



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:08 AM BST

PDB ID : 5AMO  
Title : Structure of a mouse Olfactomedin-1 disulfide-linked dimer of the Olfactomedin domain and part of the coiled coil  
Authors : Pronker, M.F.; Bos, T.G.A.A.; Sharp, T.H.; Thies-Weesie, D.M.; Janssen, B.J.C.  
Deposited on : 2015-03-11  
Resolution : 2.40 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.

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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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

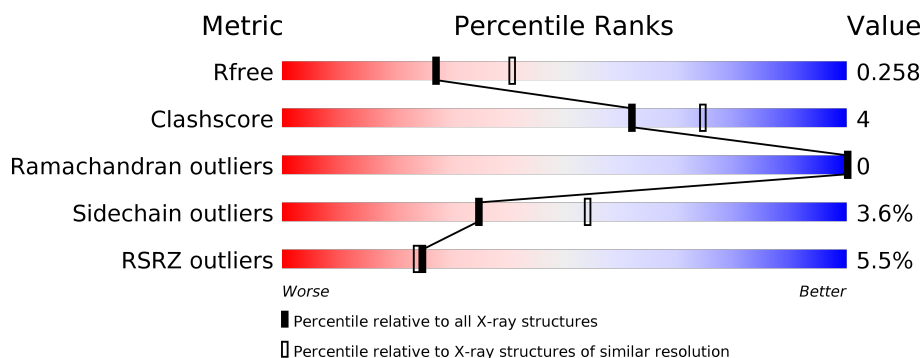
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	471	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>6%</div> <div>46%</div> </div> </div>
1	B	471	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>10%</div> <div>45%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>100%</div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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
2	NAG	E	2	-	-	-	X
3	NAG	A	1394	-	-	-	X
4	GOL	B	1483	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4304 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 NOELIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			2044	1301	347	386	10			
1	B	257	Total	C	N	O	S	0	0	0
			2075	1319	356	390	10			

There are 20 discrepancies between the modelled and reference sequences:

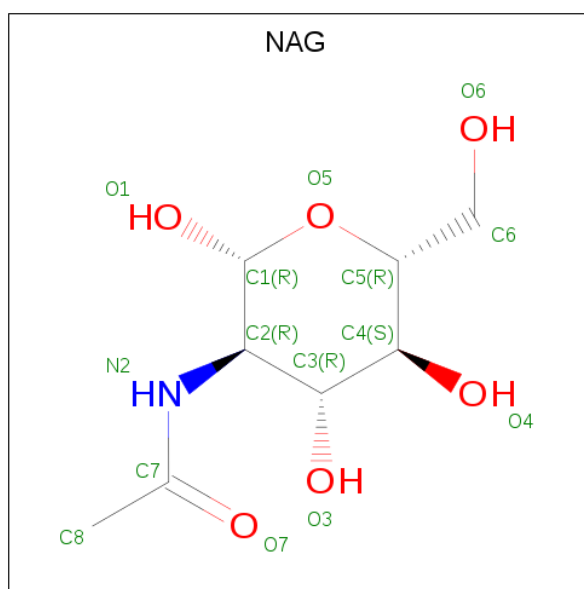
Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ALA	-	expression tag	UNP O88998
A	480	ALA	-	expression tag	UNP O88998
A	481	ALA	-	expression tag	UNP O88998
A	482	HIS	-	expression tag	UNP O88998
A	483	HIS	-	expression tag	UNP O88998
A	484	HIS	-	expression tag	UNP O88998
A	485	HIS	-	expression tag	UNP O88998
A	486	HIS	-	expression tag	UNP O88998
A	487	HIS	-	expression tag	UNP O88998
A	329	THR	ALA	variant	UNP O88998
B	479	ALA	-	expression tag	UNP O88998
B	480	ALA	-	expression tag	UNP O88998
B	481	ALA	-	expression tag	UNP O88998
B	482	HIS	-	expression tag	UNP O88998
B	483	HIS	-	expression tag	UNP O88998
B	484	HIS	-	expression tag	UNP O88998
B	485	HIS	-	expression tag	UNP O88998
B	486	HIS	-	expression tag	UNP O88998
B	487	HIS	-	expression tag	UNP O88998
B	329	THR	ALA	variant	UNP O88998

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	13	Total	O	0	0
			13	13		

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.

