



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2023 – 12:51 AM EDT

PDB ID : 2Z64  
Title : Crystal structure of mouse TLR4 and mouse MD-2 complex  
Authors : Lee, J.-O.; Kim, H.M.; Park, B.S.  
Deposited on : 2007-07-22  
Resolution : 2.84 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](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  
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

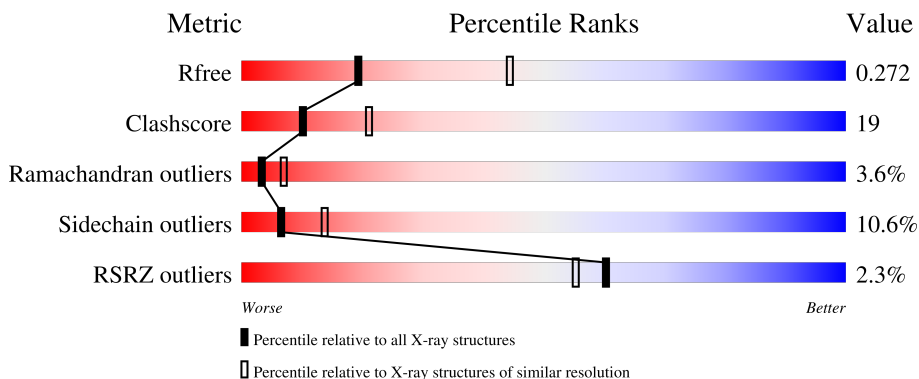
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

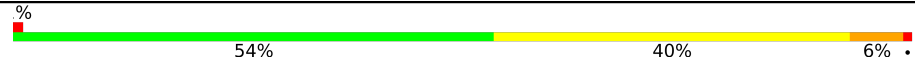

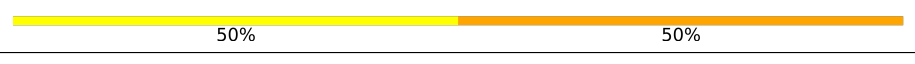
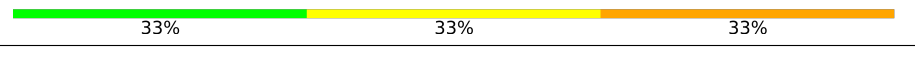
The reported resolution of this entry is 2.84 Å.

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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	599	
2	C	135	
3	B	2	
4	D	3	
4	E	3	

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Mol	Chain	Length	Quality of chain
5	F	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	1441	X	-	-	-
6	NAG	A	1451	X	-	-	-
6	NAG	A	1471	X	-	-	-
6	NAG	A	1481	X	-	-	-
6	NAG	A	1491	-	-	-	X
6	NAG	C	1511	X	-	-	-
6	NAG	C	1521	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6302 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 Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	599	4774	3055	785	906	28	0	0	0

- Molecule 2 is a protein called Lymphocyte antigen 96.

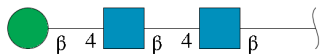
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	135	1093	706	182	198	7	0	0	0

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



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

- Molecule 4 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.



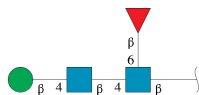
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	39	22	2	15	0	0	0

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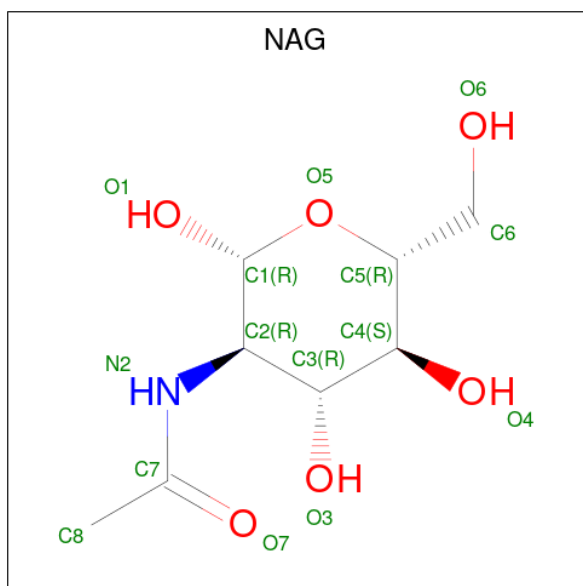
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	4	49	28	2	19	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

