



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:54 PM UTC

PDB ID : 5WL1 / pdb_00005wl1
Title : Crystal Structure of Human CD1b in Complex with PG
Authors : Shahine, A.; Gras, S.; Rossjohn, J.
Deposited on : 2017-07-25
Resolution : 1.38 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 ⓘ 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 : 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

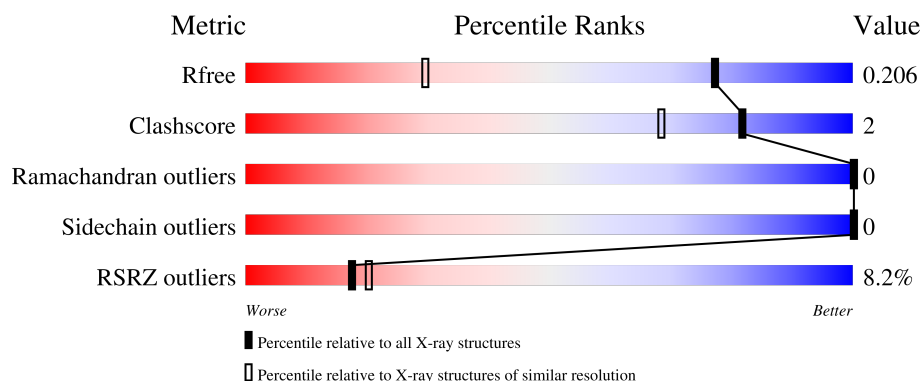
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	300	6% 88% 5% 7%
2	B	99	12% 97% ..
3	C	4	25% 75%
4	D	5	100%
5	E	7	86% 14%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7131 atoms, of which 3120 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	H	N	O	S			
1	A	280	4323	1434	2074	385	420	10	0	21	0

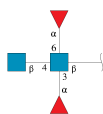
There are 23 discrepancies between the modelled and reference sequences:

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.

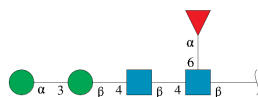
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	98	Total	C	H	N	O	S	0	4	0
			1545	519	729	139	156	2			

- Molecule 3 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.



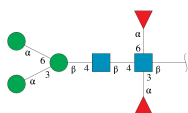
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	4	Total	C	H	N	O		0	0	0
			95	28	47	2	18				

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



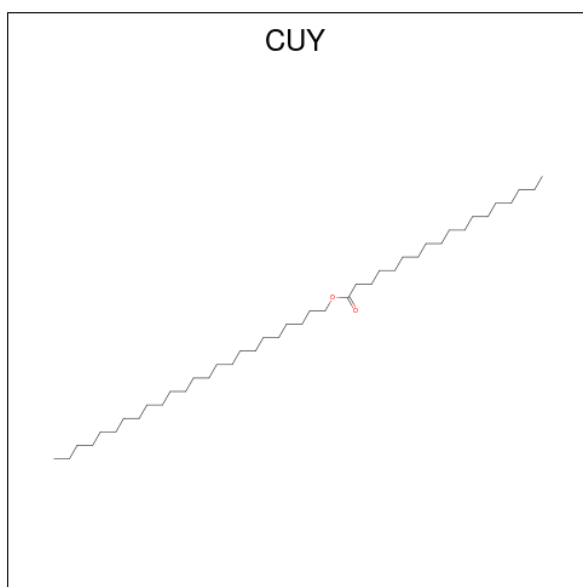
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	5	Total	C	H	N	O		0	0	0
			114	34	54	2	24				

- Molecule 5 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
5	E	7	Total	C	H	N	O		0	0	0
			156	46	75	2	33				

- Molecule 6 is tetracosyl octadecanoate (CCD ID: CUY) (formula: C₄₂H₈₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			87	33	52	2		

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

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

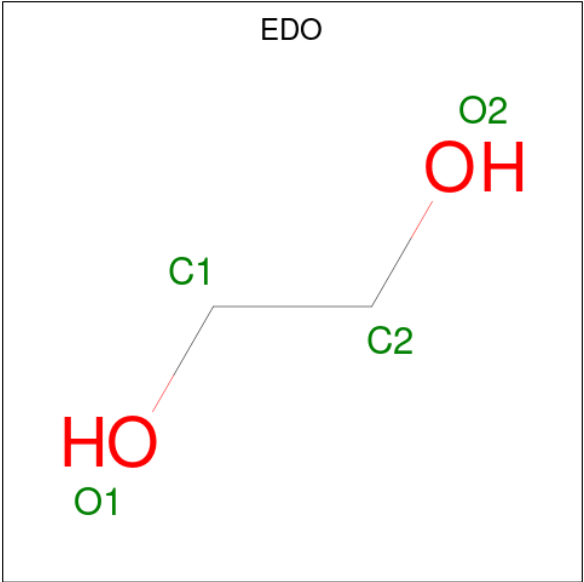
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

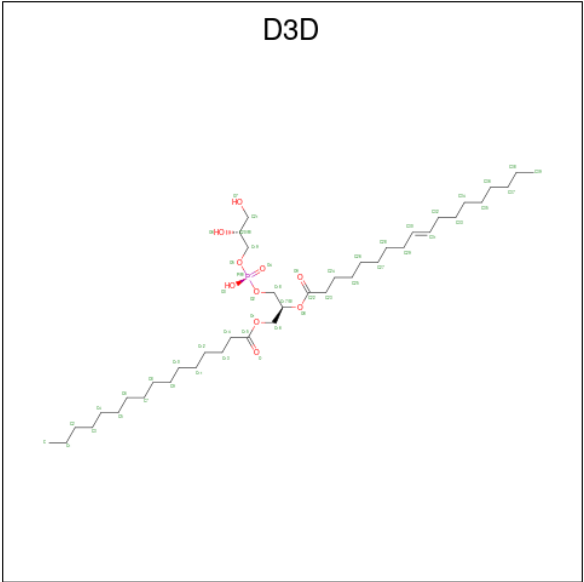
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		
9	B	1	Total	Na	0	0
			1	1		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is (19S,22R,25R)-22,25,26-trihydroxy-16,22-dioxo-17,21,23-trioxa-22lambda 5 -phosphahexacosan-19-yl (9E)-octadec-9-enoate (CCD ID: D3D) (formula: C₄₀H₇₇O₁₀P).