**Chain A:**

Amino Acid	Percentage
GLY	3%
ALA	47%
ASP	6%
GLU	46%
SER	
LEU	
VAL	
PRO	
THR	
ARG	
LYS	
ILE	
MET	
TYR	
PHE	
TRP	
HIS	
CYS	
ASN	

Chain B:

3% 45% 10% 45%

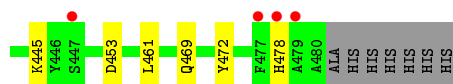
MET ILE THR ASN TRP MET SER GLN THR LEU PRO SER LEU VAL GLY ASN THR ARG LEU SER ALA GLY THR LEU ASP ARG SER THR GLY VAL LEU PRO THR ASN PRO GLU GLU SER TRP GLN VAL TYR SER ALA GLN ASP GLY ARG CYS ILE CYS THR

VAL VAL PRO GLN THR CYS SER ARG ASP GLN LEU ARG GLN MET THR LYS VAL ASP THR TYR LEU MET GLN ASN GLN ASP THR LYS GLY THR PHE

LYS GLN VAL GLU GLU SER HIS GLN HIS LEU ALA ARG ALA PHE LYS ALA ILE LYS ALA LYS MET ASP GLU LEU ARG PRO LEU ILE SER PRO VAL LEU GLU TYR LYS ASP ARG THR GLN LEU VAL THR ASP G267 G268 Y264 G267 Y268 H269 N270 R275 D282 F283 M284 D287 S299 Q303 V304

GLU GLU ILE GLY ALA TYR ASP TYR ASP GLU LEU GLN SER R2110 R2114 E215 E216 R2119 K224 C227 G228 S234 D235 P236 V239 D252 A255 P256 E257 G258 Y264 G267 Y268 H269 N270 R275 D282 F283 M284 D287 S299 Q303 V304

I340 F315 I320 F323 R334 Y338 ALA GLY TYR ASN MET TYR HIS TYR TRP GLY GLY HIS S353 D356 L357 K358 V359 D360 W365 T370 N376 Q388 P398 R399 R400 I408 Y413 V414 Y418 G421 T422 K423 Y424 H425 Y426 Y427



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

Chain C:  100%



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

Chain D:  100%



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

Chain E:  100%



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

Chain F:  50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.22Å 43.94Å 104.06Å 90.00° 114.17° 90.00°	Depositor
Resolution (Å)	50.32 – 2.40 50.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.32-2.40) 94.3 (50.32-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.237 , 0.258 0.240 , 0.258	Depositor DCC
$R_{free}$ test set	1252 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL

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	0.21	0/2098	0.38	0/2851
1	B	0.21	0/2130	0.38	0/2894
All	All	0.21	0/4228	0.38	0/5745

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

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	2044	0	1953	16	0
1	B	2075	0	1983	21	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	B	18	0	24	1	0
5	B	1	0	0	0	0
6	A	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	0	0	0
All	All	4304	0	4086	37	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 (37) 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:TYR:HB3	1:A:275:ARG:HB2	1.61	0.81
1:B:228:GLY:HA2	1:B:478:HIS:HB3	1.66	0.77
1:A:461:LEU:HB2	1:A:472:TYR:HB2	1.70	0.72
1:B:461:LEU:HB2	1:B:472:TYR:HB2	1.73	0.70
1:B:299:SER:HB2	1:B:315:PHE:HA	1.74	0.69
1:B:252:ASP:HB3	1:B:255:ALA:HB2	1.74	0.68
1:B:264:TYR:HB3	1:B:275:ARG:HB2	1.79	0.64
1:A:394:ASN:OD1	1:A:394:ASN:N	2.31	0.63
1:B:423:LYS:HE2	1:B:441:PRO:HB3	1.80	0.62
1:A:226:ALA:O	1:A:459:ARG:NH2	2.32	0.62
1:B:360:ASP:OD1	1:B:365:TRP:NE1	2.34	0.60
1:A:448:HIS:O	1:A:465:ASN:ND2	2.35	0.59
1:A:252:ASP:HB3	1:A:255:ALA:HB2	1.88	0.56
1:B:269:HIS:ND1	1:B:270:ASN:OD1	2.36	0.52
1:A:304:VAL:HG11	1:A:358:MET:HA	1.91	0.51
1:B:239:VAL:HG13	1:B:284:MET:HG2	1.94	0.50
1:B:304:VAL:HG11	1:B:358:MET:HA	1.94	0.49
1:A:327:THR:HB	1:A:329:THR:HG22	1.94	0.49
1:B:408:ILE:HB	1:B:413:TYR:HE2	1.77	0.49
1:B:414:VAL:HB	1:B:426:TYR:HB3	1.96	0.48
1:B:376:ASN:HA	1:B:398:PRO:HA	1.94	0.47
1:B:334:ARG:HH12	1:B:388:GLN:HG2	1.80	0.47
1:A:360:ASP:OD1	1:A:365:TRP:NE1	2.43	0.47
1:A:371:ASN:N	1:A:371:ASN:OD1	2.41	0.47
1:A:411:THR:HG22	1:A:429:GLN:HA	1.96	0.46
1:B:423:LYS:HG2	1:B:441:PRO:HA	1.97	0.46
1:B:236:PRO:HG2	1:B:445:LYS:HD2	1.99	0.44
1:A:368:TYR:O	1:A:378:VAL:N	2.32	0.43
1:A:332:LYS:HA	1:A:332:LYS:HD2	1.82	0.43
1:B:234:SER:OG	1:B:235:ASP:N	2.52	0.42
1:A:373:ASN:O	1:A:375:GLY:N	2.52	0.42
1:A:459:ARG:NH2	1:A:476:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HD13	1:B:357:LEU:HD21	2.02	0.41
1:B:267:GLY:HA3	4:B:1482:GOL:H11	2.02	0.41
1:A:320:ILE:HD13	1:A:357:LEU:HD21	2.01	0.41
1:B:310:ILE:HG23	1:B:323:PHE:HB3	2.04	0.40
1:B:224:LYS:O	1:B:227:CYS:HB2	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	249/471 (53%)	241 (97%)	8 (3%)	0	100	100
1	B	253/471 (54%)	244 (96%)	9 (4%)	0	100	100
All	All	502/942 (53%)	485 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/416 (54%)	216 (96%)	8 (4%)	35	54
1	B	226/416 (54%)	218 (96%)	8 (4%)	36	55
All	All	450/832 (54%)	434 (96%)	16 (4%)	35	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	THR
1	A	358	MET
1	A	371	ASN
1	A	373	ASN
1	A	394	ASN
1	A	425	HIS
1	A	458	ASP
1	A	465	ASN
1	B	227	CYS
1	B	282	ASP
1	B	287	ASP
1	B	303	GLN
1	B	356	ASP
1	B	425	HIS
1	B	453	ASP
1	B	469	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	B	223	GLN

