



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 08:39 PM BST

PDB ID : 3A79
Title : Crystal structure of TLR2-TLR6-Pam2CSK4 complex
Authors : Kang, J.Y.; Jin, M.S.; Lee, J.-O.
Deposited on : 2009-09-20
Resolution : 2.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

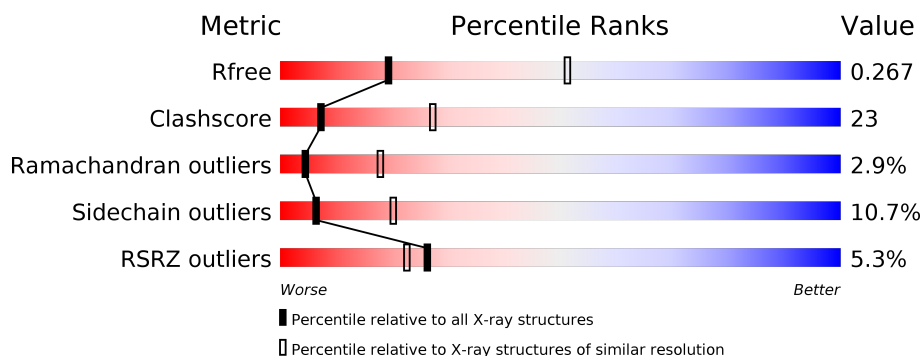
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.




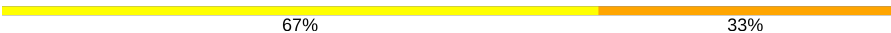

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	580	<div> <div>5%</div> <div> <div>54%</div> <div>35%</div> <div>5%</div> <div>5%</div> </div> </div>
2	B	562	<div> <div>4%</div> <div> <div>52%</div> <div>35%</div> <div>6%</div> <div>7%</div> </div> </div>
3	C	6	<div> <div>33%</div> <div> <div>33%</div> <div>50%</div> <div>17%</div> </div> </div>
4	D	2	<div> <div>50%</div> <div>50%</div> </div>
4	E	2	<div> <div>100%</div> </div>
4	I	2	<div> <div>50%</div> <div>50%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	3	 67%33%
5	G	3	 67%33%
5	H	3	 33%67%

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	NAG	I	1	X	-	-	-
6	NAG	B	981	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8906 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	550	Total	C	N	O	S	0	0	0
			4355	2771	736	828	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	ALA	-	linker	UNP Q4G1L2
A	508	SER	-	linker	UNP Q4G1L2
A	577	LEU	-	expression tag	UNP Q4G1L2
A	578	VAL	-	expression tag	UNP Q4G1L2
A	579	PRO	-	expression tag	UNP Q4G1L2
A	580	ARG	-	expression tag	UNP Q4G1L2

- Molecule 2 is a protein called Toll-like receptor 6, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	525	Total	C	N	O	S	0	0	0
			4192	2675	721	769	27			

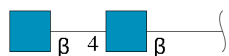
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	LEU	-	expression tag	UNP Q4G1L3
B	560	VAL	-	expression tag	UNP Q4G1L3
B	561	PRO	-	expression tag	UNP Q4G1L3
B	562	ARG	-	expression tag	UNP Q4G1L3

- Molecule 3 is a protein called Pam2CSK4.

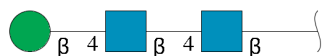
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	S	0	0	0
			49	30	10	8	1			

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



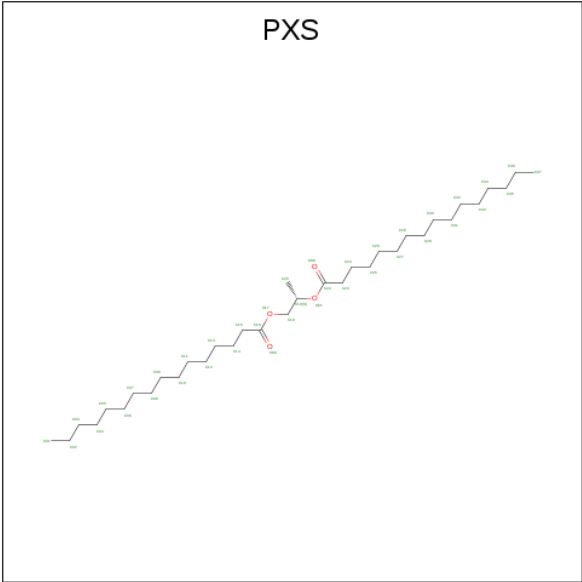
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

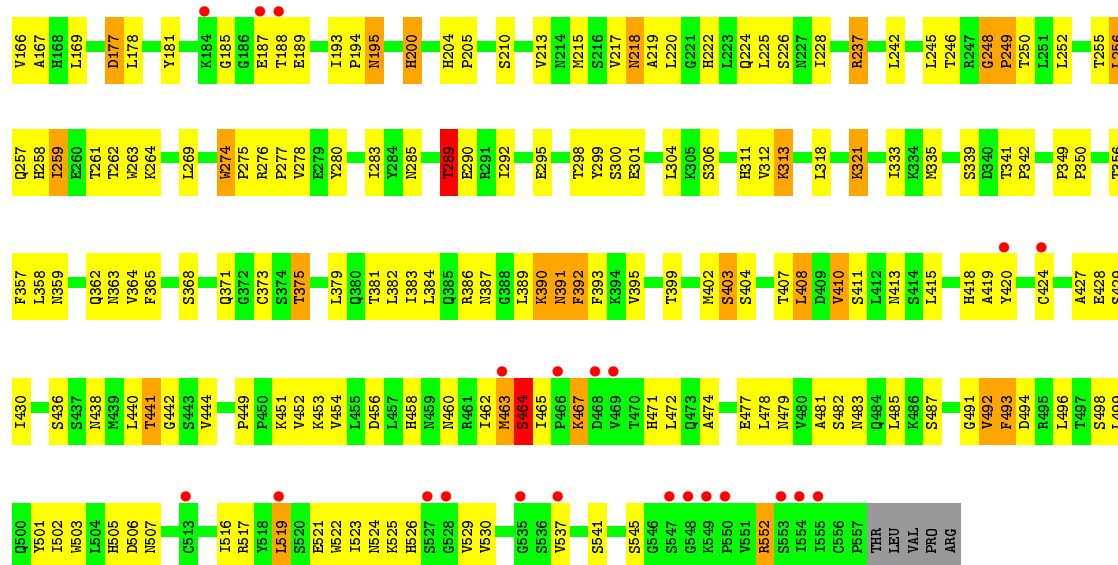


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

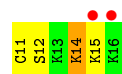
- Molecule 7 is (2S)-propane-1,2-diyl dihexadecanoate (three-letter code: PXS) (formula: C₃₅H₆₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			39	35	4		



• Molecule 3: Pam2CSK4



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



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



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




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

Chain F:  67% 33%

HA01
HA02
BU03

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

Chain G:  67% 33%

HA01
HA02
BU03

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

Chain H:  33% 67%

HA01
HA02
BU03

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.90Å 168.90Å 231.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.11 – 2.90 34.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.11-2.90) 99.7 (34.11-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.280 0.198 , 0.267	Depositor DCC
R_{free} test set	4433 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8906	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PXS, BMA, NAG

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	0.37	0/4439	0.58	0/6013
2	B	0.41	0/4286	0.60	2/5821 (0.0%)
3	C	0.44	0/48	0.47	0/57
All	All	0.39	0/8773	0.59	2/11891 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	313	LYS	CD-CE-NZ	5.86	125.18	111.70
2	B	289	THR	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4355	0	4400	198	0
2	B	4192	0	4201	198	0
3	C	49	0	60	5	0
4	D	28	0	25	2	0
4	E	28	0	25	4	0
4	I	28	0	25	0	0
5	F	39	0	34	0	0
5	G	39	0	34	1	0
5	H	39	0	34	1	0
6	A	28	0	26	0	0
6	B	42	0	39	2	0
7	C	39	0	67	12	0
All	All	8906	0	8970	403	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 23.

