



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:50 PM UTC

PDB ID : 8GLF / pdb_00008glf
Title : Crystal Structure of Human CD1b in Complex with Sphingomyelin C34:2
Authors : Shahine, A.
Deposited on : 2023-03-22
Resolution : 2.00 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 : 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

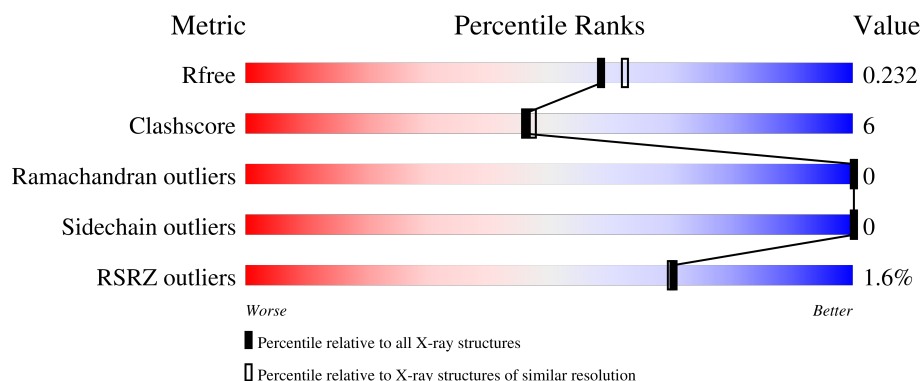
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

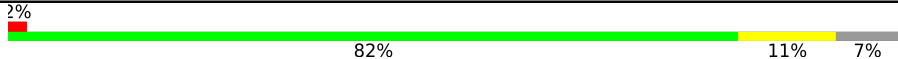
The reported resolution of this entry is 2.00 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	 2% 82% 11% 7%
2	B	101	 % 87% 11% ..
3	D	2	 50% 50%
4	C	7	 43% 57%

2 Entry composition

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	A	280	Total	C	N	O	S	0	11	0
			2238	1440	377	409	12			

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	100	Total	C	N	O	S	0	1	0
			820	523	139	156	2			

There are 2 discrepancies between the modelled and reference sequences:

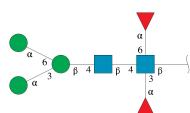
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PRO	-	expression tag	UNP P61769
B	2	LYS	-	expression tag	UNP P61769

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



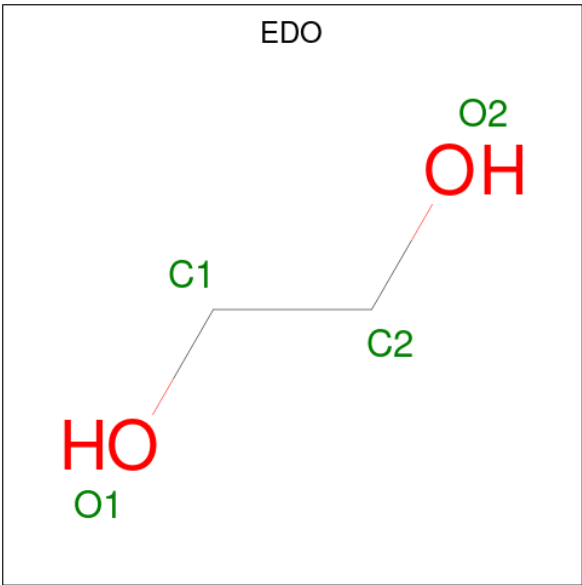
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



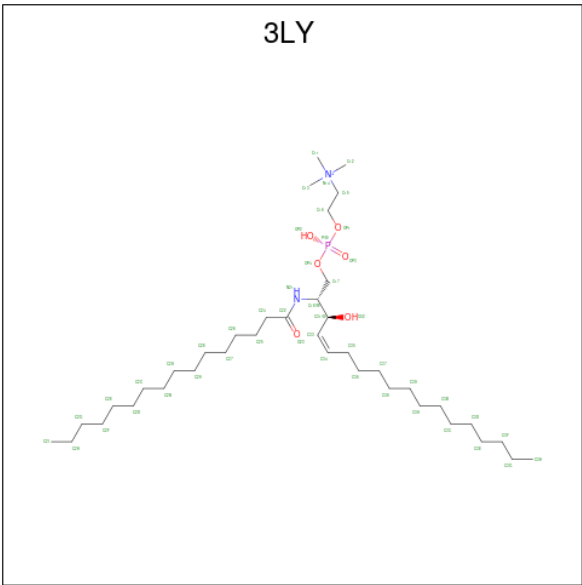
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



