Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 12:52 PM EDT

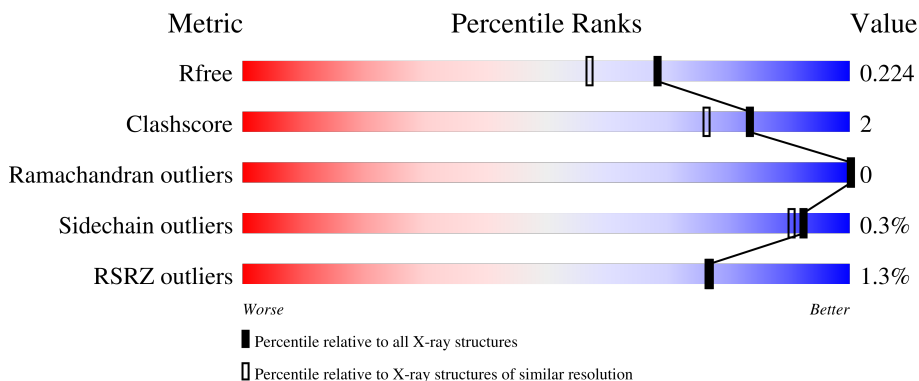|		
PDB ID	:	8GLH
Title	:	Crystal Structure of Human CD1b in Complex with Endogenous PC C40:5
Authors	:	Farquhar, R.; Rossjohn, J.; Shahine, A.
Deposited on	:	2023-03-22
Resolution	:	1.83 Å(reported)

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 1.83 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		0.224
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		1.3%

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	300	89% 5% 7%
2	B	101	92% 6% ··
3	C	7	29% 71%
4	D	5	60% 40%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 3660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2190	1403	373	404	10	3	4	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total 830	C 530	N 142	O 156	S 2	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 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-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyr anose.

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

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-aceta mido-2-deoxy-beta-D-glucopyranose.
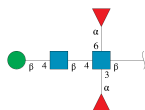
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total 59	C 34	N 2	O 23	0	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	I 1	0	0
5	B	2	Total 2	I 2	0	0

- Molecule 6 is (11E)-hexadec-11-enoic acid (three-letter code: 3IV) (formula: $C_{16}H_{30}O_2$) (labeled as "Ligand of Interest" by depositor).
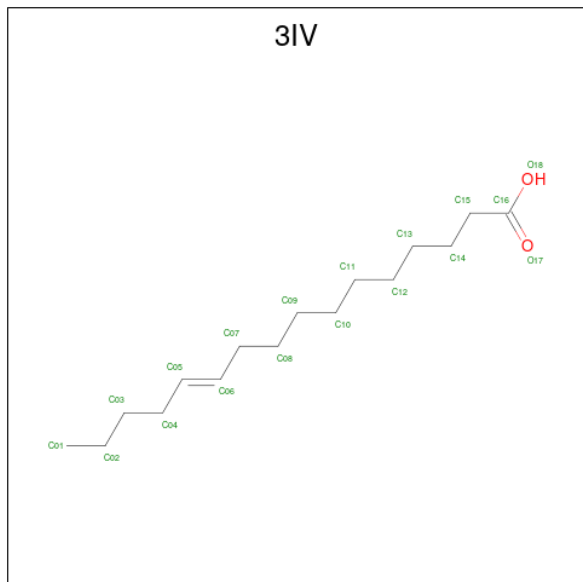
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 7 is [(2 {R})-1-dodecanoyloxy-3-[oxidanyl-[2-(trimethyl-l^{4}-azanyl)ethoxy]phosphoryl]oxy-propan-2-yl] (8 {Z},11 {Z},14 {Z},24 {Z},27 {Z})-triaconta-8,11,14,24,27-pentaenoate (three-letter code: 3IY) (formula: $C_{50}H_{91}NO_8P$) (labeled as "Ligand of Interest" by depositor).
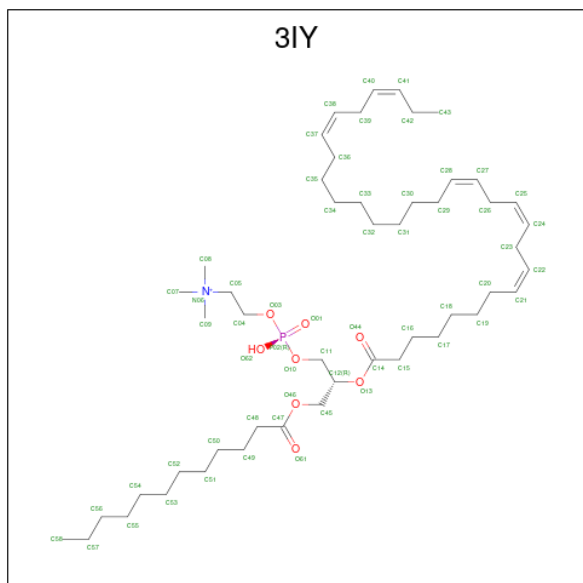
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 60	C 50	N 1	O 8	P 1	0	0

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

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	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	276	Total 276	O 276	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	126	Total 126	O 126	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
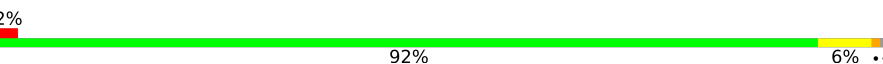
• Molecule 1: T-cell surface glycoprotein CD1b

Chain A:
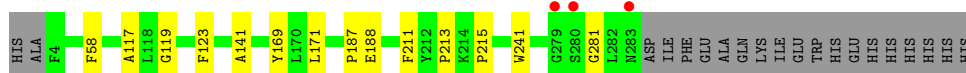
• Molecule 2: Beta-2-microglobulin

Chain B:
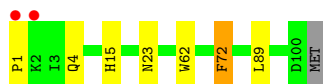
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: 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

Chain D:
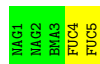
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.45Å 77.05Å 91.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.13 – 1.83 41.13 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.13-1.83) 99.8 (41.13-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.166 , 0.221 0.170 , 0.224	Depositor DCC
R_{free} test set	1820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3660	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: BMA, NAG, 3IV, NA, FUC, 3IY, MAN, IOD, EDO

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	0.39	0/2256	0.56	0/3064
2	B	0.40	0/854	0.58	0/1159
All	All	0.39	0/3110	0.57	0/4223

There are no bond length outliers.