The worst 5 of 403 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)
2:B:48:LYS:HD3	2:B:48:LYS:H	1.13	1.08
1:A:269:LEU:HB3	7:C:581:PXS:H01	1.39	1.05
2:B:389:LEU:H	2:B:413:ASN:HD22	1.03	1.02
2:B:218:ASN:OD1	6:B:981:NAG:O6	1.79	1.00
1:A:112:LEU:H	1:A:134:ASN:HD22	1.06	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	548/580 (94%)	449 (82%)	79 (14%)	20 (4%)	3	14
2	B	523/562 (93%)	430 (82%)	83 (16%)	10 (2%)	8	28
3	C	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
All	All	1075/1148 (94%)	882 (82%)	162 (15%)	31 (3%)	4	18

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	CYS
1	A	39	ARG
1	A	531	HIS
1	A	572	ILE
2	B	249	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	510/537 (95%)	457 (90%)	53 (10%)	7	21
2	B	492/525 (94%)	437 (89%)	55 (11%)	6	18
3	C	6/6 (100%)	6 (100%)	0	100	100
All	All	1008/1068 (94%)	900 (89%)	108 (11%)	6	20

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	LEU
2	B	99	ASN
2	B	464	SER
1	A	541	ARG
2	B	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	86	ASN
2	B	200	HIS
2	B	505	HIS
2	B	125	HIS
2	B	204	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 ⓘ

15 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	1,4	14,14,15	0.53	0	17,19,21	1.33	1 (5%)
4	NAG	D	2	4	14,14,15	0.62	0	17,19,21	1.02	2 (11%)
4	NAG	E	1	2,4	14,14,15	0.69	0	17,19,21	1.89	3 (17%)
4	NAG	E	2	4	14,14,15	0.59	0	17,19,21	0.94	1 (5%)
5	NAG	F	1	2,5	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
5	NAG	F	2	5	14,14,15	0.63	0	17,19,21	1.11	0
5	BMA	F	3	5	11,11,12	0.64	0	15,15,17	0.81	0
5	NAG	G	1	2,5	14,14,15	0.58	0	17,19,21	1.03	1 (5%)
5	NAG	G	2	5	14,14,15	0.60	0	17,19,21	1.56	1 (5%)
5	BMA	G	3	5	11,11,12	0.55	0	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	1	2,5	14,14,15	0.46	0	17,19,21	1.48	2 (11%)
5	NAG	H	2	5	14,14,15	0.71	0	17,19,21	1.04	2 (11%)
5	BMA	H	3	5	11,11,12	0.59	0	15,15,17	1.00	1 (6%)
4	NAG	I	1	2,4	14,14,15	0.43	0	17,19,21	2.28	5 (29%)
4	NAG	I	2	4	14,14,15	0.48	0	17,19,21	1.04	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	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
5	NAG	F	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	2,5	-	0/6/23/26	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	NAG	H	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	2,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C1-O5-C5	6.46	120.94	112.19
5	G	2	NAG	C1-O5-C5	5.30	119.38	112.19
4	E	1	NAG	C1-O5-C5	4.62	118.46	112.19
4	D	1	NAG	C1-O5-C5	4.19	117.87	112.19
5	H	1	NAG	C1-O5-C5	4.02	117.63	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	1	NAG	C1

5 of 23 torsion outliers are listed below:

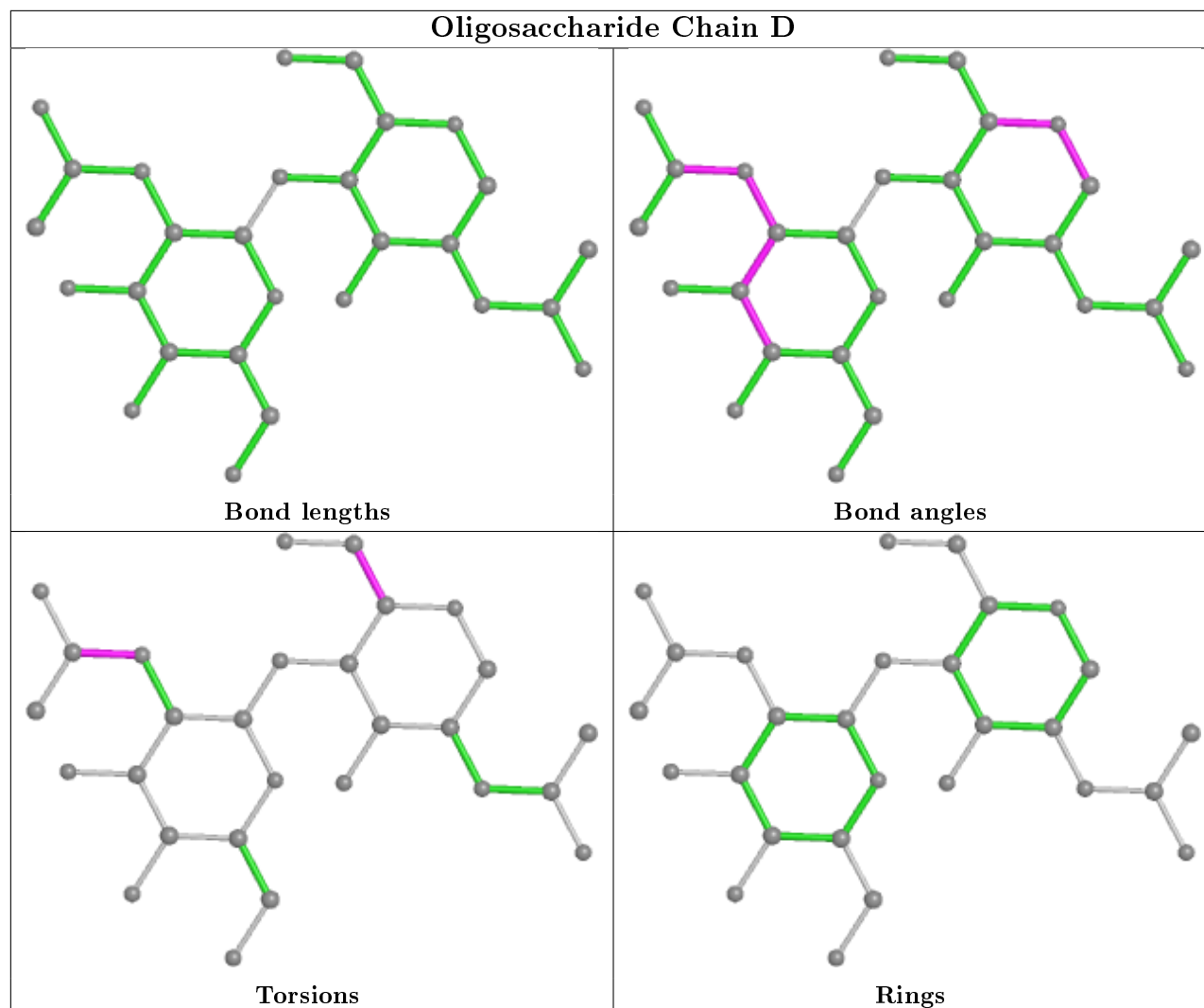
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2