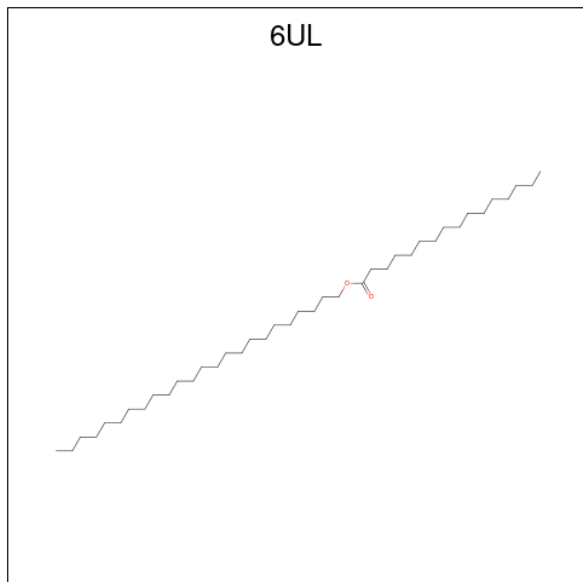
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is [({Z},2 {R},3 {S})-2-(hexadecanoylamino)-3-oxidanyl-octadec-4-enyl] 2-(tri methyl-\$l^{4}\$-azanyl)ethyl hydrogen phosphate (CCD ID: 3LY) (formula: C₃₉H₈₀N₂O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			48	39	2	6	1		

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



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

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

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

- Molecule 9 is IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 10 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

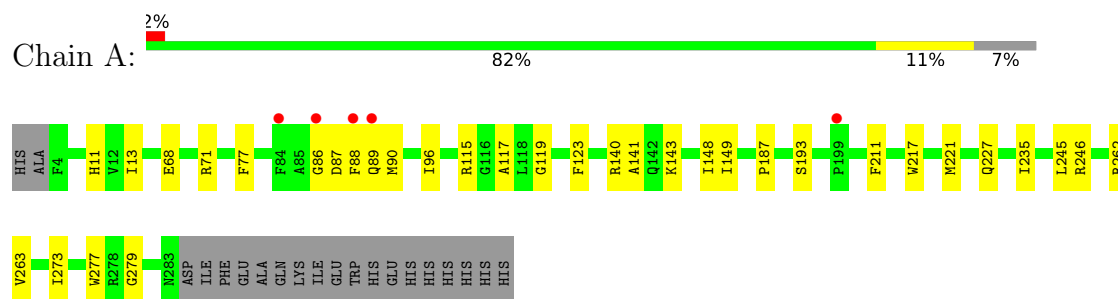
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	167	Total 167	O 167	0	0
11	B	67	Total 67	O 67	0	0

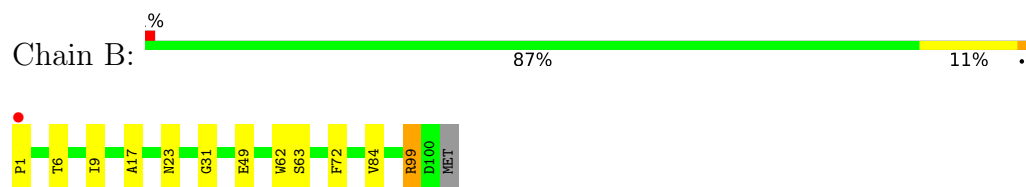
3 Residue-property plots [i](#)

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



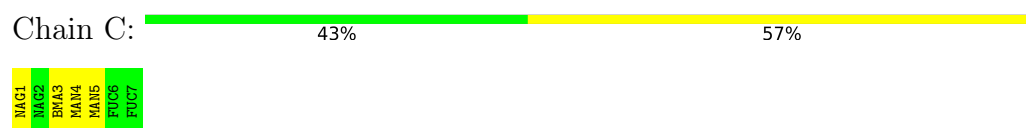
- Molecule 2: Beta-2-microglobulin



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



- Molecule 4: 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



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 77.98Å 91.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.86 – 2.00 35.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (35.86-2.00) 95.2 (35.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.176 , 0.231 0.176 , 0.232	Depositor DCC
R_{free} test set	1383 reflections (1.55%)	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)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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.*

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: NAG, 3LY, FUC, EDO, 6UL, BMA, IOD, NI, CL, 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	0.34	0/2330	0.60	4/3161 (0.1%)
2	B	0.34	0/844	0.57	2/1150 (0.2%)
All	All	0.34	0/3174	0.59	6/4311 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CA-C-N	-6.96	113.79	122.84
1	A	87	ASP	C-N-CA	-6.96	113.79	122.84
2	B	99	ARG	CA-C-N	5.43	131.47	121.70
2	B	99	ARG	C-N-CA	5.43	131.47	121.70
1	A	86	GLY	CA-C-N	5.30	127.64	120.65
1	A	86	GLY	C-N-CA	5.30	127.64	120.65

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	2238	0	2172	27	0
2	B	820	0	762	14	0
3	D	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	81	0	70	0	0
5	A	8	0	12	0	0
6	A	48	0	0	1	0
7	A	26	0	42	0	0
8	A	4	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	1	0	0	0	0
11	A	167	0	0	3	1
11	B	67	0	0	2	1
All	All	3490	0	3083	37	1

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.

