wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2023 – 12:38 PM EDT

PDB ID	:	3GMM
Title	:	Structure of mouse CD1d in complex with C8Ph
Authors	:	Schiefner, A.; Wilson, I.A.
Deposited on	:	2009-03-14
Resolution	:	1.80 Å(reported)

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

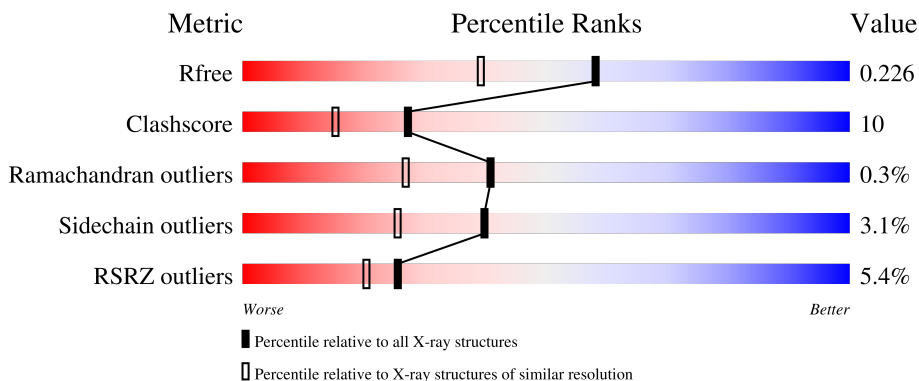|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
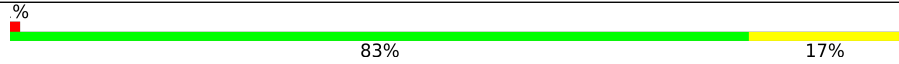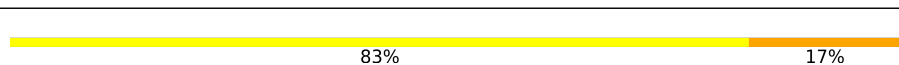*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		3.1%
RSRZ outliers		5.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	Quality of chain
1	A	287	7% / 74% 17% · 7%
2	B	99	% / 83% 17%
3	C	5	40% 60%
4	D	6	83% 17%

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	BMA	C	3	-	-	-	X
5	NAG	A	288	-	-	-	X

2 Entry composition ⓘ

There are 9 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 CD1d1.

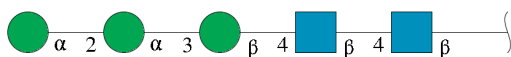| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2205	1401	383	408	13	0	5	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	expression tag	UNP P11609
A	281	SER	-	expression tag	UNP P11609
A	282	HIS	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	HIS	-	expression tag	UNP P11609
A	286	HIS	-	expression tag	UNP P11609
A	287	HIS	-	expression tag	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	833	531	140	155	7	0	2	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
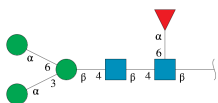
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 6 is N-{(1S,2S,3R)-1-[(alpha-D-galactopyranosyloxy)methyl]-2,3-dihydroxyheptad ecyl}-8-phenyloctanamide (three-letter code: C8P) (formula: $C_{38}H_{67}NO_9$).
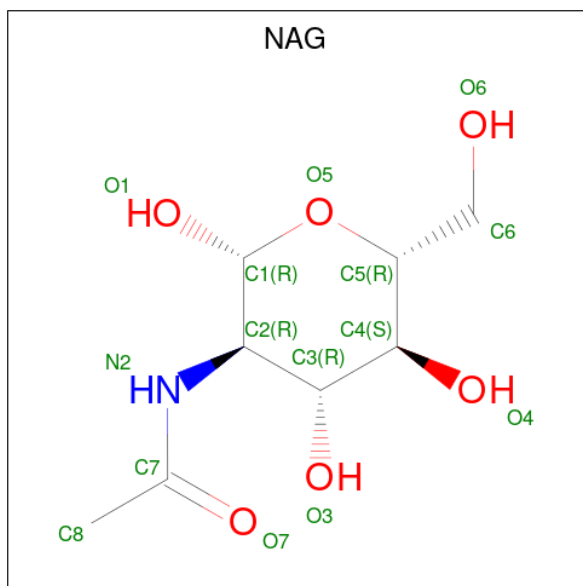
C8P