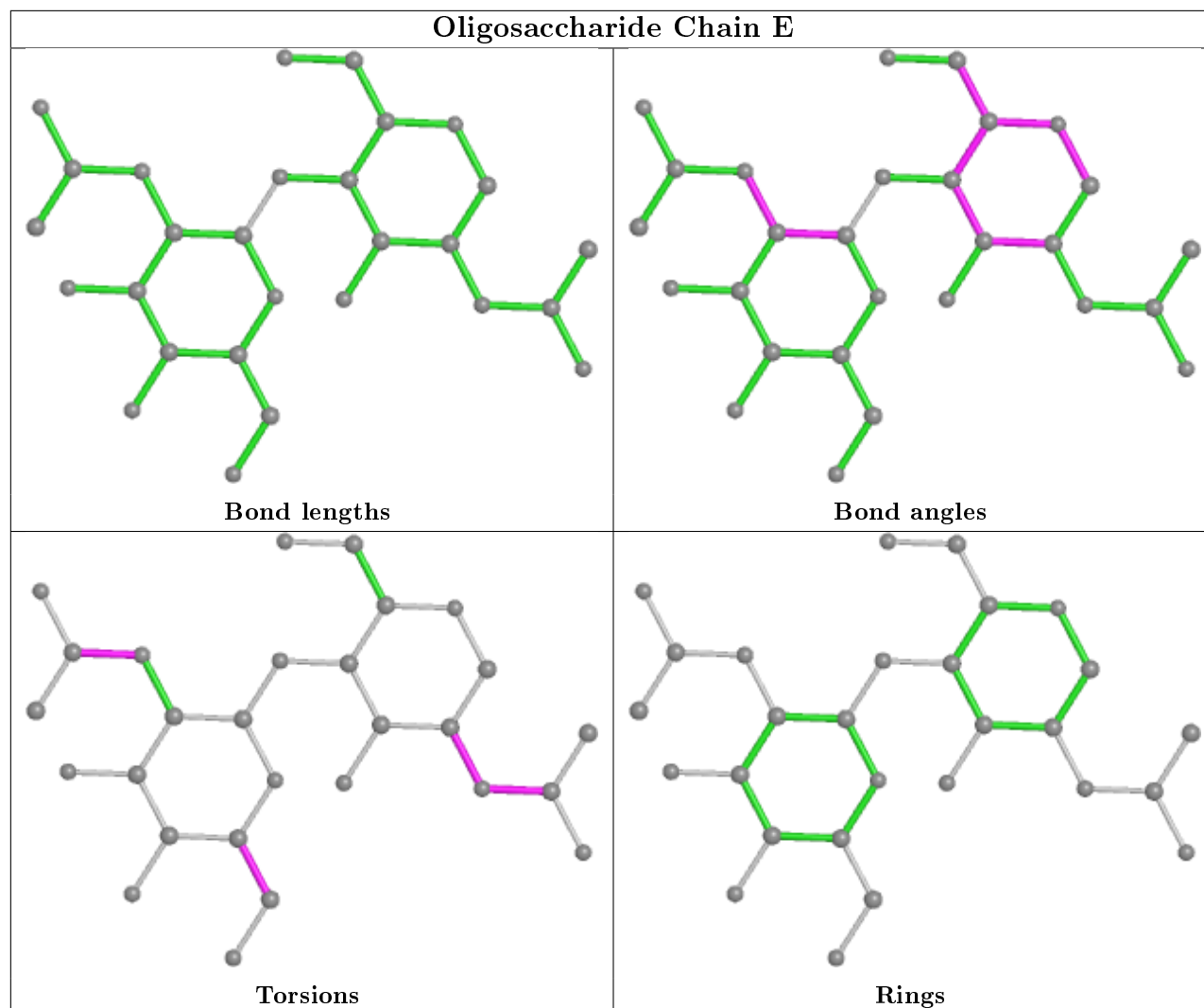
There are no ring outliers.

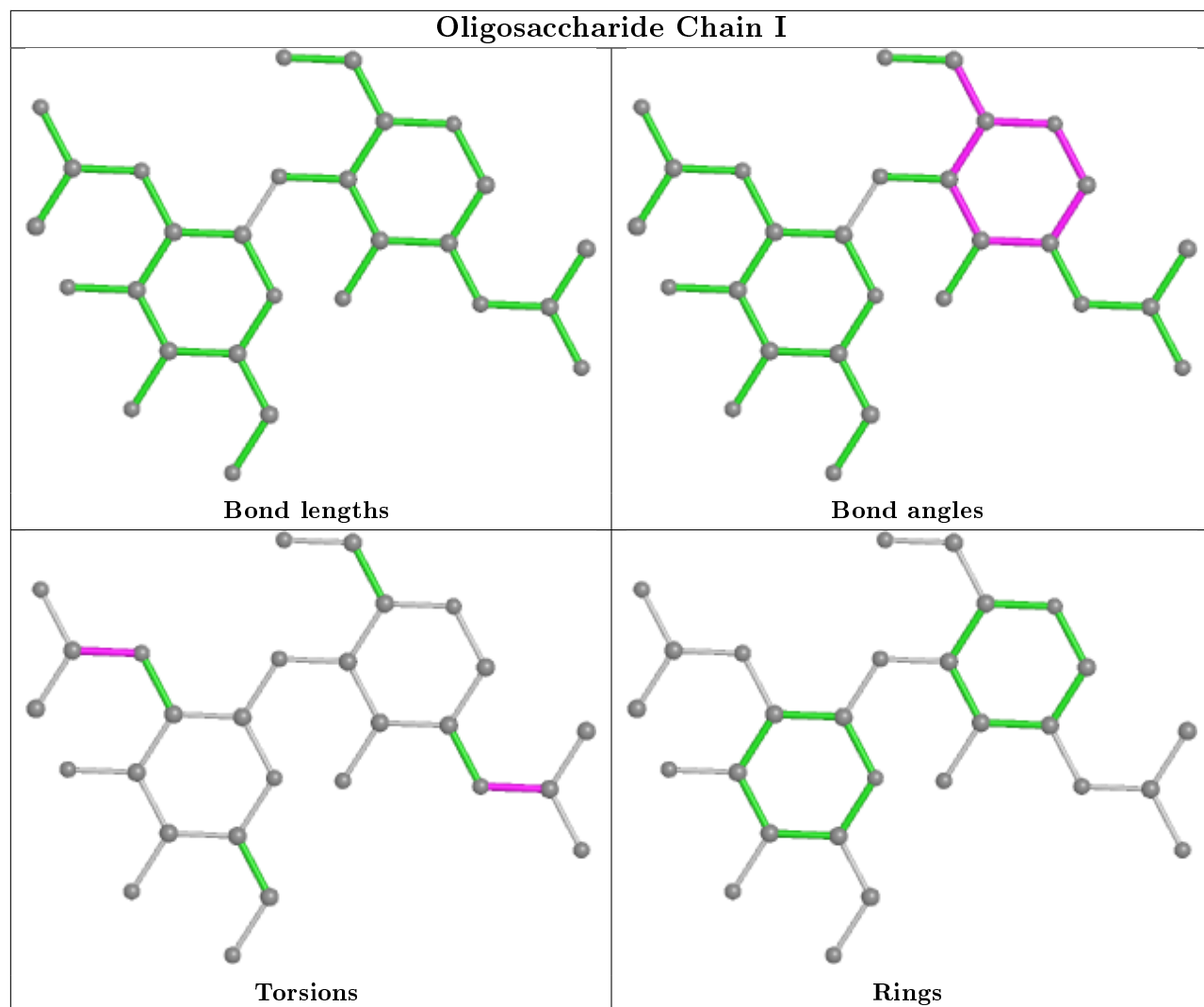
6 monomers are involved in 8 short contacts:

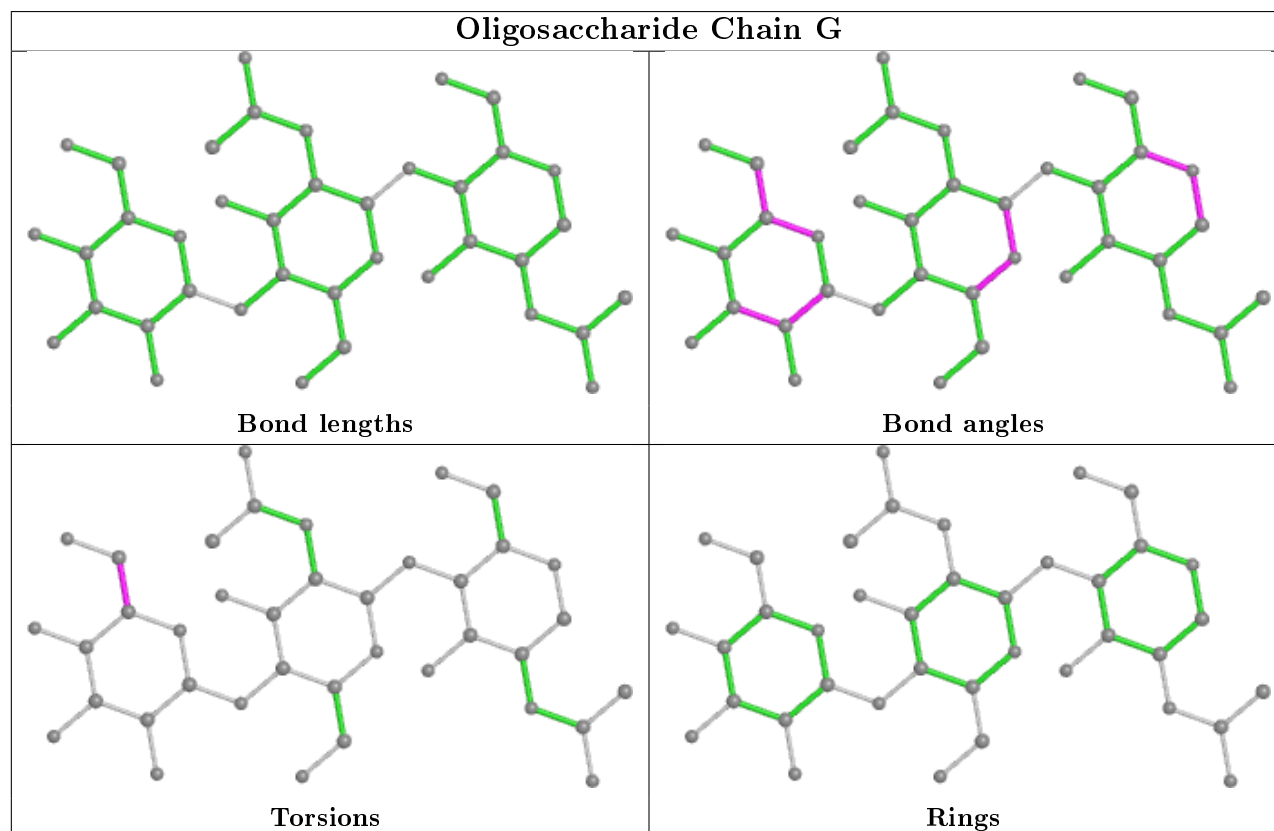
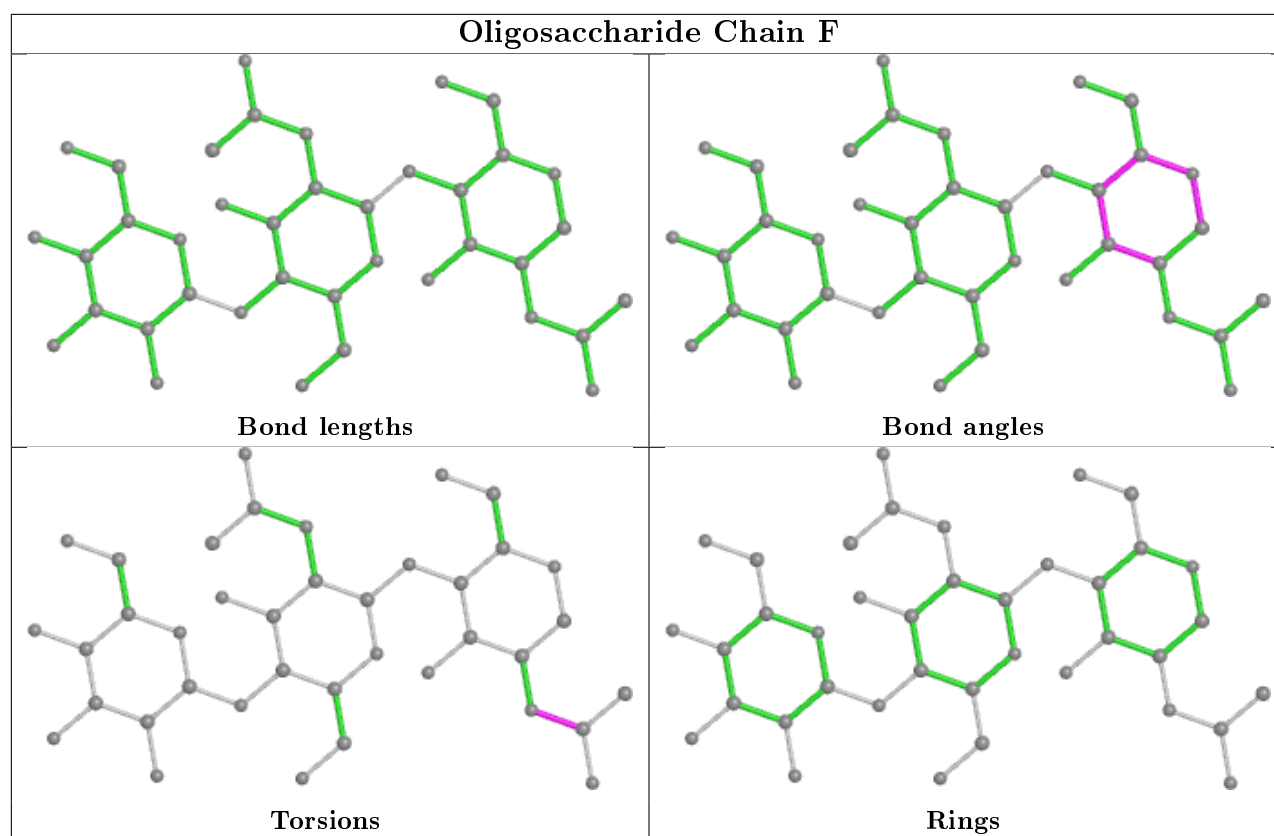
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
4	E	1	NAG	4	0
4	D	2	NAG	2	0
4	E	2	NAG	3	0
5	G	1	NAG	1	0
5	H	2	NAG	1	0