All (37) 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
1:A:88:PHE:O	1:A:90:MET:HG3	1.96	0.65
1:A:235:ILE:HD13	1:A:245:LEU:HD13	1.80	0.63
2:B:49:GLU:H	2:B:49:GLU:CD	2.08	0.62
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.83	0.61
1:A:279:GLY:N	11:A:503:HOH:O	2.33	0.61
2:B:99:ARG:O	11:B:301:HOH:O	2.17	0.57
1:A:119:GLY:HA3	2:B:1:PRO:CA	2.36	0.56
1:A:88:PHE:CD1	1:A:143:LYS:HD2	2.45	0.51
2:B:31:GLY:HA2	2:B:63:SER:HB3	1.93	0.50
1:A:148:ILE:HD12	1:A:149:ILE:N	2.28	0.49
1:A:88:PHE:CD2	1:A:140:ARG:HD3	2.48	0.48
1:A:217:TRP:HZ3	1:A:262:ARG:HG2	1.78	0.48
1:A:88:PHE:HD1	1:A:143:LYS:HD2	1.77	0.48
6:A:403:3LY:OP4	6:A:403:3LY:O32	2.33	0.47
1:A:119:GLY:HA3	2:B:1:PRO:HB3	1.97	0.46
1:A:263:VAL:HB	1:A:273:ILE:HB	1.97	0.46
1:A:123:PHE:CZ	1:A:141:ALA:HA	2.51	0.46
1:A:246:ARG:HD2	11:A:565:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLU:OE1	2:B:49:GLU:N	2.33	0.45
1:A:193:SER:HB3	1:A:277:TRP:CH2	2.51	0.44
2:B:9:ILE:HG12	2:B:84:VAL:HG21	1.99	0.44
1:A:117:ALA:HB2	2:B:62:TRP:CE2	2.52	0.44
2:B:23:ASN:HB3	2:B:72:PHE:CE2	2.53	0.44
2:B:6[B]:THR:O	11:B:302:HOH:O	2.19	0.44
1:A:119:GLY:HA3	2:B:1:PRO:CB	2.49	0.42
1:A:217:TRP:HH2	1:A:221[A]:MET:HE1	1.84	0.42
1:A:221[B]:MET:HE3	1:A:221[B]:MET:HB3	1.98	0.41
1:A:221[A]:MET:HA	1:A:227:GLN:HG2	2.02	0.41
1:A:221[A]:MET:HB3	1:A:221[A]:MET:HE2	1.73	0.41
2:B:17:ALA:CB	2:B:99:ARG:HD3	2.48	0.40
1:A:11:HIS:HD2	1:A:13:ILE:HG23	1.87	0.40
1:A:77:PHE:HZ	1:A:96:ILE:HG21	1.86	0.40

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

5.3.1 Protein backbone

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	289/300 (96%)	284 (98%)	5 (2%)	0	100	100
2	B	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	Outliers	Percentiles	
1	A	237/247 (96%)	237 (100%)	0	100	100
2	B	90/96 (94%)	90 (100%)	0	100	100
All	All	327/343 (95%)	327 (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	14	GLN
1	A	150	GLN
1	A	184	GLN
1	A	228	GLN
1	A	231	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	$\# Z > 2$
4	NAG	C	1	1,4	14,14,15	0.79	1 (7%)	17,19,21	0.93	0
4	NAG	C	2	4	14,14,15	0.53	0	17,19,21	0.41	0
4	BMA	C	3	4	11,11,12	0.62	0	15,15,17	1.18	2 (13%)
4	MAN	C	4	4	11,11,12	1.06	1 (9%)	15,15,17	1.11	2 (13%)
4	MAN	C	5	4	11,11,12	0.66	0	15,15,17	1.25	1 (6%)
4	FUC	C	6	4	10,10,11	1.01	0	14,14,16	0.86	0
4	FUC	C	7	4	10,10,11	0.95	0	14,14,16	0.63	0
3	NAG	D	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	0.51	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	C	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	FUC	C	6	4	-	-	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1
3	NAG	D	1	1,3	-	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	C	1	NAG	O5-C1	-2.86	1.38	1.43
3	D	1	NAG	O5-C1	2.18	1.47	1.43
4	C	4	MAN	O5-C5	2.05	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	MAN	C1-O5-C5	3.68	117.11	112.19
4	C	4	MAN	C1-O5-C5	3.28	116.59	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	O2-C2-C3	-2.70	104.56	110.15
3	D	1	NAG	C1-O5-C5	2.54	115.59	112.19
4	C	4	MAN	O2-C2-C3	-2.07	105.87	110.15
4	C	3	BMA	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