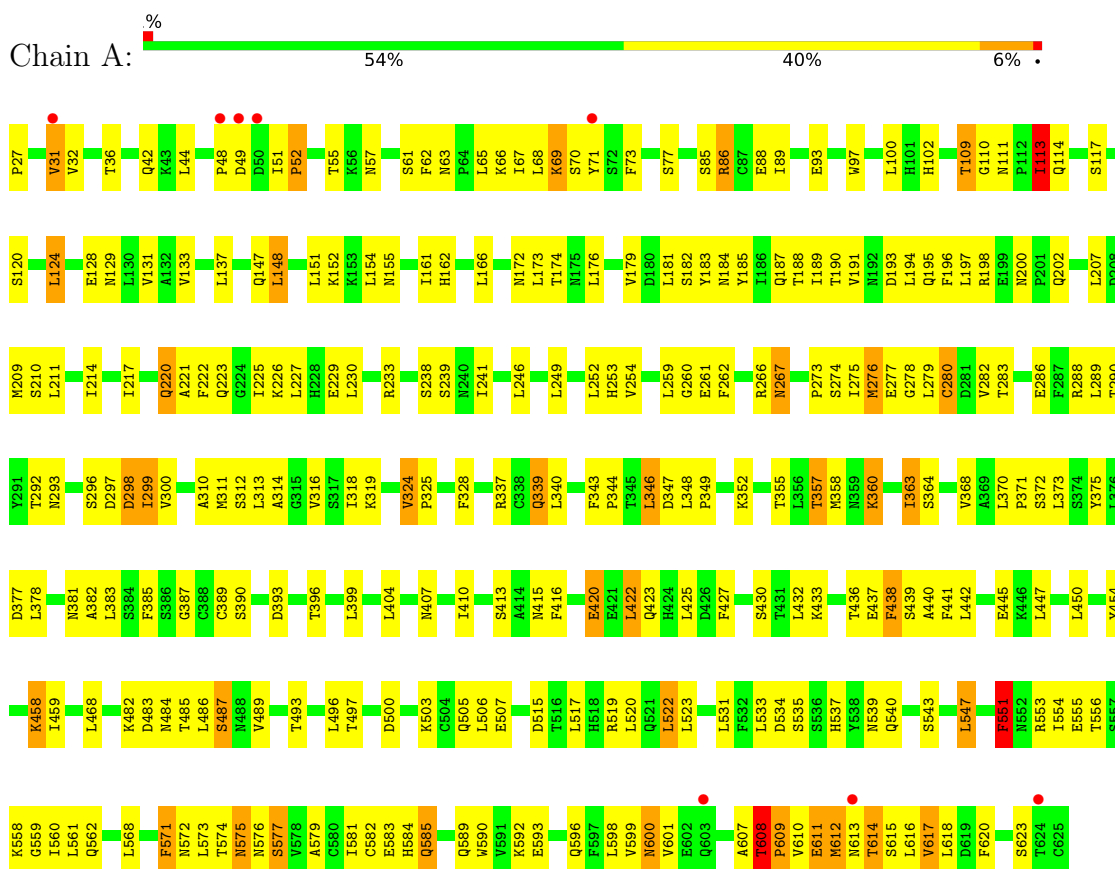
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	C	30	Total	O	0	0
			30	30		

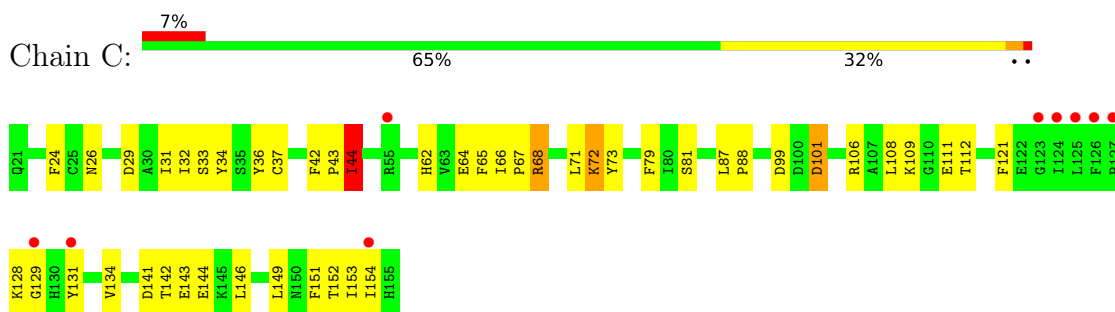
### 3 Residue-property plots i

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: Toll-like receptor 4



- Molecule 2: Lymphocyte antigen 96

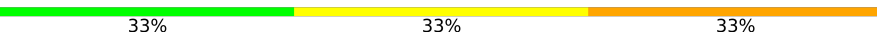


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50% 50%

MAG1  
MAG2

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

Chain D:  33% 33% 33%

MAG1  
MAG2  
BMA3

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

Chain E:  33% 67%

MAG1  
MAG2  
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 25% 50%

MAG1  
MAG2  
BMA3  
FUL4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.16Å 101.88Å 126.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.84 39.66 – 2.84	Depositor EDS
% Data completeness (in resolution range)	90.1 (20.00-2.84) 89.7 (39.66-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.242 , 0.290 0.229 , 0.272	Depositor DCC
$R_{free}$ test set	1188 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: NAG, BMA, FUL

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	0.50	0/4874	0.66	1/6604 (0.0%)
2	C	0.56	0/1124	0.65	0/1519
All	All	0.51	0/5998	0.66	1/8123 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	154	LEU	CA-CB-CG	5.84	128.74	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	608	THR	Peptide

### 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	4774	0	4729	199	0
2	C	1093	0	1048	31	0
3	B	28	0	25	1	0
4	D	39	0	34	1	0
4	E	39	0	34	2	0
5	F	49	0	43	2	0
6	A	84	0	78	0	0
6	C	42	0	39	1	0
7	A	124	0	0	7	0
7	C	30	0	0	2	0
All	All	6302	0	6030	230	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 19.

