



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:22 PM BST

PDB ID : 5WKG  
Title : Crystal Structure of Human CD1b in Complex with PA  
Authors : Shahine, A.; Gras, S.; Rossjohn, J.  
Deposited on : 2017-07-25  
Resolution : 2.06 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

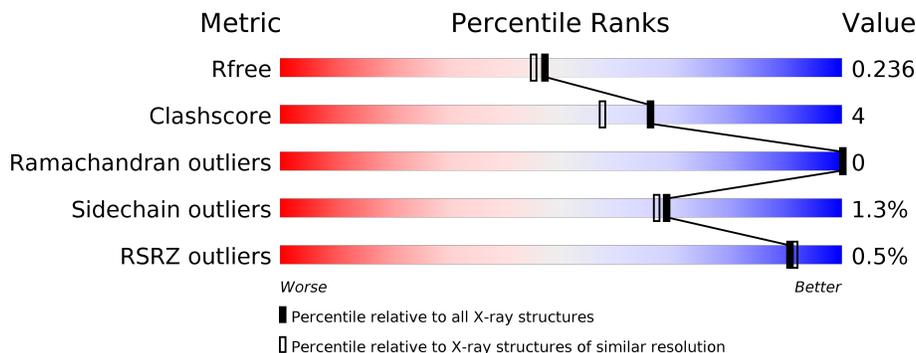
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	300	 83% 10% 7%
2	B	99	 92% 6%
3	C	7	 14% 86%
4	D	2	 50% 50%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PEG	A	413	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 3543 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	280	2213	1419	375	408	11	0	7	0

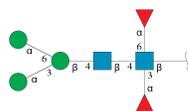
There are 23 discrepancies between the modelled and reference sequences:

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	97	818	522	138	156	2	0	2	0

- 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.



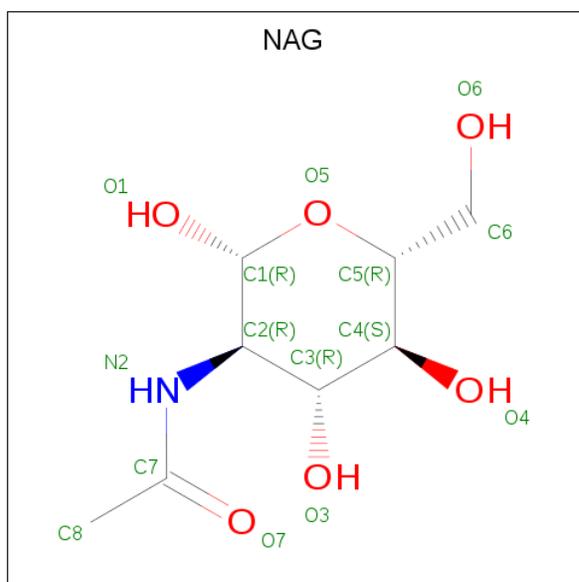
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	7	81	46	2	33	0	0	0

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



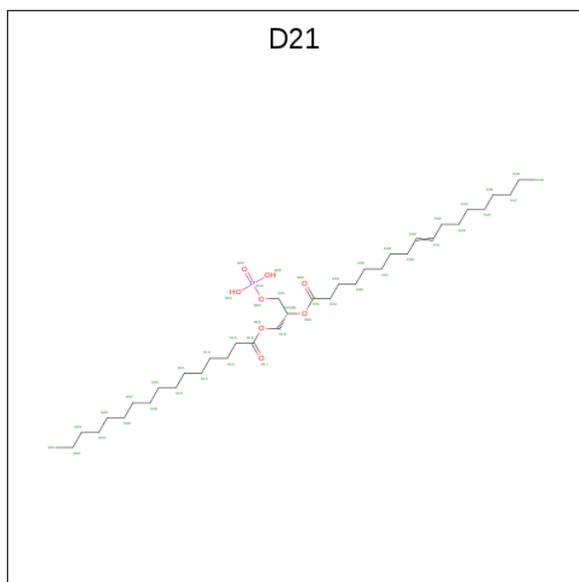
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	24	14	1	9	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



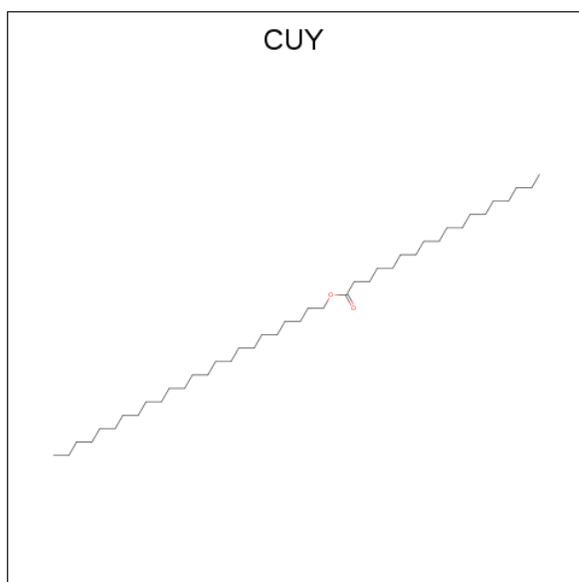
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

- Molecule 6 is (2R)-1-(hexadecanoyloxy)-3-(phosphonoxy)propan-2-yl (9Z)-octadec-9-enoate (three-letter code: D21) (formula:  $C_{37}H_{71}O_8P$ ).



