



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 26, 2020 – 12:12 PM JST

PDB ID : 7BU7  
Title : Structure of human beta1 adrenergic receptor bound to BI-167107 and nanobody 6B9  
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Deposited on : 2020-04-04  
Resolution : 2.60 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 : 2.14.6  
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) : 2.14.6

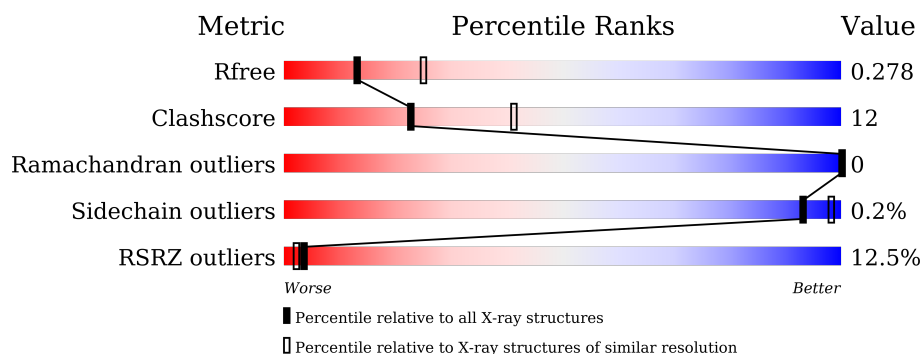
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	516	<div> <div>5%</div> <div> <div>72%</div> <div>15%</div> <div>13%</div> </div> </div>
2	B	128	<div> <div>34%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>100%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	P6G	A	1414	-	-	X	X
3	GLC	C	1	-	-	-	X
3	GLC	C	2	-	-	X	X
3	GLC	D	2	-	-	-	X
4	SO4	A	1406	-	-	X	-
6	1WV	A	1410	-	-	-	X
8	EPE	A	1412	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4669 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 Endolysin,Beta-1 adrenergic receptor chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3553	2304	607	620	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	884	ASP	-	expression tag	UNP D9IEF7
A	885	TYR	-	expression tag	UNP D9IEF7
A	886	LYS	-	expression tag	UNP D9IEF7
A	887	ASP	-	expression tag	UNP D9IEF7
A	888	ASP	-	expression tag	UNP D9IEF7
A	889	ASP	-	expression tag	UNP D9IEF7
A	890	ASP	-	expression tag	UNP D9IEF7
A	891	ALA	-	expression tag	UNP D9IEF7
A	944	THR	CYS	engineered mutation	UNP D9IEF7
A	987	ALA	CYS	engineered mutation	UNP D9IEF7
A	1052	ALA	-	linker	UNP D9IEF7
A	1053	ALA	-	linker	UNP D9IEF7

- Molecule 2 is a protein called camelid antibody fragment.

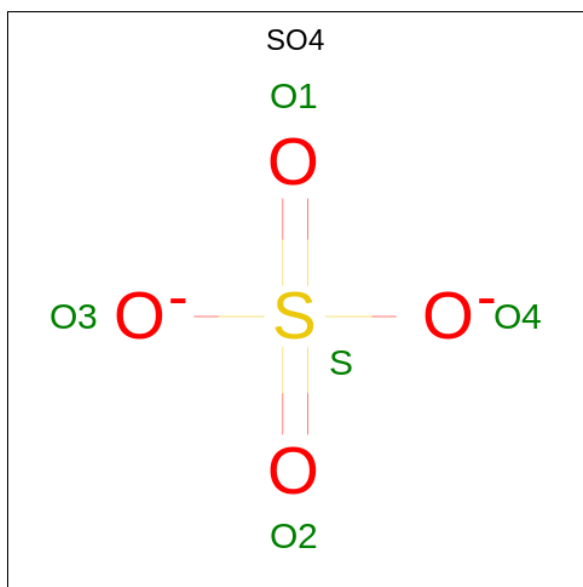
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			910	569	159	178	4			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



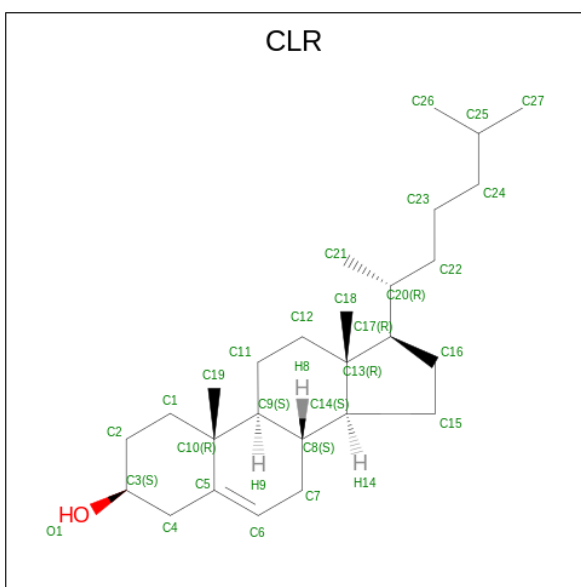
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			
3	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



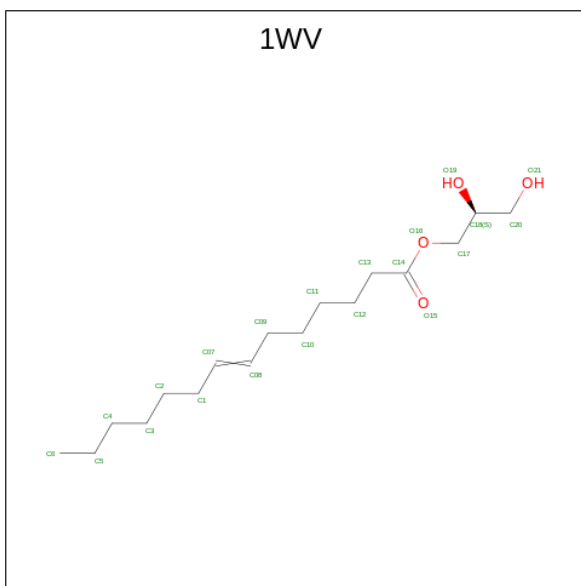
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 6 is (2S)-2,3-dihydroxypropyl (7Z)-tetradec-7-enoate (three-letter code: 1WV) (formula:  $C_{17}H_{32}O_4$ ).