The worst 5 of 230 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:383:LEU:HB3	1:A:407:ASN:HD22	1.00	1.16
1:A:608:THR:HB	1:A:609:PRO:HD3	1.21	1.12
1:A:109:THR:HG23	1:A:133:VAL:HB	1.25	1.10
1:A:383:LEU:HB3	1:A:407:ASN:ND2	1.68	1.06
1:A:608:THR:HB	1:A:609:PRO:CD	2.01	0.91

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	597/599 (100%)	495 (83%)	79 (13%)	23 (4%)	<b>3</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	6	13
All	All	730/734 (100%)	610 (84%)	94 (13%)	26 (4%)	3	7

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	ALA
1	A	440	ALA
1	A	608	THR
2	C	143	GLU
1	A	347	ASP

### 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	558/558 (100%)	498 (89%)	60 (11%)	6	13
2	C	122/122 (100%)	110 (90%)	12 (10%)	8	16
All	All	680/680 (100%)	608 (89%)	72 (11%)	6	14

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	614	THR
2	C	152	THR
1	A	620	PHE
2	C	72	LYS
1	A	297	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	521	GLN

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Mol	Chain	Res	Type
1	A	600	ASN
1	A	484	ASN
1	A	537	HIS

### 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 [i](#)

12 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	$\# Z  > 2$
3	NAG	B	1	3,1	14,14,15	0.58	0	17,19,21	1.67	5 (29%)
3	NAG	B	2	3	14,14,15	0.55	0	17,19,21	2.54	3 (17%)
4	NAG	D	1	1,4	14,14,15	0.55	0	17,19,21	1.45	2 (11%)
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	0.81	0
4	BMA	D	3	4	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.65	0	17,19,21	1.54	4 (23%)
4	NAG	E	2	4	14,14,15	0.42	0	17,19,21	1.33	2 (11%)
4	BMA	E	3	4	11,11,12	0.63	0	15,15,17	0.57	0
5	NAG	F	1	5	14,14,15	0.56	0	17,19,21	1.14	1 (5%)
5	NAG	F	2	5	14,14,15	0.58	0	17,19,21	1.44	3 (17%)
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.91	0
5	FUL	F	4	5	10,10,11	0.68	0	14,14,16	1.47	2 (14%)

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
3	NAG	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	FUL	F	4	5	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C1-O5-C5	8.52	123.73	112.19
3	B	2	NAG	O5-C1-C2	4.52	118.42	111.29
4	E	1	NAG	C4-C3-C2	4.36	117.41	111.02
4	D	1	NAG	O5-C1-C2	-4.28	104.53	111.29
5	F	4	FUL	C1-C2-C3	4.19	114.82	109.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

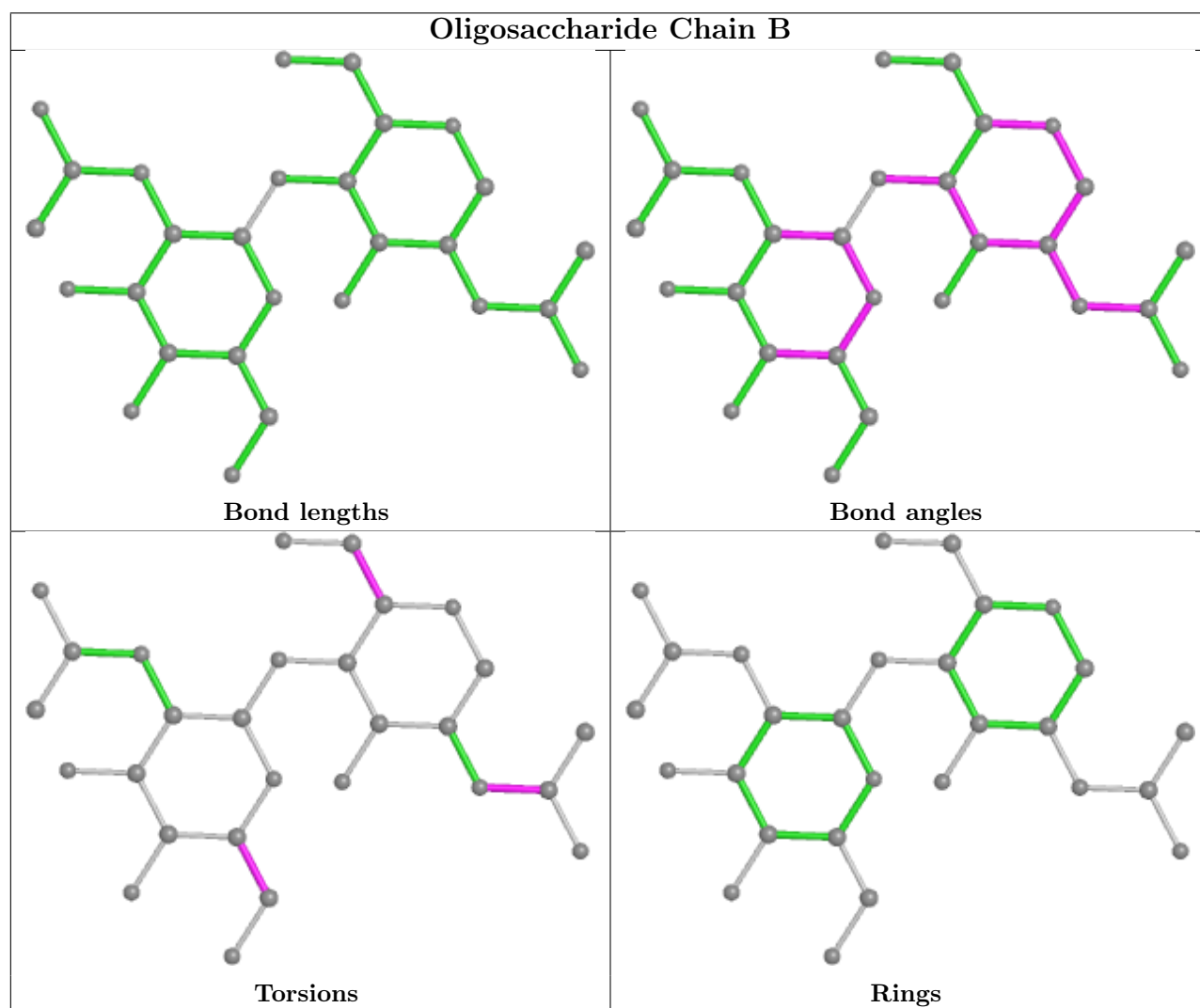
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2