There are no bond angle outliers.

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	2190	0	2095	12	0
2	B	830	0	783	8	0
3	C	81	0	70	1	0
4	D	59	0	52	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	18	0	0	0	0
7	A	60	0	0	0	0
8	A	16	0	24	0	0
9	B	1	0	0	0	0
10	A	276	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	126	0	0	2	0
All	All	3660	0	3024	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLY:HA3	2:B:1:PRO:HA	1.32	1.07
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.51	0.91
1:A:119:GLY:HA3	2:B:1:PRO:CA	2.09	0.82
2:B:89:LEU:O	10:B:301:HOH:O	2.16	0.62
1:A:119:GLY:CA	2:B:1:PRO:HA	2.18	0.62
1:A:188:GLU:OE2	2:B:15:HIS:ND1	2.30	0.60
1:A:281:GLY:HA2	10:A:1000:HOH:O	2.03	0.57
1:A:171:LEU:HD12	3:C:2:NAG:H82	1.88	0.55
2:B:4:GLN:OE1	10:B:302:HOH:O	2.18	0.55
1:A:117:ALA:HB2	2:B:62:TRP:CE2	2.51	0.45
2:B:23:ASN:HB3	2:B:72:PHE:CE2	2.52	0.45
1:A:123:PHE:CZ	1:A:141:ALA:HA	2.54	0.43
1:A:241:TRP:N	1:A:241:TRP:CD1	2.87	0.42
1:A:213:PRO:HB2	1:A:215:PRO:HD2	2.02	0.42
1:A:58:PHE:CZ	1:A:169:TYR:HB2	2.56	0.41

There are no symmetry-related clashes.

