

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 11, 2023 – 01:13 PM EDT

PDB ID	:	8GLF
Title	:	Crystal Structure of Human CD1b in Complex with Sphingomyelin C34:2
Authors	:	Shahine, A.
Deposited on		
Resolution	:	2.00  Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

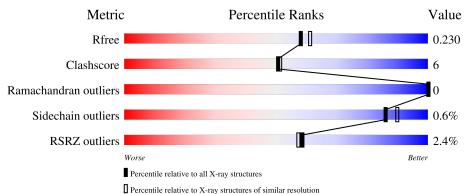
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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		of chain	
1	А	300	<sup>2%</sup> 83%		10% 7%
2	В	101	4%		11% ••
3	D	2	50%	50%	
4	С	7	29%	71%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	2	-	-	-	Х



# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3490 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
1	А	280	Total 2238	C 1440	N 377	O 409	S 12	0	11	0

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

There are 23 discrepancies between the modelled and reference sequences:

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 820	C 523	N 139	O 156	S 2	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

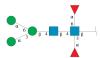
Chain	Residue	Modelled	Actual	Comment	Reference
В	1	PRO	-	expression tag	UNP P61769
В	2	LYS	-	expression tag	UNP P61769

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0	0

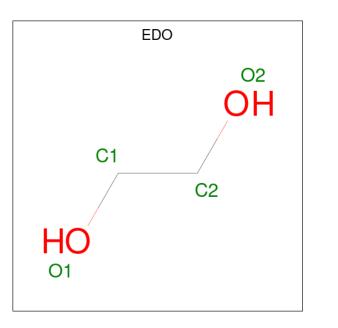
• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyr anose.



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

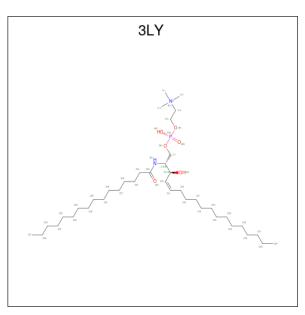
• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

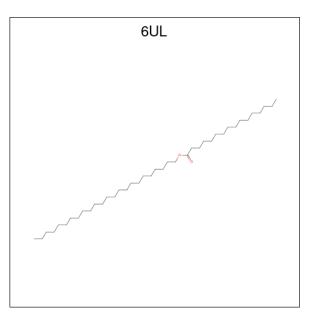
• Molecule 6 is [( {Z},2 {R},3 {S})-2-(hexadecanoylamino)-3-oxidanyl-octadec-4-enyl] 2-(trimethyl- $1^{4}-azanyl$ )ethyl hydrogen phosphate (three-letter code: 3LY) (formula:  $C_{39}H_{80}N_2O_6P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
6	Δ	1	Total	С	Ν	0	Р	0	0
0	Л	1	48	39	2	6	1	0	0



• Molecule 7 is TETRACOSYL PALMITATE (three-letter code: 6UL) (formula:  $C_{40}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	А	1	Total 26	C 24	O 2	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	4	Total Cl 4 4	0	0

• Molecule 9 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total I 1 1	0	0
9	В	1	Total I 1 1	0	0

• Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total Ni 1 1	0	0

• Molecule 11 is water.

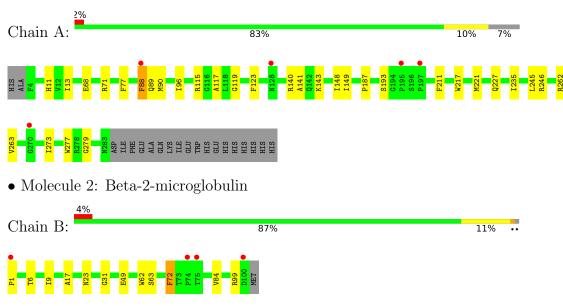


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	167	Total O 167 167	0	0
11	В	67	Total         O           67         67	0	0



# 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 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:	50%	50%
NAG1 NAG2		

 $\label{eq:mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]} beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-6)] beta-D-glucopyranose-(1-6)] beta-D-gluco$ 





