



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:37 AM EDT

PDB ID : 2Q7Y
Title : Structure of the endogenous iNKT cell ligand iGb3 bound to mCD1d
Authors : Zajonc, D.M.; Wilson, I.A.; Teyton, L.
Deposited on : 2007-06-07
Resolution : 1.95 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 : 4.02b-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

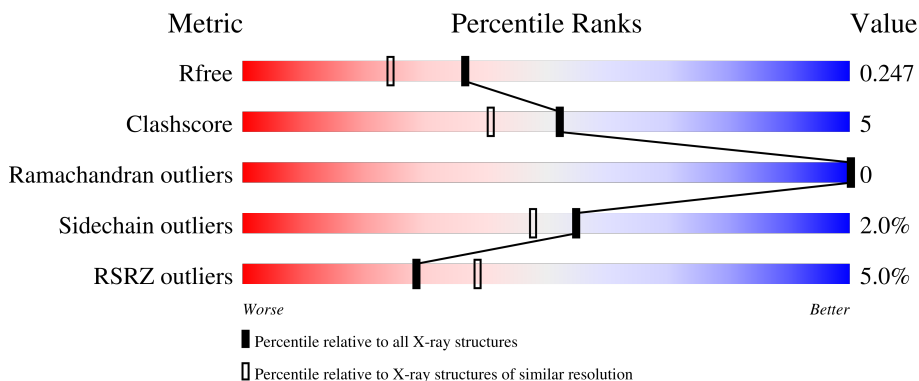
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



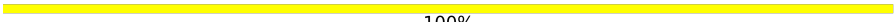

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	285	 6% 78% 16% • 6%
1	C	285	 5% 82% 12% • 6%
2	B	99	 2% 83% 14% ••
2	D	99	 2% 85% 13% ••
3	E	2	 100%

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
4	F	5	 20% 80%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6589 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	269	2165	1381	372	399	13	0	0	0
1	C	269	2165	1381	372	399	13	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
A	280	HIS	-	expression tag	UNP P11609
A	281	HIS	-	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
C	201	HIS	ASP	conflict	UNP P11609
C	280	HIS	-	expression tag	UNP P11609
C	281	HIS	-	expression tag	UNP P11609
C	282	HIS	-	expression tag	UNP P11609
C	283	HIS	-	expression tag	UNP P11609
C	284	HIS	-	expression tag	UNP P11609
C	285	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	98	810	517	137	149	7	0	0	0
2	D	98	810	517	137	149	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

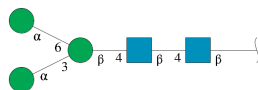
Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	variant	UNP P01887
D	85	ALA	ASP	variant	UNP P01887

- 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
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



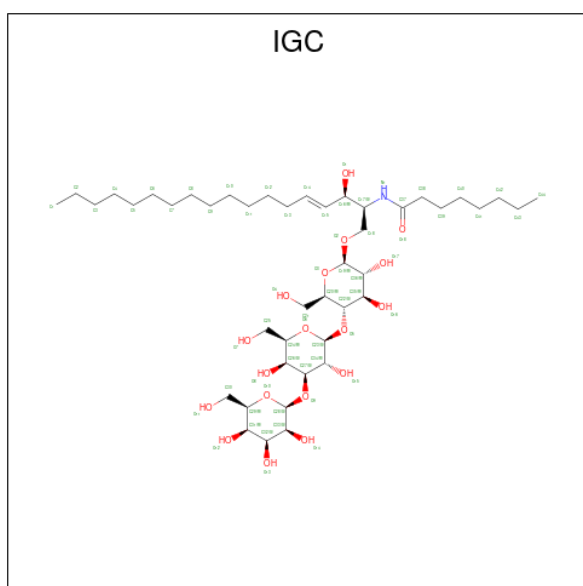
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	5	61	34	2	25	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



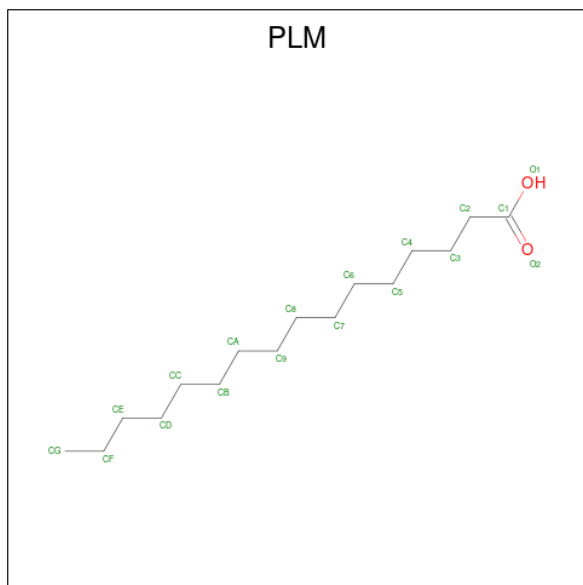
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0

- Molecule 6 is N-[(1S,2R,3E)-1-({[ALPHA-D-GALACTOPYRANOSYL-(1->3)-BETA-D-GALACTOPYRANOSYL-(1->4)-BETA-D-GLUCOPYRANOSYL]OXY}METHYL)-2-H YDROXYHEPTADEC-3-EN-1-YL]OCTANAMIDE (three-letter code: IGC) (formula: $C_{44}H_{81}NO_{18}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			41	32	1	8		
6	C	1	Total	C	N	O	0	0
			52	38	1	13		

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



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

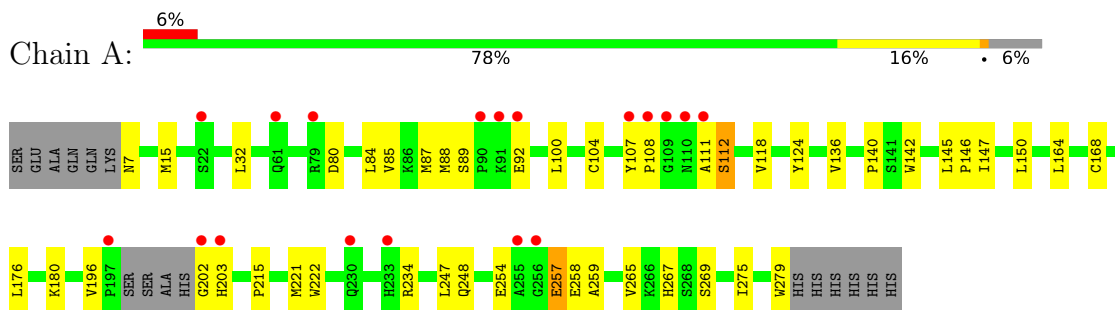
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	96	Total	O	0	0
			96	96		
8	B	52	Total	O	0	0
			52	52		
8	C	145	Total	O	0	0
			145	145		
8	D	58	Total	O	0	0
			58	58		

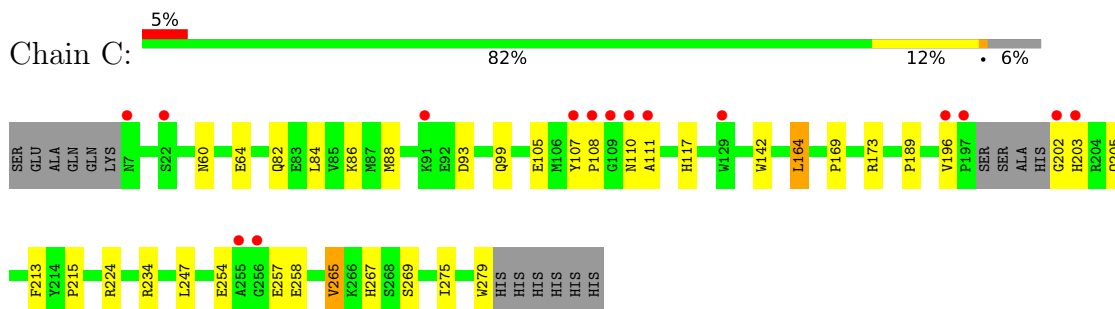
3 Residue-property plots [i](#)

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.