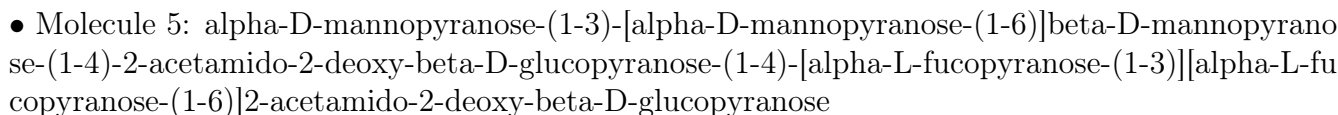
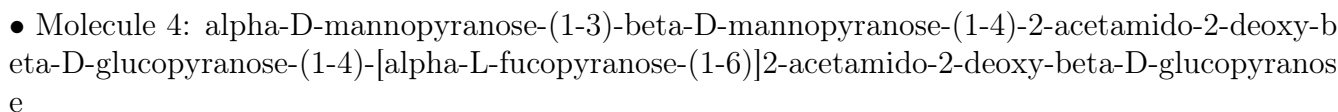
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	H	O	P	0	0
			120	38	71	10	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	496	Total	O	0	0
			496	496		
12	B	161	Total	O	0	0
			161	161		

i

- Molecule 1: T-cell surface glycoprotein CD1b



Chain E:

86%

14%

HA01
HA02
HA03
HA04
HA05
HA06
HA07

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.89Å 80.28Å 92.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.34 – 1.38 30.34 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.34-1.38) 98.1 (30.34-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.38Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.188 , 0.206 0.190 , 0.206	Depositor DCC
R_{free} test set	4336 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7131	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, D3D, FUC, CUY, MAN, CL, NAG, BMA, NA, IOD

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	0.77	2/2375 (0.1%)	0.93	5/3224 (0.2%)
2	B	0.67	0/860	0.92	0/1167
All	All	0.75	2/3235 (0.1%)	0.92	5/4391 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219[A]	MET	SD-CE	-6.44	1.63	1.79
1	A	219[B]	MET	SD-CE	-6.44	1.63	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	LEU	CA-C-N	6.38	133.18	121.70
1	A	282	LEU	C-N-CA	6.38	133.18	121.70
1	A	43[A]	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	43[B]	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	33	ASP	CA-CB-CG	5.24	117.84	112.60

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	2249	2074	2091	11	0
2	B	816	729	743	2	0
3	C	48	47	43	2	0
4	D	60	54	52	0	0
5	E	81	75	70	0	0
6	A	35	52	0	1	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	8	12	12	1	0
10	B	4	6	0	0	0
11	A	49	71	0	4	0
12	A	496	0	0	7	0
12	B	161	0	0	0	0
All	All	4011	3120	3011	16	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 2.

The worst 5 of 16 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:283:ASN:C	12:A:502:HOH:O	2.18	0.87
1:A:228:GLN:HG3	12:A:804:HOH:O	1.79	0.81
11:A:423:D3D:C16	12:A:501:HOH:O	2.29	0.79
1:A:269:GLU:HG3	12:A:503:HOH:O	1.95	0.67
11:A:423:D3D:O2	12:A:501:HOH:O	2.15	0.63

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	299/300 (100%)	297 (99%)	2 (1%)	0	100	100
2	B	100/99 (101%)	100 (100%)	0	0	100	100
All	All	399/399 (100%)	397 (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	242/247 (98%)	242 (100%)	0	100	100
2	B	93/94 (99%)	93 (100%)	0	100	100
All	All	335/341 (98%)	335 (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	36	GLN
1	A	150	GLN
1	A	184	GLN
1	A	203	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

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	1,3	14,14,15	0.55	0	17,19,21	2.65	5 (29%)
3	FUC	C	2	3	10,10,11	0.27	0	14,14,16	0.37	0
3	NAG	C	3	3	14,14,15	0.37	0	17,19,21	1.15	1 (5%)
3	FUC	C	4	3	10,10,11	0.57	0	14,14,16	0.92	1 (7%)
4	NAG	D	1	4,1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.33	0	17,19,21	0.86	0
4	BMA	D	3	4	11,11,12	0.21	0	15,15,17	0.74	0
4	MAN	D	4	4	11,11,12	0.25	0	15,15,17	0.52	0
4	FUC	D	5	4	10,10,11	0.30	0	14,14,16	0.79	0
5	NAG	E	1	1,5	14,14,15	0.34	0	17,19,21	1.05	1 (5%)
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.73	0
5	BMA	E	3	5	11,11,12	0.21	0	15,15,17	0.80	0
5	MAN	E	4	5	11,11,12	0.24	0	15,15,17	0.59	0
5	MAN	E	5	5	11,11,12	0.25	0	15,15,17	0.67	0
5	FUC	E	6	5	10,10,11	0.25	0	14,14,16	0.30	0
5	FUC	E	7	5	10,10,11	0.31	0	14,14,16	0.41	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	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	NAG	C	3	3	-	2/6/23/26	0/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	8.72	123.88	112.19
3	C	3	NAG	O5-C1-C2	-4.11	104.92	111.29
3	C	1	NAG	O5-C1-C2	-3.97	105.14	111.29
3	C	1	NAG	C1-C2-N2	-2.82	105.98	110.43
3	C	1	NAG	O5-C5-C6	-2.49	102.82	107.66