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	57.57Å 77.98Å 91.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	35.86 - 2.00	Depositor
Resolution (A)	35.86 - 2.00	EDS
% Data completeness	95.2 (35.86-2.00)	Depositor
(in resolution range)	95.2(35.86-2.00)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.26 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.176 , $0.231$	Depositor
$R, R_{free}$	0.176 , $0.230$	DCC
$R_{free}$ test set	1383 reflections $(5.10\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.8	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 49.2	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3490	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CL, NAG, IOD, 3LY, EDO, BMA, 6UL, MAN, NI, FUC

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		lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.40	0/2330	0.57	0/3161
2	В	0.41	0/844	0.59	0/1150
All	All	0.40	0/3174	0.57	0/4311

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	А	2238	0	2172	26	0
2	В	820	0	762	14	0
3	D	28	0	25	0	0
4	С	81	0	70	0	0
5	А	8	0	12	0	0
6	А	48	0	0	1	0
7	А	26	0	42	0	0
8	А	4	0	0	0	0
9	А	1	0	0	0	0
9	В	1	0	0	0	0
10	В	1	0	0	0	0

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001000	Continued from precious page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
11	А	167	0	0	3	1		
11	В	67	0	0	2	1		
All	All	3490	0	3083	36	1		

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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 6.

The worst 5 of 36 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:68:GLU:OE2	1:A:71[A]:ARG:NH1	2.14	0.80
1:A:115:ARG:NH1	11:A:501:HOH:O	2.21	0.73
1:A:119:GLY:HA3	2:B:1:PRO:HA	1.72	0.70
2:B:17:ALA:HB3	2:B:99:ARG:HD3	1.77	0.66
1:A:89:GLN:HA	1:A:89:GLN:OE1	1.95	0.66

All (1) 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)	
11:A:533:HOH:O	11:B:304:HOH:O[4_445]	2.19	0.01	

### 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	Favoured Allowed		Percentiles		
1	А	289/300~(96%)	284 (98%)	5(2%)	0	100	100	
2	В	99/101~(98%)	99 (100%)	0	0	100	100	
All	All	388/401~(97%)	383~(99%)	5 (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	Rotameric Outliers		
1	А	237/247~(96%)	236 (100%)	1 (0%)	91 93	
2	В	90/96~(94%)	89~(99%)	1 (1%)	73 78	
All	All	327/343~(95%)	325~(99%)	2(1%)	86 90	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	88	PHE
2	В	72	PHE

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

#### 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	Turne	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	NAG	С	1	4,1	$14,\!14,\!15$	0.84	1 (7%)	17,19,21	0.91	0
4	NAG	С	2	4	14,14,15	0.50	0	17,19,21	0.40	0
4	BMA	С	3	4	11,11,12	0.64	0	15,15,17	1.21	1 (6%)
4	MAN	С	4	4	11,11,12	1.08	0	15,15,17	1.15	2 (13%)
4	MAN	С	5	4	11,11,12	0.68	0	15,15,17	1.29	1 (6%)
4	FUC	С	6	4	10,10,11	1.03	1 (10%)	14,14,16	0.90	0
4	FUC	С	7	4	10,10,11	0.95	0	14,14,16	0.68	0
3	NAG	D	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	0.50	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	1	NAG	O5-C1	-3.02	1.38	1.43
3	D	1	NAG	O5-C1	2.28	1.47	1.43
4	С	6	FUC	C2-C3	2.02	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	С	5	MAN	C1-O5-C5	3.63	117.11	112.19
4	С	4	MAN	C1-O5-C5	3.24	116.59	112.19
4	С	3	BMA	O2-C2-C3	-2.78	104.56	110.14
3	D	1	NAG	C1-O5-C5	2.51	115.59	112.19
4	С	4	MAN	O2-C2-C3	-2.13	105.87	110.14



There are no chirality outliers.

