



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2025 – 10:15 AM EST

PDB ID : 9OI0 / pdb_00009oi0
Title : Crystal structure of CD1b presenting ganglioside GD3
Authors : Chen, Y.; Cao, T.P.; Farquhar, R.; Rossjohn, J.; Shahine, A.
Deposited on : 2025-05-05
Resolution : 1.84 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

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>.

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)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

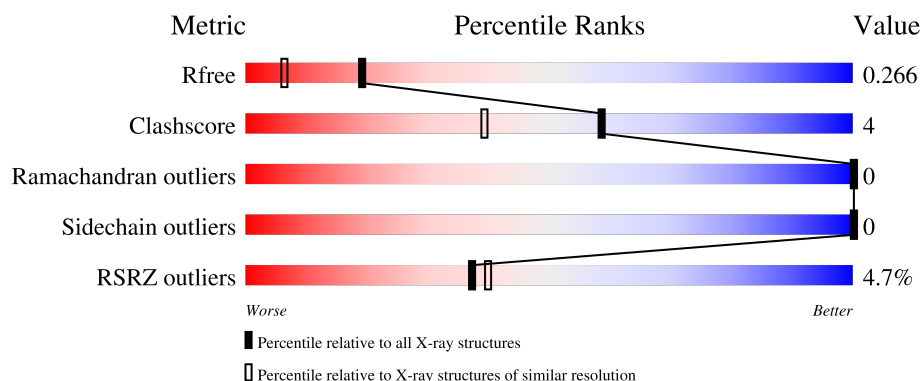
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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 $\leq 5\%$. 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	280	
2	B	100	
3	C	7	
4	D	3	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 3590 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	2223	1420	381	412	10	0	7	0

There are 5 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

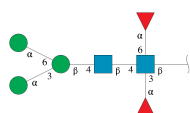
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	826	525	141	158	2	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

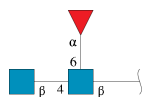
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP P61769
B	0	LYS	-	expression tag	UNP P61769

- 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
3	C	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 4 is an oligosaccharide called 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
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	I	0	0
			3	3		
5	B	1	Total	I	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

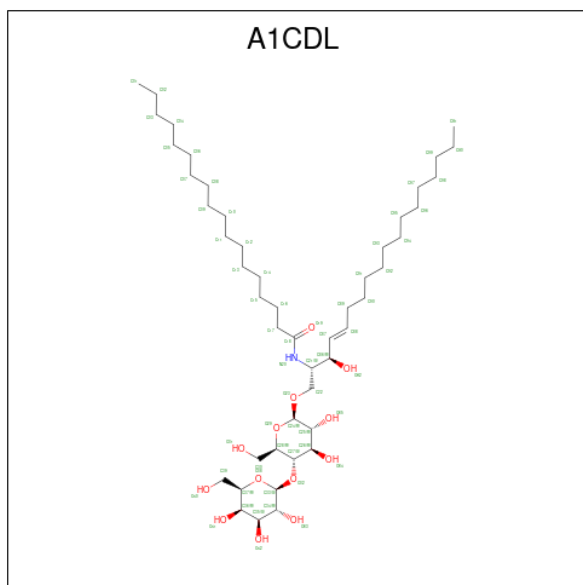
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Cl	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



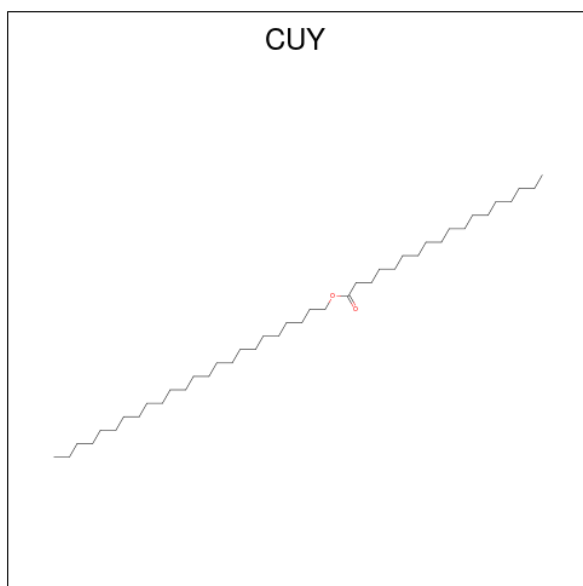
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is N-[(2S,3R,4E)-1-[(4-O-beta-D-galactopyranosyl-beta-D-glucopyranosyl)oxy]-3-hydroxyoctadec-4-en-2-yl]octadecanamide (CCD ID: A1CDL) (formula: $C_{48}H_{91}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			62	48	1	13		

- Molecule 9 is tetracosyl octadecanoate (CCD ID: CUY) (formula: $C_{42}H_{84}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			35	33	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		

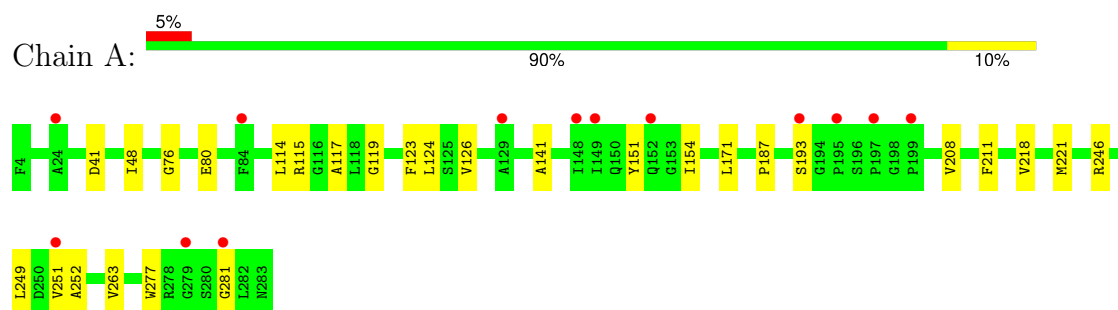
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	235	Total	O	0	0
			235	235		
11	B	71	Total	O	0	0
			71	71		

