



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 03:32 PM EDT

PDB ID : 7RC9  
Title : Crystal structure of human TLR8 ectodomain bound to small molecule antagonist 21  
Authors : Critton, D.A.  
Deposited on : 2021-07-07  
Resolution : 2.76 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 : 2.28.1  
buster-report : 1.1.7 (2018)  
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) : 2.28.1

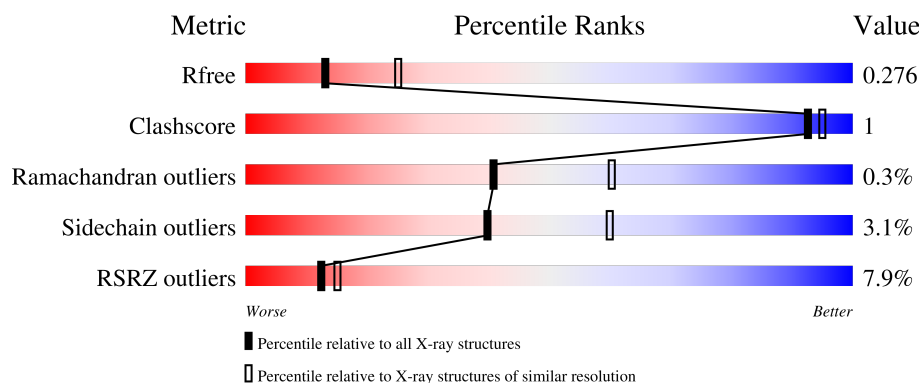
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	811	<div> <div>3%</div> <div>84%</div> <div>6%</div> <div>9%</div> </div>
1	B	811	<div> <div>11%</div> <div>84%</div> <div>6%</div> <div>9%</div> </div>
2	C	3	<div> <div>100%</div> </div>
2	D	3	<div> <div>67%</div> <div>33%</div> </div>
3	E	5	<div> <div>20%</div> <div>80%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	5	
3	H	5	
4	G	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
5	NAG	A	903	-	-	-	X
5	NAG	B	901	-	-	-	X
5	NAG	B	903	-	-	-	X
5	NAG	B	904	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12205 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.

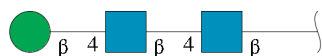
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	2	0
			5725	3683	956	1067	19			
1	B	737	Total	C	N	O	S	0	2	0
			5729	3685	957	1068	19			

There are 20 discrepancies between the modelled and reference sequences:

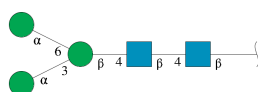
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



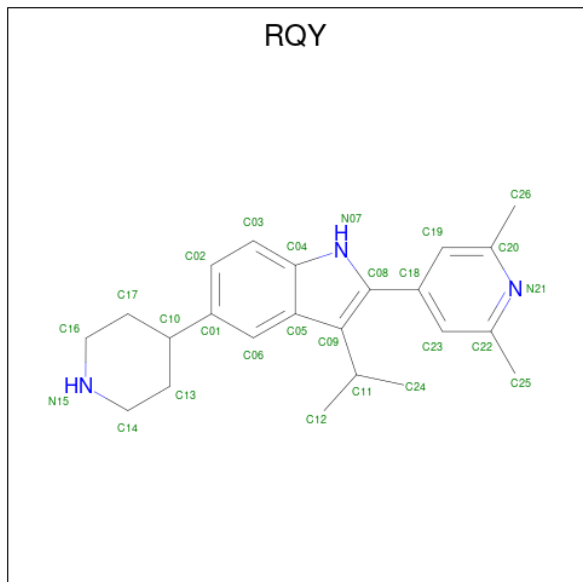
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 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
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 2-(2,6-dimethylpyridin-4-yl)-5-(piperidin-4-yl)-3-(propan-2-yl)-1H-indole (three-letter code: RQY) (formula: C<sub>23</sub>H<sub>29</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			26	23	3		
6	B	1	Total	C	N	0	0
			26	23	3		

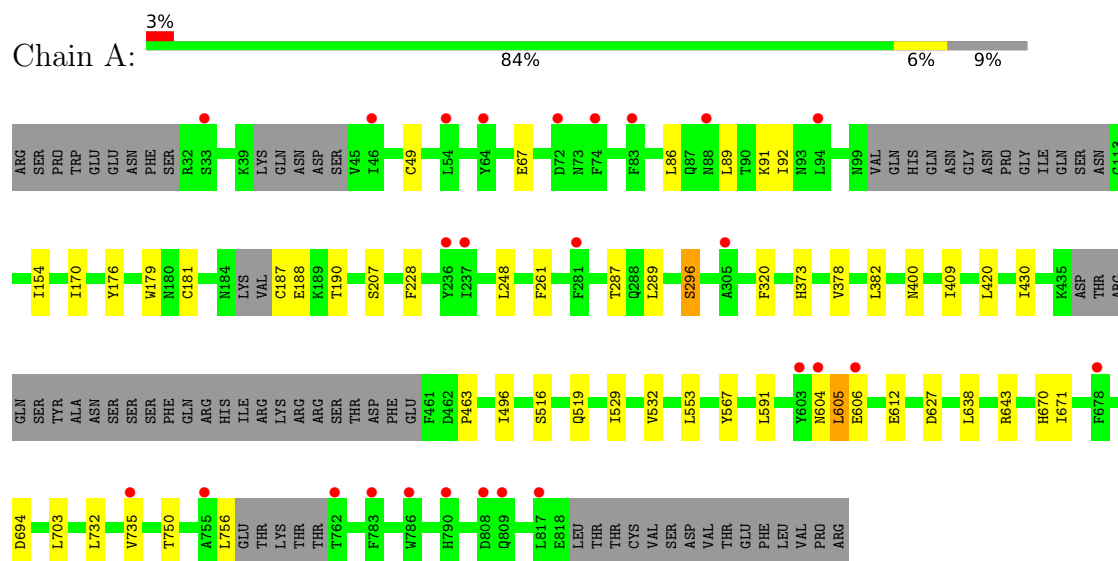
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	110	Total	O	0	0
			110	110		
7	B	82	Total	O	0	0
			82	82		

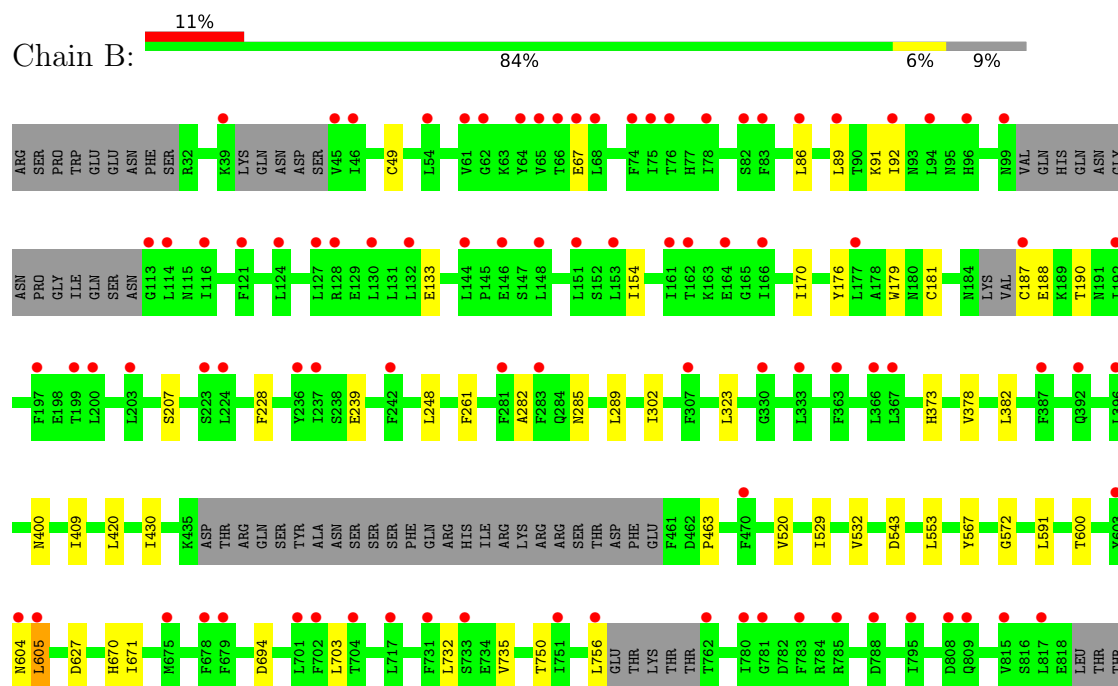
### 3 Residue-property plots

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 8



#### • Molecule 1: Toll-like receptor 8



CYS	VAL	SER	ASP	VAL	THR	GLU	PHE	LEU	VAL	PRO	ARG
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- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

NAG1	NAG2	BMA3
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- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

NAG1	NAG2	BMA3
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- Molecule 3: 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 E:  20% 80%

NAG1	NAG2	BMA3	MAN4	MAN5
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- Molecule 3: 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 F:  60% 40%

NAG1	NAG2	BMA3	MAN4	MAN5
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- Molecule 3: 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:  40% 60%

NAG1	NAG2	BMA3	MAN4	MAN5
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- 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:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.89Å 83.88Å 153.52Å 90.00° 119.72° 90.00°	Depositor
Resolution (Å)	40.41 – 2.76 40.01 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.41-2.76) 99.5 (40.01-2.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.234 , 0.262 0.247 , 0.276	Depositor DCC
$R_{free}$ test set	2331 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, BMA, NAG, RQY

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	0.39	0/5852	0.59	1/7979 (0.0%)
1	B	0.39	0/5856	0.58	1/7984 (0.0%)
All	All	0.39	0/11708	0.59	2/15963 (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	604	ASN	C-N-CA	5.23	134.78	121.70
1	B	604	ASN	C-N-CA	5.22	134.75	121.70

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	5725	0	5496	16	0
1	B	5729	0	5502	19	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	E	61	0	52	0	0
3	F	61	0	52	0	0
3	H	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	50	0	43	0	0
5	A	98	0	91	0	0
5	B	98	0	91	0	0
6	A	26	0	0	0	0
6	B	26	0	0	1	0
7	A	110	0	0	0	0
7	B	82	0	0	0	0
All	All	12205	0	11447	35	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 1.