### 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 ⓘ

8 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	C	1	1,2	14,14,15	0.22	0	17,19,21	0.39	0
2	NAG	C	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.36	0
2	NAG	E	1	1,2	14,14,15	0.36	0	17,19,21	0.35	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	F	1	1,2	14,14,15	0.43	0	17,19,21	0.67	1 (5%)
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	2.22	115.19	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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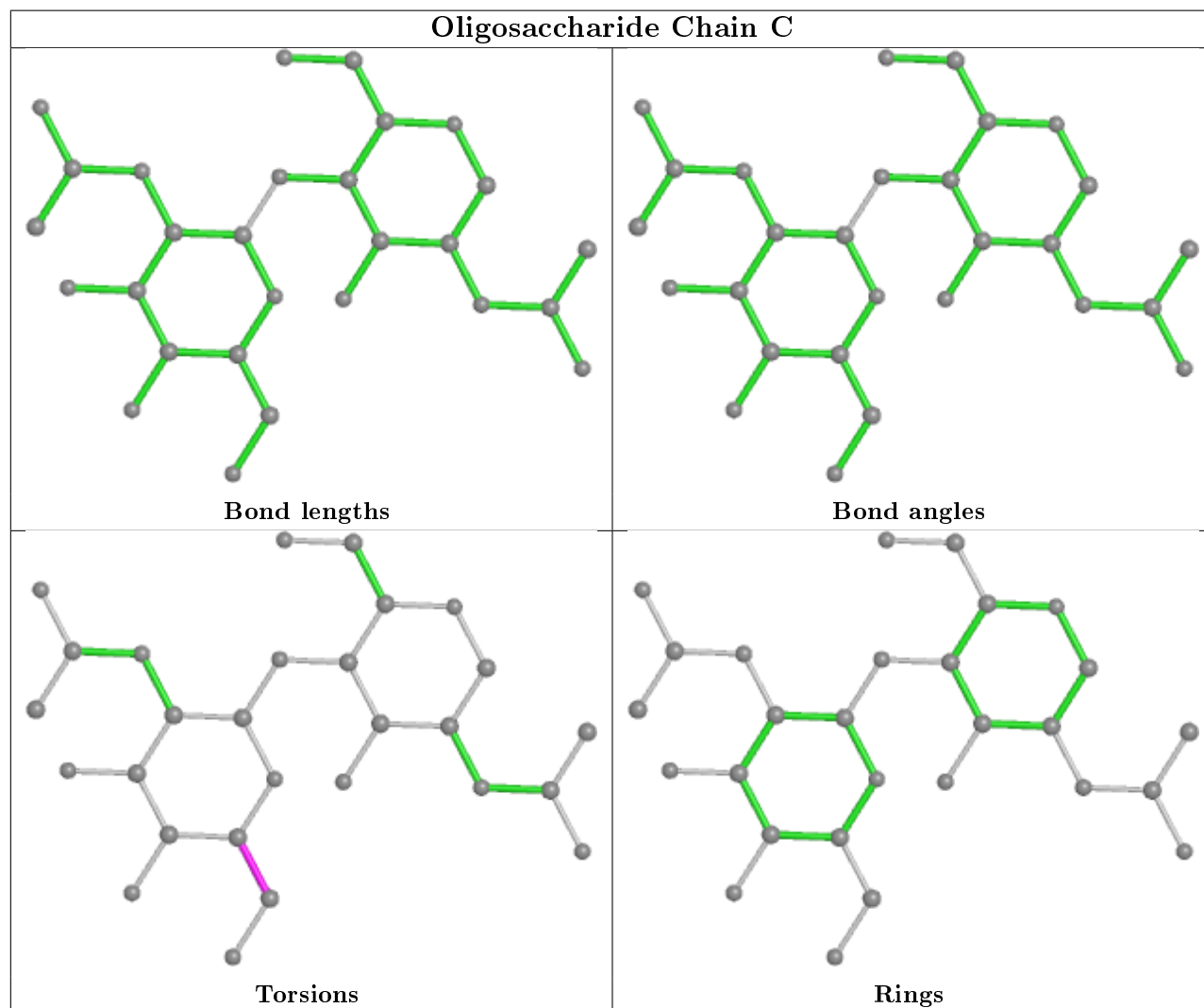
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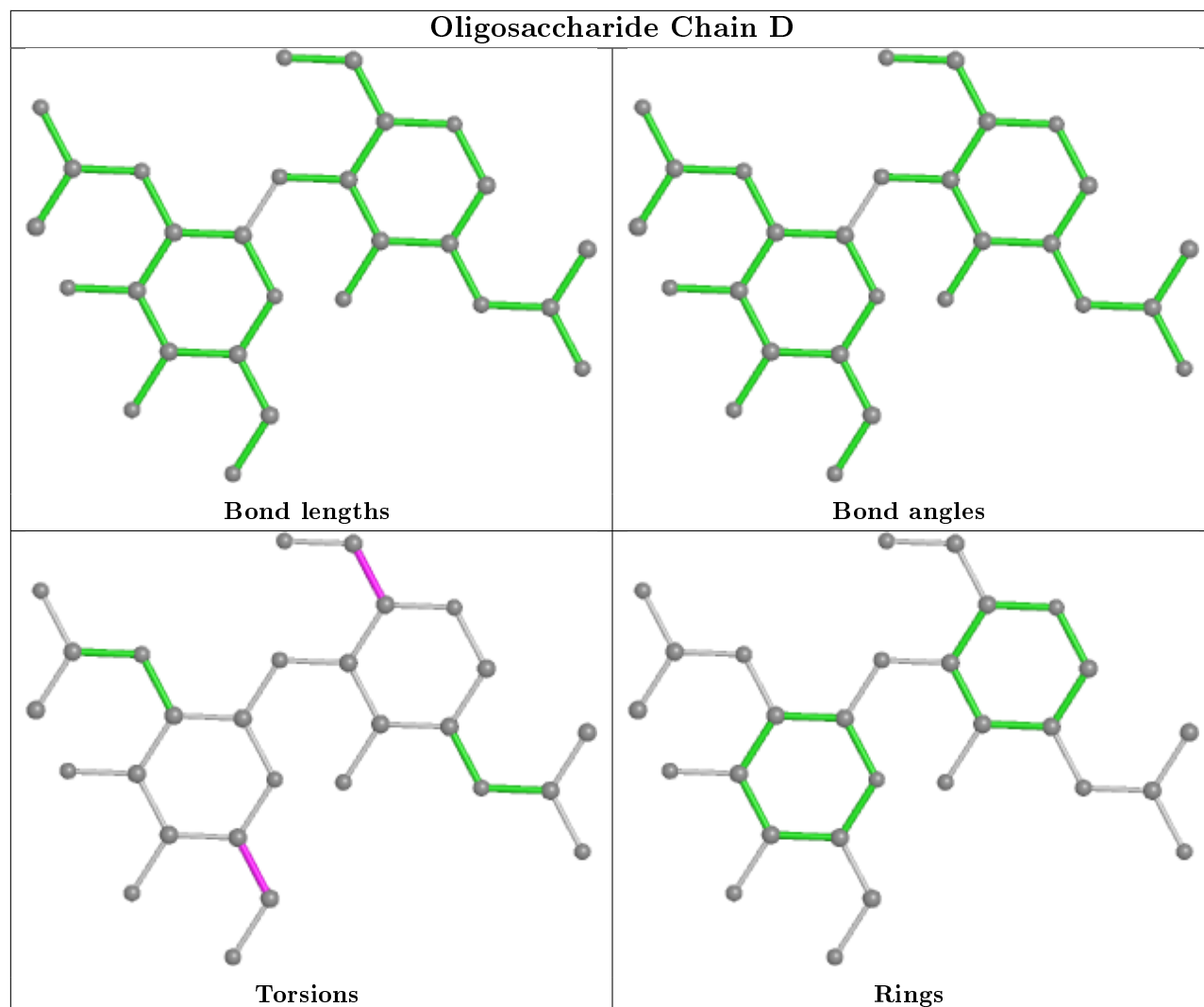
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