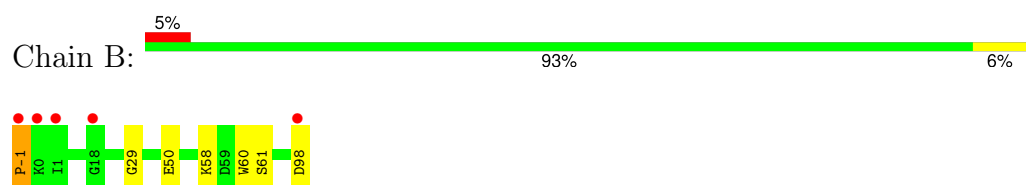
3 Residue-property plots

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.

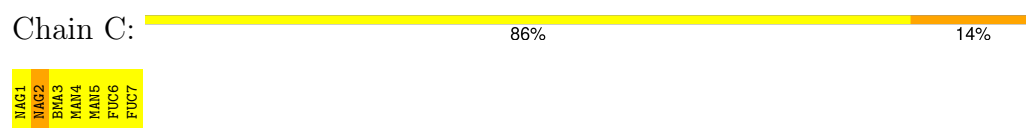
- Molecule 1: T-cell surface glycoprotein CD1b



- 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: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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, α , β , γ	57.57Å 77.85Å 92.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.29 – 1.84 46.29 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-1.84) 100.0 (46.29-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.211 , 0.266 0.213 , 0.266	Depositor DCC
R_{free} test set	1832 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EDO, A1CDL, CUY, IOD, FUC, NAG, CL, BMA, 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	0.48	0/2283	0.79	0/3100
2	B	0.46	0/849	0.80	1/1154 (0.1%)
All	All	0.48	0/3132	0.79	1/4254 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	-1	PRO	N-CA-CB	6.94	110.63	103.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2223	0	2119	23	0
2	B	826	0	764	7	0
3	C	81	0	70	2	0
4	D	38	0	34	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
7	A	12	0	16	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	62	0	0	0	0
9	A	35	0	0	0	0
10	A	1	0	0	0	0
11	A	235	0	0	1	0
11	B	71	0	0	2	0
All	All	3590	0	3003	27	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 (27) 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:119:GLY:HA3	2:B:-1:PRO:HA	1.56	0.87
1:A:115[A]:ARG:HD3	7:A:308:EDO:H12	1.80	0.63
1:A:171:LEU:HD12	3:C:2:NAG:H82	1.81	0.62
1:A:208:VAL:HG21	1:A:218[B]:VAL:HG11	1.82	0.61
2:B:29:GLY:HA2	2:B:61[A]:SER:HB3	1.83	0.60
1:A:218[B]:VAL:HG12	1:A:263:VAL:HG22	1.88	0.56
2:B:98:ASP:HB2	11:B:240:HOH:O	2.07	0.53
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.90	0.53
1:A:41:ASP:HB2	1:A:48:ILE:HD11	1.92	0.50
1:A:193[B]:SER:HB3	1:A:277:TRP:CH2	2.46	0.50
2:B:50:GLU:HG3	11:B:232:HOH:O	2.13	0.48
1:A:151:TYR:HB3	1:A:154:ILE:HG12	1.97	0.47
1:A:221:MET:HE3	1:A:221:MET:HB3	1.76	0.47
7:A:308:EDO:H11	2:B:60:TRP:CZ2	2.50	0.46
1:A:115[A]:ARG:NH1	2:B:58:LYS:HZ3	2.14	0.46
1:A:246:ARG:HD2	11:A:454:HOH:O	2.16	0.45
1:A:76:GLY:O	1:A:80:GLU:HG2	2.17	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:A:249:LEU:HG	1:A:251[A]:VAL:HG23	1.99	0.43
1:A:171:LEU:CD1	3:C:2:NAG:H82	2.49	0.43
1:A:115[B]:ARG:HG2	7:A:306:EDO:H11	1.84	0.42
1:A:114:LEU:HB3	1:A:126:VAL:HB	2.01	0.42
1:A:114:LEU:C	1:A:114:LEU:HD23	2.45	0.41
1:A:123:PHE:CZ	1:A:141:ALA:HA	2.55	0.41
1:A:124:LEU:HD12	1:A:124:LEU:C	2.45	0.41
1:A:251[A]:VAL:HG12	1:A:252:ALA:O	2.20	0.40
1:A:281:GLY:HA2	7:A:305:EDO:C1	2.51	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	285/280 (102%)	281 (99%)	4 (1%)	0	100	100
2	B	100/100 (100%)	99 (99%)	1 (1%)	0	100	100
All	All	385/380 (101%)	380 (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	Outliers	Percentiles	
1	A	232/229 (101%)	232 (100%)	0	100	100
2	B	91/95 (96%)	91 (100%)	0	100	100
All	All	323/324 (100%)	323 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	14	GLN
1	A	175	ASN

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Mol	Chain	Res	Type
1	A	184	GLN
2	B	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

10 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	1.06	2 (14%)	17,19,21	1.66	6 (35%)
3	NAG	C	2	3	14,14,15	1.39	1 (7%)	17,19,21	1.43	3 (17%)
3	BMA	C	3	3	11,11,12	0.80	0	15,15,17	1.57	2 (13%)
3	MAN	C	4	3	11,11,12	0.70	0	15,15,17	1.13	2 (13%)
3	MAN	C	5	3	11,11,12	0.68	0	15,15,17	1.33	2 (13%)
3	FUC	C	6	3	10,10,11	0.78	0	14,14,16	1.15	1 (7%)
3	FUC	C	7	3	10,10,11	0.78	0	14,14,16	1.53	3 (21%)
4	NAG	D	1	4,1	14,14,15	0.93	0	17,19,21	1.35	3 (17%)
4	NAG	D	2	4	14,14,15	0.78	0	17,19,21	0.98	1 (5%)
4	FUC	D	3	4	10,10,11	0.77	0	14,14,16	1.57	3 (21%)