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

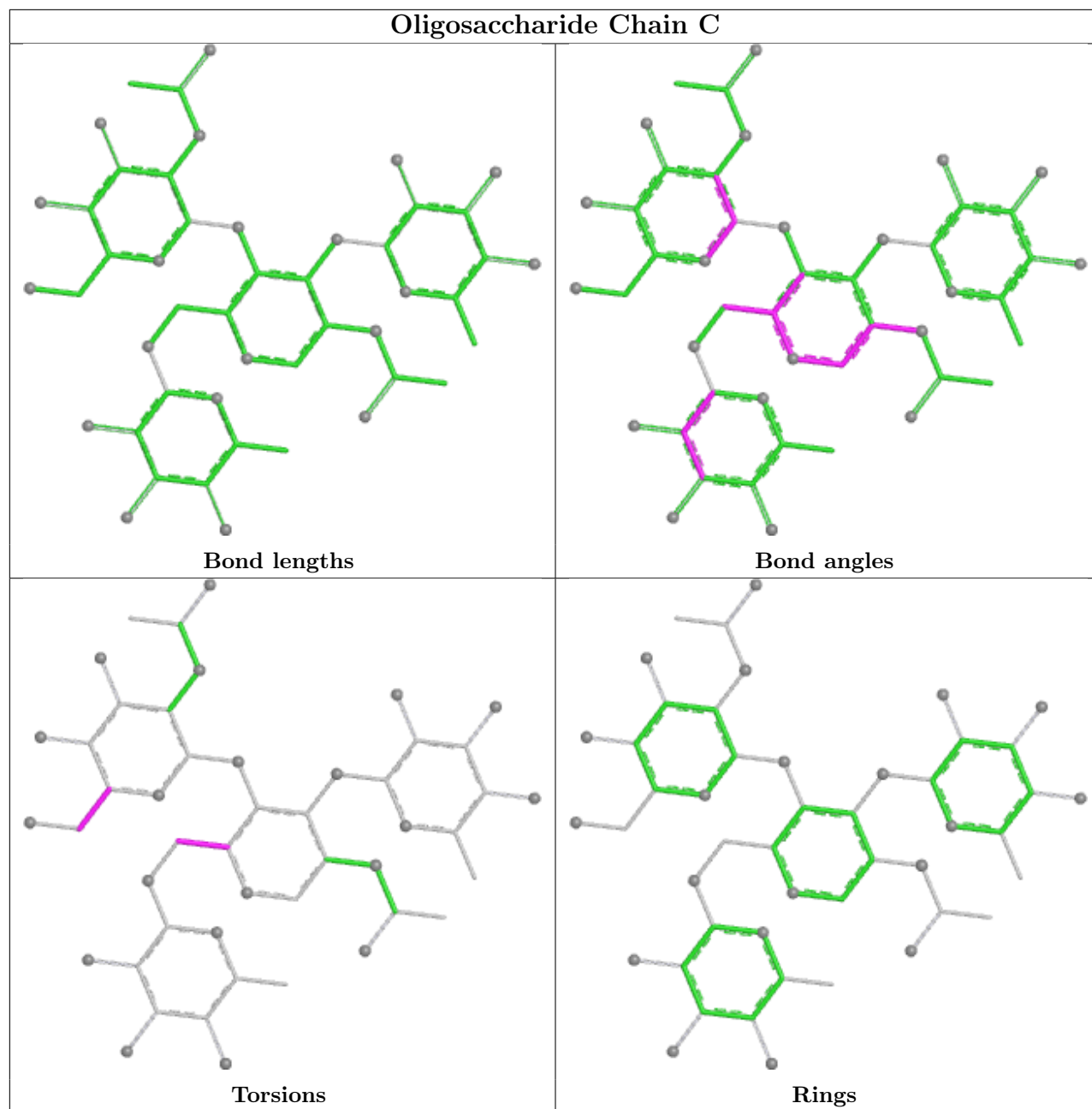
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	3	NAG	C4-C5-C6-O6
3	C	3	NAG	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

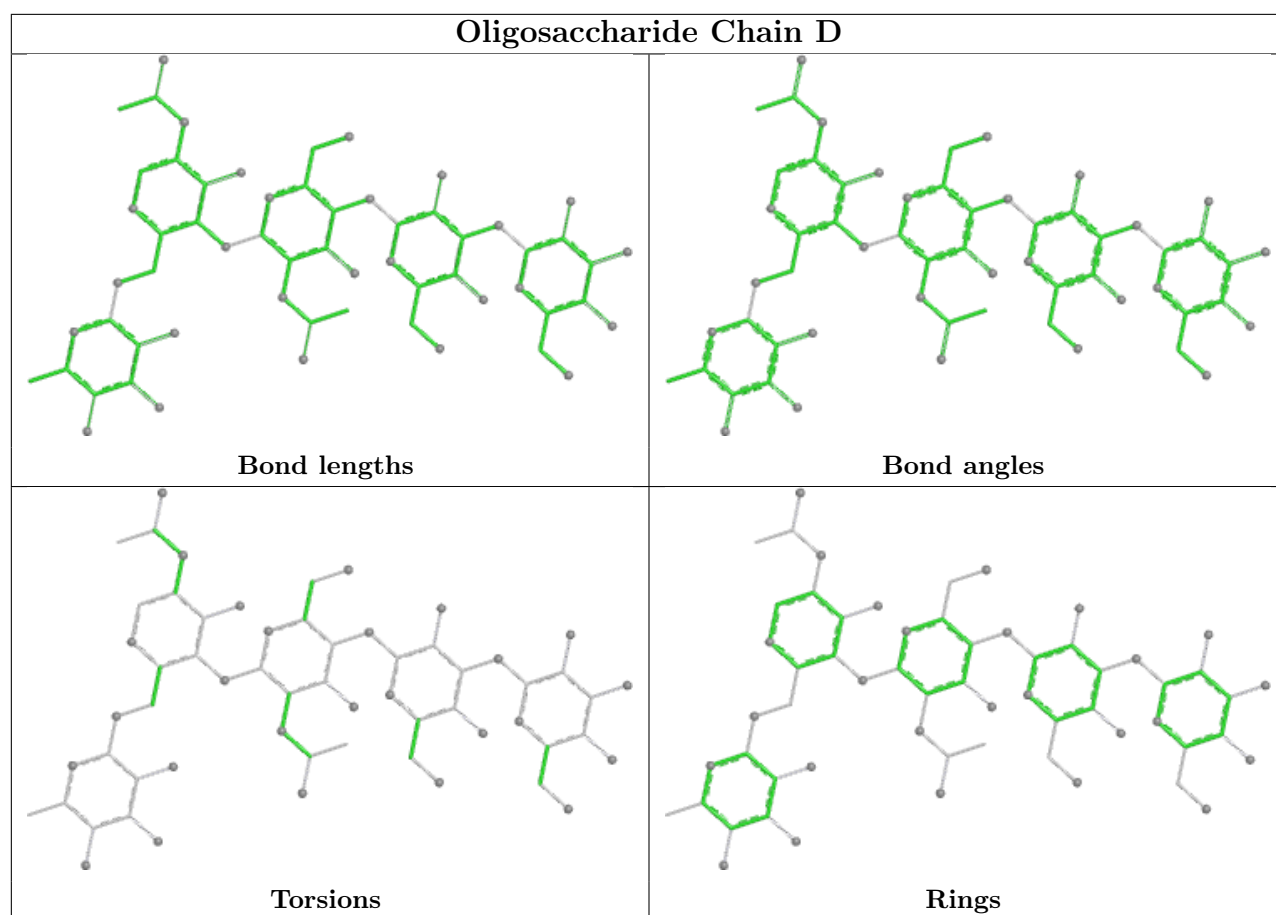
There are no ring outliers.