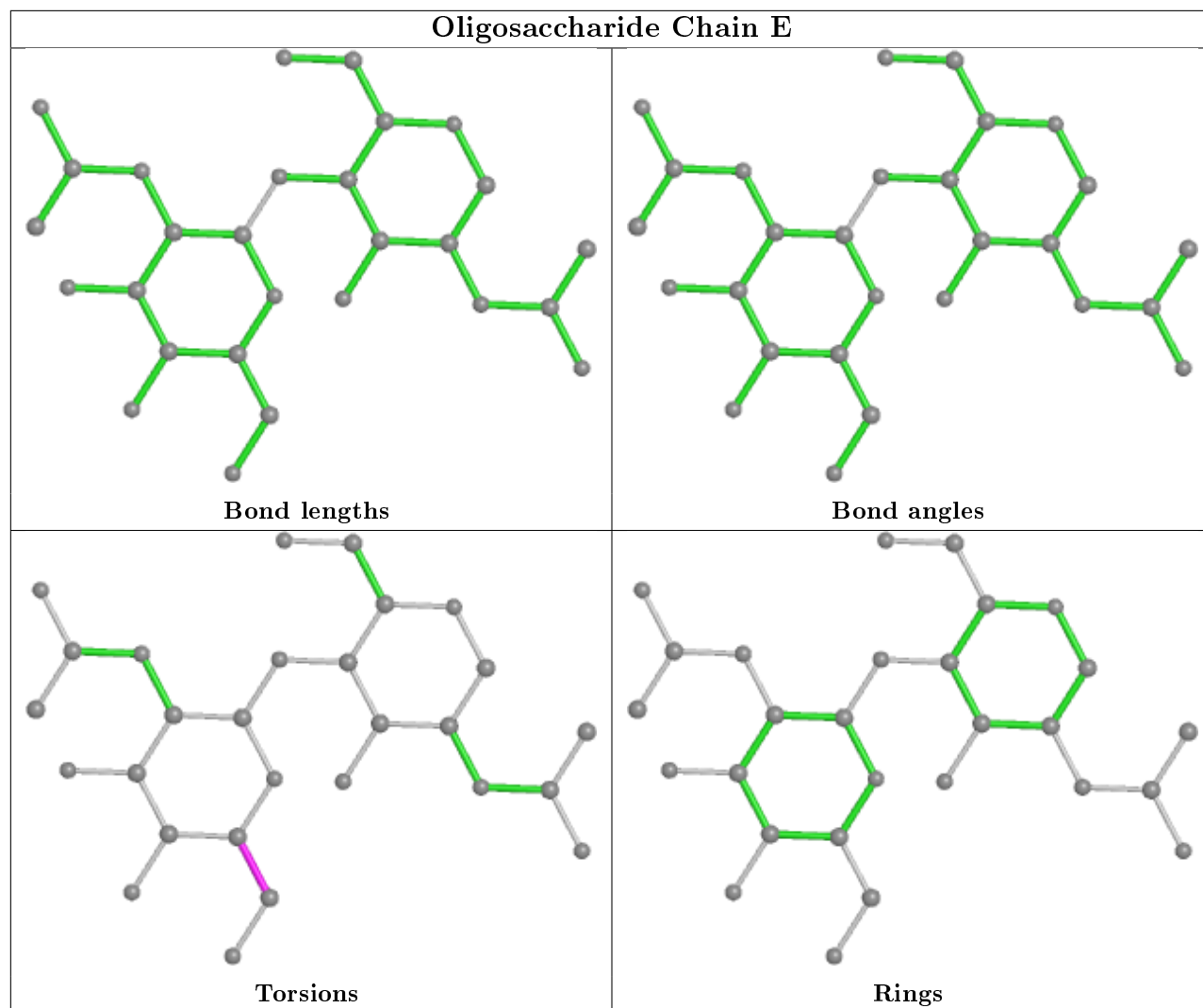
No monomer is involved in short contacts.