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
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	-	1/2/19/22	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	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	4.39	1.58	1.52
3	C	1	NAG	C1-C2	2.34	1.55	1.52
3	C	1	NAG	O5-C1	-2.04	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	4.48	118.18	112.19
3	C	7	FUC	C1-C2-C3	3.80	115.18	109.64
4	D	3	FUC	C1-C2-C3	3.57	114.84	109.64
3	C	2	NAG	O5-C5-C6	3.13	113.75	107.66
3	C	1	NAG	C1-O5-C5	3.06	116.28	112.19
3	C	5	MAN	C1-O5-C5	3.01	116.21	112.19
3	C	1	NAG	O5-C5-C6	-2.75	102.31	107.66
4	D	1	NAG	C2-N2-C7	2.49	126.24	122.90
3	C	7	FUC	C1-O5-C5	2.49	118.84	112.97
3	C	1	NAG	O6-C6-C5	-2.47	102.91	111.33
3	C	3	BMA	C3-C4-C5	2.44	114.65	110.23
4	D	3	FUC	C3-C4-C5	-2.40	106.17	109.81
4	D	1	NAG	C6-C5-C4	2.37	118.84	113.02
3	C	5	MAN	O5-C5-C6	2.35	112.23	107.66
3	C	4	MAN	O4-C4-C3	-2.29	104.98	110.38
3	C	1	NAG	O4-C4-C3	-2.28	105.00	110.38
4	D	3	FUC	O3-C3-C2	-2.27	105.42	110.05
3	C	7	FUC	O3-C3-C2	-2.21	105.55	110.05
3	C	1	NAG	C1-C2-N2	-2.11	107.10	110.43
3	C	1	NAG	C2-N2-C7	2.11	125.72	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	O7-C7-N2	-2.10	118.28	121.98
4	D	2	NAG	O5-C1-C2	-2.09	108.05	111.29
3	C	6	FUC	C1-O5-C5	2.09	117.90	112.97
4	D	1	NAG	O3-C3-C4	2.06	115.23	110.38
3	C	4	MAN	C6-C5-C4	-2.01	108.08	113.02
3	C	2	NAG	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

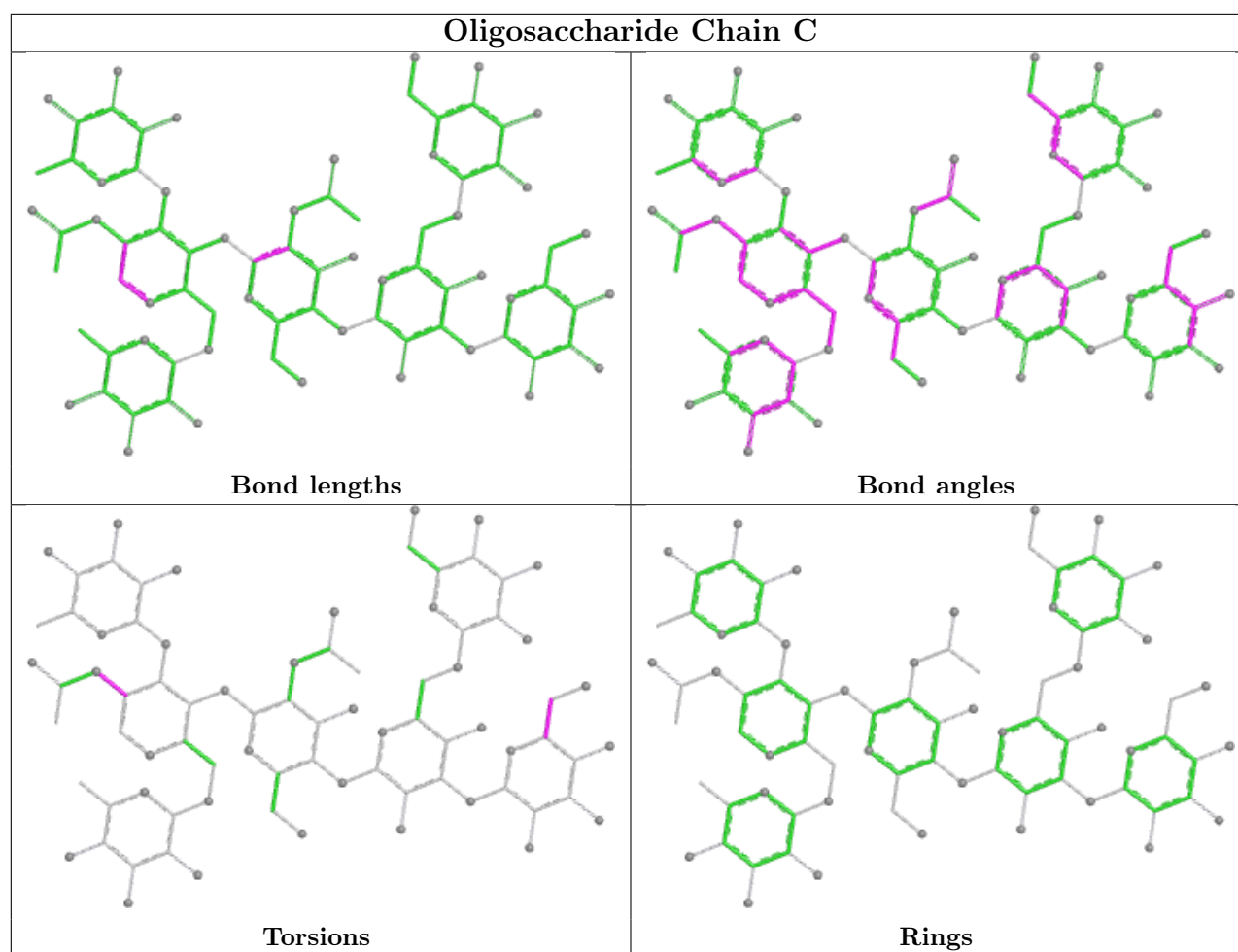
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	C	4	MAN	C4-C5-C6-O6