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	48	38	1	9	0	0

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

PLM
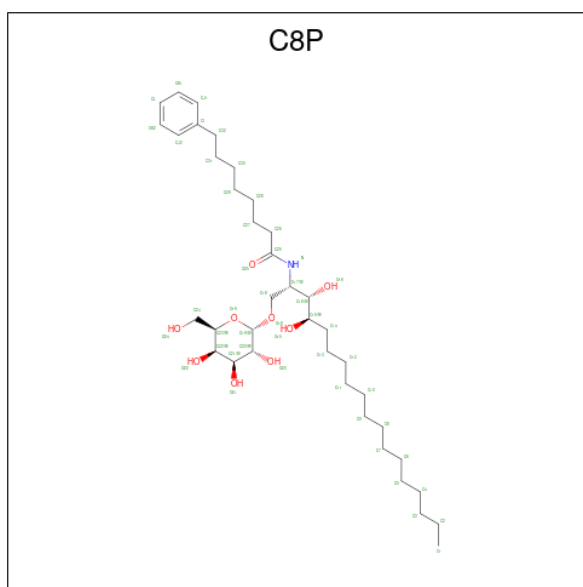
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	18	16	2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
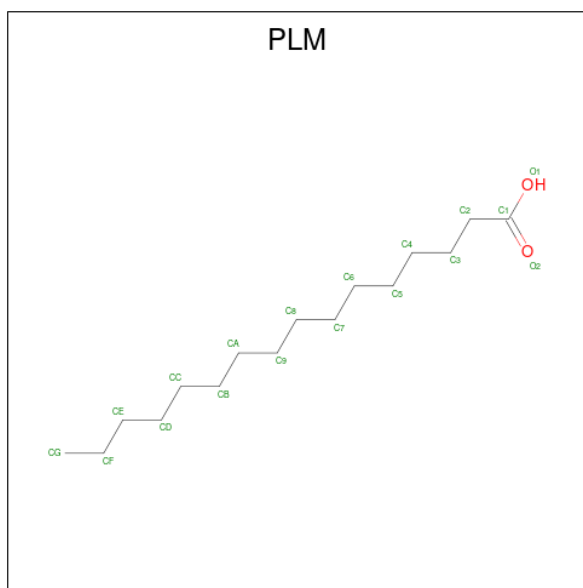
EDO

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 8	C 4	O 4	0	1

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	218	Total 223	O 223	0	5
9	B	96	Total 97	O 97	0	1

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 CD1d1

Chain A:
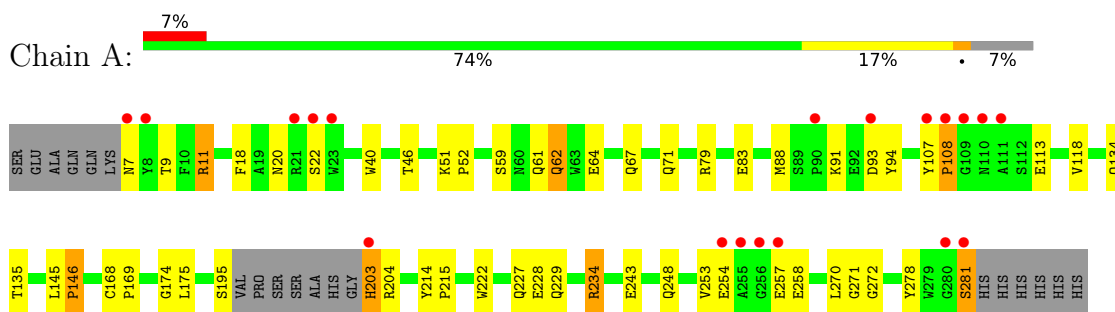
• Molecule 2: Beta-2 microglobulin

Chain B:
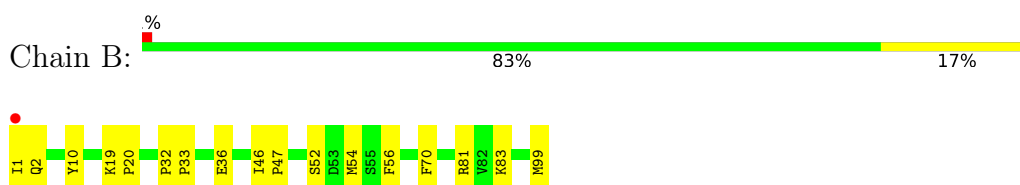
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• 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-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:
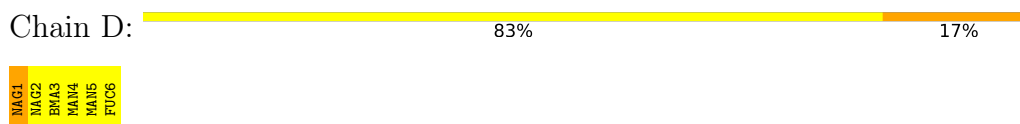
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.74Å　　97.90Å　　55.42Å 90.00°　　106.57°　　90.00°	Depositor
Resolution (Å)	29.77　－　1.80 29.77　－　1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.77-1.80) 99.6 (29.77-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.175　,　0.219 0.182　,　0.226	Depositor DCC
R_{free} test set	1993 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PLM, EDO, C8P, NAG, BMA, FUC, 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	1.09	2/2268 (0.1%)	0.98	2/3079 (0.1%)
2	B	1.22	3/859 (0.3%)	1.03	0/1164
All	All	1.13	5/3127 (0.2%)	0.99	2/4243 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	MET	CG-SD	-7.23	1.62	1.81
2	B	10	TYR	CD1-CE1	5.79	1.48	1.39
2	B	56	PHE	CE2-CZ	5.34	1.47	1.37
1	A	40	TRP	CE3-CZ3	5.20	1.47	1.38
1	A	222	TRP	CB-CG	5.03	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	GLY	N-CA-C	-5.29	99.89	113.10
1	A	175	LEU	CB-CG-CD2	5.18	119.81	111.00

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	2205	0	2097	48	0
2	B	833	0	806	14	1
3	C	61	0	52	2	0
4	D	71	0	61	1	0
5	A	14	0	13	1	0
6	A	48	0	67	2	0
7	A	18	0	31	2	0
8	A	8	0	12	1	0
8	B	12	0	18	2	0
9	A	223	0	0	12	0
9	B	97	0	0	6	1
All	All	3590	0	3157	65	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 10.