All (35) 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:187:CYS:N	1:B:188:GLU:HA	2.07	0.69
1:A:187:CYS:N	1:A:188:GLU:HA	2.07	0.68
1:B:409:ILE:HD12	1:B:430:ILE:HD11	1.86	0.58
1:A:732:LEU:HD12	1:A:756:LEU:HA	1.84	0.57
1:B:732:LEU:HD12	1:B:756:LEU:HA	1.85	0.57
1:A:409:ILE:HD12	1:A:430:ILE:HD11	1.88	0.56
1:B:382:LEU:HB3	1:B:409:ILE:HG12	1.92	0.52
1:A:382:LEU:HB3	1:A:409:ILE:HG12	1.92	0.52
1:A:532:VAL:HB	1:A:553:LEU:HD22	1.94	0.50
1:B:532:VAL:HB	1:B:553:LEU:HD22	1.94	0.48
1:B:154:ILE:HD11	1:B:176:TYR:HB3	1.97	0.47
1:A:86:LEU:HB3	1:A:89:LEU:HD12	1.97	0.46
1:A:179:TRP:NE1	1:A:463:PRO:HB3	2.31	0.46
1:B:86:LEU:HB3	1:B:89:LEU:HD12	1.97	0.45
1:B:179:TRP:NE1	1:B:463:PRO:HB3	2.31	0.45
1:B:520:VAL:HA	1:B:543:ASP:HB3	1.99	0.45
1:A:67:GLU:HG2	1:A:91:LYS:HB3	1.99	0.45
1:A:89:LEU:HD13	1:A:92:ILE:HD11	1.99	0.45
1:B:67:GLU:HG2	1:B:91:LYS:HB3	1.99	0.44
1:A:612:GLU:HG3	1:A:643:ARG:HB3	1.98	0.44
1:A:154:ILE:HD11	1:A:176:TYR:HB3	1.98	0.44
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.99	0.44
1:A:207:SER:HA	1:A:228:PHE:HB2	2.00	0.44
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.99	0.44
1:B:89:LEU:HD13	1:B:92:ILE:HD11	2.00	0.44
1:B:302:ILE:HD11	1:B:323:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.99	0.43
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.99	0.43
1:B:239:GLU:HA	1:B:282:ALA:HA	2.01	0.43
1:A:296:SER:HA	1:A:320:PHE:O	2.19	0.42
1:B:207:SER:HA	1:B:228:PHE:HB2	2.01	0.41
1:B:572:GLY:C	1:B:600:THR:HG21	2.41	0.41
1:A:496:ILE:HD12	1:A:519:GLN:HG2	2.04	0.40
1:B:261:PHE:HZ	6:B:908:RQY:C24	2.35	0.40
1:B:133:GLU:HG2	1:B:154:ILE:HB	2.04	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	727/811 (90%)	673 (93%)	51 (7%)	3 (0%)	34	53
1	B	727/811 (90%)	671 (92%)	54 (7%)	2 (0%)	41	60
All	All	1454/1622 (90%)	1344 (92%)	105 (7%)	5 (0%)	41	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	LEU
1	B	605	LEU
1	A	606	GLU
1	A	378	VAL
1	B	378	VAL

### 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	624/755 (83%)	603 (97%)	21 (3%)	37	58
1	B	625/755 (83%)	608 (97%)	17 (3%)	44	65
All	All	1249/1510 (83%)	1211 (97%)	38 (3%)	40	61

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	170	ILE
1	A	181	CYS
1	A	190	THR
1	A	248	LEU
1	A	261	PHE
1	A	287	THR
1	A	289	LEU
1	A	296	SER
1	A	420	LEU
1	A	516	SER
1	A	529	ILE
1	A	567	TYR
1	A	591	LEU
1	A	605	LEU
1	A	627	ASP
1	A	638	LEU
1	A	671	ILE
1	A	703	LEU
1	A	735	VAL
1	A	750	THR
1	B	49	CYS
1	B	170	ILE
1	B	181	CYS
1	B	190	THR
1	B	248	LEU
1	B	285	ASN

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Mol	Chain	Res	Type
1	B	289	LEU
1	B	420	LEU
1	B	529	ILE
1	B	567	TYR
1	B	591	LEU
1	B	605	LEU
1	B	627	ASP
1	B	671	ILE
1	B	703	LEU
1	B	735	VAL
1	B	750	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	135	ASN
1	B	97	ASN
1	B	135	ASN
1	B	388	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 ⓘ

25 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	0.29	0	17,19,21	0.59	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.67	0
2	BMA	C	3	2	11,11,12	0.33	0	15,15,17	0.54	0
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.53	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	1.58	2 (11%)
2	BMA	D	3	2	11,11,12	0.37	0	15,15,17	0.42	0
3	NAG	E	1	1,3	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
3	BMA	E	3	3	11,11,12	0.29	0	15,15,17	0.56	0
3	MAN	E	4	3	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
3	MAN	E	5	3	11,11,12	0.36	0	15,15,17	0.84	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.58	0
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.65	0
3	MAN	F	4	3	11,11,12	0.42	0	15,15,17	0.87	2 (13%)
3	MAN	F	5	3	11,11,12	0.37	0	15,15,17	0.81	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.57	0
4	BMA	G	3	4	11,11,12	0.40	0	15,15,17	0.77	0
4	MAN	G	4	4	11,11,12	0.39	0	15,15,17	1.01	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
3	NAG	H	2	3	14,14,15	0.27	0	17,19,21	0.56	0
3	BMA	H	3	3	11,11,12	0.29	0	15,15,17	0.57	0
3	MAN	H	4	3	11,11,12	0.37	0	15,15,17	0.89	1 (6%)
3	MAN	H	5	3	11,11,12	0.40	0	15,15,17	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	O5-C1-C2	-5.87	102.02	111.29
4	G	4	MAN	C1-O5-C5	3.50	116.94	112.19
3	H	5	MAN	C1-O5-C5	3.32	116.68	112.19
3	H	4	MAN	C1-O5-C5	2.97	116.21	112.19
3	E	5	MAN	C1-O5-C5	2.49	115.57	112.19
3	F	5	MAN	C1-O5-C5	2.48	115.56	112.19
3	E	4	MAN	C1-O5-C5	2.47	115.54	112.19
3	F	4	MAN	C1-O5-C5	2.26	115.25	112.19
2	D	2	NAG	O4-C4-C3	-2.11	105.47	110.35
3	H	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	F	4	MAN	C1-C2-C3	2.07	112.22	109.67
3	E	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	E	1	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

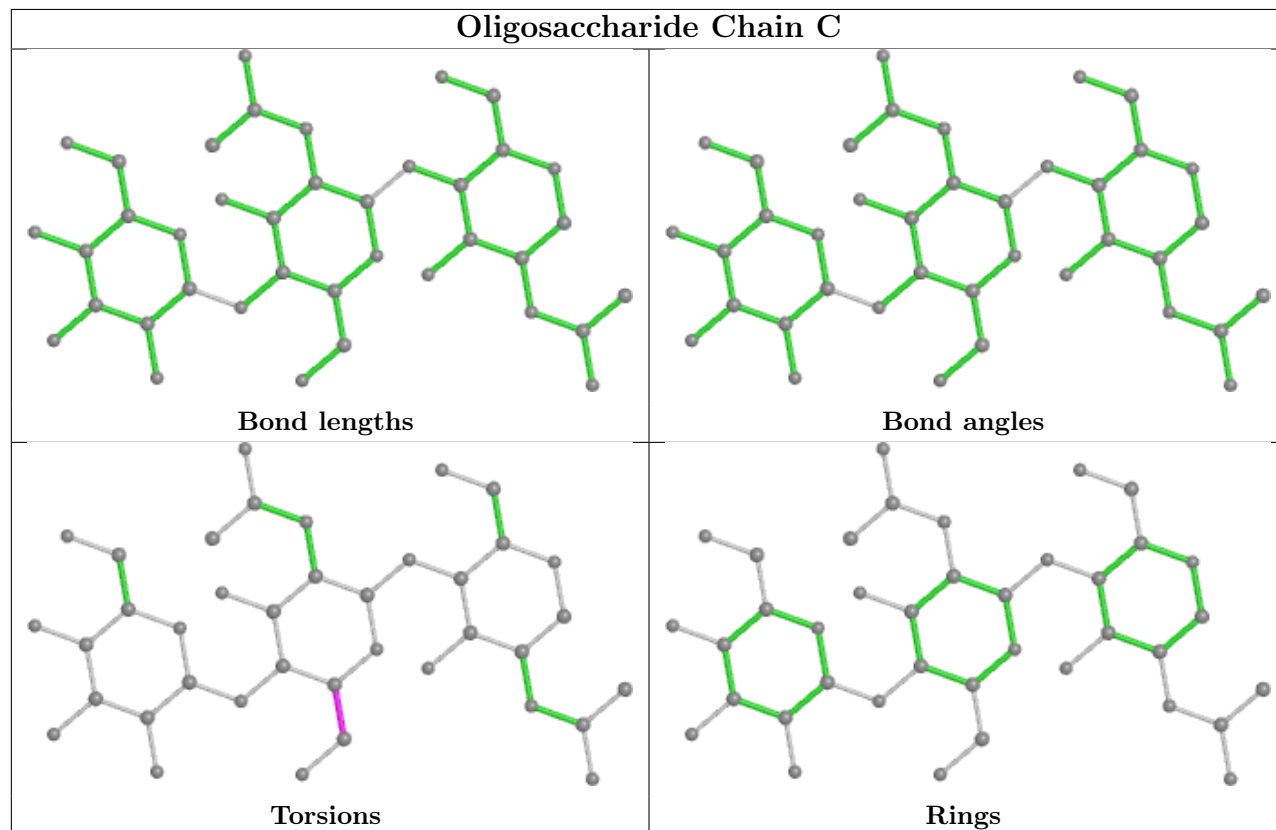
All (1) torsion outliers are listed below:

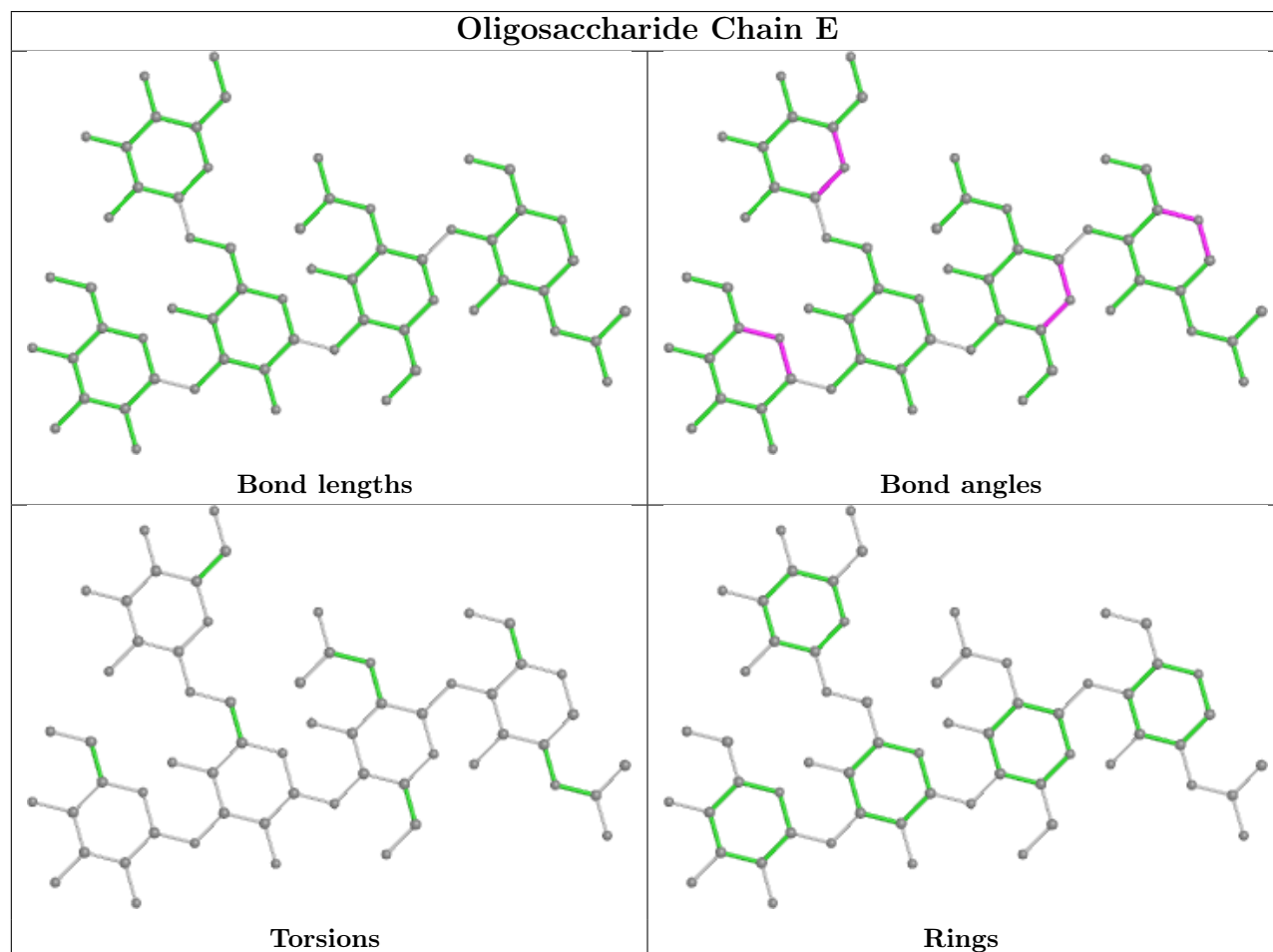
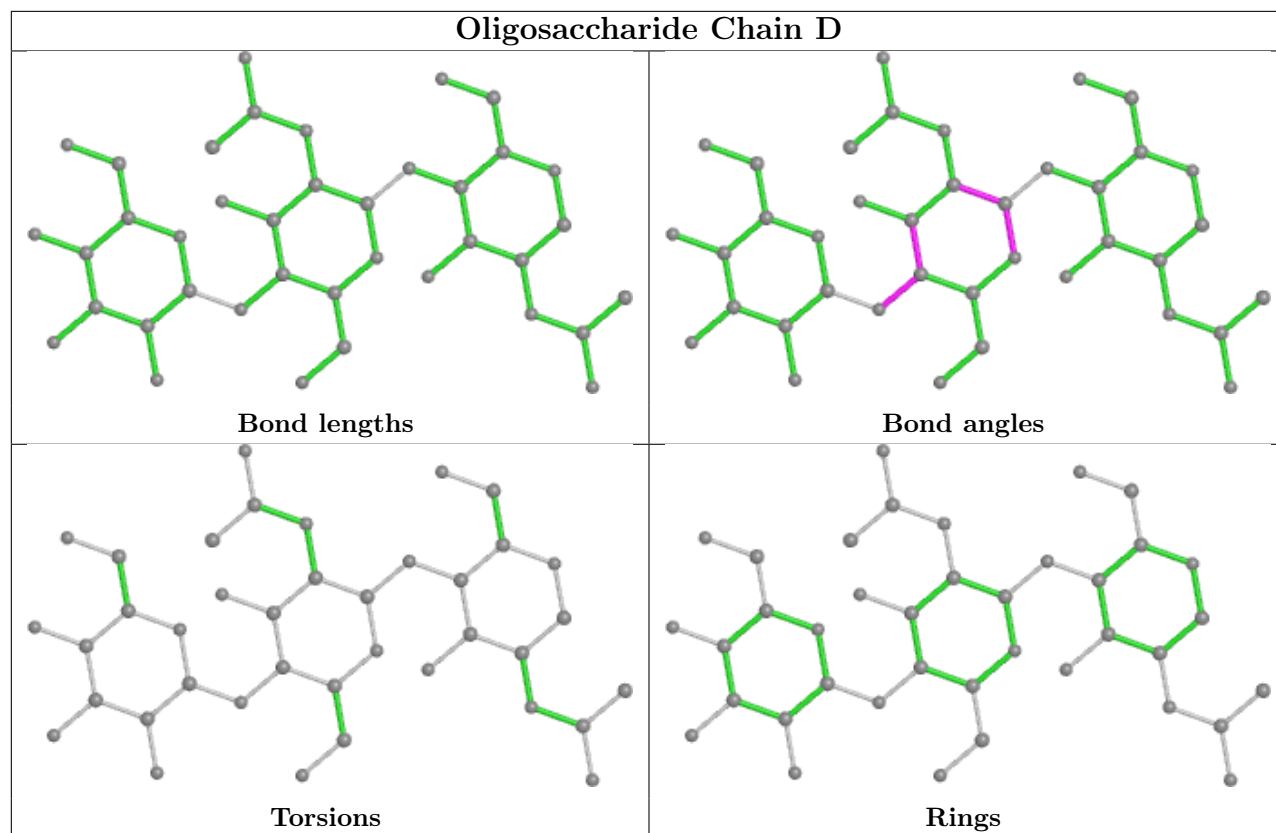
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6