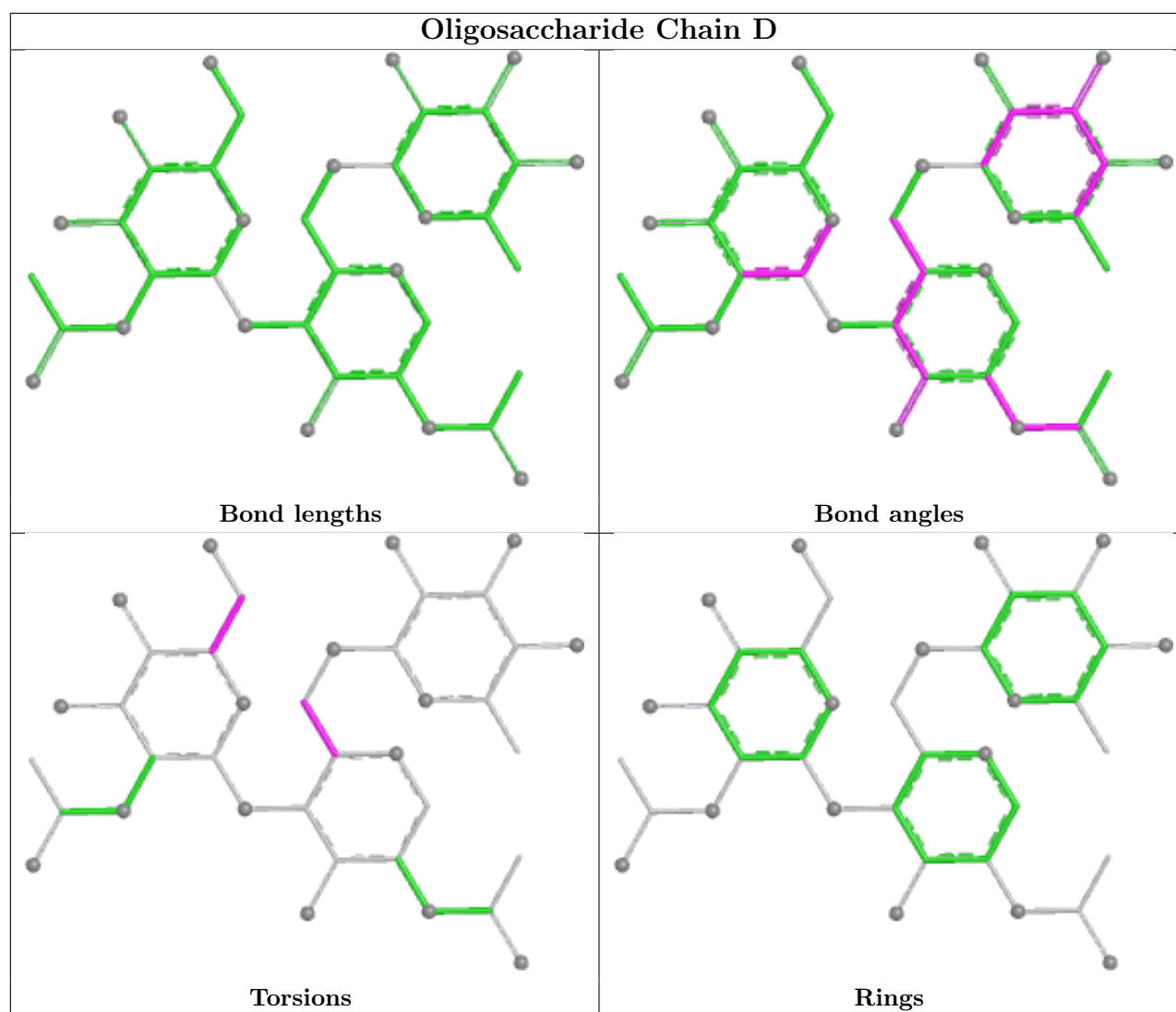
There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

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





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 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	$\# Z > 2$
8	A1CDL	A	309	-	62,63,63	1.62	10 (16%)	75,77,77	1.63	14 (18%)
9	CUY	A	310	-	34,34,43	0.62	1 (2%)	34,34,43	1.22	2 (5%)
7	EDO	A	306	-	3,3,3	0.50	0	2,2,2	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	305	-	3,3,3	0.43	0	2,2,2	0.40	0
7	EDO	A	308	-	3,3,3	0.39	0	2,2,2	0.20	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
8	A1CDL	A	309	-	-	33/53/93/93	0/2/2/2
9	CUY	A	310	-	-	20/33/33/42	-
7	EDO	A	306	-	-	1/1/1/1	-
7	EDO	A	305	-	-	1/1/1/1	-
7	EDO	A	308	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	309	A1CDL	C18-N20	7.25	1.49	1.34
8	A	309	A1CDL	O29-C24	4.23	1.52	1.41
8	A	309	A1CDL	C22-C21	2.91	1.57	1.51
8	A	309	A1CDL	C86-C87	2.86	1.54	1.50
8	A	309	A1CDL	C21-N20	2.73	1.50	1.46
8	A	309	A1CDL	O23-C24	2.48	1.44	1.40
8	A	309	A1CDL	C26-C25	-2.39	1.46	1.52
8	A	309	A1CDL	O32-C27	2.19	1.49	1.43
8	A	309	A1CDL	C17-C18	2.18	1.55	1.51
9	A	310	CUY	OAQ-CAP	2.10	1.39	1.33
8	A	309	A1CDL	O19-C18	-2.05	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	309	A1CDL	C22-C21-N20	5.06	116.85	109.66
8	A	309	A1CDL	C10-C09-C08	4.47	136.95	114.37
8	A	309	A1CDL	C21-N20-C18	4.13	130.29	123.40
8	A	309	A1CDL	C86-C87-C88	-3.90	116.60	124.69
8	A	309	A1CDL	O19-C18-C17	-3.29	116.07	122.02
8	A	309	A1CDL	O29-C28-C27	3.15	116.24	109.72
8	A	309	A1CDL	C33-O32-C27	-3.09	110.65	117.98
9	A	310	CUY	OAQ-CAP-CAO	2.97	120.89	111.83
8	A	309	A1CDL	C22-C21-C86	-2.90	106.43	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	309	A1CDL	O23-C24-C25	-2.76	104.09	108.27
8	A	309	A1CDL	C25-C26-C27	2.56	115.49	109.68
8	A	309	A1CDL	O84-C26-C25	-2.39	104.75	110.38
8	A	309	A1CDL	C24-C25-C26	2.27	114.80	110.01
9	A	310	CUY	CAW-CBM-CBL	-2.21	103.19	114.37
8	A	309	A1CDL	C17-C18-N20	2.14	119.63	115.86
8	A	309	A1CDL	C35-C36-C37	2.05	113.95	110.23