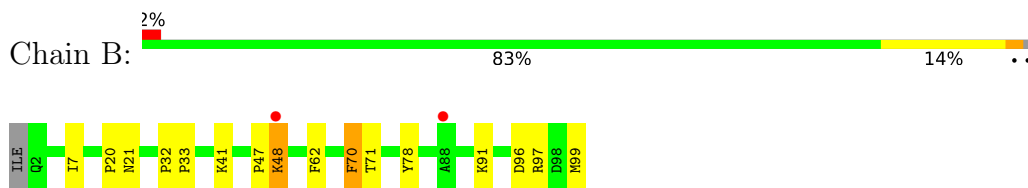
- Molecule 1: T-cell surface glycoprotein CD1d1



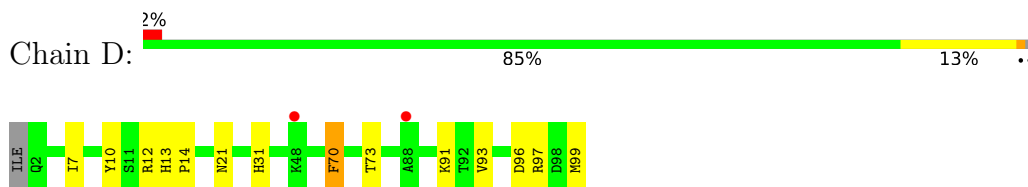
- Molecule 1: T-cell surface glycoprotein CD1d1



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




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

Chain E:  100%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  20% 80%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.94Å 96.22Å 77.93Å 90.00° 106.23° 90.00°	Depositor
Resolution (Å)	27.91 – 1.95 27.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (27.91-1.95) 97.5 (27.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.245 0.198 , 0.247	Depositor DCC
R_{free} test set	1219 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6589	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9034e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BMA, NAG, PLM, MAN, IGC

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	0.72	4/2228 (0.2%)	0.75	1/3028 (0.0%)
1	C	0.72	1/2228 (0.0%)	0.75	1/3028 (0.0%)
2	B	0.67	0/836	0.75	0/1133
2	D	0.76	0/836	0.89	2/1133 (0.2%)
All	All	0.72	5/6128 (0.1%)	0.77	4/8322 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLY	N-CA	9.46	1.60	1.46
1	C	202	GLY	N-CA	8.54	1.58	1.46
1	A	257	GLU	CD-OE2	7.72	1.34	1.25
1	A	257	GLU	CD-OE1	6.06	1.32	1.25
1	A	259	ALA	C-N	5.44	1.42	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	112	SER	N-CA-C	5.74	126.49	111.00
2	D	12	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	164	LEU	CB-CG-CD1	5.47	120.30	111.00

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	2165	0	2073	31	0
1	C	2165	0	2071	19	0
2	B	810	0	783	10	0
2	D	810	0	783	8	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
4	F	61	0	52	0	0
5	A	14	0	13	0	0
5	C	28	0	26	0	0
6	A	41	0	60	0	0
6	C	52	0	70	3	0
7	A	18	0	31	0	0
7	C	18	0	31	0	0
8	A	96	0	0	0	0
8	B	52	0	0	0	0
8	C	145	0	0	0	0
8	D	58	0	0	0	0
All	All	6589	0	6043	67	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 5.

All (67) 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:111:ALA:O	1:A:112:SER:HB3	1.59	1.02
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.48	0.92
2:D:7:ILE:HD12	2:D:91:LYS:HD3	1.52	0.92
6:C:602:IGC:H23	6:C:602:IGC:O16	1.77	0.85
2:D:96:ASP:O	2:D:96:ASP:OD1	1.94	0.83
2:B:96:ASP:OD1	2:B:96:ASP:O	2.05	0.75
1:A:221:MET:HE3	1:A:222:TRP:O	1.86	0.74
1:C:258:GLU:HB3	1:C:279:TRP:CD1	2.23	0.73
1:C:110:ASN:HA	1:C:173:ARG:NH2	2.05	0.71
1:A:88:MET:HE3	1:A:146:PRO:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.77	0.66
2:B:47:PRO:HG2	2:B:48:LYS:HD3	1.78	0.63
1:A:100:LEU:HG	1:A:118:VAL:HG22	1.81	0.63
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.64	0.62
1:C:107:TYR:HB3	1:C:108:PRO:HD2	1.82	0.61
1:C:107:TYR:HB2	1:C:111:ALA:HB3	1.81	0.60
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.27	0.60
2:D:7:ILE:CD1	2:D:91:LYS:HD3	2.28	0.60
1:C:60:ASN:O	1:C:64:GLU:HG2	2.02	0.59
1:A:32:LEU:HD21	1:A:176:LEU:HD23	1.83	0.58
1:A:215:PRO:O	1:A:267:HIS:HE1	1.86	0.58
2:D:10:TYR:HB3	2:D:99:MET:HG2	1.86	0.58
2:B:20:PRO:HA	2:B:71:THR:HG22	1.89	0.55
1:A:267:HIS:HD2	1:A:269:SER:OG	1.90	0.55
1:C:265:VAL:HG13	1:C:275:ILE:HB	1.89	0.54
1:A:147:ILE:HD13	1:A:150:LEU:HD12	1.89	0.54
1:A:254:GLU:O	1:A:257:GLU:HB3	2.07	0.54
1:A:87:MET:HG2	1:A:88:MET:HE2	1.91	0.53
1:A:111:ALA:O	1:A:112:SER:CB	2.38	0.52
1:A:267:HIS:CD2	1:A:269:SER:H	2.28	0.52
1:C:267:HIS:CD2	1:C:269:SER:H	2.27	0.52
1:A:104:CYS:SG	1:A:168:CYS:SG	3.08	0.52
1:A:92:GLU:HG3	1:A:142:TRP:CE2	2.46	0.51
1:A:258:GLU:HB3	1:A:279:TRP:CD1	2.47	0.50
1:C:215:PRO:O	1:C:267:HIS:HE1	1.93	0.50
1:A:203:HIS:CD2	1:A:254:GLU:HG2	2.47	0.50
1:C:88:MET:HE1	1:C:142:TRP:HB2	1.93	0.50
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.47	0.49
1:C:189:PRO:HB3	1:C:213:PHE:HB3	1.94	0.49
1:C:82:GLN:O	1:C:86:LYS:HG3	2.13	0.49
1:A:248:GLN:OE1	2:B:99:MET:SD	2.71	0.49
1:A:85:VAL:O	1:A:89:SER:HB2	2.14	0.48
2:B:96:ASP:C	2:B:97:ARG:HG3	2.32	0.48
1:C:196:VAL:HG23	1:C:205:GLN:HB3	1.94	0.48
1:C:203:HIS:NE2	1:C:254:GLU:HG2	2.29	0.47
1:A:80:ASP:O	1:A:84:LEU:HG	2.14	0.47
1:A:221:MET:CE	1:A:222:TRP:O	2.62	0.47
1:C:267:HIS:HD2	1:C:269:SER:OG	1.98	0.45
1:A:107:TYR:O	1:A:111:ALA:HB2	2.16	0.45
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.52	0.45
1:C:224:ARG:NH2	1:C:257:GLU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:THR:O	2:D:97:ARG:NH2	2.50	0.44
2:B:41:LYS:HG3	2:B:78:TYR:CE2	2.52	0.44
1:A:265:VAL:HB	1:A:275:ILE:HB	2.00	0.44
6:C:602:IGC:O16	6:C:602:IGC:C23	2.59	0.43
1:A:234:ARG:HG2	1:A:247:LEU:HD11	2.01	0.42
1:A:221:MET:HE2	1:A:221:MET:HB3	1.91	0.42
1:A:140:PRO:HB2	1:A:142:TRP:CD1	2.55	0.42
1:A:88:MET:HE1	1:A:145:LEU:HB3	2.02	0.42
1:C:99:GLN:OE1	2:D:31:HIS:HE1	2.01	0.42
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.54	0.42
1:C:84:LEU:HD23	6:C:602:IGC:H22A	2.02	0.41
2:D:13:HIS:HB3	2:D:14:PRO:HD2	2.02	0.41
1:A:92:GLU:HG3	1:A:142:TRP:CZ2	2.56	0.41
1:C:169:PRO:O	1:C:173:ARG:HG2	2.20	0.40
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.03	0.40
1:C:234:ARG:CG	1:C:247:LEU:HD11	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	265/285 (93%)	259 (98%)	6 (2%)	0	100	100
1	C	265/285 (93%)	261 (98%)	4 (2%)	0	100	100
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	D	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
All	All	722/768 (94%)	708 (98%)	14 (2%)	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	235/249 (94%)	231 (98%)	4 (2%)	60	55
1	C	235/249 (94%)	230 (98%)	5 (2%)	53	46
2	B	92/93 (99%)	90 (98%)	2 (2%)	52	44
2	D	92/93 (99%)	90 (98%)	2 (2%)	52	44
All	All	654/684 (96%)	641 (98%)	13 (2%)	55	48