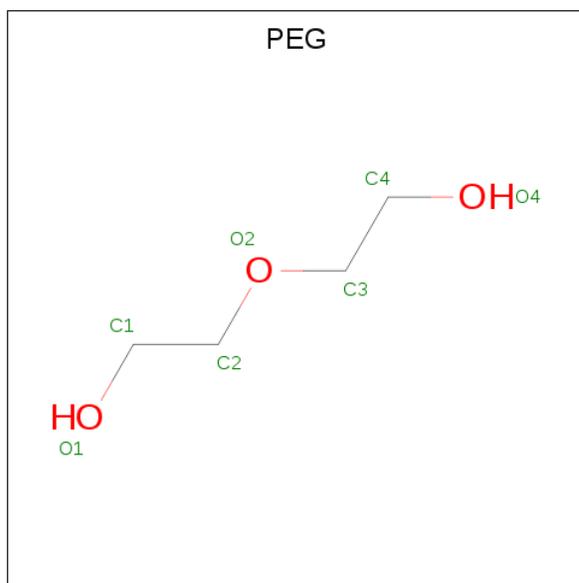
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
6	A	1	46	37	8	1	0	0

- Molecule 7 is tetracosyl octadecanoate (three-letter code: CUY) (formula:  $C_{42}H_{84}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			36	34	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

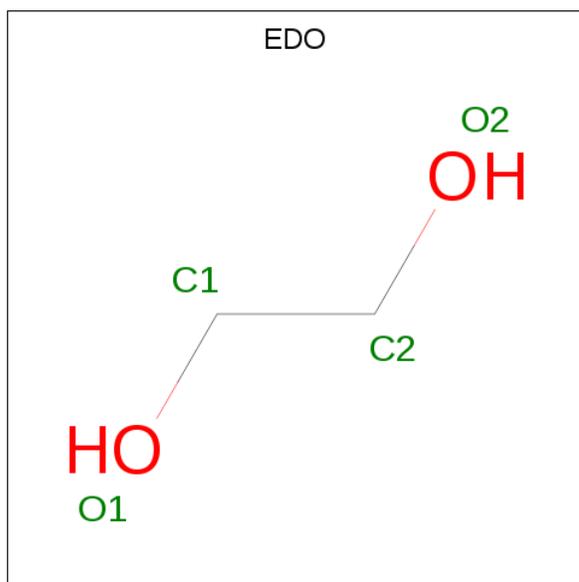


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0
9	A	3	Total Cl 3 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 11 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total I 1 1	0	0
11	A	2	Total I 2 2	0	0

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total Na 1 1	0	0

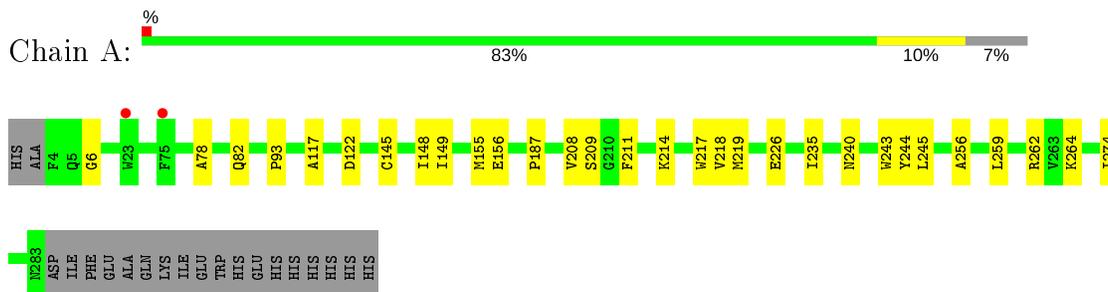
- Molecule 13 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
13	A	203	Total 203	O 203	0	0
13	B	89	Total 89	O 89	0	0

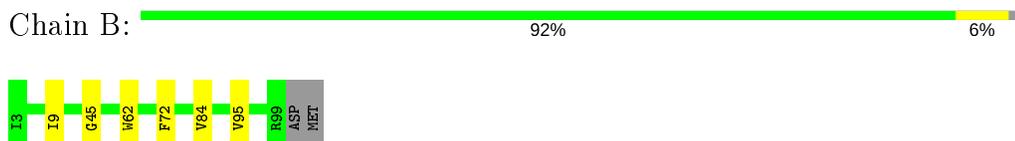
### 3 Residue-property plots [i](#)

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.19Å 78.53Å 84.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.58 – 2.06 32.37 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.58-2.06) 100.0 (32.37-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.06Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.171 , 0.224 0.184 , 0.236	Depositor DCC
$R_{free}$ test set	1259 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: IOD, BMA, NAG, CL, D21, NA, EDO, CUY, FUC, PEG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.62	0/2291	0.69	0/3107
2	B	0.63	0/844	0.70	0/1146
All	All	0.62	0/3135	0.69	0/4253

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	2213	0	2136	22	0
2	B	818	0	779	4	0
3	C	81	0	70	0	0
4	D	24	0	22	0	0
5	A	14	0	13	0	0
6	A	46	0	0	0	0
7	A	36	0	0	0	0
8	A	7	0	10	7	0
9	A	3	0	0	0	0
9	B	1	0	0	0	0
10	A	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	2	0	0	0	0
11	B	1	0	0	1	0
12	B	1	0	0	0	0
13	A	203	0	0	0	0
13	B	89	0	0	0	0
All	All	3543	0	3036	25	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 4.