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	309	A1CDL	C86-C21-C22-O23
8	A	309	A1CDL	N20-C21-C22-O23
8	A	309	A1CDL	C22-C21-C86-C87
8	A	309	A1CDL	C22-C21-C86-OA2
8	A	309	A1CDL	N20-C21-C86-C87
8	A	309	A1CDL	N20-C21-C86-OA2
8	A	309	A1CDL	C22-C21-N20-C18
8	A	309	A1CDL	C15-C16-C17-C18
8	A	309	A1CDL	O29-C28-C30-O31
9	A	310	CUY	CAK-CAL-CAM-CAN
9	A	310	CUY	CAO-CAP-OAQ-CAR
8	A	309	A1CDL	C92-C93-C94-C95
8	A	309	A1CDL	C94-C95-C96-C97
8	A	309	A1CDL	C89-C90-C91-C92
8	A	309	A1CDL	C96-C97-C98-C99
8	A	309	A1CDL	O38-C37-C39-O40
8	A	309	A1CDL	C36-C37-C39-O40
9	A	310	CUY	OBO-CAP-OAQ-CAR
8	A	309	A1CDL	C16-C17-C18-N20
8	A	309	A1CDL	C16-C17-C18-O19
9	A	310	CUY	CAG-CAH-CAI-CAJ
8	A	309	A1CDL	C05-C06-C07-C08
9	A	310	CUY	CAF-CAG-CAH-CAI
8	A	309	A1CDL	C11-C12-C13-C14
8	A	309	A1CDL	C98-C99-CA0-CA1
8	A	309	A1CDL	C95-C96-C97-C98
9	A	310	CUY	CAC-CAD-CAE-CAF
9	A	310	CUY	CBF-CBG-CBH-CBI
9	A	310	CUY	CBK-CBL-CBM-CAW
9	A	310	CUY	CBD-CBE-CBF-CBG

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Mol	Chain	Res	Type	Atoms
7	A	305	EDO	O1-C1-C2-O2
9	A	310	CUY	CAM-CAN-CAO-CAP
8	A	309	A1CDL	C02-C03-C04-C05
9	A	310	CUY	CAB-CAC-CAD-CAE
8	A	309	A1CDL	C25-C24-O23-C22
8	A	309	A1CDL	C13-C14-C15-C16
9	A	310	CUY	CAR-CAS-CAT-CAU
9	A	310	CUY	CAV-CAW-CBM-CBL
8	A	309	A1CDL	C27-C28-C30-O31
8	A	309	A1CDL	C97-C98-C99-CA0
8	A	309	A1CDL	C03-C04-C05-C06
7	A	306	EDO	O1-C1-C2-O2
9	A	310	CUY	CBI-CBJ-CBK-CBL
9	A	310	CUY	CAE-CAF-CAG-CAH
9	A	310	CUY	CAD-CAE-CAF-CAG
9	A	310	CUY	C1-CBD-CBE-CBF
8	A	309	A1CDL	C04-C05-C06-C07
8	A	309	A1CDL	C90-C91-C92-C93
8	A	309	A1CDL	C08-C09-C10-C11
8	A	309	A1CDL	C93-C94-C95-C96
8	A	309	A1CDL	C01-C02-C03-C04
9	A	310	CUY	OAQ-CAR-CAS-CAT
9	A	310	CUY	CAS-CAT-CAU-CAV
9	A	310	CUY	CAI-CAJ-CAK-CAL
8	A	309	A1CDL	C06-C07-C08-C09