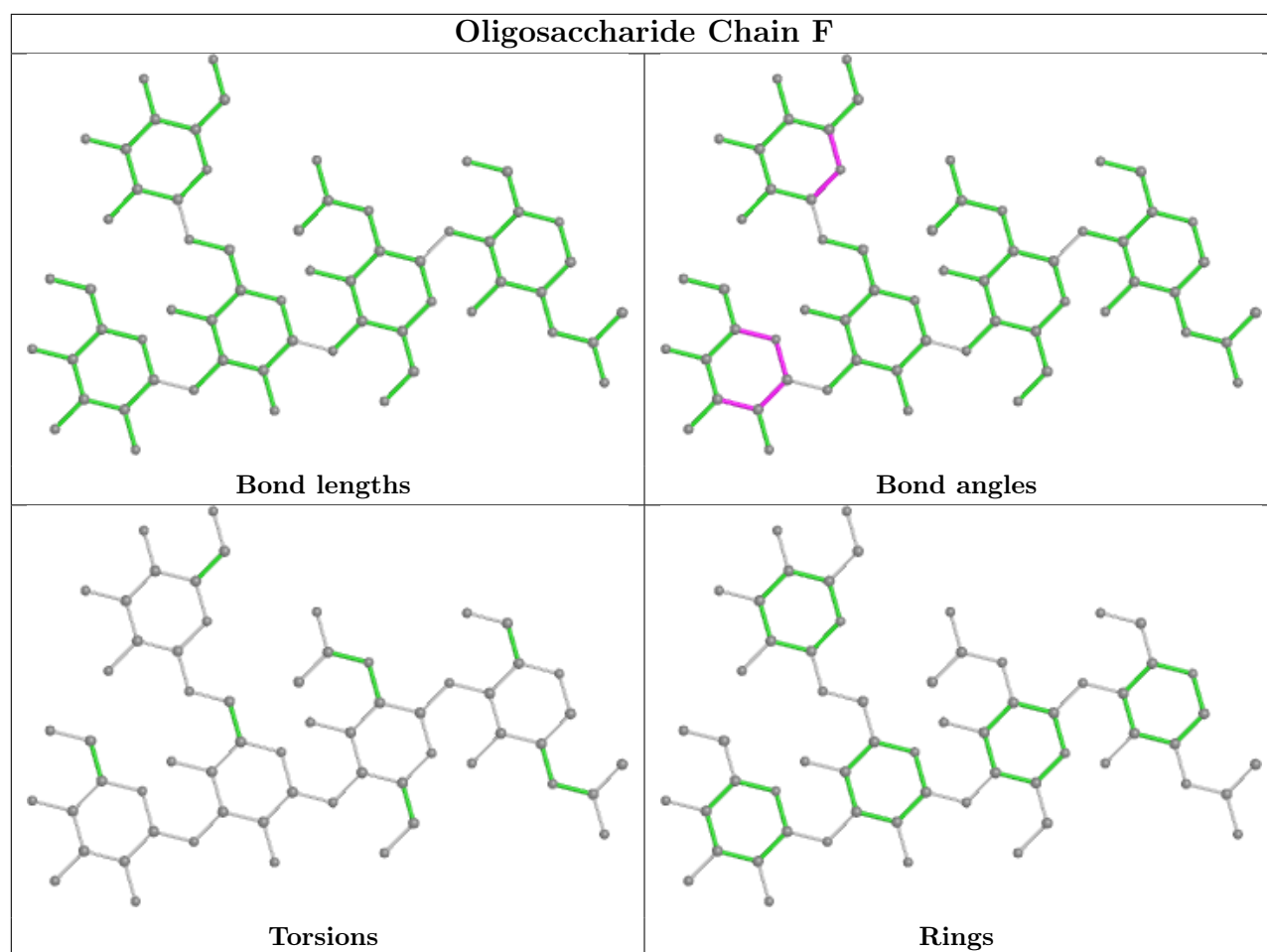
There are no ring outliers.

No monomer is involved in short contacts.

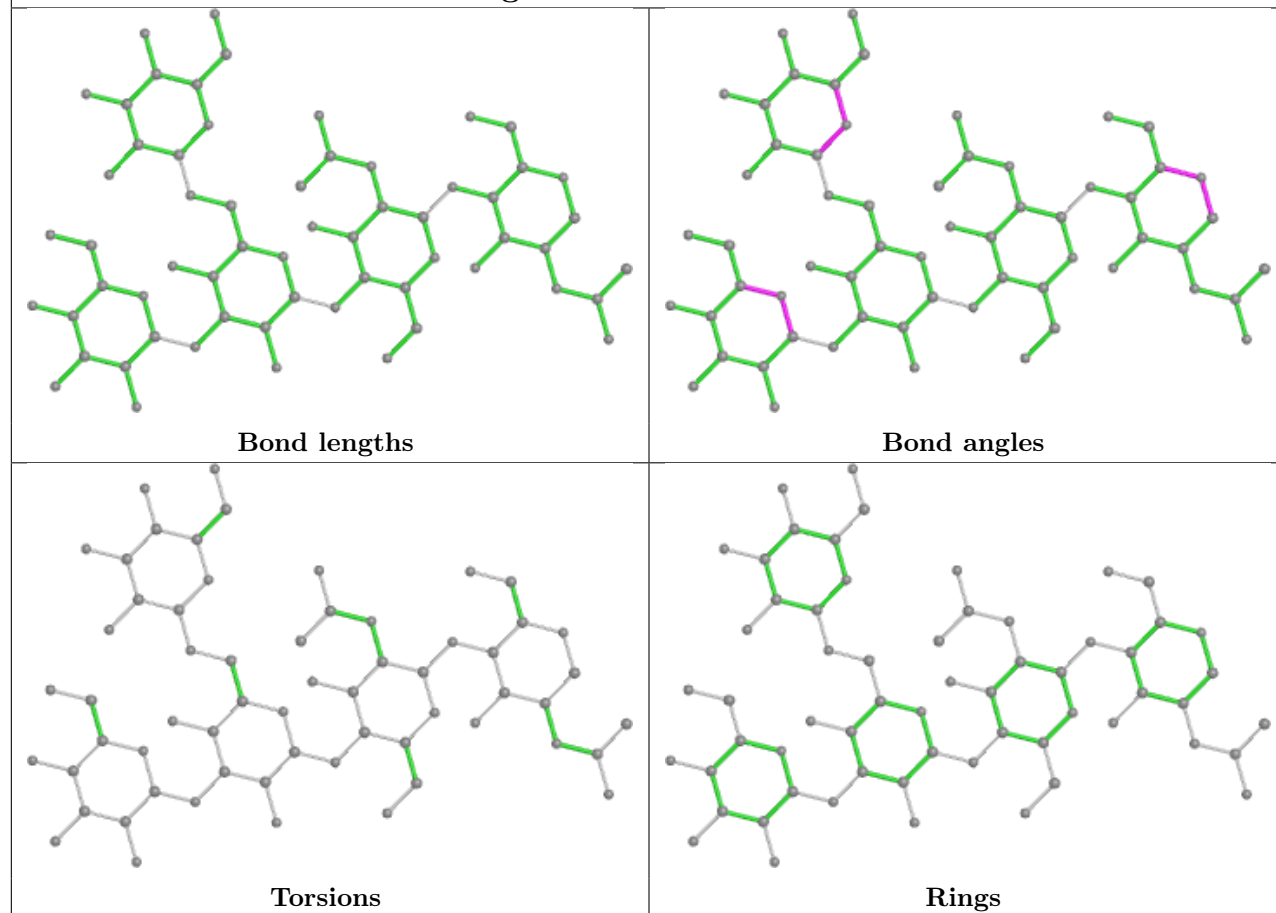
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



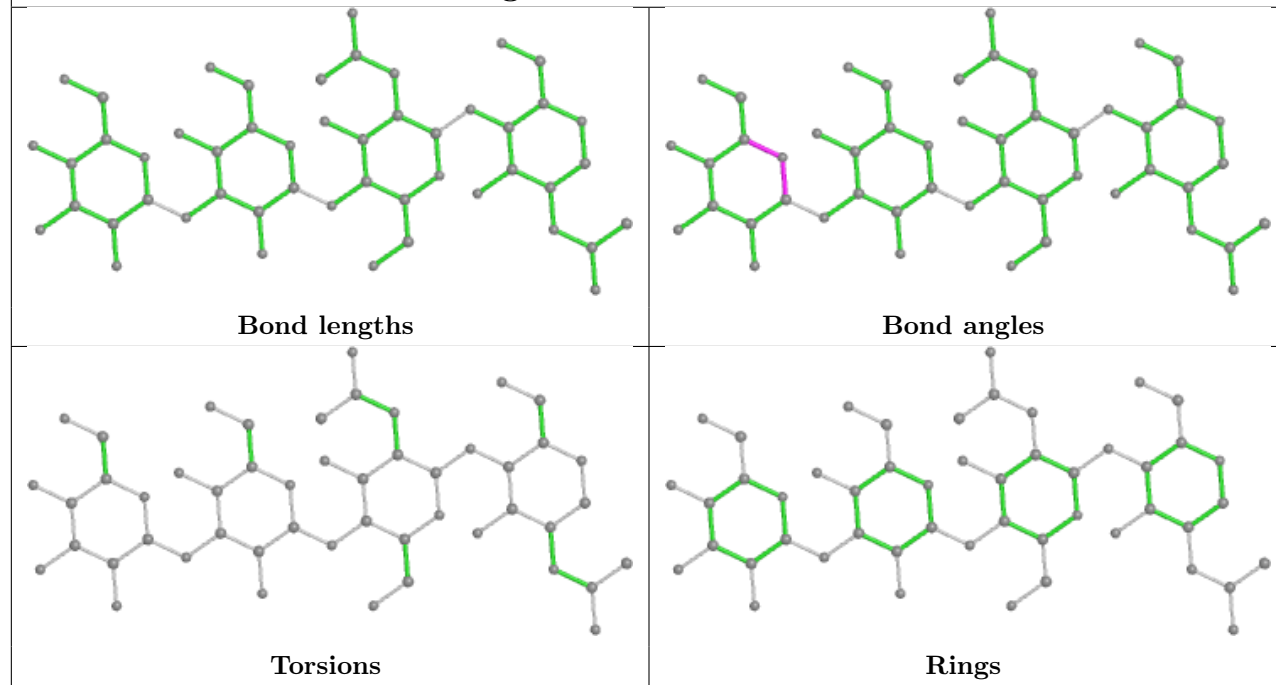




## Oligosaccharide Chain H



## Oligosaccharide Chain G



## 5.6 Ligand geometry

16 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	NAG	B	906	1	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
5	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	A	903	1	14,14,15	0.31	0	17,19,21	0.61	0
5	NAG	A	905	1	14,14,15	0.29	0	17,19,21	0.52	0
5	NAG	B	904	1	14,14,15	0.32	0	17,19,21	0.75	0
5	NAG	A	902	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	B	905	1	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	A	906	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	B	903	1	14,14,15	0.31	0	17,19,21	0.63	0
6	RQY	A	908	-	29,29,29	4.64	14 (48%)	33,42,42	1.44	7 (21%)
5	NAG	A	904	1	14,14,15	0.30	0	17,19,21	0.71	0
5	NAG	B	901	1	14,14,15	0.29	0	17,19,21	0.50	0
6	RQY	B	908	-	29,29,29	4.64	14 (48%)	33,42,42	1.30	5 (15%)
5	NAG	B	907	1	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
5	NAG	B	902	1	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
5	NAG	A	907	1	14,14,15	0.30	0	17,19,21	0.74	2 (11%)

