



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:34 AM BST

PDB ID : 4PE5  
Title : Crystal Structure of GluN1a/GluN2B NMDA Receptor Ion Channel  
Authors : Karakas, E.; Furukawa, H.  
Deposited on : 2014-04-22  
Resolution : 3.96 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)

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  
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) : 2.13.1

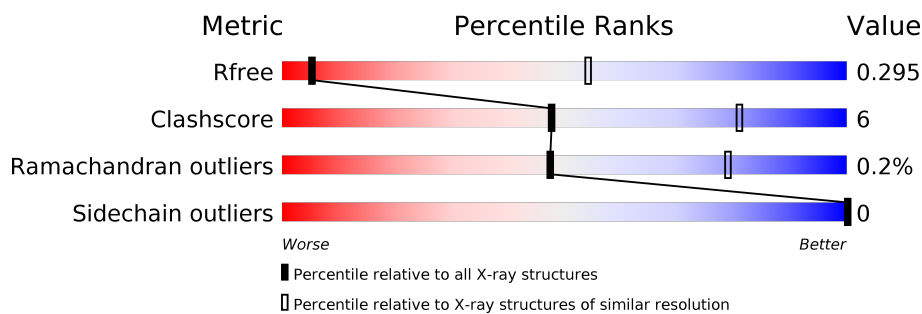
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.96 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.




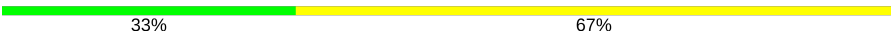

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	825	79% 11% 10%
1	C	825	82% 10% 9%
2	B	820	78% 10% 12%
2	D	820	79% 10% 11%
3	E	4	75% 25%
3	I	4	25% 75%
3	J	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	F	6	 17%83%
5	G	6	 33%67%
6	H	2	 50%50%

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	MAN	G	5	-	-	X	-
5	MAN	G	6	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20246 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5049	3173	884	967	25			
1	C	754	Total	C	N	O	S	0	0	0
			5026	3175	874	954	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP P35439
A	239	ASP	ASN	engineered mutation	UNP P35439
A	350	GLN	ASN	engineered mutation	UNP P35439
A	471	GLN	ASN	engineered mutation	UNP P35439
A	491	GLN	ASN	engineered mutation	UNP P35439
A	561	CYS	THR	engineered mutation	UNP P35439
A	594	GLN	GLU	engineered mutation	UNP P35439
A	595	SER	GLU	engineered mutation	UNP P35439
A	597	SER	GLU	engineered mutation	UNP P35439
A	598	THR	GLU	engineered mutation	UNP P35439
A	771	GLN	ASN	engineered mutation	UNP P35439
A	810	CYS	PHE	engineered mutation	UNP P35439
A	844	ASN	ARG	engineered mutation	UNP P35439
A	845	GLY	ARG	engineered mutation	UNP P35439
A	846	ALA	LYS	engineered mutation	UNP P35439
C	61	GLN	ASN	engineered mutation	UNP P35439
C	239	ASP	ASN	engineered mutation	UNP P35439
C	350	GLN	ASN	engineered mutation	UNP P35439
C	471	GLN	ASN	engineered mutation	UNP P35439
C	491	GLN	ASN	engineered mutation	UNP P35439
C	561	CYS	THR	engineered mutation	UNP P35439
C	594	GLN	GLU	engineered mutation	UNP P35439
C	595	SER	GLU	engineered mutation	UNP P35439
C	597	SER	GLU	engineered mutation	UNP P35439
C	598	THR	GLU	engineered mutation	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	GLN	ASN	engineered mutation	UNP P35439
C	810	CYS	PHE	engineered mutation	UNP P35439
C	844	ASN	ARG	engineered mutation	UNP P35439
C	845	GLY	ARG	engineered mutation	UNP P35439
C	846	ALA	LYS	engineered mutation	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	720	Total	C	N	O	S	0	0	0
			4798	3048	788	933	29			
2	D	727	Total	C	N	O	S	0	0	0
			4777	3027	809	912	29			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	214	CYS	SER	engineered mutation	UNP Q00960
B	348	ASP	ASN	engineered mutation	UNP Q00960
B	?	-	CYS	deletion	UNP Q00960
B	?	-	PRO	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	557	CYS	ASP	engineered mutation	UNP Q00960
B	588	SER	CYS	engineered mutation	UNP Q00960
B	815	CYS	ILE	engineered mutation	UNP Q00960
B	838	SER	CYS	engineered mutation	UNP Q00960
B	849	SER	CYS	engineered mutation	UNP Q00960
D	214	CYS	SER	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960
D	?	-	CYS	deletion	UNP Q00960
D	?	-	PRO	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	557	CYS	ASP	engineered mutation	UNP Q00960
D	588	SER	CYS	engineered mutation	UNP Q00960
D	815	CYS	ILE	engineered mutation	UNP Q00960
D	838	SER	CYS	engineered mutation	UNP Q00960

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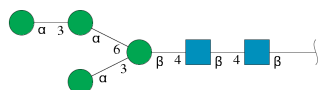
Chain	Residue	Modelled	Actual	Comment	Reference
D	849	SER	CYS	engineered mutation	UNP Q00960

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

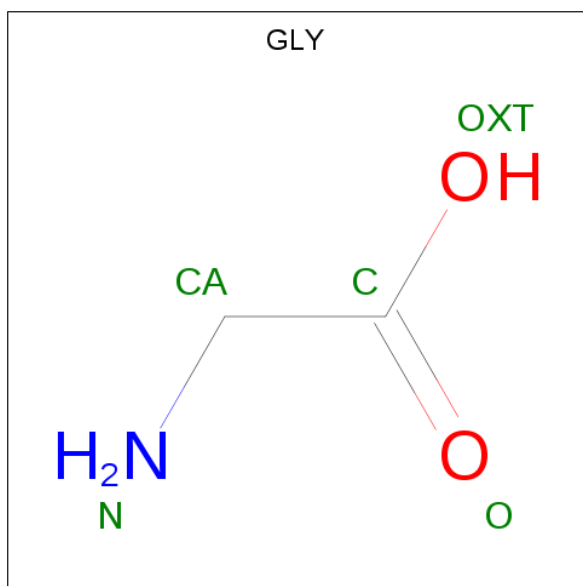


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is TUNGSTEN ION (three-letter code: W) (formula: W).

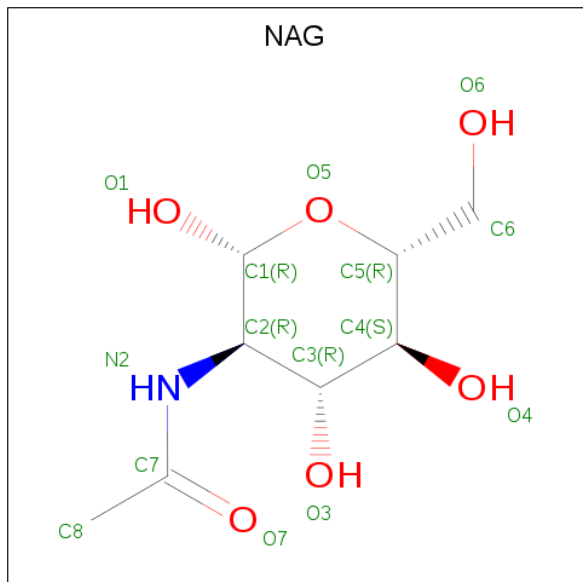
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total	W	0	0
			11	11		
7	A	37	Total	W	0	0
			37	37		
7	C	36	Total	W	0	0
			36	36		

- Molecule 8 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			5	2	1	2		
8	C	1	Total	C	N	O	0	0
			5	2	1	2		

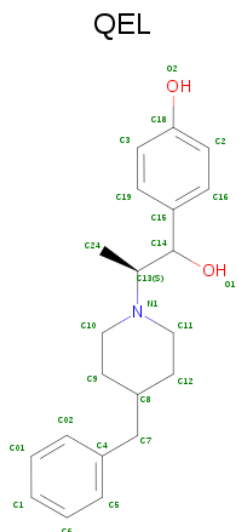
- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

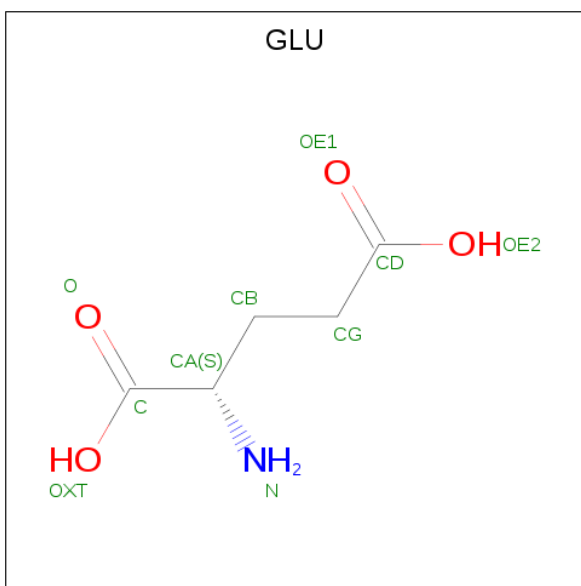
- Molecule 10 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (three-letter code: QEL) (formula:  $C_{21}H_{27}NO_2$ ).





