WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 11:12 PM EDT

PDB ID	:	3T8X
Title	:	Crystal structure of human CD1b in complex with synthetic antigenic diacyls ulfoglycolipid SGL12 and endogenous spacer
Authors	:	Garcia-Alles, L.F.; Maveyraud, L.; Mourey, L.; Julien, S.
Deposited on	:	2011-08-02
Resolution	:	1.90 Å(reported)

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 ⓘ

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

The reported resolution of this entry is 1.90 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.
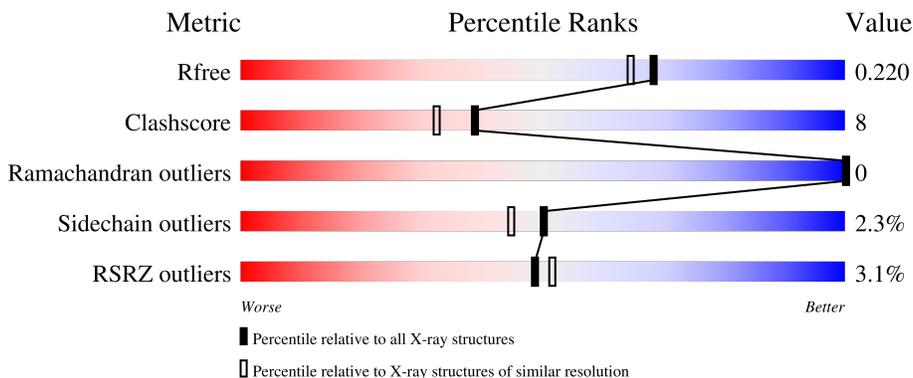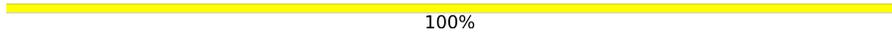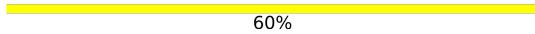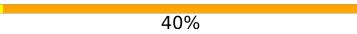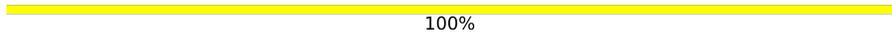

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	301	3% ... 77% ... 13% · 9%
1	C	301	3% ... 80% ... 11% · 8%
2	B	99	2% ... 92% ... 7% ·
2	D	99	3% ... 91% ... 8% ·
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	2	100%
4	F	5	60% 40%
5	H	3	100%

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	FUC	E	2	X	-	-	-
3	FUC	G	2	X	-	-	-
8	T8X	A	304	-	-	X	-

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 6803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2147	1379	365	393	10			
1	C	277	Total	C	N	O	S	0	3	0
			2138	1376	357	395	10			