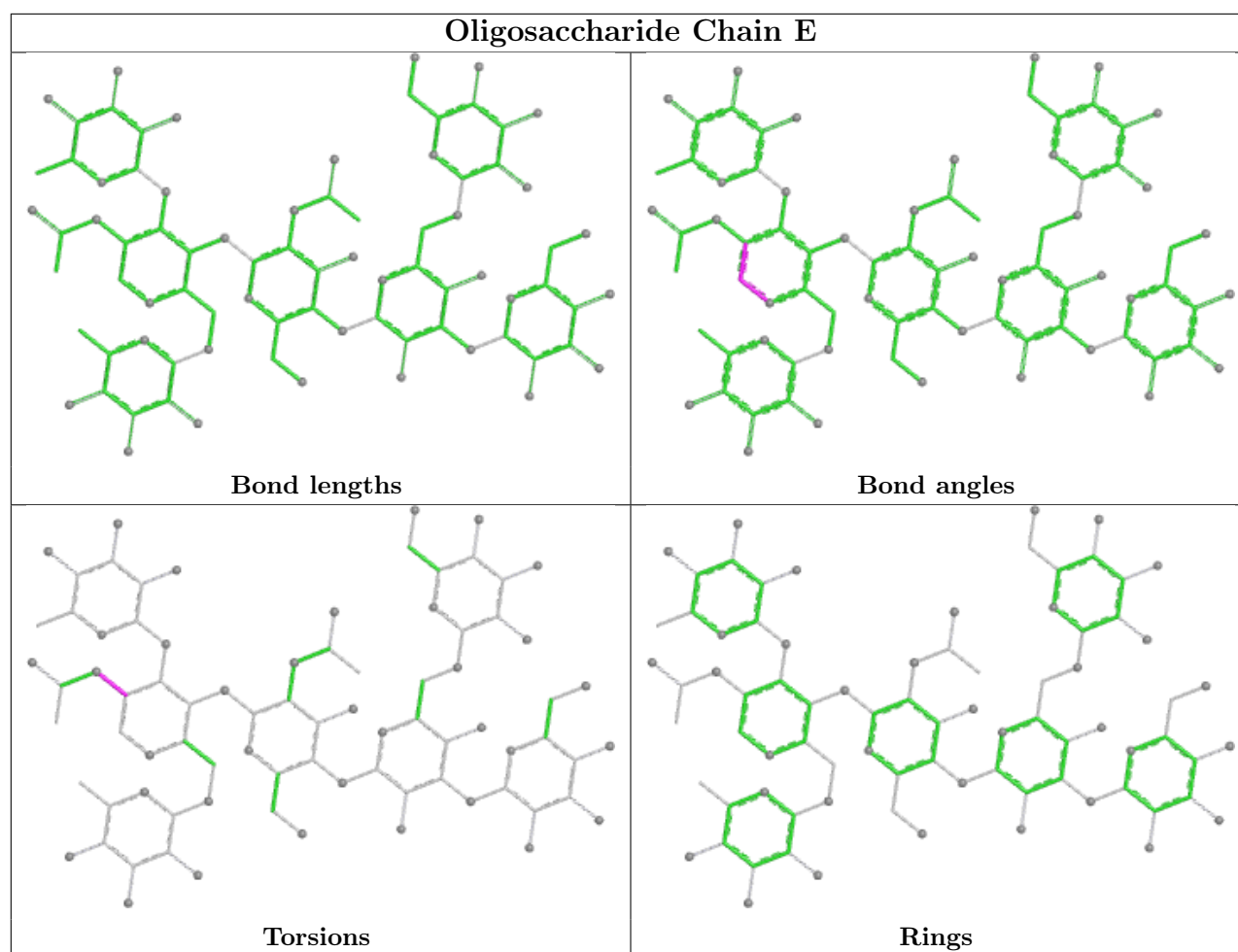
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	NAG	1	0
3	C	1	NAG	1	0
3	C	4	FUC	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 9 ligands modelled in this entry, 4 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	$\# Z > 2$
11	D3D	A	423	-	48,48,50	0.98	4 (8%)	51,54,56	1.17	3 (5%)
10	EDO	A	421	-	3,3,3	0.61	0	2,2,2	0.31	0
10	EDO	B	101	-	3,3,3	3.38	2 (66%)	2,2,2	0.73	0
6	CUY	A	401	-	34,34,43	0.69	1 (2%)	34,34,43	0.85	1 (2%)
10	EDO	A	422	-	3,3,3	0.51	0	2,2,2	0.36	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
11	D3D	A	423	-	-	13/53/53/55	-
10	EDO	A	421	-	-	1/1/1/1	-
10	EDO	B	101	-	-	0/1/1/1	-
6	CUY	A	401	-	-	10/33/33/42	-
10	EDO	A	422	-	-	1/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	101	EDO	O1-C1	-4.25	1.20	1.42
10	B	101	EDO	C2-C1	-3.79	1.18	1.48
6	A	401	CUY	OAQ-CAP	2.80	1.41	1.33
11	A	423	D3D	O1-C16	-2.74	1.39	1.45
11	A	423	D3D	O8-C22	2.72	1.42	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	423	D3D	C18-C17-C16	-4.91	100.35	111.78
6	A	401	CUY	OAQ-CAP-CAO	2.76	120.24	111.83
11	A	423	D3D	O1-C16-C17	2.72	116.25	108.40
11	A	423	D3D	O8-C22-C23	2.58	117.07	111.48