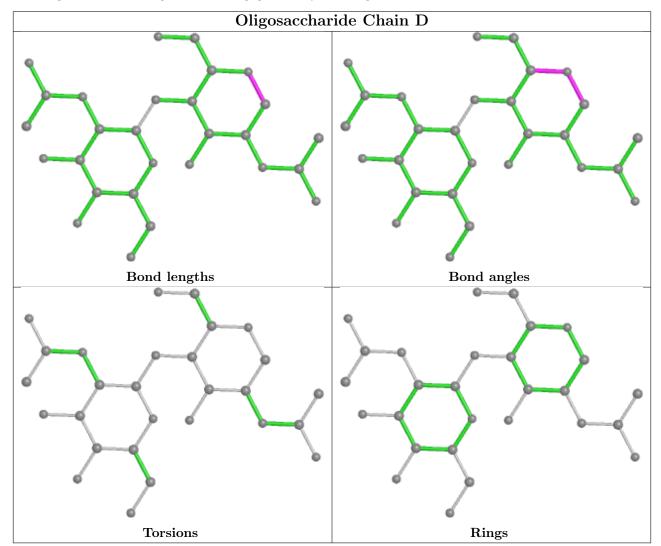
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C3-C2-N2-C7

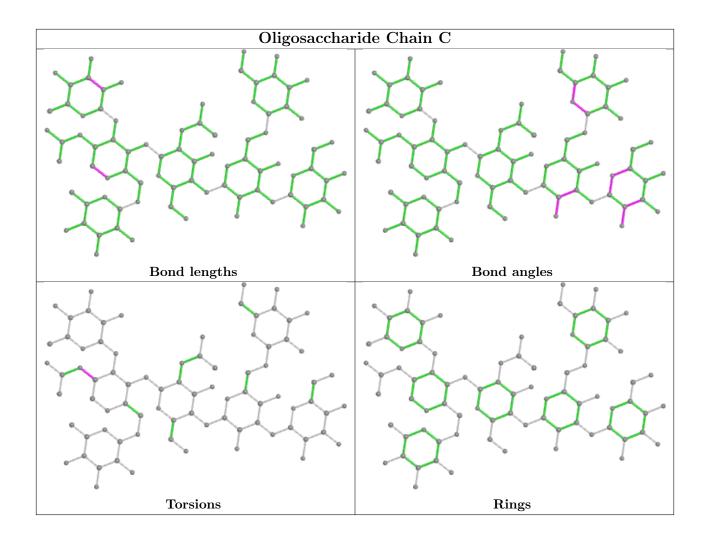
There are no ring outliers.

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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	lol Type Chain Res		Res	Link	Bo	ond leng	$\mathbf{ths}$	Bond angles			
10101	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
7	6UL	А	404	-	$25,\!25,\!41$	0.76	1 (4%)	$25,\!25,\!41$	1.00	1 (4%)	
5	EDO	А	402	-	$3,\!3,\!3$	0.46	0	2,2,2	0.27	0	
6	3LY	А	403	-	46,47,47	1.24	3 (6%)	$52,\!55,\!55$	1.04	3 (5%)	
5	EDO	А	401	-	3,3,3	0.46	0	$2,\!2,\!2$	0.37	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
7	6UL	А	404	-	-	10/24/24/40	-
5	EDO	А	402	-	-	0/1/1/1	-
6	3LY	А	403	-	-	27/52/52/52	-
5	EDO	А	401	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	403	3LY	C22-N21	5.87	1.46	1.34
7	А	404	6UL	OAQ-CAP	2.60	1.40	1.33
6	А	403	3LY	O23-C22	-2.44	1.18	1.23
6	А	403	3LY	C31-C33	2.14	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	А	403	3LY	O32-C31-C18	4.73	120.48	107.93
6	А	403	3LY	C24-C22-N21	3.45	121.81	115.83
7	А	404	6UL	OAQ-CAP-CAO	2.84	120.83	111.91
6	А	403	3LY	O23-C22-C24	-2.23	117.94	122.02

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	403	3LY	OP4-C17-C18-N21
6	А	403	3LY	OP4-C17-C18-C31
6	А	403	3LY	N21-C18-C31-O32
6	А	403	3LY	N21-C18-C31-C33
6	А	403	3LY	C17-C18-C31-O32