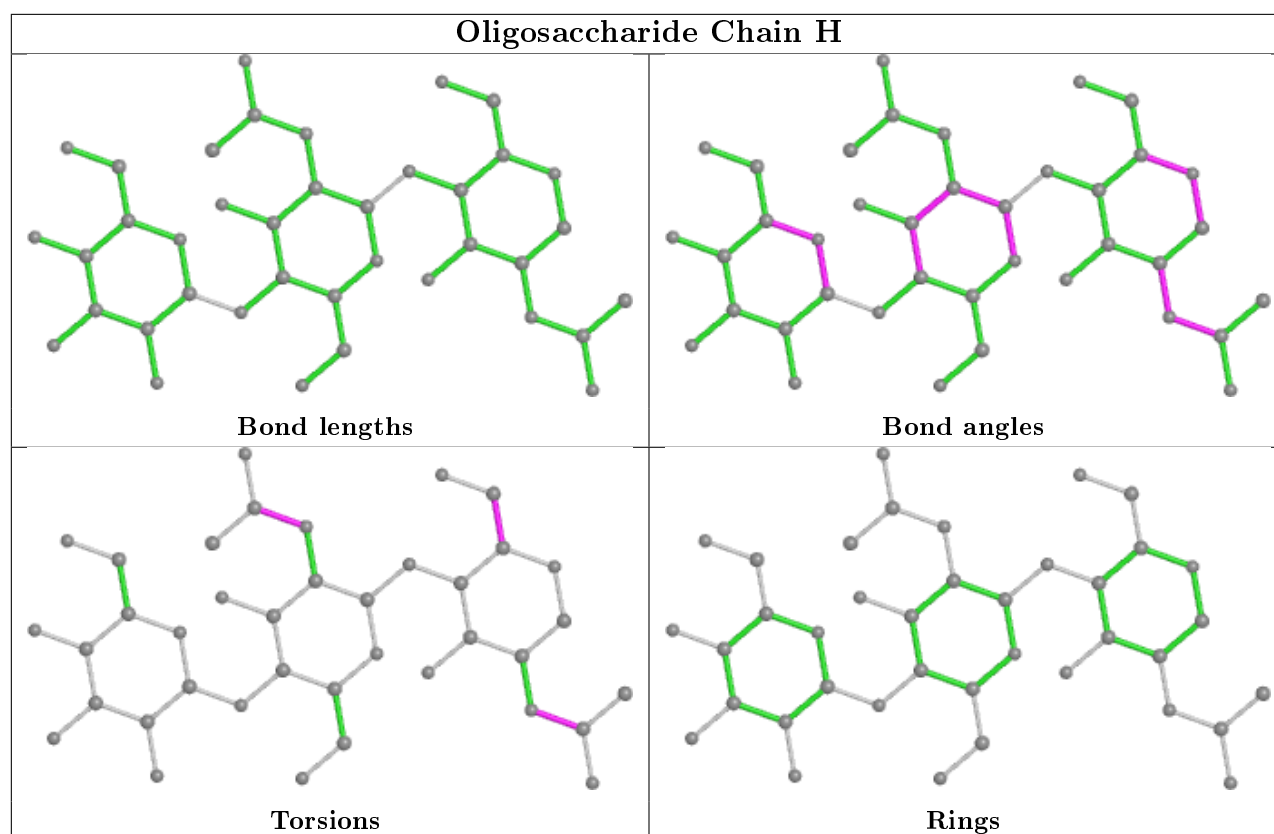
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	811	1	14,14,15	0.45	0	17,19,21	1.49	2 (11%)
6	NAG	B	981	2	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
6	NAG	A	821	1	14,14,15	0.50	0	17,19,21	1.07	1 (5%)
7	PXS	C	581	3	38,38,38	1.85	4 (10%)	40,40,40	0.99	3 (7%)
6	NAG	B	911	2	14,14,15	0.66	0	17,19,21	1.81	4 (23%)
6	NAG	B	921	2	14,14,15	0.52	0	17,19,21	2.28	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	811	1	-	3/6/23/26	0/1/1/1
6	NAG	B	981	2	-	3/6/23/26	0/1/1/1
6	NAG	A	821	1	-	3/6/23/26	0/1/1/1
7	PXS	C	581	3	-	19/39/39/39	-
6	NAG	B	911	2	-	3/6/23/26	0/1/1/1
6	NAG	B	921	2	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	581	PXS	O21-C19	-9.52	1.30	1.47
7	C	581	PXS	C20-C19	-2.81	1.39	1.51
7	C	581	PXS	O17-C16	2.77	1.41	1.33
7	C	581	PXS	O21-C22	2.23	1.40	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	921	NAG	C1-O5-C5	6.98	121.65	112.19
6	B	981	NAG	C1-O5-C5	6.94	121.60	112.19
6	B	911	NAG	C1-O5-C5	5.50	119.64	112.19
6	A	811	NAG	C1-O5-C5	4.35	118.09	112.19
6	B	981	NAG	C1-C2-N2	3.41	116.31	110.49