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	282/300 (94%)	278 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	100/101 (99%)	99 (99%)	1 (1%)	0	100	100
All	All	382/401 (95%)	377 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	227/247 (92%)	227 (100%)	0	100	100
2	B	92/96 (96%)	91 (99%)	1 (1%)	73	64
All	All	319/343 (93%)	318 (100%)	1 (0%)	92	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	72	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	C	1	1,3	14,14,15	0.33	0	17,19,21	1.03	1 (5%)
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	0.61	0
3	BMA	C	3	3	11,11,12	1.01	1 (9%)	15,15,17	0.93	1 (6%)
3	MAN	C	4	3	11,11,12	0.78	0	15,15,17	1.02	1 (6%)
3	MAN	C	5	3	11,11,12	0.77	0	15,15,17	0.97	2 (13%)
3	FUC	C	6	3	10,10,11	0.84	0	14,14,16	0.86	0
3	FUC	C	7	3	10,10,11	0.87	0	14,14,16	0.90	0
4	NAG	D	1	4,1	14,14,15	0.49	0	17,19,21	0.43	0
4	NAG	D	2	4	14,14,15	0.35	0	17,19,21	0.44	0
4	BMA	D	3	4	11,11,12	0.65	0	15,15,17	0.74	0
4	FUC	D	4	4	10,10,11	0.72	0	14,14,16	1.12	2 (14%)
4	FUC	D	5	4	10,10,11	0.69	0	14,14,16	0.91	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	O5-C1	-2.86	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-O5-C5	2.83	116.03	112.19
4	D	4	FUC	C1-O5-C5	2.53	118.51	112.78
3	C	4	MAN	C1-O5-C5	2.25	115.25	112.19
3	C	5	MAN	C1-O5-C5	2.22	115.20	112.19
4	D	5	FUC	C1-O5-C5	2.21	117.78	112.78
3	C	3	BMA	C1-O5-C5	2.14	115.10	112.19
4	D	4	FUC	O5-C5-C4	2.07	113.24	109.52
3	C	5	MAN	O2-C2-C3	-2.00	106.12	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C3-C2-N2-C7
4	D	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
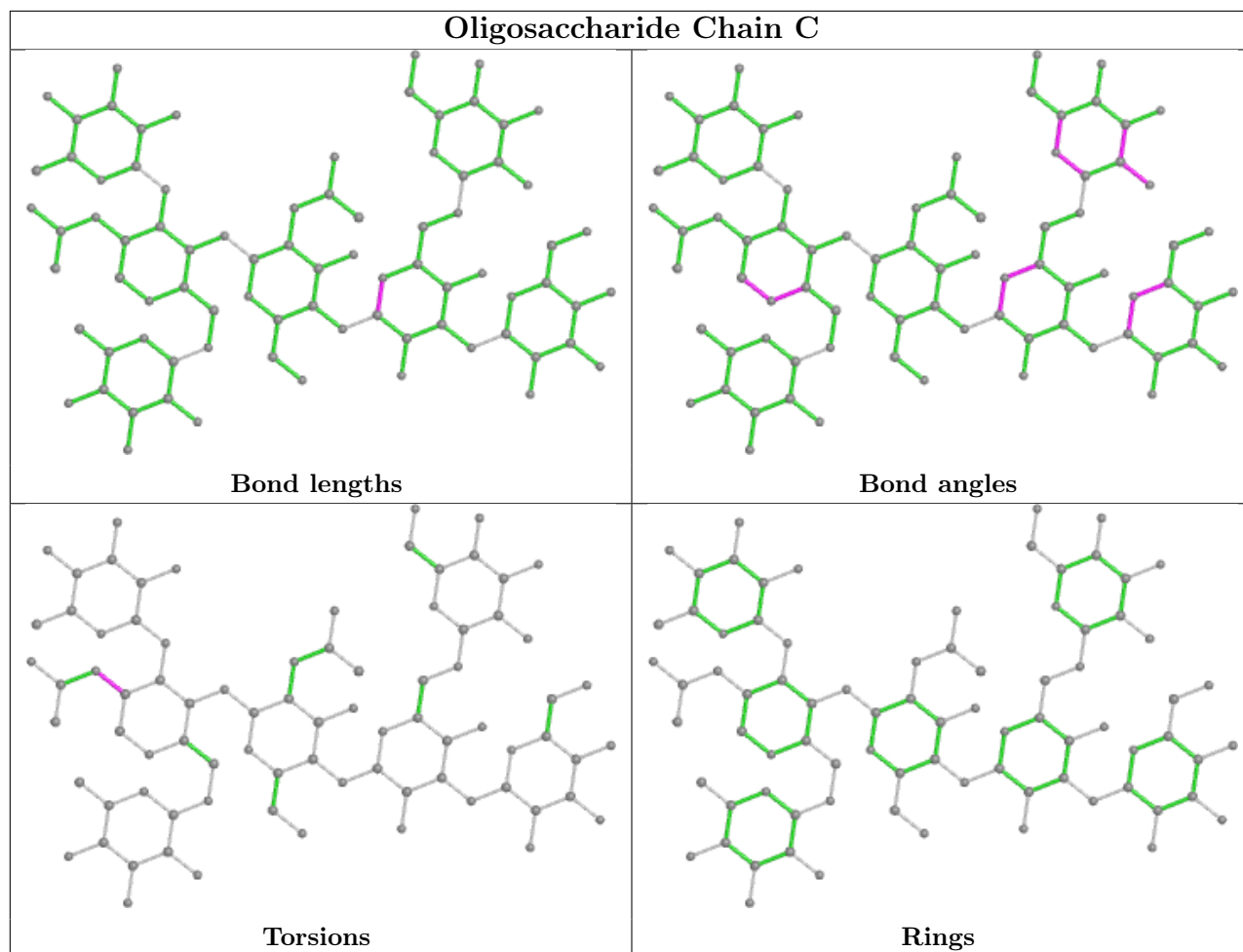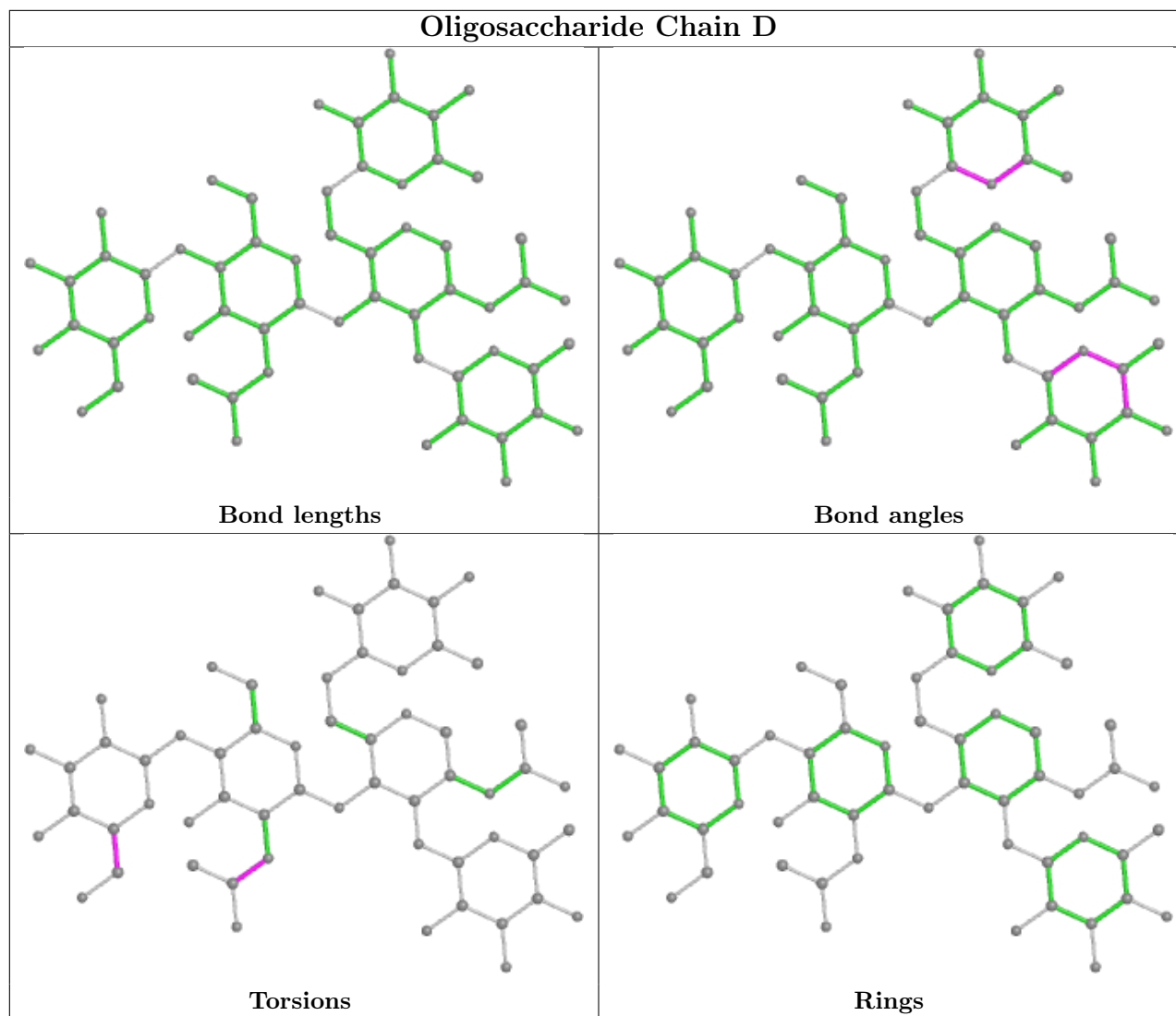
5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
8	EDO	A	707	-	3,3,3	0.47	0	2,2,2	0.40	0
8	EDO	A	704	-	3,3,3	0.07	0	2,2,2	0.35	0
6	3IV	A	702	-	17,17,17	0.58	0	17,17,17	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
8	EDO	A	705	-	3,3,3	0.55	0	2,2,2	0.11	0
8	EDO	A	706	-	3,3,3	0.41	0	2,2,2	0.35	0
7	3IY	A	703	-	59,59,59	1.00	3 (5%)	64,67,67	0.81	2 (3%)

