	SO4	B	403	5/5	0.93	0.20	87,94,96,96	0
7	SO4	B	404	5/5	0.94	0.16	111,114,115,117	0
6	NA	C	405	1/1	0.95	0.18	57,57,57,57	0
6	NA	A	402	1/1	0.95	0.32	65,65,65,65	0
6	NA	D	402	1/1	0.96	0.17	66,66,66,66	0
7	SO4	B	401	5/5	0.97	0.14	96,98,98,102	0
7	SO4	C	402	5/5	0.97	0.12	78,80,82,85	0
6	NA	B	408	1/1	0.98	0.30	92,92,92,92	0
7	SO4	B	402	5/5	0.98	0.24	80,86,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	A	401	1/1	0.99	0.28	69,69,69,69	0
6	NA	C	404	1/1	0.99	0.10	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.