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

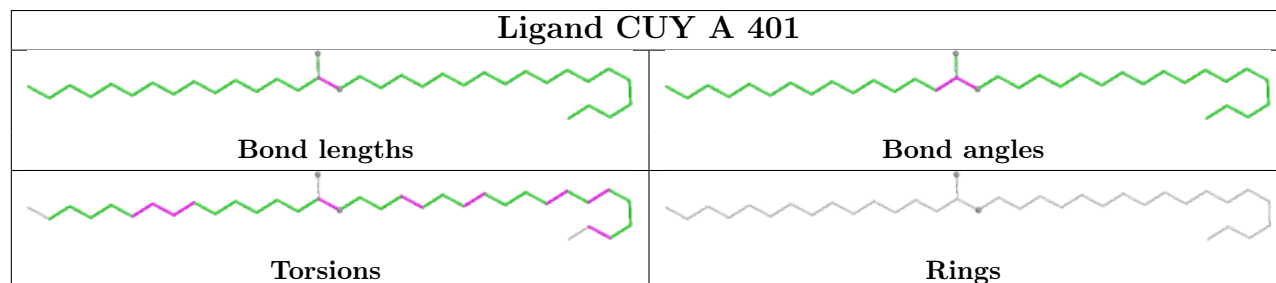
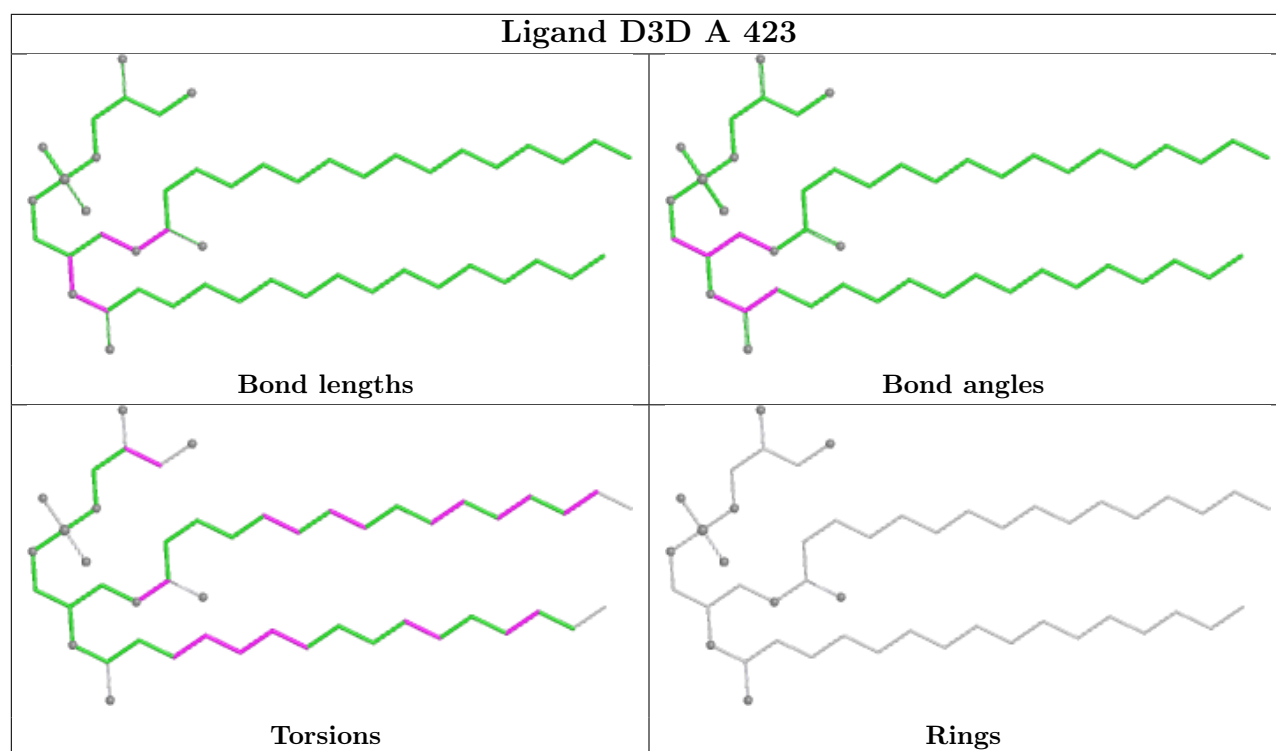
Mol	Chain	Res	Type	Atoms
6	A	401	CUY	CAF-CAG-CAH-CAI
11	A	423	D3D	C7-C8-C9-C10
11	A	423	D3D	C23-C24-C25-C26
11	A	423	D3D	C25-C26-C27-C28
6	A	401	CUY	CAG-CAH-CAI-CAJ

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	423	D3D	4	0
6	A	401	CUY	1	0
10	A	422	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	280/300 (93%)	0.21	19 (6%) 23 27	7, 16, 35, 63	11 (3%)
2	B	98/99 (98%)	0.55	12 (12%) 8 10	6, 21, 43, 55	2 (2%)
All	All	378/399 (94%)	0.30	31 (8%) 17 20	6, 17, 40, 63	13 (3%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLN	5.8
1	A	151	TYR	5.3
2	B	1	ILE	5.2
1	A	283	ASN	4.9
1	A	88	PHE	3.4

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, 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.