There are 42 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 810	C 518	N 135	O 154	S 3	0	0	0
2	D	99	Total 807	C 515	N 137	O 152	S 3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total 24	C 14	N 1	O 9	0	0	0
3	G	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 4 is an oligosaccharide called 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.
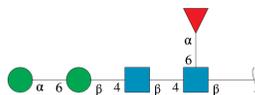
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
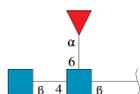
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
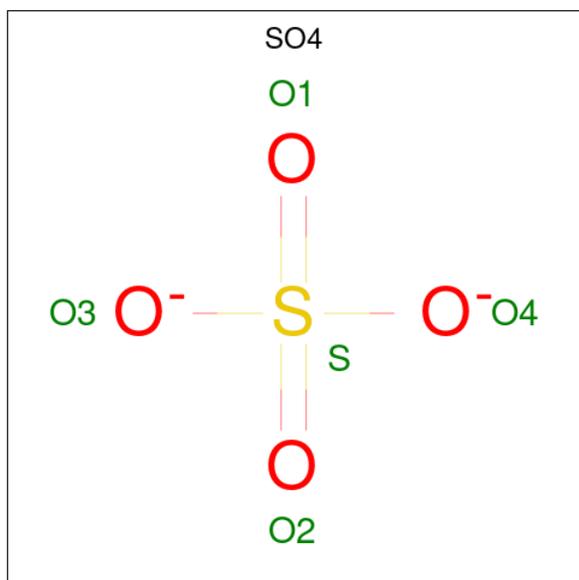
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0
6	D	1	Total 5	O 4	S 1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
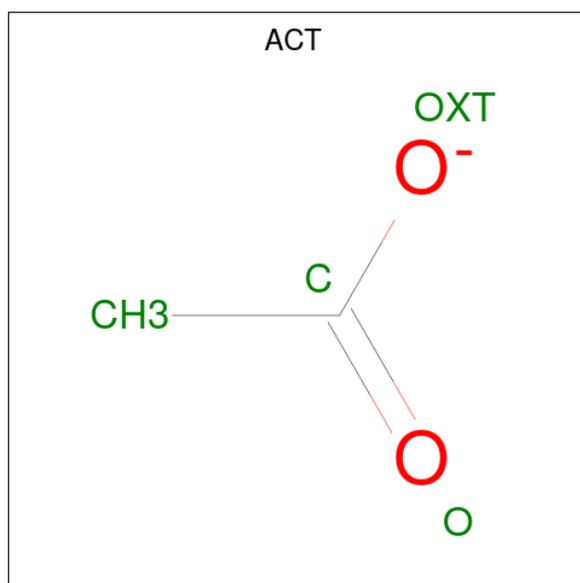
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0

- Molecule 8 is 2-O-sulfo-alpha-D-glucopyranosyl 2-O-hexadecanoyl-3-O-[(2E,4S,6S,8S)-2,4,6, 8-tetramethyltetracos-2-enoyl]-alpha-D-glucopyranoside (three-letter code: T8X) (formula: $C_{56}H_{104}O_{16}S$).
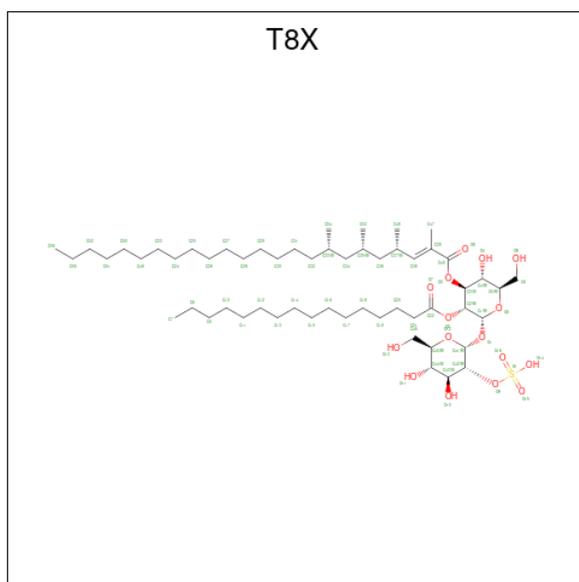
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 73	C 56	O 16	S 1	0	0
8	C	1	Total 31	C 31			0	0