The worst 5 of 65 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:234:ARG:HG2	1:A:234:ARG:HH11	1.14	1.08
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.26	1.08
1:A:59:SER:OG	1:A:62:GLN:HG3	1.69	0.91
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.00	0.91
1:A:228:GLU:HG3	9:A:397:HOH:O	1.73	0.86

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)
2:B:1:ILE:CD1	9:B:392:HOH:O[1_655]	1.33	0.87

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	269/287 (94%)	262 (97%)	6 (2%)	1 (0%)	34	21
2	B	99/99 (100%)	96 (97%)	3 (3%)	0	100	100
All	All	368/386 (95%)	358 (97%)	9 (2%)	1 (0%)	41	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	PRO

5.3.2   Protein sidechains ⓘ

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	239/250 (96%)	229 (96%)	10 (4%)	30	15
2	B	95/93 (102%)	94 (99%)	1 (1%)	73	68
All	All	334/343 (97%)	323 (97%)	11 (3%)	40	23

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	234	ARG
2	B	70	PHE
1	A	281	SER
1	A	93	ASP

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

Mol	Chain	Res	Type
1	A	203	HIS

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 ⓘ

11 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	3,1	14,14,15	0.86	1 (7%)	17,19,21	2.28	7 (41%)
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	1.20	2 (11%)
3	BMA	C	3	3	11,11,12	0.59	0	15,15,17	1.93	3 (20%)
3	MAN	C	4	3	11,11,12	0.60	0	15,15,17	1.36	2 (13%)
3	MAN	C	5	3	11,11,12	0.61	0	15,15,17	1.44	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	1.99	3 (17%)
4	NAG	D	2	4	14,14,15	0.58	0	17,19,21	1.77	6 (35%)
4	BMA	D	3	4	11,11,12	0.63	0	15,15,17	1.61	5 (33%)
4	MAN	D	4	4	11,11,12	0.64	0	15,15,17	2.09	7 (46%)
4	MAN	D	5	4	11,11,12	0.84	1 (9%)	15,15,17	1.29	1 (6%)
4	FUC	D	6	4	10,10,11	1.14	0	14,14,16	2.18	6 (42%)

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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	FUC	D	6	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	1	NAG	O3-C3	-2.30	1.37	1.43
4	D	1	NAG	O5-C5	-2.05	1.39	1.43
4	D	5	MAN	O5-C1	-2.04	1.40	1.43

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C3-C4-C5	-6.14	99.29	110.24
3	C	3	BMA	C1-C2-C3	4.78	115.54	109.67
4	D	1	NAG	C8-C7-N2	4.54	123.78	116.10
3	C	5	MAN	O5-C5-C6	4.22	113.82	107.20
4	D	4	MAN	C2-C3-C4	-3.99	104.00	110.89

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	MAN	1	0
3	C	4	MAN	1	0
4	D	1	NAG	1	0
3	C	2	NAG	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
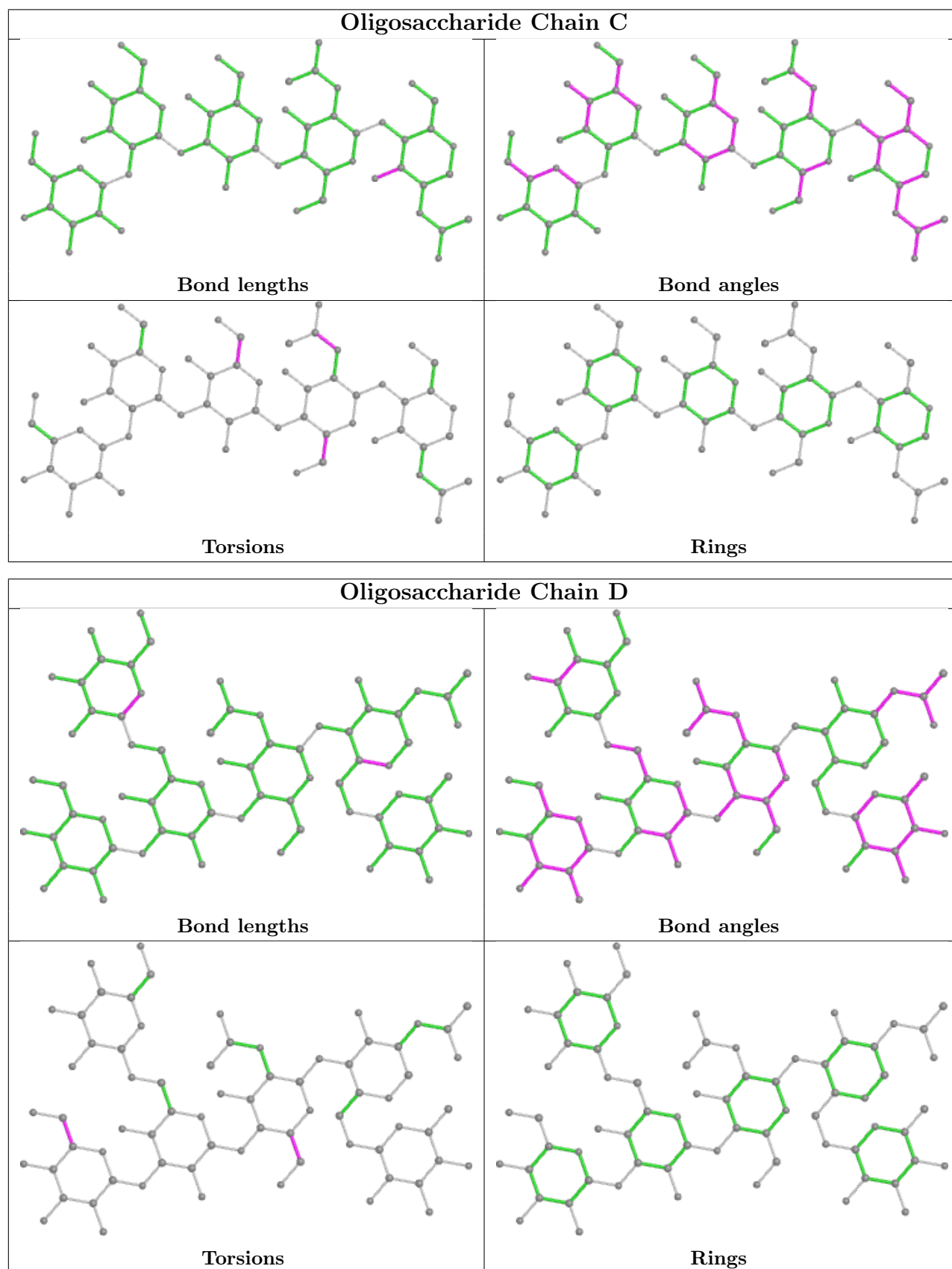
5.6 Ligand geometry (i)