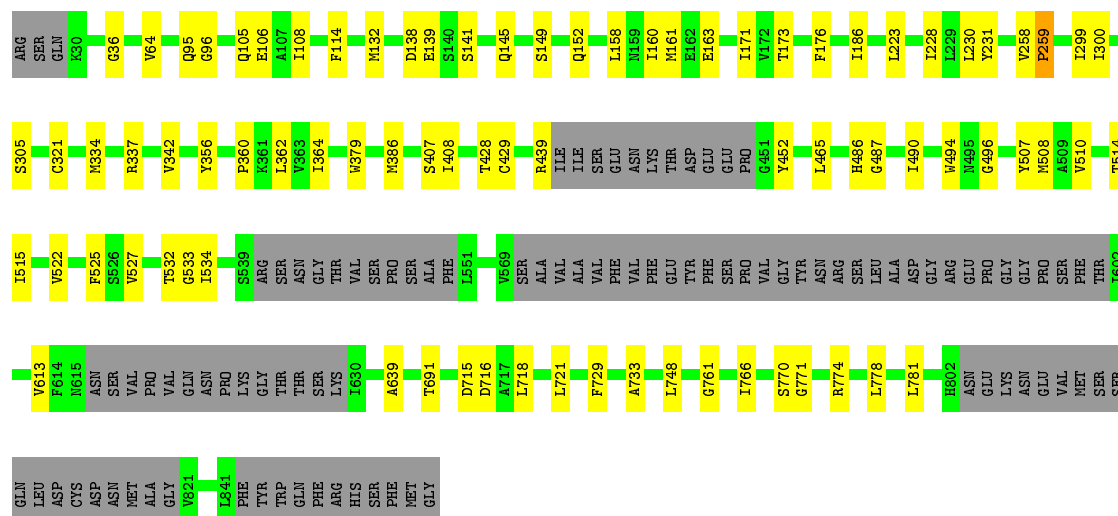
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total 24	C 21	N 1	O 2	0	0
10	C	1	Total 24	C 21	N 1	O 2	0	0

- Molecule 11 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $\text{C}_5\text{H}_9\text{NO}_4$ ).

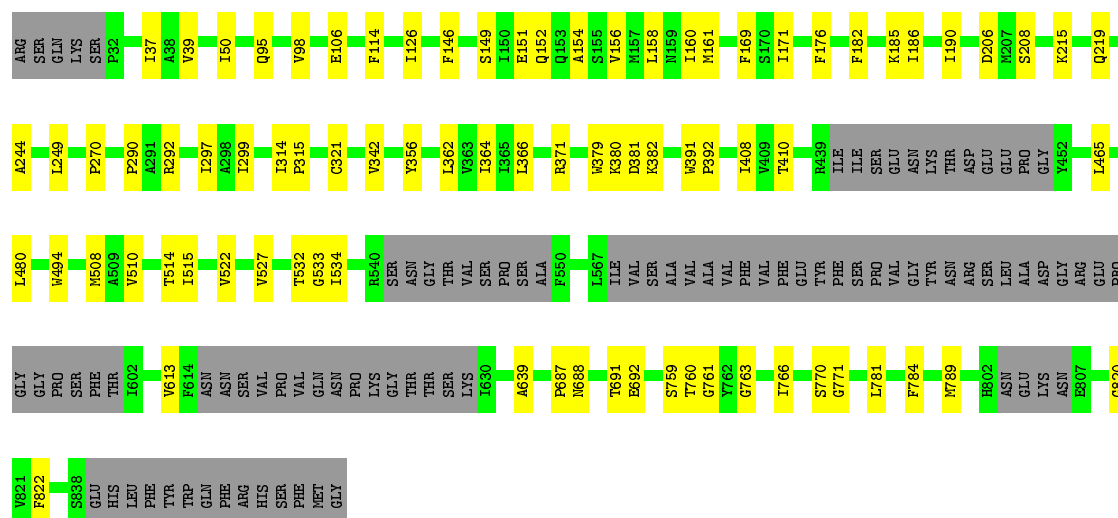
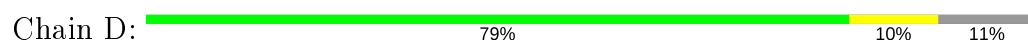


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total 10	C 5	N 1	O 4	0	0
11	D	1	Total 10	C 5	N 1	O 4	0	0





- Molecule 2: Glutamate receptor ionotropic, NMDA 2B



- Molecule 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



- Molecule 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



- Molecule 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 J:  75% 25%



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 F:  17% 83%



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.83Å 163.19Å 163.14Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	29.72 – 3.96 47.55 – 3.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.72-3.96) 98.2 (47.55-3.96)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.256 , 0.295 0.260 , 0.295	Depositor DCC
$R_{free}$ test set	2627 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	196.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 268.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	20246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: QEL, BMA, NAG, W, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.22	0/5138	0.42	0/7050
1	C	0.21	0/5118	0.41	0/7035
2	B	0.20	0/4884	0.35	0/6718
2	D	0.21	0/4862	0.40	0/6682
All	All	0.21	0/20002	0.40	0/27485

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5049	0	4271	55	0
1	C	5026	0	4204	49	0
2	B	4798	0	3981	51	0
2	D	4777	0	3881	56	0
3	E	50	0	43	1	0
3	I	50	0	43	4	0
3	J	50	0	43	1	0
4	F	72	0	61	0	0
5	G	72	0	61	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	28	0	25	2	0
7	A	37	0	0	0	0
7	B	11	0	0	0	0
7	C	36	0	0	0	0
8	A	5	0	2	2	0
8	C	5	0	2	0	0
9	A	42	0	39	0	0
9	B	28	0	26	0	0
9	C	14	0	13	0	0
9	D	28	0	26	0	0
10	B	24	0	26	6	0
10	C	24	0	26	6	0
11	B	10	0	5	2	0
11	D	10	0	5	1	0
All	All	20246	0	16783	224	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 6.