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	A	707	-	-	0/1/1/1	-
8	EDO	A	704	-	-	0/1/1/1	-
6	3IV	A	702	-	-	9/15/15/15	-
8	EDO	A	705	-	-	0/1/1/1	-
8	EDO	A	706	-	-	1/1/1/1	-
7	3IY	A	703	-	-	40/63/63/63	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	703	3IY	O46-C47	2.87	1.41	1.33
7	A	703	3IY	O13-C12	-2.35	1.40	1.46
7	A	703	3IY	O13-C14	2.09	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	703	3IY	O13-C14-C15	3.55	119.14	111.50
7	A	703	3IY	O46-C47-C48	2.64	120.19	111.91
6	A	702	3IV	O18-C16-C15	2.03	120.55	114.03

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	703	3IY	C11-C12-O13-C14
7	A	703	3IY	C38-C39-C40-C41
7	A	703	3IY	C40-C41-C42-C43
7	A	703	3IY	C04-O03-P02-O01
7	A	703	3IY	C11-O10-P02-O01

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Mol	Chain	Res	Type	Atoms
7	A	703	3IY	C11-O10-P02-O03
7	A	703	3IY	C11-O10-P02-O62
7	A	703	3IY	O44-C14-O13-C12
7	A	703	3IY	O61-C47-O46-C45
7	A	703	3IY	C48-C47-O46-C45
7	A	703	3IY	C15-C14-O13-C12
6	A	702	3IV	C11-C12-C13-C14
6	A	702	3IV	C07-C08-C09-C10
7	A	703	3IY	C17-C18-C19-C20
6	A	702	3IV	C02-C03-C04-C05
7	A	703	3IY	C29-C30-C31-C32
7	A	703	3IY	C28-C29-C30-C31
7	A	703	3IY	C47-C48-C49-C50
7	A	703	3IY	C18-C19-C20-C21
7	A	703	3IY	C54-C55-C56-C57
7	A	703	3IY	C11-C12-C45-O46
7	A	703	3IY	C51-C52-C53-C54
7	A	703	3IY	C50-C51-C52-C53
7	A	703	3IY	O10-C11-C12-O13
7	A	703	3IY	O10-C11-C12-C45
7	A	703	3IY	C55-C56-C57-C58
7	A	703	3IY	C30-C31-C32-C33
6	A	702	3IV	C12-C13-C14-C15
7	A	703	3IY	C15-C16-C17-C18
7	A	703	3IY	O03-C04-C05-N06
7	A	703	3IY	O13-C12-C45-O46
7	A	703	3IY	C33-C34-C35-C36
7	A	703	3IY	C53-C54-C55-C56
7	A	703	3IY	C21-C22-C23-C24
7	A	703	3IY	C22-C23-C24-C25
7	A	703	3IY	C25-C26-C27-C28
7	A	703	3IY	C37-C38-C39-C40
6	A	702	3IV	C08-C09-C10-C11
7	A	703	3IY	C31-C32-C33-C34
6	A	702	3IV	C14-C15-C16-O17
8	A	706	EDO	O1-C1-C2-O2
7	A	703	3IY	C32-C33-C34-C35
6	A	702	3IV	C09-C10-C11-C12
7	A	703	3IY	O13-C14-C15-C16
7	A	703	3IY	C04-O03-P02-O10
7	A	703	3IY	C19-C20-C21-C22
7	A	703	3IY	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
6	A	702	3IV	C03-C04-C05-C06
6	A	702	3IV	C14-C15-C16-O18
7	A	703	3IY	C48-C49-C50-C51

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 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 3IV A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand 3IY A 703