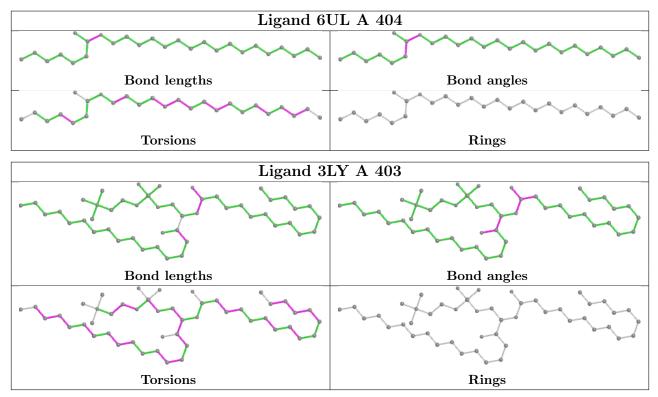
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	403	3LY	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 then 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 sufficient 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	280/300~(93%)	-0.13	5 (1%) 68 66	14, 26, 53, 82	0
2	В	100/101~(99%)	0.06	4 (4%) 38 37	15, 32, 55, 70	0
All	All	380/401~(94%)	-0.08	9 (2%) 59 57	14, 27, 54, 82	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	1	PRO	4.2
1	А	197	PRO	3.0
1	А	128	ASN	2.9
2	В	75	THR	2.8
1	А	270	GLY	2.5

### 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	NAG	D	2	14/15	0.36	0.46	92,102,110,113	0
3	NAG	D	1	14/15	0.77	0.24	49,60,81,85	0
4	FUC	С	6	10/11	0.89	0.14	$28,\!36,\!42,\!43$	0
4	MAN	С	4	11/12	0.93	0.10	27,30,35,38	0
4	FUC	С	7	10/11	0.93	0.11	33,36,40,41	0

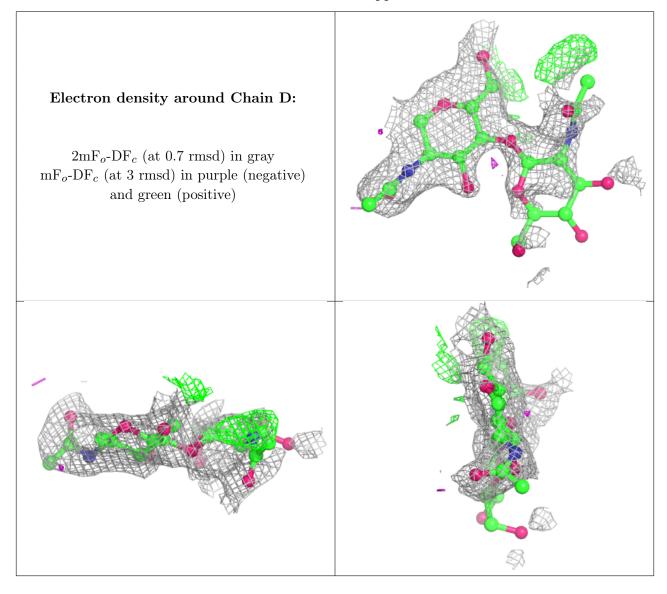
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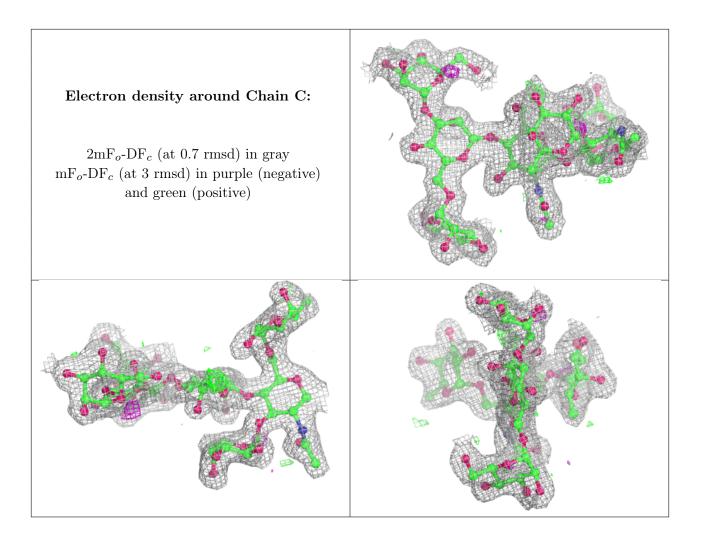
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	С	2	14/15	0.95	0.09	14,22,28,34	0
4	MAN	С	5	11/12	0.96	0.15	16,23,30,31	0
4	NAG	С	1	14/15	0.97	0.08	15,20,22,26	0
4	BMA	С	3	11/12	0.97	0.09	16,22,26,29	0

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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.