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	164	LEU
1	A	180	LYS
1	A	196	VAL
2	B	48	LYS
2	B	70	PHE
1	C	93	ASP
1	C	105	GLU
1	C	117	HIS
1	C	164	LEU
1	C	265	VAL
2	D	70	PHE
2	D	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	267	HIS
1	C	267	HIS
2	D	31	HIS

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
3	NAG	E	1	1,3	14,14,15	0.70	0	17,19,21	1.09	1 (5%)
3	NAG	E	2	3	14,14,15	0.64	0	17,19,21	1.74	4 (23%)
4	NAG	F	1	4,1	14,14,15	0.69	0	17,19,21	1.15	2 (11%)
4	NAG	F	2	4	14,14,15	0.57	0	17,19,21	1.19	1 (5%)
4	BMA	F	3	4	11,11,12	0.63	0	15,15,17	0.87	0
4	MAN	F	4	4	11,11,12	0.52	0	15,15,17	1.18	1 (6%)
4	MAN	F	5	4	11,11,12	0.45	0	15,15,17	1.19	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.82	0	17,19,21	0.96	2 (11%)
3	NAG	G	2	3	14,14,15	0.59	0	17,19,21	1.32	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
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C5-C6	4.23	113.84	107.20
3	G	2	NAG	C1-O5-C5	3.90	117.47	112.19
4	F	4	MAN	C1-O5-C5	3.76	117.28	112.19
4	F	5	MAN	C1-O5-C5	3.67	117.17	112.19
4	F	2	NAG	O5-C5-C6	3.64	112.91	107.20
3	E	2	NAG	C2-N2-C7	2.92	127.06	122.90
3	G	2	NAG	C2-N2-C7	-2.90	118.77	122.90
3	E	2	NAG	C3-C4-C5	-2.69	105.44	110.24
4	F	1	NAG	O5-C5-C6	2.40	110.97	107.20
4	F	1	NAG	C1-C2-N2	2.33	114.47	110.49
3	E	2	NAG	O7-C7-N2	2.21	126.01	121.95
3	G	1	NAG	C1-C2-N2	2.15	114.16	110.49
3	E	1	NAG	C4-C3-C2	2.14	114.16	111.02
3	G	1	NAG	O5-C1-C2	-2.13	107.92	111.29

There are no chirality outliers.

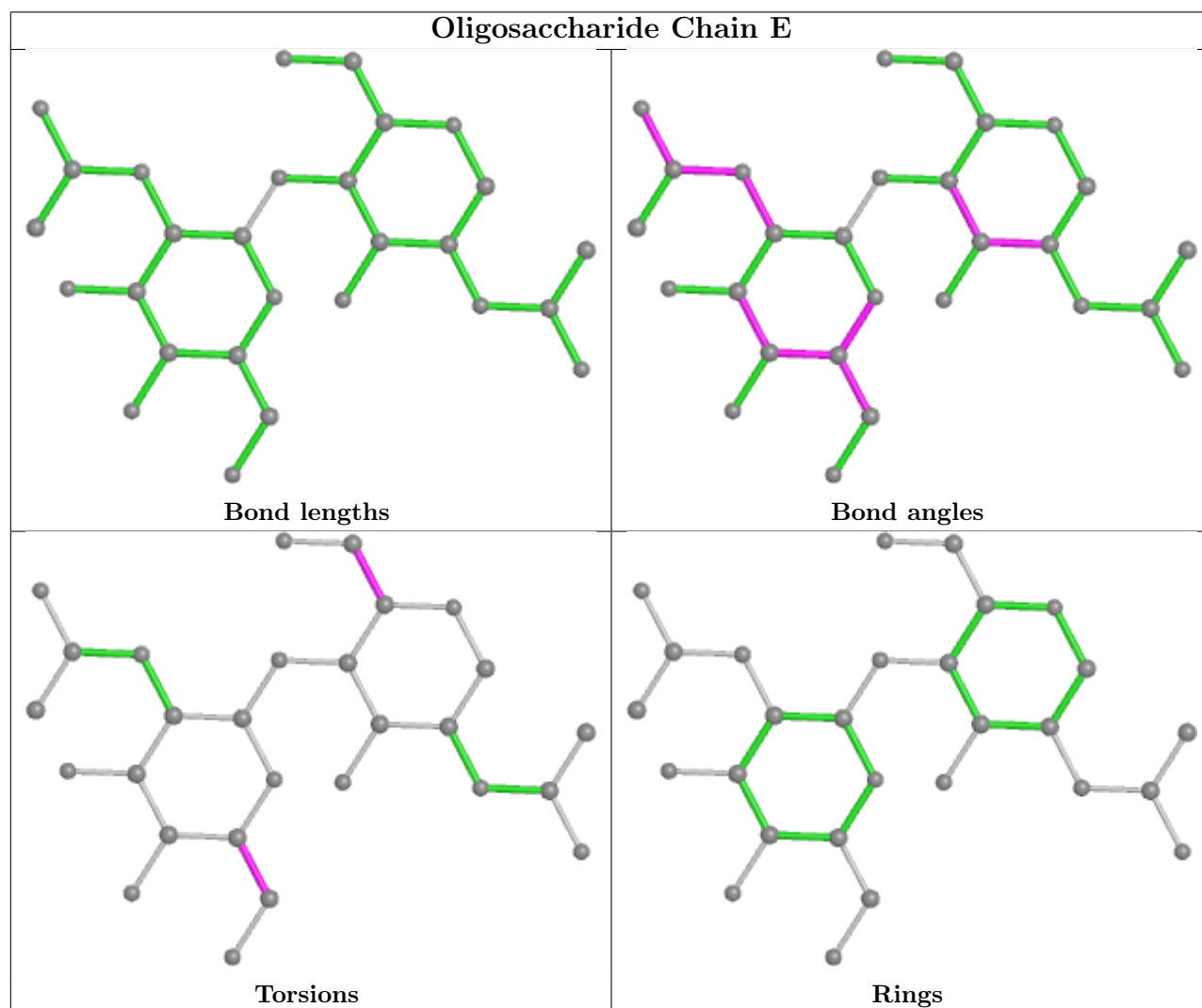
All (8) torsion outliers are listed below:

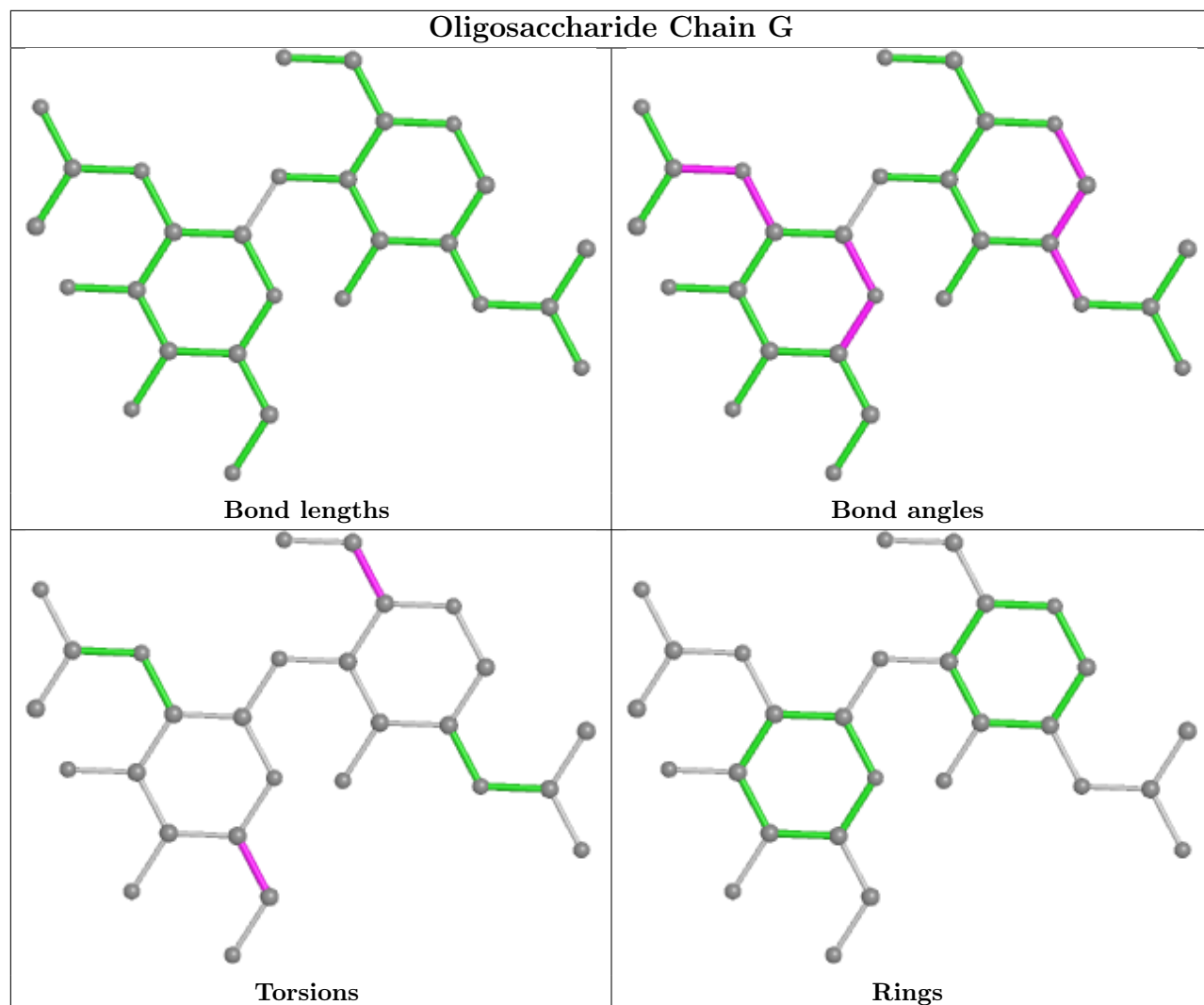
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