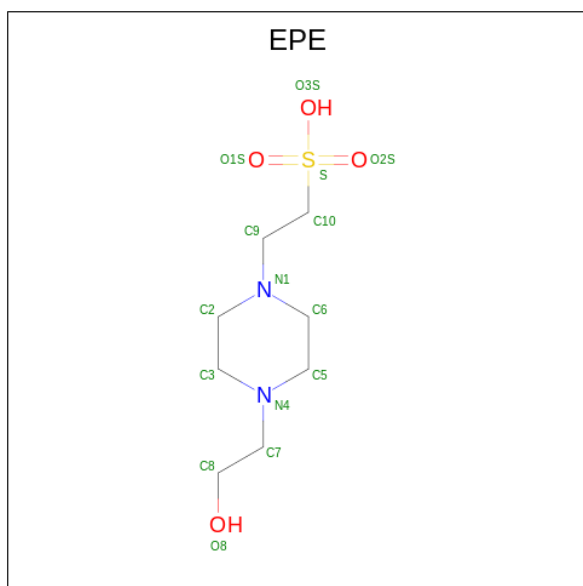


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

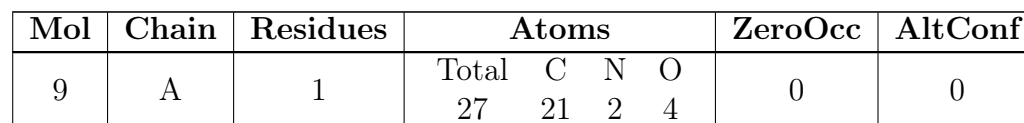
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is 8-[(1R)-2-{[1,1-dimethyl-2-(2-methylphenyl)ethyl]amino}-1-hydroxyethyl]-5-hydroxy-2H-1,4-benzoxazin-3(4H)-one (three-letter code: P0G) (formula: C<sub>21</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



- P6G
- 
- Chemical structure of P6G (poly(6-geranyl glycidyl ether)) showing a linear chain of six repeating units. The structure is labeled with atom numbers: O1, C2, C3, O4, C5, C6, O7, C8, C9, O10, C11, C12, O13, C14, C15, O16, C17, C18, and OH19.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 11 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	25	Total 25	O 25	0	0



Chain D:

100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	377.98Å 66.22Å 47.86Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	19.98 – 2.60 49.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.98-2.60) 96.4 (49.76-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.243 , 0.270 0.249 , 0.278	Depositor DCC
$R_{free}$ test set	2000 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.5	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	0.89	EDS
Total number of atoms	4669	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: P0G, NA, GLC, SO4, P6G, 1WV, EPE, CLR

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	0.40	0/3632	0.48	0/4931
2	B	0.33	0/927	0.50	0/1256
All	All	0.39	0/4559	0.48	0/6187

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	3553	0	3608	68	0
2	B	910	0	878	28	0
3	C	23	0	20	6	0
3	D	23	0	20	2	0
4	A	30	0	0	3	0
5	A	28	0	46	1	0
6	A	15	0	18	0	0
7	A	1	0	0	0	0
8	A	15	0	17	1	0
9	A	27	0	25	5	0
10	A	19	0	26	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	25	0	0	0	0
All	All	4669	0	4658	107	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 12.

The worst 5 of 107 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:1028:TRP:HA	3:C:2:GLC:O3	1.57	1.03
1:A:1360:VAL:HG22	9:A:1413:P0G:HAH	1.51	0.91
1:A:1028:TRP:CA	3:C:2:GLC:O3	2.20	0.89
1:A:1107:MET:HE2	1:A:1142:VAL:HG23	1.56	0.88
1:A:1107:MET:CE	1:A:1142:VAL:HG23	2.12	0.79

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	443/516 (86%)	437 (99%)	6 (1%)	0	100	100
2	B	118/128 (92%)	117 (99%)	1 (1%)	0	100	100
All	All	561/644 (87%)	554 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/426 (88%)	375 (100%)	1 (0%)	92	98
2	B	94/102 (92%)	94 (100%)	0	100	100
All	All	470/528 (89%)	469 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1363	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

4 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	GLC	C	1	3	12,12,12	1.21	1 (8%)	17,17,17	2.54	9 (52%)
3	GLC	C	2	3	11,11,12	2.04	5 (45%)	15,15,17	5.01	10 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	D	1	3	12,12,12	1.53	3 (25%)	17,17,17	2.70	9 (52%)
3	GLC	D	2	3	11,11,12	1.71	2 (18%)	15,15,17	2.53	5 (33%)

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	GLC	C	1	3	-	2/2/22/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	1	3	-	1/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	GLC	O3-C3	4.49	1.53	1.43
3	D	2	GLC	O5-C1	3.88	1.49	1.43
3	D	2	GLC	C2-C3	-2.89	1.48	1.52
3	D	1	GLC	O5-C1	2.76	1.49	1.42
3	C	2	GLC	C2-C3	2.60	1.56	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	GLC	O2-C2-C1	-10.94	86.76	109.15
3	C	2	GLC	O5-C5-C6	-9.87	91.73	107.20
3	D	2	GLC	C1-C2-C3	7.03	118.31	109.67
3	C	2	GLC	C1-C2-C3	6.90	118.15	109.67
3	C	2	GLC	O3-C3-C2	6.16	121.79	109.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	GLC	O5-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
3	C	2	GLC	C4-C5-C6-O6