All (25) 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:93:PRO:HB2	10:A:417:EDO:H22	1.38	1.04
1:A:243[B]:TRP:CH2	8:A:413:PEG:H22	2.18	0.79
1:A:243[B]:TRP:HH2	8:A:413:PEG:H22	1.51	0.74
1:A:93:PRO:HB2	10:A:417:EDO:C2	2.17	0.74
1:A:209:SER:HB2	1:A:244:TYR:HD1	1.66	0.61
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.86	0.57
2:B:9:ILE:HD12	2:B:84:VAL:HG21	1.87	0.56
1:A:262:ARG:HH21	1:A:274:ILE:HD11	1.71	0.56
1:A:235:ILE:HG13	1:A:245:LEU:HD13	1.88	0.56
1:A:243[B]:TRP:CH2	8:A:413:PEG:C2	2.89	0.54
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.90	0.54
1:A:214:LYS:HB2	8:A:413:PEG:H21	1.90	0.53
2:B:45:GLY:N	11:B:203:IOD:I	3.15	0.50
1:A:214:LYS:H	8:A:413:PEG:H32	1.78	0.46
1:A:145:CYS:HA	1:A:148:ILE:HG22	1.99	0.45
1:A:219[A]:MET:HE2	1:A:226:GLU:HB3	1.98	0.45
1:A:208:VAL:HG21	1:A:218:VAL:HG21	1.98	0.44
1:A:256:ALA:HA	1:A:259:LEU:HD12	2.00	0.44
1:A:78:ALA:O	1:A:82:GLN:HG2	2.18	0.43
1:A:149:ILE:HG22	1:A:155:MET:CE	2.49	0.42
1:A:209:SER:HB2	1:A:244:TYR:CD1	2.50	0.42
1:A:117:ALA:HB2	2:B:62:TRP:CE2	2.54	0.41
2:B:9:ILE:HB	2:B:95:VAL:HG21	2.01	0.41
1:A:6:GLY:CA	8:A:413:PEG:H41	2.50	0.41
1:A:214:LYS:HB2	8:A:413:PEG:H31	2.03	0.40

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	285/300 (95%)	283 (99%)	2 (1%)	0	100	100
2	B	97/99 (98%)	97 (100%)	0	0	100	100
All	All	382/399 (96%)	380 (100%)	2 (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	234/247 (95%)	231 (99%)	3 (1%)	69	67
2	B	93/94 (99%)	92 (99%)	1 (1%)	73	72
All	All	327/341 (96%)	323 (99%)	4 (1%)	69	69

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	156	GLU
1	A	240	ASN
2	B	72	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	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](#)

9 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	1,3	14,14,15	1.43	3 (21%)	17,19,21	2.23	3 (17%)
3	NAG	C	2	3	14,14,15	1.52	2 (14%)	17,19,21	1.52	1 (5%)
3	BMA	C	3	3	11,11,12	0.32	0	15,15,17	0.56	0
3	MAN	C	4	3	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
3	MAN	C	5	3	11,11,12	0.29	0	15,15,17	0.99	1 (6%)
3	FUC	C	6	3	10,10,11	1.15	1 (10%)	14,14,16	1.25	2 (14%)
3	FUC	C	7	3	10,10,11	1.28	1 (10%)	14,14,16	1.28	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.30	0	17,19,21	1.42	3 (17%)
4	FUC	D	2	4	10,10,11	0.47	0	14,14,16	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O7-C7	-4.26	1.13	1.23
3	C	1	NAG	O7-C7	-2.92	1.16	1.23
3	C	1	NAG	O5-C1	-2.43	1.39	1.43
3	C	6	FUC	O5-C1	-2.35	1.40	1.43
3	C	2	NAG	O5-C5	-2.25	1.38	1.43
3	C	1	NAG	C2-N2	-2.21	1.42	1.46
3	C	7	FUC	O5-C1	-2.13	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	6.94	121.59	112.19
3	C	2	NAG	C1-O5-C5	4.21	117.90	112.19
4	D	1	NAG	C1-O5-C5	4.13	117.79	112.19
3	C	1	NAG	C2-N2-C7	3.85	128.38	122.90
3	C	7	FUC	C1-C2-C3	3.54	114.01	109.67
3	C	6	FUC	O3-C3-C2	3.36	116.42	109.99
3	C	5	MAN	C1-O5-C5	3.28	116.63	112.19
3	C	4	MAN	C1-O5-C5	2.64	115.77	112.19
3	C	1	NAG	C8-C7-N2	-2.59	111.71	116.10
4	D	1	NAG	O5-C1-C2	-2.42	107.47	111.29
4	D	1	NAG	C3-C4-C5	2.24	114.24	110.24
3	C	6	FUC	O2-C2-C3	2.22	114.58	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6