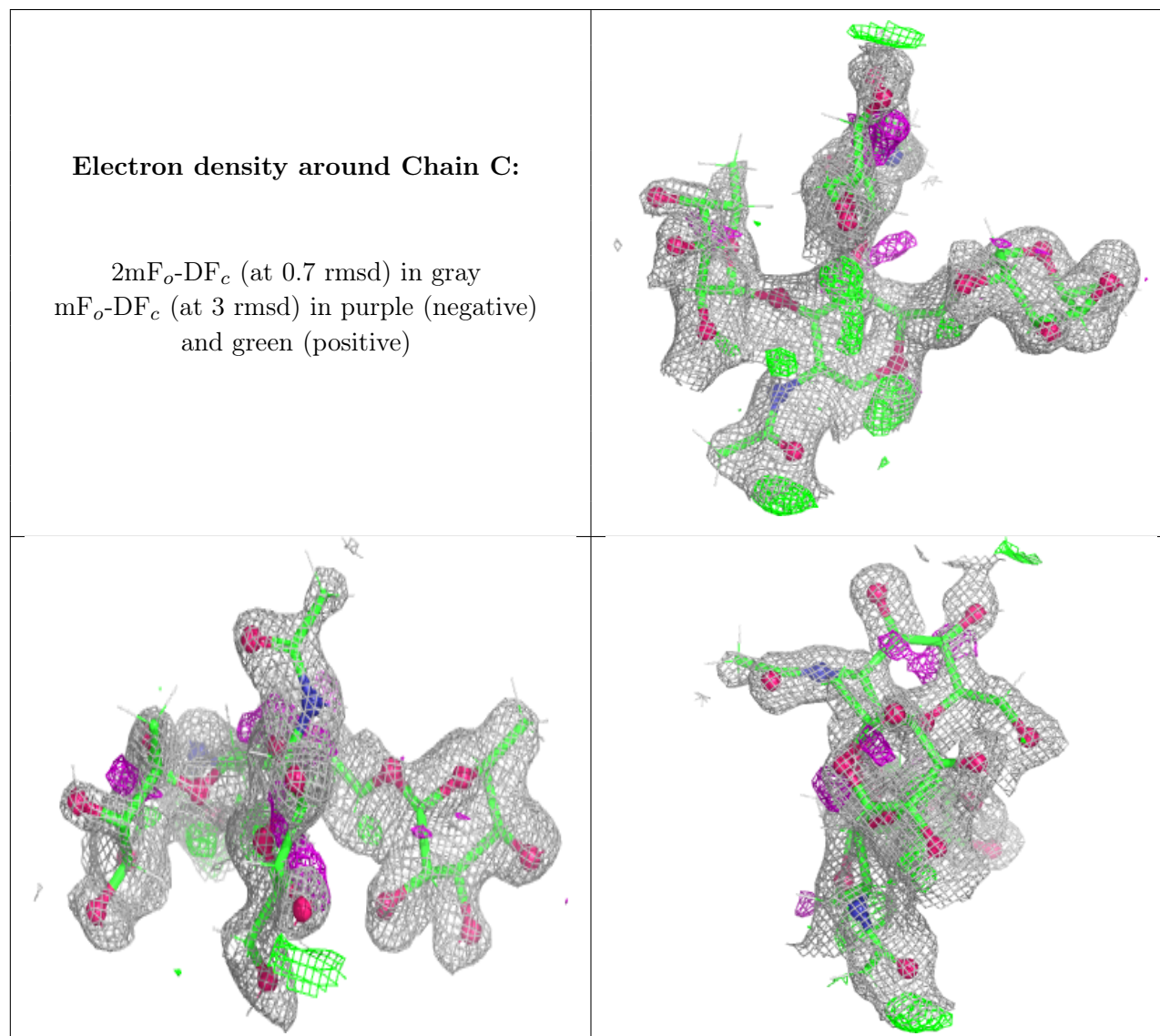
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	0.60	0.19	42,44,48,55	0
3	FUC	C	2	10/11	0.60	0.19	60,65,66,66	0
4	FUC	D	5	10/11	0.66	0.13	45,48,50,51	0
4	NAG	D	2	14/15	0.73	0.13	39,42,45,47	0
4	NAG	D	1	14/15	0.73	0.14	39,44,50,50	0