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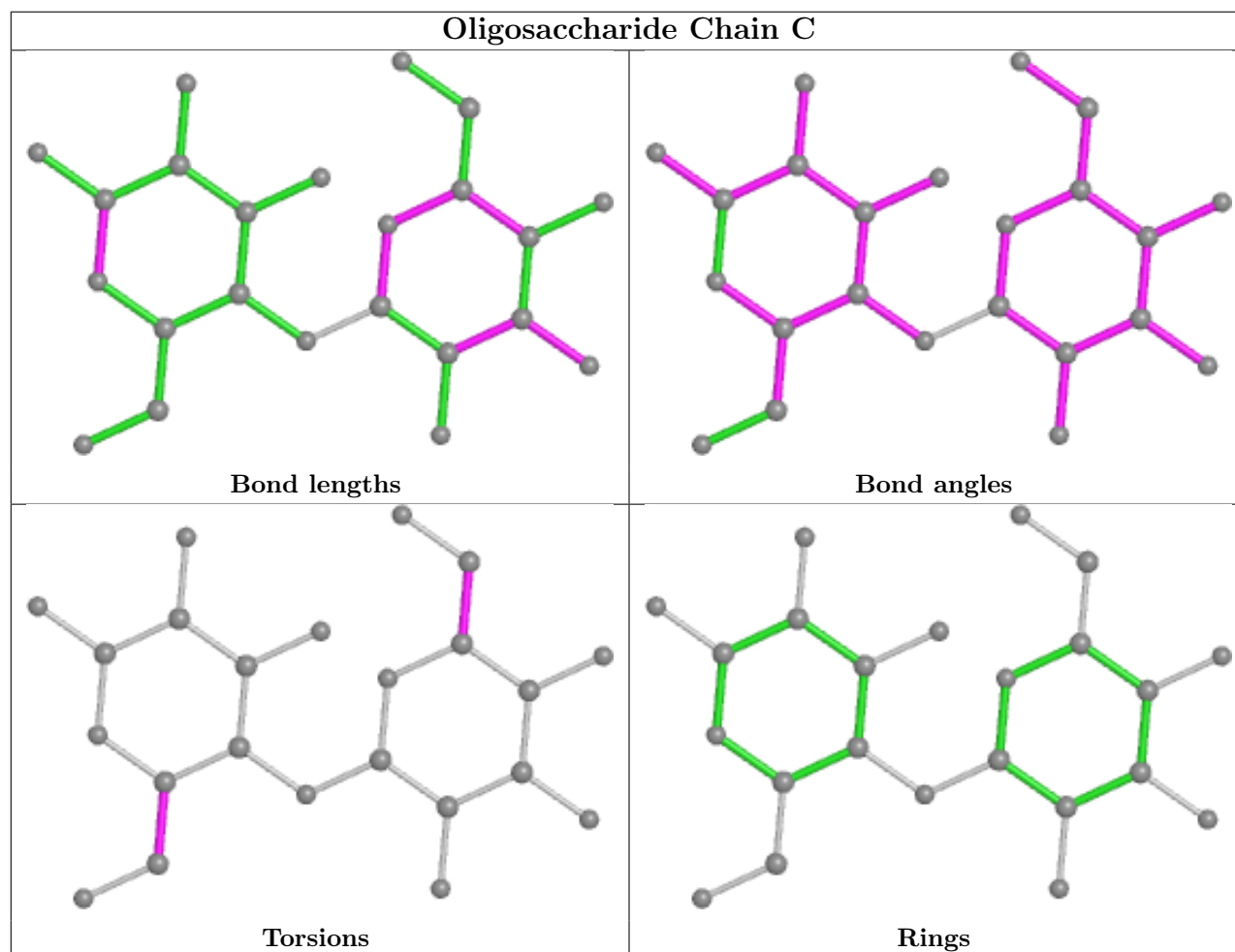
Mol	Chain	Res	Type	Atoms
3	D	1	GLC	C4-C5-C6-O6

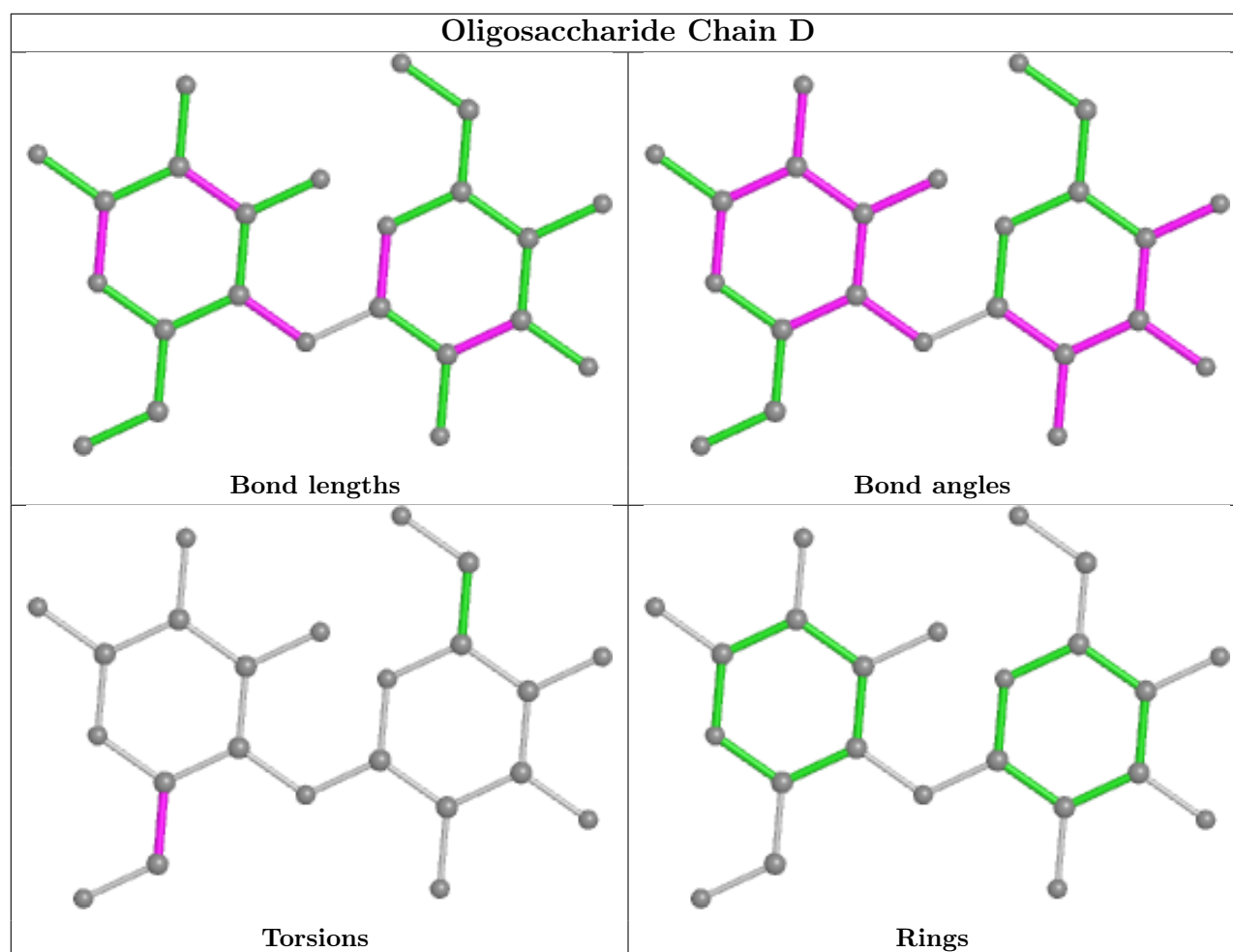
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	GLC	2	0
3	C	2	GLC	6	0
3	D	1	GLC	2	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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z  > 2$
4	SO4	A	1403	-	4,4,4	0.11	0	6,6,6	0.09	0
4	SO4	A	1408	-	4,4,4	0.14	0	6,6,6	0.07	0
9	P0G	A	1413	-	27,29,29	1.25	2 (7%)	32,42,42	1.37	3 (9%)
4	SO4	A	1407	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	1406	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CLR	A	1409	-	31,31,31	0.69	0	48,48,48	1.14	5 (10%)
6	1WV	A	1410	-	14,14,20	1.91	3 (21%)	15,15,21	2.37	4 (26%)
4	SO4	A	1405	-	4,4,4	0.14	0	6,6,6	0.06	0
10	P6G	A	1414	-	18,18,18	0.72	0	17,17,17	0.73	0
8	EPE	A	1412	-	15,15,15	2.20	1 (6%)	18,20,20	2.14	6 (33%)
4	SO4	A	1404	-	4,4,4	0.16	0	6,6,6	0.12	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	P0G	A	1413	-	-	4/15/24/24	0/3/3/3
5	CLR	A	1409	-	-	3/10/68/68	0/4/4/4
10	P6G	A	1414	-	-	13/16/16/16	-
8	EPE	A	1412	-	-	5/9/19/19	0/1/1/1
6	1WV	A	1410	-	-	8/14/14/20	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1412	EPE	C10-S	-8.43	1.65	1.77
6	A	1410	1WV	O15-C14	5.18	1.37	1.22
9	A	1413	P0G	CBA-NAP	-4.18	1.45	1.49
9	A	1413	P0G	CAW-CAZ	-3.71	1.49	1.52
6	A	1410	1WV	C07-C08	3.45	1.51	1.28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1410	1WV	O16-C14-O15	-7.36	105.01	123.59
8	A	1412	EPE	O2S-S-C10	5.01	112.95	106.92
9	A	1413	P0G	OAR-CAY-CAW	4.53	123.12	116.75
6	A	1410	1WV	O15-C14-C13	-4.17	107.45	123.73
9	A	1413	P0G	OAR-CAY-CAX	-3.94	116.18	121.22