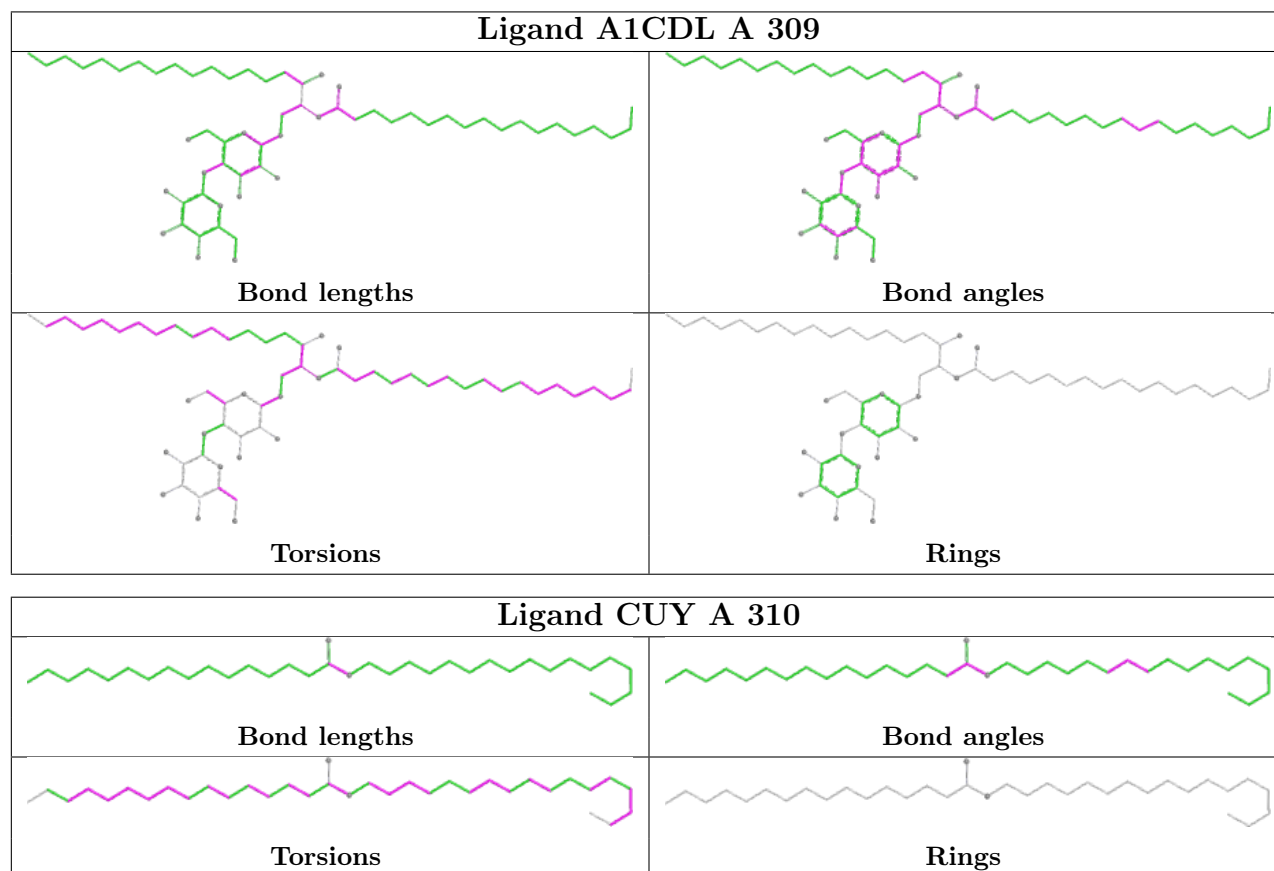
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	306	EDO	1	0
7	A	305	EDO	1	0
7	A	308	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/280 (100%)	0.28	13 (4%) 38 41	9, 23, 44, 55	7 (2%)
2	B	100/100 (100%)	0.59	5 (5%) 35 37	9, 29, 46, 56	2 (2%)
All	All	380/380 (100%)	0.36	18 (4%) 37 40	9, 24, 45, 56	9 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	-1	PRO	5.6
1	A	193[A]	SER	5.5
1	A	279	GLY	4.3
1	A	197	PRO	3.4
1	A	199	PRO	3.0
1	A	195	PRO	3.0
2	B	0	LYS	2.9
1	A	129	ALA	2.9
1	A	251[A]	VAL	2.8
1	A	148	ILE	2.7
1	A	149	ILE	2.7
1	A	84	PHE	2.6
2	B	1	ILE	2.3
1	A	152	GLN	2.3
2	B	98	ASP	2.3
1	A	281	GLY	2.2
1	A	24	ALA	2.1
2	B	18	GLY	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

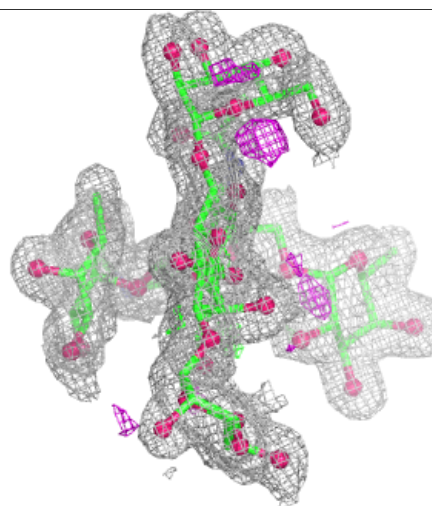
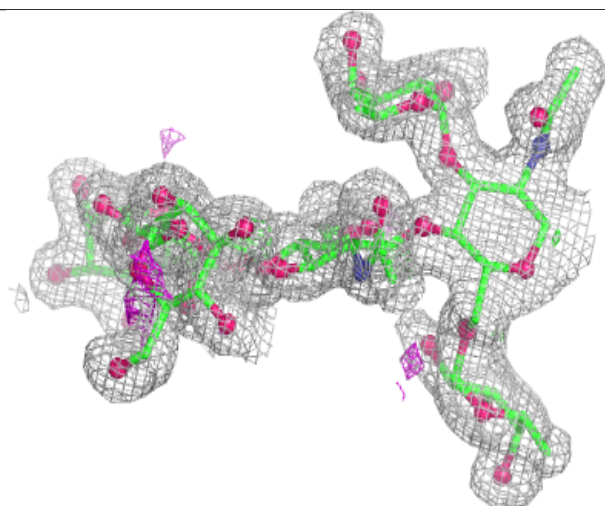
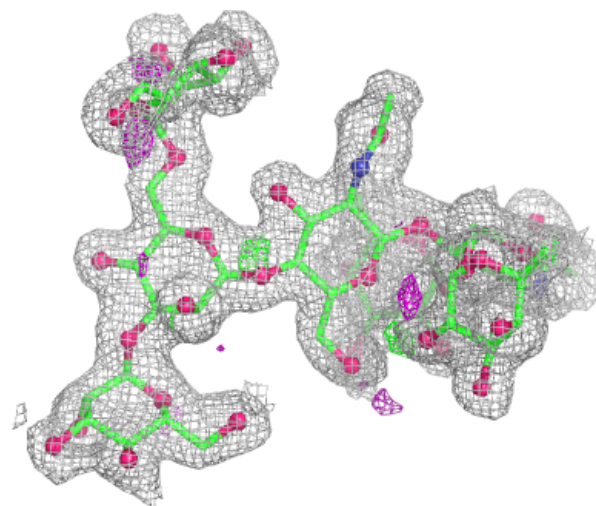
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