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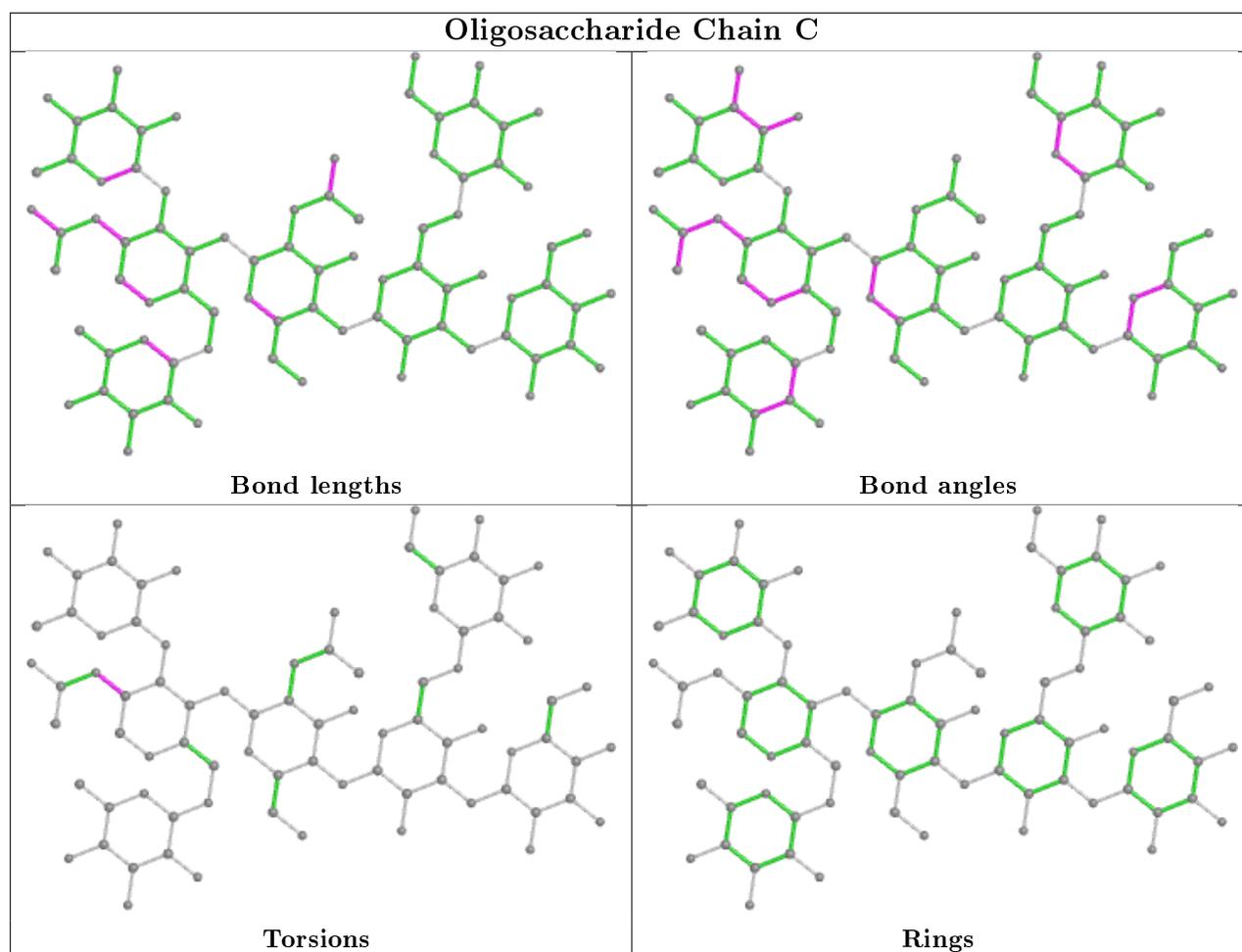
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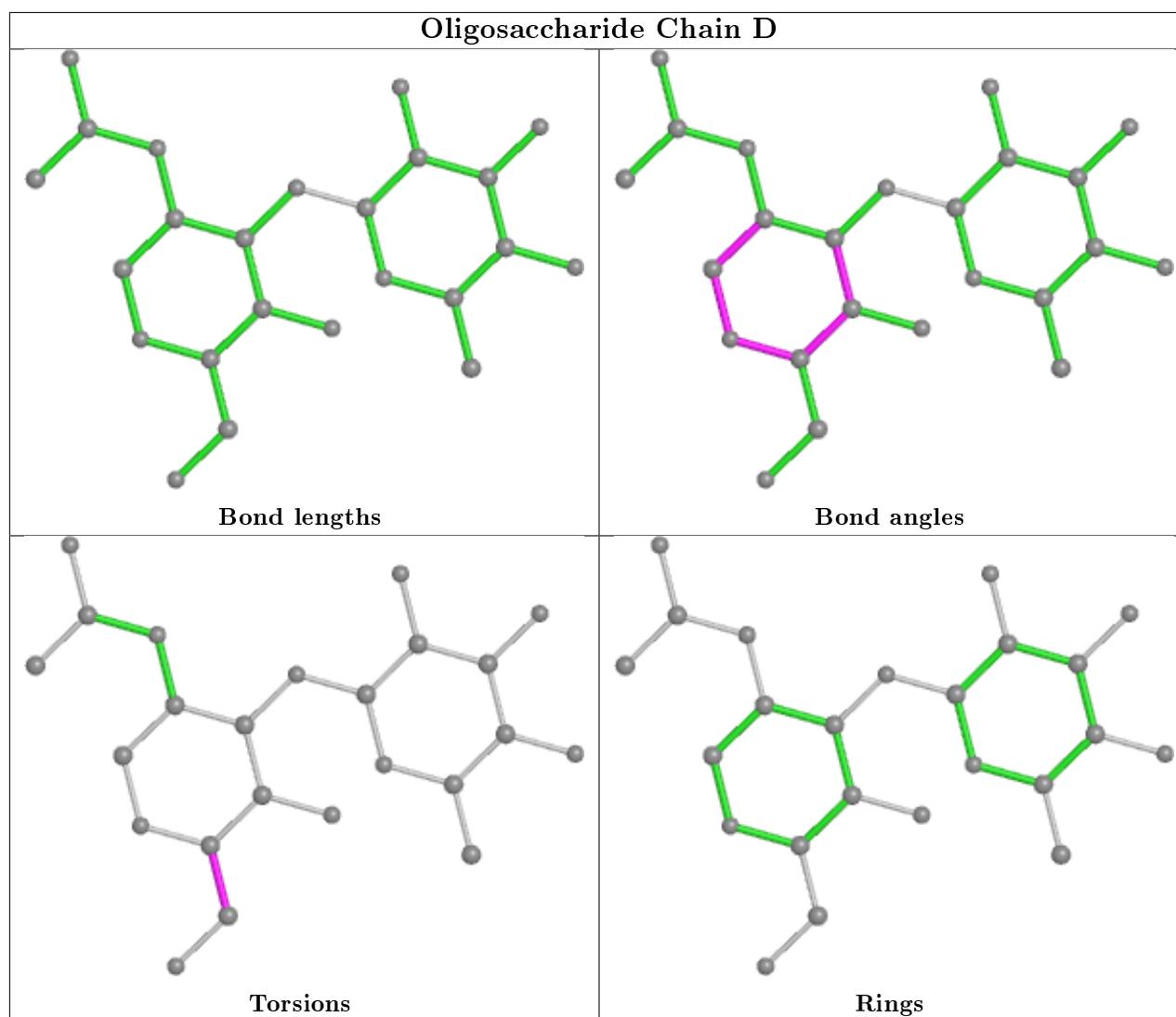
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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 13 ligands modelled in this entry, 8 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	$\# Z  > 2$
10	EDO	A	417	-	3,3,3	0.63	0	2,2,2	0.29	0
7	CUY	A	412	-	35,35,43	0.38	0	35,35,43	0.34	0
8	PEG	A	413	-	6,6,6	0.41	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	D21	A	411	-	45,45,45	0.78	2 (4%)	49,50,50	1.04	4 (8%)
5	NAG	A	408	1	14,14,15	0.57	0	17,19,21	1.45	2 (11%)