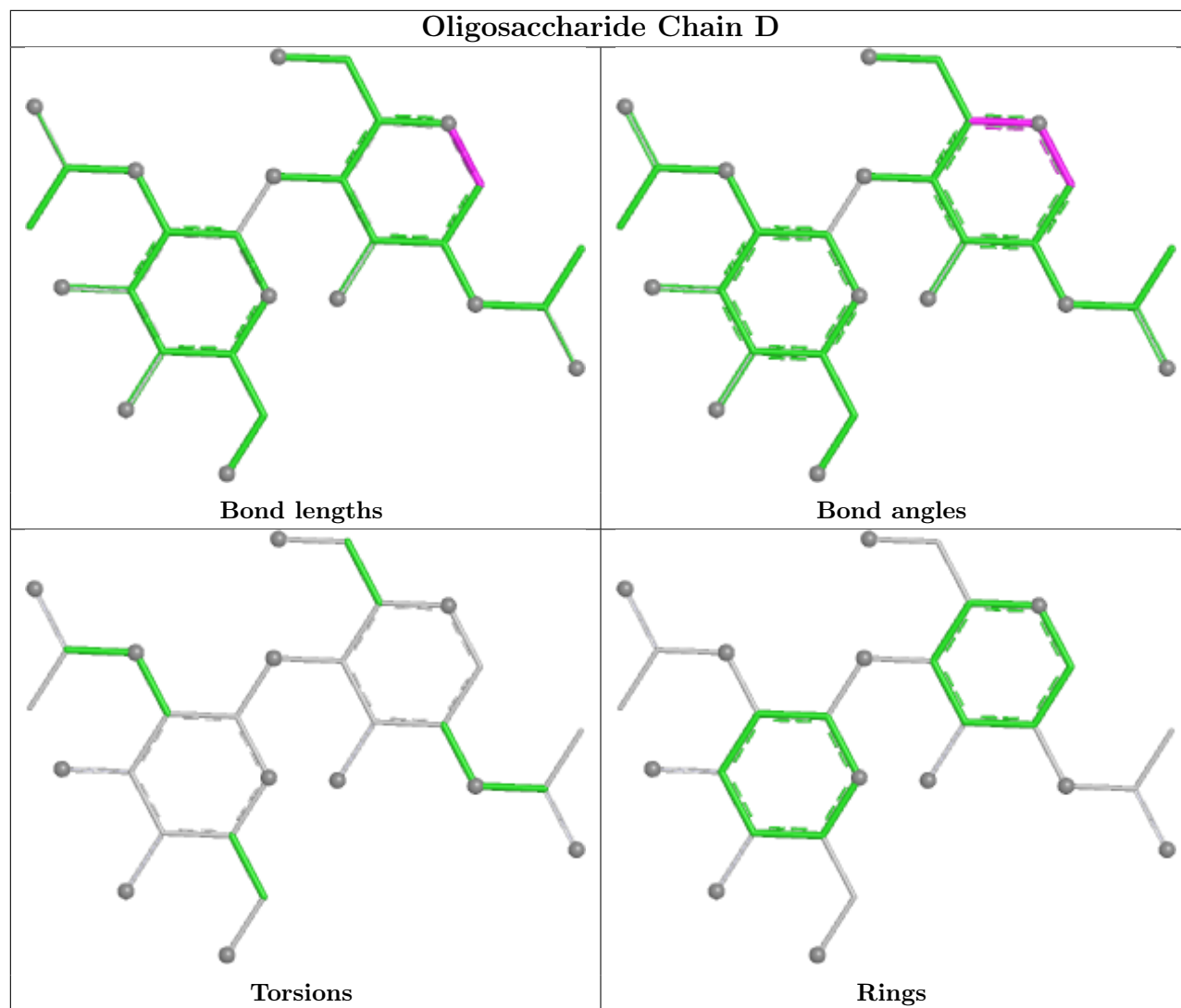
All (1) torsion outliers are listed below:

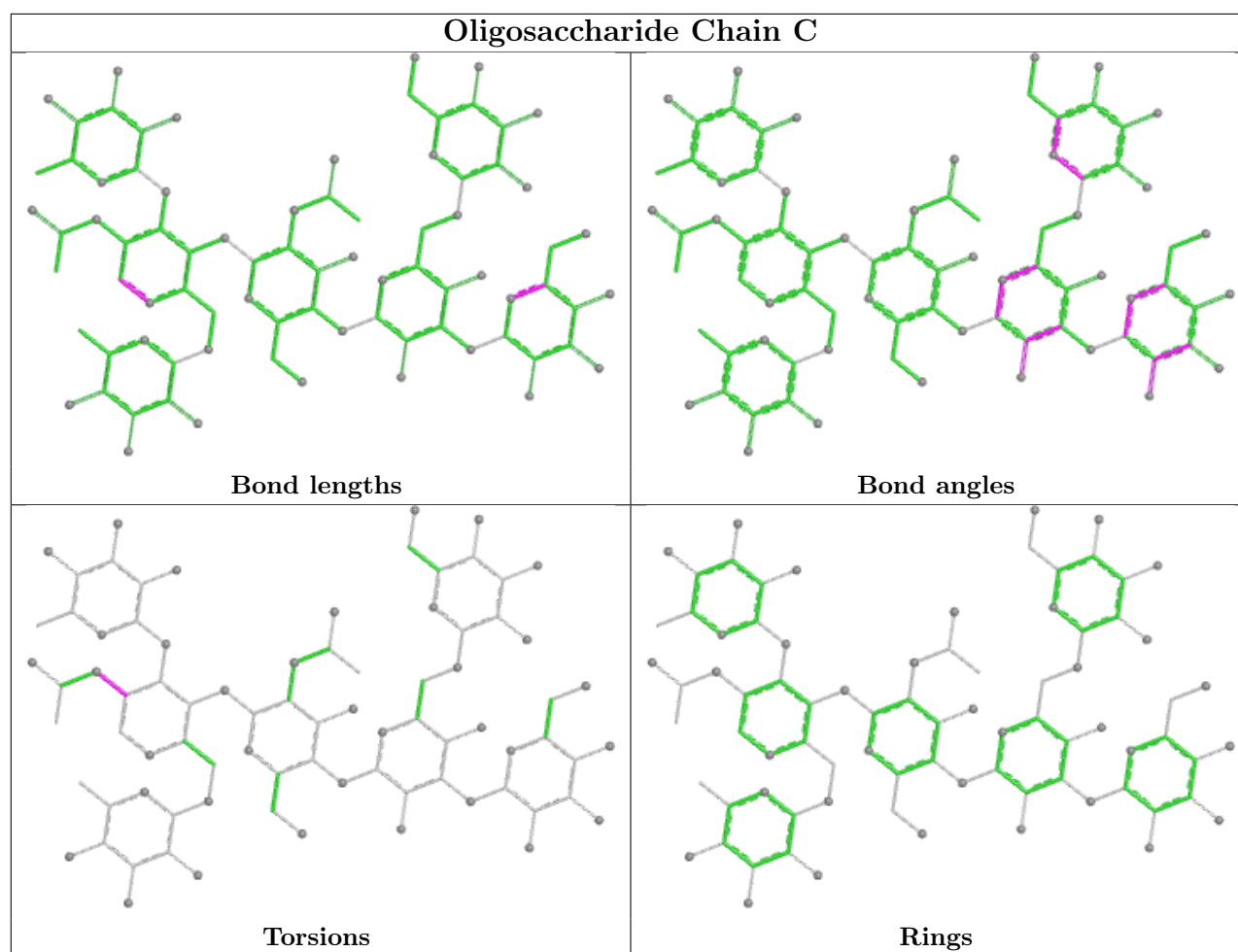
Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C3-C2-N2-C7