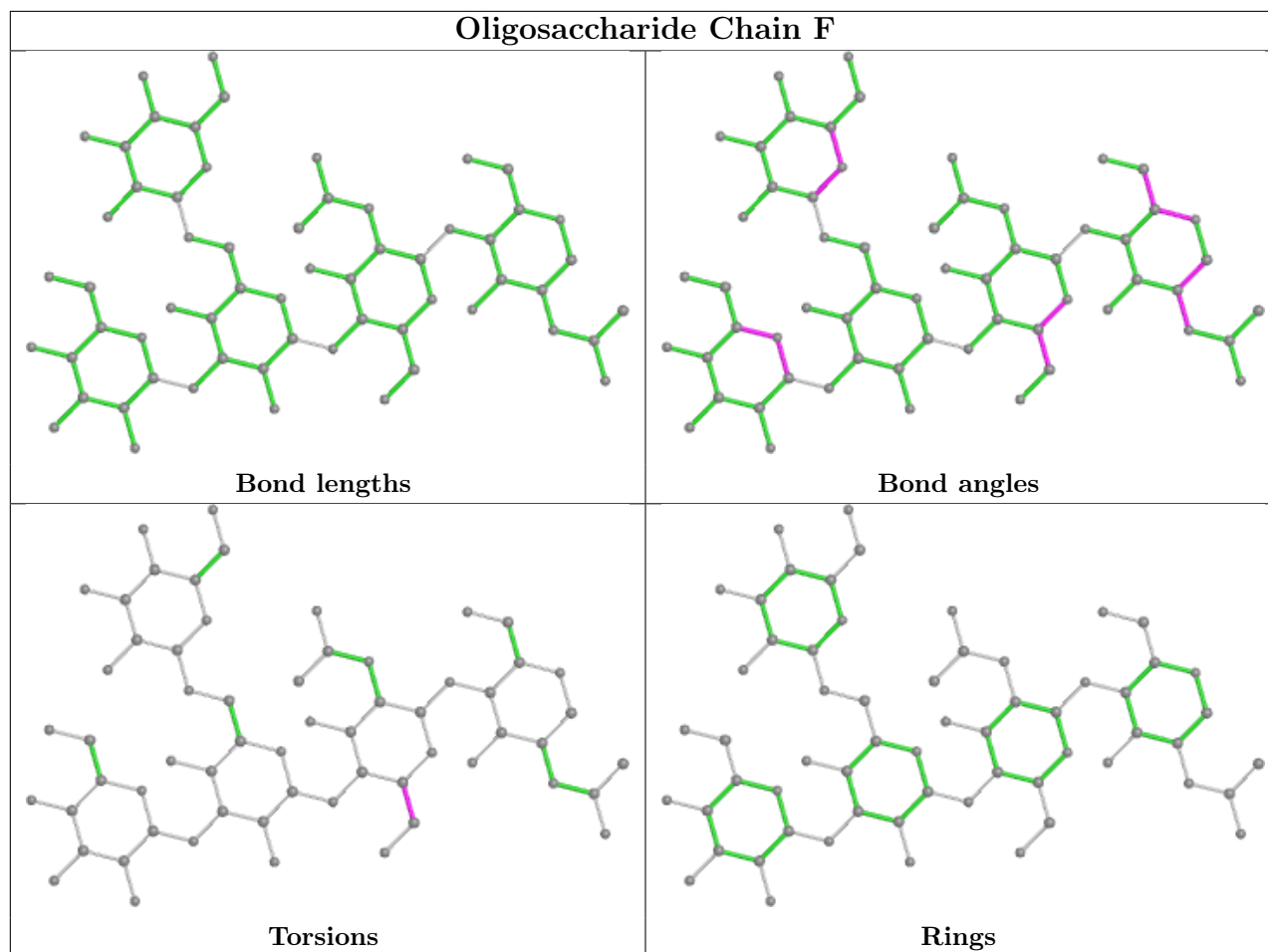
There are no ring outliers.

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](#)

7 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$
5	NAG	C	500	1	14,14,15	0.57	0	17,19,21	1.03	2 (11%)
6	IGC	A	601	-	40,41,65	1.20	4 (10%)	47,49,85	1.72	3 (6%)
7	PLM	C	702	-	17,17,17	0.75	0	17,17,17	0.79	1 (5%)
6	IGC	C	602	-	52,53,65	1.43	8 (15%)	65,67,85	1.22	7 (10%)
5	NAG	C	501	1	14,14,15	0.66	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PLM	A	701	-	17,17,17	0.77	1 (5%)	17,17,17	0.76	0
5	NAG	A	500	1	14,14,15	0.62	0	17,19,21	1.32	4 (23%)

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
5	NAG	C	500	1	-	4/6/23/26	0/1/1/1
6	IGC	A	601	-	-	12/37/57/109	0/1/1/3
7	PLM	C	702	-	-	9/15/15/15	-
6	IGC	C	602	-	-	18/43/83/109	0/2/2/3
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
7	PLM	A	701	-	-	10/15/15/15	-
5	NAG	A	500	1	-	3/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	IGC	O2-C19	5.45	1.49	1.40
6	A	601	IGC	O2-C19	4.57	1.48	1.40
6	C	602	IGC	O6-C23	3.01	1.49	1.41
6	C	602	IGC	O3-C19	2.57	1.48	1.41
6	C	602	IGC	C18-C17	2.52	1.56	1.51
6	C	602	IGC	O3-C20	2.47	1.50	1.44
6	C	602	IGC	C16-C15	2.16	1.53	1.50
6	C	602	IGC	C15-C14	2.12	1.40	1.31
6	A	601	IGC	O3-C19	2.10	1.47	1.41
7	A	701	PLM	C2-C1	2.07	1.55	1.50
6	A	601	IGC	C38-C37	2.04	1.55	1.51
6	C	602	IGC	O5-C23	2.04	1.47	1.41
6	A	601	IGC	C13-C14	-2.02	1.38	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	IGC	O2-C19-C36	9.11	122.53	108.30
6	A	601	IGC	C16-C15-C14	-5.00	113.64	124.79
6	C	602	IGC	O5-C22-C35	3.67	117.04	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	IGC	C35-C22-C20	-3.56	102.75	110.93
6	C	602	IGC	O5-C23-C34	3.19	116.37	108.10
5	A	500	NAG	C1-C2-N2	3.08	115.75	110.49
5	C	501	NAG	O5-C1-C2	-2.99	106.57	111.29
6	C	602	IGC	O3-C20-C21	2.68	113.11	106.44
6	A	601	IGC	C18-C17-C16	-2.58	106.89	112.92
6	C	602	IGC	O1-C16-C15	-2.51	104.13	110.85
6	C	602	IGC	O6-C24-C25	2.48	112.60	106.44
5	A	500	NAG	C2-N2-C7	2.30	126.17	122.90
6	C	602	IGC	C19-C36-C35	2.11	114.39	110.00
5	A	500	NAG	O5-C1-C2	-2.10	107.97	111.29
5	C	500	NAG	O5-C5-C6	2.07	110.45	107.20
7	C	702	PLM	O2-C1-C2	-2.05	116.49	123.08
5	C	500	NAG	C1-O5-C5	2.05	114.97	112.19
5	C	501	NAG	C1-O5-C5	2.00	114.90	112.19
5	A	500	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	500	NAG	C8-C7-N2-C2
5	A	500	NAG	O7-C7-N2-C2
5	C	500	NAG	C8-C7-N2-C2
5	C	500	NAG	O7-C7-N2-C2
6	C	602	IGC	C15-C16-C17-C18
6	C	602	IGC	C15-C16-C17-N1
6	C	602	IGC	O1-C16-C17-C18
6	C	602	IGC	O1-C16-C17-N1
6	C	602	IGC	C35-C22-O5-C23
6	C	602	IGC	O3-C20-C21-O4
6	C	602	IGC	C22-C20-C21-O4
6	A	601	IGC	C36-C19-O2-C18
5	A	500	NAG	C1-C2-N2-C7
7	A	701	PLM	C5-C6-C7-C8
7	C	702	PLM	CC-CD-CE-CF
7	C	702	PLM	CA-CB-CC-CD
6	A	601	IGC	C4-C5-C6-C7
7	C	702	PLM	C6-C7-C8-C9
7	C	702	PLM	C2-C3-C4-C5
6	A	601	IGC	C5-C6-C7-C8
6	A	601	IGC	C7-C8-C9-C10