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
10	EDO	A	417	-	-	1/1/1/1	-
7	CUY	A	412	-	-	16/34/34/42	-
8	PEG	A	413	-	-	3/4/4/4	-
6	D21	A	411	-	-	13/47/47/47	-
5	NAG	A	408	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	411	D21	C41-C40	3.30	1.50	1.31
6	A	411	D21	C42-C41	-3.13	1.32	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	NAG	C1-O5-C5	4.53	118.33	112.19
6	A	411	D21	P23-O22-C21	3.71	128.51	118.30
6	A	411	D21	O30-C20-C19	2.92	118.99	108.40
6	A	411	D21	C43-C42-C41	2.87	128.87	112.43
5	A	408	NAG	C2-N2-C7	2.39	126.31	122.90
6	A	411	D21	O30-C20-C21	2.28	116.67	108.40

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	408	NAG	C3-C2-N2-C7
5	A	408	NAG	C8-C7-N2-C2
5	A	408	NAG	O7-C7-N2-C2
6	A	411	D21	C13-C14-C15-C16
6	A	411	D21	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
7	A	412	CUY	CAM-CAN-CAO-CAP
6	A	411	D21	C39-C40-C41-C42
7	A	412	CUY	CBK-CBL-CBM-CAW
7	A	412	CUY	CAG-CAH-CAI-CAJ
7	A	412	CUY	CAH-CAI-CAJ-CAK
7	A	412	CUY	CAS-CAT-CAU-CAV
7	A	412	CUY	CAJ-CAK-CAL-CAM
7	A	412	CUY	CAL-CAM-CAN-CAO
10	A	417	EDO	O1-C1-C2-O2
7	A	412	CUY	C40-CAA-CAB-CAC
6	A	411	D21	C35-C36-C37-C38
6	A	411	D21	C36-C37-C38-C39
7	A	412	CUY	CAR-CAS-CAT-CAU
7	A	412	CUY	C41-C40-CAA-CAB
7	A	412	CUY	CBE-CBF-CBG-CBH
8	A	413	PEG	C4-C3-O2-C2
7	A	412	CUY	CAT-CAU-CAV-CAW
6	A	411	D21	O18-C19-C20-O30
6	A	411	D21	C41-C42-C43-C44
8	A	413	PEG	C1-C2-O2-C3
6	A	411	D21	C40-C41-C42-C43
7	A	412	CUY	CAD-CAE-CAF-CAG
7	A	412	CUY	CAA-CAB-CAC-CAD
6	A	411	D21	C07-C08-C09-C10
7	A	412	CUY	CAV-CAW-CBM-CBL
7	A	412	CUY	CAI-CAJ-CAK-CAL
6	A	411	D21	C38-C39-C40-C41
8	A	413	PEG	O1-C1-C2-O2
6	A	411	D21	C14-C15-C16-O18
6	A	411	D21	C06-C07-C08-C09
6	A	411	D21	C14-C15-C16-O17

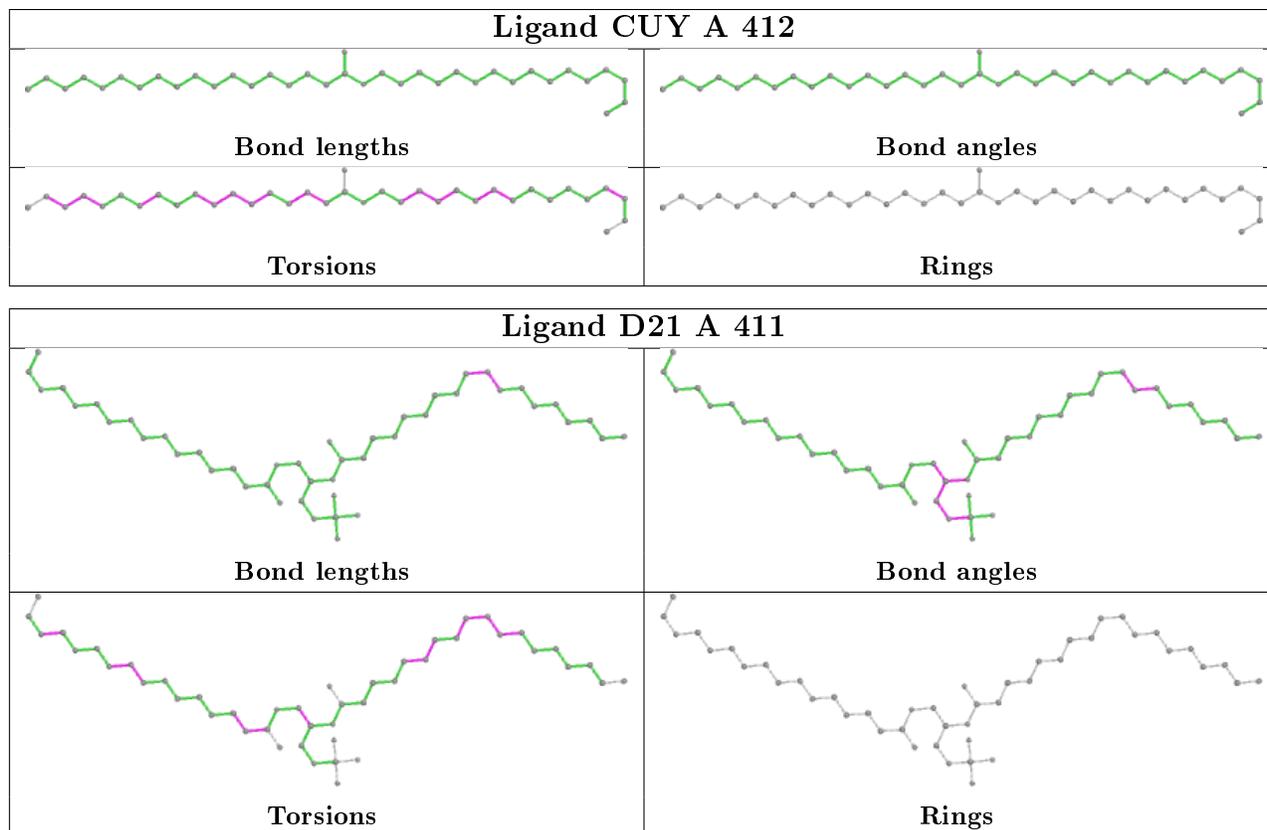
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	417	EDO	2	0
8	A	413	PEG	7	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	280/300 (93%)	-0.50	2 (0%) 87 88	9, 17, 37, 55	0
2	B	97/99 (97%)	-0.59	0 100 100	10, 18, 38, 55	0
All	All	377/399 (94%)	-0.52	2 (0%) 91 91	9, 18, 38, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	PHE	2.2
1	A	23	TRP	2.1