8 ligands 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	#$\|Z\| > 2$
8	EDO	B	101[B]	-	3,3,3	0.56	0	2,2,2	0.55	0
6	C8P	A	300	-	49,49,49	0.86	2 (4%)	56,60,60	1.38	8 (14%)
8	EDO	A	303	-	3,3,3	0.81	0	2,2,2	0.57	0
5	NAG	A	288	1	14,14,15	0.95	1 (7%)	17,19,21	1.50	3 (17%)
8	EDO	B	100	-	3,3,3	0.71	0	2,2,2	0.76	0
8	EDO	B	101[A]	-	3,3,3	0.52	0	2,2,2	0.62	0
8	EDO	A	302	-	3,3,3	0.50	0	2,2,2	0.55	0
7	PLM	A	301	-	17,17,17	0.41	0	17,17,17	1.13	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	101[B]	-	-	0/1/1/1	-
6	C8P	A	300	-	-	6/43/63/63	0/2/2/2
8	EDO	A	303	-	-	0/1/1/1	-
5	NAG	A	288	1	-	0/6/23/26	0/1/1/1
8	EDO	B	100	-	-	0/1/1/1	-
8	EDO	B	101[A]	-	-	1/1/1/1	-
8	EDO	A	302	-	-	1/1/1/1	-
7	PLM	A	301	-	-	7/15/15/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	300	C8P	O18-C19	3.23	1.45	1.40
6	A	300	C8P	C18-C17	2.50	1.56	1.51
5	A	288	NAG	C1-C2	2.31	1.55	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	288	NAG	C1-O5-C5	-3.47	107.49	112.19
7	A	301	PLM	O1-C1-C2	3.14	124.11	114.03
6	A	300	C8P	C18-C17-N	-2.98	105.22	109.61
6	A	300	C8P	O19-C23-C22	2.92	115.00	109.69
5	A	288	NAG	C4-C3-C2	2.90	115.26	111.02