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

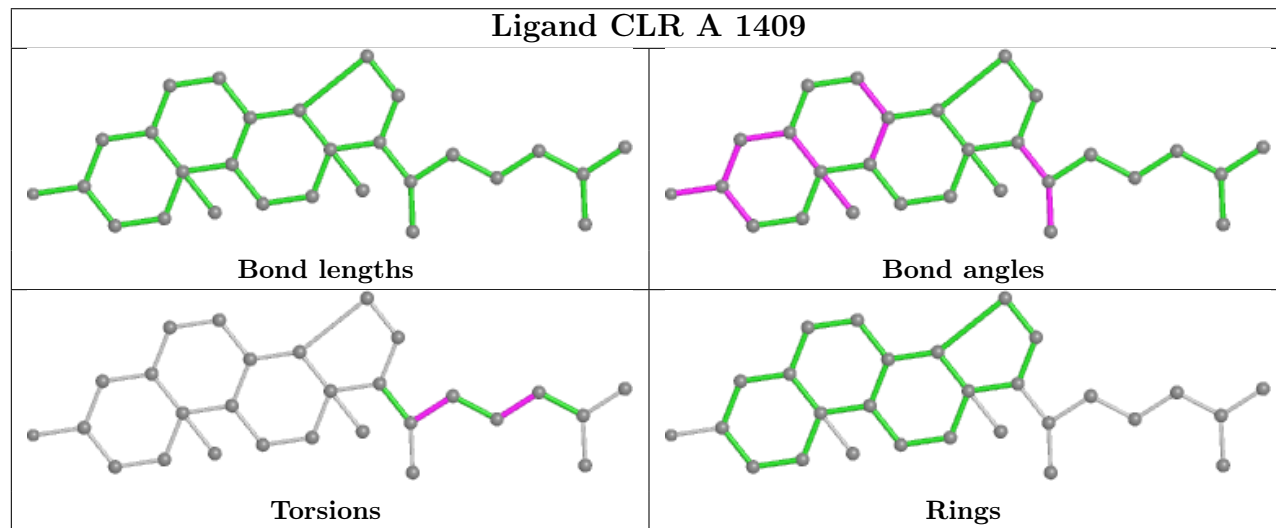
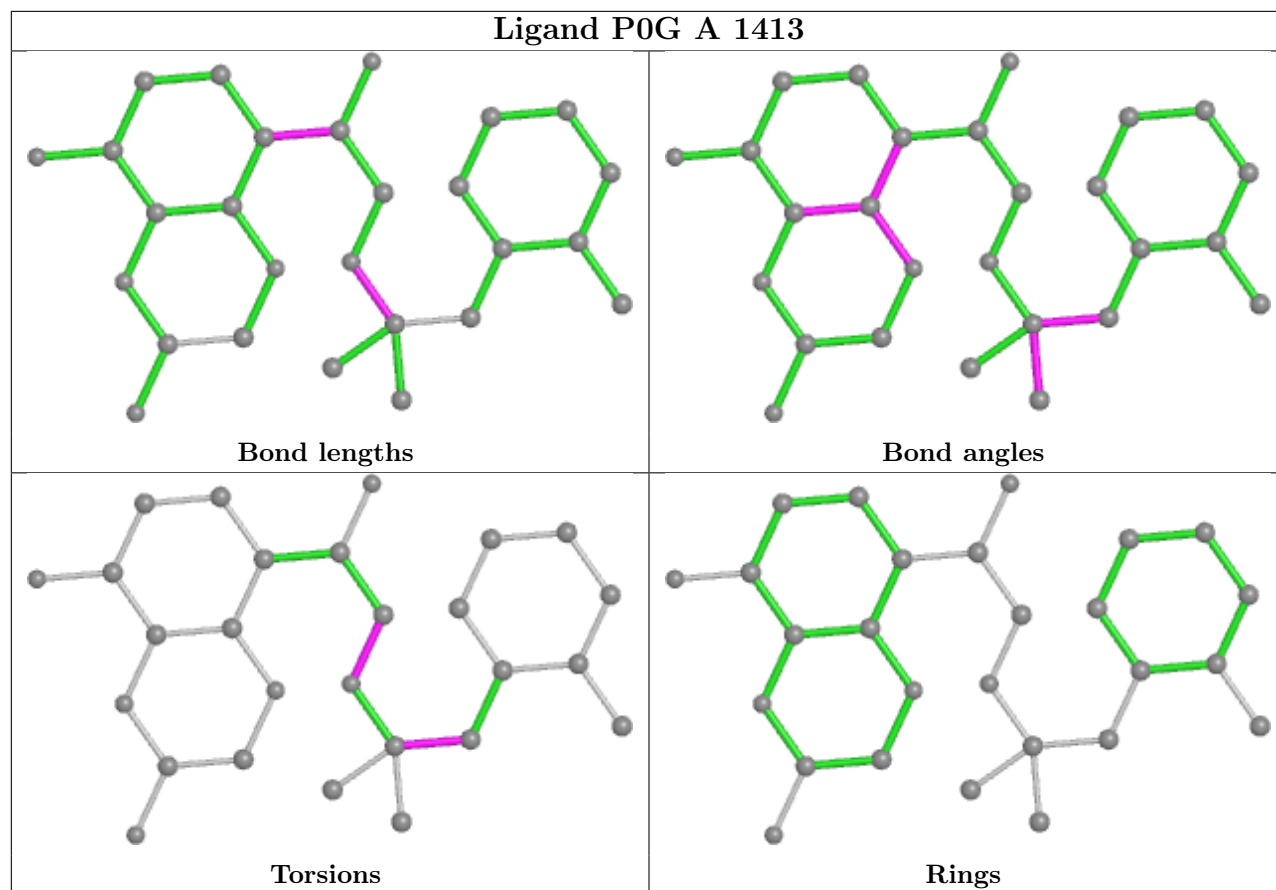
Mol	Chain	Res	Type	Atoms
9	A	1413	P0G	CAV-CAO-CBA-CAB
9	A	1413	P0G	CAV-CAO-CBA-CAC
9	A	1413	P0G	CAV-CAO-CBA-NAP
8	A	1412	EPE	C9-C10-S-O2S
10	A	1414	P6G	O10-C11-C12-O13