The worst 5 of 224 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)
5:G:5:MAN:H61	5:G:6:MAN:H3	1.37	1.00
2:D:514:THR:HG1	11:D:907:GLU:N	1.69	0.90
5:G:5:MAN:H61	5:G:6:MAN:C3	2.00	0.86
2:B:114:PHE:CB	10:B:920:QEL:H6	2.10	0.80
3:I:2:NAG:C3	3:I:3:BMA:H2	2.16	0.75

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	727/825 (88%)	667 (92%)	59 (8%)	1 (0%)	51	83
1	C	742/825 (90%)	681 (92%)	58 (8%)	3 (0%)	34	70
2	B	708/820 (86%)	656 (93%)	50 (7%)	2 (0%)	41	74
2	D	715/820 (87%)	656 (92%)	58 (8%)	1 (0%)	51	83
All	All	2892/3290 (88%)	2660 (92%)	225 (8%)	7 (0%)	47	79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	547	PRO
2	B	490	ILE
2	D	381	ASP
2	B	259	PRO
1	C	516	PRO

### 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	422/710 (59%)	422 (100%)	0	100	100
1	C	402/710 (57%)	402 (100%)	0	100	100
2	B	394/716 (55%)	394 (100%)	0	100	100
2	D	368/716 (51%)	368 (100%)	0	100	100
All	All	1586/2852 (56%)	1586 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	355	ASN
2	D	486	HIS
2	D	180	GLN

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Mol	Chain	Res	Type
1	A	355	ASN
2	D	311	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

26 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	E	1	1,3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.61	0
3	BMA	E	3	3	11,11,12	0.27	0	15,15,17	0.64	0
3	MAN	E	4	3	11,11,12	0.26	0	15,15,17	0.63	0
4	NAG	F	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.35	0
4	BMA	F	3	4	11,11,12	1.07	1 (9%)	15,15,17	2.04	4 (26%)
4	MAN	F	4	4	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
4	MAN	F	5	4	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
4	MAN	F	6	4	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
5	NAG	G	1	2,5	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.26	0	17,19,21	0.37	0
5	BMA	G	3	5	11,11,12	0.27	0	15,15,17	0.64	0
5	MAN	G	4	5	11,11,12	0.26	0	15,15,17	0.64	0
5	MAN	G	5	5	11,11,12	0.28	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	G	6	5	11,11,12	0.25	0	15,15,17	0.76	0
6	NAG	H	1	1,6	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
6	NAG	H	2	6	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	I	1	1,3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.92	0
3	BMA	I	3	3	11,11,12	0.27	0	15,15,17	0.82	0
3	MAN	I	4	3	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
3	NAG	J	1	3,2	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	0.62	0
3	BMA	J	3	3	11,11,12	0.27	0	15,15,17	0.64	0
3	MAN	J	4	3	11,11,12	0.26	0	15,15,17	0.64	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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
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
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C4-C5	2.37	1.58	1.53
4	F	1	NAG	C1-C2	2.09	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	O5-C5-C6	4.56	114.36	107.20
4	F	3	BMA	O2-C2-C1	3.08	115.46	109.15
6	H	1	NAG	C1-O5-C5	2.84	116.04	112.19
4	F	1	NAG	C1-O5-C5	2.79	115.97	112.19
4	F	3	BMA	O2-C2-C3	2.70	115.56	110.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	6	MAN	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 20 short contacts:

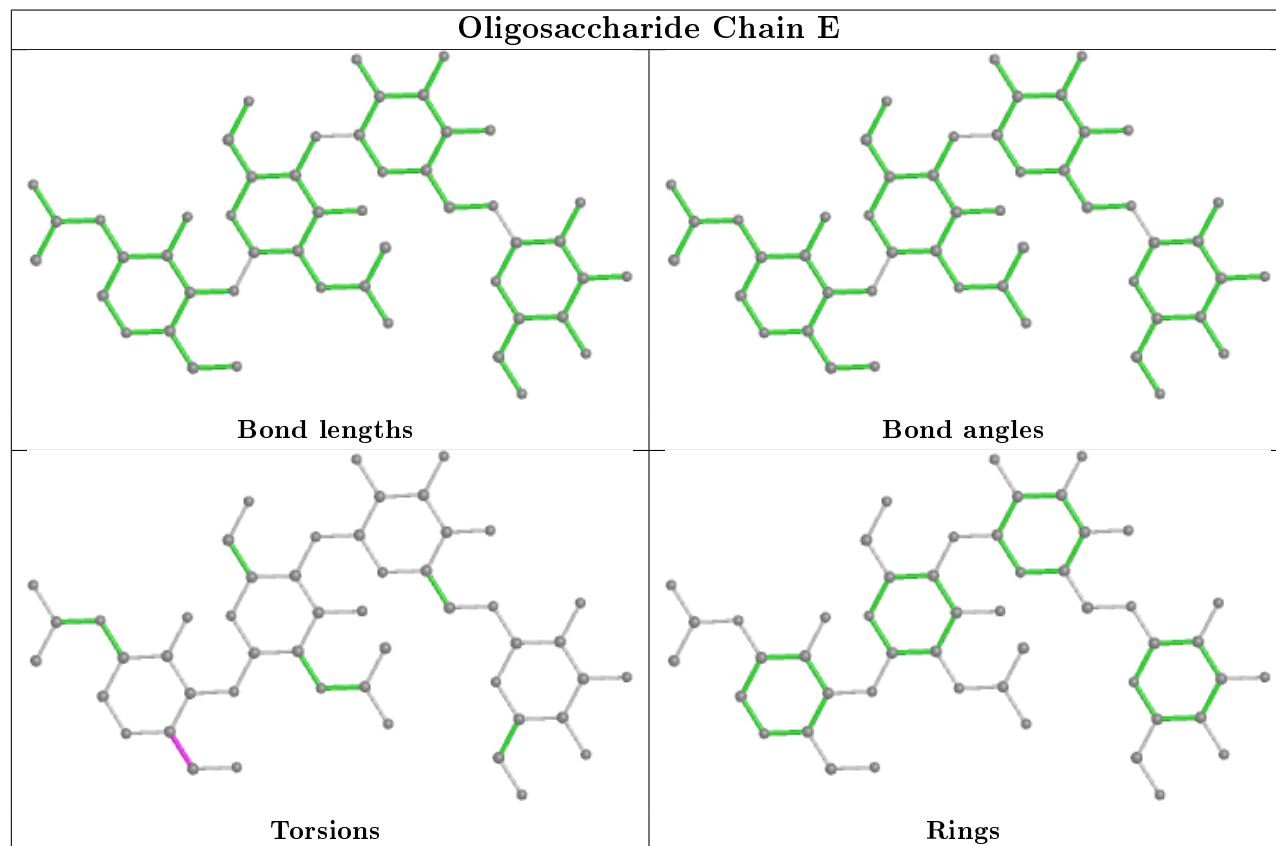
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	BMA	4	0
3	J	1	NAG	1	0
5	G	5	MAN	10	0
6	H	1	NAG	2	0
5	G	6	MAN	10	0
5	G	4	MAN	2	0
5	G	3	BMA	2	0

