



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 11:52 AM BST

PDB ID : 2Z7X  
Title : Crystal structure of the TLR1-TLR2 heterodimer induced by binding of a tri-acylated lipopeptide  
Authors : Lee, J.O.; Jin, M.S.; Kim, S.E.; Heo, J.Y.  
Deposited on : 2007-08-29  
Resolution : 2.10 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

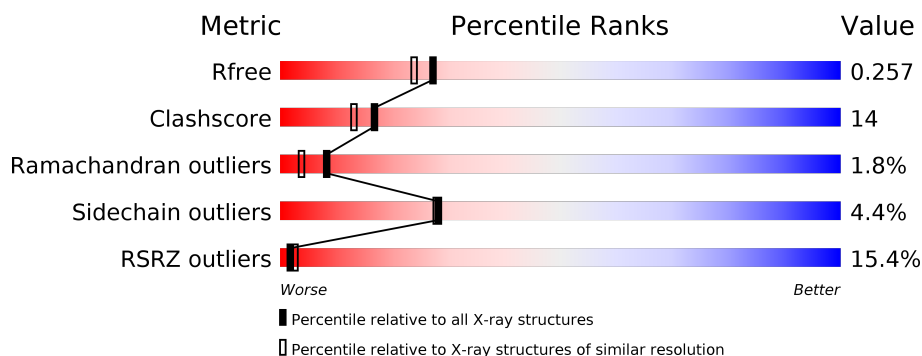
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



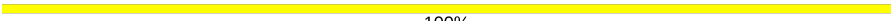
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	549	<div> <div>28%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
2	B	520	<div> <div>2%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
3	C	5	<div> <div>20%</div> <div>80%</div> <div>20%</div> </div>
4	D	3	<div> <div>33%</div> <div>67%</div> </div>
5	E	3	<div> <div>33%</div> <div>67%</div> </div>
6	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	2	 100%

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
4	MAN	D	3	-	-	-	X
5	MAN	E	3	-	-	-	X
8	NAG	A	901	X	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9088 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 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4366	2766	735	844	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	SER	-	linker	UNP O60603
A	508	ARG	-	linker	UNP O60603

- Molecule 2 is a protein called Toll-like receptor 1, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	S	0	0	0
			4172	2671	697	784	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	ALA	-	linker	UNP Q15399
B	477	SER	-	linker	UNP Q15399

- Molecule 3 is a protein called Pam3CSK4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			43	27	9	7			

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



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

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



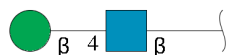
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

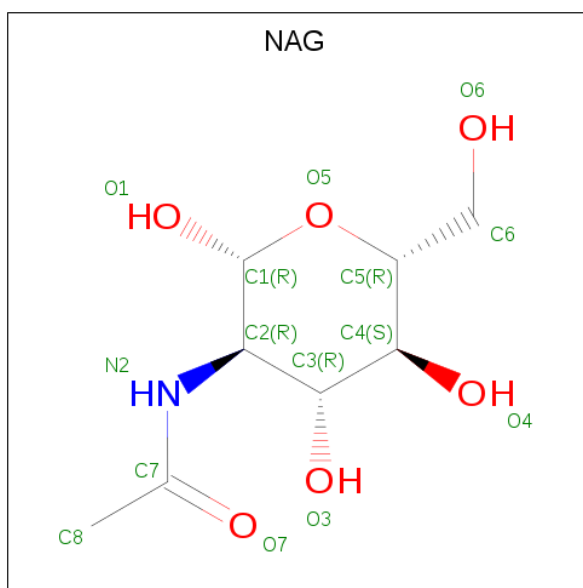
- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			25	14	1	10			

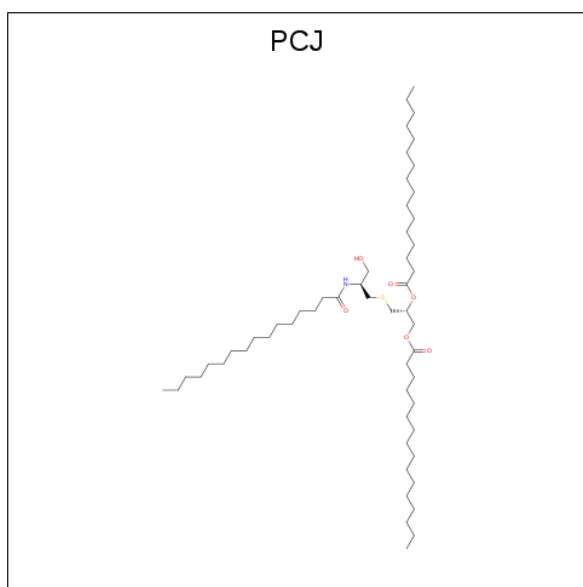
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 9 is (2R)-3-[[[(2S)-3-HYDROXY-2-(PALMITOYLAMINO)PROPYL]THIO}PROPANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PCJ) (formula: C<sub>54</sub>H<sub>105</sub>NO<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	S	0	0
			62	54	1	6	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	70	Total O 70 70	0	0
10	B	175	Total O 175 175	0	0
10	C	2	Total O 2 2	0	0

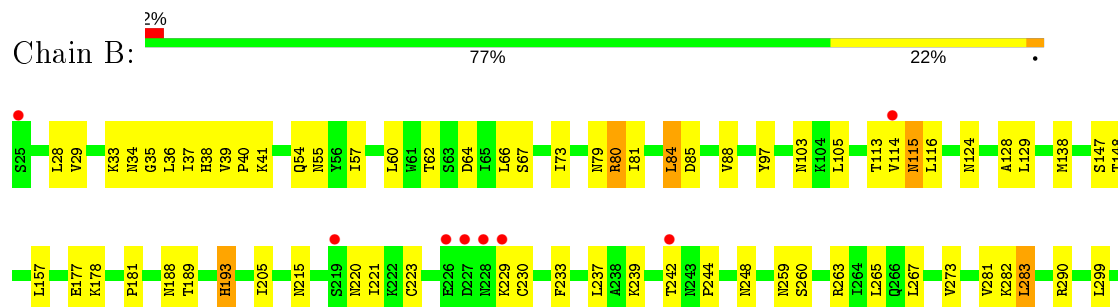
### 3 Residue-property plots

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.