### 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.

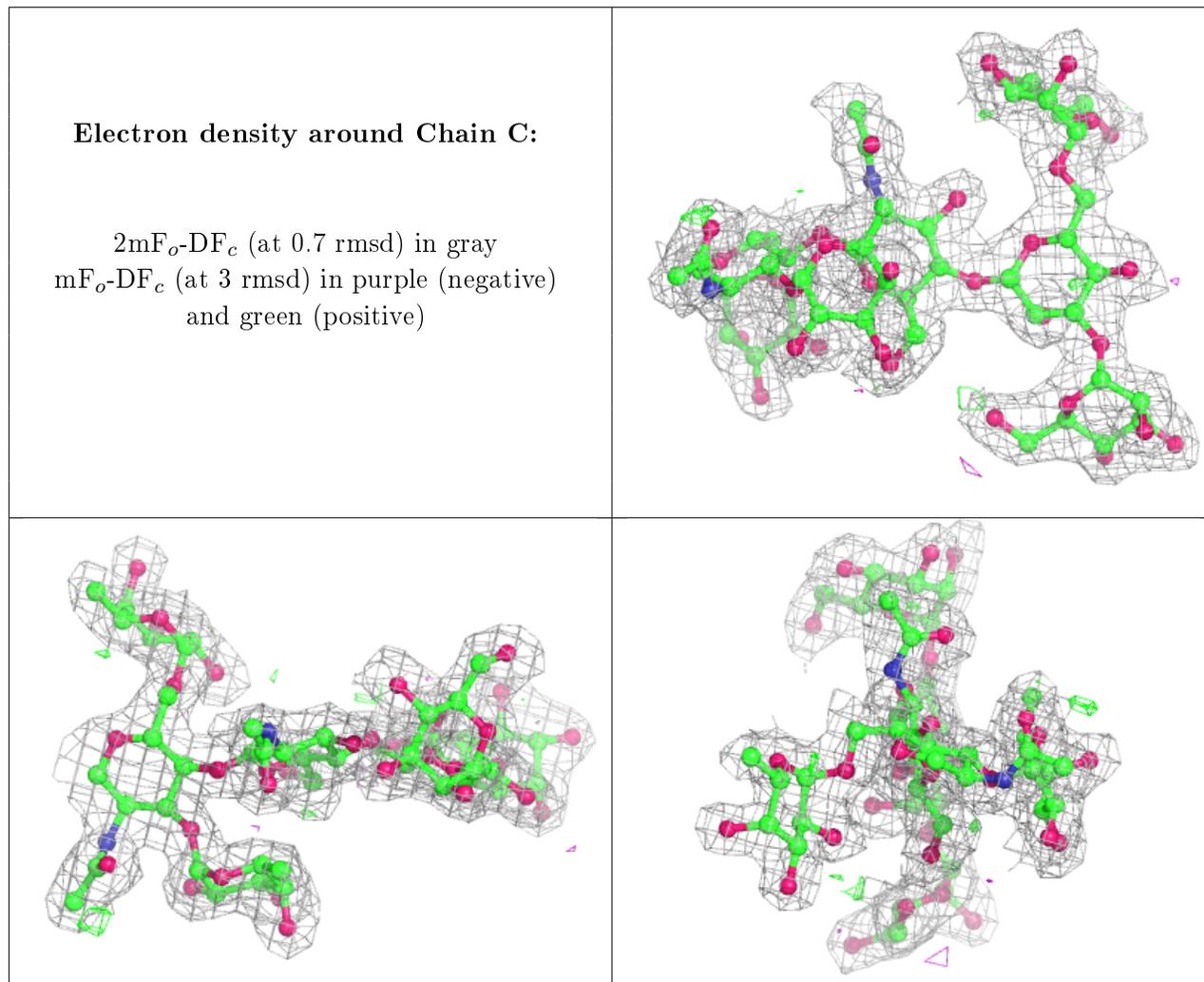
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	D	1	14/15	0.78	0.28	42,46,49,50	0
4	FUC	D	2	10/11	0.83	0.29	36,39,41,42	0
3	MAN	C	4	11/12	0.91	0.09	25,27,30,33	0
3	FUC	C	7	10/11	0.94	0.11	18,21,26,27	0
3	BMA	C	3	11/12	0.94	0.08	18,19,21,26	0
3	FUC	C	6	10/11	0.95	0.08	19,21,23,24	0
3	MAN	C	5	11/12	0.95	0.09	10,16,23,24	0