There are no chirality outliers.
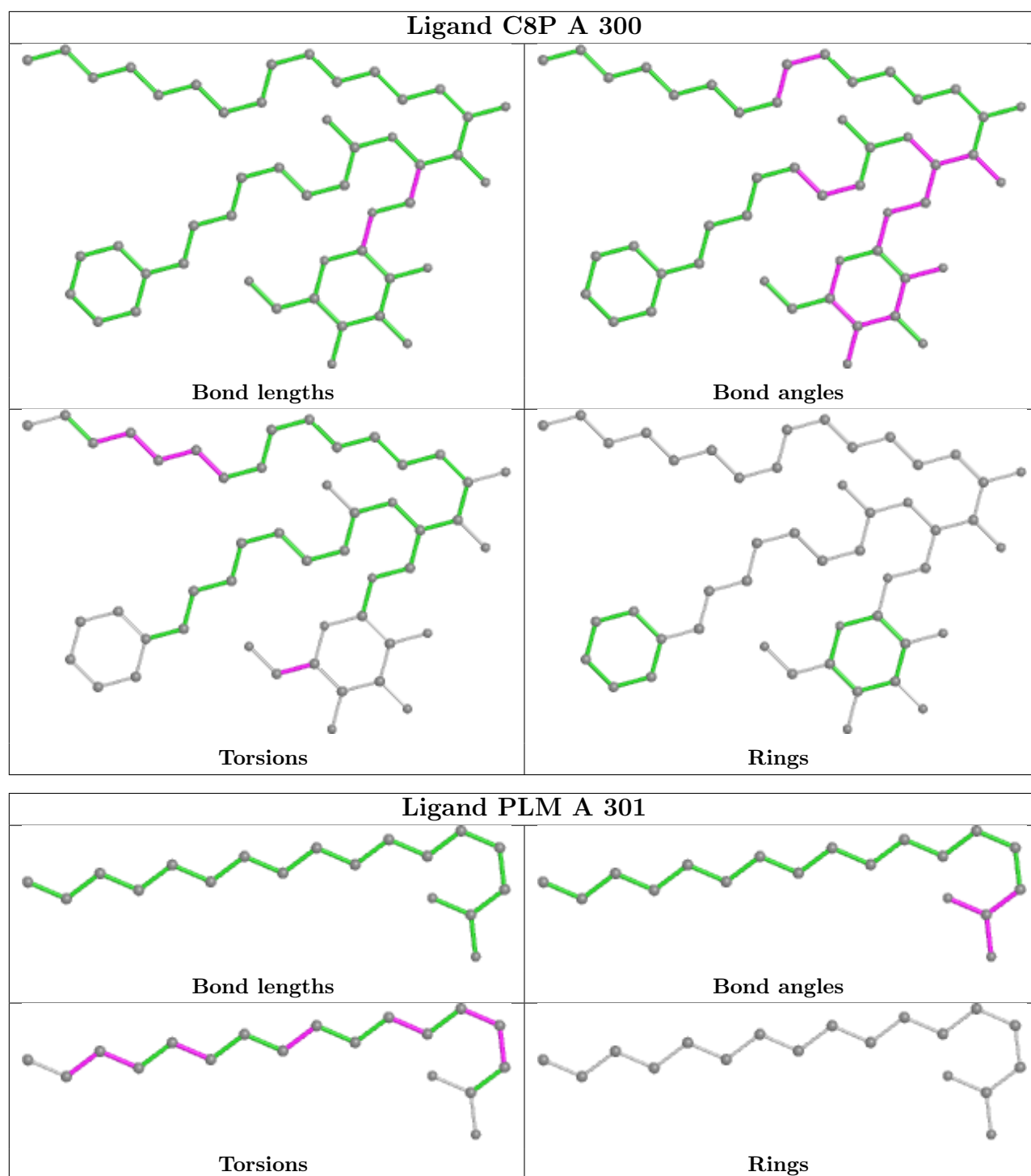
5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	301	PLM	C4-C5-C6-C7
6	A	300	C8P	O19-C23-C24-O24
6	A	300	C8P	C22-C23-C24-O24
7	A	301	PLM	CC-CD-CE-CF
6	A	300	C8P	C5-C6-C7-C8

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	300	C8P	2	0
8	A	303	EDO	1	0
5	A	288	NAG	1	0
8	B	101[A]	EDO	2	0
7	A	301	PLM	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 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 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.

Ligand C8P A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM A 301

Bond lengths

Bond angles

Torsions

Rings

5.7   Other polymers ⓘ

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   ⓘ

6.1   Protein, DNA and RNA chains   ⓘ

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	268/287 (93%)	0.14	19 (7%)	16	12	13, 21, 42, 57	0
2	B	99/99 (100%)	-0.22	1 (1%)	82	80	14, 20, 31, 40	0
All	All	367/386 (95%)	0.04	20 (5%)	25	20	13, 21, 40, 57	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	6.5
1	A	109	GLY	6.2
1	A	203	HIS	5.7
1	A	255	ALA	5.1
1	A	110	ASN	4.9