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

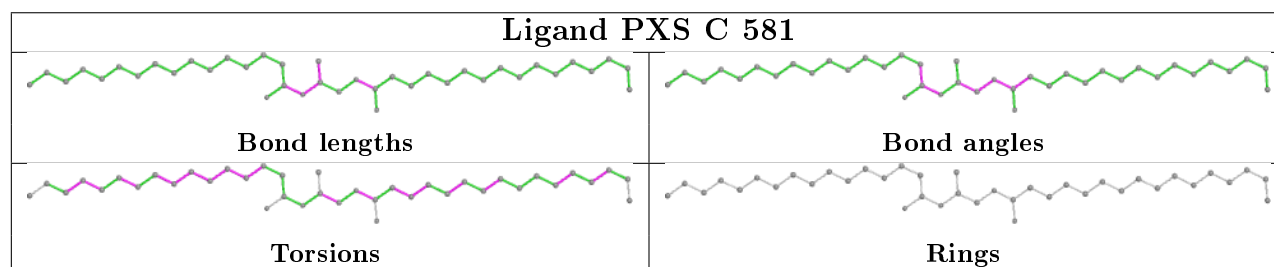
Mol	Chain	Res	Type	Atoms
6	A	811	NAG	C8-C7-N2-C2
6	A	811	NAG	O7-C7-N2-C2
6	B	981	NAG	C1-C2-N2-C7
6	B	981	NAG	C8-C7-N2-C2
6	B	981	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	981	NAG	2	0
7	C	581	PXS	12	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, 95th 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 ²)	Q<0.9
1	A	550/580 (94%)	-0.08	30 (5%) 25 21	43, 78, 165, 240	0
2	B	525/562 (93%)	0.00	25 (4%) 30 27	48, 78, 137, 202	0
3	C	6/6 (100%)	1.60	2 (33%) 0 0	67, 99, 139, 143	0
All	All	1081/1148 (94%)	-0.03	57 (5%) 26 22	43, 78, 151, 240	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	ILE	6.6
1	A	572	ILE	5.6
3	C	16	LYS	5.4
1	A	538	SER	4.9
2	B	469	VAL	4.8

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, 95th 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.

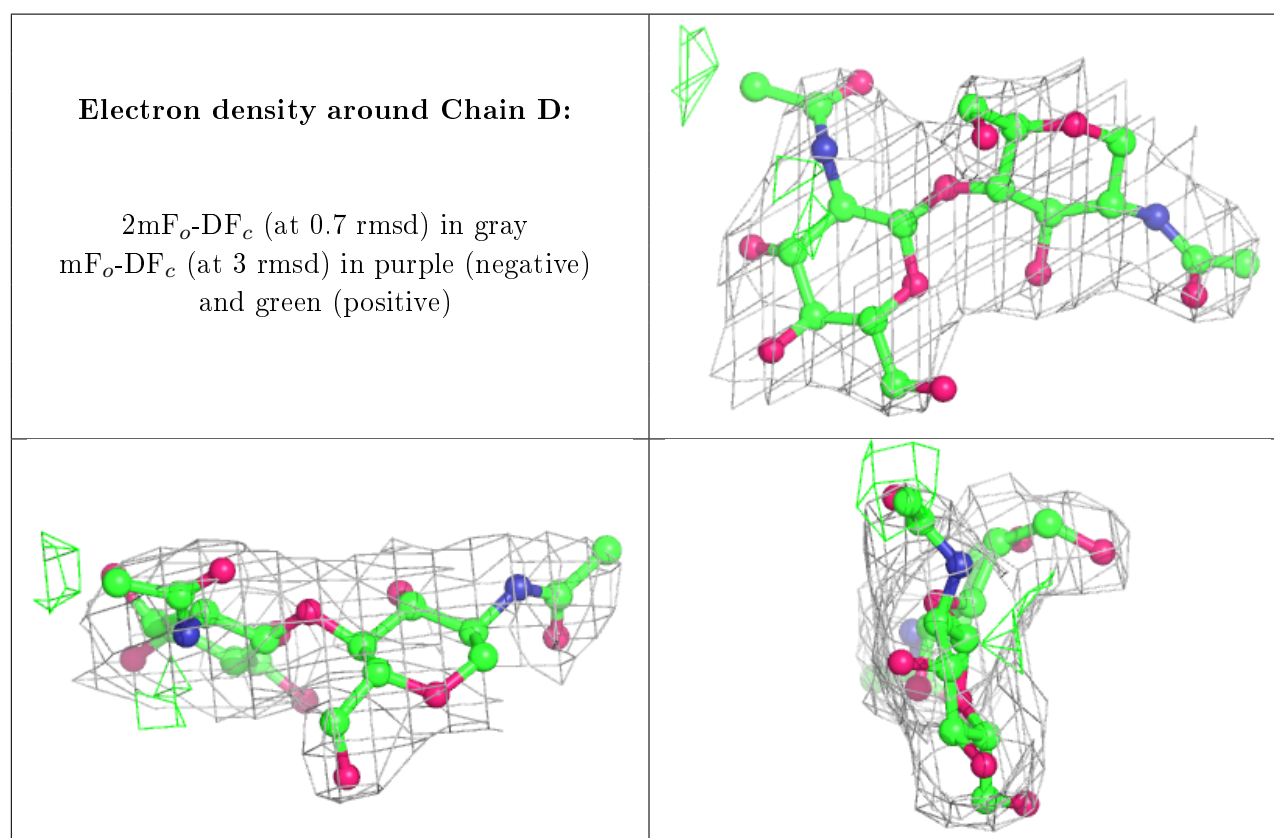
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	H	3	11/12	0.72	0.40	154,164,174,175	0
5	BMA	F	3	11/12	0.79	0.27	86,104,110,112	0
5	NAG	H	2	14/15	0.79	0.32	94,147,165,175	0

Continued on next page...

Continued from previous page...

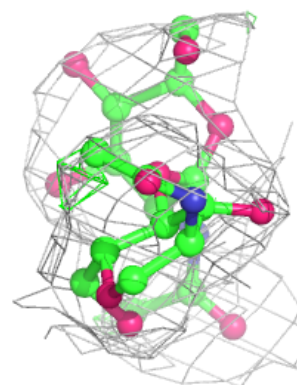
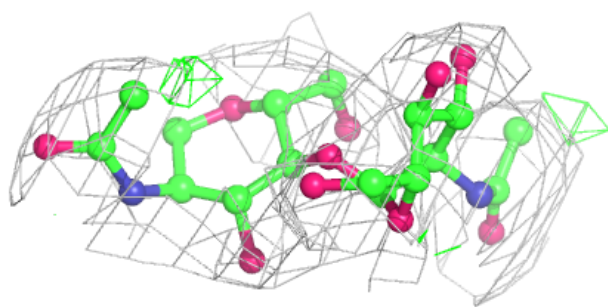
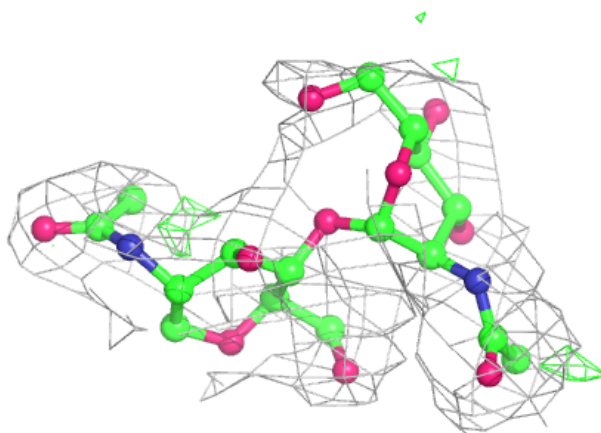
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	I	2	14/15	0.82	0.39	104,126,137,139	0
5	BMA	G	3	11/12	0.83	0.38	95,124,136,138	0
5	NAG	H	1	14/15	0.86	0.26	98,116,136,148	0
4	NAG	E	2	14/15	0.89	0.24	87,135,145,145	0
4	NAG	I	1	14/15	0.89	0.29	89,104,118,119	0
4	NAG	E	1	14/15	0.92	0.18	89,104,121,124	0
4	NAG	D	2	14/15	0.94	0.29	93,111,122,126	0
5	NAG	G	1	14/15	0.95	0.19	57,64,76,81	0
5	NAG	G	2	14/15	0.96	0.30	61,71,91,101	0
5	NAG	F	1	14/15	0.96	0.14	58,67,79,80	0
4	NAG	D	1	14/15	0.96	0.16	71,84,92,97	0
5	NAG	F	2	14/15	0.97	0.23	63,76,86,89	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.