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	NAG	B	906	1	-	0/6/23/26	0/1/1/1
5	NAG	A	901	1	-	1/6/23/26	0/1/1/1
5	NAG	A	903	1	-	0/6/23/26	0/1/1/1
5	NAG	A	905	1	-	0/6/23/26	0/1/1/1
5	NAG	B	904	1	-	0/6/23/26	0/1/1/1
5	NAG	A	902	1	-	0/6/23/26	0/1/1/1
5	NAG	B	905	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	906	1	-	1/6/23/26	0/1/1/1
5	NAG	B	903	1	-	0/6/23/26	0/1/1/1
6	RQY	A	908	-	-	3/12/20/20	0/4/4/4
5	NAG	A	904	1	-	0/6/23/26	0/1/1/1
5	NAG	B	901	1	-	1/6/23/26	0/1/1/1
6	RQY	B	908	-	-	2/12/20/20	0/4/4/4
5	NAG	B	907	1	-	0/6/23/26	0/1/1/1
5	NAG	B	902	1	-	0/6/23/26	0/1/1/1
5	NAG	A	907	1	-	0/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	908	RQY	C03-C04	9.21	1.57	1.41
6	B	908	RQY	C03-C04	9.21	1.57	1.41
6	A	908	RQY	C06-C05	8.53	1.59	1.42
6	B	908	RQY	C06-C05	8.41	1.58	1.42
6	B	908	RQY	C19-C20	7.69	1.53	1.38
6	A	908	RQY	C23-C22	7.64	1.53	1.38
6	A	908	RQY	C20-N21	7.58	1.49	1.34
6	B	908	RQY	C20-N21	7.47	1.49	1.34
6	B	908	RQY	C22-N21	7.47	1.49	1.34
6	B	908	RQY	C23-C22	7.46	1.53	1.38
6	A	908	RQY	C22-N21	7.46	1.49	1.34
6	A	908	RQY	C19-C20	7.27	1.52	1.38
6	A	908	RQY	C06-C01	6.98	1.51	1.37
6	B	908	RQY	C06-C01	6.90	1.51	1.37
6	B	908	RQY	C03-C02	6.86	1.51	1.36
6	A	908	RQY	C03-C02	6.78	1.50	1.36
6	A	908	RQY	C02-C01	6.46	1.49	1.39
6	B	908	RQY	C02-C01	6.41	1.49	1.39
6	A	908	RQY	C23-C18	5.91	1.50	1.39
6	A	908	RQY	C19-C18	5.90	1.50	1.39
6	B	908	RQY	C19-C18	5.84	1.49	1.39
6	B	908	RQY	C23-C18	5.75	1.49	1.39
6	B	908	RQY	C18-C08	3.71	1.53	1.49
6	A	908	RQY	C01-C10	3.59	1.59	1.52
6	B	908	RQY	C01-C10	3.58	1.59	1.52
6	A	908	RQY	C18-C08	3.55	1.53	1.49
6	B	908	RQY	C09-C05	-2.28	1.38	1.40
6	A	908	RQY	C09-C05	-2.15	1.38	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	908	RQY	C17-C10-C13	2.85	115.51	109.56
6	A	908	RQY	C26-C20-N21	2.75	120.95	116.56
6	B	908	RQY	C25-C22-N21	2.55	120.62	116.56
5	B	906	NAG	C1-O5-C5	2.53	115.63	112.19
6	A	908	RQY	C01-C06-C05	-2.44	120.38	122.00
6	A	908	RQY	C24-C11-C09	-2.43	107.47	112.94
6	B	908	RQY	C26-C20-N21	2.32	120.26	116.56
6	B	908	RQY	C08-C09-C11	-2.32	124.95	129.63
5	B	902	NAG	O5-C1-C2	-2.31	107.63	111.29
6	A	908	RQY	C08-C09-C11	-2.30	124.98	129.63
6	B	908	RQY	C17-C10-C13	2.19	114.13	109.56
6	A	908	RQY	C08-N07-C04	2.19	108.41	103.90
6	A	908	RQY	C25-C22-N21	2.16	120.00	116.56
5	B	907	NAG	C1-O5-C5	2.05	114.98	112.19
6	B	908	RQY	C08-N07-C04	2.05	108.12	103.90
5	A	907	NAG	C1-O5-C5	2.02	114.92	112.19
5	A	907	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	908	RQY	N07-C08-C18-C19
6	B	908	RQY	N07-C08-C18-C19
6	A	908	RQY	N07-C08-C18-C23
6	B	908	RQY	N07-C08-C18-C23
5	B	901	NAG	O5-C5-C6-O6
5	A	901	NAG	O5-C5-C6-O6
5	A	906	NAG	O5-C5-C6-O6
6	A	908	RQY	C08-C09-C11-C12

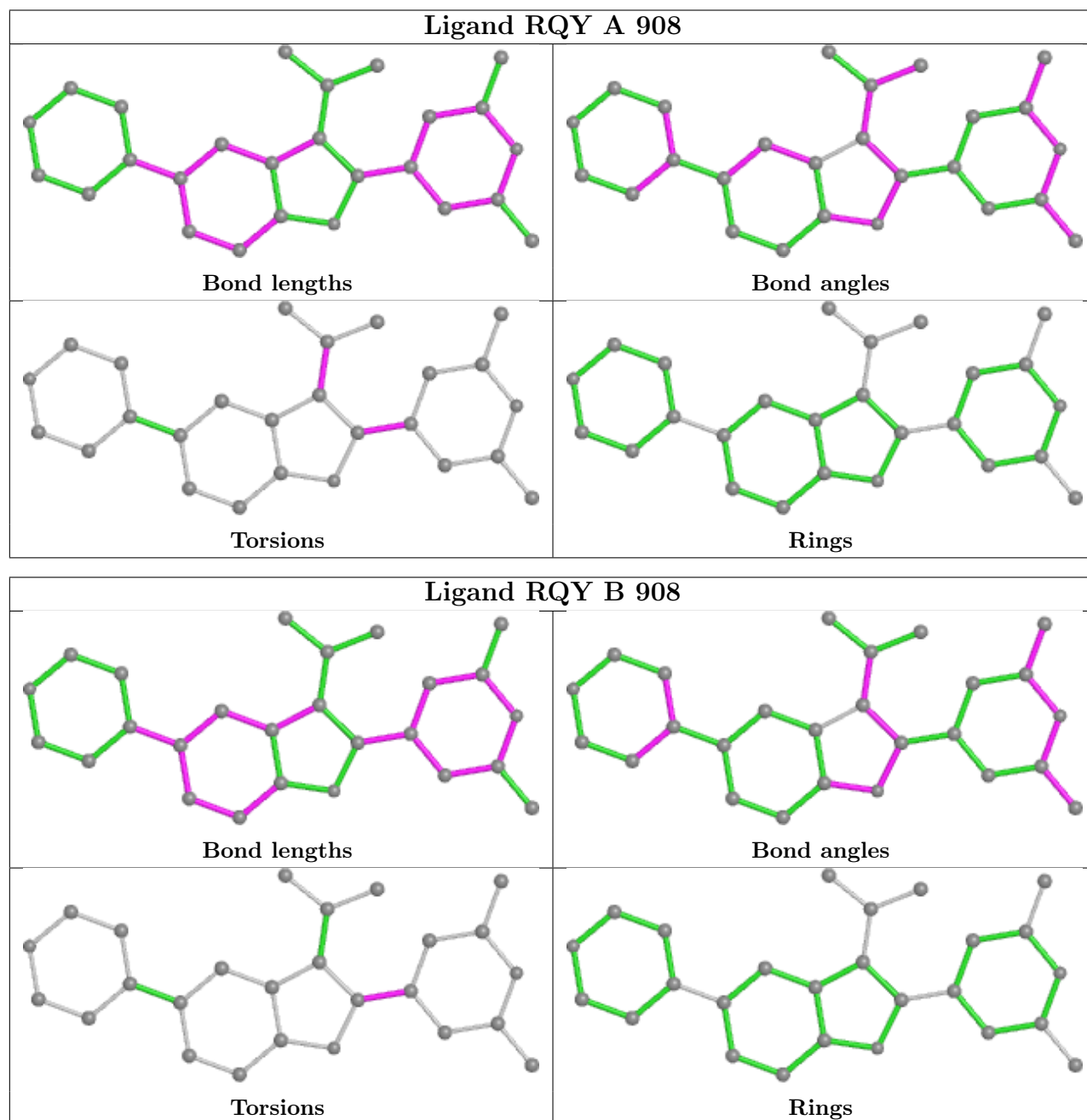
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	908	RQY	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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