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

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.
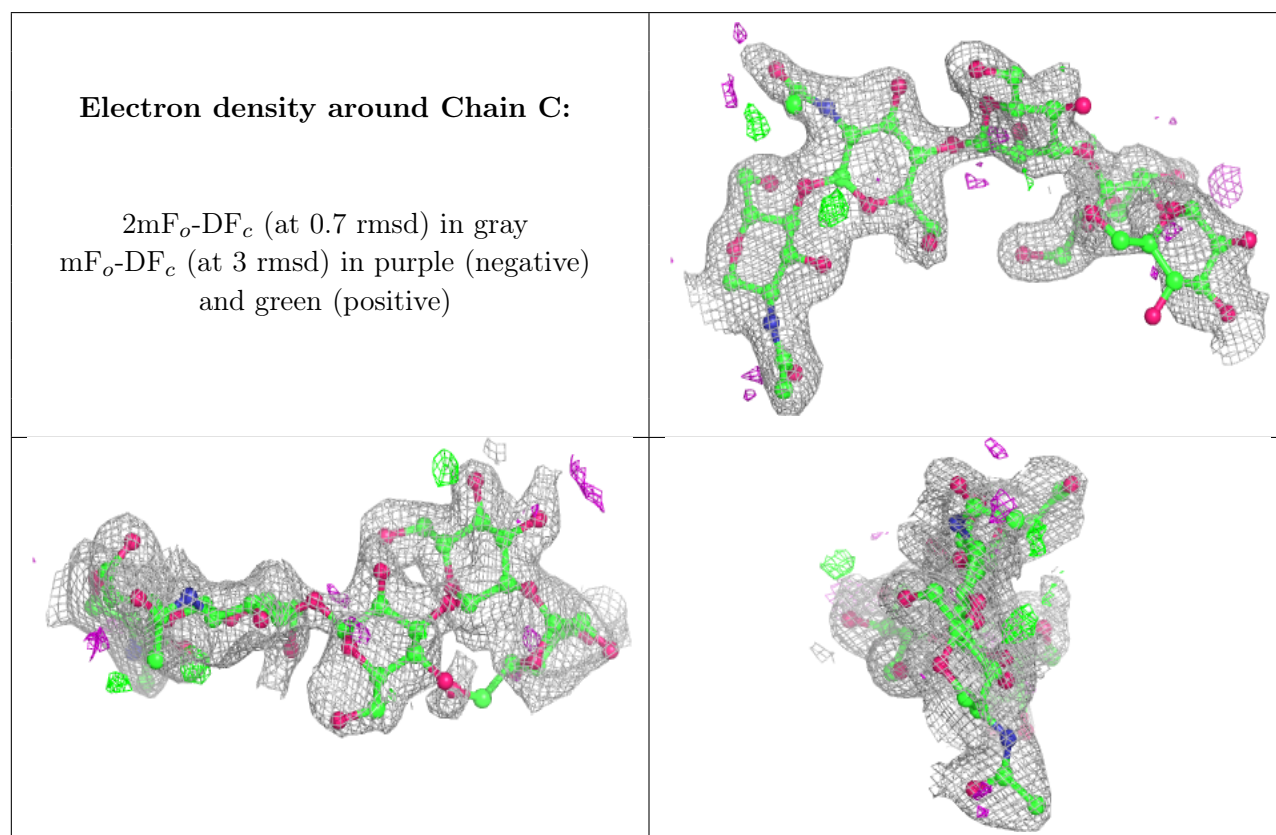
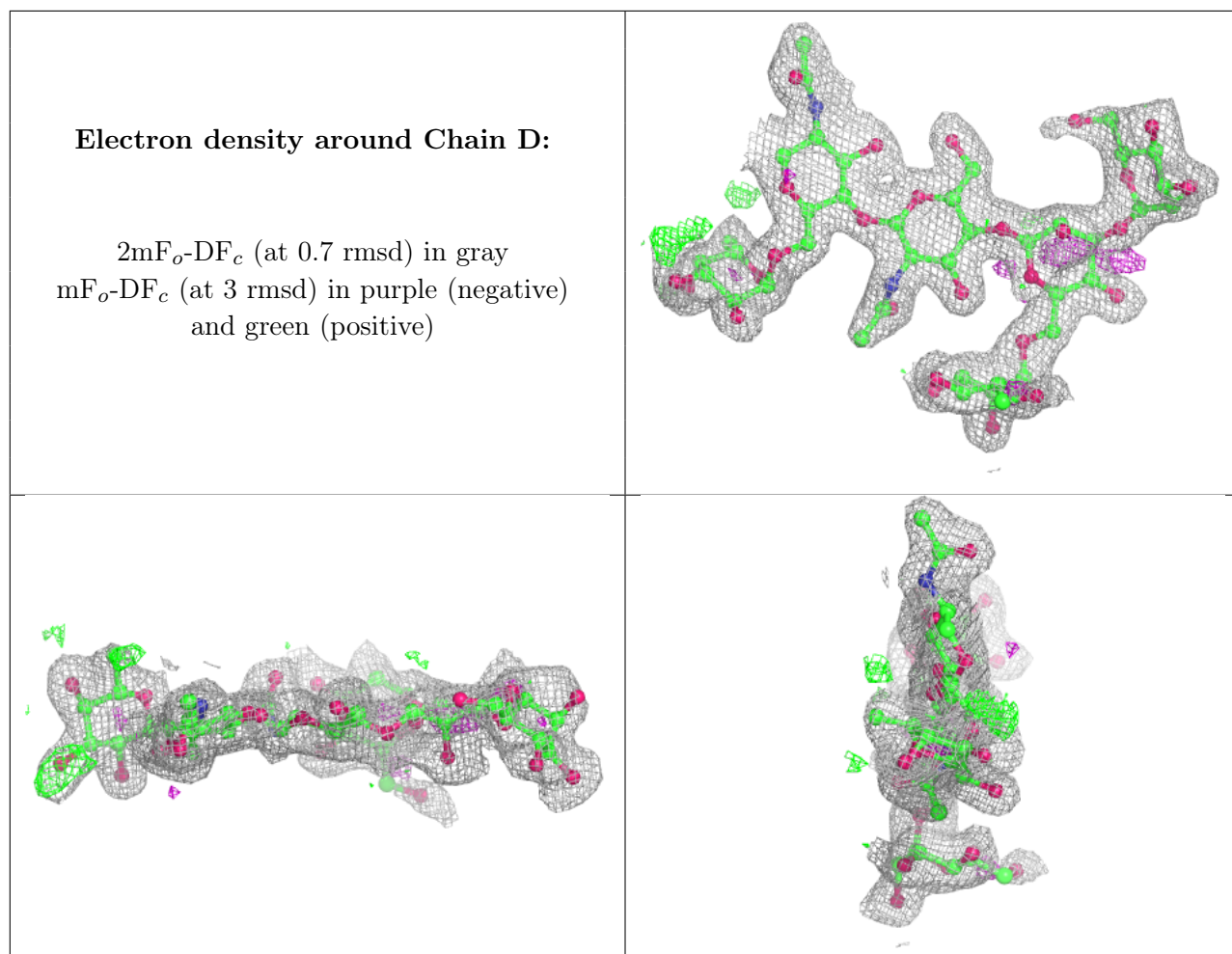| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	5	11/12	0.63	0.38	75,78,81,82	0
3	MAN	C	4	11/12	0.69	0.23	46,54,63,68	0
3	BMA	C	3	11/12	0.69	0.42	67,71,74,76	0
3	NAG	C	2	14/15	0.70	0.32	62,65,69,71	0