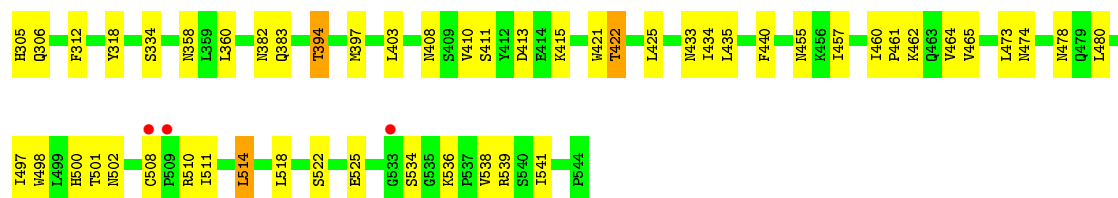
- Molecule 1: Toll-like receptor 2, Variable lymphocyte receptor B



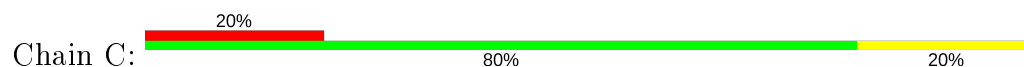
- Molecule 2: Toll-like receptor 1, Variable lymphocyte receptor B







- Molecule 3: Pam3CSK4



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



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



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



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.30 Å   120.14 Å   74.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	45.85 – 2.10 45.85 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.5 (45.85-2.10) 93.0 (45.85-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.08 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.244   ,   0.270 0.234   ,   0.257	Depositor DCC
$R_{free}$ test set	5025 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: PCJ, BMA, NAG, NDG, 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	0.32	0/4442	0.60	2/6014 (0.0%)
2	B	0.38	0/4257	0.63	0/5766
3	C	0.38	0/42	0.50	0/49
All	All	0.35	0/8741	0.61	2/11829 (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	425	PHE	N-CA-C	-5.74	95.51	111.00
1	A	351	VAL	N-CA-C	-5.03	97.41	111.00

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	4366	0	4418	155	0
2	B	4172	0	4221	91	0
3	C	43	0	56	0	0
4	D	39	0	33	4	0
5	E	39	0	34	0	0
6	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	25	0	22	2	0
8	A	42	0	39	1	0
8	B	14	0	13	0	0
9	C	62	0	102	4	0
10	A	70	0	0	3	0
10	B	175	0	0	3	0
10	C	2	0	0	0	0
All	All	9088	0	8972	251	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 14.

The worst 5 of 251 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:511:LEU:H	1:A:533:ASN:HD22	1.01	0.95
2:B:229:LYS:HD2	2:B:263:ARG:HE	1.32	0.94
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.59	0.84
1:A:372:MET:H	1:A:397:ASN:HD22	1.25	0.84
2:B:81:ILE:H	2:B:103:ASN:HD22	1.27	0.81

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	547/549 (100%)	458 (84%)	72 (13%)	17 (3%)	<b>4</b> <b>1</b>
2	B	518/520 (100%)	480 (93%)	36 (7%)	2 (0%)	34 32
3	C	3/5 (60%)	3 (100%)	0	0	<b>100</b> <b>100</b>
All	All	1068/1074 (99%)	941 (88%)	108 (10%)	19 (2%)	<b>8</b> <b>4</b>

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	143	SER
1	A	241	GLU
1	A	572	ILE
1	A	85	SER

### 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	518/518 (100%)	492 (95%)	26 (5%)	24	23
2	B	494/494 (100%)	476 (96%)	18 (4%)	35	36
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	1017/1017 (100%)	972 (96%)	45 (4%)	28	28

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	LEU
1	A	523	THR
2	B	422	THR
1	A	490	MET
2	B	41	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	557	GLN
2	B	92	ASN
2	B	478	ASN
2	B	38	HIS
2	B	55	ASN

### 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 ⓘ

11 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	$\# Z  > 2$
4	NAG	D	1	2,4	14,14,15	0.77	0	17,19,21	0.71	0
4	NDG	D	2	4	14,14,15	0.90	0	17,19,21	0.83	0
4	MAN	D	3	4	11,11,12	0.77	0	15,15,17	0.82	0
5	NAG	E	1	2,5	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	14,14,15	0.69	0	17,19,21	0.73	1 (5%)
5	MAN	E	3	5	11,11,12	0.71	0	15,15,17	0.71	0
6	NAG	F	1	2,6	14,14,15	0.61	0	17,19,21	0.74	0
6	NAG	F	2	6	14,14,15	0.63	0	17,19,21	0.61	0
6	BMA	F	3	6	11,11,12	0.52	0	15,15,17	0.27	0
7	NAG	G	1	7	14,14,15	0.74	0	17,19,21	0.88	0
7	BMA	G	2	7	11,11,12	0.67	0	15,15,17	0.34	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
4	NAG	D	1	2,4	-	3/6/23/26	0/1/1/1
4	NDG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	MAN	E	3	5	-	2/2/19/22	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
7	NAG	G	1	7	-	2/6/23/26	0/1/1/1
7	BMA	G	2	7	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C2-N2-C7	-2.62	119.17	122.90
5	E	2	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