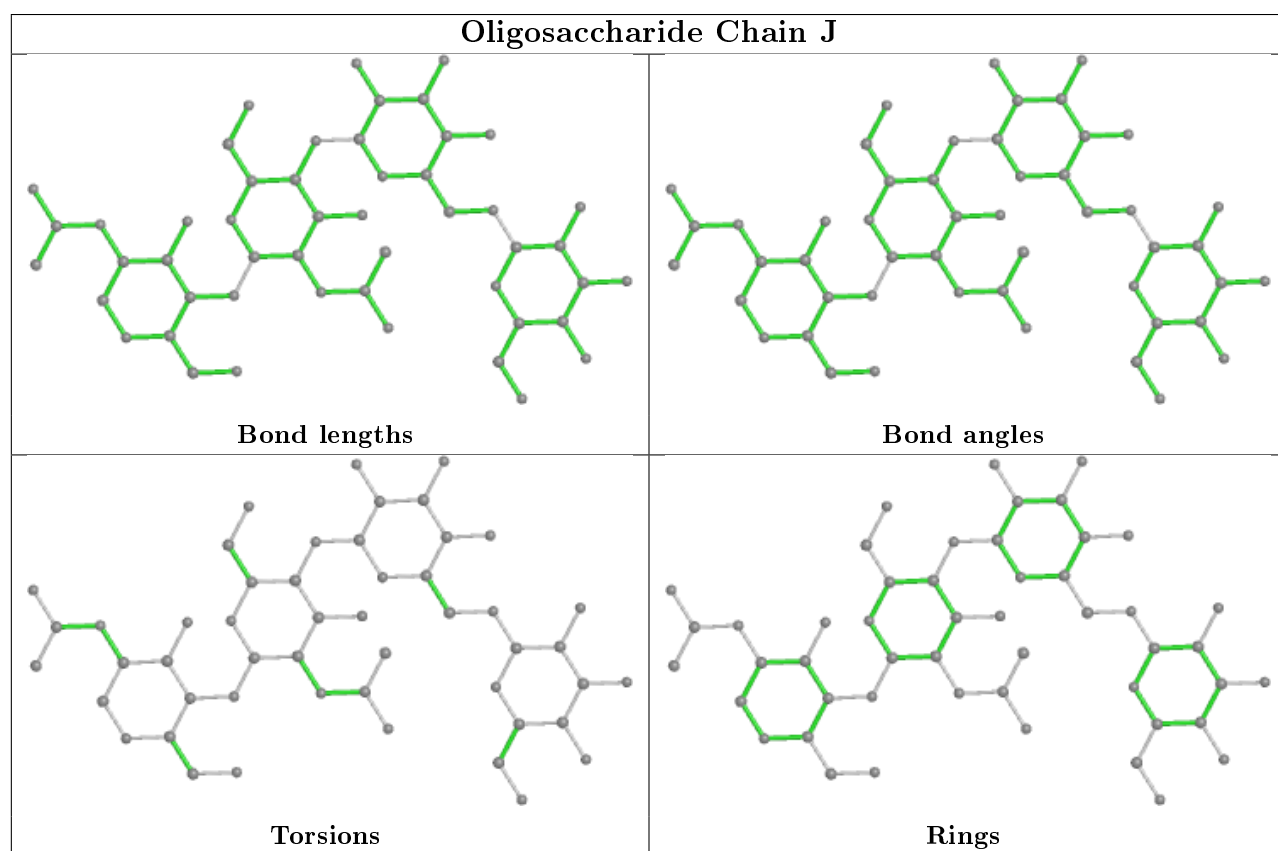
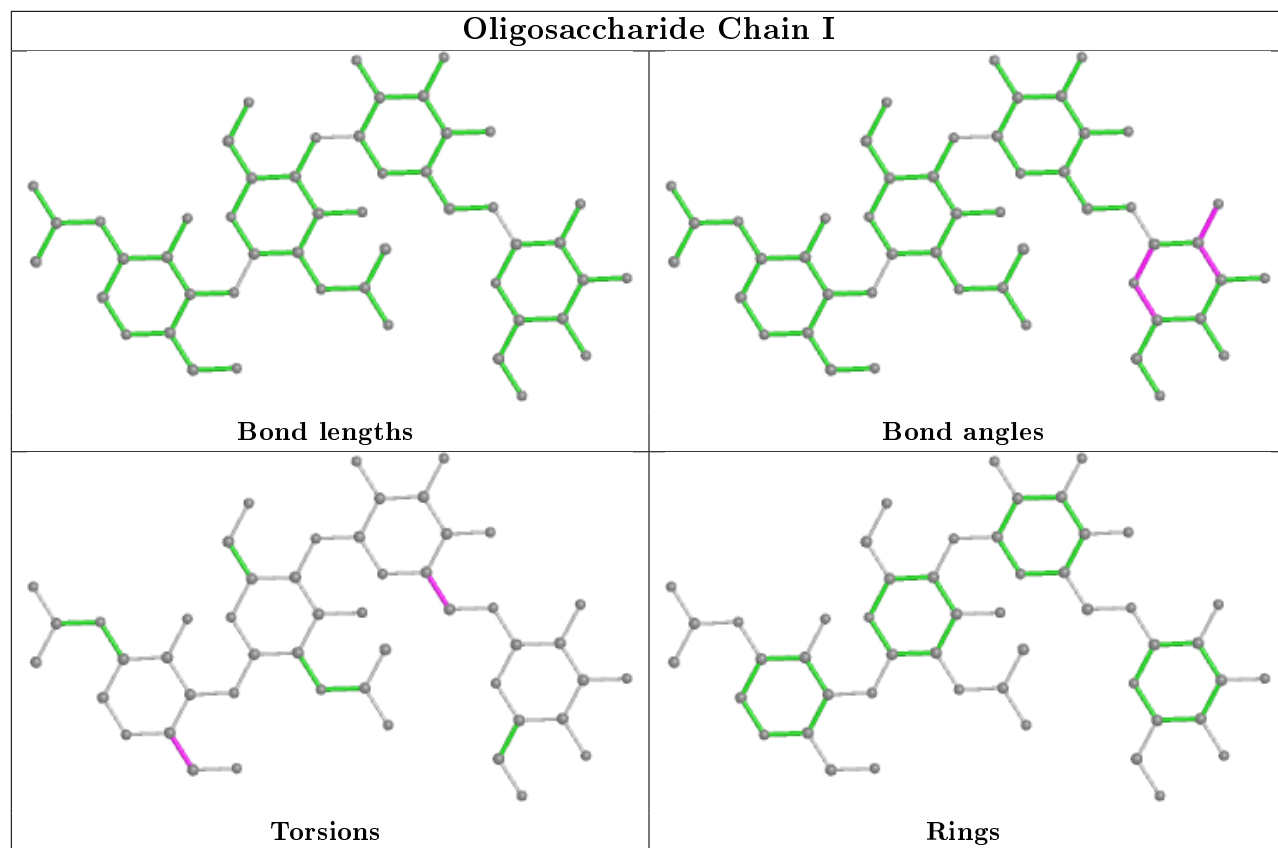
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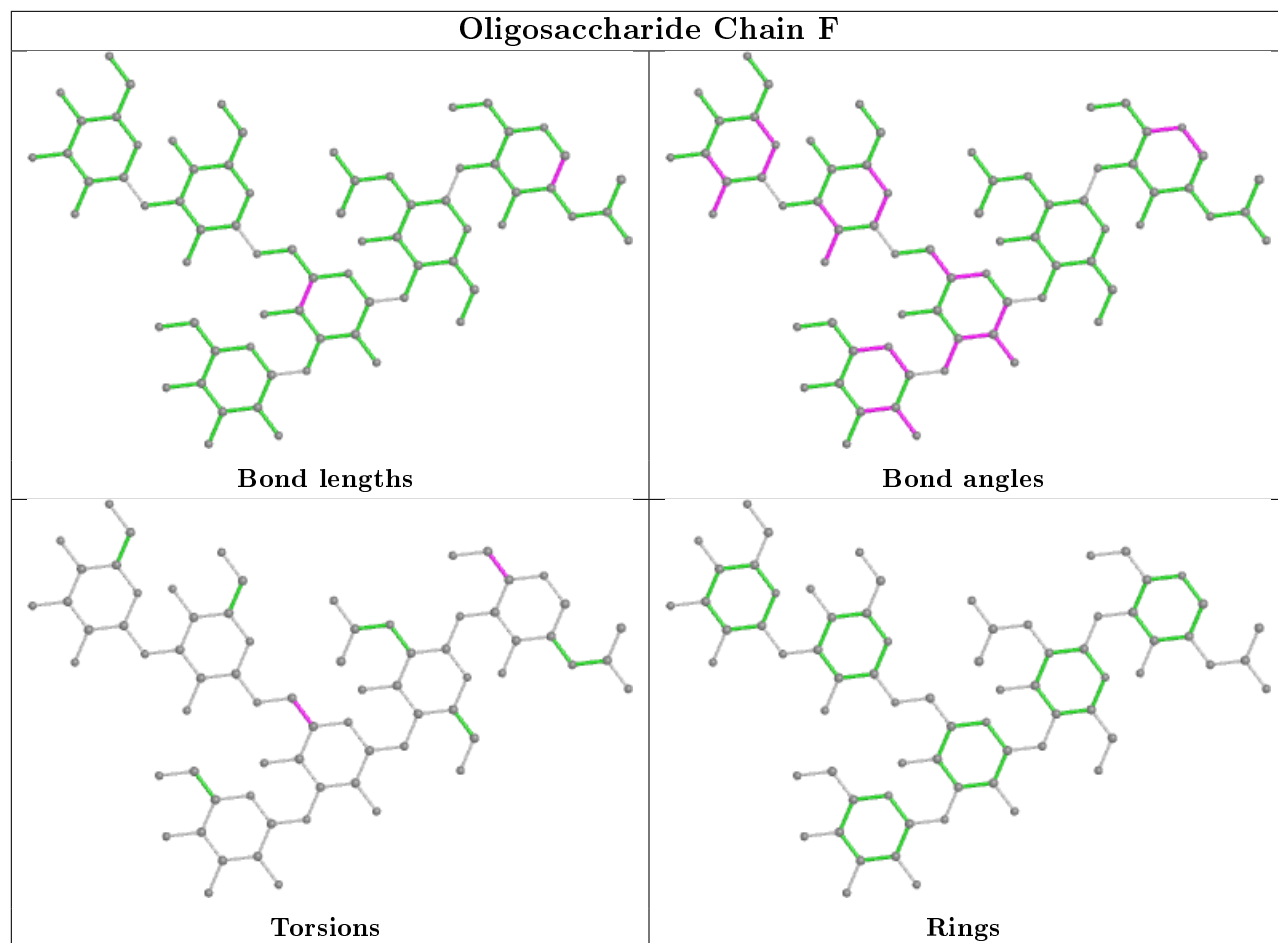
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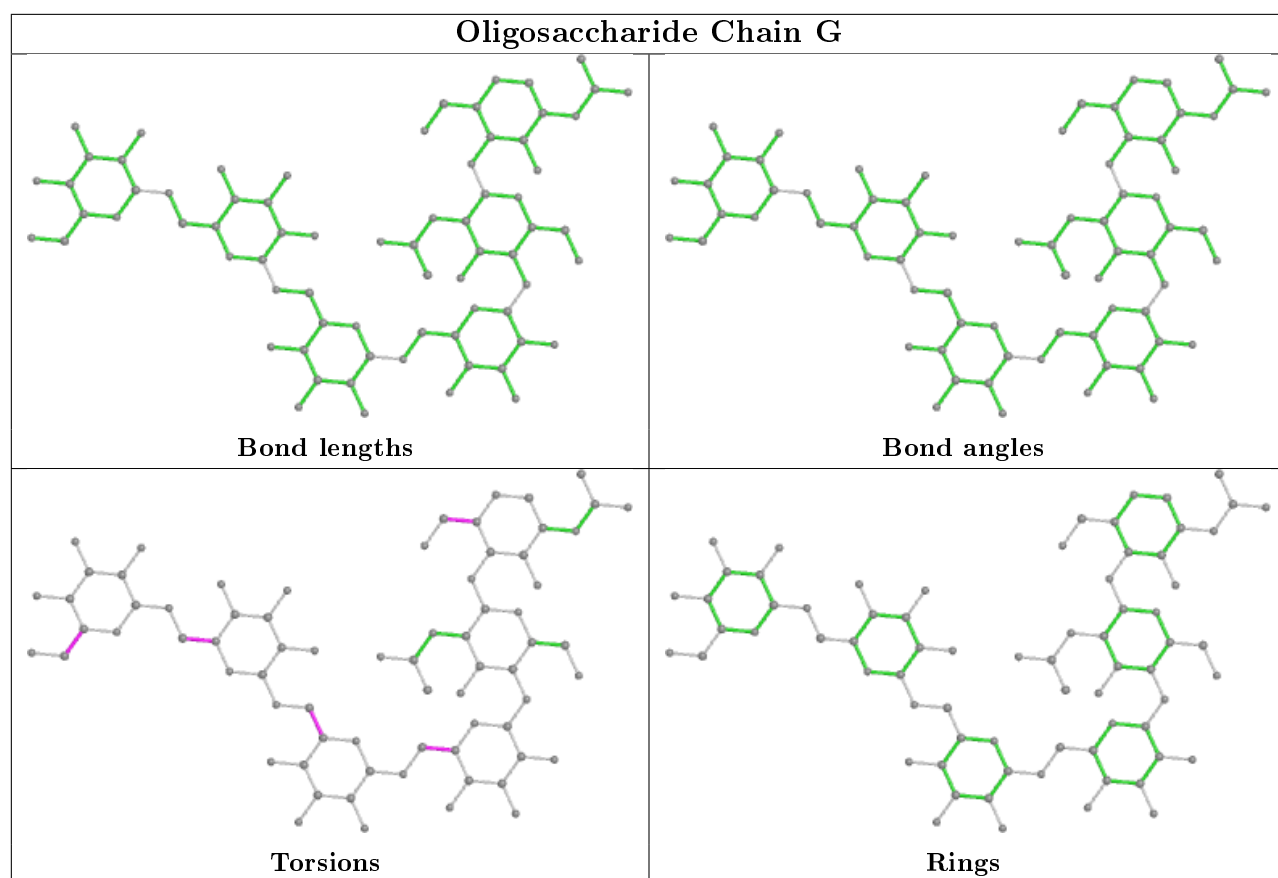
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
3	I	2	NAG	4	0