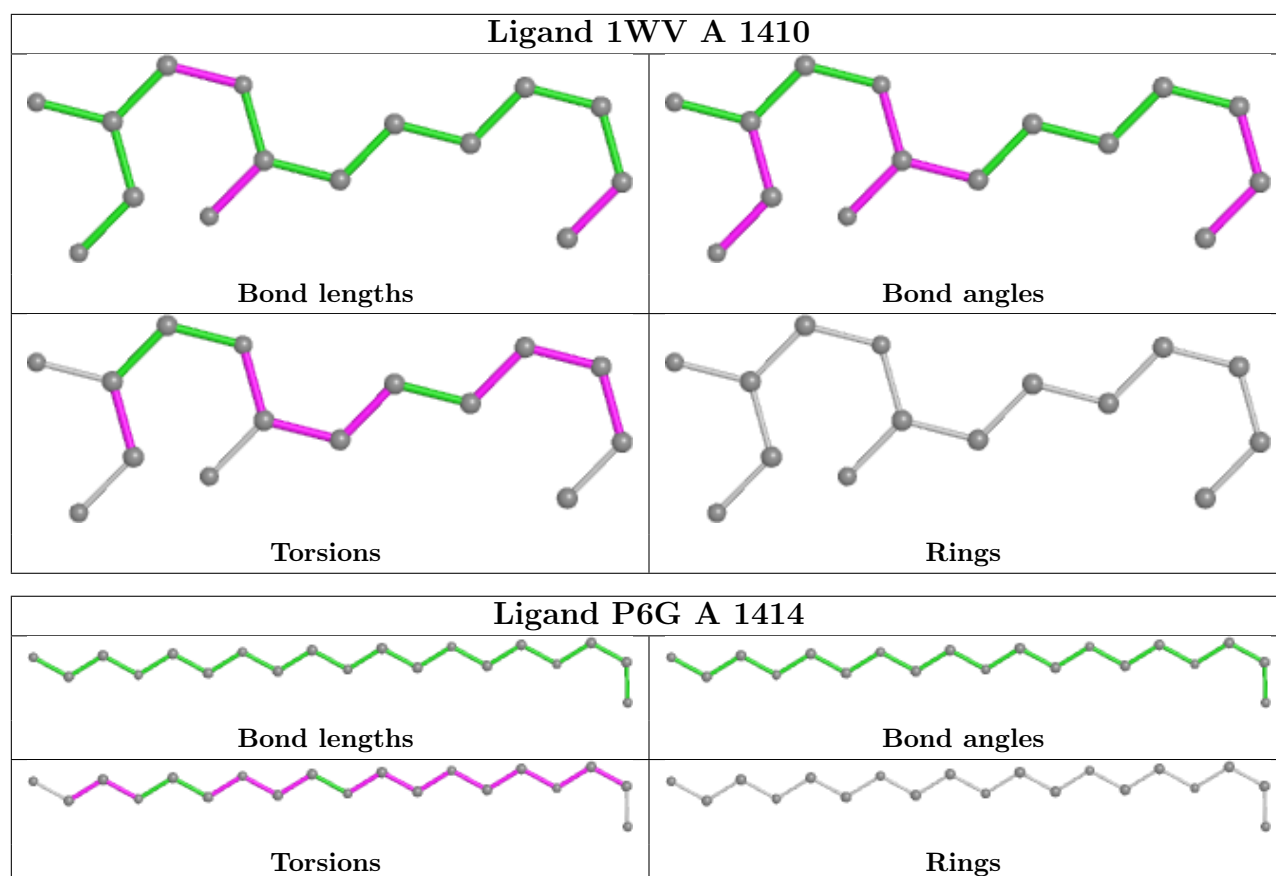
There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1413	P0G	5	0
4	A	1406	SO4	2	0
5	A	1409	CLR	1	0
10	A	1414	P6G	11	0
8	A	1412	EPE	1	0
4	A	1404	SO4	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	447/516 (86%)	0.53	28 (6%) 20 15	39, 72, 115, 145	0
2	B	120/128 (93%)	1.60	43 (35%) 0 0	89, 118, 132, 139	0
All	All	567/644 (88%)	0.76	71 (12%) 3 2	39, 78, 125, 145	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1255	VAL	9.9
2	B	74	ALA	9.2
2	B	107	TYR	7.1
1	A	1252	GLN	7.0
1	A	1169	LEU	6.9

