



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 AM UTC

PDB ID : 6D64 / pdb\_00006d64  
Title : Crystal Structure of Human CD1b in Complex with POPC  
Authors : Shahine, A.E.; Rossjohn, J.  
Deposited on : 2018-04-20  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

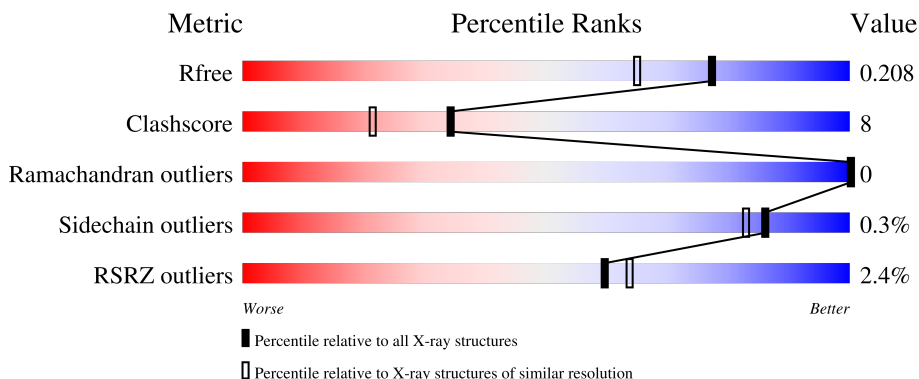
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	 2% 82% 11% 6%
2	B	101	 3% 93% 6%
3	C	7	 43% 57%
4	D	4	 75% 25%
5	E	5	 40% 60%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
8	CL	A	423	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 3933 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 T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2269	1450	385	424	10	0	11	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

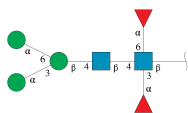
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	825	527	140	156	2	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

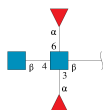
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PRO	-	expression tag	UNP P61769
B	2	LYS	-	expression tag	UNP P61769

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



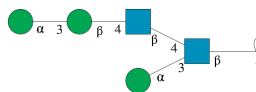
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	7	81	46	2	33	0	0	0

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



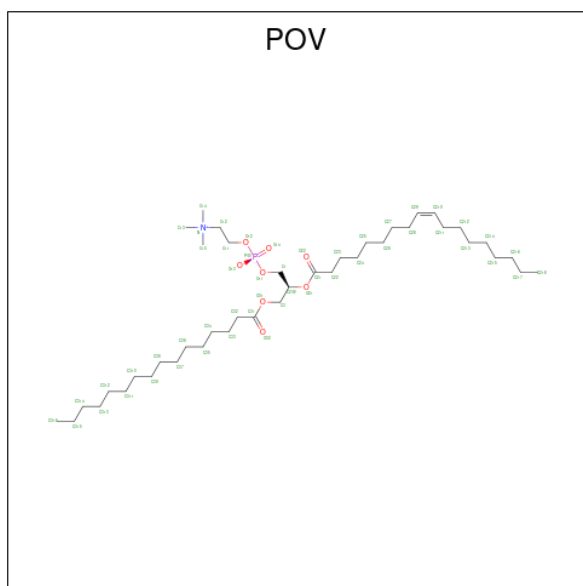
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	48	28	2	18	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



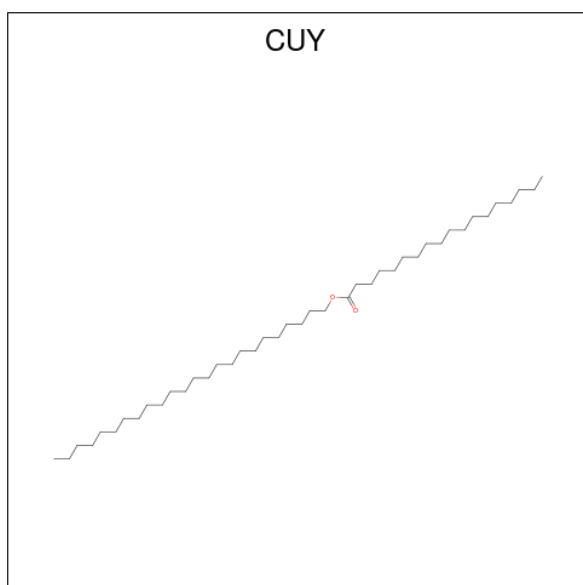
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	5	61	34	2	25	0	0	0

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	52	42	1	8	1	0	0

- Molecule 7 is tetracosyl octadecanoate (CCD ID: CUY) (formula: C<sub>42</sub>H<sub>84</sub>O<sub>2</sub>).

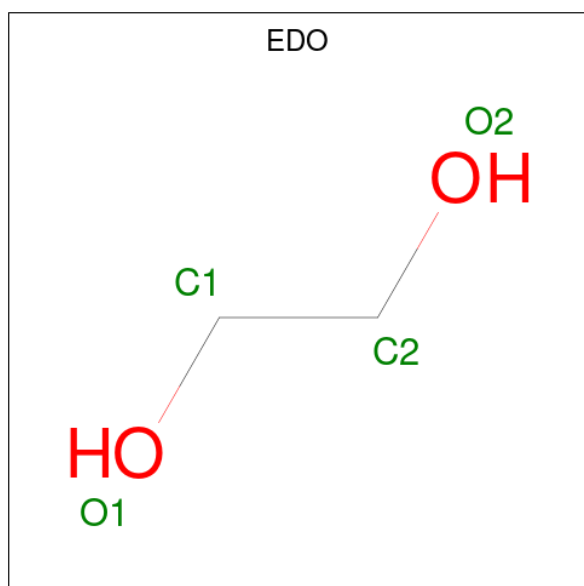


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			37	35	2		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	6	Total	Cl		0	0
			6	6			
8	B	1	Total	Cl		0	0
			1	1			

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 11 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total I 2 2	0	0

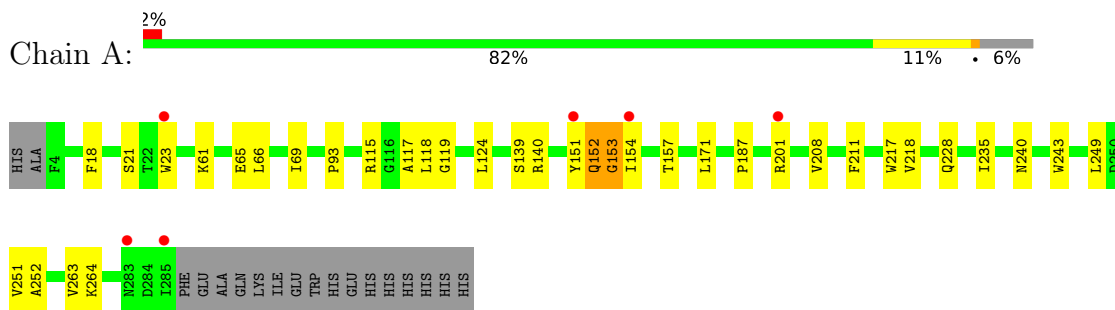
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	423	Total O 423 423	0	0
12	B	115	Total O 115 115	0	0

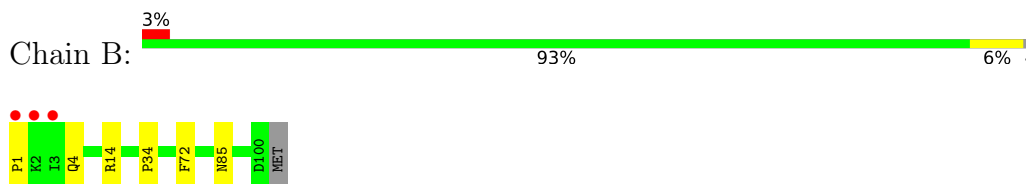
### 3 Residue-property plots [i](#)

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.