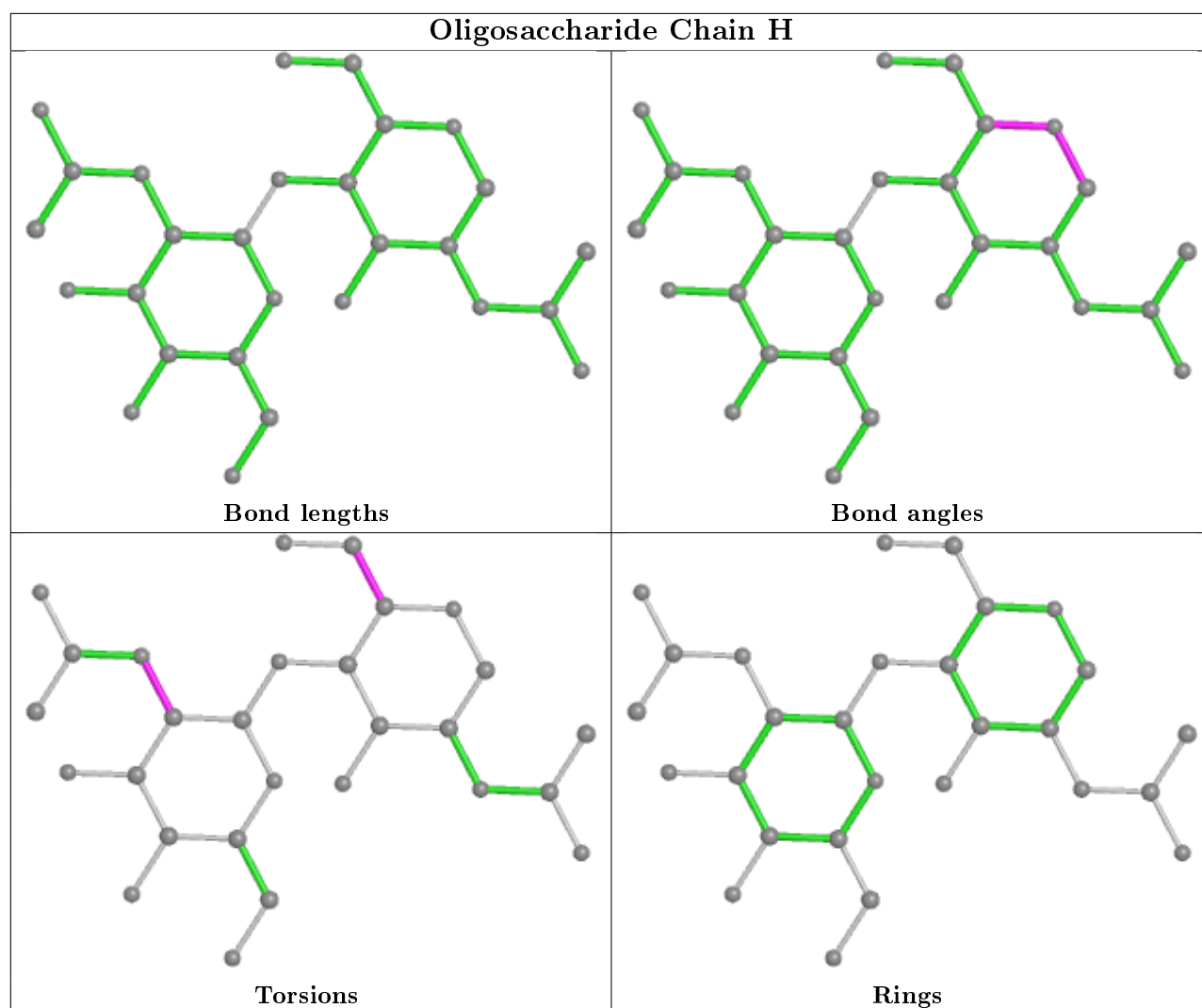
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 84 are monoatomic - leaving 14 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	$\# Z  > 2$
9	NAG	B	912	2	14,14,15	0.21	0	17,19,21	0.34	0
9	NAG	C	941	1	14,14,15	0.23	0	17,19,21	0.42	0
10	QEL	B	920	-	26,26,26	2.67	9 (34%)	35,35,35	1.78	8 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	B	913	2	14,14,15	0.23	0	17,19,21	0.41	0
9	NAG	D	901	2	14,14,15	0.28	0	17,19,21	0.33	0
9	NAG	A	944	1	14,14,15	0.22	0	17,19,21	0.37	0
9	NAG	D	902	2	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
10	QEL	C	939	-	26,26,26	2.52	9 (34%)	35,35,35	1.88	7 (20%)
9	NAG	A	945	1	14,14,15	0.24	0	17,19,21	0.61	1 (5%)
9	NAG	A	943	1	14,14,15	0.28	0	17,19,21	0.46	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
9	NAG	B	912	2	-	2/6/23/26	0/1/1/1
9	NAG	C	941	1	-	2/6/23/26	0/1/1/1
10	QEL	B	920	-	-	6/16/26/26	0/3/3/3
9	NAG	B	913	2	-	2/6/23/26	0/1/1/1
9	NAG	D	901	2	-	2/6/23/26	0/1/1/1
9	NAG	A	944	1	-	2/6/23/26	0/1/1/1
9	NAG	D	902	2	-	3/6/23/26	0/1/1/1
10	QEL	C	939	-	-	6/16/26/26	0/3/3/3
9	NAG	A	945	1	-	0/6/23/26	0/1/1/1
9	NAG	A	943	1	-	2/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	920	QEL	O1-C14	-10.32	1.22	1.42
10	C	939	QEL	O1-C14	-9.29	1.24	1.42
10	B	920	QEL	C14-C13	-3.53	1.49	1.54
10	C	939	QEL	C14-C13	-3.51	1.49	1.54
10	B	920	QEL	C3-C18	-3.28	1.32	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	939	QEL	O1-C14-C15	5.10	122.32	111.19
10	C	939	QEL	C24-C13-C14	-4.80	104.64	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	920	QEL	C24-C13-C14	-4.76	104.70	111.92
10	B	920	QEL	C12-C8-C7	-4.17	102.14	111.88
10	C	939	QEL	C12-C8-C7	-4.16	102.16	111.88