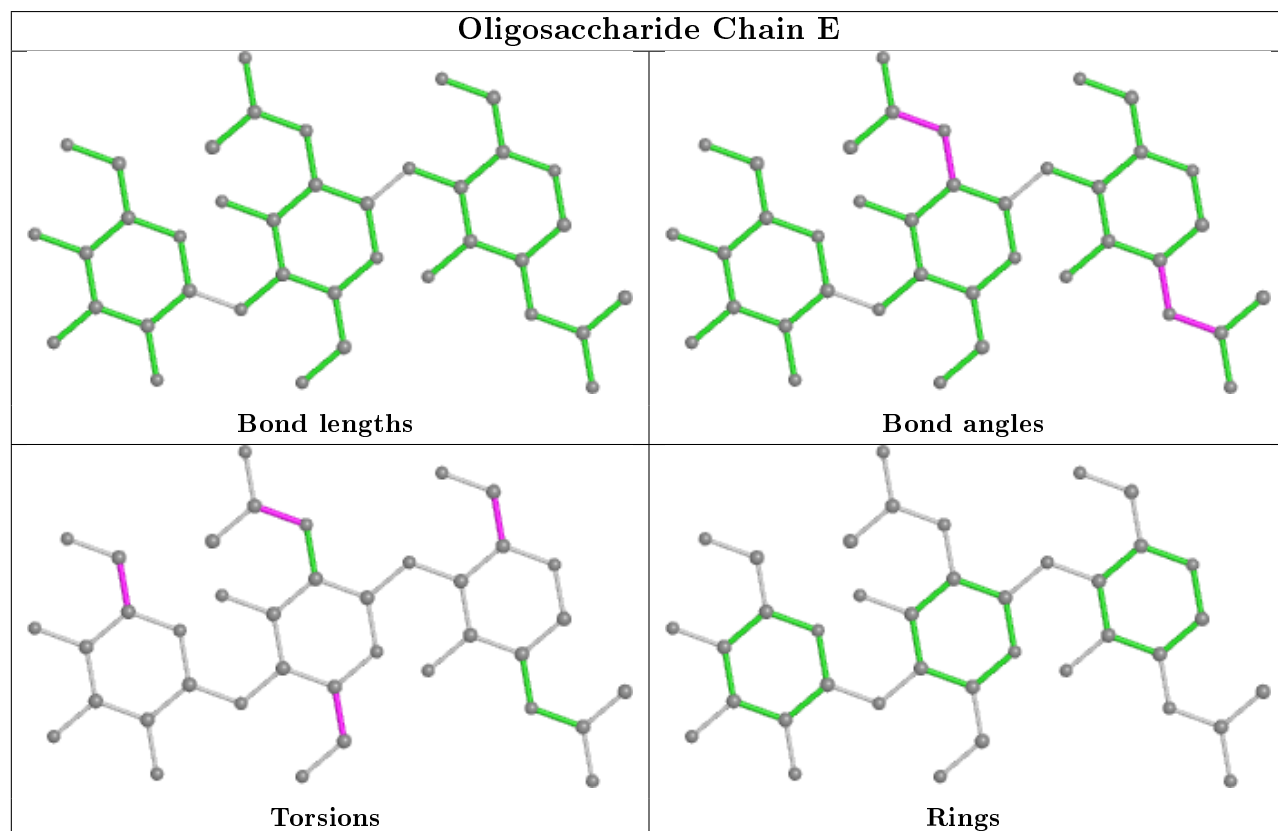
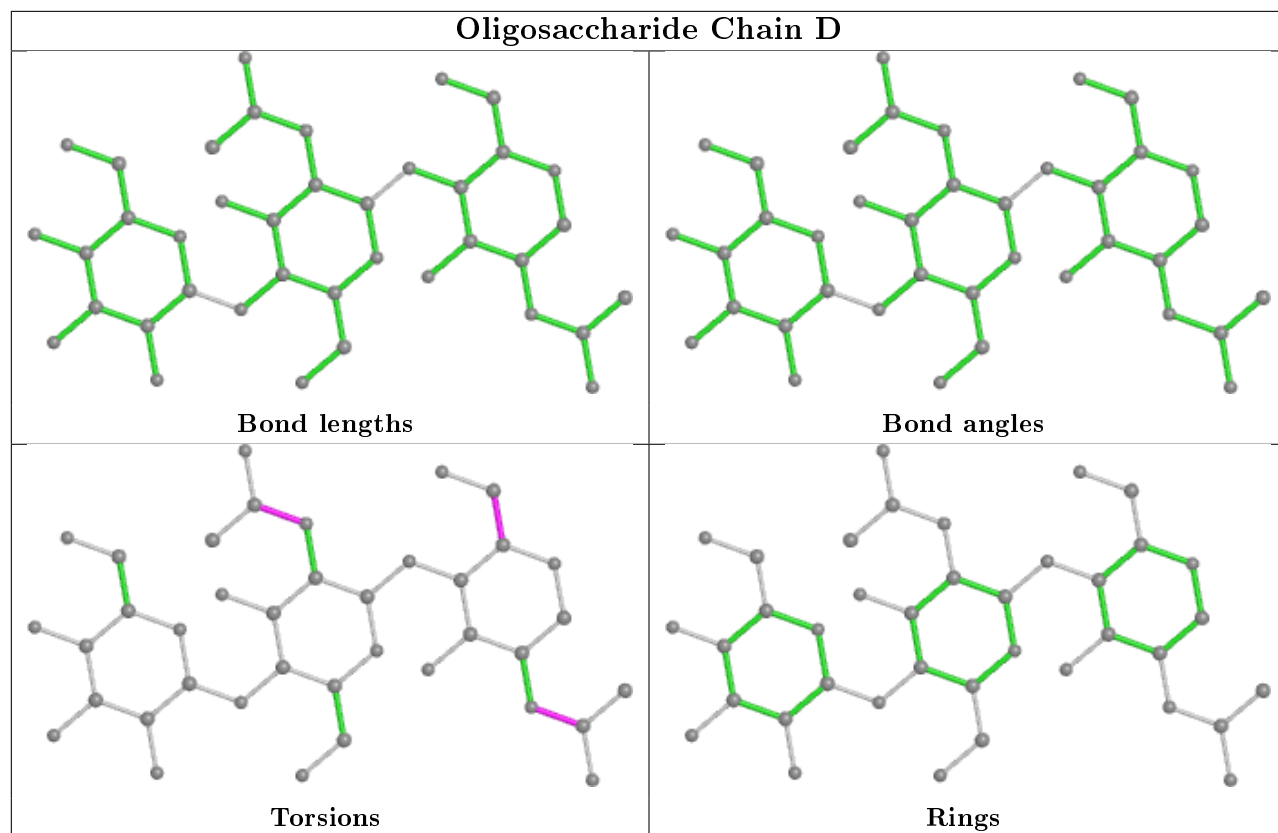
Mol	Chain	Res	Type	Atoms
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
5	E	3	MAN	O5-C5-C6-O6

There are no ring outliers.