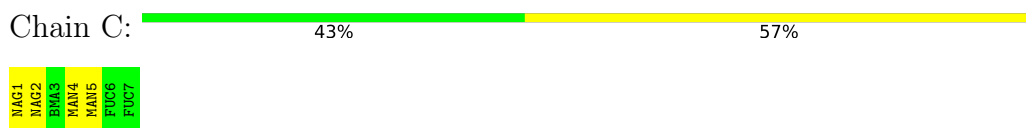
- Molecule 1: T-cell surface glycoprotein CD1b



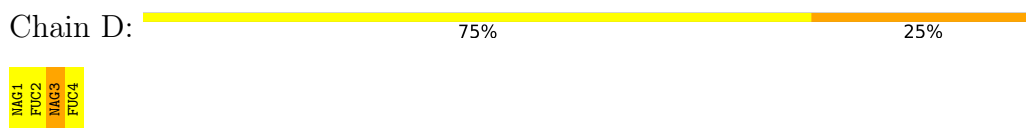
- Molecule 2: Beta-2-microglobulin



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.98Å 80.03Å 92.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.13 – 1.70 40.13 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.13-1.70) 99.9 (40.13-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.179 , 0.211 0.179 , 0.208	Depositor DCC
$R_{free}$ test set	2417 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: NA, MAN, FUC, IOD, CUY, CL, POV, EDO, 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	0.62	8/2332 (0.3%)	0.59	1/3167 (0.0%)
2	B	0.57	0/849	0.59	0/1154
All	All	0.60	8/3181 (0.3%)	0.59	1/4321 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	TRP	C-O	-6.62	1.16	1.23
1	A	118	LEU	C-O	-6.46	1.16	1.23
1	A	152	GLN	N-CA	-6.30	1.38	1.46
1	A	153	GLY	C-O	-6.09	1.16	1.23
1	A	117	ALA	C-O	-5.93	1.16	1.23
1	A	18	PHE	C-O	-5.69	1.17	1.24
1	A	139	SER	C-O	-5.53	1.17	1.24
1	A	140	ARG	C-O	-5.01	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	SER	N-CA-C	6.79	121.02	112.87

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	2269	0	2173	35	0
2	B	825	0	767	5	0
3	C	81	0	70	1	0
4	D	48	0	43	2	0
5	E	61	0	52	1	0
6	A	52	0	82	17	0
7	A	37	0	0	3	0
8	A	6	0	0	4	0
8	B	1	0	0	0	0
9	A	8	0	12	3	0
9	B	4	0	6	1	0
10	A	1	0	0	0	0
11	A	2	0	0	1	0
12	A	423	0	0	11	3
12	B	115	0	0	4	0
All	All	3933	0	3205	50	3

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 8.

All (50) 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:153:GLY:C	6:A:417:POV:H15	1.86	1.01
1:A:228:GLN:NE2	8:A:423:CL:CL	2.36	0.95
1:A:119:GLY:HA3	2:B:1:PRO:HA	1.47	0.93
1:A:153:GLY:O	6:A:417:POV:H15	1.81	0.81
1:A:228:GLN:NE2	12:A:501:HOH:O	1.97	0.80
12:A:502:HOH:O	4:D:3:NAG:O3	2.01	0.78
6:A:417:POV:O13	12:A:503:HOH:O	2.03	0.77
1:A:153:GLY:HA3	6:A:417:POV:C14	2.16	0.74
1:A:208:VAL:HG21	1:A:218[B]:VAL:HG11	1.70	0.73
1:A:61:LYS:NZ	1:A:65:GLU:OE2	2.22	0.72
1:A:228:GLN:HG2	12:A:501:HOH:O	1.87	0.72
1:A:153:GLY:HA3	6:A:417:POV:H14	1.71	0.72
11:A:429:IOD:I	12:A:508:HOH:O	2.79	0.71
1:A:151:TYR:OH	12:A:504:HOH:O	2.10	0.69
1:A:66:LEU:HD13	6:A:417:POV:H216	1.80	0.62
1:A:228:GLN:CD	8:A:423:CL:CL	2.82	0.60
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HD11	6:A:417:POV:H32	1.87	0.57
1:A:115:ARG:HD2	8:A:421:CL:CL	2.42	0.56
1:A:228:GLN:OE1	8:A:423:CL:CL	2.60	0.56
6:A:417:POV:C218	7:A:418:CUY:C3	2.85	0.54
1:A:153:GLY:CA	6:A:417:POV:H15	2.38	0.52
9:A:425:EDO:H22	2:B:34:PRO:CB	2.39	0.52
1:A:69:ILE:HG12	6:A:417:POV:O14	2.11	0.51
9:B:202:EDO:H12	12:B:359:HOH:O	2.10	0.51
12:A:506:HOH:O	5:E:1:NAG:O6	2.19	0.50
1:A:171:LEU:HD12	3:C:2:NAG:H82	1.94	0.49
1:A:228:GLN:CG	12:A:501:HOH:O	2.51	0.49
6:A:417:POV:H21G	7:A:418:CUY:C3	2.44	0.48
1:A:93:PRO:HB2	9:A:425:EDO:H12	1.96	0.47
1:A:201[B]:ARG:NE	12:A:520:HOH:O	2.44	0.46
1:A:251[A]:VAL:HG12	1:A:252:ALA:O	2.15	0.46
1:A:240:ASN:ND2	12:A:525:HOH:O	2.48	0.46
2:B:85:ASN:ND2	12:B:304:HOH:O	2.39	0.45
4:D:3:NAG:H82	4:D:3:NAG:H2	1.70	0.45
6:A:417:POV:H21H	7:A:418:CUY:C3	2.47	0.44
1:A:157:THR:OG1	6:A:417:POV:H15A	2.16	0.44
1:A:208:VAL:HG21	1:A:218[B]:VAL:CG1	2.45	0.44
1:A:218[B]:VAL:HG12	1:A:263:VAL:HG22	1.99	0.44
1:A:154:ILE:HG12	6:A:417:POV:H13	2.00	0.44
1:A:153:GLY:HA3	6:A:417:POV:H14A	1.96	0.43
2:B:14:ARG:NH2	12:B:309:HOH:O	2.49	0.43
1:A:235:ILE:HD11	1:A:243:TRP:HB3	2.02	0.42
6:A:417:POV:O21	6:A:417:POV:H13B	2.19	0.41
2:B:4:GLN:NE2	12:B:312:HOH:O	2.53	0.41
1:A:124:LEU:HD12	1:A:124:LEU:C	2.46	0.41
1:A:249:LEU:HG	1:A:251[A]:VAL:HG23	2.03	0.41
1:A:217:TRP:HB3	1:A:264:LYS:HB2	2.02	0.41
9:A:425:EDO:H21	12:A:617:HOH:O	2.20	0.40
1:A:152:GLN:O	6:A:417:POV:H14	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:797:HOH:O	12:A:880:HOH:O[1_455]	1.83	0.37
12:A:835:HOH:O	12:A:842:HOH:O[2_454]	2.07	0.13
12:A:660:HOH:O	12:A:899:HOH:O[2_455]	2.13	0.07