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

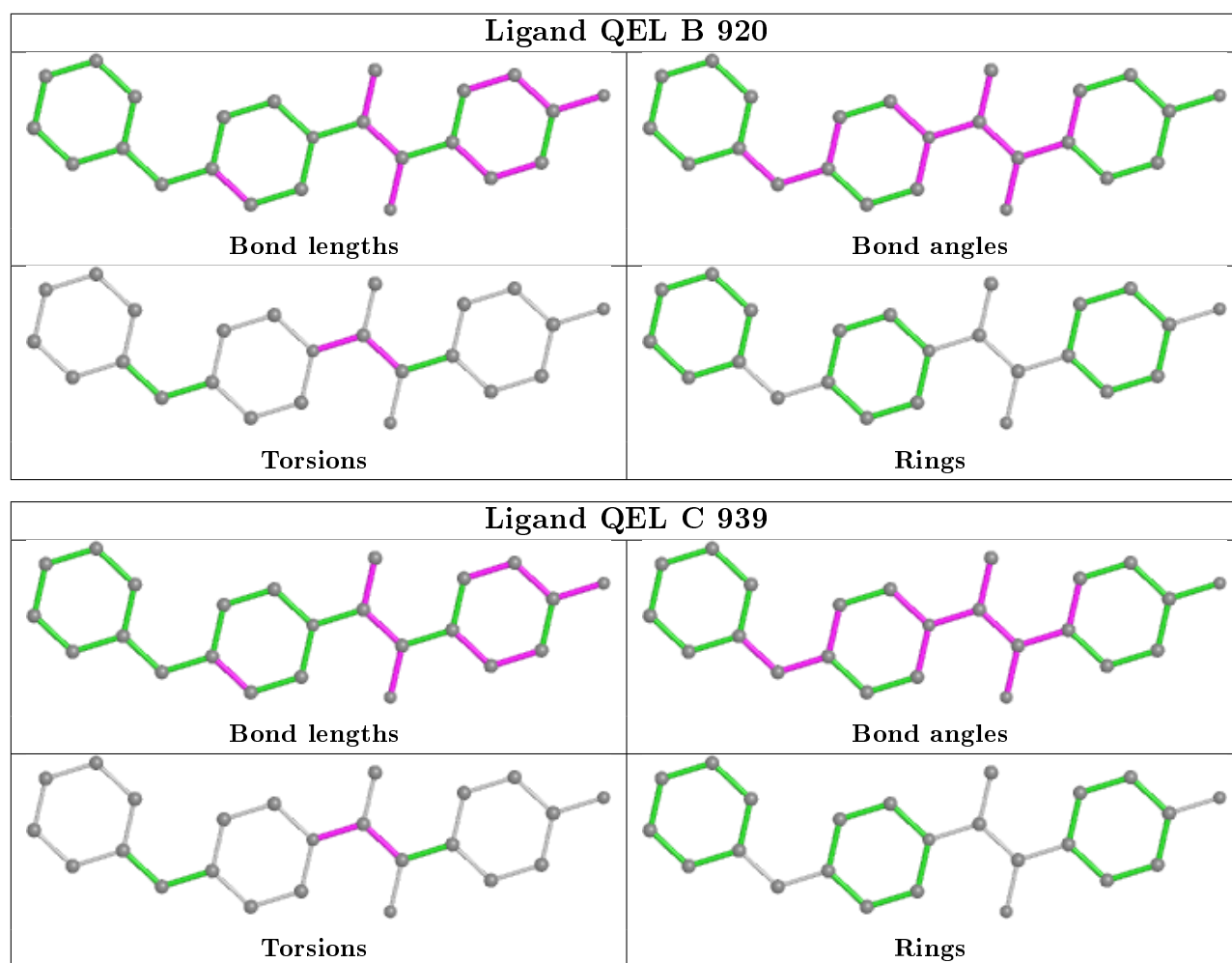
Mol	Chain	Res	Type	Atoms
10	B	920	QEL	C24-C13-N1-C10
10	C	939	QEL	C24-C13-N1-C10
9	B	913	NAG	C4-C5-C6-O6
9	B	912	NAG	O5-C5-C6-O6
9	A	943	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	920	QEL	6	0
10	C	939	QEL	6	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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