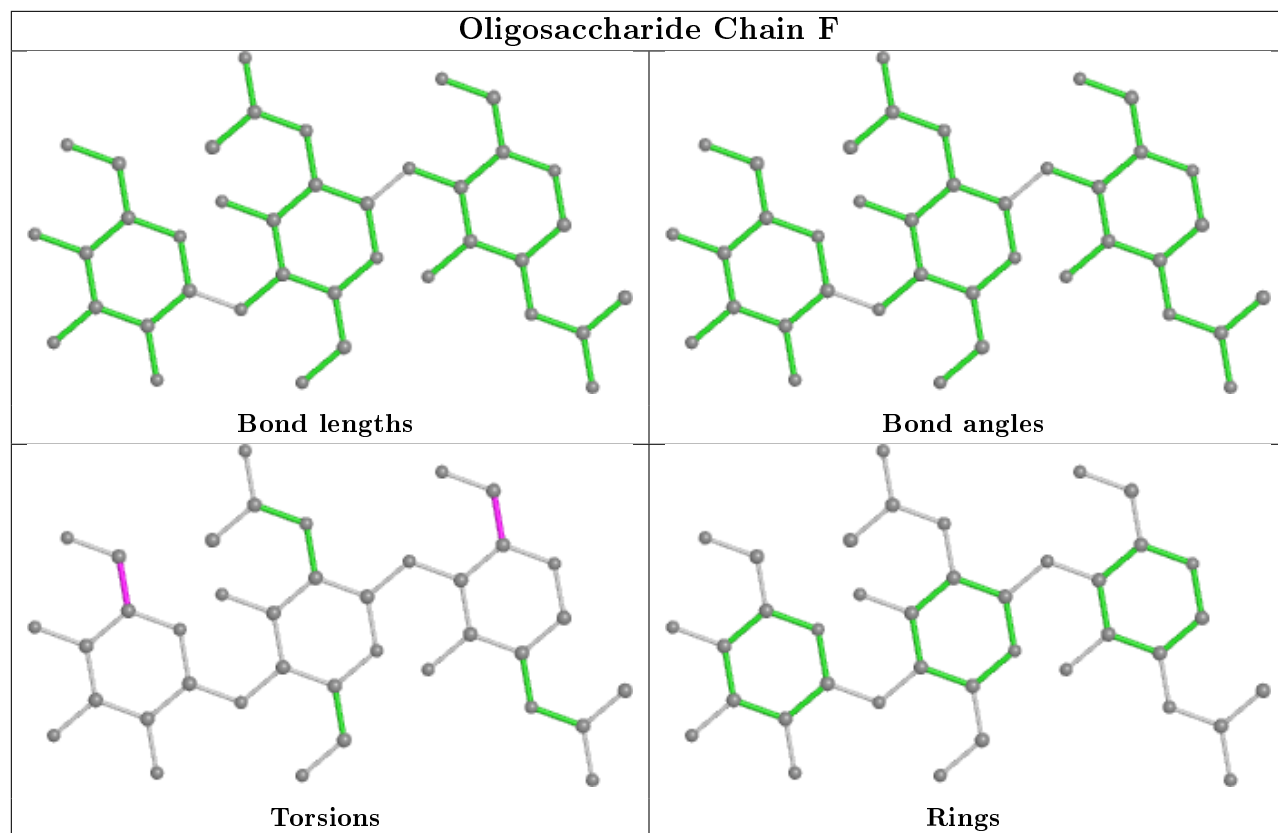
4 monomers are involved in 6 short contacts:

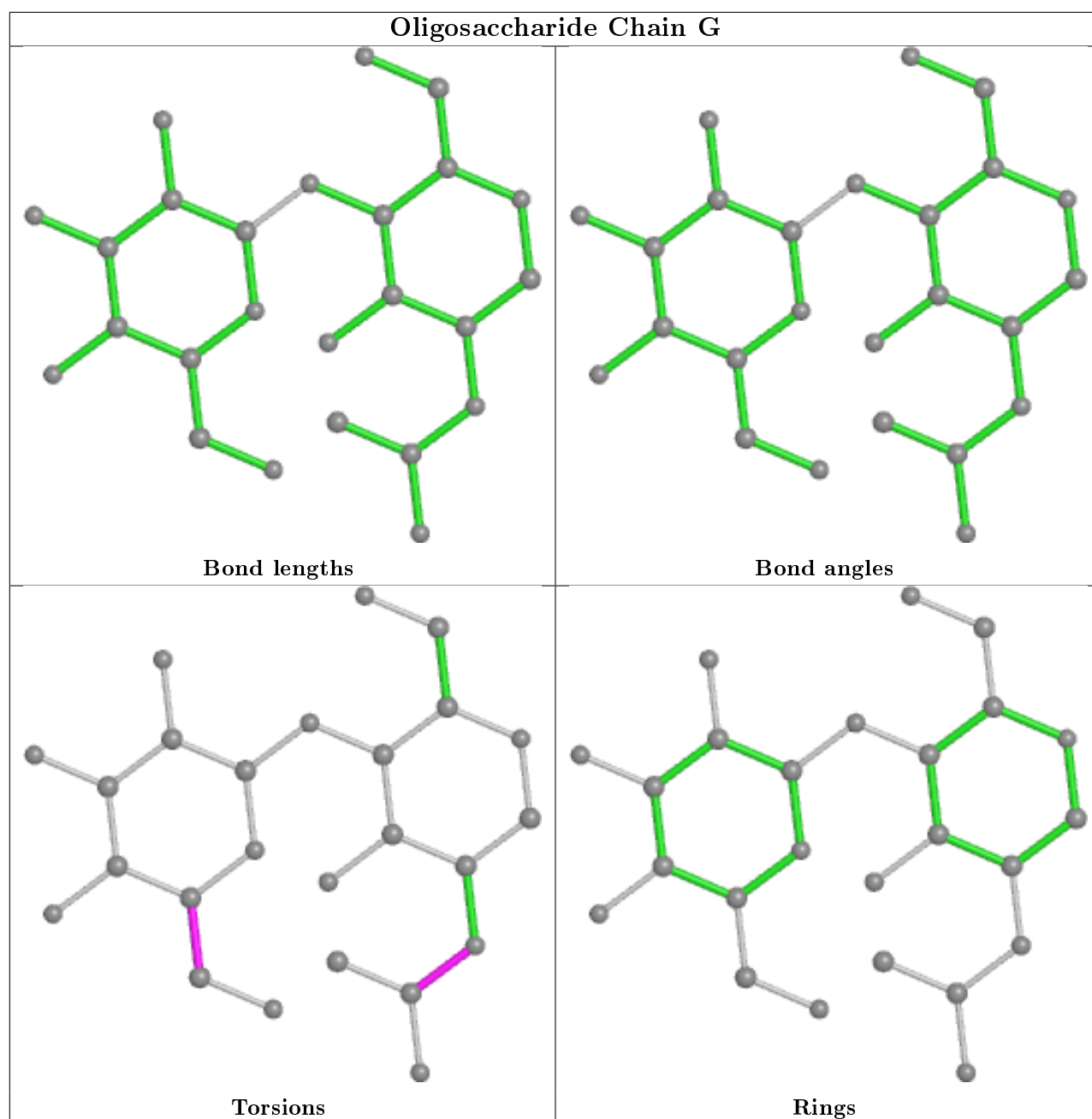
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	BMA	2	0
7	G	1	NAG	2	0
4	D	1	NAG	2	0
4	D	2	NDG	3	0

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](#)

5 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
9	PCJ	C	1	3	60,61,61	0.75	1 (1%)	59,65,65	1.05	4 (6%)
8	NAG	B	811	2	14,14,15	0.57	0	17,19,21	0.67	1 (5%)
8	NAG	A	921	1	14,14,15	0.56	0	17,19,21	0.62	0
8	NAG	A	911	1	14,14,15	0.63	0	17,19,21	0.57	0
8	NAG	A	901	1	14,14,15	0.59	0	17,19,21	0.61	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	PCJ	C	1	3	-	17/66/66/66	-
8	NAG	B	811	2	-	2/6/23/26	0/1/1/1
8	NAG	A	921	1	-	0/6/23/26	0/1/1/1
8	NAG	A	911	1	-	4/6/23/26	0/1/1/1
8	NAG	A	901	1	1/1/5/7	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1	PCJ	O-C	-4.68	1.22	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1	PCJ	O2-C46-C45	3.58	119.22	111.50
9	C	1	PCJ	O-C-CA	3.32	120.54	111.95
9	C	1	PCJ	C2-O2-C46	-2.80	110.91	117.79
9	C	1	PCJ	O3-C26-C25	2.57	119.97	111.91
8	B	811	NAG	C2-N2-C7	-2.15	119.84	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	901	NAG	C1

5 of 26 torsion outliers are listed below:

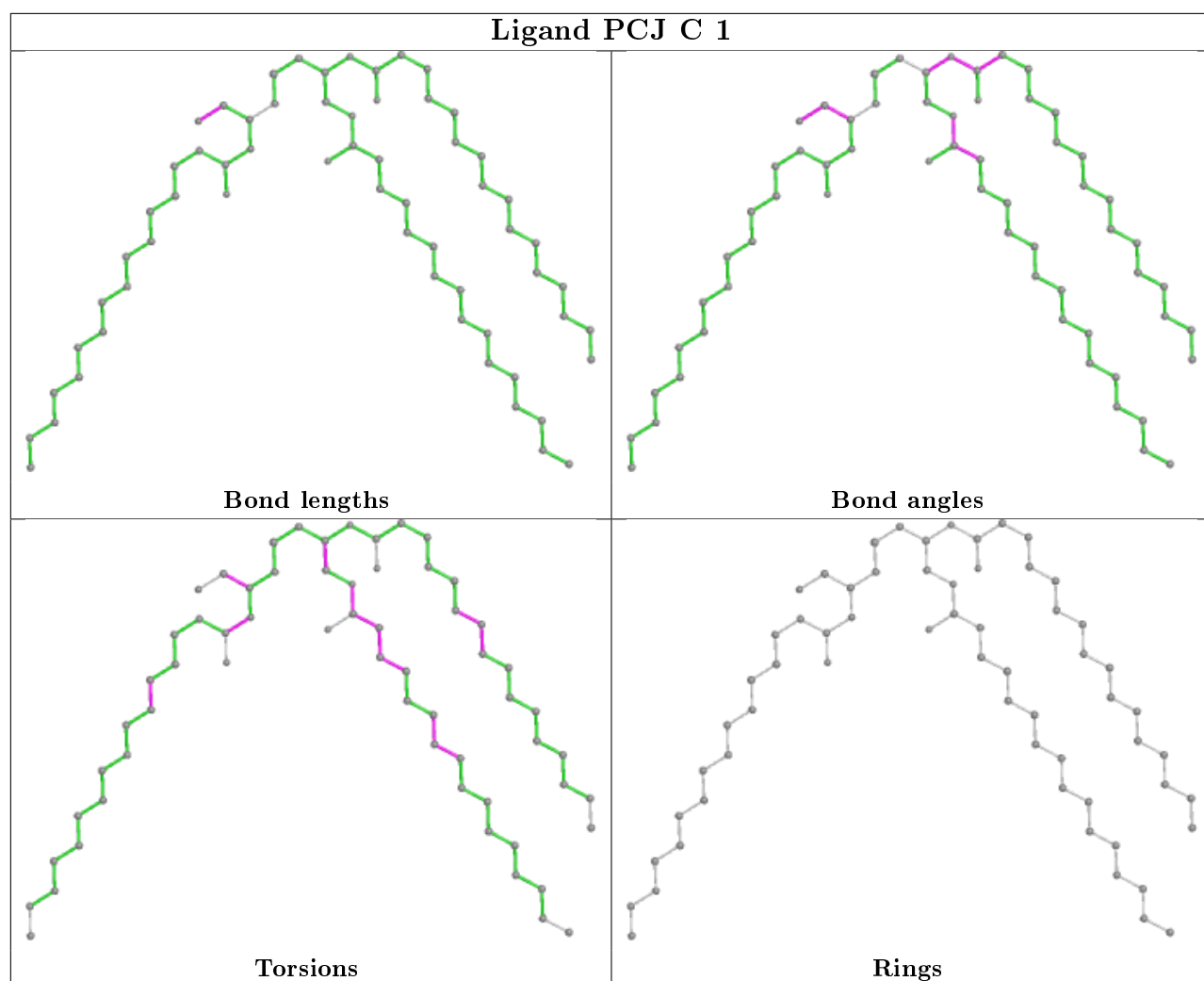
Mol	Chain	Res	Type	Atoms
9	C	1	PCJ	O-C-CA-CB
9	C	1	PCJ	O-C-CA-N
8	B	811	NAG	C8-C7-N2-C2
8	B	811	NAG	O7-C7-N2-C2
8	A	911	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1	PCJ	4	0
8	A	911	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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](#)