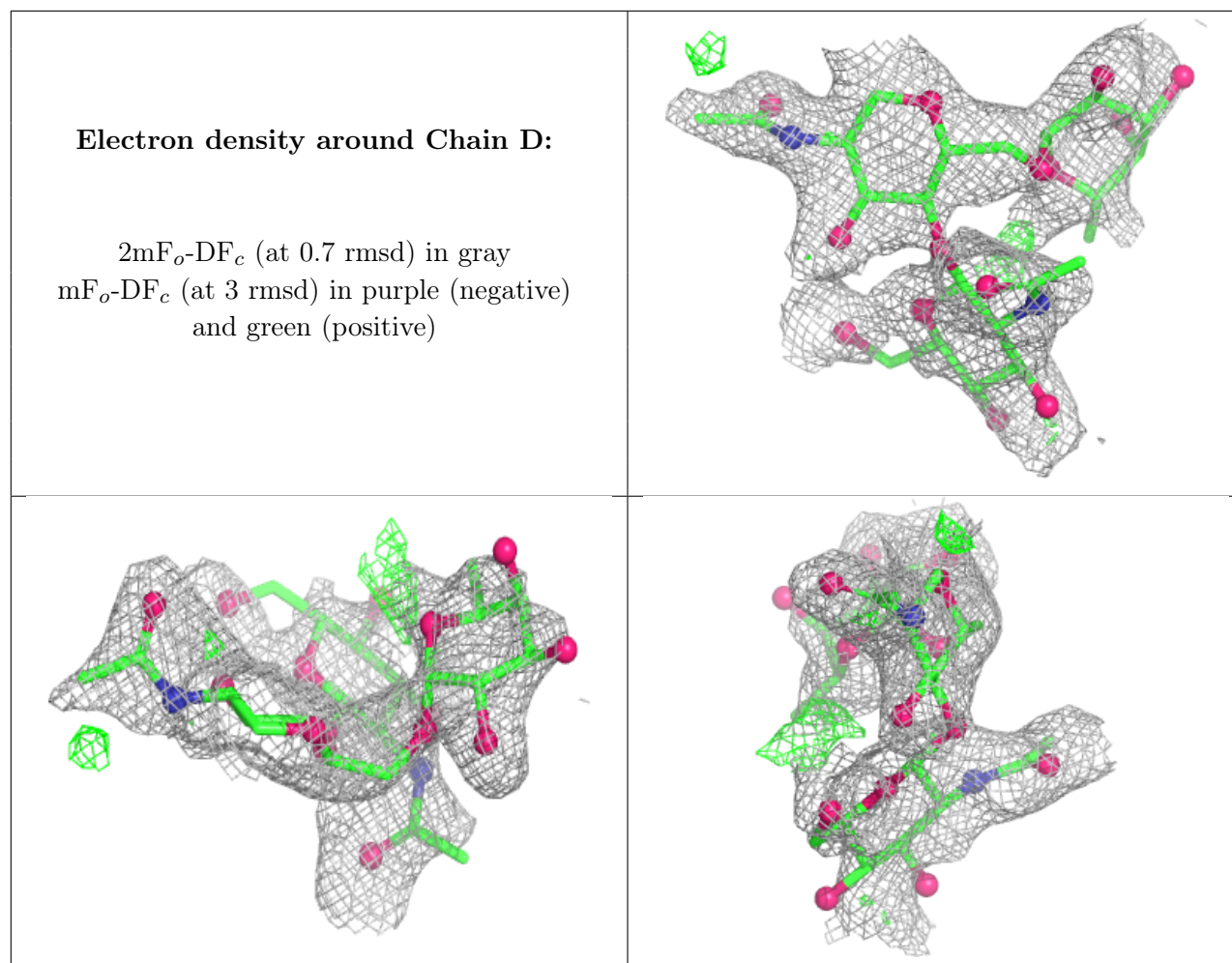
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	2	14/15	0.61	0.17	59,67,77,80	0
4	FUC	D	3	10/11	0.67	0.19	51,69,75,76	0
4	NAG	D	1	14/15	0.82	0.12	41,52,69,69	0
3	MAN	C	5	11/12	0.89	0.11	22,25,32,35	0
3	FUC	C	7	10/11	0.90	0.10	27,31,37,39	0
3	NAG	C	2	14/15	0.90	0.09	21,24,28,29	0
3	FUC	C	6	10/11	0.91	0.10	27,32,39,42	0
3	NAG	C	1	14/15	0.94	0.07	20,22,24,26	0
3	BMA	C	3	11/12	0.94	0.07	25,27,29,30	0
3	MAN	C	4	11/12	0.94	0.07	30,33,35,38	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)





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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	A1CDL	A	309	62/62	0.73	0.18	21,50,75,79	3
7	EDO	A	305	4/4	0.76	0.18	41,50,53,54	0
7	EDO	A	306	4/4	0.80	0.17	32,38,40,40	0
9	CUY	A	310	35/44	0.83	0.15	17,32,44,48	0
7	EDO	A	308	4/4	0.89	0.17	17,26,29,31	0
10	NA	A	311	1/1	0.95	0.12	28,28,28,28	0
5	IOD	A	302	1/1	0.97	0.19	67,67,67,67	0
6	CL	A	304	1/1	0.97	0.10	31,31,31,31	0
6	CL	A	307	1/1	0.97	0.05	28,28,28,28	0
5	IOD	A	303	1/1	0.98	0.13	66,66,66,66	0