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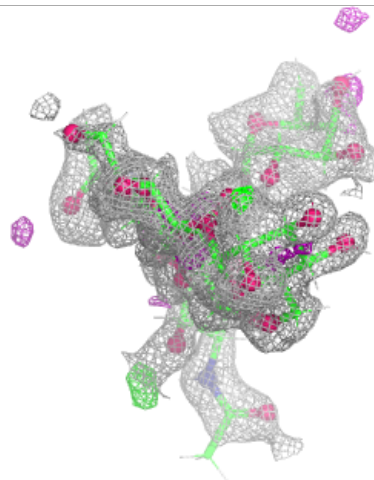
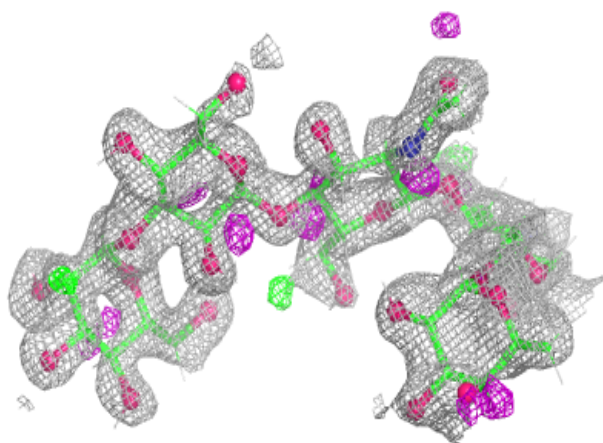
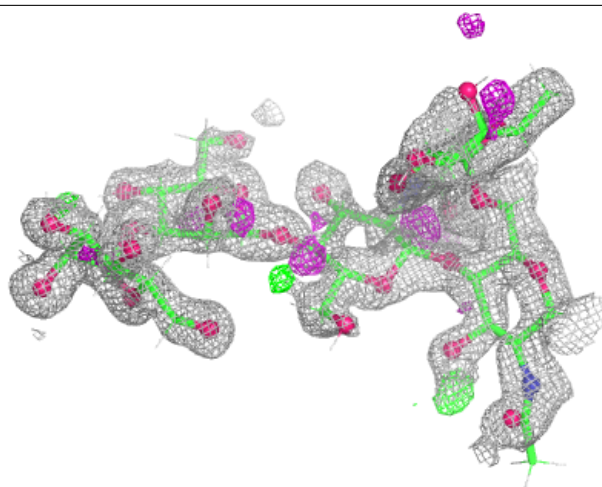
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	C	4	10/11	0.77	0.12	41,42,46,46	0
3	NAG	C	3	14/15	0.79	0.14	36,39,41,43	0
4	BMA	D	3	11/12	0.82	0.10	37,42,47,48	0
4	MAN	D	4	11/12	0.84	0.10	33,37,40,41	0
5	FUC	E	6	10/11	0.91	0.09	15,20,24,24	0
5	MAN	E	4	11/12	0.96	0.06	15,18,20,21	0
5	FUC	E	7	10/11	0.96	0.07	15,18,21,22	0
5	NAG	E	2	14/15	0.97	0.05	7,12,17,23	0
5	MAN	E	5	11/12	0.97	0.06	12,15,18,19	0
5	NAG	E	1	14/15	0.98	0.05	8,12,15,16	0
5	BMA	E	3	11/12	0.98	0.04	11,13,16,18	0

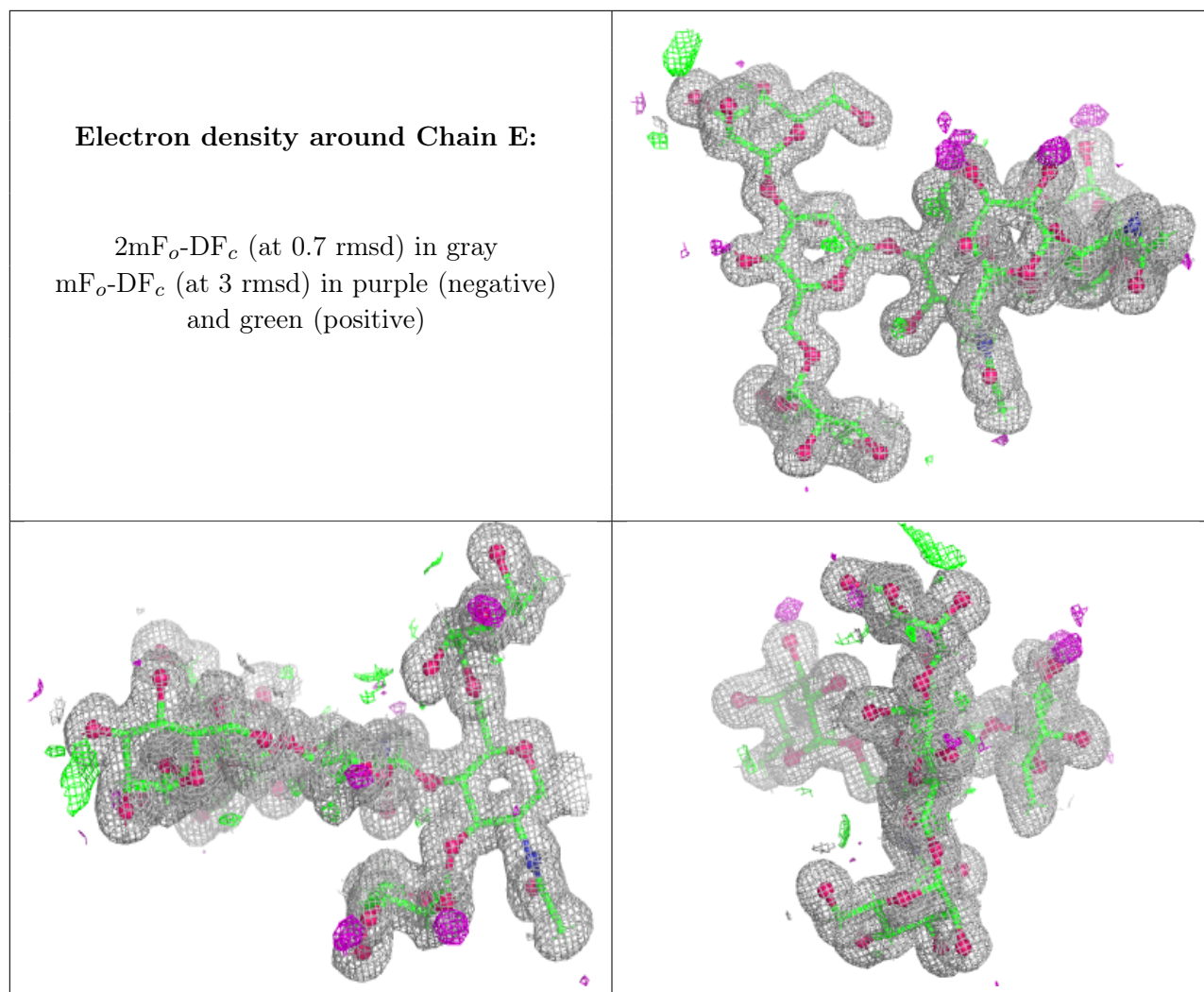
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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](#)