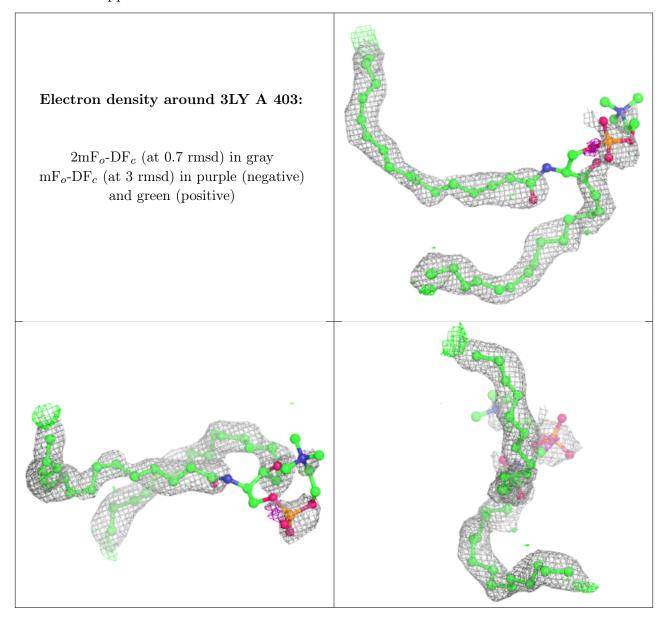
### 6.4 Ligands (i)

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,  $95^{th}$  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.

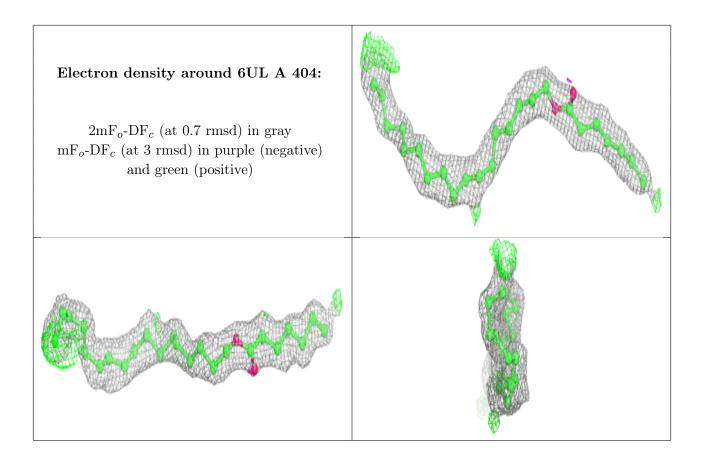
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
6	3LY	А	403	48/48	0.70	0.29	$24,\!55,\!119,\!121$	0
8	CL	А	405	1/1	0.79	0.09	56, 56, 56, 56	0
5	EDO	А	401	4/4	0.84	0.26	$53,\!54,\!59,\!62$	0
7	$6 \mathrm{UL}$	А	404	26/42	0.89	0.22	20,35,42,55	0
10	NI	В	202	1/1	0.94	0.09	43,43,43,43	0
5	EDO	А	402	4/4	0.97	0.12	43,44,45,47	0
9	IOD	В	201	1/1	0.98	0.05	48,48,48,48	1
8	CL	А	407	1/1	0.98	0.10	40,40,40,40	0
8	CL	А	406	1/1	0.99	0.11	30,30,30,30	0
8	CL	А	408	1/1	0.99	0.25	$19,\!19,\!19,\!19$	0
9	IOD	А	409	1/1	1.00	0.09	22,22,22,22	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.