## 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	291/300 (97%)	290 (100%)	1 (0%)	0	100	100
2	B	100/101 (99%)	100 (100%)	0	0	100	100
All	All	391/401 (98%)	390 (100%)	1 (0%)	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	240/247 (97%)	240 (100%)	0	100	100
2	B	90/96 (94%)	89 (99%)	1 (1%)	65	54
All	All	330/343 (96%)	329 (100%)	1 (0%)	86	83

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

Mol	Chain	Res	Type
2	B	72	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	184	GLN

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Mol	Chain	Res	Type
2	B	4	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

16 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	C	1	3,1	14,14,15	0.76	1 (7%)	17,19,21	0.93	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.59	0
3	BMA	C	3	3	11,11,12	0.63	0	15,15,17	0.85	0
3	MAN	C	4	3	11,11,12	0.95	0	15,15,17	0.95	1 (6%)
3	MAN	C	5	3	11,11,12	0.62	0	15,15,17	1.01	1 (6%)
3	FUC	C	6	3	10,10,11	0.80	0	14,14,16	0.54	0
3	FUC	C	7	3	10,10,11	0.68	0	14,14,16	0.82	0
4	NAG	D	1	1,4	14,14,15	1.45	2 (14%)	17,19,21	2.20	7 (41%)
4	FUC	D	2	4	10,10,11	0.53	0	14,14,16	1.58	4 (28%)
4	NAG	D	3	4	14,14,15	1.09	2 (14%)	17,19,21	2.43	9 (52%)
4	FUC	D	4	4	10,10,11	0.80	0	14,14,16	1.58	3 (21%)
5	NAG	E	1	5,1	14,14,15	0.50	0	17,19,21	0.62	0
5	NAG	E	2	5	14,14,15	0.37	0	17,19,21	0.52	0
5	BMA	E	3	5	11,11,12	0.79	0	15,15,17	1.09	0
5	MAN	E	4	5	11,11,12	0.70	0	15,15,17	1.14	2 (13%)
5	MAN	E	5	5	11,11,12	1.60	1 (9%)	15,15,17	1.63	2 (13%)

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	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
4	NAG	D	3	4	-	4/6/23/26	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5	MAN	C4-C5	3.89	1.61	1.53
4	D	1	NAG	O5-C1	-3.20	1.38	1.43
4	D	1	NAG	C1-C2	2.49	1.55	1.52
4	D	3	NAG	O5-C5	-2.10	1.39	1.43
3	C	1	NAG	O5-C1	-2.01	1.40	1.43
4	D	3	NAG	C3-C2	-2.00	1.48	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	NAG	O5-C5-C6	5.13	117.65	107.66
4	D	1	NAG	C4-C3-C2	-4.57	104.32	111.02
4	D	1	NAG	O7-C7-C8	-3.92	115.07	122.05
4	D	4	FUC	O5-C1-C2	-3.69	101.99	110.79
4	D	1	NAG	C1-C2-N2	3.68	116.23	110.43
5	E	5	MAN	C3-C4-C5	3.66	116.88	110.23
4	D	3	NAG	O4-C4-C5	-3.58	100.50	109.32
3	C	5	MAN	C1-O5-C5	3.41	116.76	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	4	MAN	C1-O5-C5	3.27	116.57	112.19
4	D	2	FUC	C1-C2-C3	3.21	114.32	109.64
5	E	5	MAN	C1-C2-C3	-3.12	105.10	109.64
4	D	3	NAG	O4-C4-C3	-3.03	103.24	110.38
4	D	3	NAG	O5-C1-C2	2.97	115.89	111.29
4	D	1	NAG	O7-C7-N2	2.95	127.20	121.98
4	D	3	NAG	O7-C7-N2	2.94	127.17	121.98
4	D	3	NAG	C8-C7-N2	-2.88	111.34	116.12
4	D	2	FUC	C6-C5-C4	-2.72	108.11	113.08
4	D	3	NAG	O6-C6-C5	2.66	120.40	111.33
4	D	3	NAG	C3-C4-C5	2.51	114.79	110.23
4	D	1	NAG	O5-C5-C6	2.38	112.29	107.66
4	D	4	FUC	C6-C5-C4	-2.37	108.75	113.08
3	C	4	MAN	O2-C2-C3	-2.30	105.38	110.15
4	D	4	FUC	C1-C2-C3	-2.19	106.45	109.64
4	D	1	NAG	O4-C4-C3	-2.15	105.31	110.38
4	D	2	FUC	O5-C5-C4	2.12	113.36	109.55
4	D	3	NAG	O3-C3-C2	-2.06	105.11	109.40
4	D	2	FUC	O5-C5-C6	2.06	111.87	107.40
4	D	1	NAG	C1-O5-C5	-2.04	109.45	112.19
5	E	4	MAN	O2-C2-C3	-2.02	105.96	110.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	NAG	O5-C5-C6-O6
4	D	3	NAG	C4-C5-C6-O6
4	D	3	NAG	C8-C7-N2-C2
4	D	3	NAG	O7-C7-N2-C2
5	E	5	MAN	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
3	C	1	NAG	C3-C2-N2-C7
4	D	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