### 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	737/811 (90%)	0.24	26 (3%) 44 52	45, 78, 122, 165	0
1	B	737/811 (90%)	0.68	90 (12%) 4 4	53, 101, 149, 182	0
All	All	1474/1622 (90%)	0.46	116 (7%) 12 15	45, 87, 140, 182	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	9.1
1	B	603	TYR	8.2
1	B	236	TYR	6.3
1	B	89	LEU	6.1
1	B	121	PHE	5.7
1	B	702	PHE	5.6
1	B	92	ILE	5.4
1	B	604	ASN	5.3
1	B	678	PHE	5.3
1	B	45	VAL	5.2
1	B	203	LEU	5.0
1	B	96	HIS	5.0
1	A	755	ALA	4.9
1	B	127	LEU	4.7
1	B	679	PHE	4.6
1	B	83	PHE	4.4
1	A	786	TRP	4.2
1	B	68	LEU	4.2
1	B	200	LEU	4.1
1	B	124	LEU	4.0
1	B	78	ILE	3.9
1	A	783	PHE	3.9
1	B	61	VAL	3.9
1	B	130	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	46	ILE	3.8
1	B	751	ILE	3.8
1	B	86	LEU	3.8
1	B	74	PHE	3.7
1	B	333	LEU	3.7
1	B	187	CYS	3.6
1	B	46	ILE	3.6
1	B	199	THR	3.6
1	A	33	SER	3.6
1	B	67	GLU	3.5
1	B	76	THR	3.5
1	B	144	LEU	3.4
1	A	305	ALA	3.4
1	B	756	LEU	3.4
1	B	808	ASP	3.4
1	A	236	TYR	3.3
1	A	817	LEU	3.2
1	A	74	PHE	3.2
1	B	470	PHE	3.2
1	B	151	LEU	3.2
1	B	75	ILE	3.1
1	B	192	ILE	3.1
1	B	363	PHE	3.1
1	B	161	ILE	3.1
1	B	113	GLY	3.0
1	A	64	TYR	3.0
1	B	54	LEU	3.0
1	B	197	PHE	3.0
1	B	166	ILE	2.9
1	B	128	ARG	2.9
1	B	148	LEU	2.9
1	B	164	GLU	2.9
1	B	64	TYR	2.9
1	B	783	PHE	2.8
1	B	283	PHE	2.8
1	B	815	VAL	2.8
1	A	94	LEU	2.8
1	B	780	ILE	2.8
1	B	785	ARG	2.8
1	A	83	PHE	2.7
1	B	99	ASN	2.7
1	A	606	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	701	LEU	2.7
1	A	72	ASP	2.6
1	B	162	THR	2.6
1	B	114	LEU	2.6
1	B	132	LEU	2.6
1	B	116	ILE	2.6
1	A	790	HIS	2.5
1	B	153	LEU	2.5
1	A	678	PHE	2.5
1	B	39	LYS	2.5
1	A	88	ASN	2.5
1	B	307	PHE	2.4
1	B	177	LEU	2.4
1	A	237	ILE	2.4
1	A	809	GLN	2.3
1	B	396	LEU	2.3
1	B	809	GLN	2.3
1	A	54	LEU	2.3
1	B	788	ASP	2.3
1	A	281	PHE	2.3
1	B	731	PHE	2.3
1	B	330	GLY	2.3
1	B	366	LEU	2.3
1	A	735	VAL	2.3
1	B	781	GLY	2.2
1	B	82	SER	2.2
1	B	704	THR	2.2
1	B	717	LEU	2.2
1	B	675	MET	2.2
1	B	223	SER	2.2
1	B	817	LEU	2.2
1	B	733	SER	2.2
1	B	367	LEU	2.2
1	B	242	PHE	2.2
1	A	604	ASN	2.2
1	B	605	LEU	2.1
1	B	62	GLY	2.1
1	B	762	THR	2.1
1	B	387	PHE	2.1
1	B	94	LEU	2.1
1	A	762	THR	2.1
1	B	66	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	603	TYR	2.1
1	B	146	GLU	2.1
1	B	237	ILE	2.1
1	B	392	GLN	2.1
1	B	224	LEU	2.0
1	B	795	ILE	2.0
1	A	808	ASP	2.0
1	B	281	PHE	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.

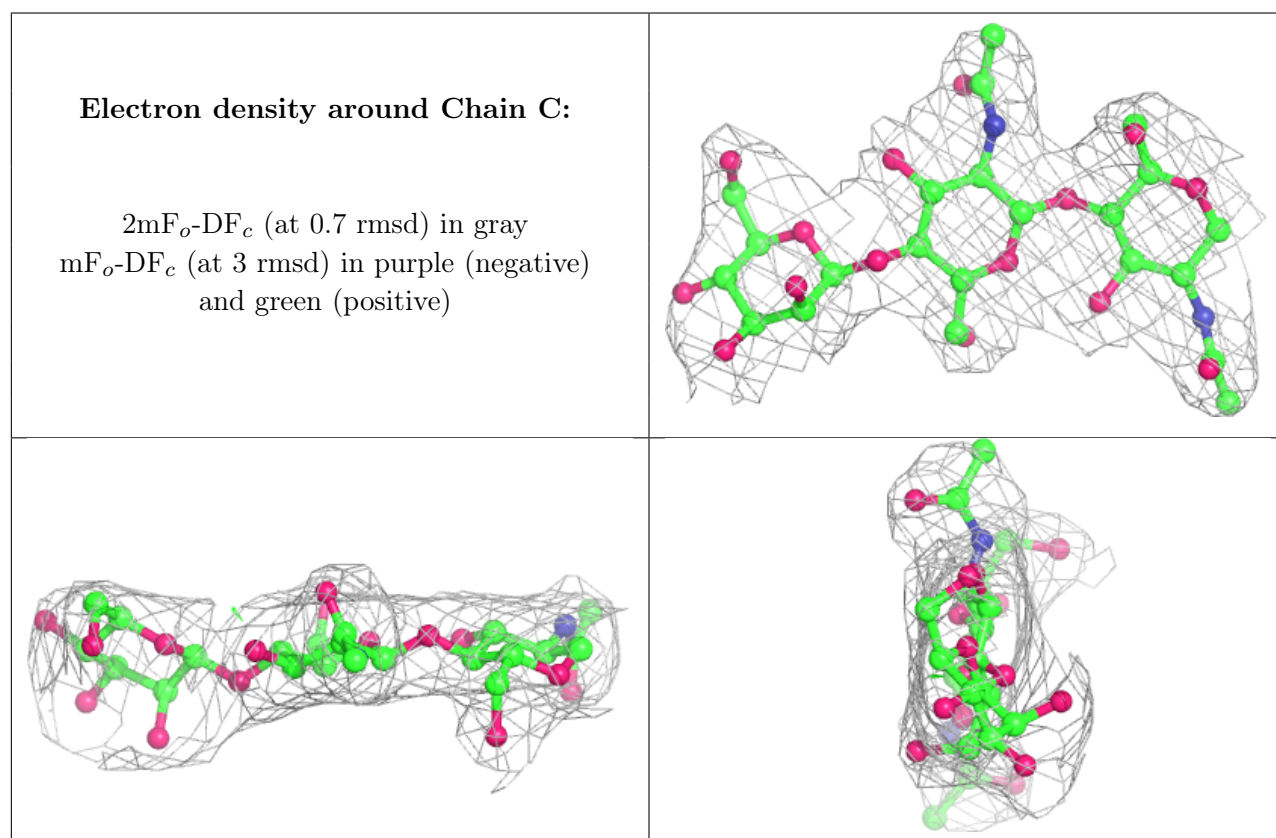
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	G	4	11/12	0.67	0.31	119,123,124,126	0
3	MAN	F	5	11/12	0.69	0.20	123,126,132,133	0
3	MAN	F	4	11/12	0.70	0.16	115,118,121,122	0
4	BMA	G	3	11/12	0.72	0.24	102,106,110,115	0
2	BMA	D	3	11/12	0.77	0.33	92,95,97,97	0
3	BMA	F	3	11/12	0.79	0.15	110,116,122,123	0
3	MAN	E	5	11/12	0.81	0.15	98,100,104,106	0
4	NAG	G	2	14/15	0.81	0.16	81,85,90,97	0
3	MAN	H	5	11/12	0.85	0.24	117,120,123,125	0
3	BMA	H	3	11/12	0.85	0.22	97,105,109,113	0
3	MAN	E	4	11/12	0.86	0.12	92,97,98,100	0
3	MAN	H	4	11/12	0.89	0.24	109,112,117,119	0
3	BMA	E	3	11/12	0.90	0.14	81,88,92,95	0
2	NAG	D	2	14/15	0.90	0.21	73,79,84,87	0
2	BMA	C	3	11/12	0.90	0.16	78,80,84,85	0
4	NAG	G	1	14/15	0.92	0.17	63,67,69,74	0
3	NAG	H	1	14/15	0.93	0.16	64,67,73,74	0
3	NAG	F	2	14/15	0.94	0.19	93,97,100,103	0
3	NAG	H	2	14/15	0.95	0.19	73,78,84,90	0
2	NAG	D	1	14/15	0.96	0.16	52,55,59,66	0