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	549/549 (100%)	1.54	153 (27%) <b>0</b> <b>0</b>	22, 59, 130, 137	0
2	B	520/520 (100%)	0.15	11 (2%) 63 68	20, 35, 60, 83	0
3	C	5/5 (100%)	1.26	1 (20%) <b>1</b> <b>1</b>	41, 57, 74, 83	0
All	All	1074/1074 (100%)	0.87	165 (15%) <b>2</b> <b>2</b>	20, 43, 125, 137	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LEU	11.3
1	A	244	THR	11.3
1	A	67	ILE	10.9
1	A	35	ILE	10.7
1	A	46	ILE	10.3

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

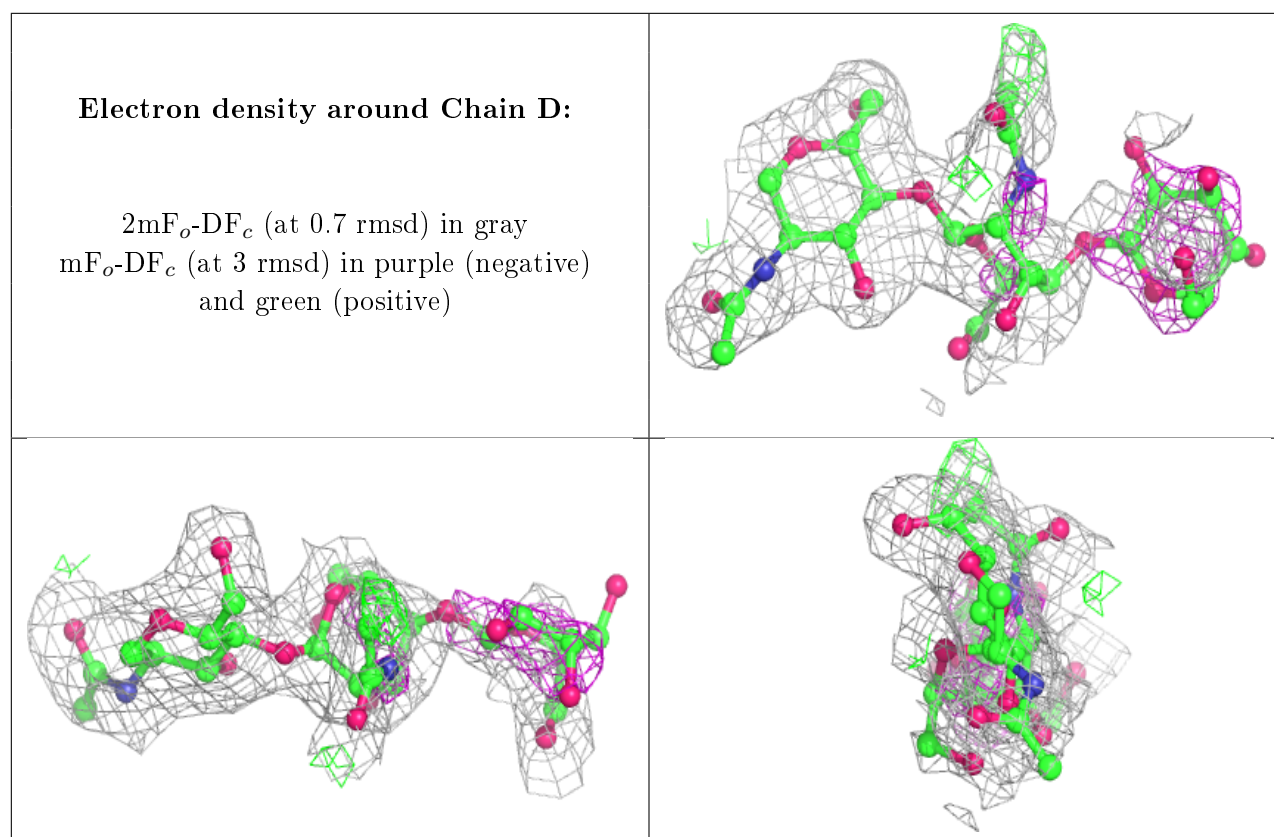
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	D	3	11/12	<b>0.36</b>	<b>0.70</b>	98,100,102,102	0
7	NAG	G	1	14/15	0.44	0.28	90,93,96,96	0
7	BMA	G	2	11/12	0.47	0.31	96,98,99,99	0