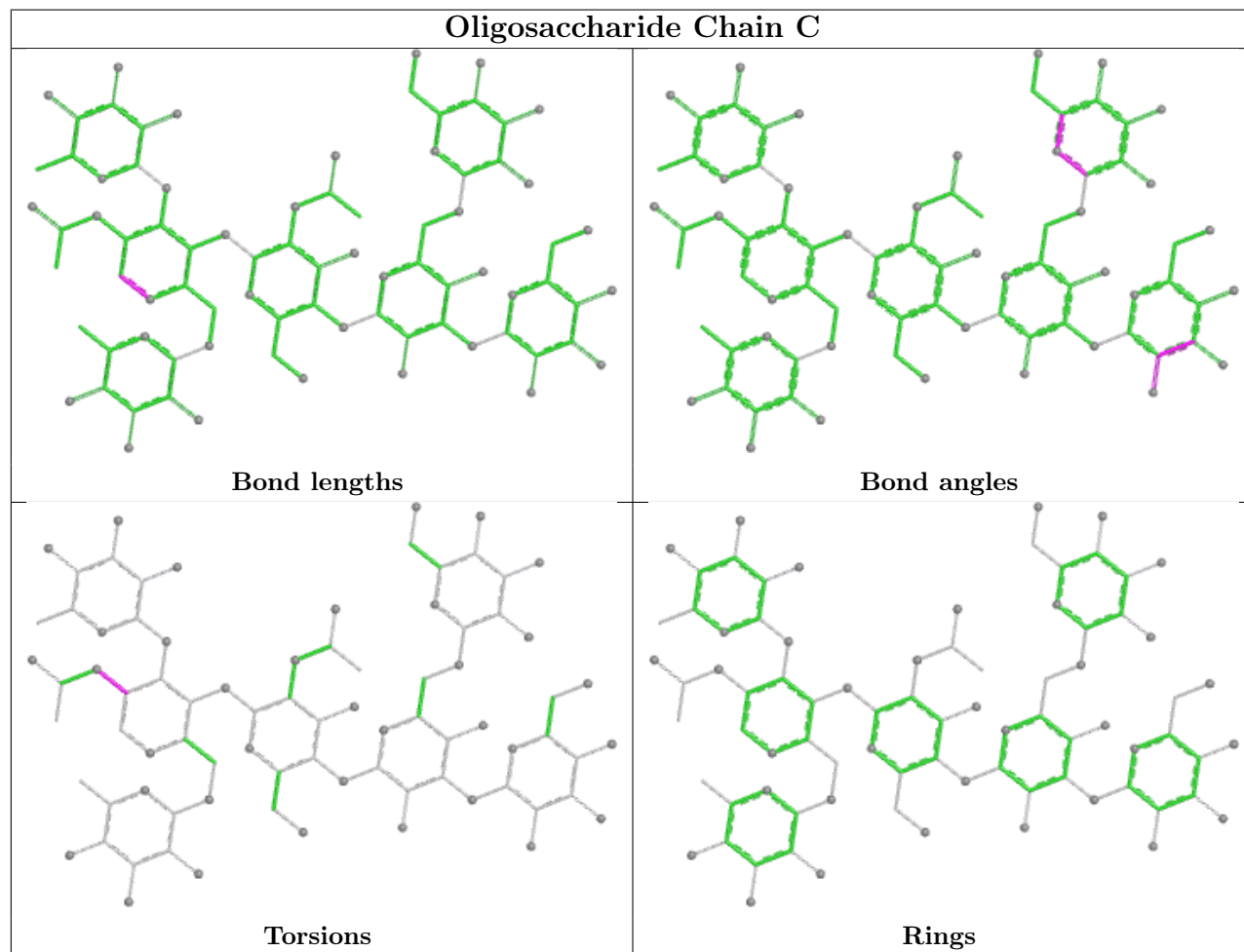
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0

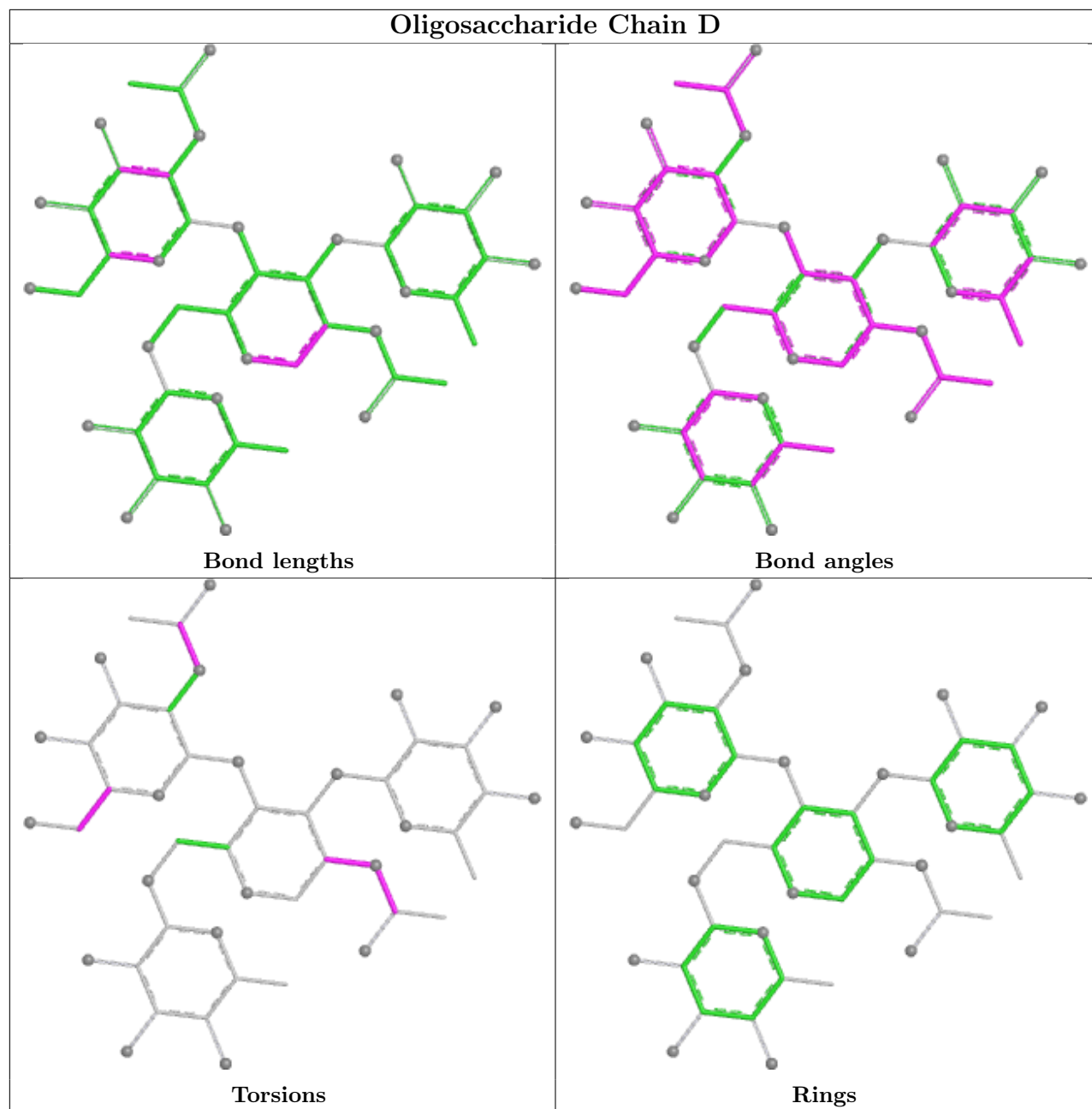
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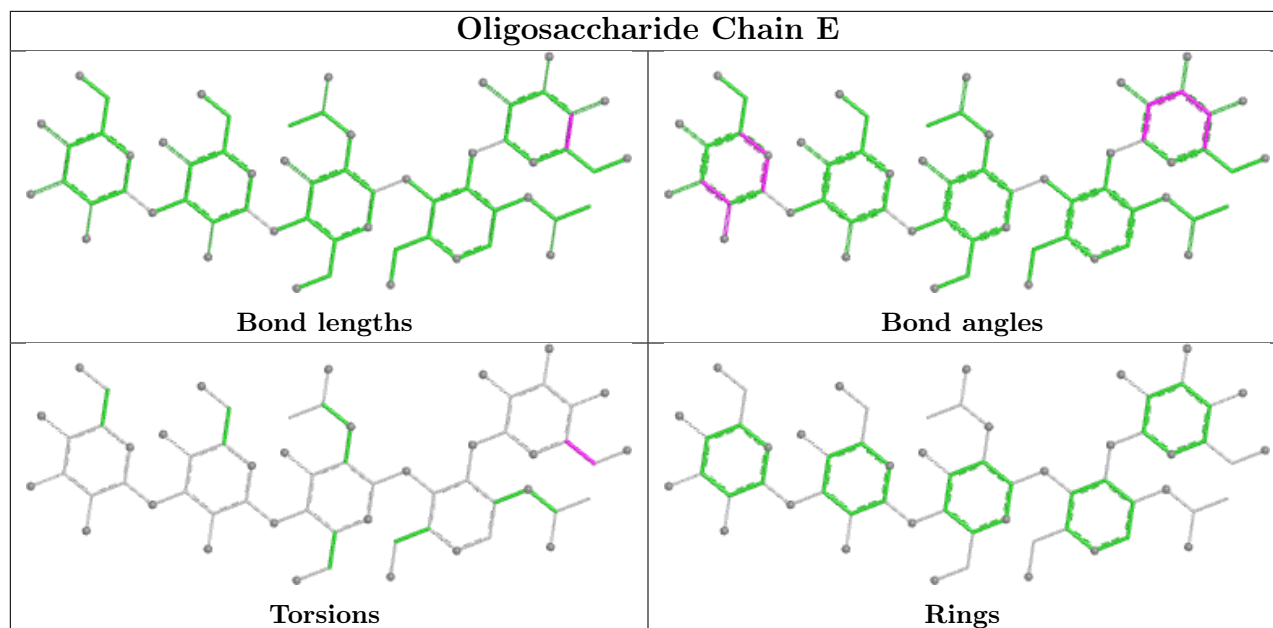
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	NAG	2	0
5	E	1	NAG	1	0