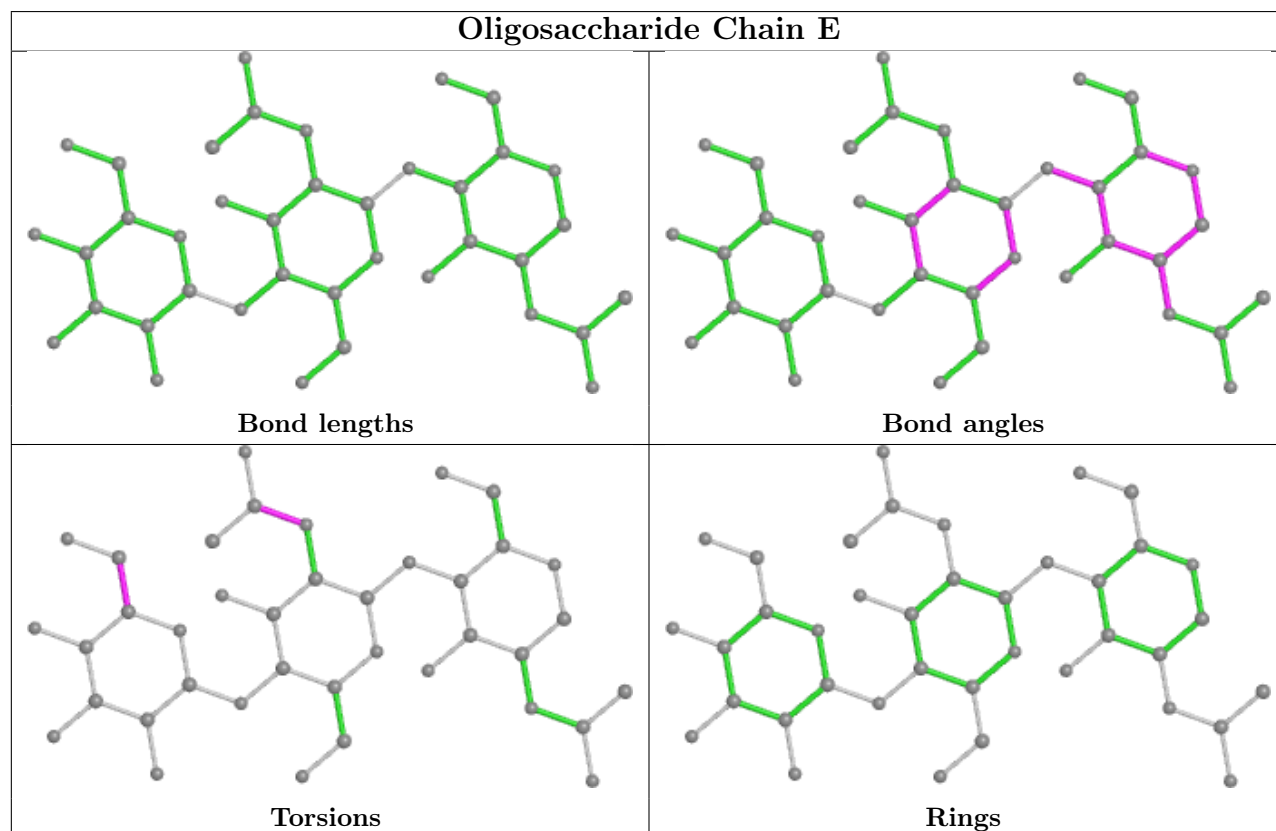
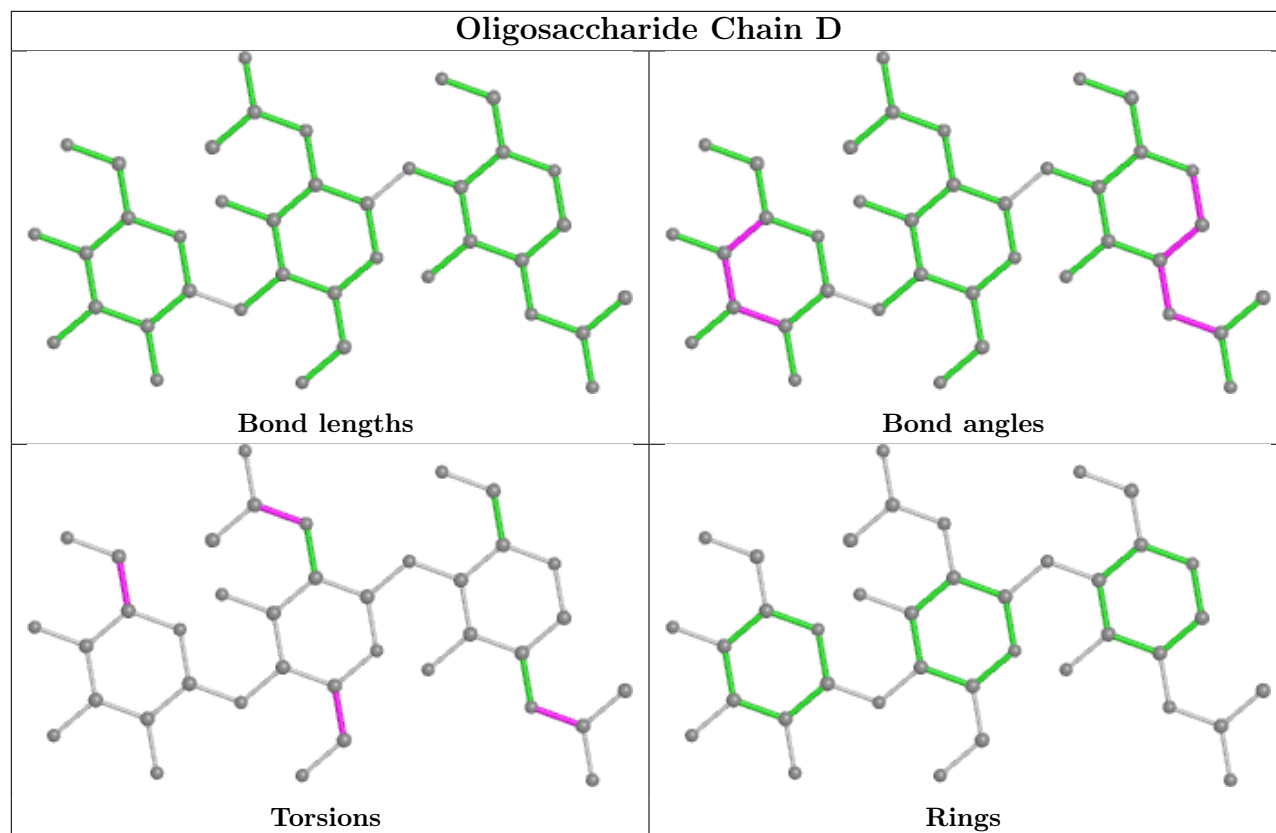
There are no ring outliers.