4	MAN	D	4	11/12	0.74	0.26	63,67,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	FUC	D	6	10/11	0.78	0.14	39,42,45,45	0
4	BMA	D	3	11/12	0.79	0.22	42,45,52,57	0
4	MAN	D	5	11/12	0.85	0.22	41,45,50,52	0
4	NAG	D	2	14/15	0.92	0.10	35,37,41,42	0
3	NAG	C	1	14/15	0.94	0.11	33,42,48,52	0
4	NAG	D	1	14/15	0.95	0.07	26,30,33,35	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.
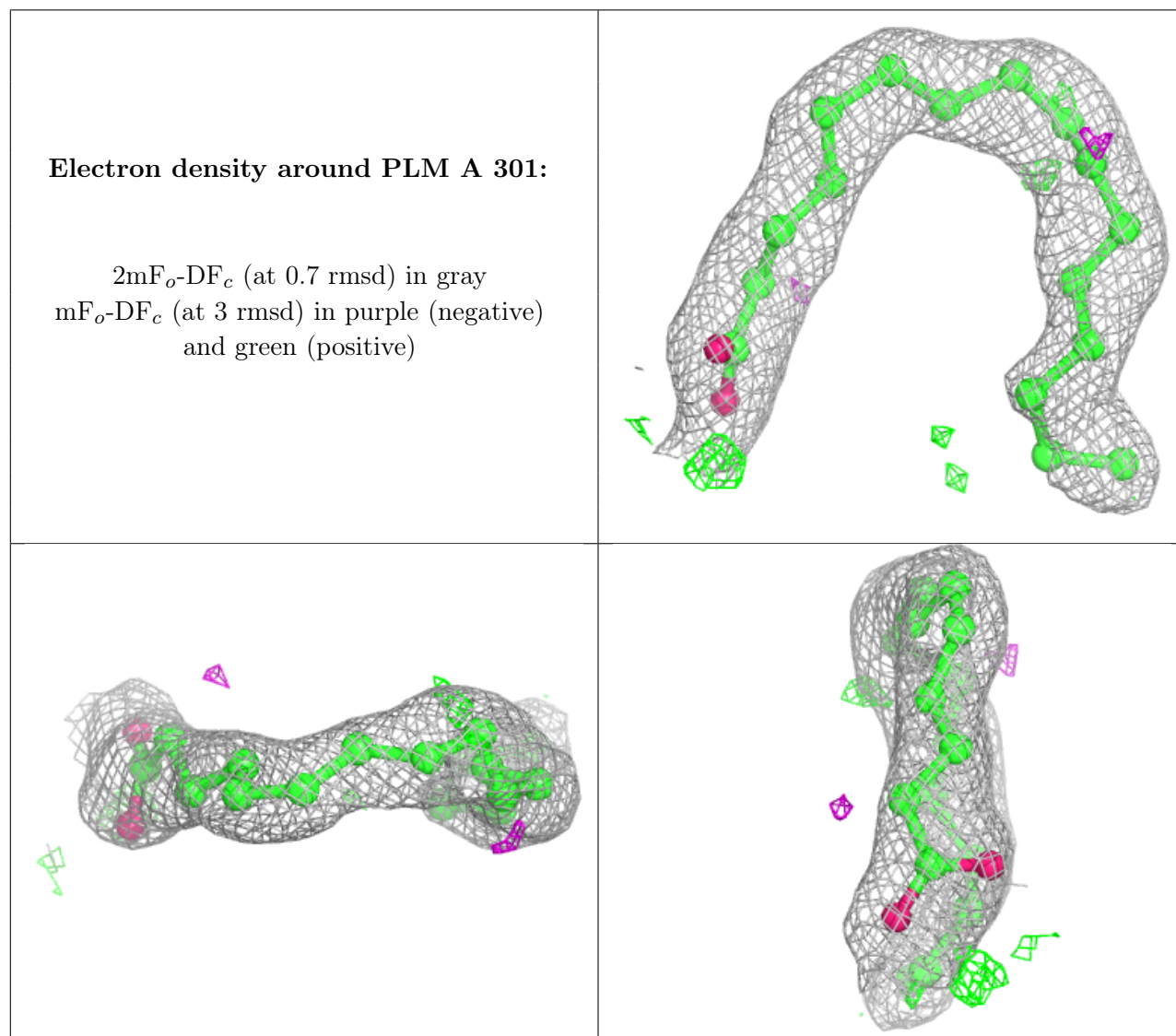