• Molecule 9 is tetracontane (three-letter code: ULI) (formula: $C_{40}H_{82}$).
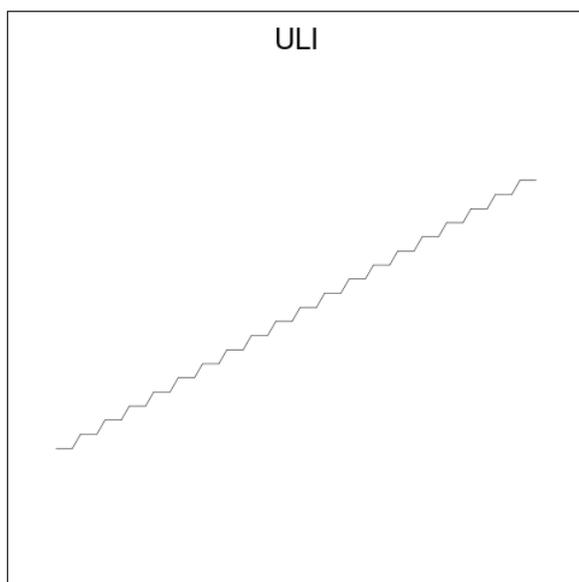
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 40	C 40	0	0
9	C	1	Total 39	C 39	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
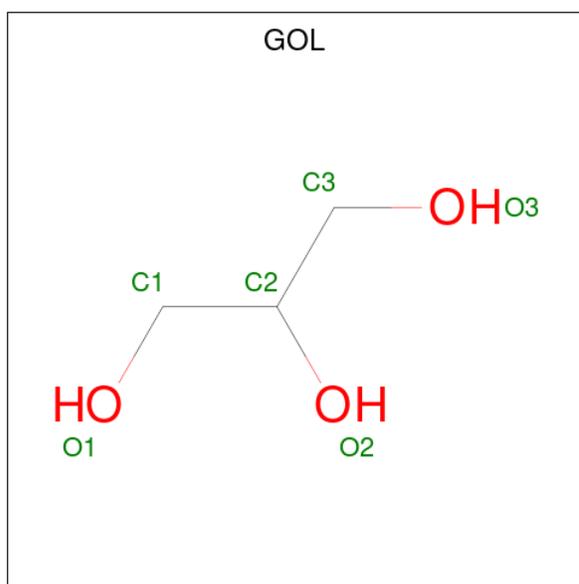
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total 6	C 3	O 3	0	0
10	B	1	Total 6	C 3	O 3	0	0
10	D	1	Total 6	C 3	O 3	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	194	Total 194	O 194	0	0
11	B	97	Total 97	O 97	0	0
11	C	162	Total 162	O 162	0	0
11	D	72	Total 72	O 72	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 1: T-cell surface glycoprotein CD1b

Chain C:

- Molecule 2: Beta-2-microglobulin

Chain B:

- Molecule 2: Beta-2-microglobulin

Chain D:

- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

NAG1
FUC2

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

100%

NAG1
FUC2

• Molecule 4: 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 F:

60%   40%

NAG1
NAG2
BMA3
MAN4
FUC5

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

NAG1
NAG2
FUC3

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.25Å 67.58Å 88.19Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-1.90) 92.6 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.165 , 0.211 0.173 , 0.220	Depositor DCC
R_{free} test set	4044 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 60.3	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SO4, ULI, T8X, ACT, NAG, FUC, GOL, 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	1.27	6/2207 (0.3%)	1.06	11/2998 (0.4%)
1	C	1.17	6/2198 (0.3%)	1.01	7/2992 (0.2%)
2	B	1.22	1/833 (0.1%)	1.00	1/1131 (0.1%)
2	D	1.03	1/830 (0.1%)	0.93	1/1127 (0.1%)
All	All	1.20	14/6068 (0.2%)	1.02	20/8248 (0.2%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	TRP	CD2-CE2	6.79	1.49	1.41
2	B	60	TRP	CD2-CE2	6.06	1.48	1.41
1	A	53	TRP	CD2-CE2	6.00	1.48	1.41
1	C	241	TRP	CD2-CE2	5.93	1.48	1.41
2	D	95	TRP	CD2-CE2	5.86	1.48	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	D	59	ASP	CB-CG-OD1	7.55	125.09	118.30
1	A	34	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	83	ASP	CB-CG-OD2	7.49	125.05	118.30
1	A	272	ASP	CB-CG-OD2	6.73	124.36	118.30

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	2147	0	2051	27	0
1	C	2138	0	2014	22	0
2	B	810	0	749	5	0
2	D	807	0	753	7	0
3	E	24	0	22	0	0
3	G	24	0	22	0	0
4	F	60	0	52	2	0
5	H	38	0	34	0	0
6	A	5	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
7	A	4	0	3	0	0
8	A	73	0	103	33	0
8	C	31	0	61	4	0
9	A	40	0	82	16	0
9	C	39	0	77	8	0
10	B	12	0	16	4	0
10	D	6	0	8	0	0
11	A	194	0	0	1	1
11	B	97	0	0	1	0
11	C	162	0	0	10	1
11	D	72	0	0	3	0
All	All	6803	0	6047	91	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 8.