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	3LY	A	403	-	46,47,47	1.27	3 (6%)	52,55,55	1.05	3 (5%)
5	EDO	A	401	-	3,3,3	0.43	0	2,2,2	0.41	0
5	EDO	A	402	-	3,3,3	0.43	0	2,2,2	0.32	0
7	6UL	A	404	-	25,25,41	0.77	1 (4%)	25,25,41	1.02	1 (4%)

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
6	3LY	A	403	-	-	25/52/52/52	-
5	EDO	A	401	-	-	1/1/1/1	-
5	EDO	A	402	-	-	0/1/1/1	-
7	6UL	A	404	-	-	10/24/24/40	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	3LY	C22-N21	5.91	1.46	1.34
7	A	404	6UL	OAQ-CAP	2.60	1.40	1.33
6	A	403	3LY	O23-C22	-2.50	1.18	1.23
6	A	403	3LY	C31-C33	2.23	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	403	3LY	O32-C31-C18	4.79	120.48	107.85
6	A	403	3LY	C24-C22-N21	3.37	121.81	115.86
7	A	404	6UL	OAQ-CAP-CAO	2.95	120.83	111.83
6	A	403	3LY	O23-C22-C24	-2.25	117.94	122.02

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	403	3LY	OP4-C17-C18-N21
6	A	403	3LY	OP4-C17-C18-C31
6	A	403	3LY	N21-C18-C31-O32
6	A	403	3LY	N21-C18-C31-C33
6	A	403	3LY	C17-C18-C31-O32
6	A	403	3LY	C17-C18-C31-C33
6	A	403	3LY	C17-OP4-P-OP3
6	A	403	3LY	N14-C15-C16-OP1
6	A	403	3LY	C3A-C3B-C3C-C3D
7	A	404	6UL	CAU-CAV-CAW-CBM
7	A	404	6UL	CBF-CBG-CBH-CBI
7	A	404	6UL	CAV-CAW-CBM-CBL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	403	3LY	C2D-C2E-C2F-C2G
6	A	403	3LY	C2C-C2D-C2E-C2F
6	A	403	3LY	C29-C2A-C2B-C2C
6	A	403	3LY	C34-C35-C36-C37
6	A	403	3LY	C2E-C2F-C2G-C2H
7	A	404	6UL	CBI-CBJ-CBK-CBL
7	A	404	6UL	CBD-CBE-CBF-CBG
7	A	404	6UL	CAT-CAU-CAV-CAW
6	A	403	3LY	C24-C25-C26-C27
6	A	403	3LY	C22-C24-C25-C26
6	A	403	3LY	C3C-C3D-C3E-C3F
6	A	403	3LY	C3E-C3F-C3G-C3H
6	A	403	3LY	C3D-C3E-C3F-C3G
7	A	404	6UL	CBJ-CBK-CBL-CBM
6	A	403	3LY	C37-C38-C39-C3A
7	A	404	6UL	CBC-CBD-CBE-CBF
6	A	403	3LY	C2F-C2G-C2H-C2I
6	A	403	3LY	C38-C39-C3A-C3B
5	A	401	EDO	O1-C1-C2-O2
7	A	404	6UL	OAQ-CAR-CAS-CAT
7	A	404	6UL	CAL-CAM-CAN-CAO
6	A	403	3LY	C33-C34-C35-C36
6	A	403	3LY	O32-C31-C33-C34
6	A	403	3LY	C27-C28-C29-C2A