Bond lengths

Bond angles

Torsions

Rings
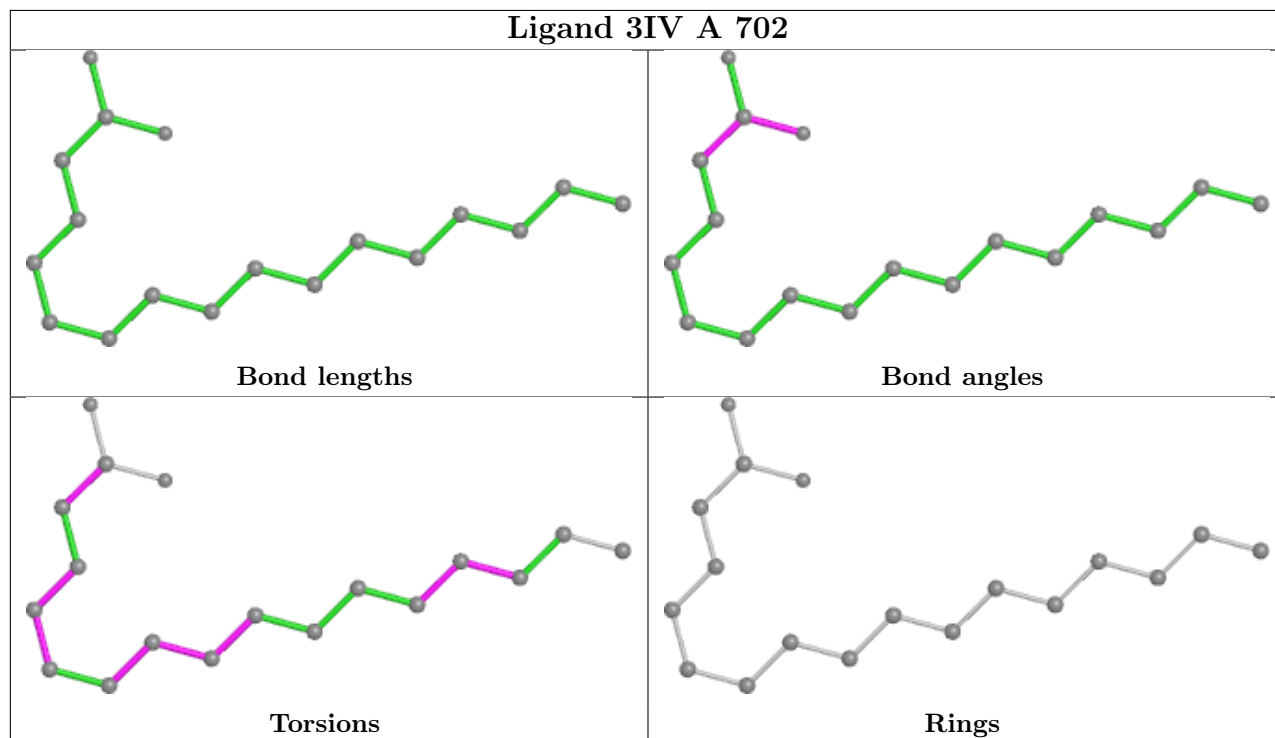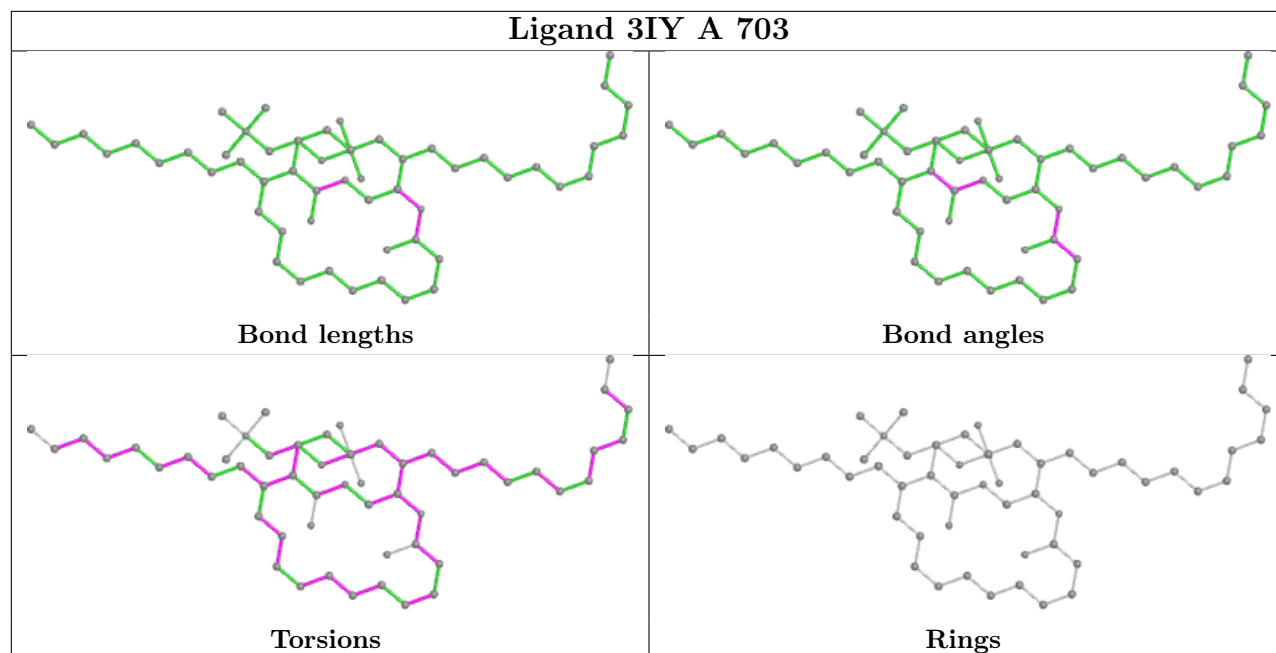
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	280/300 (93%)	-0.38	3 (1%)	80	80	14, 24, 47, 75	1 (0%)
2	B	100/101 (99%)	-0.35	2 (2%)	65	64	15, 27, 46, 69	0
All	All	380/401 (94%)	-0.37	5 (1%)	77	77	14, 25, 47, 75	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	4.7
1	A	279	GLY	4.4
1	A	280	SER	3.7
1	A	283	ASN	3.5
2	B	2	LYS	2.1