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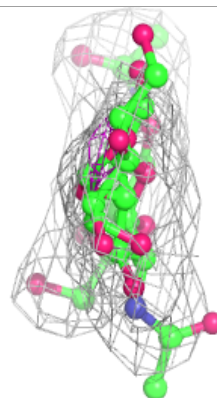
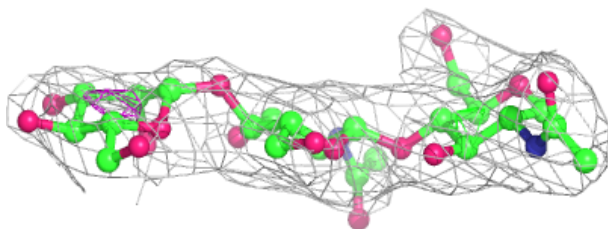
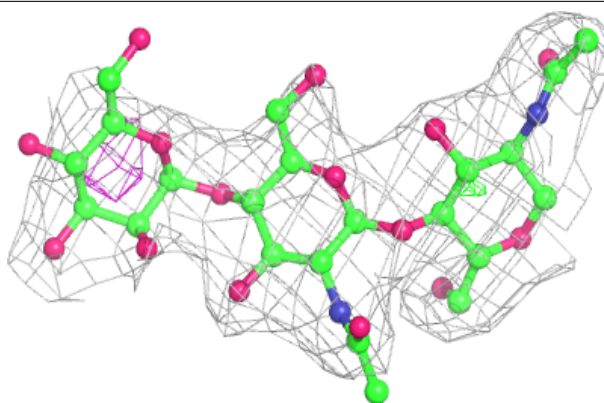
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	2	14/15	0.96	0.14	60,66,69,75	0
2	NAG	C	2	14/15	0.96	0.19	63,67,69,73	0
3	NAG	E	1	14/15	0.97	0.15	49,53,57,58	0
3	NAG	F	1	14/15	0.97	0.22	81,85,91,91	0
2	NAG	C	1	14/15	0.97	0.20	51,56,59,60	0

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.

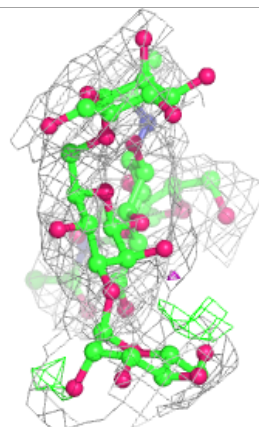
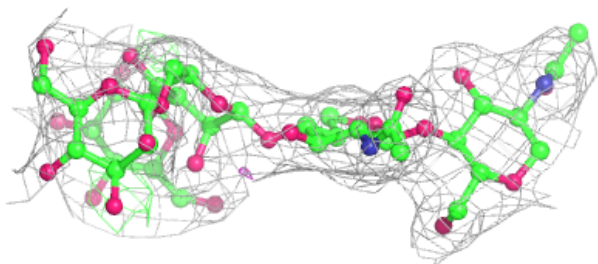
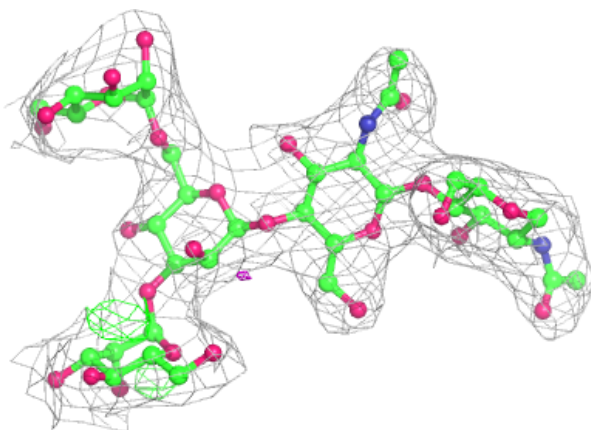


**Electron density around Chain D:**

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

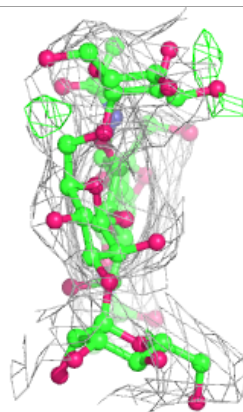
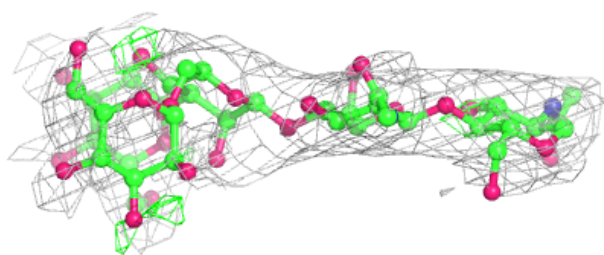
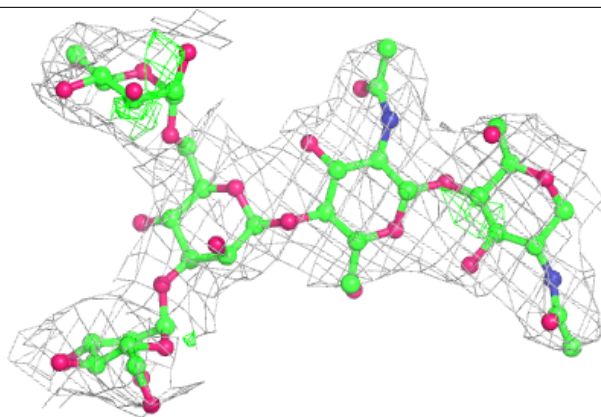
**Electron density around Chain E:**

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

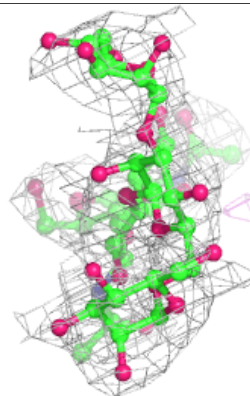
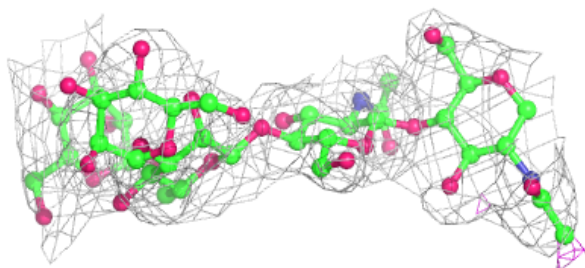
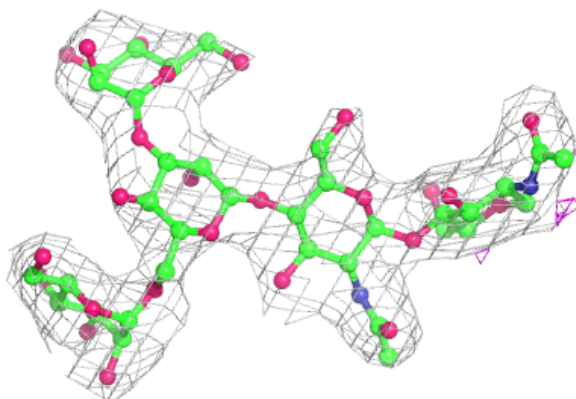


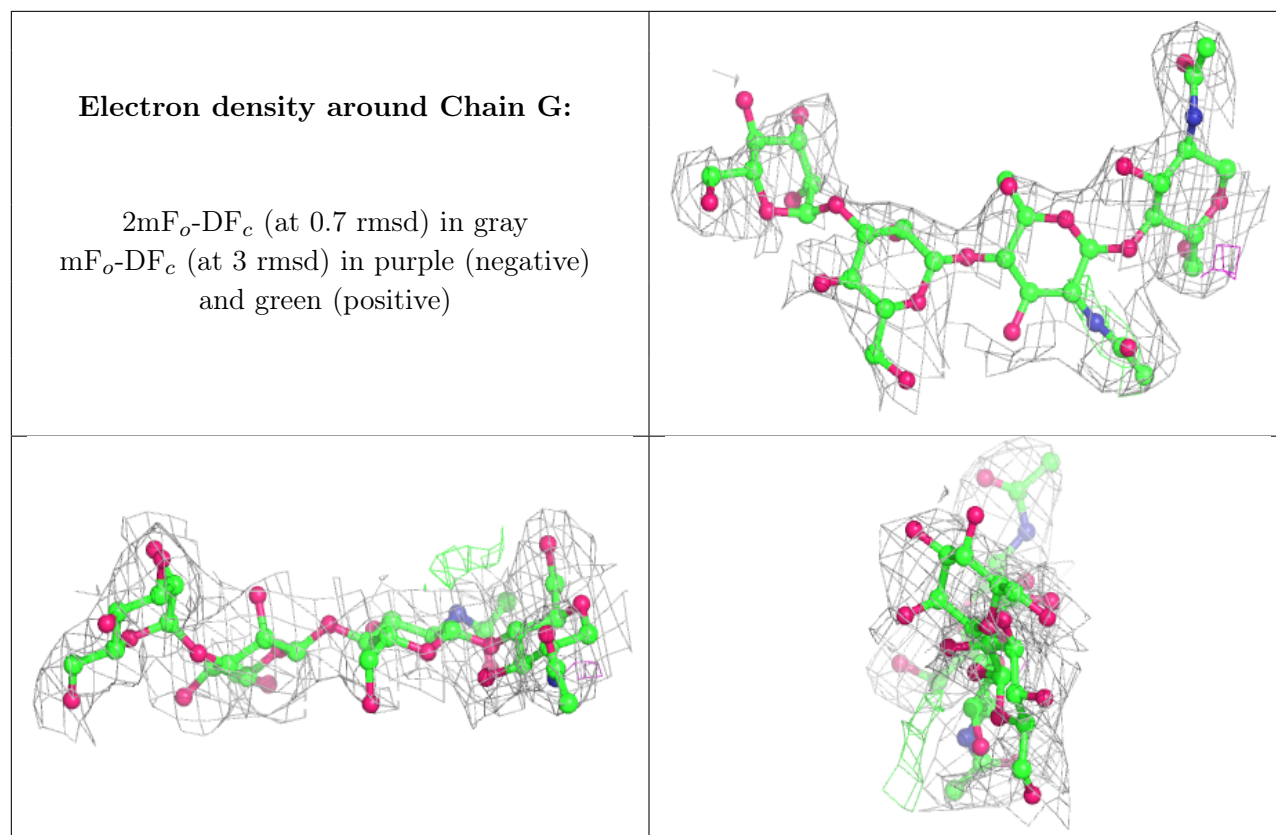
**Electron density around Chain F:**

$2mF_o-DF_c$  (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.