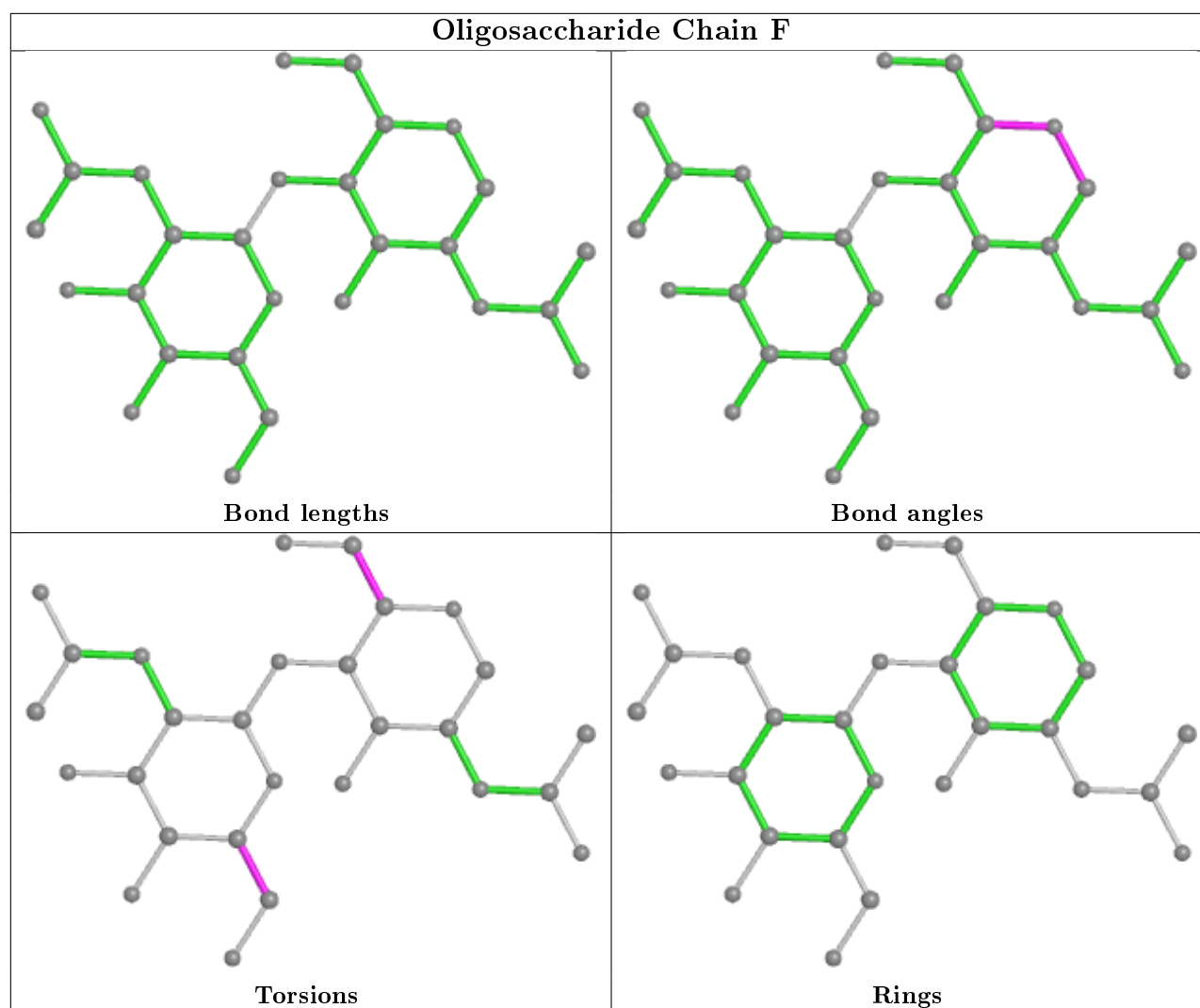
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z  > 2$
3	NAG	B	1473	1	14,14,15	0.21	0	17,19,21	0.42	0
4	GOL	B	1483	-	5,5,5	0.36	0	5,5,5	0.48	0
4	GOL	B	1481	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	B	1482	-	5,5,5	0.25	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1394	1	14,14,15	0.25	0	17,19,21	0.40	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
3	NAG	B	1473	1	-	0/6/23/26	0/1/1/1
4	GOL	B	1483	-	-	3/4/4/4	-
4	GOL	B	1481	-	-	0/4/4/4	-
4	GOL	B	1482	-	-	2/4/4/4	-
3	NAG	A	1394	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1483	GOL	C1-C2-C3-O3
4	B	1482	GOL	C1-C2-C3-O3
4	B	1483	GOL	O2-C2-C3-O3
4	B	1483	GOL	O1-C1-C2-O2
4	B	1482	GOL	O2-C2-C3-O3
3	A	1394	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1482	GOL	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	253/471 (53%)	0.36	13 (5%) 28 26	44, 67, 93, 133	0
1	B	257/471 (54%)	0.54	15 (5%) 23 22	48, 67, 98, 119	0
All	All	510/942 (54%)	0.45	28 (5%) 25 24	44, 67, 96, 133	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	GLY	6.2
1	A	211	VAL	5.8
1	B	478	HIS	5.6
1	B	214	LEU	5.2
1	A	212	SER	4.7
1	B	418	TYR	4.5
1	A	477	PHE	3.9
1	B	338	TYR	3.6
1	A	216	GLU	3.5
1	B	257	GLU	3.4
1	B	211	VAL	3.2
1	B	258	GLY	3.2
1	A	338	TYR	3.2
1	A	213	ASN	3.1
1	B	477	PHE	3.0
1	B	400	ARG	3.0
1	A	214	LEU	3.0
1	B	216	GLU	2.9
1	A	400	ARG	2.6
1	A	281	VAL	2.5
1	B	447	SER	2.4
1	B	219	ARG	2.4
1	A	219	ARG	2.4
1	B	479	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	2.2
1	A	286	THR	2.2
1	A	474	VAL	2.1
1	B	370	THR	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](#)