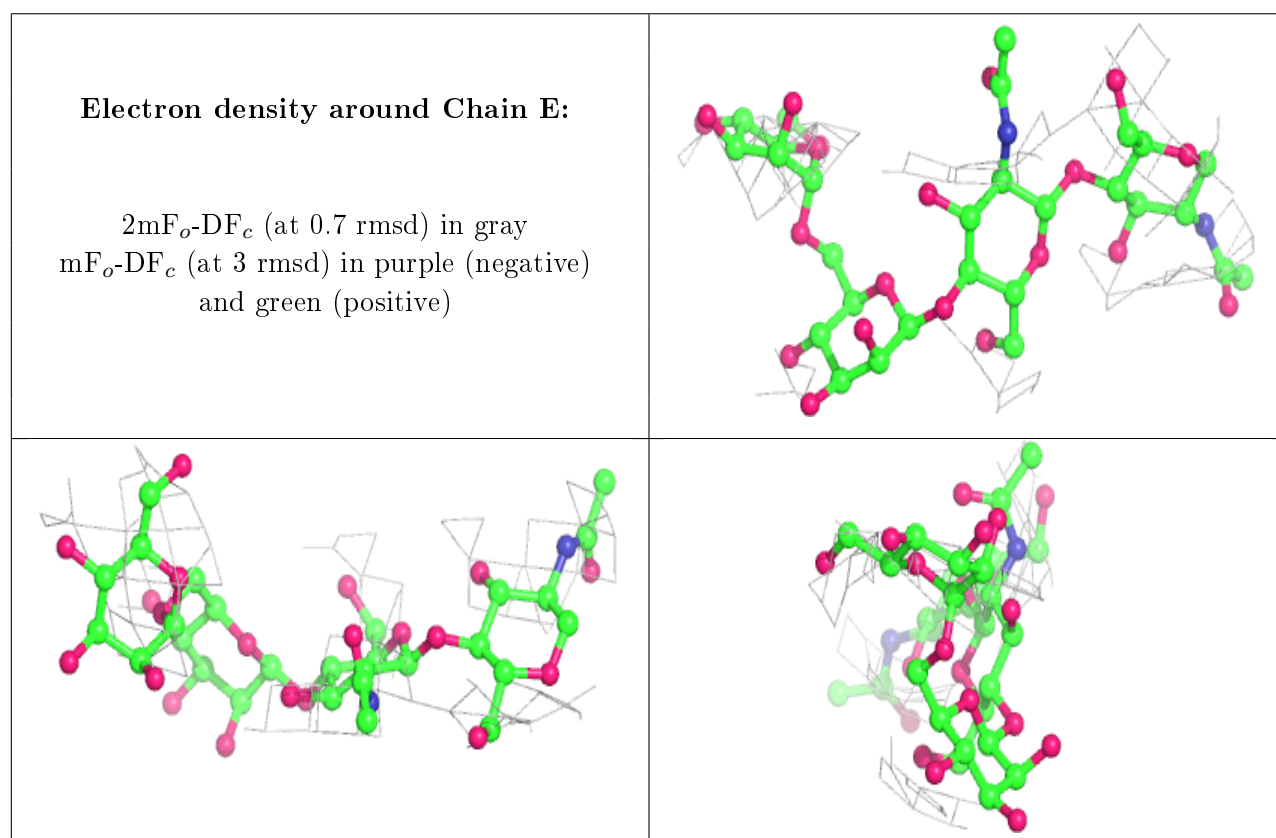
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

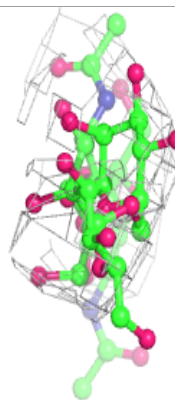
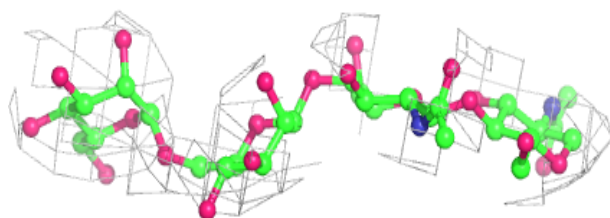
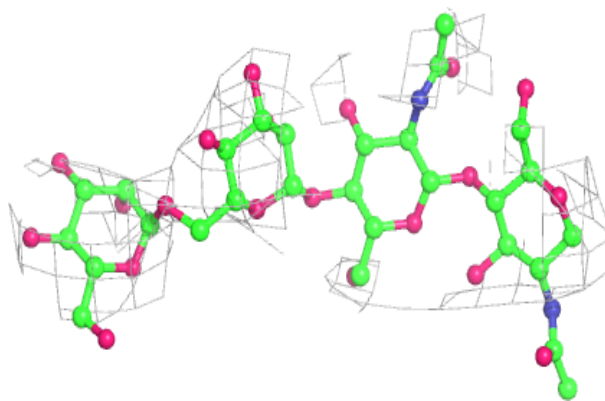
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

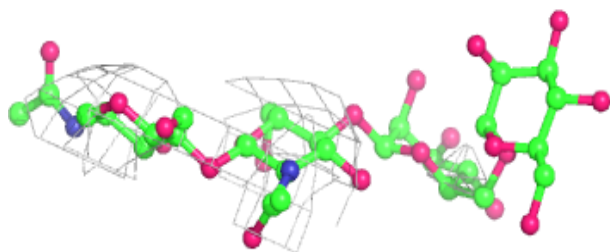
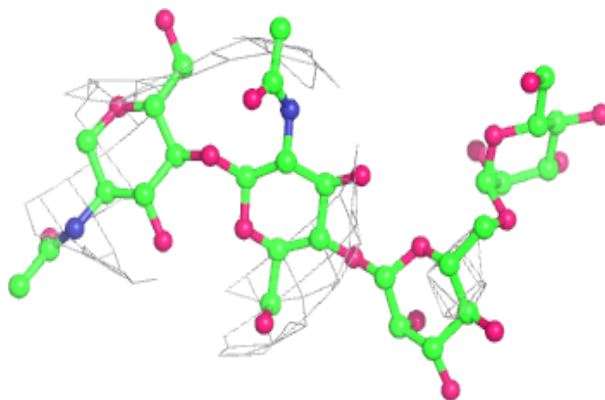


**Electron density around Chain I:**

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

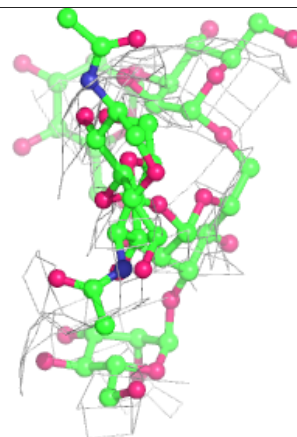
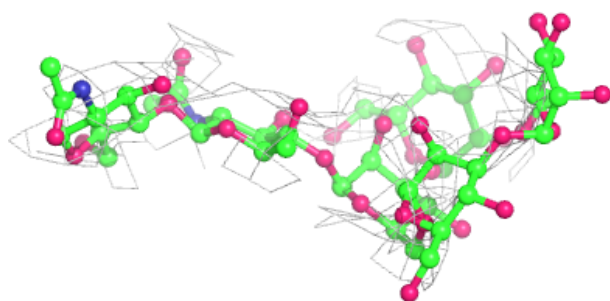
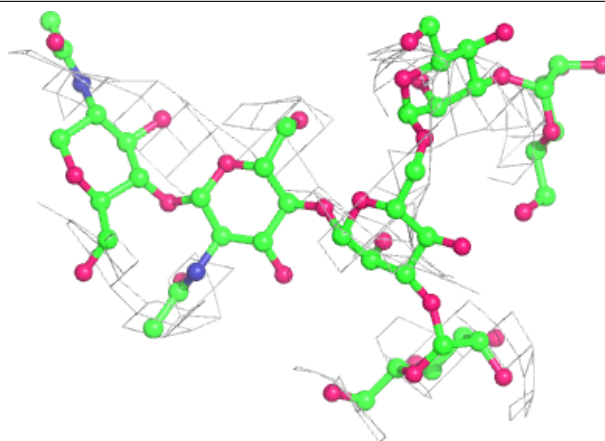
**Electron density around Chain J:**

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

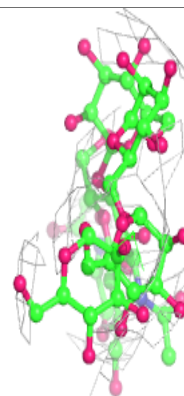
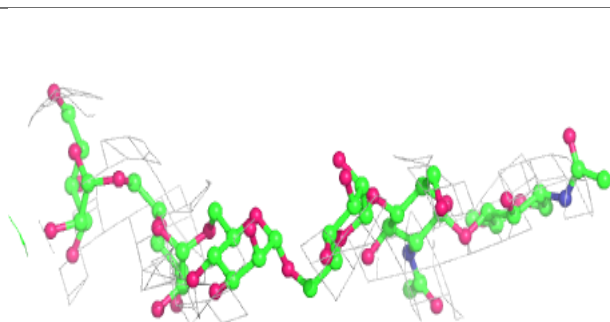
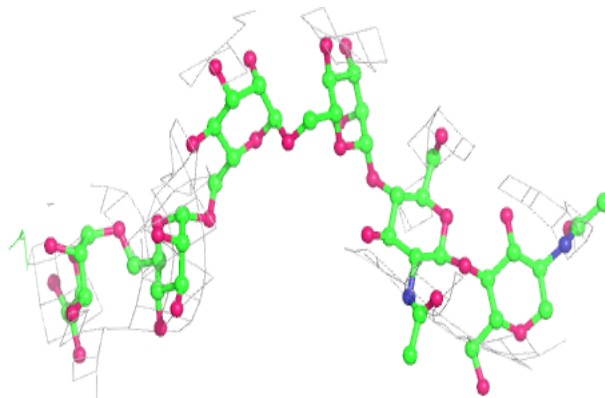