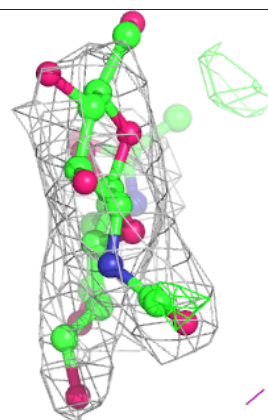
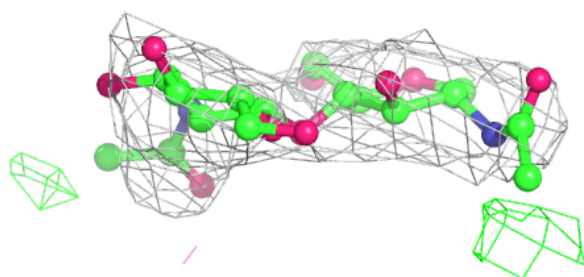
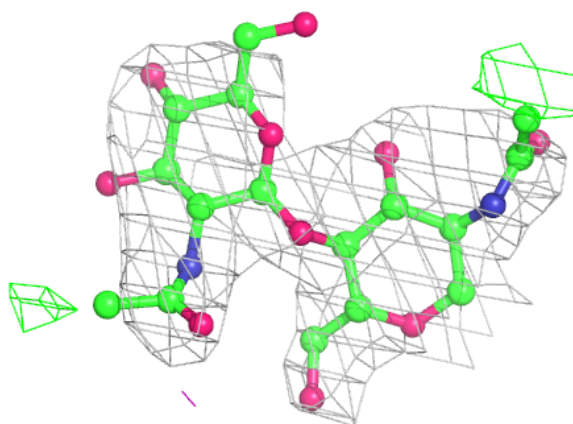
Electron density around Chain E:

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

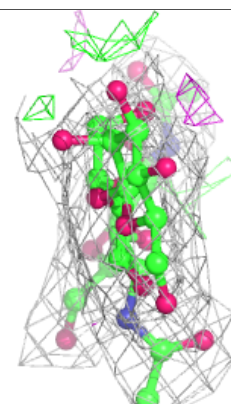
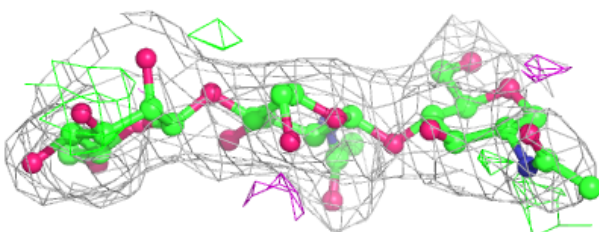
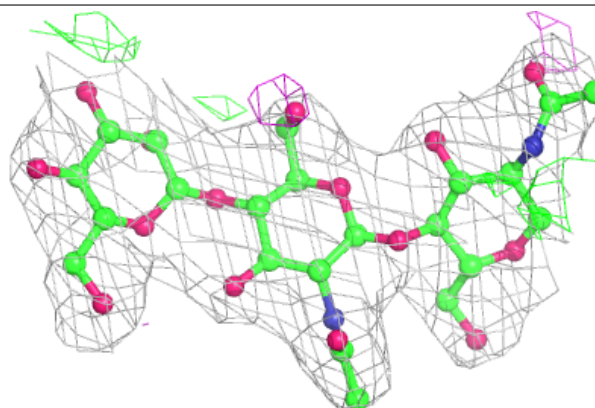


Electron density around Chain I:

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

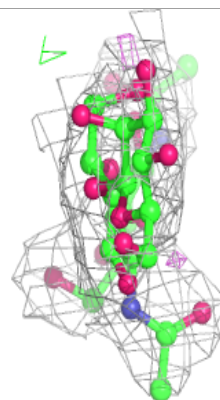
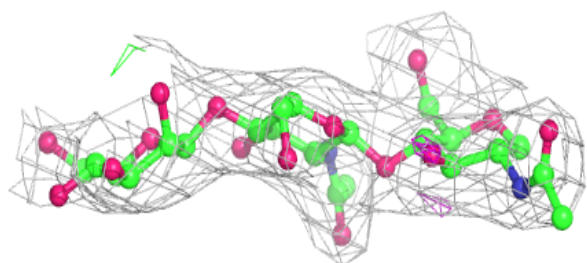
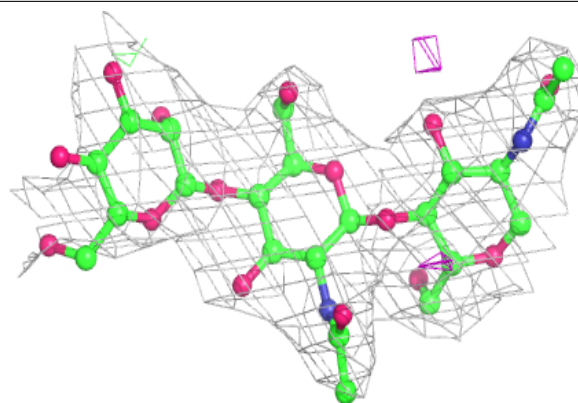
**Electron density around Chain F:**