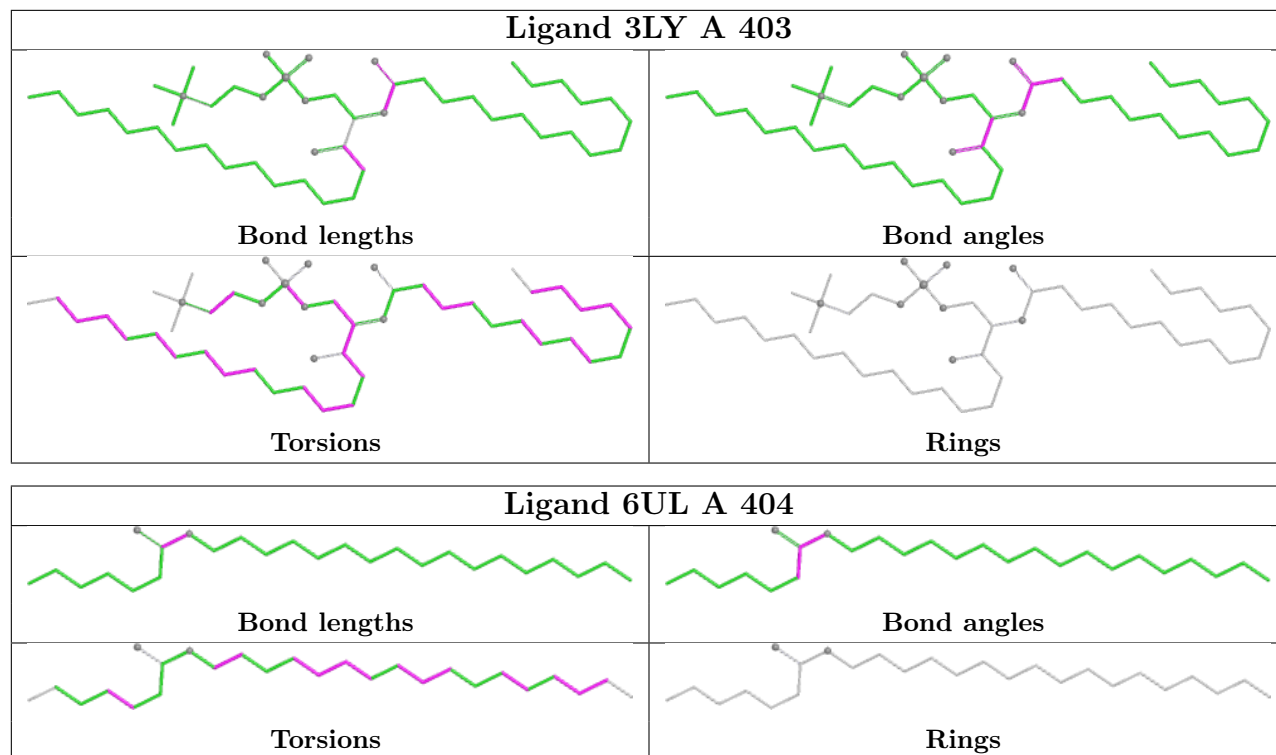
There are no ring outliers.

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 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%)	-0.24	5 (1%) 67 67	11, 25, 53, 82	11 (3%)
2	B	100/101 (99%)	-0.15	1 (1%) 79 79	14, 32, 55, 70	1 (1%)
All	All	380/401 (94%)	-0.21	6 (1%) 70 70	11, 26, 54, 82	12 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	3.6
1	A	88	PHE	2.6
1	A	199	PRO	2.3
1	A	89	GLN	2.2
1	A	86	GLY	2.1
1	A	84	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