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.
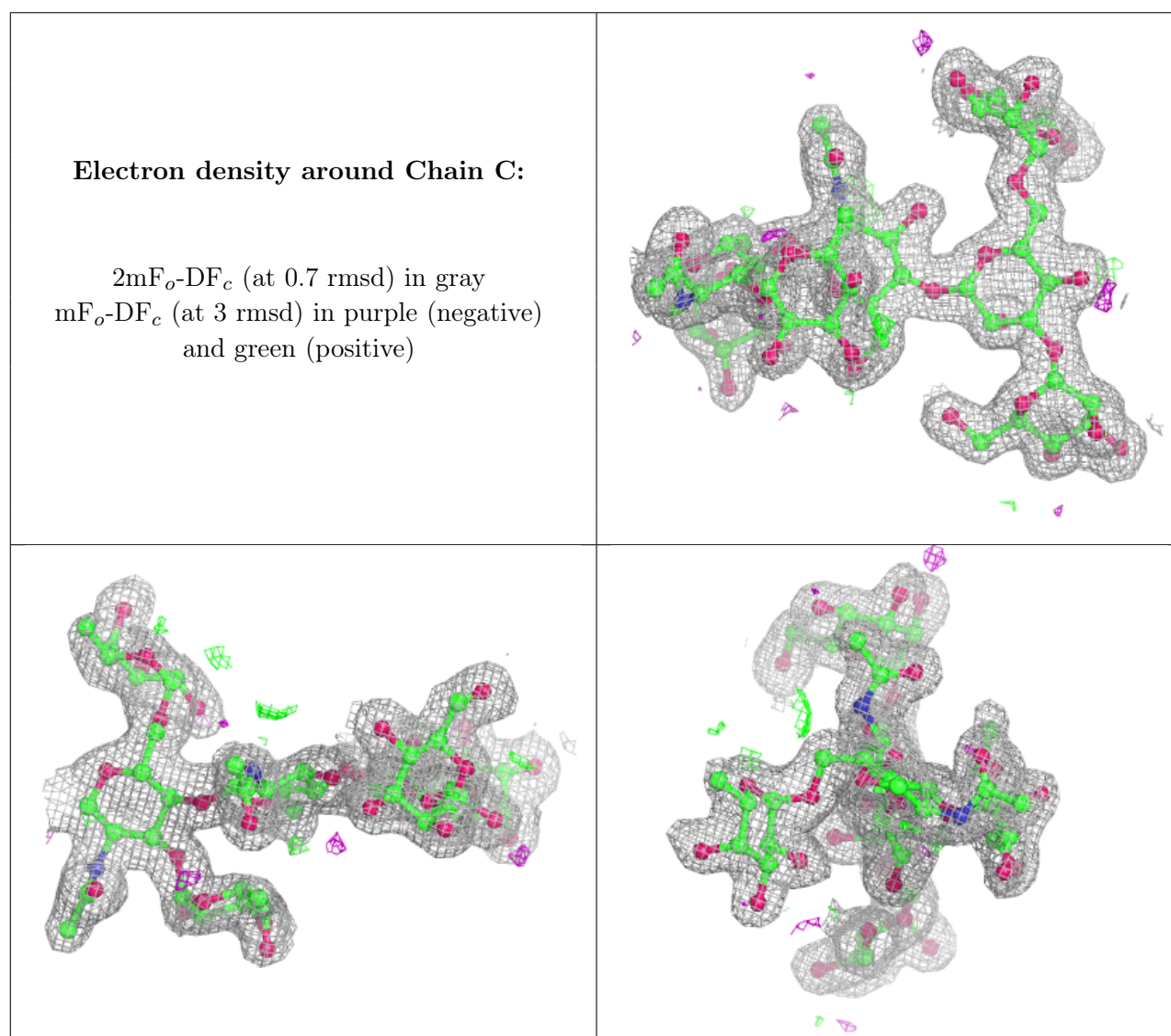
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	D	4	10/11	0.48	0.35	78,82,91,95	0
4	BMA	D	3	11/12	0.68	0.28	67,77,84,85	0
4	NAG	D	2	14/15	0.75	0.22	73,85,92,98	0
4	NAG	D	1	14/15	0.79	0.21	43,54,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	C	6	10/11	0.83	0.18	39,44,54,59	0