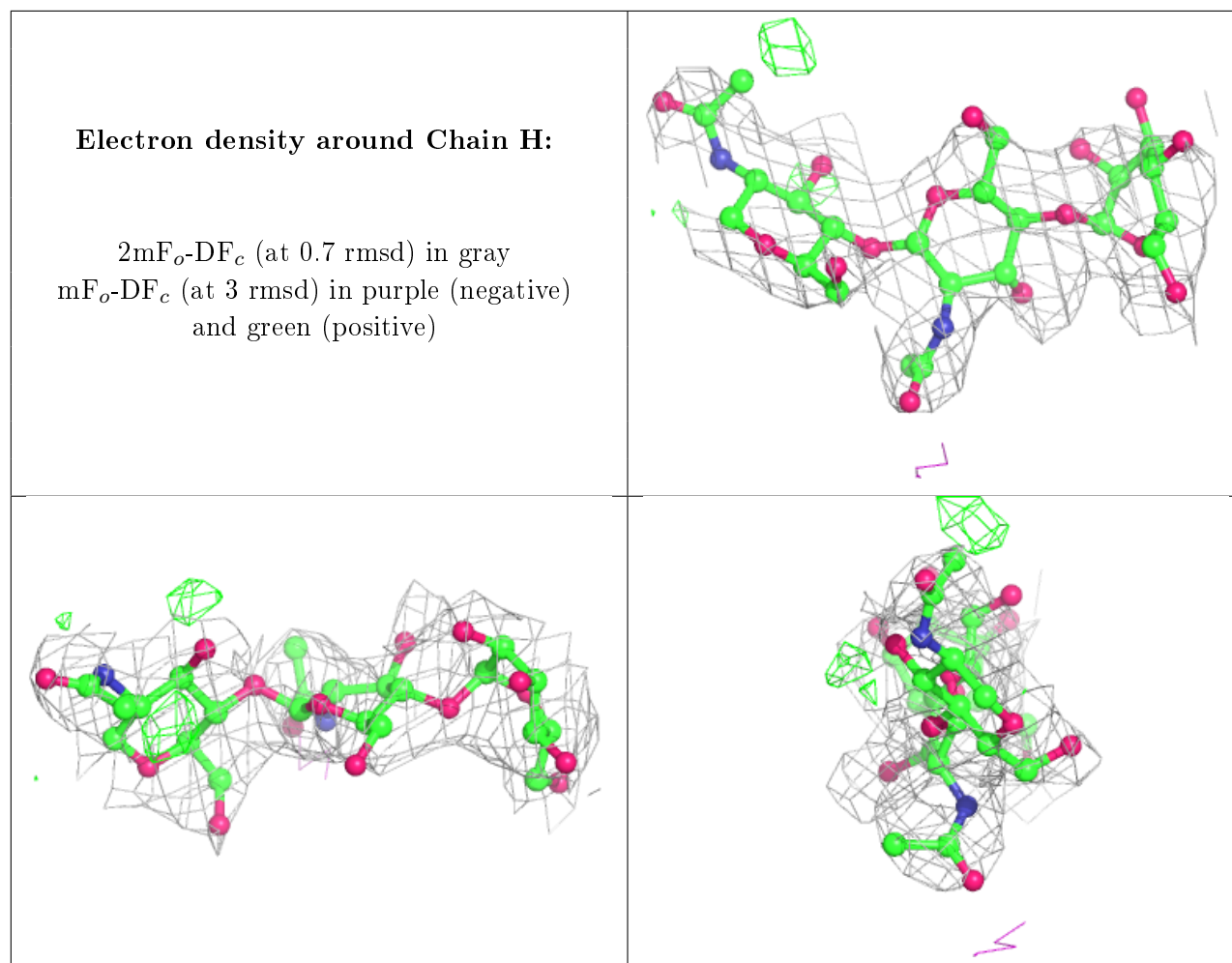
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)



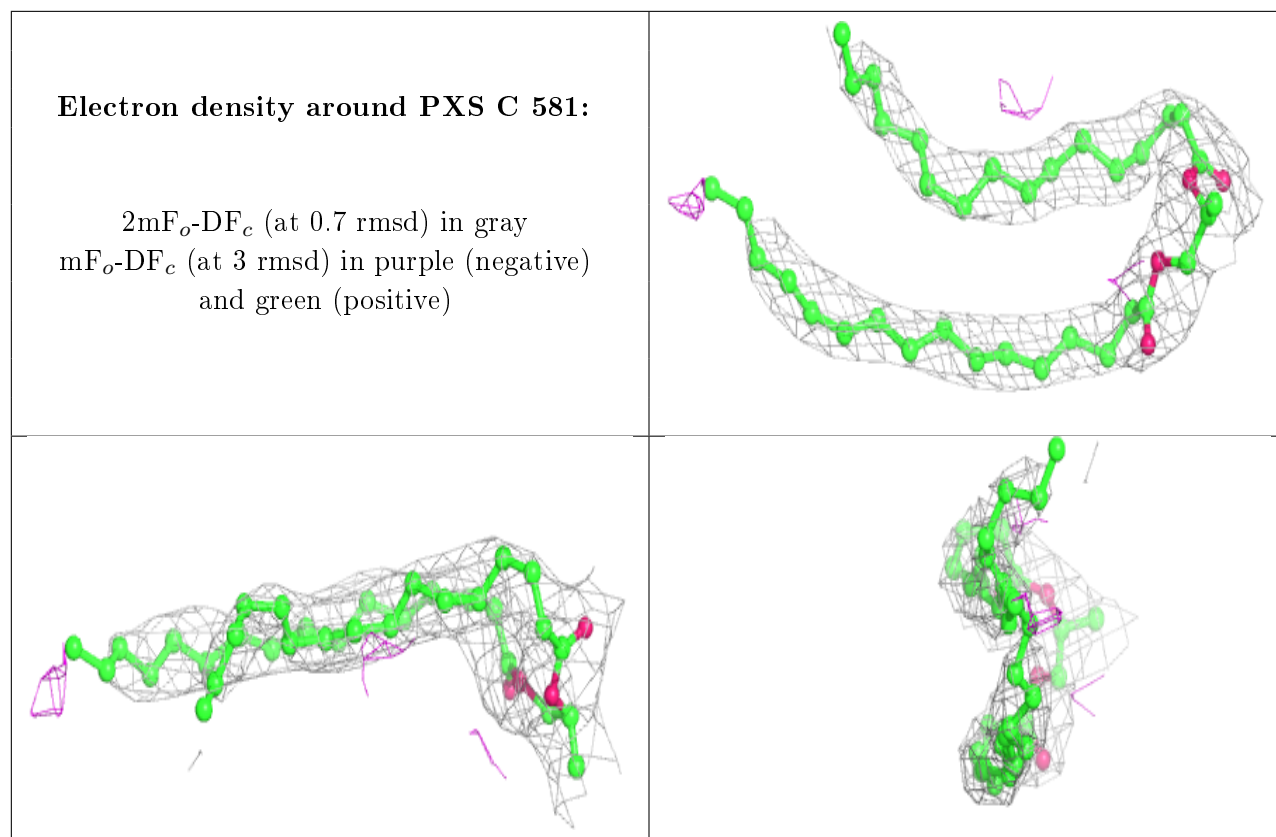


6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
6	NAG	B	981	14/15	0.53	0.53	117,139,157,157	0
6	NAG	A	811	14/15	0.70	0.28	96,140,149,153	0
6	NAG	B	921	14/15	0.85	0.34	91,132,147,149	0
6	NAG	A	821	14/15	0.89	0.23	95,109,122,122	0
6	NAG	B	911	14/15	0.92	0.17	64,80,99,110	0
7	PXS	C	581	39/39	0.95	0.25	52,64,96,120	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.