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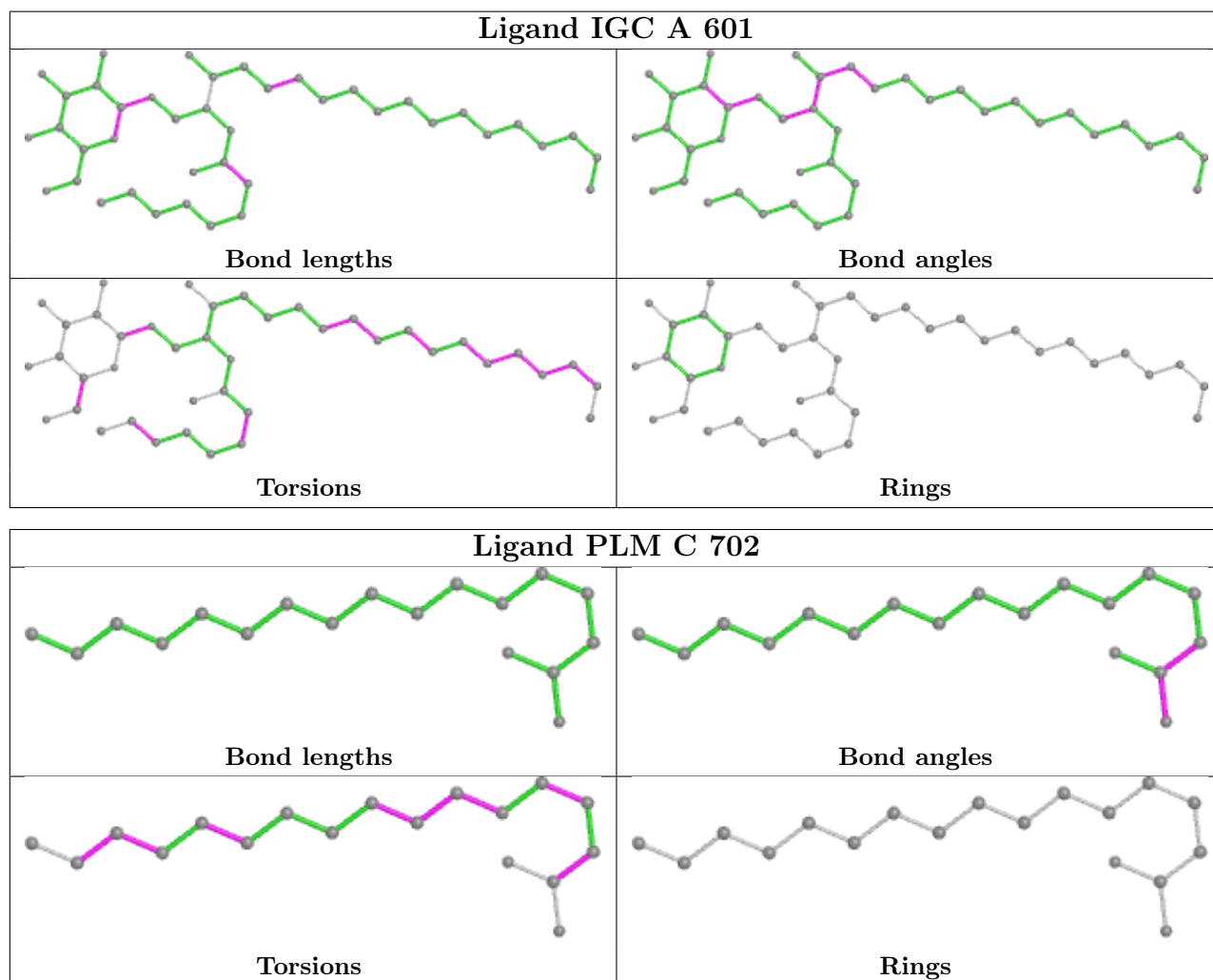
Mol	Chain	Res	Type	Atoms
6	C	602	IGC	C9-C10-C11-C12
7	C	702	PLM	C5-C6-C7-C8
6	C	602	IGC	O6-C24-C25-O7
6	A	601	IGC	C3-C4-C5-C6
7	A	701	PLM	C4-C5-C6-C7
7	A	701	PLM	CC-CD-CE-CF
6	C	602	IGC	C10-C11-C12-C13
6	A	601	IGC	C9-C10-C11-C12
7	A	701	PLM	C7-C8-C9-CA
6	A	601	IGC	C1-C2-C3-C4
6	C	602	IGC	C7-C8-C9-C10
7	A	701	PLM	CA-CB-CC-CD
6	C	602	IGC	C41-C42-C43-C44
7	A	701	PLM	C6-C7-C8-C9
7	C	702	PLM	C4-C5-C6-C7
5	C	500	NAG	C4-C5-C6-O6
7	A	701	PLM	C9-CA-CB-CC
6	C	602	IGC	C6-C7-C8-C9
7	A	701	PLM	C2-C3-C4-C5
6	C	602	IGC	C14-C15-C16-C17
7	C	702	PLM	O2-C1-C2-C3
6	A	601	IGC	C10-C11-C12-C13
7	A	701	PLM	O2-C1-C2-C3
6	C	602	IGC	C40-C41-C42-C43
6	C	602	IGC	C14-C15-C16-O1
7	A	701	PLM	O1-C1-C2-C3
7	C	702	PLM	O1-C1-C2-C3
6	A	601	IGC	C37-C38-C39-C40
6	A	601	IGC	C41-C42-C43-C44
6	A	601	IGC	C2-C3-C4-C5
6	C	602	IGC	C12-C13-C14-C15
6	C	602	IGC	C20-C22-O5-C23
5	C	500	NAG	O5-C5-C6-O6
7	C	702	PLM	CD-CE-CF-CG
6	A	601	IGC	O3-C20-C21-O4