6 monomers are involved in 5 short contacts:

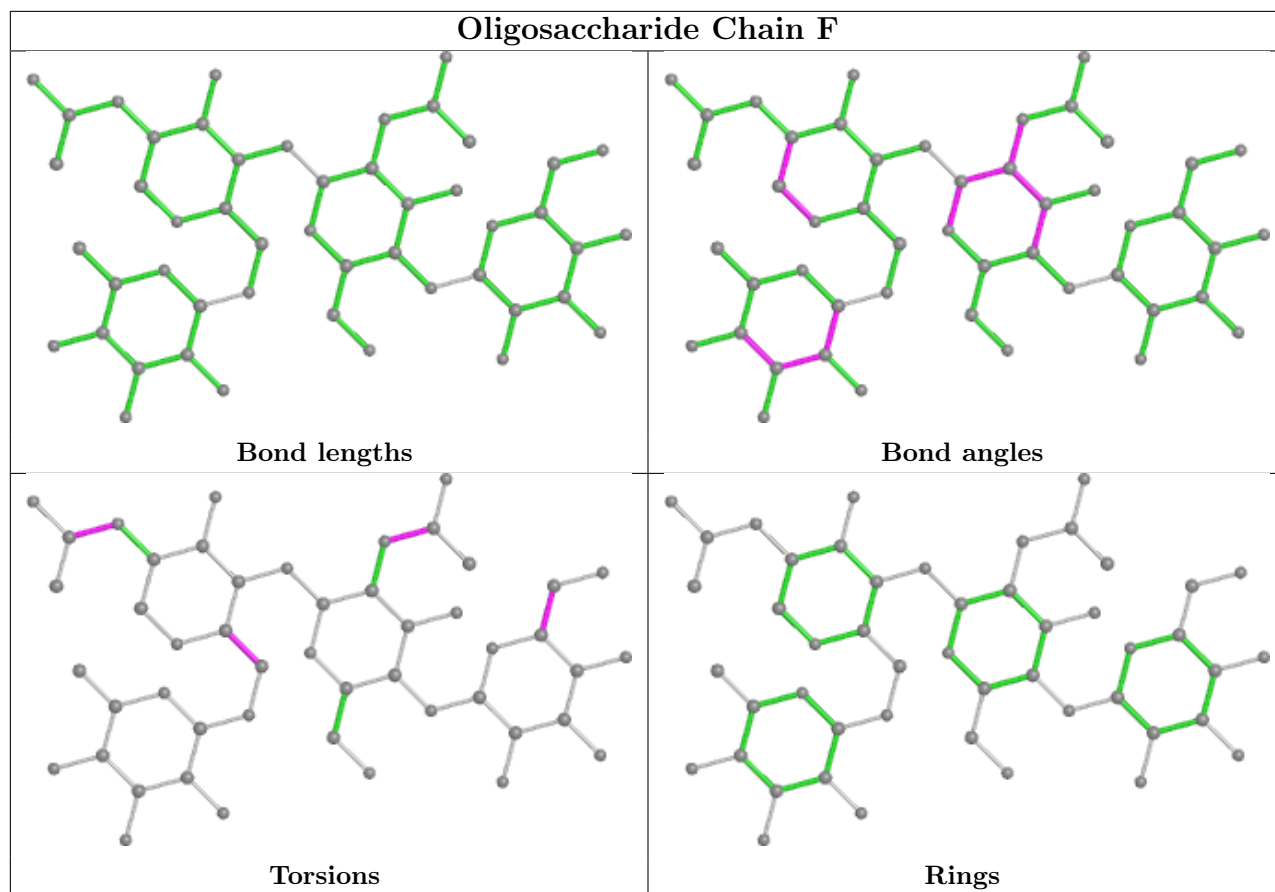
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
5	F	2	NAG	1	0
3	B	1	NAG	1	0
5	F	1	NAG	1	0
4	E	1	NAG	2	0
4	D	1	NAG	1	0