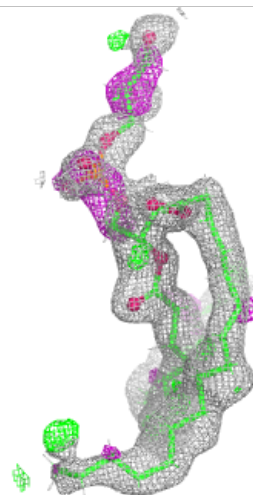
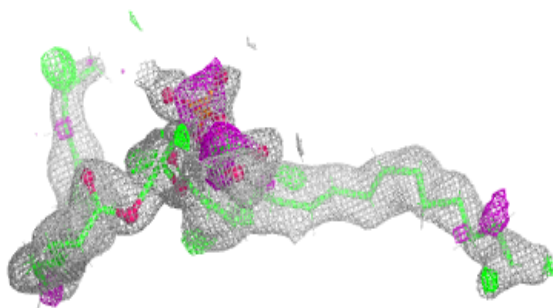
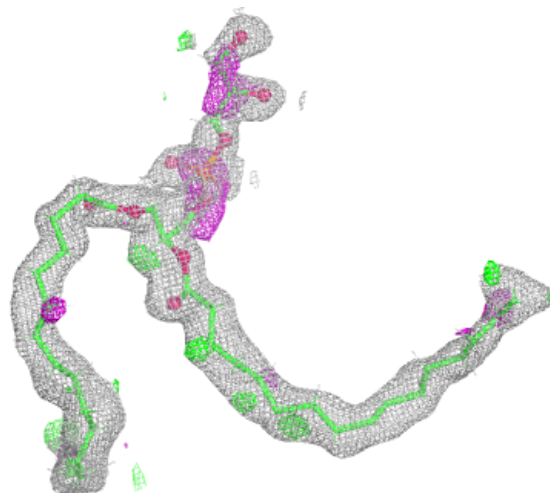
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

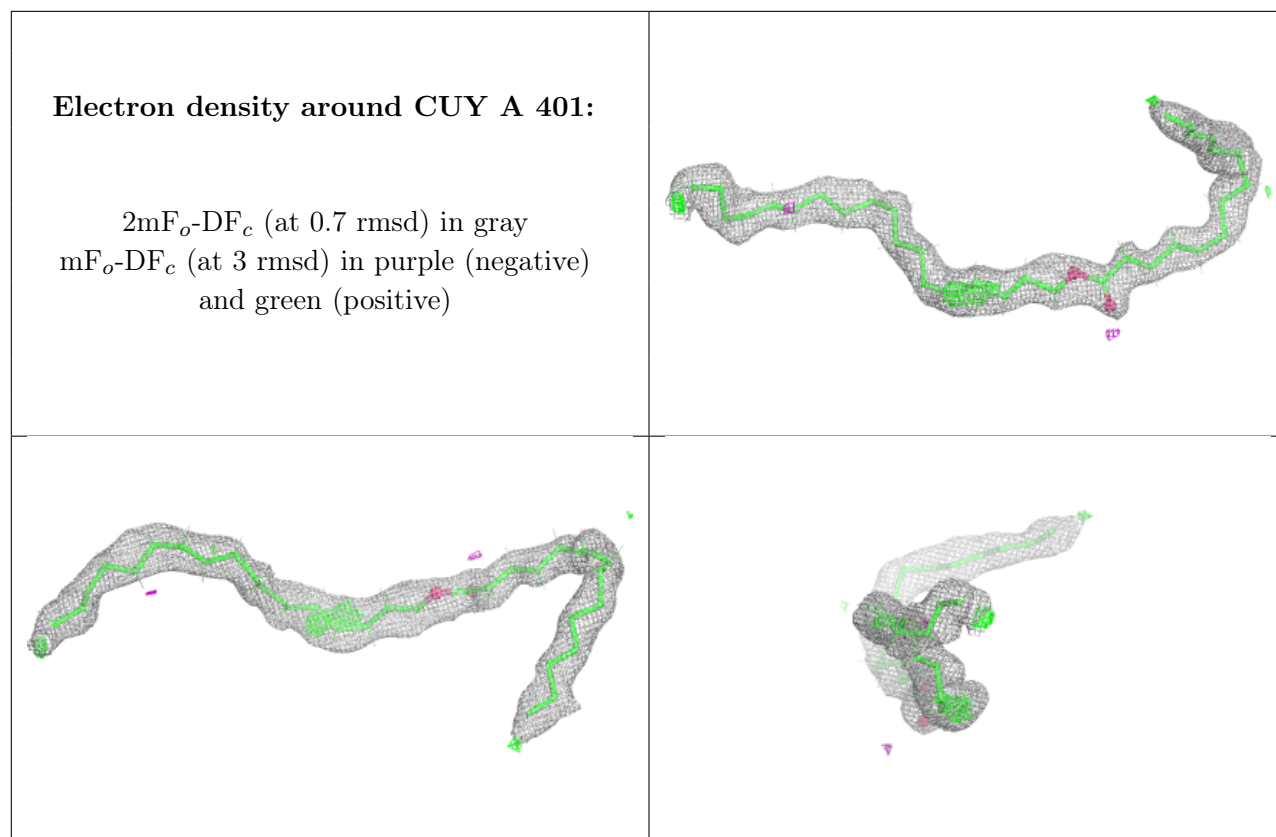
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	EDO	A	421	4/4	0.74	0.14	39,40,40,40	0
11	D3D	A	423	49/51	0.74	0.13	29,30,34,38	0
10	EDO	A	422	4/4	0.82	0.14	41,43,43,43	0
6	CUY	A	401	35/44	0.83	0.14	31,35,38,39	0
10	EDO	B	101	4/4	0.90	0.22	3,12,25,26	0
9	NA	A	420	1/1	0.97	0.06	23,23,23,23	0
8	CL	A	419	1/1	0.98	0.05	17,17,17,17	0
7	IOD	A	402	1/1	0.98	0.14	6,6,6,6	1
9	NA	B	102	1/1	0.99	0.04	16,16,16,16	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 D3D A 423:

$2mF_o-DF_c$ (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.