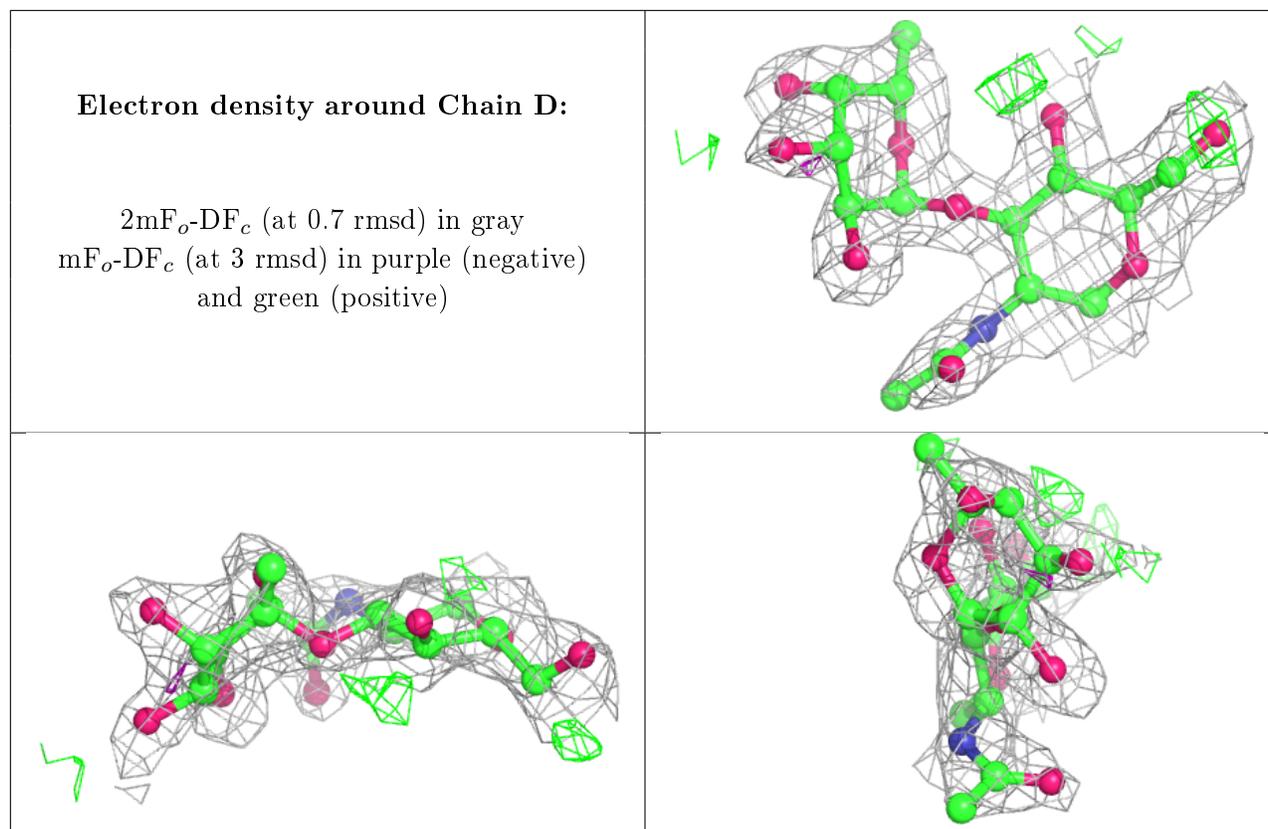
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	2	14/15	0.96	0.08	8,14,16,19	0
3	NAG	C	1	14/15	0.97	0.07	10,15,17,18	0

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.





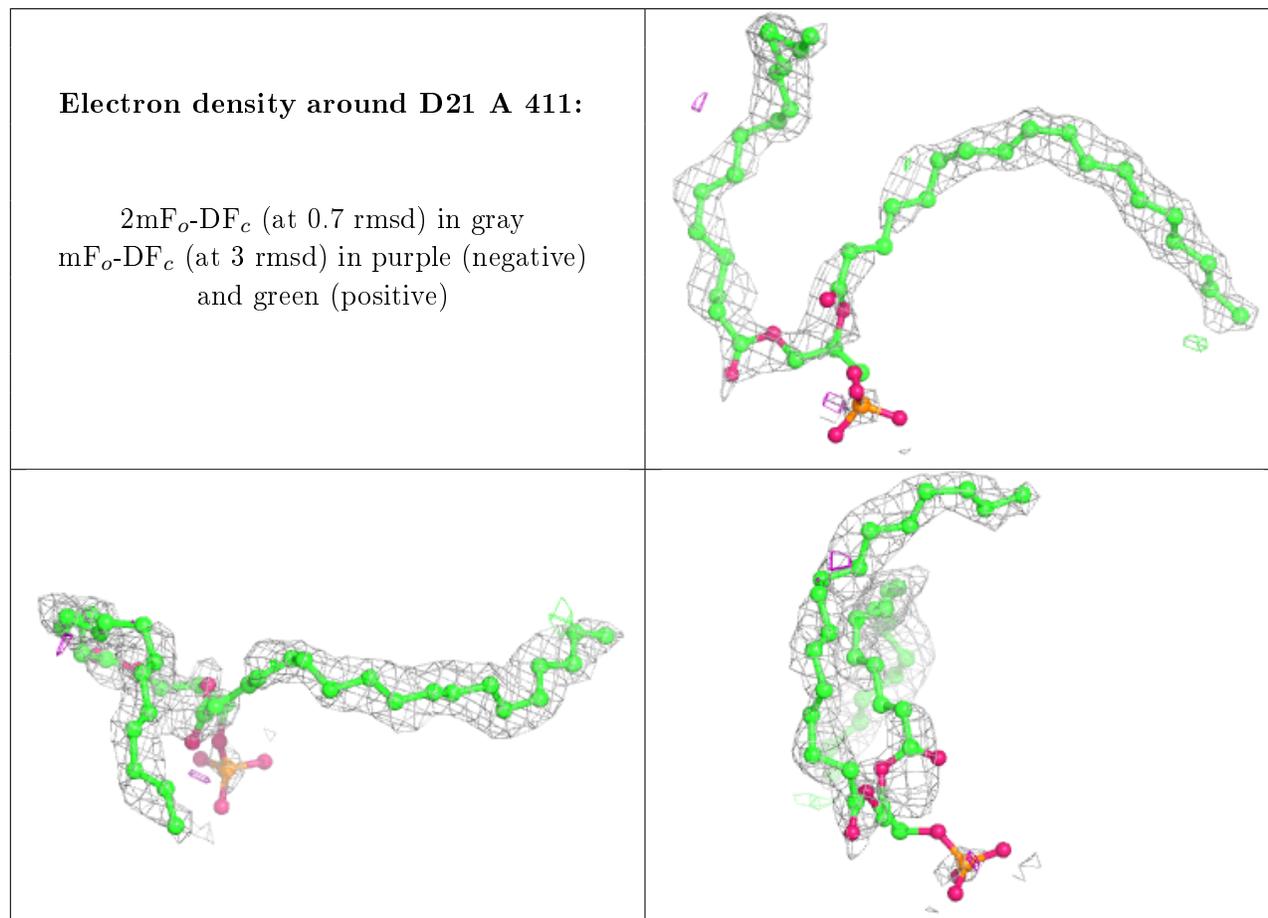
## 6.4 Ligands [i](#)