The worst 5 of 91 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)
8:A:304:T8X:C56	9:A:305:ULI:HAA	1.47	1.41
8:A:304:T8X:C56	9:A:305:ULI:CAA	2.11	1.28
1:C:22[A]:THR:HG22	11:C:311:HOH:O	1.03	1.21
1:C:219:MET:HE1	11:C:472:HOH:O	1.04	1.20
8:A:304:T8X:HCTA	9:A:305:ULI:HAA	1.31	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:490:HOH:O	11:C:479:HOH:O[4_546]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/301 (91%)	272 (99%)	2 (1%)	0	100	100
1	C	278/301 (92%)	274 (99%)	4 (1%)	0	100	100
2	B	97/99 (98%)	97 (100%)	0	0	100	100
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
All	All	746/800 (93%)	738 (99%)	8 (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	221/247 (90%)	217 (98%)	4 (2%)	59	55
1	C	216/247 (87%)	210 (97%)	6 (3%)	43	36
2	B	87/94 (93%)	85 (98%)	2 (2%)	50	45
2	D	88/94 (94%)	86 (98%)	2 (2%)	50	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	612/682 (90%)	598 (98%)	14 (2%)	50 45

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	155	MET
1	C	168	ARG
2	D	70	PHE
1	C	281	ILE
2	D	69	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	C	227	GLN
2	D	51	HIS
1	C	240	ASN
1	A	203	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	E	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	2.18	7 (41%)
3	FUC	E	2	3	10,10,11	1.52	2 (20%)	14,14,16	2.61	8 (57%)
4	NAG	F	1	1,4	14,14,15	0.75	0	17,19,21	1.81	5 (29%)
4	NAG	F	2	4	14,14,15	0.77	0	17,19,21	2.04	5 (29%)
4	BMA	F	3	4	11,11,12	0.83	0	15,15,17	1.95	5 (33%)
4	MAN	F	4	4	11,11,12	0.84	0	15,15,17	2.35	4 (26%)
4	FUC	F	5	4	10,10,11	1.97	1 (10%)	14,14,16	2.39	4 (28%)
3	NAG	G	1	1,3	14,14,15	0.75	0	17,19,21	2.38	6 (35%)
3	FUC	G	2	3	10,10,11	1.33	1 (10%)	14,14,16	3.12	6 (42%)
5	NAG	H	1	1,5	14,14,15	0.99	1 (7%)	17,19,21	1.61	4 (23%)
5	NAG	H	2	5	14,14,15	0.92	0	17,19,21	1.87	5 (29%)
5	FUC	H	3	5	10,10,11	1.66	1 (10%)	14,14,16	3.28	7 (50%)

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	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	1/1/4/5	-	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	FUC	F	5	4	-	-	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	G	2	3	1/1/4/5	-	0/1/1/1
5	NAG	H	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	FUC	H	3	5	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	FUC	O5-C1	-5.28	1.35	1.43
5	H	3	FUC	O5-C1	-4.19	1.37	1.43
3	E	2	FUC	O5-C1	-3.70	1.37	1.43
3	G	2	FUC	O5-C1	-3.26	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	3.10	1.57	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	FUC	C1-C2-C3	-8.03	99.80	109.67
3	G	2	FUC	C1-C2-C3	-7.93	99.92	109.67
4	F	5	FUC	C1-C2-C3	-7.05	101.00	109.67
4	F	4	MAN	C1-C2-C3	6.77	117.98	109.67
5	H	3	FUC	C3-C4-C5	5.52	118.37	109.77