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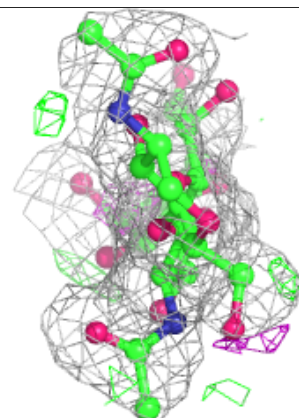
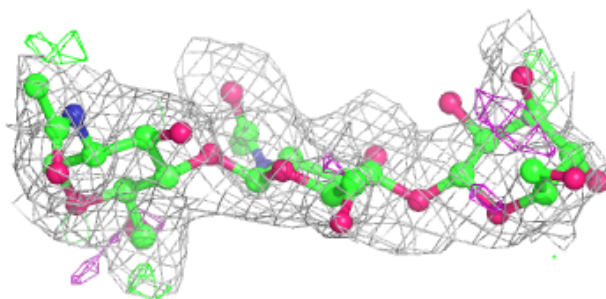
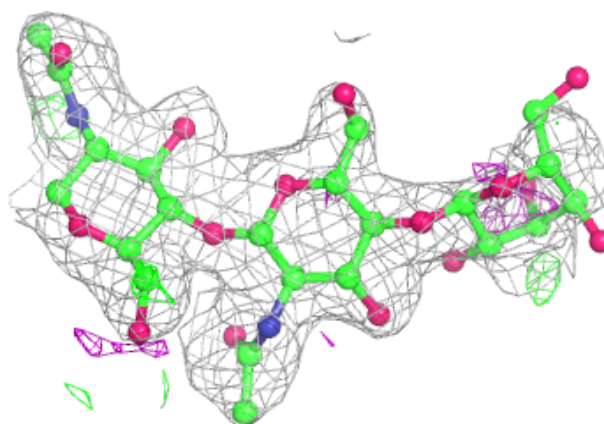
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NDG	D	2	14/15	0.61	0.29	80,85,89,94	0
5	MAN	E	3	11/12	0.72	0.46	81,84,86,88	0
6	BMA	F	3	11/12	0.78	0.18	68,72,74,77	0
5	NAG	E	2	14/15	0.84	0.19	55,65,71,75	0
5	NAG	E	1	14/15	0.91	0.11	41,46,52,56	0
4	NAG	D	1	14/15	0.93	0.09	53,58,62,72	0
6	NAG	F	2	14/15	0.93	0.10	35,48,54,62	0
6	NAG	F	1	14/15	0.95	0.10	24,30,33,40	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.

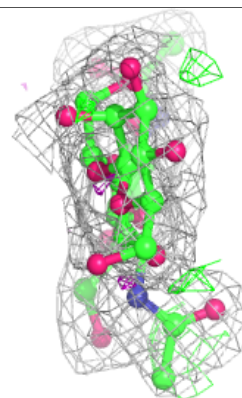
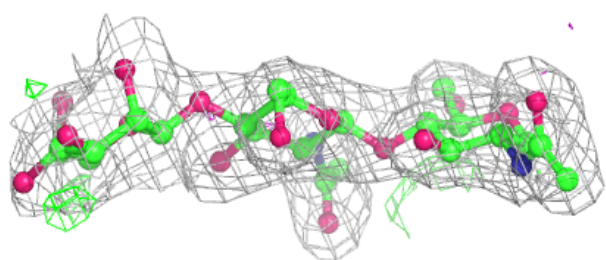
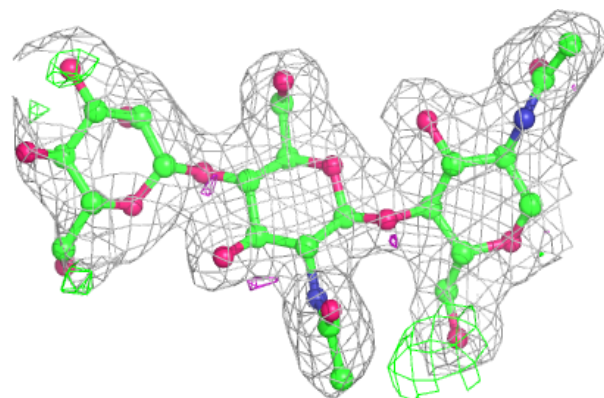