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](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	EDO	A	425	-	3,3,3	0.44	0	2,2,2	0.30	0
9	EDO	B	202	-	3,3,3	0.47	0	2,2,2	0.26	0
6	POV	A	417	-	51,51,51	1.30	4 (7%)	57,59,59	1.29	3 (5%)
9	EDO	A	426	-	3,3,3	0.44	0	2,2,2	0.37	0
7	CUY	A	418	-	36,36,43	1.38	3 (8%)	36,36,43	1.65	5 (13%)

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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	425	-	-	0/1/1/1	-
9	EDO	B	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	A	417	-	-	24/55/55/55	-
9	EDO	A	426	-	-	0/1/1/1	-
7	CUY	A	418	-	-	19/35/35/42	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	418	CUY	CAU-CAV	-4.56	1.29	1.51
7	A	418	CUY	CBG-CBF	-4.37	1.30	1.51
7	A	418	CUY	OAQ-CAP	4.37	1.46	1.33
6	A	417	POV	O21-C21	3.44	1.44	1.34
6	A	417	POV	O31-C31	3.44	1.43	1.33
6	A	417	POV	P-O11	2.48	1.69	1.59
6	A	417	POV	C15-N	-2.09	1.43	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	417	POV	O21-C21-C22	4.78	121.83	111.48
7	A	418	CUY	CAU-CAV-CAW	4.43	136.78	114.37
7	A	418	CUY	OAQ-CAP-CAO	4.30	124.93	111.83
7	A	418	CUY	CAT-CAU-CAV	3.97	134.42	114.37
6	A	417	POV	O31-C31-C32	3.18	121.54	111.83
7	A	418	CUY	CAR-OAQ-CAP	2.51	124.76	116.90
7	A	418	CUY	OBO-CAP-CAO	-2.35	114.60	123.78
6	A	417	POV	O21-C2-C1	2.07	115.75	108.34

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	417	POV	C11-O12-P-O11
6	A	417	POV	C11-O12-P-O14
6	A	417	POV	O12-C11-C12-N
7	A	418	CUY	CBE-CBF-CBG-CBH
7	A	418	CUY	CAT-CAU-CAV-CAW
7	A	418	CUY	OBO-CAP-OAQ-CAR
7	A	418	CUY	CAO-CAP-OAQ-CAR
6	A	417	POV	C32-C31-O31-C3
7	A	418	CUY	OAQ-CAR-CAS-CAT
6	A	417	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	A	417	POV	C311-C310-C39-C38
7	A	418	CUY	CBH-CBI-CBJ-CBK
7	A	418	CUY	CAS-CAT-CAU-CAV
7	A	418	CUY	CAJ-CAK-CAL-CAM
7	A	418	CUY	CAE-CAF-CAG-CAH
6	A	417	POV	C310-C311-C312-C313
7	A	418	CUY	CAF-CAG-CAH-CAI
6	A	417	POV	C32-C33-C34-C35
7	A	418	CUY	CAR-CAS-CAT-CAU
7	A	418	CUY	CAH-CAI-CAJ-CAK
7	A	418	CUY	CBF-CBG-CBH-CBI
6	A	417	POV	C210-C211-C212-C213
7	A	418	CUY	CAU-CAV-CAW-CBM
6	A	417	POV	C35-C36-C37-C38
7	A	418	CUY	CBD-CBE-CBF-CBG
7	A	418	CUY	CBG-CBH-CBI-CBJ
6	A	417	POV	C213-C214-C215-C216
6	A	417	POV	C22-C23-C24-C25
6	A	417	POV	C2-C1-O11-P
6	A	417	POV	C212-C213-C214-C215
6	A	417	POV	O11-C1-C2-O21
6	A	417	POV	C211-C212-C213-C214
7	A	418	CUY	CAK-CAL-CAM-CAN
7	A	418	CUY	CAI-CAJ-CAK-CAL
6	A	417	POV	C214-C215-C216-C217
6	A	417	POV	C11-O12-P-O13
6	A	417	POV	C1-C2-O21-C21
9	B	202	EDO	O1-C1-C2-O2
7	A	418	CUY	C1-CBD-CBE-CBF
6	A	417	POV	C312-C313-C314-C315
6	A	417	POV	C27-C28-C29-C210
6	A	417	POV	O11-C1-C2-C3
6	A	417	POV	C29-C210-C211-C212
6	A	417	POV	O31-C31-C32-C33

There are no ring outliers.

4 monomers are involved in 21 short contacts:

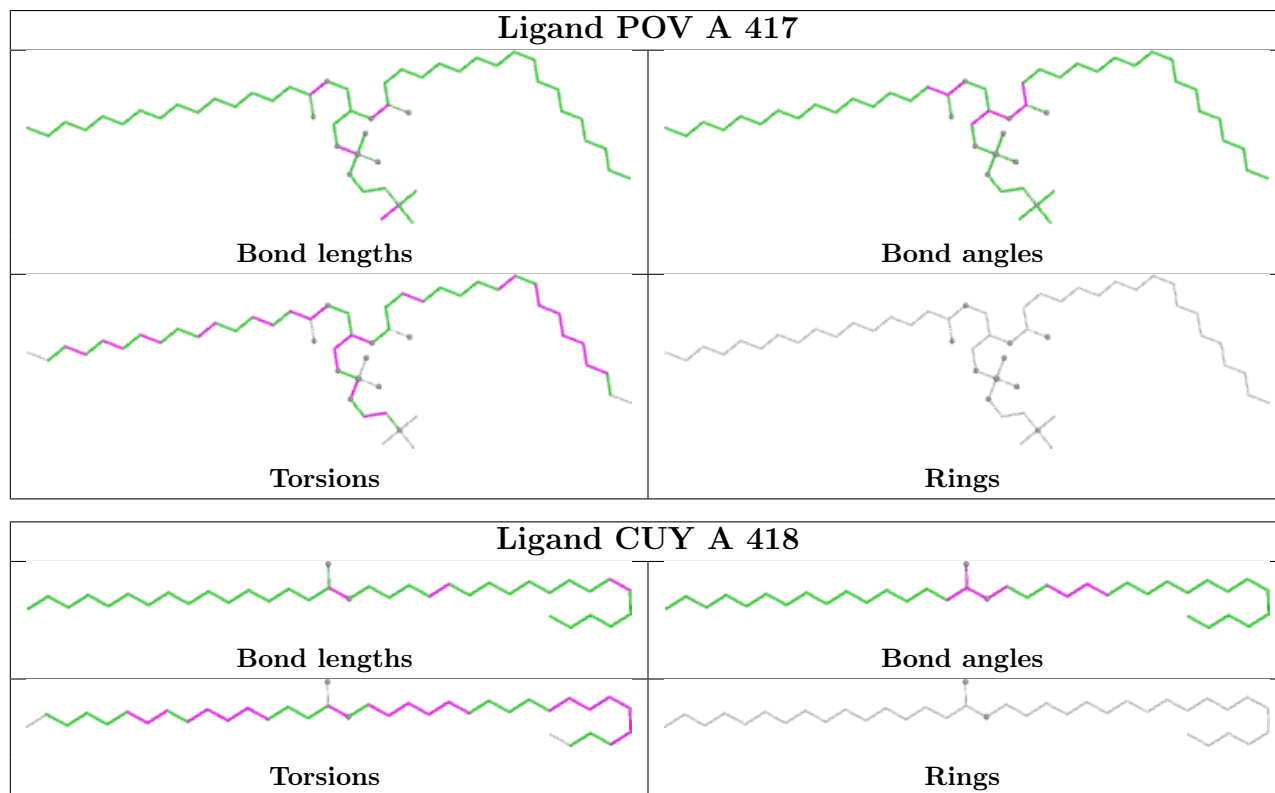
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	425	EDO	3	0
9	B	202	EDO	1	0
6	A	417	POV	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	418	CUY	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 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	282/300 (94%)	-0.11	6 (2%) 63 68	9, 20, 41, 49	13 (4%)
2	B	100/101 (99%)	0.28	3 (3%) 52 56	7, 26, 51, 62	3 (3%)
All	All	382/401 (95%)	-0.00	9 (2%) 59 64	7, 21, 44, 62	16 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ILE	3.1
2	B	3	ILE	3.0
1	A	283	ASN	2.9
2	B	2	LYS	2.8
2	B	1	PRO	2.8
1	A	151	TYR	2.7
1	A	201[A]	ARG	2.3
1	A	154	ILE	2.2
1	A	23	TRP	2.0

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUC	D	2	10/11	0.56	0.17	68,76,85,87	0

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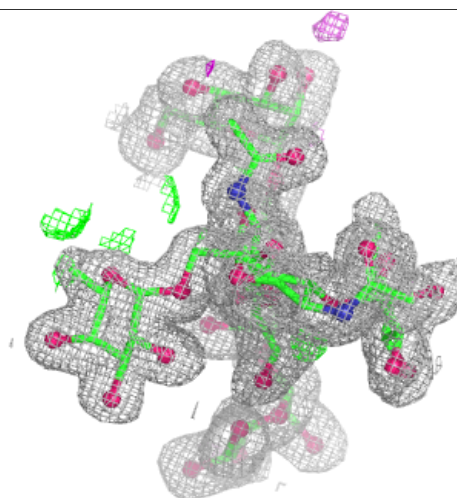
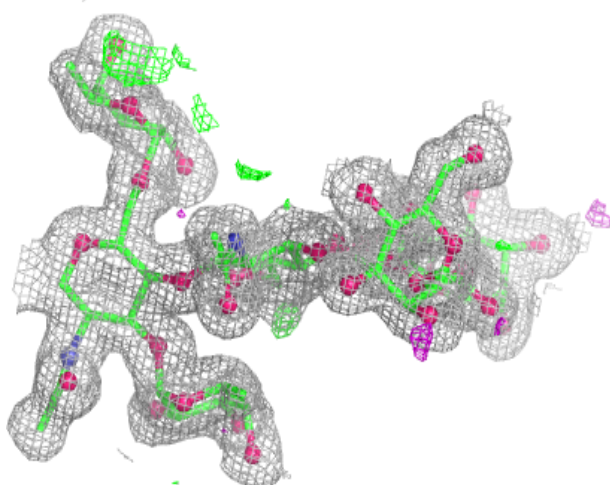
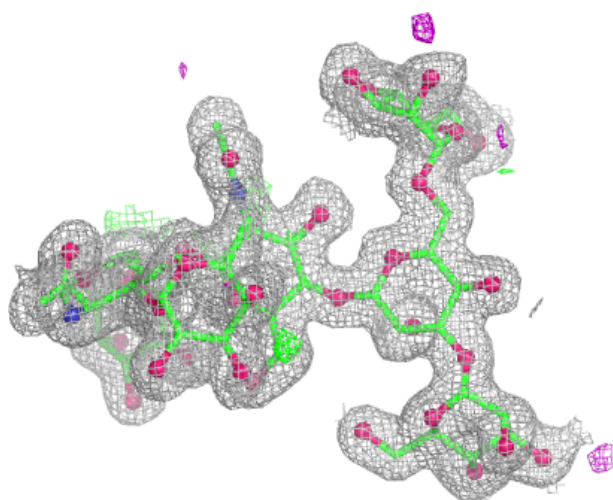
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	2	14/15	0.58	0.17	52,67,75,75	2
5	MAN	E	5	11/12	0.66	0.15	66,70,75,75	0
5	NAG	E	1	14/15	0.71	0.15	47,59,66,66	0
5	BMA	E	3	11/12	0.74	0.14	48,60,69,72	1
4	NAG	D	3	14/15	0.76	0.15	53,63,76,81	0
4	FUC	D	4	10/11	0.79	0.13	47,59,65,72	0
4	NAG	D	1	14/15	0.80	0.14	39,56,63,73	0
5	MAN	E	4	11/12	0.81	0.13	44,50,58,61	1
3	MAN	C	4	11/12	0.95	0.07	20,25,27,27	0
3	FUC	C	6	10/11	0.95	0.07	19,31,33,34	0
3	FUC	C	7	10/11	0.95	0.07	20,25,28,33	0
3	MAN	C	5	11/12	0.96	0.05	14,17,21,23	0
3	NAG	C	2	14/15	0.96	0.06	13,17,26,28	0
3	BMA	C	3	11/12	0.97	0.05	13,18,19,21	0
3	NAG	C	1	14/15	0.97	0.06	13,16,20,21	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.