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

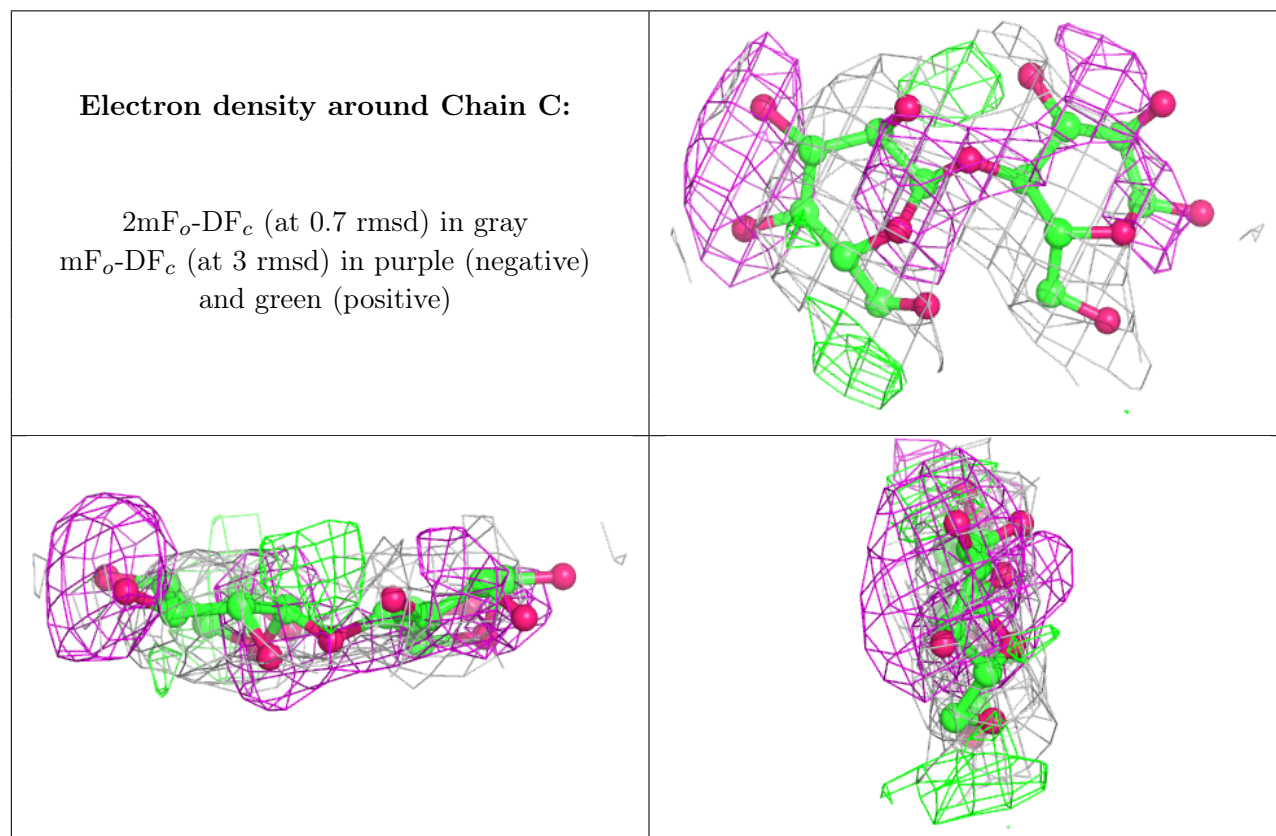
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