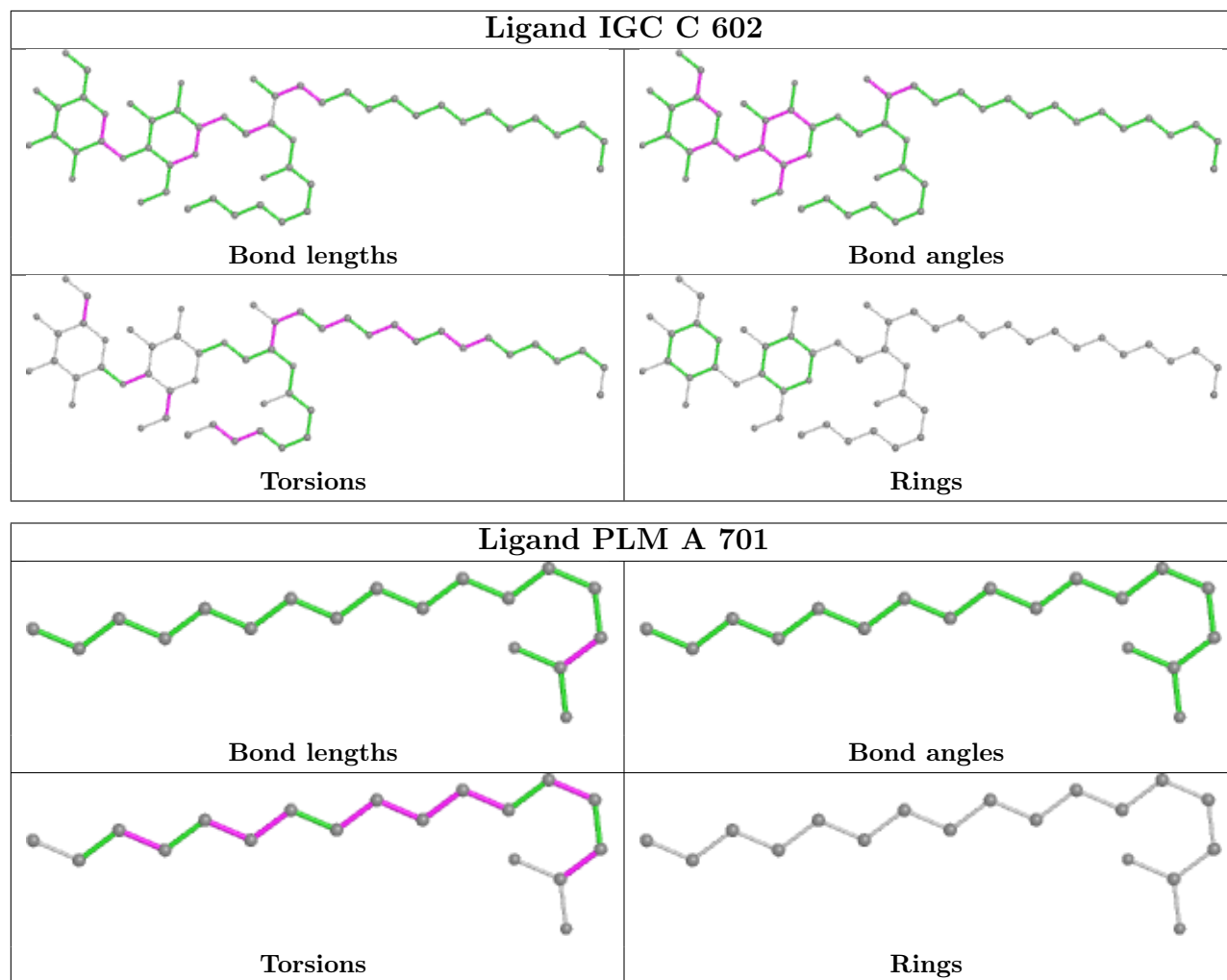
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	IGC	3	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

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	269/285 (94%)	0.36	18 (6%) 17 26	16, 30, 63, 91	0
1	C	269/285 (94%)	0.21	15 (5%) 24 33	15, 26, 55, 78	0
2	B	98/99 (98%)	0.07	2 (2%) 65 73	18, 31, 50, 57	0
2	D	98/99 (98%)	-0.05	2 (2%) 65 73	15, 27, 45, 57	0
All	All	734/768 (95%)	0.21	37 (5%) 28 39	15, 28, 57, 91	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	7.6
1	C	110	ASN	6.6
1	A	255	ALA	6.2
1	C	108	PRO	5.7
1	C	109	GLY	5.7
1	A	202	GLY	5.1
1	A	108	PRO	5.1
1	A	109	GLY	5.0
1	A	110	ASN	4.9
1	C	255	ALA	4.8
1	C	107	TYR	4.4
2	B	48	LYS	4.2
1	C	197	PRO	4.0
1	A	107	TYR	3.9
1	A	203	HIS	3.8
1	A	197	PRO	3.8
1	A	256	GLY	3.8
1	C	203	HIS	3.5
1	C	111	ALA	3.1
2	D	48	LYS	3.1
1	A	230	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	22	SER	3.0
1	A	91	LYS	2.9
1	A	22	SER	2.9
1	C	196	VAL	2.8
1	C	129	TRP	2.8
2	B	88	ALA	2.8
1	A	233	HIS	2.7
1	C	7	ASN	2.6
1	A	92	GLU	2.6
1	C	202	GLY	2.5
1	A	90	PRO	2.4
1	C	256	GLY	2.2
1	A	79	ARG	2.1
2	D	88	ALA	2.1
1	A	61	GLN	2.0
1	C	91	LYS	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](#)

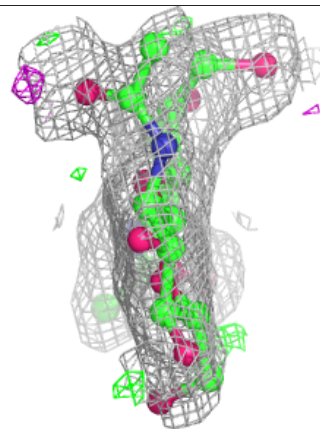
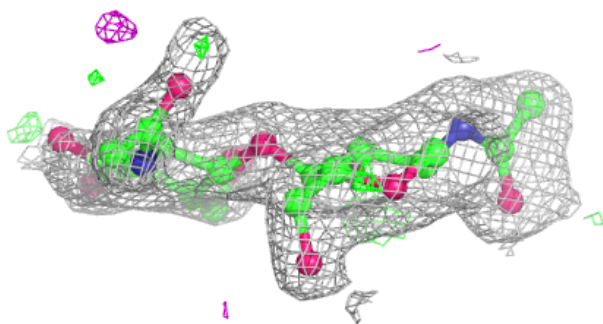
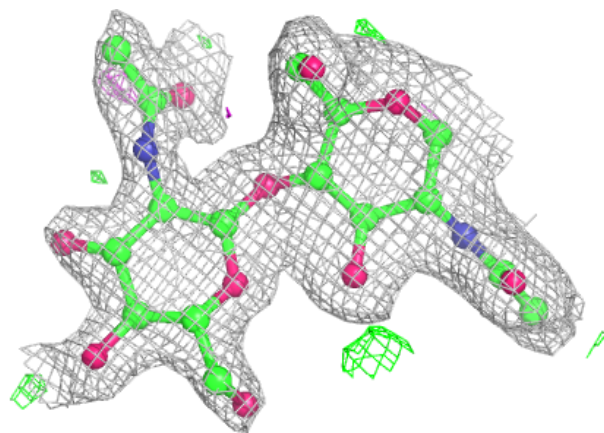
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	BMA	F	3	11/12	0.80	0.27	48,55,61,66	0
3	NAG	E	2	14/15	0.81	0.36	50,55,59,60	0
3	NAG	G	1	14/15	0.82	0.12	32,36,41,41	0
4	MAN	F	4	11/12	0.83	0.28	68,71,76,79	0
3	NAG	G	2	14/15	0.86	0.25	48,51,59,60	0
4	NAG	F	2	14/15	0.86	0.23	43,47,52,53	0
4	NAG	F	1	14/15	0.88	0.13	34,38,43,43	0
4	MAN	F	5	11/12	0.89	0.19	44,48,51,53	0
3	NAG	E	1	14/15	0.95	0.09	27,33,40,41	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.