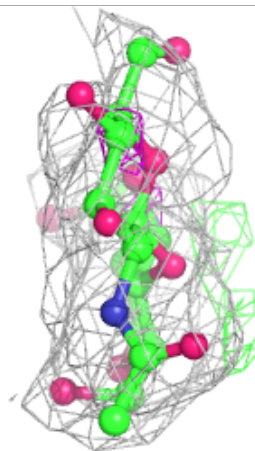
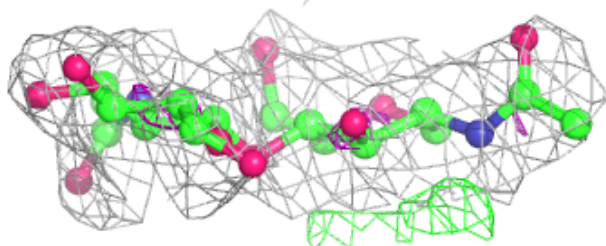
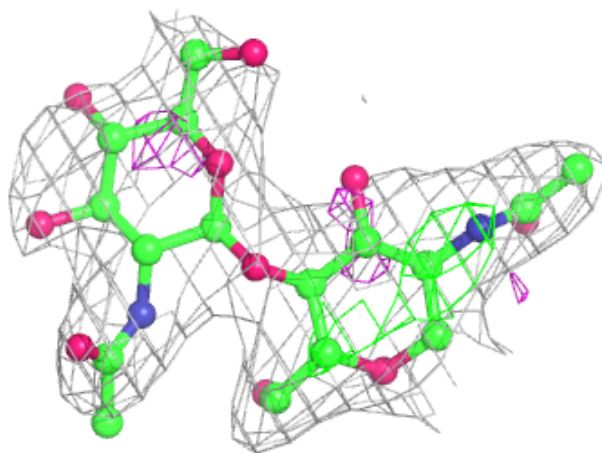
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	NAG	E	2	14/15	0.69	0.47	89,96,98,99	0
2	NAG	F	2	14/15	0.76	0.24	85,88,91,92	0
2	NAG	D	2	14/15	0.76	0.37	92,97,100,101	0
2	NAG	F	1	14/15	0.77	0.22	70,74,78,82	0
2	NAG	E	1	14/15	0.78	0.25	68,72,76,83	0
2	NAG	C	1	14/15	0.79	0.25	67,72,77,84	0
2	NAG	C	2	14/15	0.81	0.29	89,91,93,94	0
2	NAG	D	1	14/15	0.86	0.25	73,77,80,86	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.

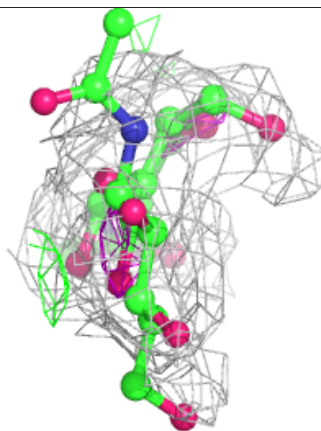
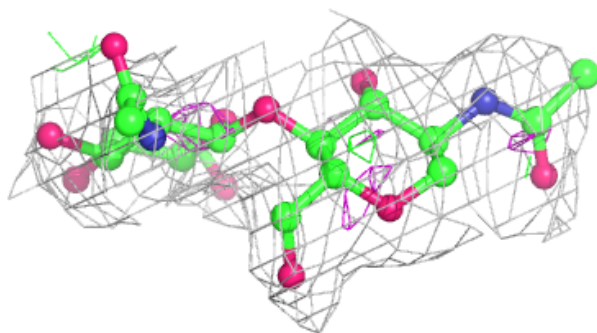
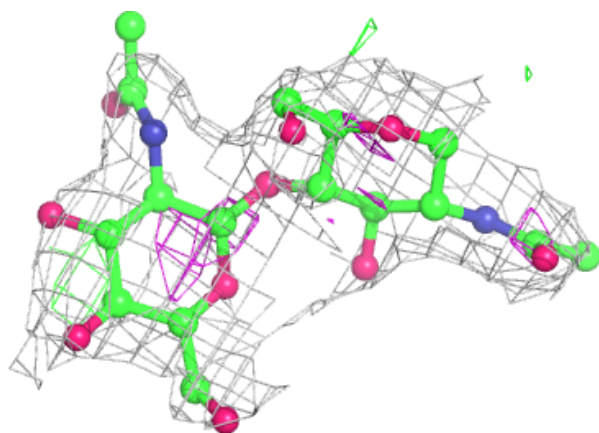
**Electron density around Chain C:**

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



**Electron density around Chain D:**

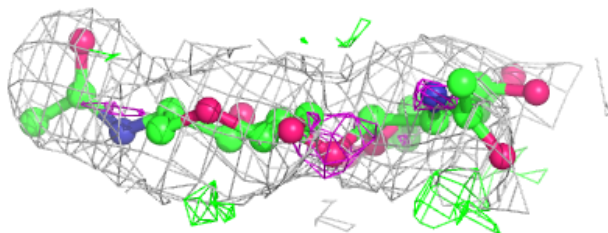
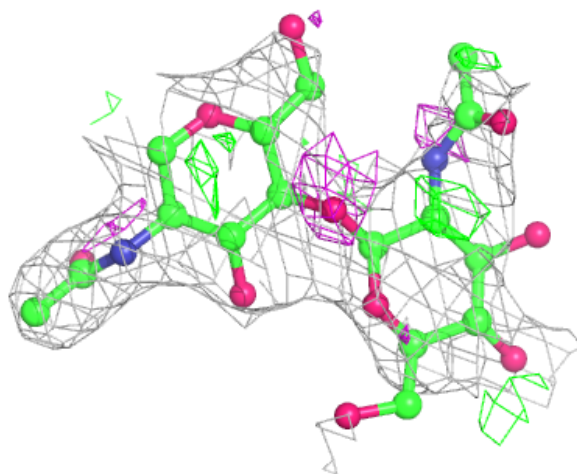
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