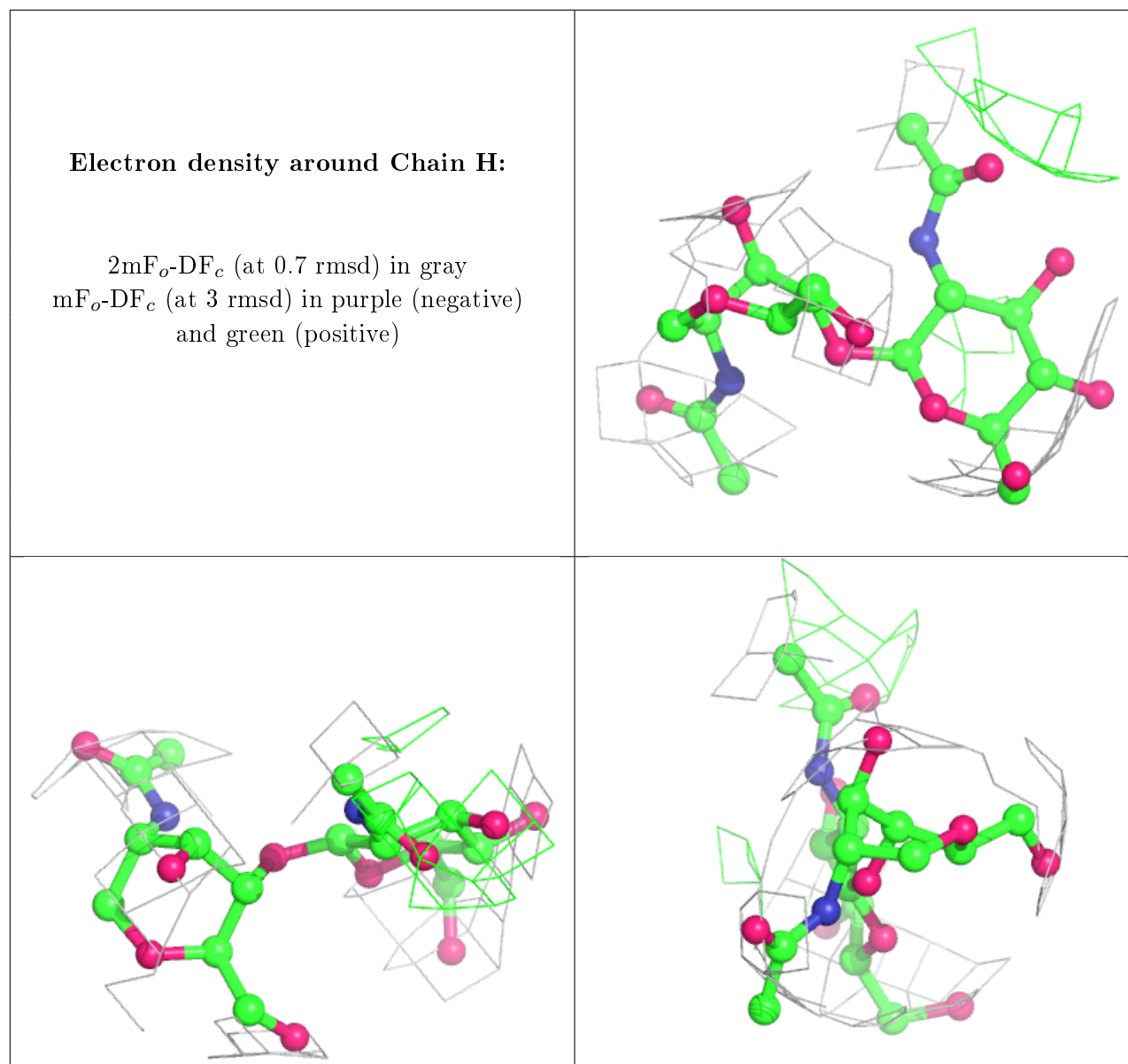
**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





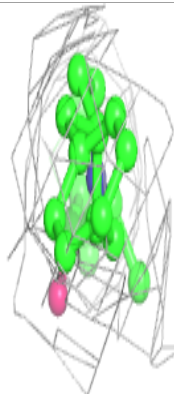
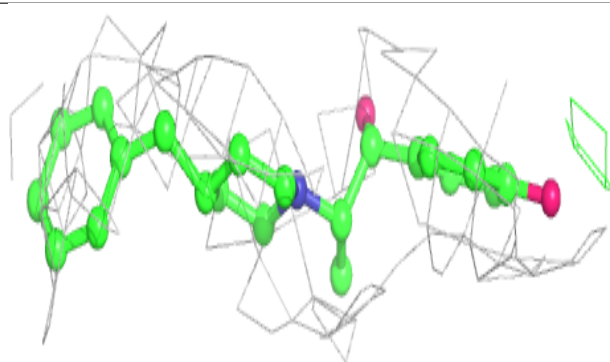
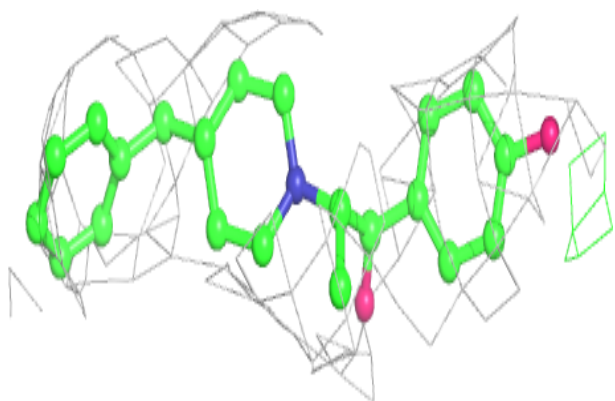
## 6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

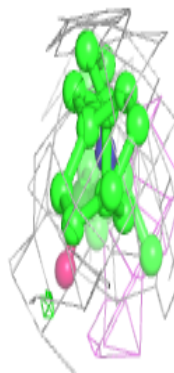
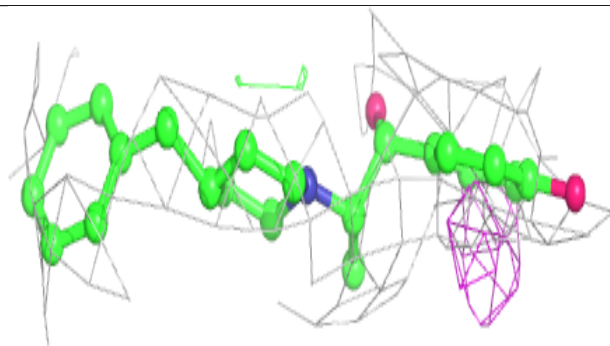
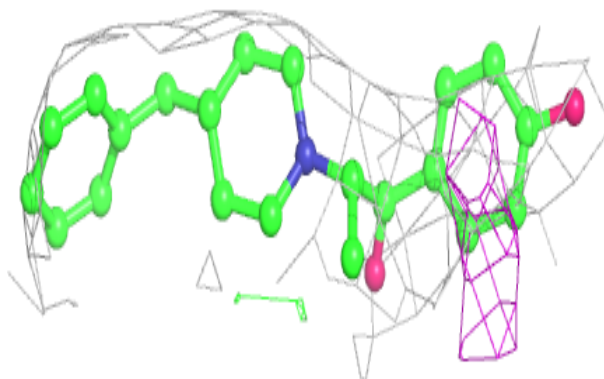
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around QEL B 920:**

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

**Electron density around QEL C 939:**

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





## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.