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](#)

9 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	$\# Z  > 2$
6	NAG	A	1431	1	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
6	NAG	A	1471	1	14,14,15	0.52	0	17,19,21	1.15	1 (5%)
6	NAG	A	1451	1	14,14,15	0.49	0	17,19,21	1.37	2 (11%)
6	NAG	C	1521	2	14,14,15	0.75	0	17,19,21	1.17	1 (5%)
6	NAG	A	1491	1	14,14,15	0.62	0	17,19,21	1.13	2 (11%)
6	NAG	C	1501	2	14,14,15	0.74	1 (7%)	17,19,21	1.30	1 (5%)
6	NAG	A	1481	1	14,14,15	0.68	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1441	1	14,14,15	0.52	0	17,19,21	1.35	3 (17%)
6	NAG	C	1511	2	14,14,15	0.50	0	17,19,21	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1431	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1471	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	1451	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	C	1521	2	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	1491	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1501	2	-	3/6/23/26	0/1/1/1
6	NAG	A	1481	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	1441	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	C	1511	2	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1501	NAG	C1-C2	2.19	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1501	NAG	C1-O5-C5	3.77	117.30	112.19
6	A	1451	NAG	O5-C1-C2	-3.49	105.78	111.29
6	A	1471	NAG	O5-C1-C2	-3.29	106.10	111.29
6	A	1431	NAG	C1-O5-C5	3.07	116.35	112.19
6	A	1491	NAG	C2-N2-C7	2.95	127.11	122.90

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1441	NAG	C1
6	A	1451	NAG	C1
6	A	1471	NAG	C1

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Mol	Chain	Res	Type	Atom
6	A	1481	NAG	C1
6	C	1511	NAG	C1

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1431	NAG	C8-C7-N2-C2
6	A	1431	NAG	O7-C7-N2-C2
6	A	1441	NAG	C8-C7-N2-C2
6	A	1441	NAG	O7-C7-N2-C2
6	A	1451	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1501	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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	599/599 (100%)	-0.00	8 (1%) 77 74	8, 28, 46, 66	0
2	C	135/135 (100%)	0.30	9 (6%) 17 12	4, 30, 44, 69	2 (1%)
All	All	734/734 (100%)	0.05	17 (2%) 60 55	4, 28, 45, 69	2 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	126	PHE	5.5
2	C	124	ILE	4.6
2	C	125	LEU	4.4
2	C	55	ARG	3.4
1	A	48	PRO	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, 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.

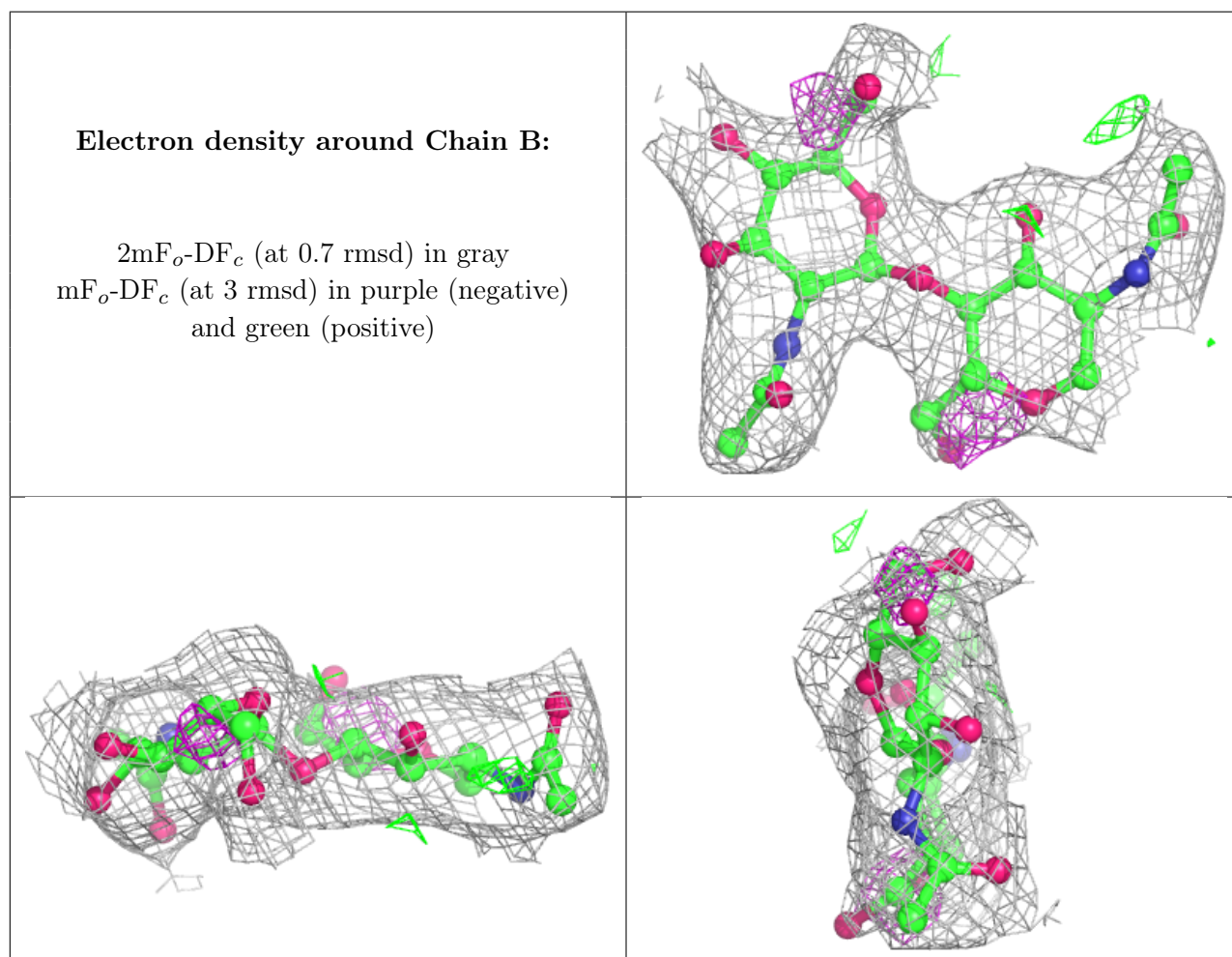
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	D	3	11/12	0.54	0.25	90,95,96,97	0
4	BMA	E	3	11/12	0.70	0.26	94,97,101,102	0
5	FUL	F	4	10/11	0.76	0.31	87,92,94,96	0
5	NAG	F	2	14/15	0.78	0.17	74,78,80,87	0
5	BMA	F	3	11/12	0.80	0.18	87,92,94,95	0