Electron density around Chain C:

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

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)
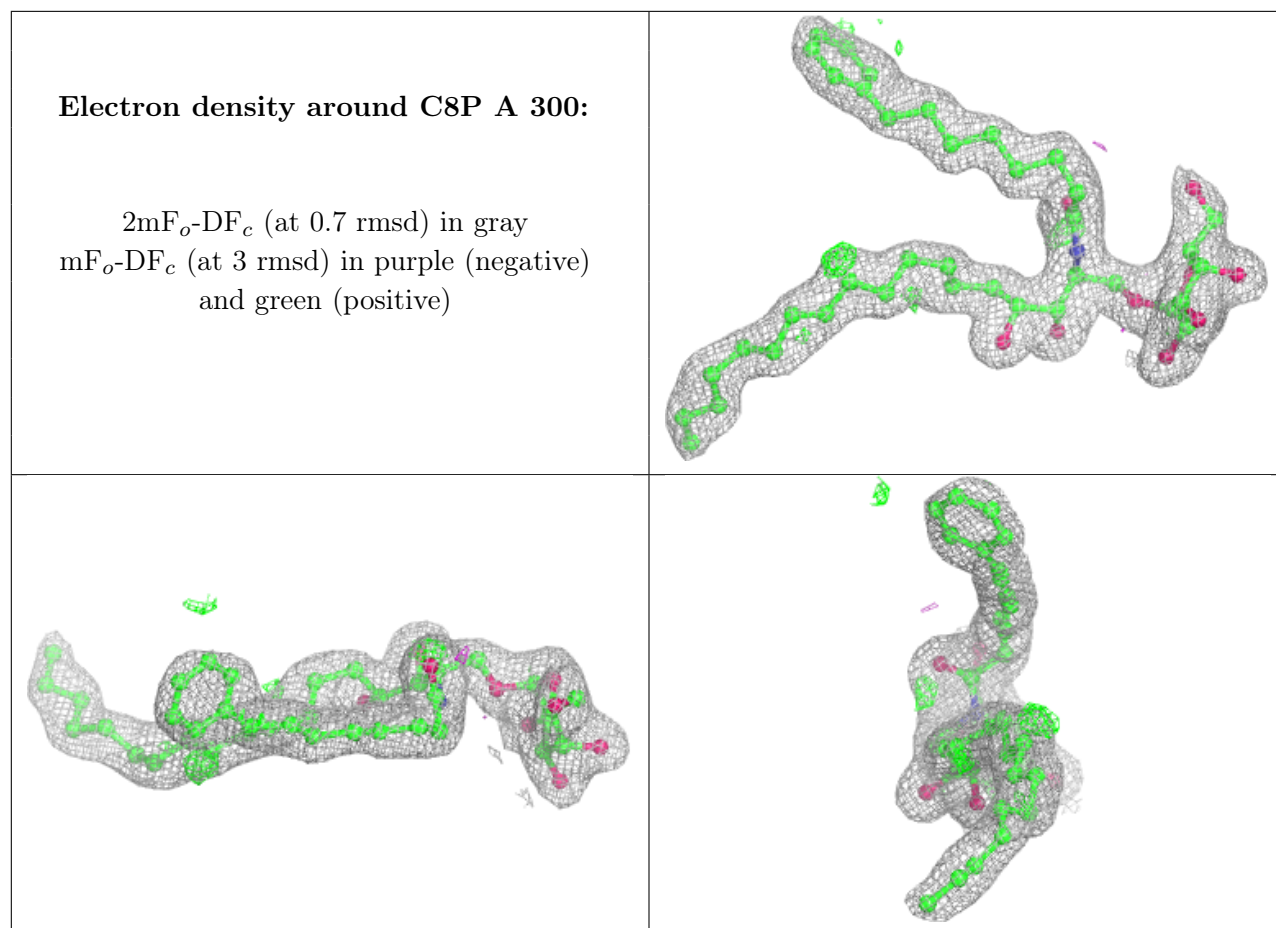and green (positive)

6.4 Ligands ⓘ

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
5	NAG	A	288	14/15	0.69	0.46	59,66,74,75	0
7	PLM	A	301	18/18	0.87	0.29	41,46,52,53	0
6	C8P	A	300	48/48	0.91	0.12	23,33,42,54	0
8	EDO	A	302	4/4	0.92	0.14	27,28,29,33	0
8	EDO	B	100	4/4	0.95	0.13	22,28,30,32	0
8	EDO	A	303	4/4	0.96	0.12	24,34,36,45	0
8	EDO	B	101[A]	4/4	0.97	0.14	30,31,31,38	4
8	EDO	B	101[B]	4/4	0.97	0.14	21,22,25,29	4

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 PLM A 301:

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

Electron density around C8P A 300:

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 ⓘ

There are no such residues in this entry.