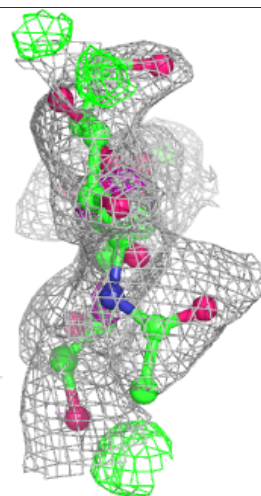
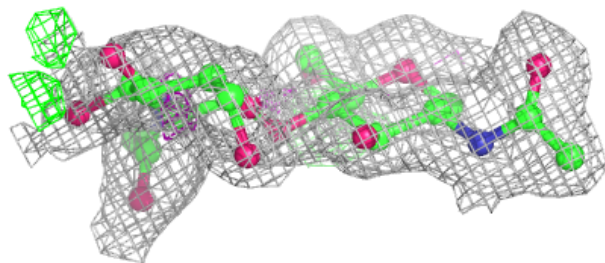
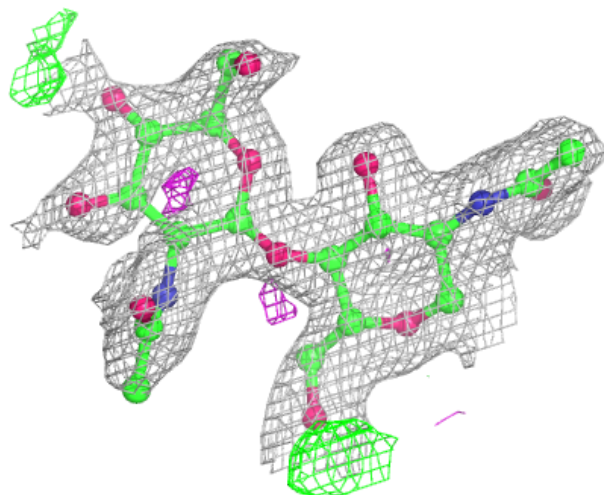
Electron density around Chain E:

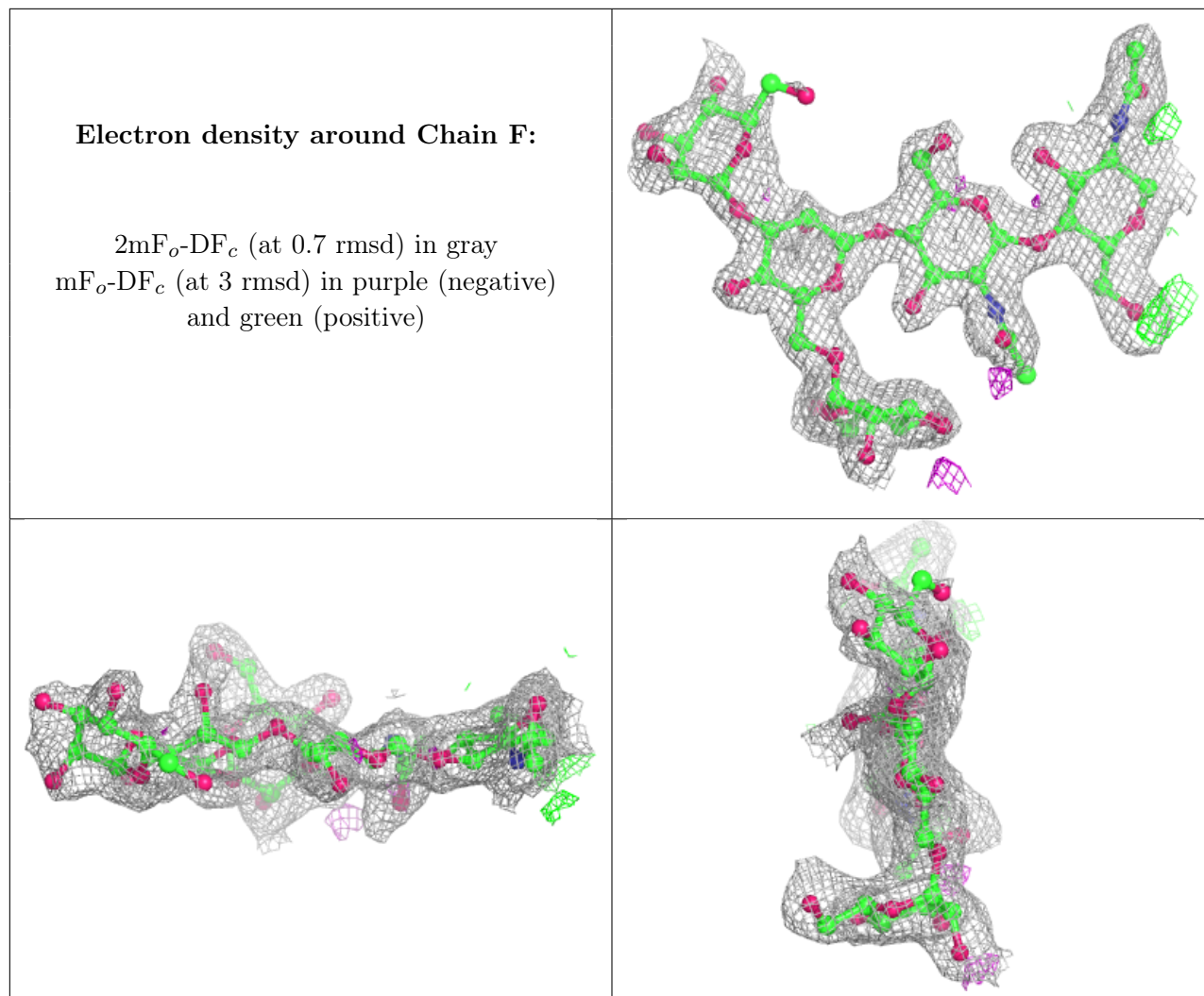
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





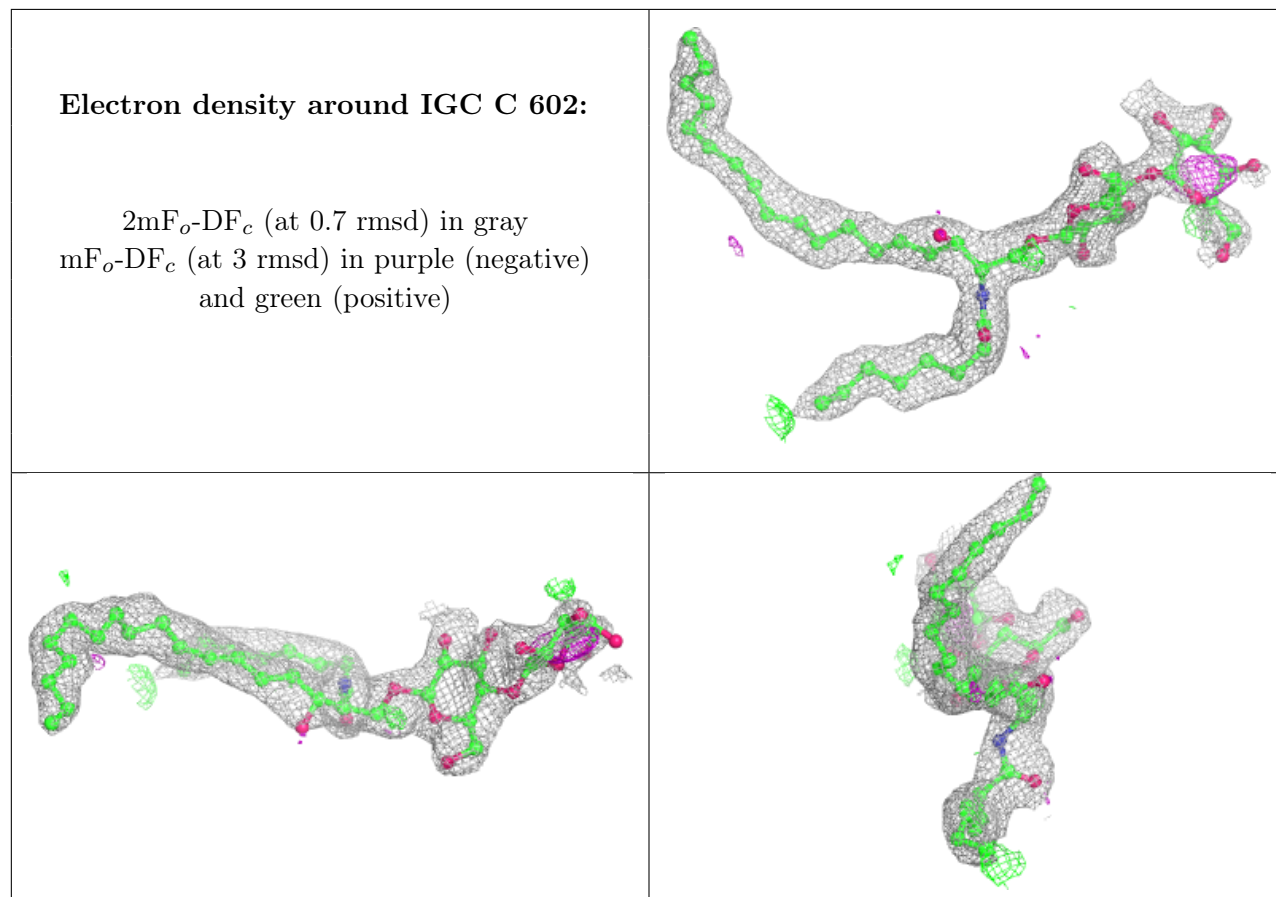
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
6	IGC	C	602	52/63	0.63	0.24	34,50,81,85	0
6	IGC	A	601	41/63	0.66	0.23	41,48,70,73	0
5	NAG	A	500	14/15	0.84	0.24	47,50,58,58	0
7	PLM	A	701	18/18	0.84	0.33	40,47,58,58	0
5	NAG	C	500	14/15	0.85	0.27	54,60,67,71	0
7	PLM	C	702	18/18	0.91	0.28	37,39,53,55	0
5	NAG	C	501	14/15	0.97	0.09	29,33,40,41	0