4	FUC	D	5	10/11	0.84	0.19	49,66,69,73	0
3	FUC	C	7	10/11	0.92	0.15	28,36,43,45	0
3	MAN	C	5	11/12	0.94	0.13	18,24,27,28	0
3	NAG	C	2	14/15	0.95	0.09	18,24,31,31	0
3	BMA	C	3	11/12	0.95	0.09	20,22,24,24	0
3	NAG	C	1	14/15	0.96	0.08	16,20,27,28	0
3	MAN	C	4	11/12	0.96	0.11	22,26,34,37	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.
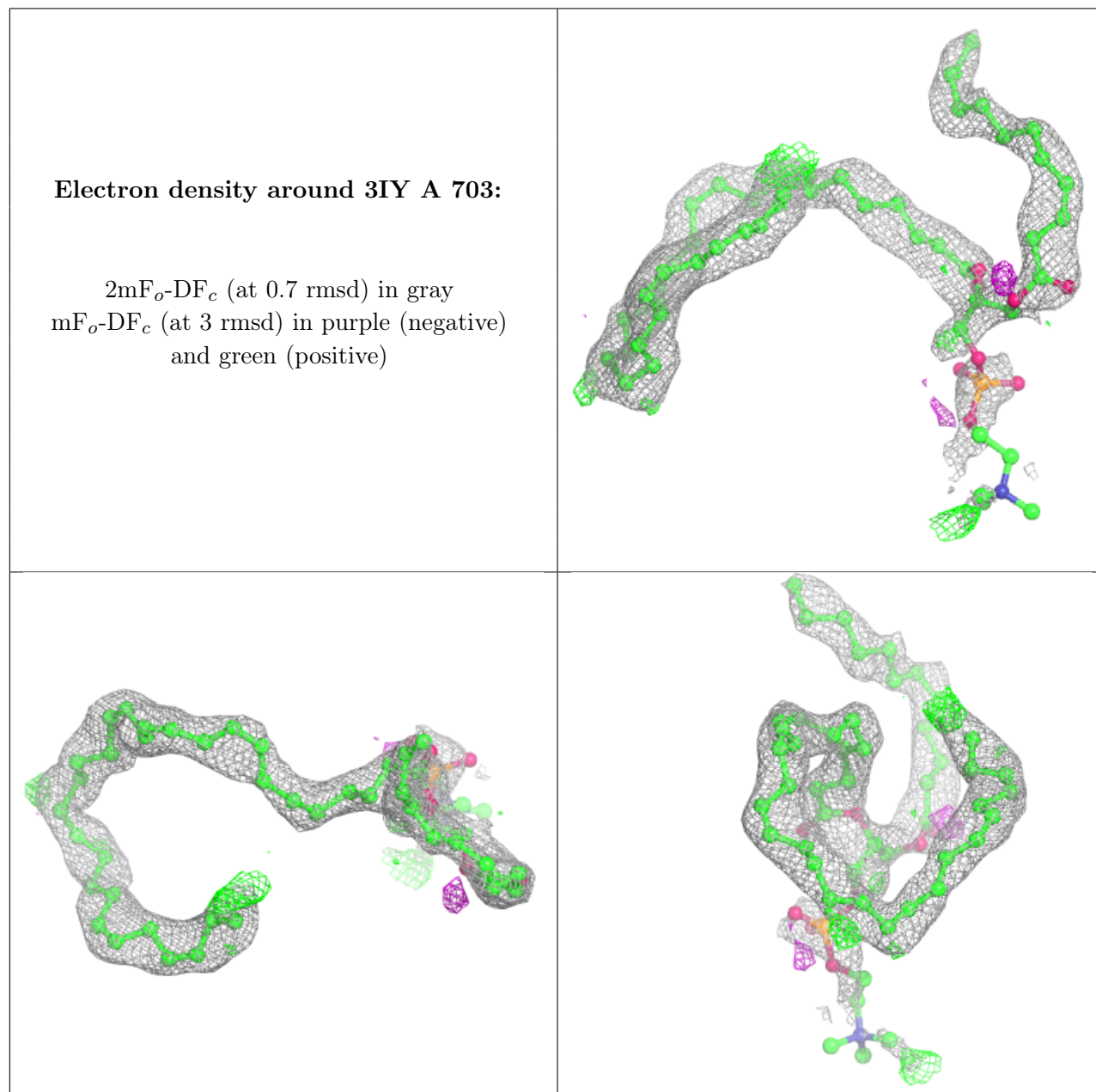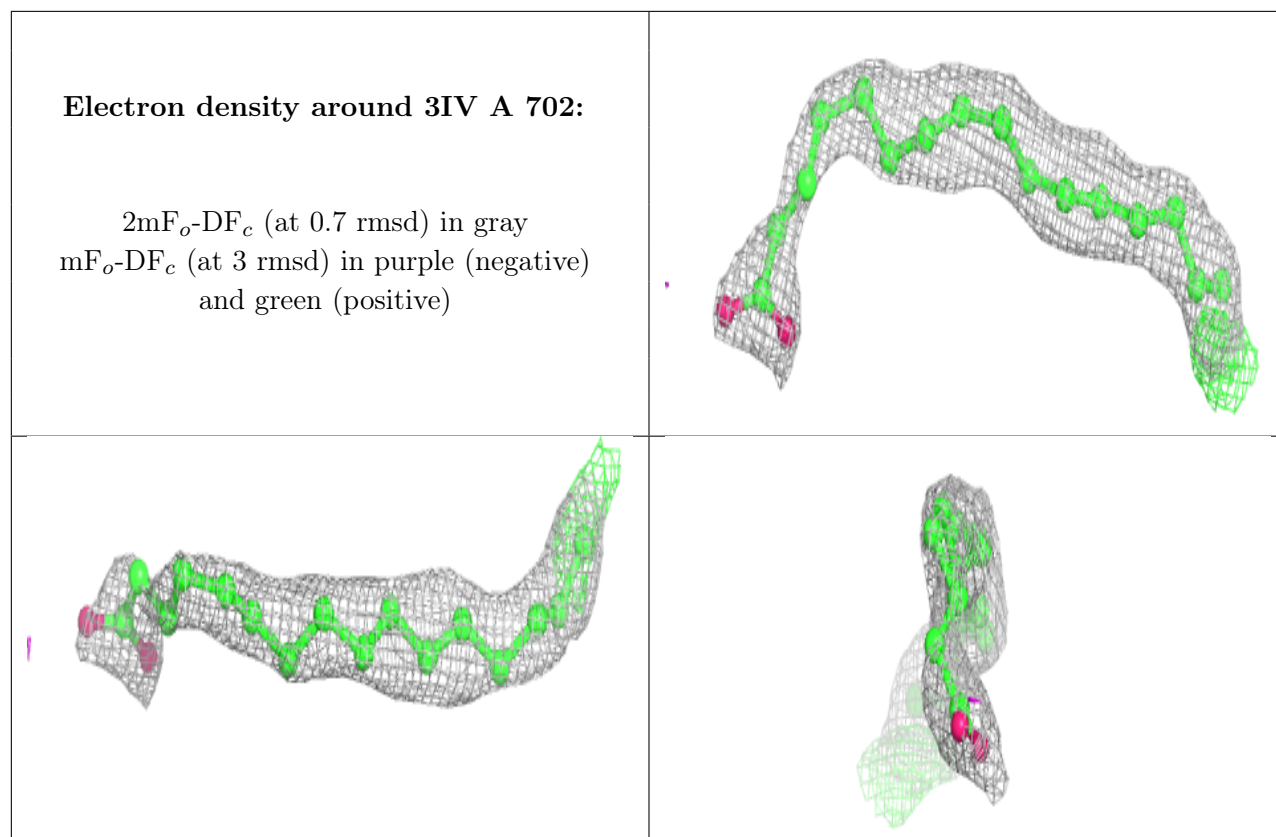