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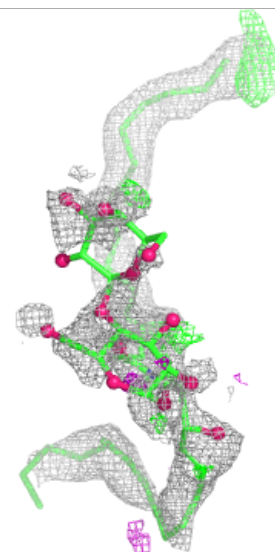
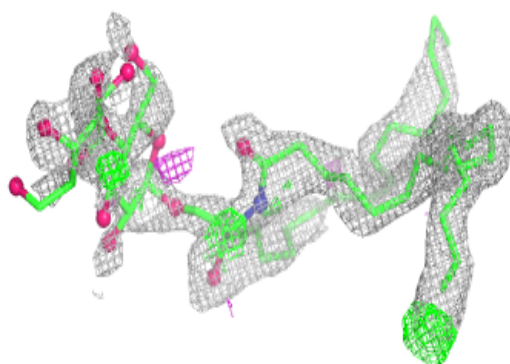
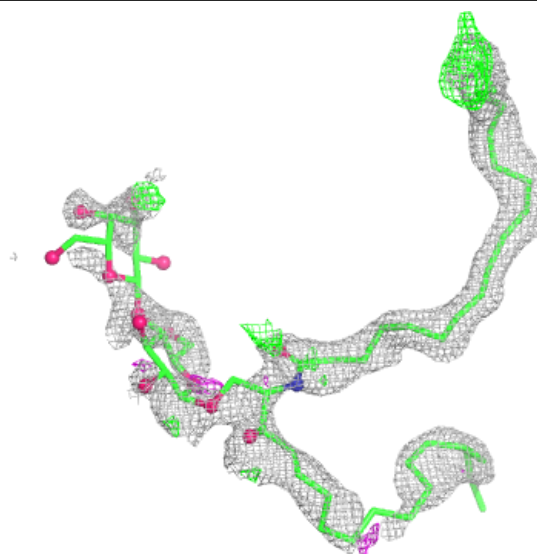
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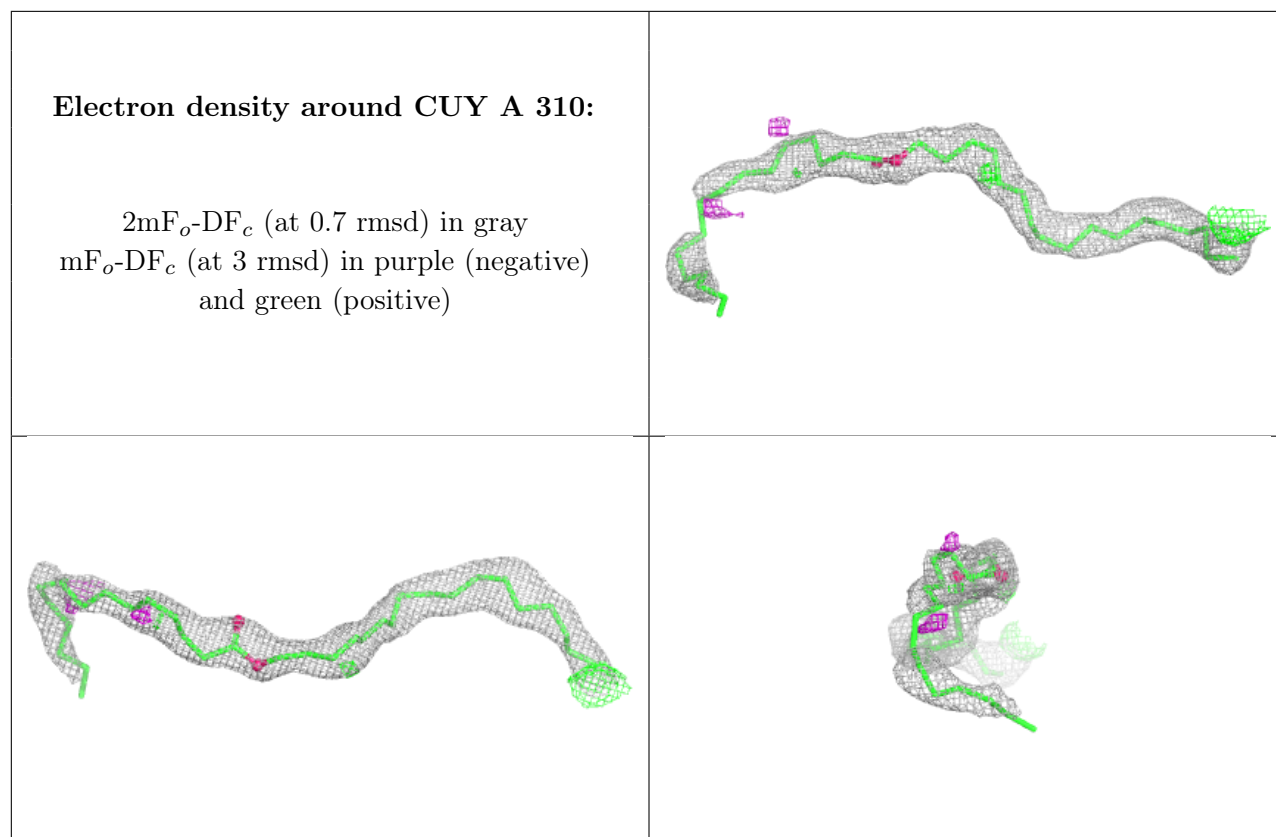
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	A	301	1/1	0.99	0.02	23,23,23,23	0
5	IOD	B	101	1/1	0.99	0.09	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CDL A 309:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.