**Electron density around Chain E:**

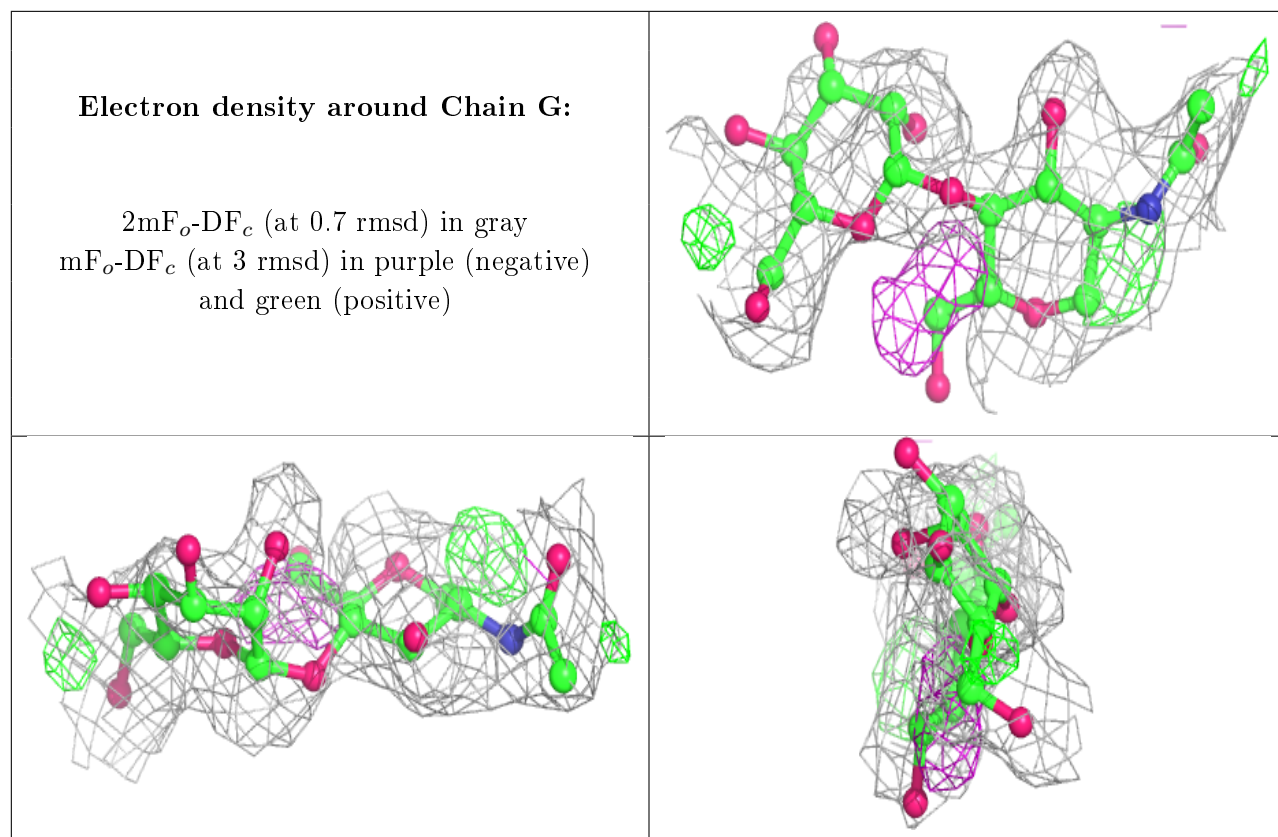
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)





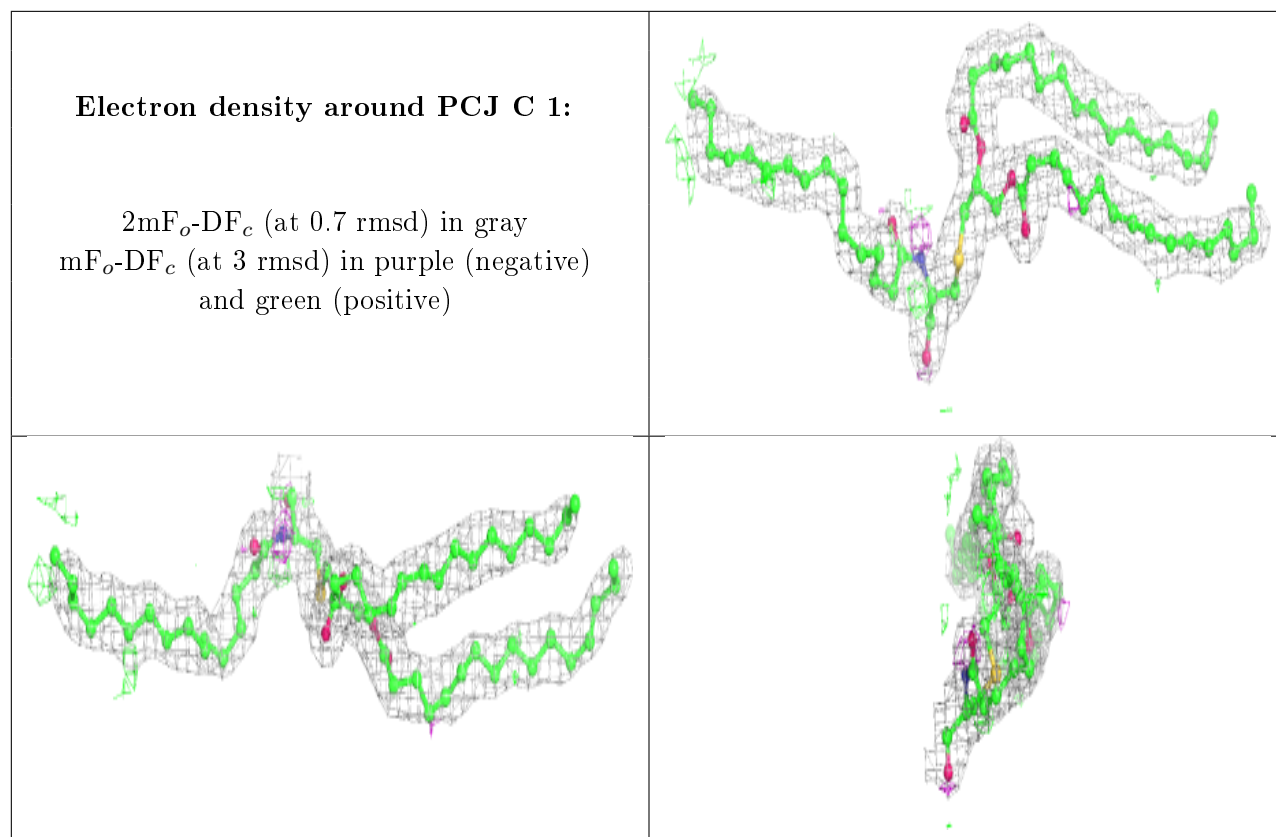


## 6.4 Ligands [i](#)

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
8	NAG	A	911	14/15	0.55	0.22	71,74,77,78	0
8	NAG	A	901	14/15	0.67	0.46	104,106,107,107	0
8	NAG	B	811	14/15	0.70	0.28	74,78,80,81	0
9	PCJ	C	1	62/62	0.93	0.20	28,37,53,56	0
8	NAG	A	921	14/15	0.94	0.08	31,34,37,37	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.