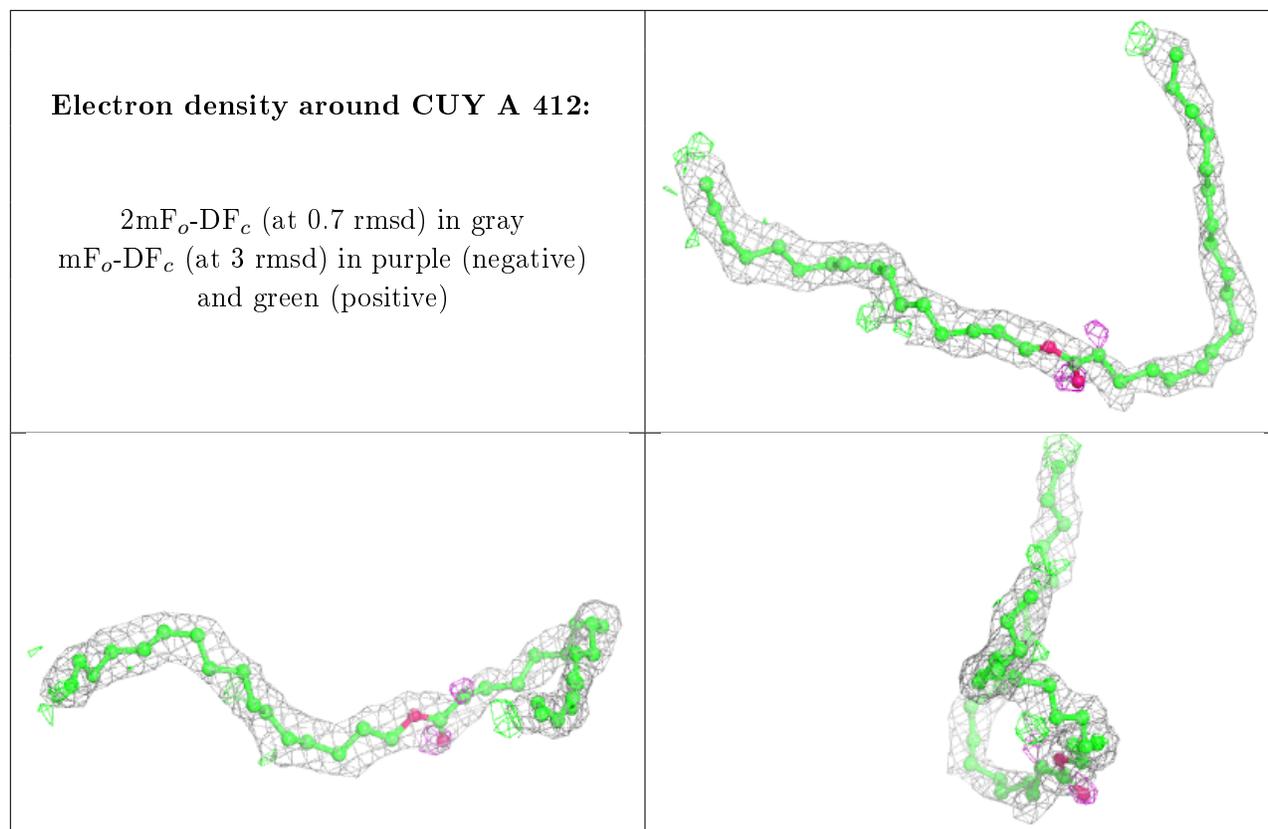
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	NAG	A	408	14/15	0.65	0.24	51,55,62,64	0
6	D21	A	411	46/46	0.74	0.25	29,43,89,90	1
7	CUY	A	412	36/44	0.81	0.20	24,31,43,48	0
9	CL	A	414	1/1	0.86	0.08	42,42,42,42	0
9	CL	A	416	1/1	0.89	0.11	85,85,85,85	0
10	EDO	A	417	4/4	0.92	0.19	19,22,25,27	0
8	PEG	A	413	7/7	0.94	0.19	4,16,23,32	0
11	IOD	B	203	1/1	0.95	0.05	37,37,37,37	1
9	CL	B	202	1/1	0.96	0.13	42,42,42,42	0
11	IOD	A	418	1/1	0.98	0.05	39,39,39,39	1
9	CL	A	415	1/1	0.98	0.09	18,18,18,18	0
12	NA	B	201	1/1	0.99	0.03	15,15,15,15	0
11	IOD	A	419	1/1	0.99	0.06	15,15,15,15	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.