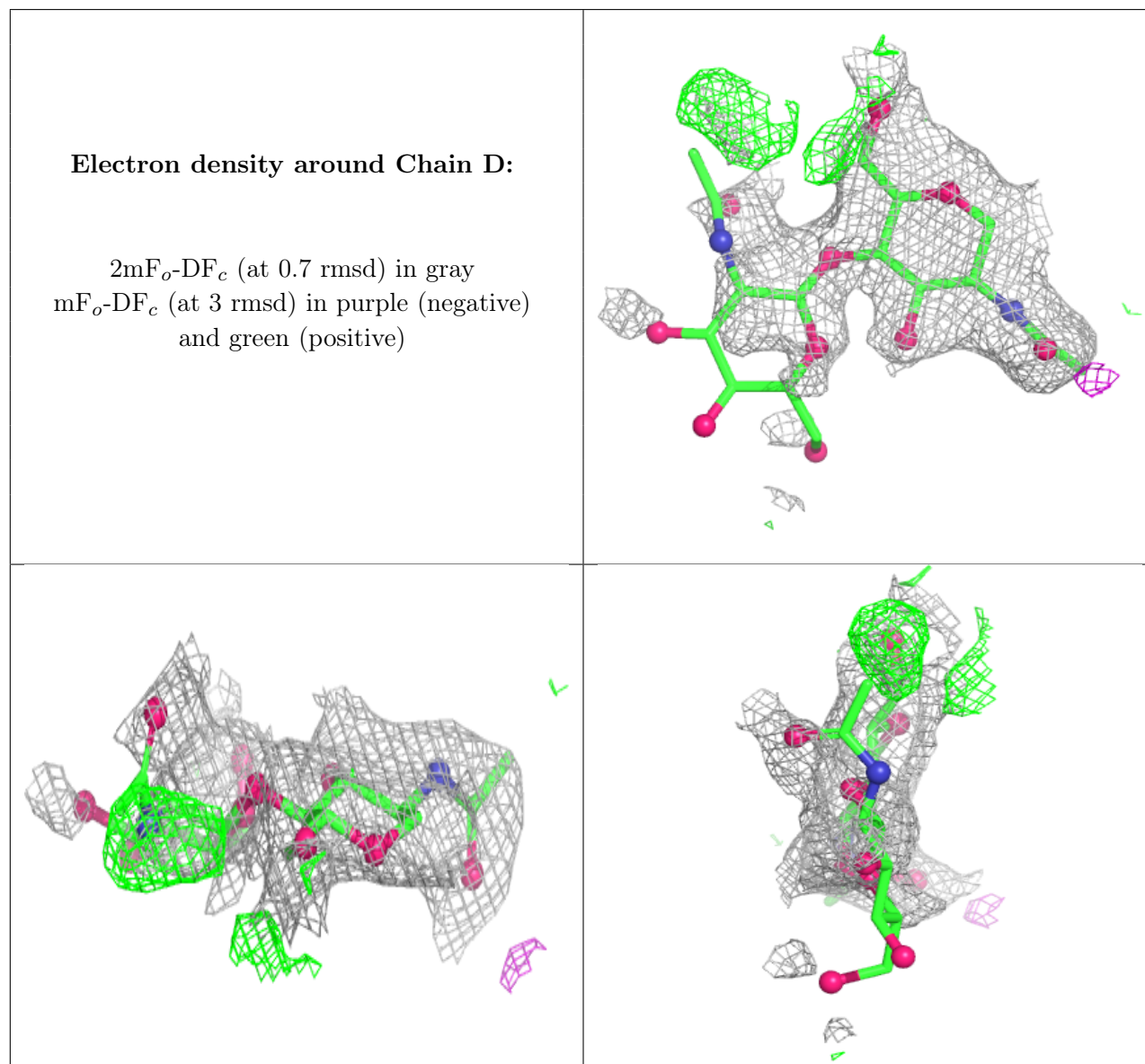
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	2	14/15	0.23	0.19	14,22,28,34	0
4	NAG	C	1	14/15	0.75	0.14	15,20,22,26	0
3	NAG	D	2	14/15	0.94	0.06	92,102,110,113	0

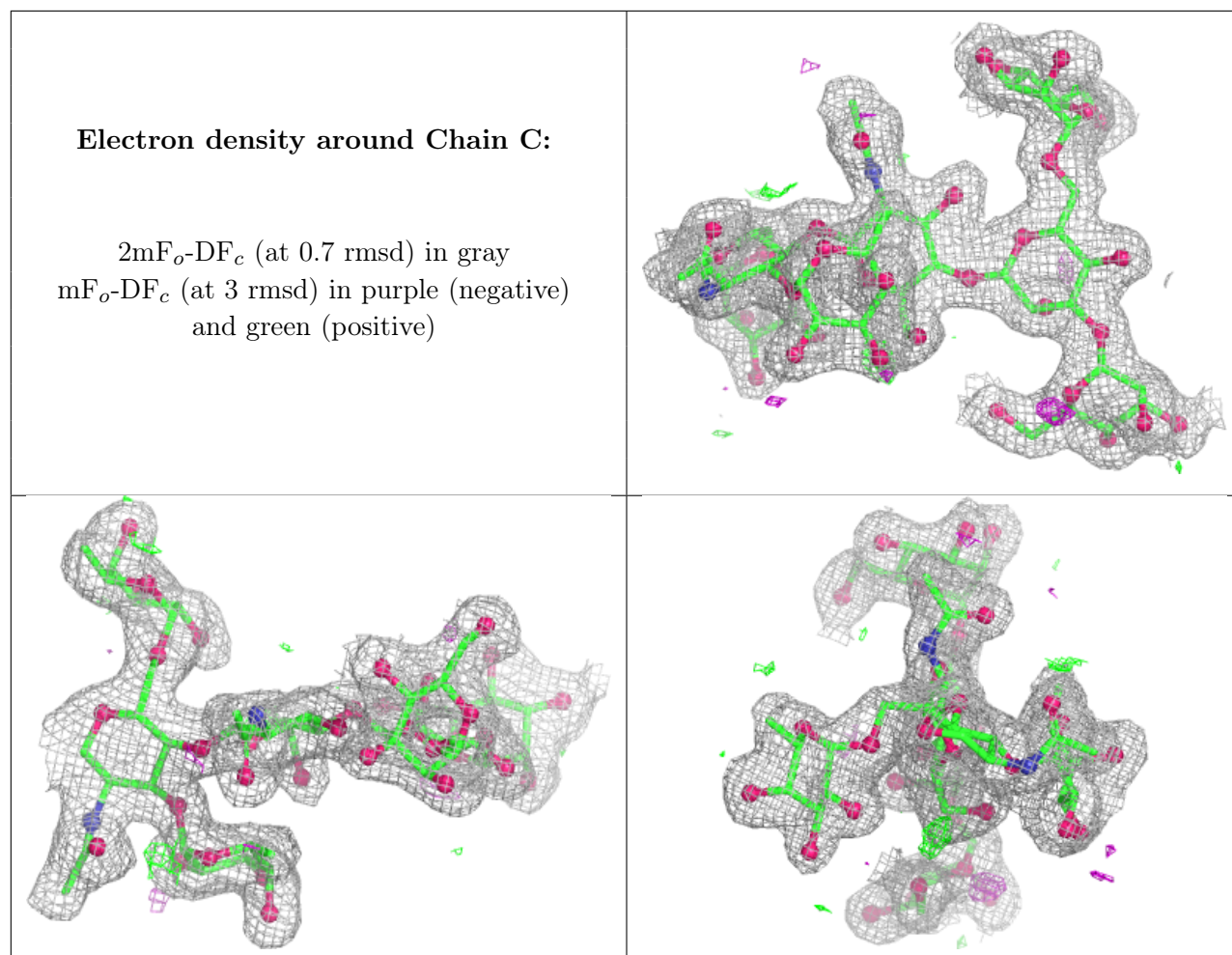
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	1	14/15	0.96	0.06	49,60,81,85	0
4	BMA	C	3	11/12	-	-	16,22,26,29	0
4	MAN	C	4	11/12	-	-	27,30,35,38	0
4	MAN	C	5	11/12	-	-	16,23,30,31	0
4	FUC	C	6	10/11	-	-	28,36,42,43	0
4	FUC	C	7	10/11	-	-	33,36,40,41	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, 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
6	3LY	A	403	48/48	0.83	0.16	24,55,119,121	0
8	CL	A	405	1/1	0.87	0.10	56,56,56,56	0
7	6UL	A	404	26/42	0.88	0.12	20,35,42,55	0
5	EDO	A	401	4/4	0.89	0.12	53,54,59,62	0
5	EDO	A	402	4/4	0.90	0.08	43,44,45,47	0
10	NI	B	202	1/1	0.95	0.06	43,43,43,43	0
8	CL	A	407	1/1	0.98	0.04	40,40,40,40	0
9	IOD	B	201	1/1	0.98	0.05	48,48,48,48	1
8	CL	A	406	1/1	0.98	0.05	30,30,30,30	0
8	CL	A	408	1/1	0.99	0.10	19,19,19,19	0