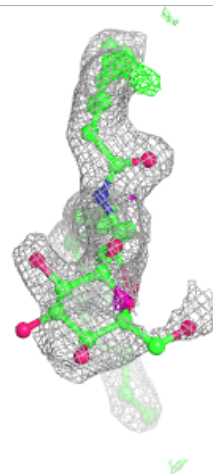
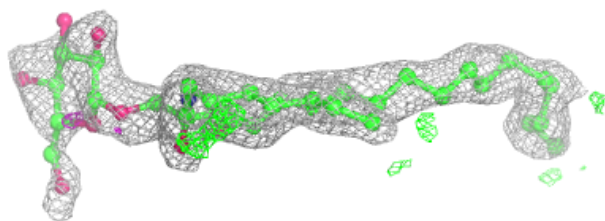
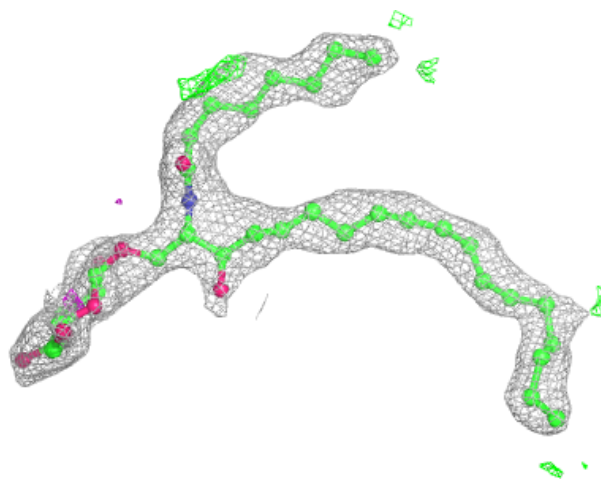
The following is a graphical depiction of the model fit to experimental electron density of all

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.



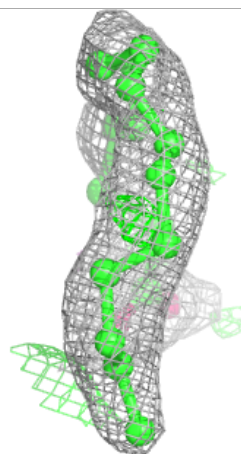
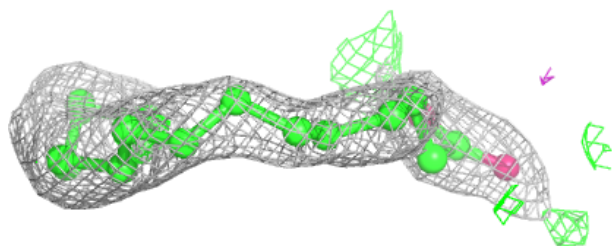
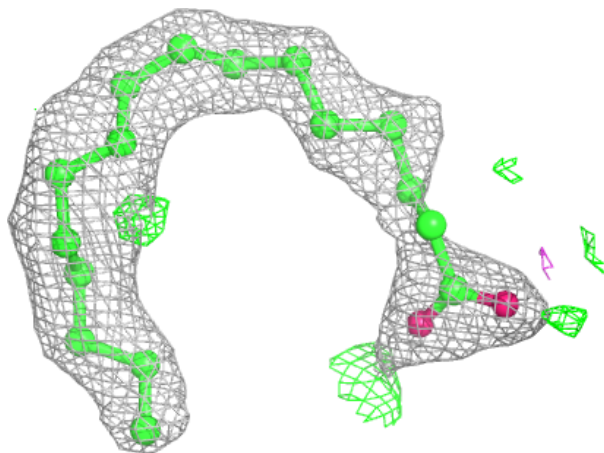
Electron density around IGC A 601:

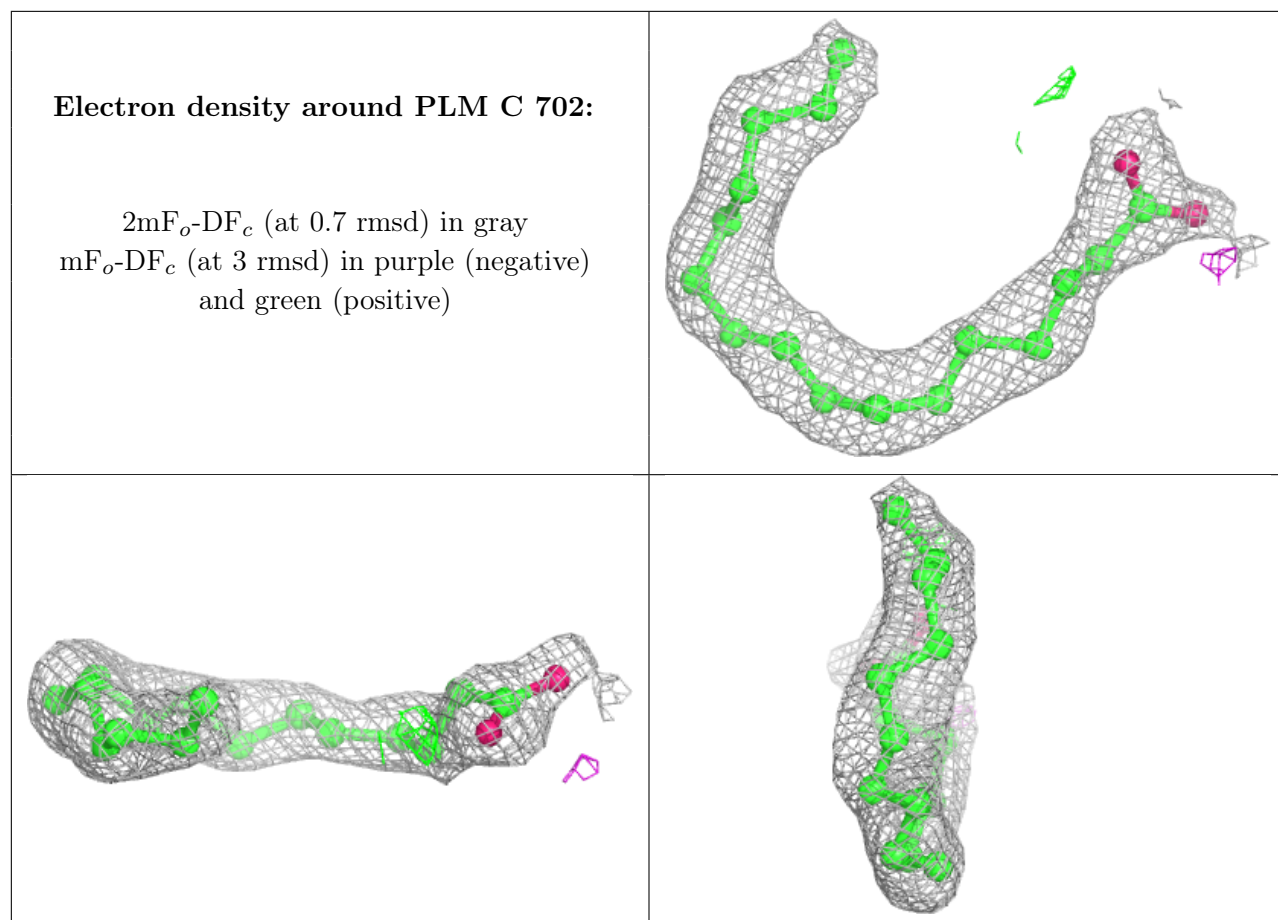
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLM A 701:

$2mF_o-DF_c$ (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.