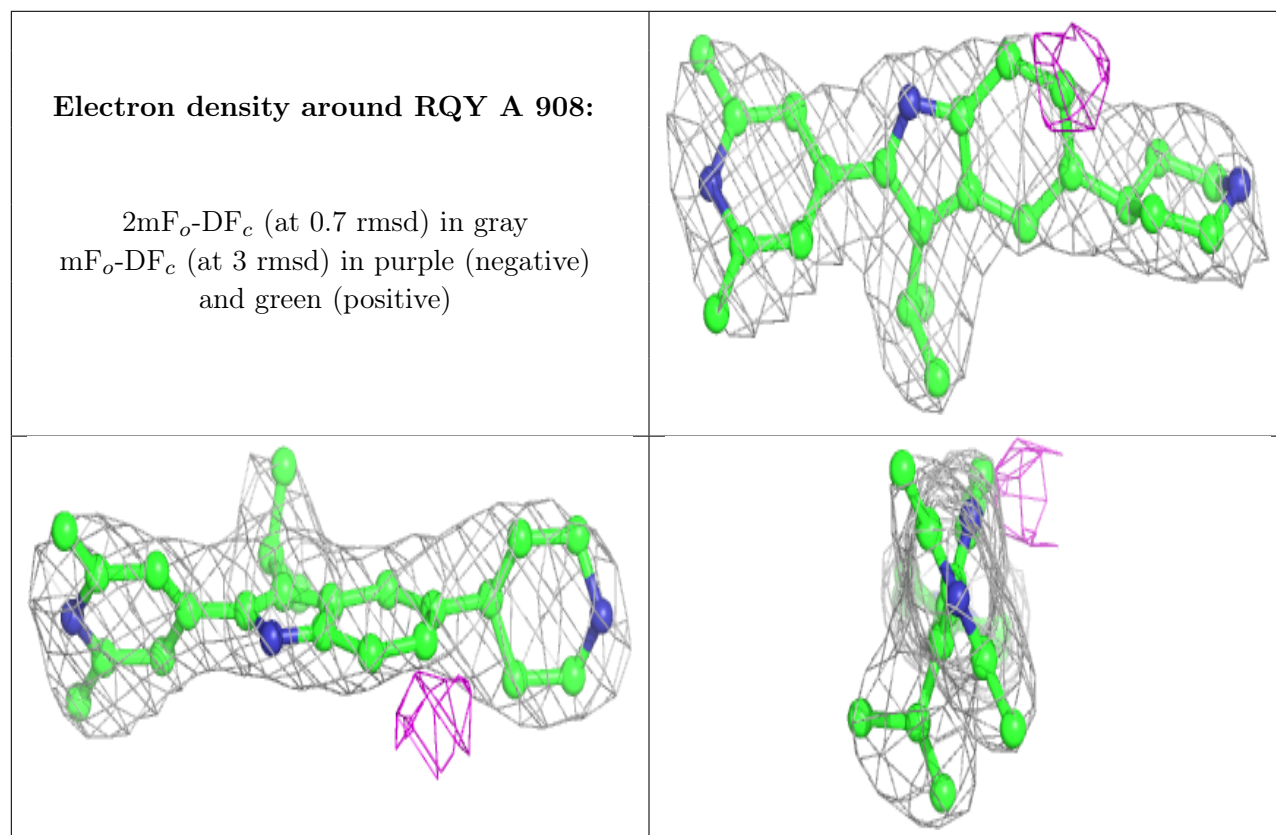
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	904	14/15	0.42	0.47	147,152,158,158	0
5	NAG	B	901	14/15	0.63	0.42	181,186,196,197	0
5	NAG	A	903	14/15	0.63	0.52	120,124,128,129	0
5	NAG	B	907	14/15	0.63	0.30	141,144,149,152	0
5	NAG	A	904	14/15	0.68	0.36	126,132,139,141	0
5	NAG	B	903	14/15	0.68	0.40	142,148,154,158	0
5	NAG	B	906	14/15	0.71	0.30	132,137,141,142	0
5	NAG	B	902	14/15	0.72	0.35	159,164,170,174	0
5	NAG	B	905	14/15	0.77	0.28	99,102,106,109	0
5	NAG	A	905	14/15	0.79	0.32	112,113,121,121	0
5	NAG	A	906	14/15	0.82	0.27	103,119,127,132	0
5	NAG	A	901	14/15	0.83	0.15	125,129,138,139	0
5	NAG	A	902	14/15	0.84	0.26	120,123,129,130	0
5	NAG	A	907	14/15	0.90	0.16	101,107,112,115	0

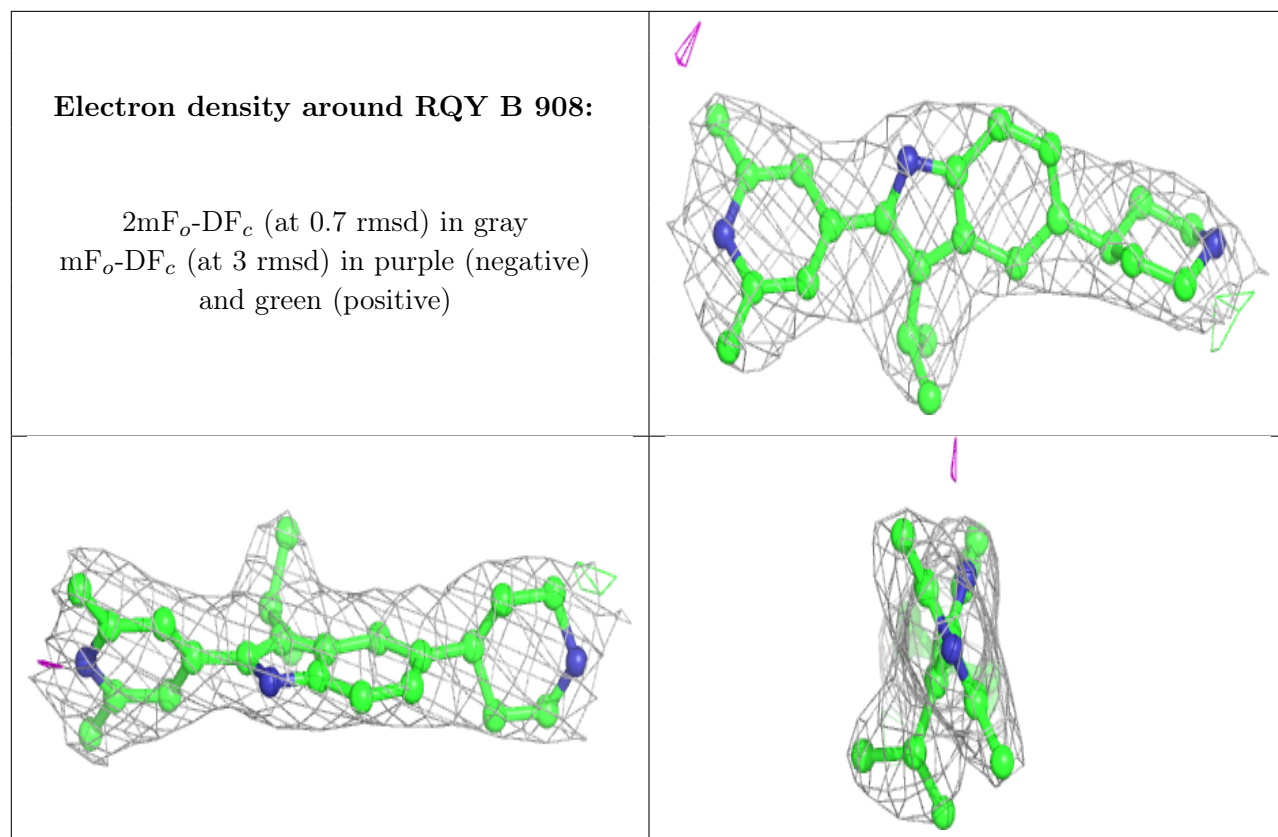
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	RQY	A	908	26/26	0.94	0.22	46,50,55,56	0
6	RQY	B	908	26/26	0.95	0.22	43,51,58,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.