Continued on next page...

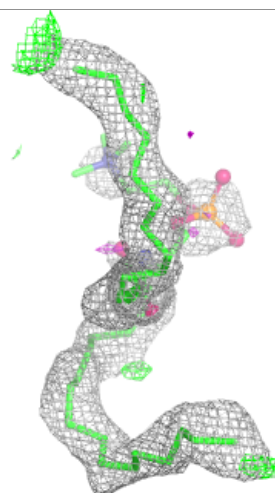
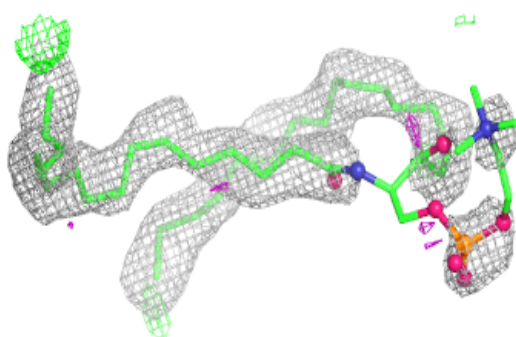
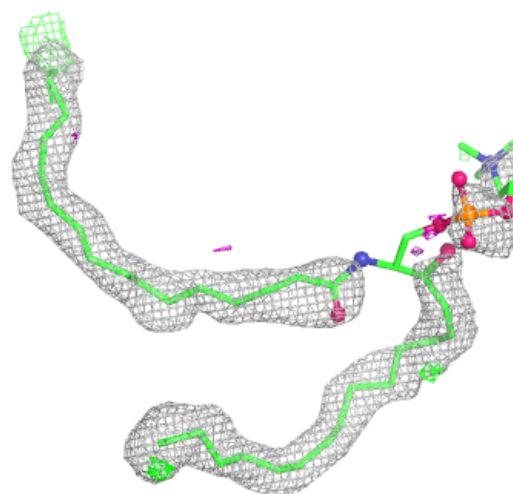
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	IOD	A	409	1/1	1.00	0.01	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.

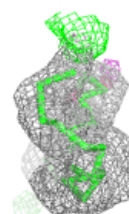
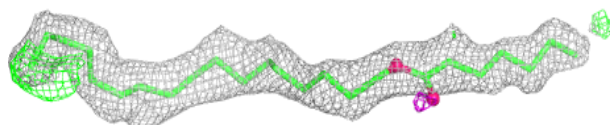
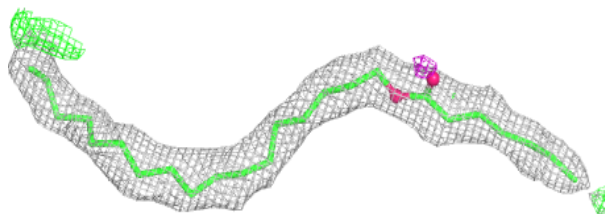
Electron density around 3LY A 403:

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



Electron density around 6UL A 404:

$2mF_o-DF_c$ (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.