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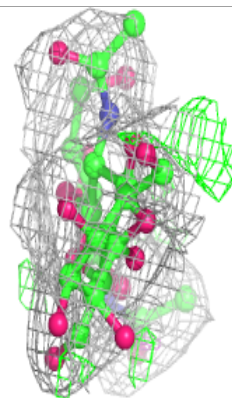
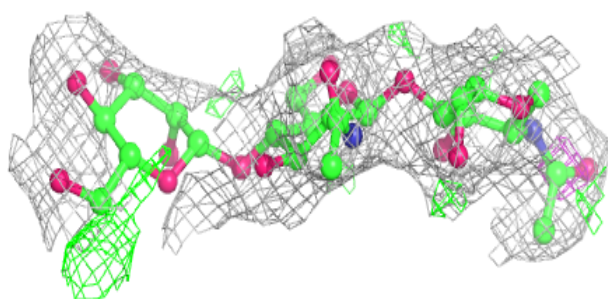
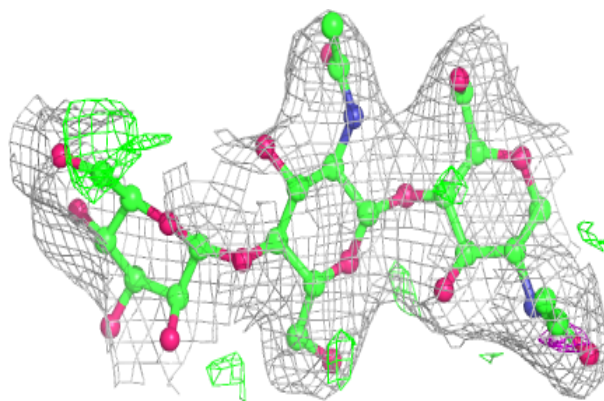
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	F	1	14/15	0.80	0.16	67,72,77,82	0
4	NAG	E	2	14/15	0.84	0.19	72,82,86,93	0
3	NAG	B	2	14/15	0.91	0.19	41,47,54,61	0
4	NAG	E	1	14/15	0.92	0.21	39,45,63,67	0
3	NAG	B	1	14/15	0.93	0.16	28,38,47,54	0
4	NAG	D	2	14/15	0.95	0.20	51,56,68,81	0
4	NAG	D	1	14/15	0.96	0.10	18,28,33,43	0

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

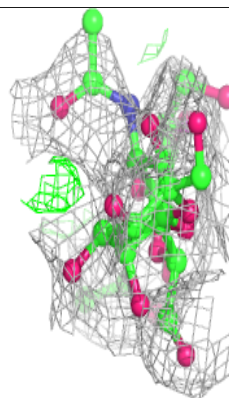
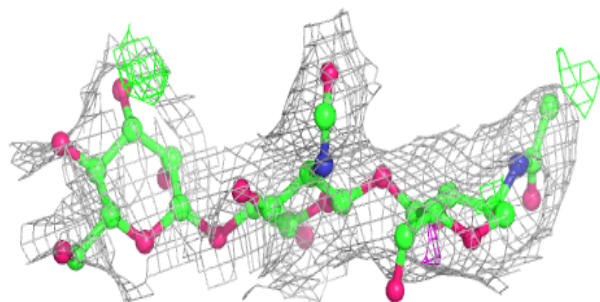
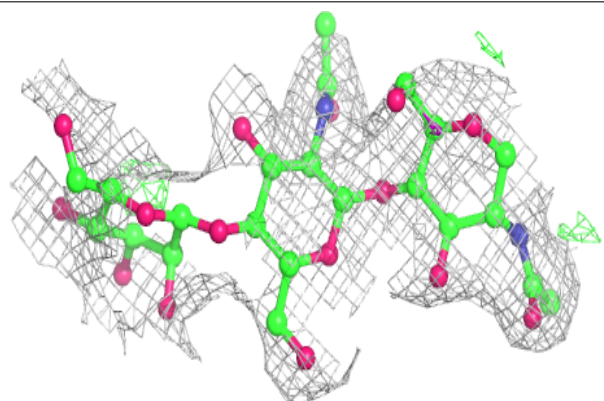