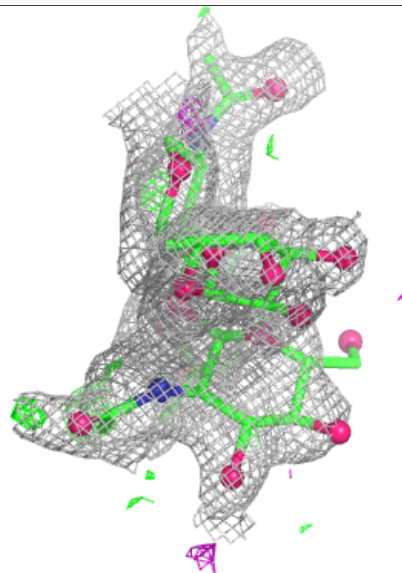
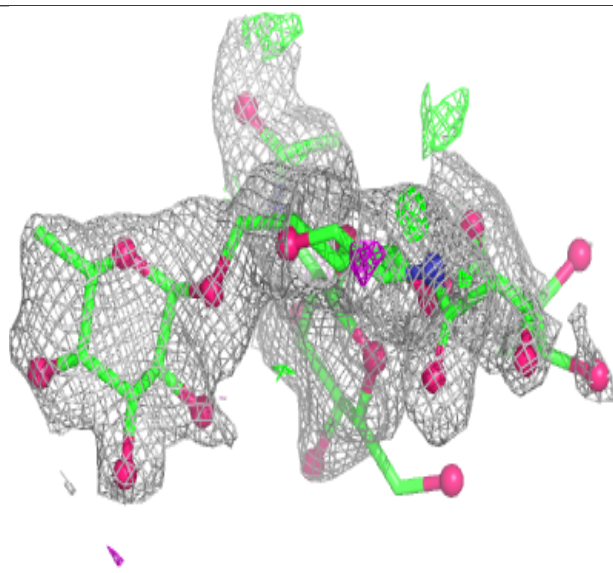
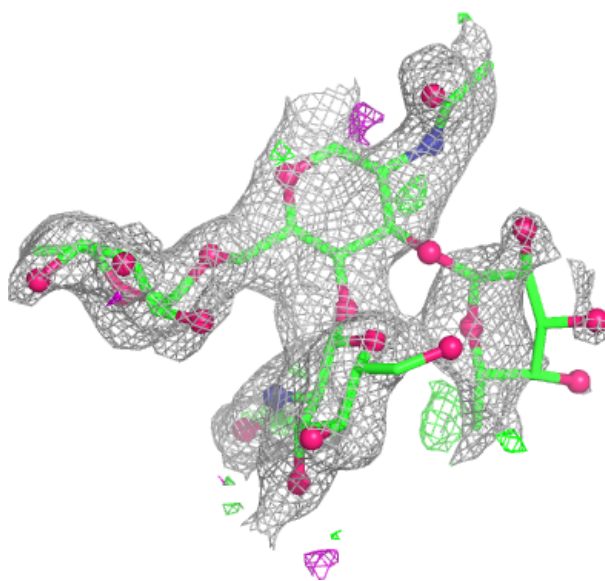
**Electron density around Chain C:**

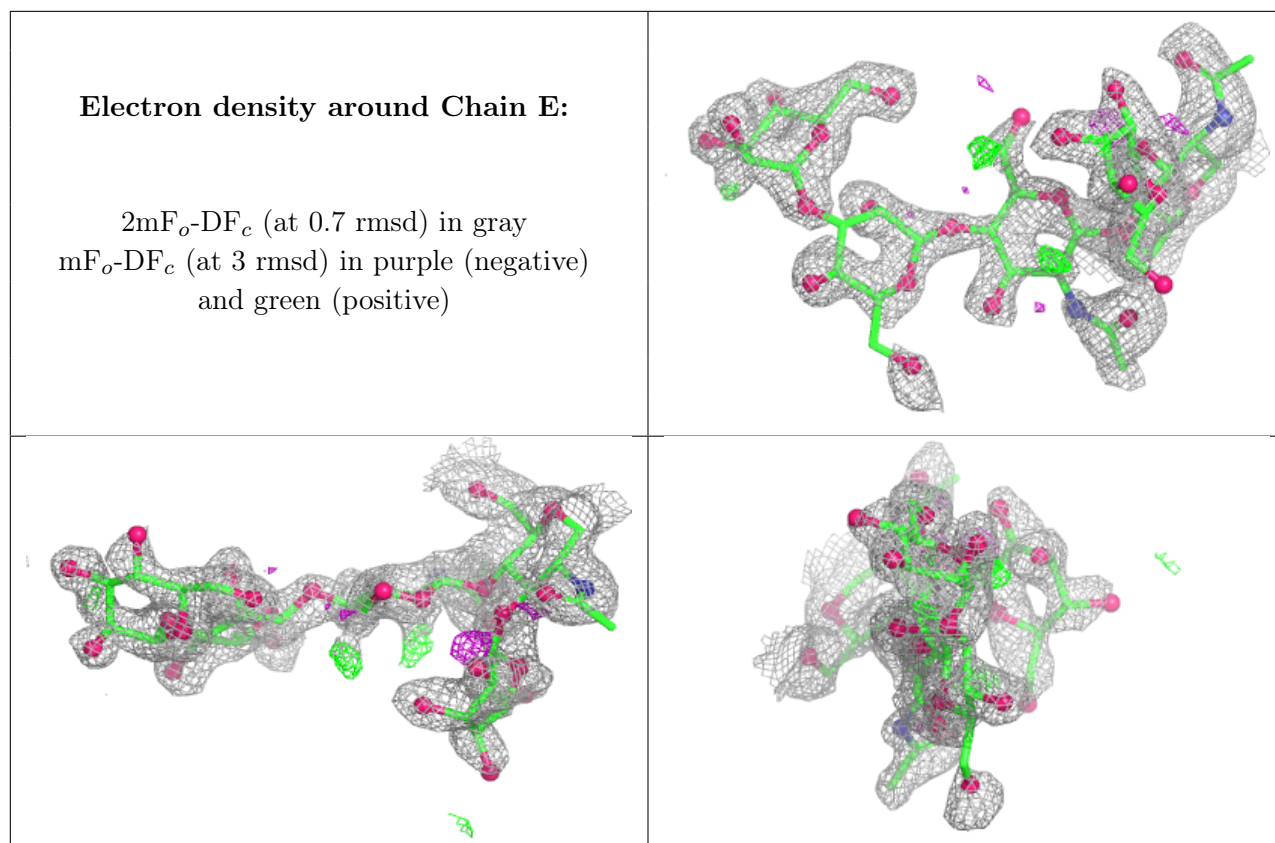
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

$2mF_o-DF_c$  (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.