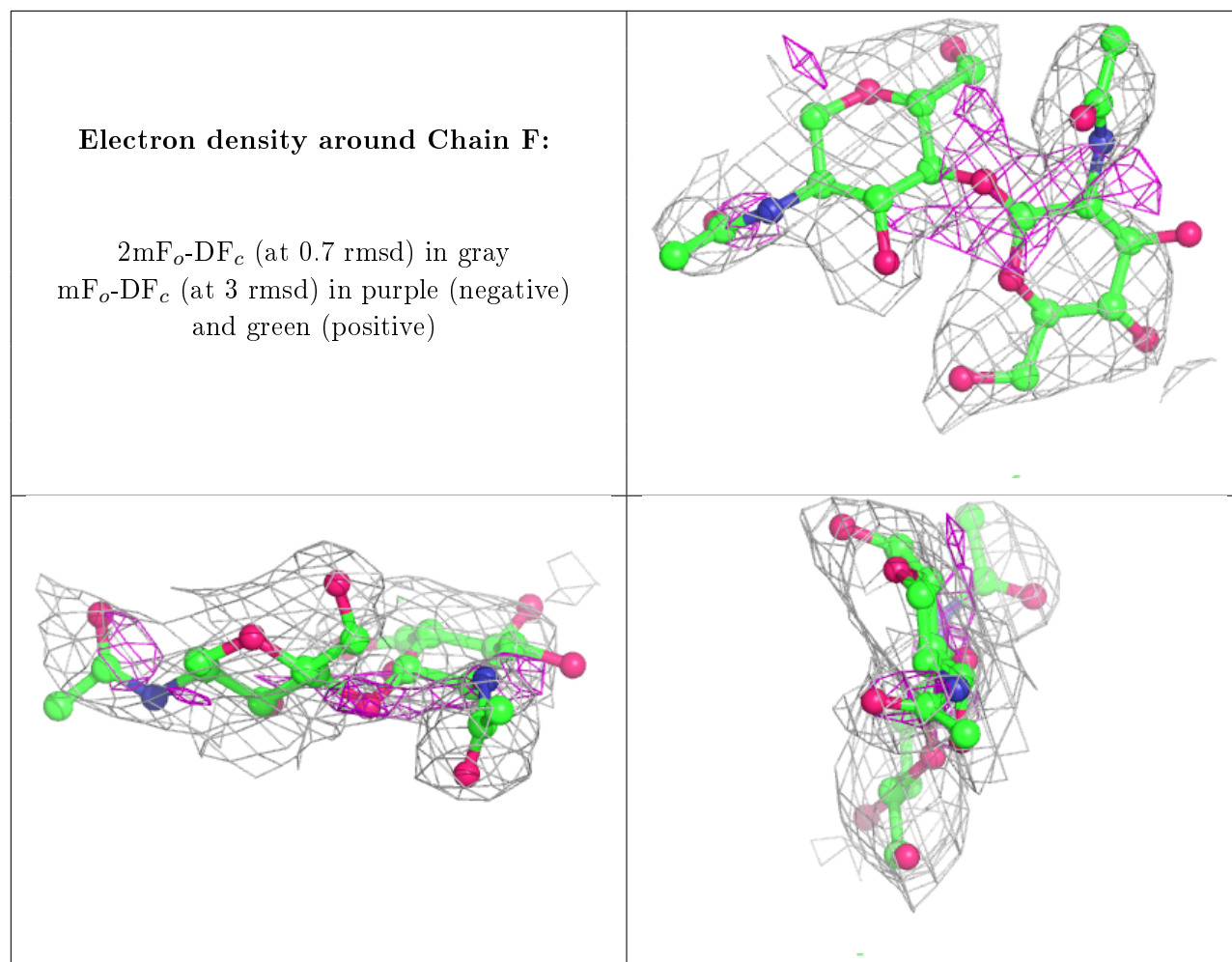




**Electron density around Chain E:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	1483	6/6	0.47	0.41	106,107,108,108	0
4	GOL	B	1482	6/6	0.63	0.34	95,95,99,100	0
3	NAG	A	1394	14/15	0.78	0.50	69,78,81,84	0
5	CL	B	1484	1/1	0.81	0.16	91,91,91,91	0
3	NAG	B	1473	14/15	0.82	0.36	68,74,77,77	0
4	GOL	B	1481	6/6	0.87	0.20	71,72,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.