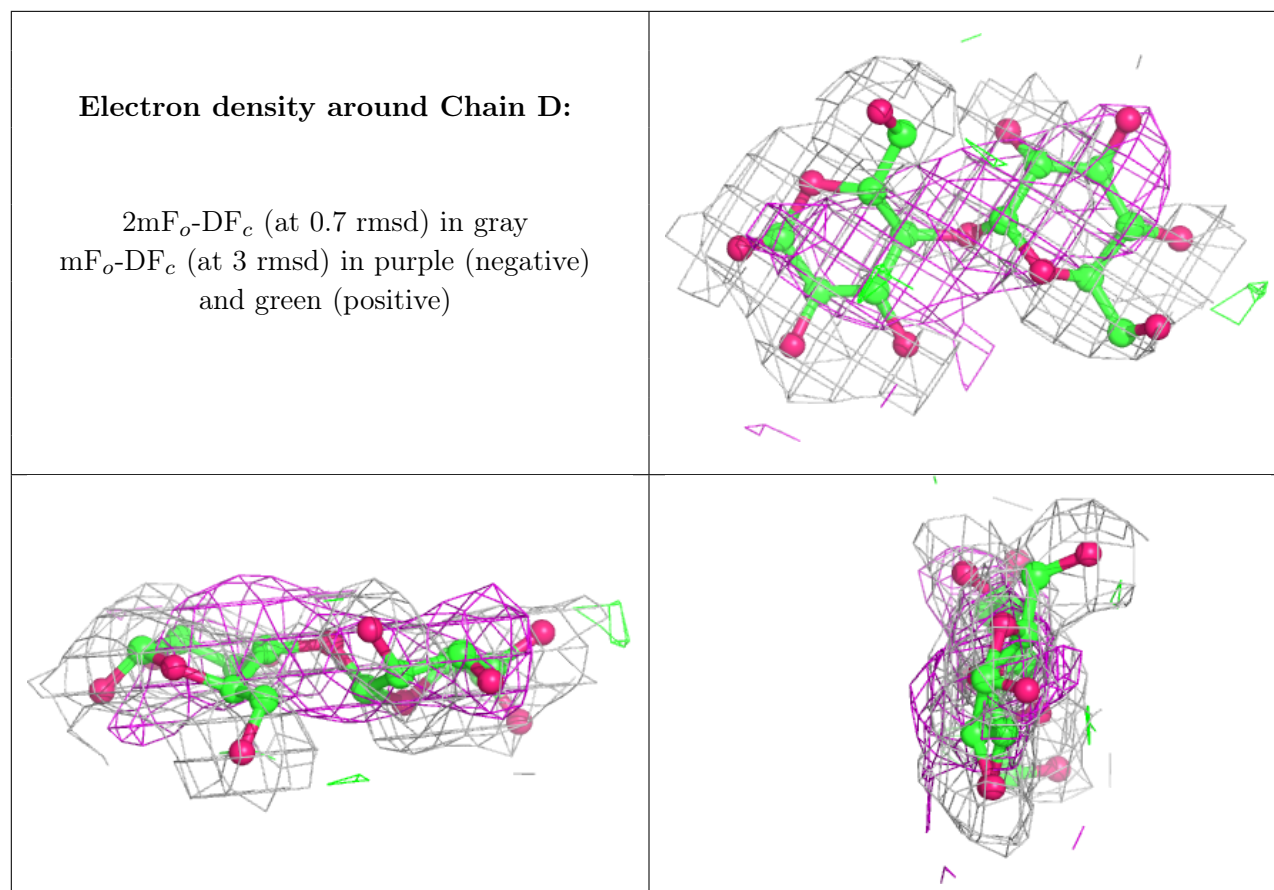
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
3	GLC	C	1	12/12	0.53	0.41	87,112,122,124	0
3	GLC	C	2	11/12	0.56	0.54	75,84,103,110	0
3	GLC	D	2	11/12	0.57	0.42	71,84,94,101	0
3	GLC	D	1	12/12	0.61	0.39	59,69,80,82	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.





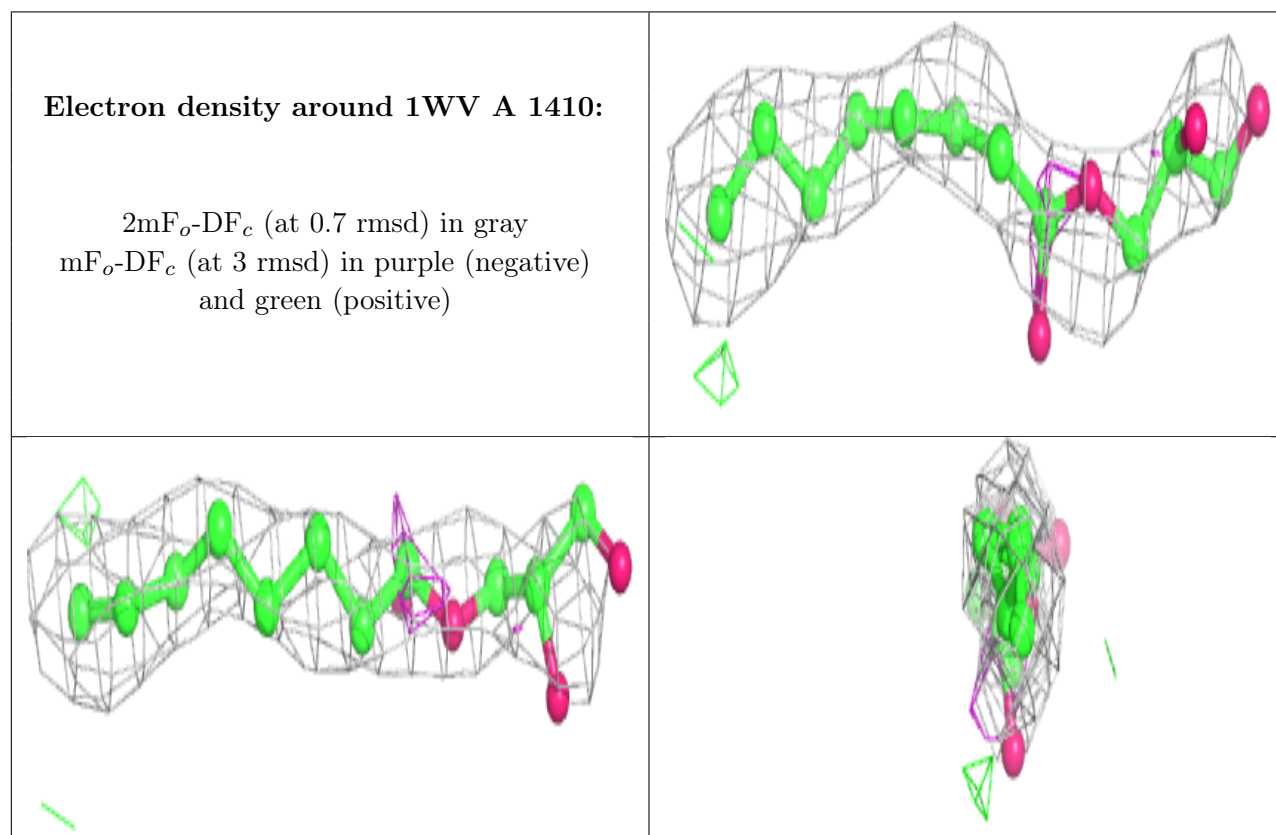


## 6.4 Ligands ⓘ

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, 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.