**Electron density around Chain D:**

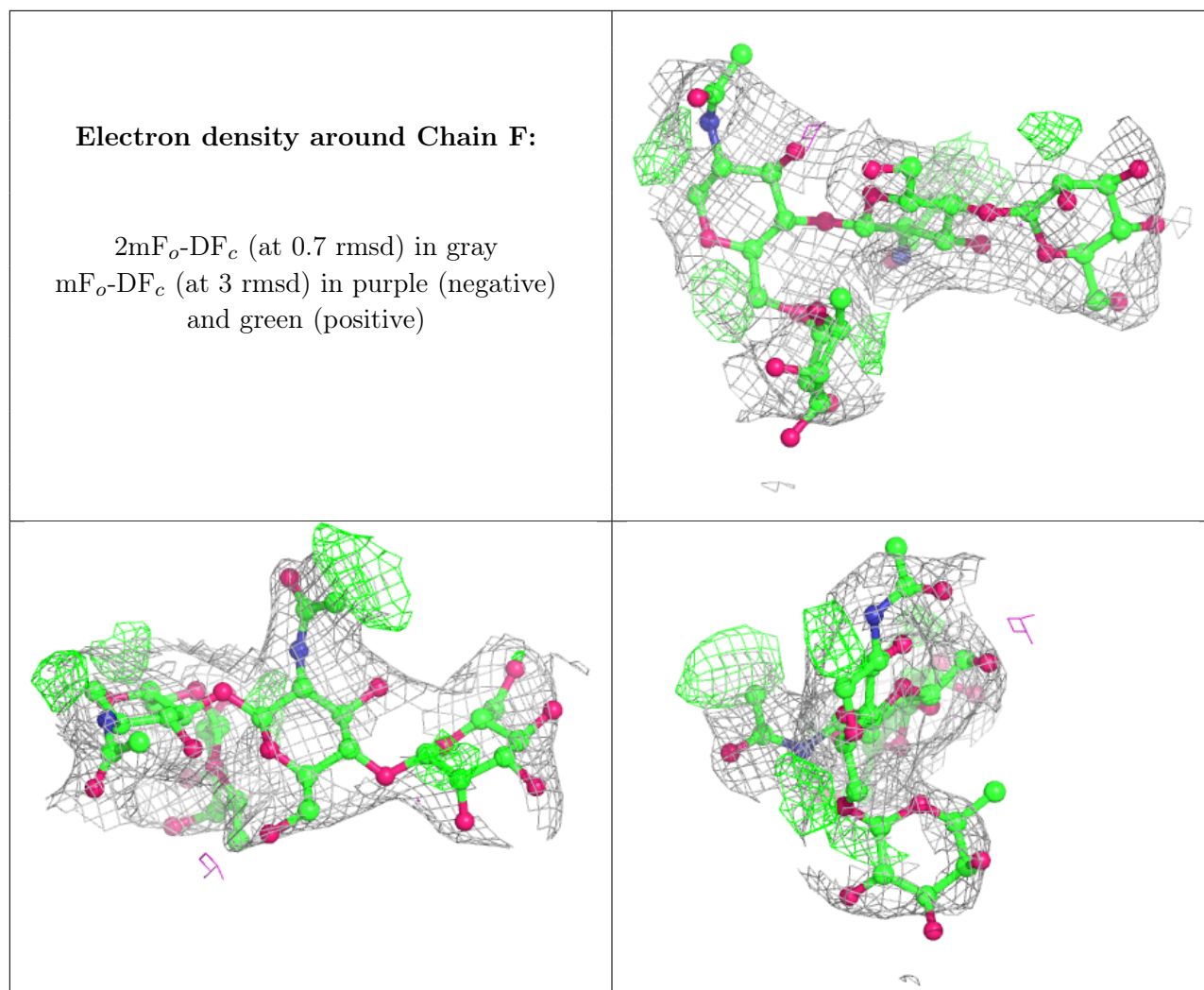
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$  (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	NAG	A	1491	14/15	0.55	0.44	80,88,94,96	0
6	NAG	A	1451	14/15	0.68	0.35	79,85,88,89	0
6	NAG	A	1431	14/15	0.71	0.22	82,91,94,95	0
6	NAG	A	1481	14/15	0.76	0.31	57,65,69,70	0
6	NAG	A	1441	14/15	0.76	0.37	48,59,65,66	0
6	NAG	C	1521	14/15	0.83	0.27	22,49,73,76	0
6	NAG	C	1501	14/15	0.85	0.16	65,71,85,86	0
6	NAG	A	1471	14/15	0.85	0.23	54,63,72,75	0
6	NAG	C	1511	14/15	0.91	0.33	38,42,44,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.