Electron density around Chain C:

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

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
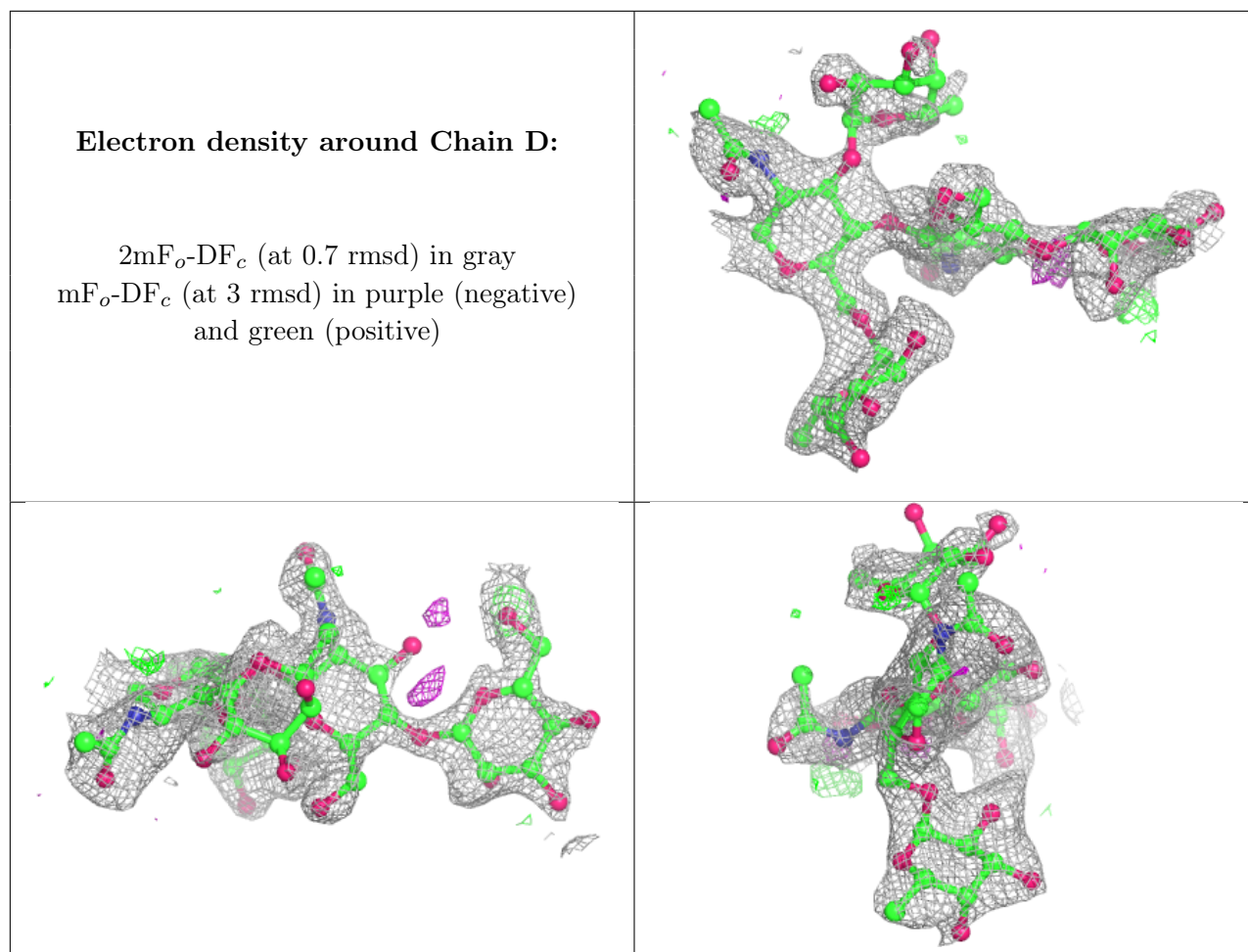
6.4 Ligands (i)

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
7	3IY	A	703	60/60	0.84	0.19	29,50,129,133	0
8	EDO	A	704	4/4	0.86	0.15	50,54,54,56	0
6	3IV	A	702	18/18	0.87	0.20	34,41,64,70	0
8	EDO	A	707	4/4	0.91	0.14	38,44,45,46	0
8	EDO	A	705	4/4	0.95	0.10	22,28,35,39	0
5	IOD	B	201	1/1	0.96	0.07	29,29,29,29	1
8	EDO	A	706	4/4	0.97	0.15	18,30,38,41	0
5	IOD	B	203	1/1	0.97	0.06	38,38,38,38	1
5	IOD	A	701	1/1	0.99	0.09	16,16,16,16	1
9	NA	B	202	1/1	0.99	0.09	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 3IY A 703:

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

Electron density around 3IV A 702:

$2mF_o$-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.