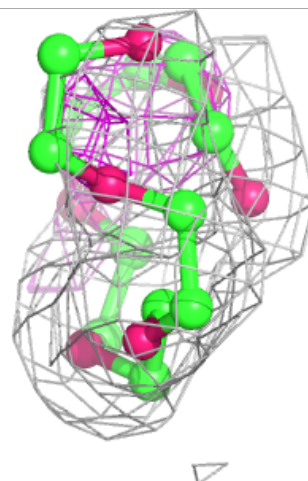
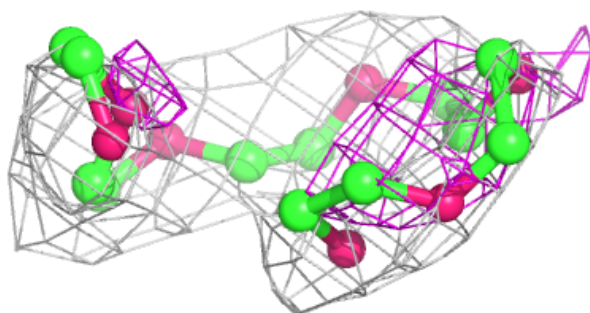
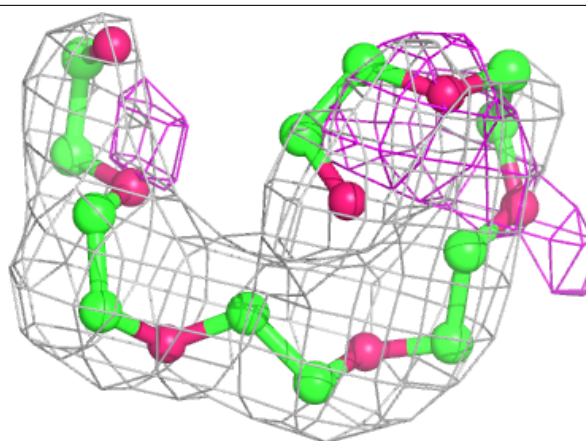
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	1WV	A	1410	15/21	0.70	0.45	69,85,104,106	0
8	EPE	A	1412	15/15	0.73	0.53	63,87,116,125	0
4	SO4	A	1407	5/5	0.76	0.27	81,89,125,128	0
10	P6G	A	1414	19/19	0.80	0.44	67,83,97,99	0
5	CLR	A	1409	28/28	0.86	0.41	72,88,92,94	0
4	SO4	A	1408	5/5	0.89	0.21	90,92,104,104	0
9	P0G	A	1413	27/27	0.90	0.22	62,78,83,88	0
7	NA	A	1411	1/1	0.92	0.10	70,70,70,70	0
4	SO4	A	1405	5/5	0.96	0.13	62,70,79,85	0
4	SO4	A	1404	5/5	0.97	0.23	52,54,57,65	0
4	SO4	A	1406	5/5	0.98	0.12	74,75,81,87	0
4	SO4	A	1403	5/5	0.98	0.21	57,59,60,66	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.



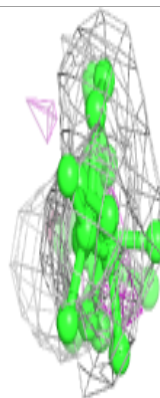
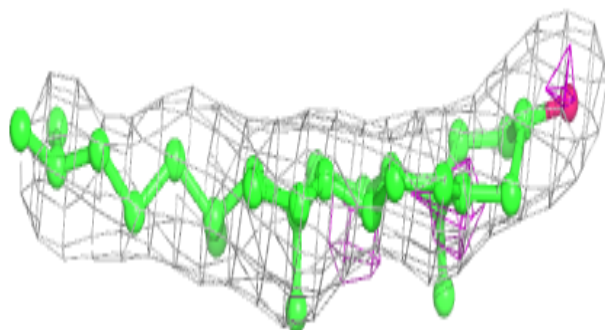
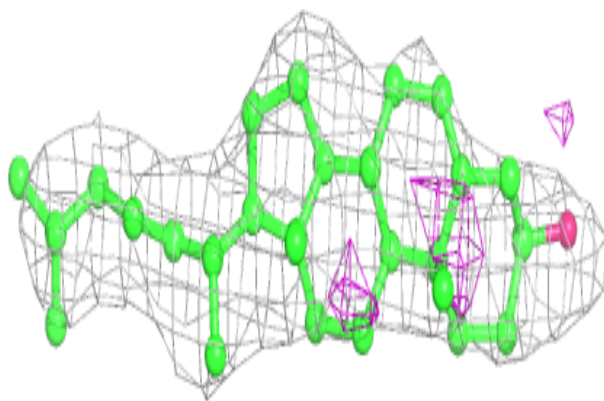
**Electron density around P6G A 1414:**

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

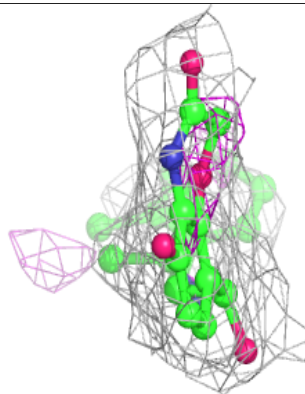
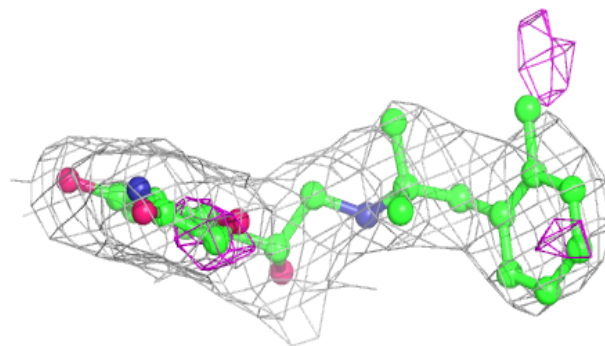
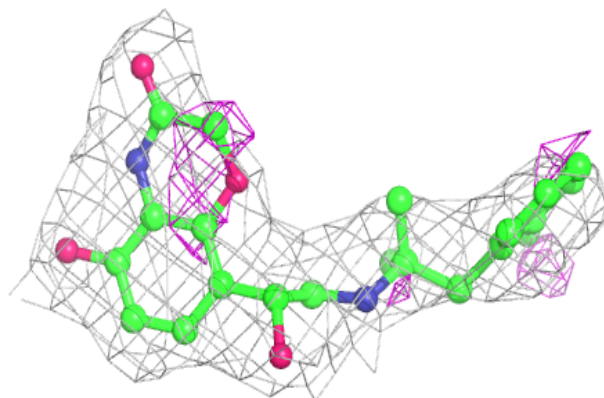


**Electron density around CLR A 1409:**

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

**Electron density around P0G A 1413:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.