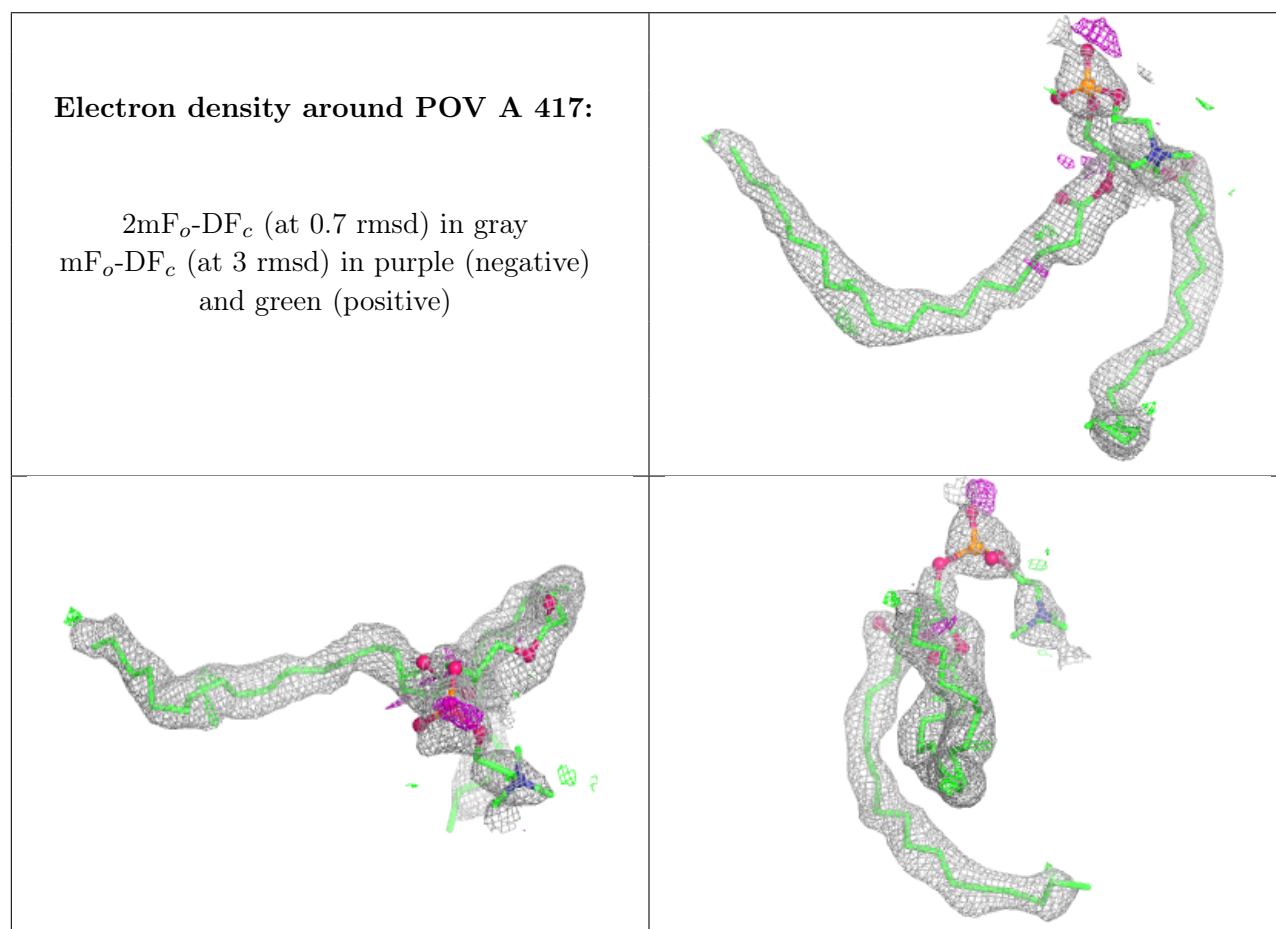
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NA	A	427	1/1	0.77	0.20	54,54,54,54	0
9	EDO	A	426	4/4	0.78	0.17	52,55,55,59	0
9	EDO	B	202	4/4	0.84	0.14	40,42,46,47	0
6	POV	A	417	52/52	0.84	0.16	28,42,82,85	2
8	CL	A	421	1/1	0.85	0.20	65,65,65,65	0
8	CL	B	201	1/1	0.89	0.17	20,20,20,20	0
7	CUY	A	418	37/44	0.89	0.13	25,38,47,52	0
9	EDO	A	425	4/4	0.94	0.17	12,19,30,39	0
8	CL	A	424	1/1	0.96	0.13	19,19,19,19	0
11	IOD	A	429	1/1	0.97	0.04	17,17,17,17	1
8	CL	A	422	1/1	0.98	0.05	27,27,27,27	0
8	CL	A	423	1/1	0.98	0.04	18,18,18,18	0
8	CL	A	420	1/1	0.98	0.05	27,27,27,27	0
11	IOD	A	428	1/1	0.99	0.02	13,13,13,13	1

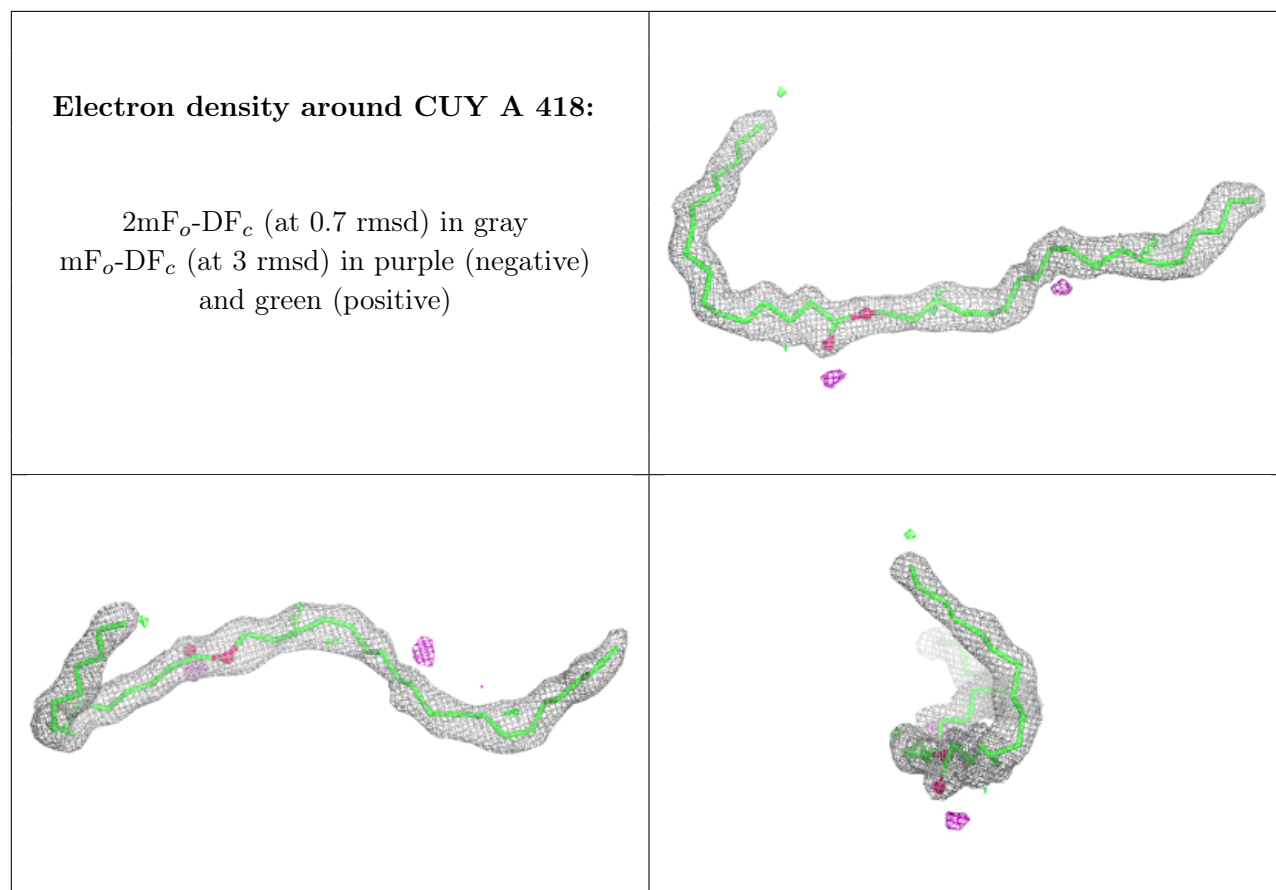
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CL	A	419	1/1	0.99	0.04	20,20,20,20	0

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.