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	FUC	C1
3	G	2	FUC	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	1	NAG	C3-C2-N2-C7
5	H	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	F	4	MAN	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 E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
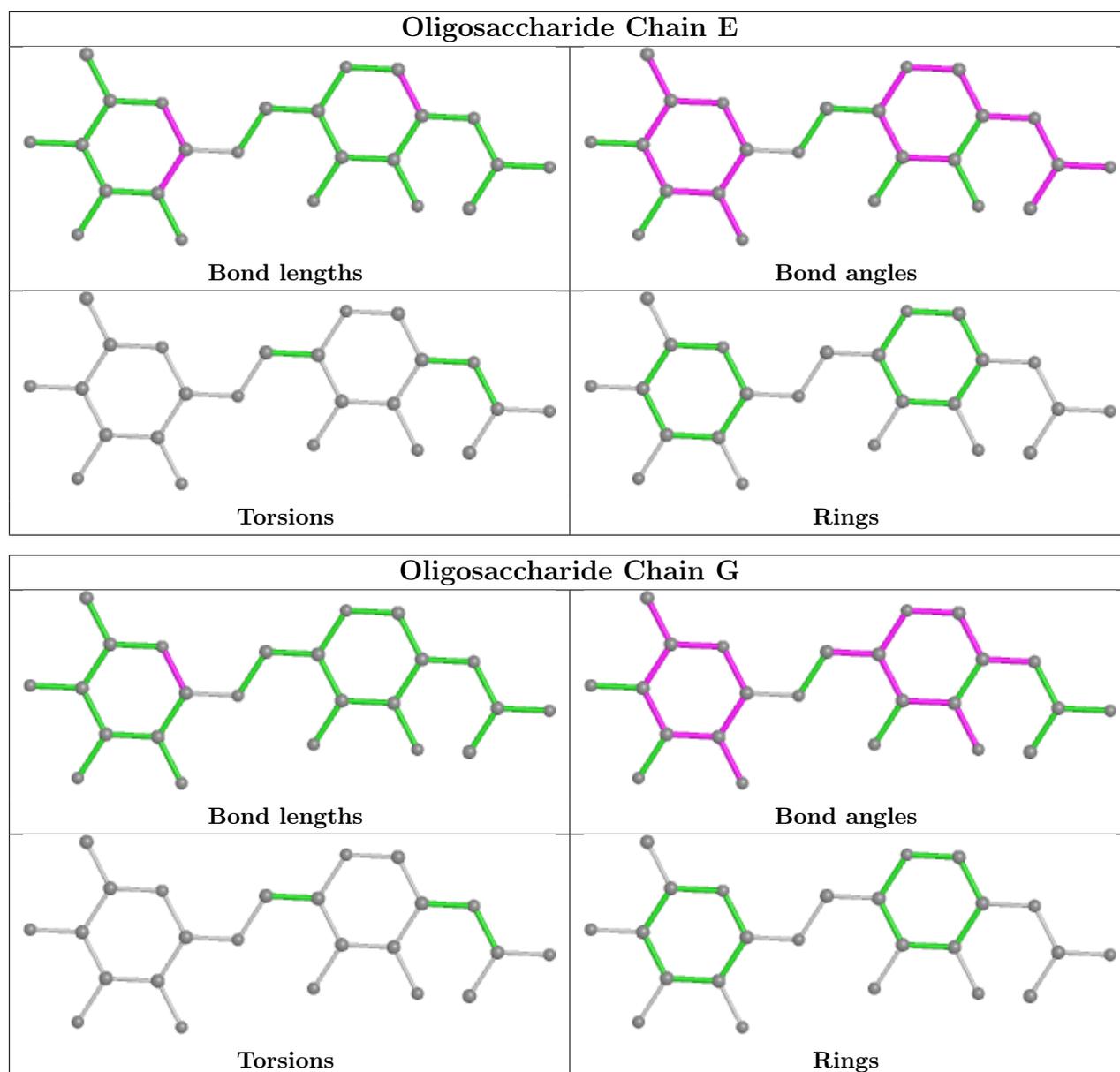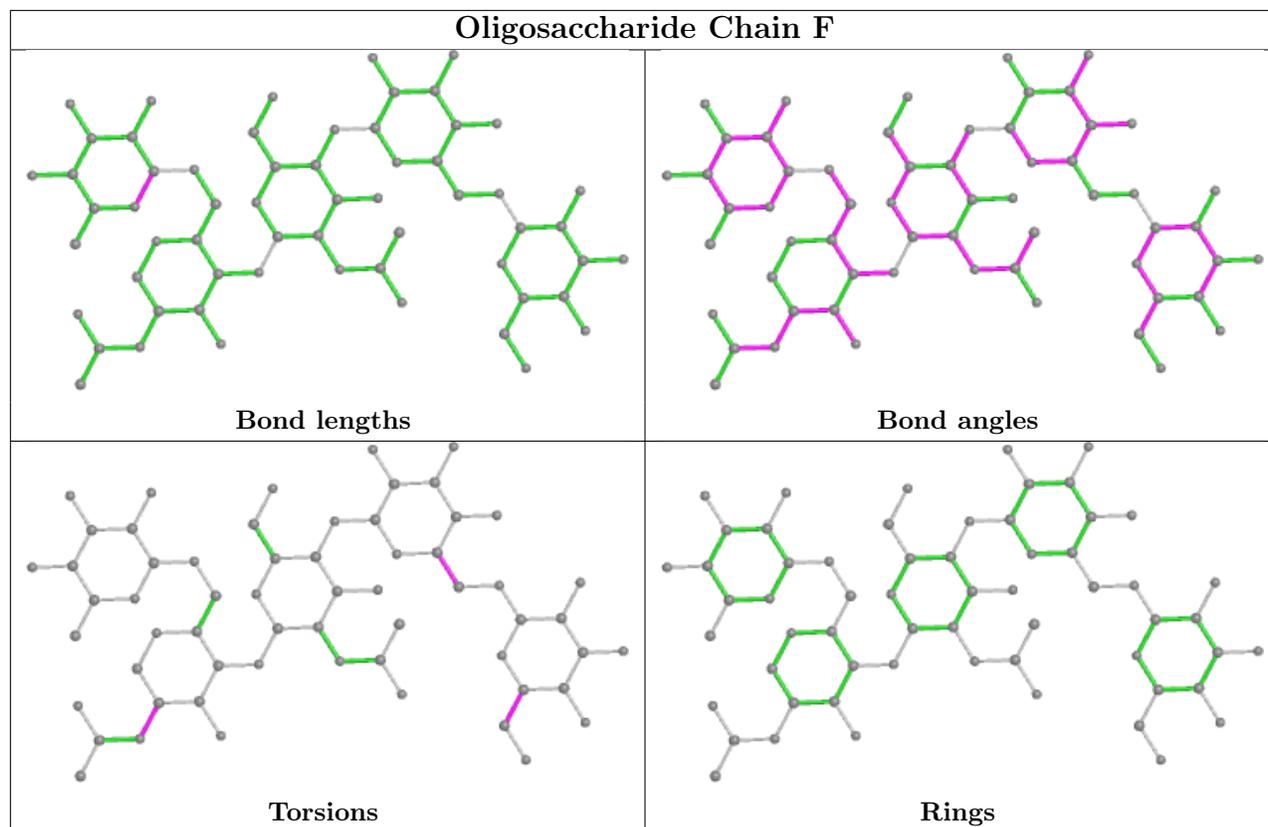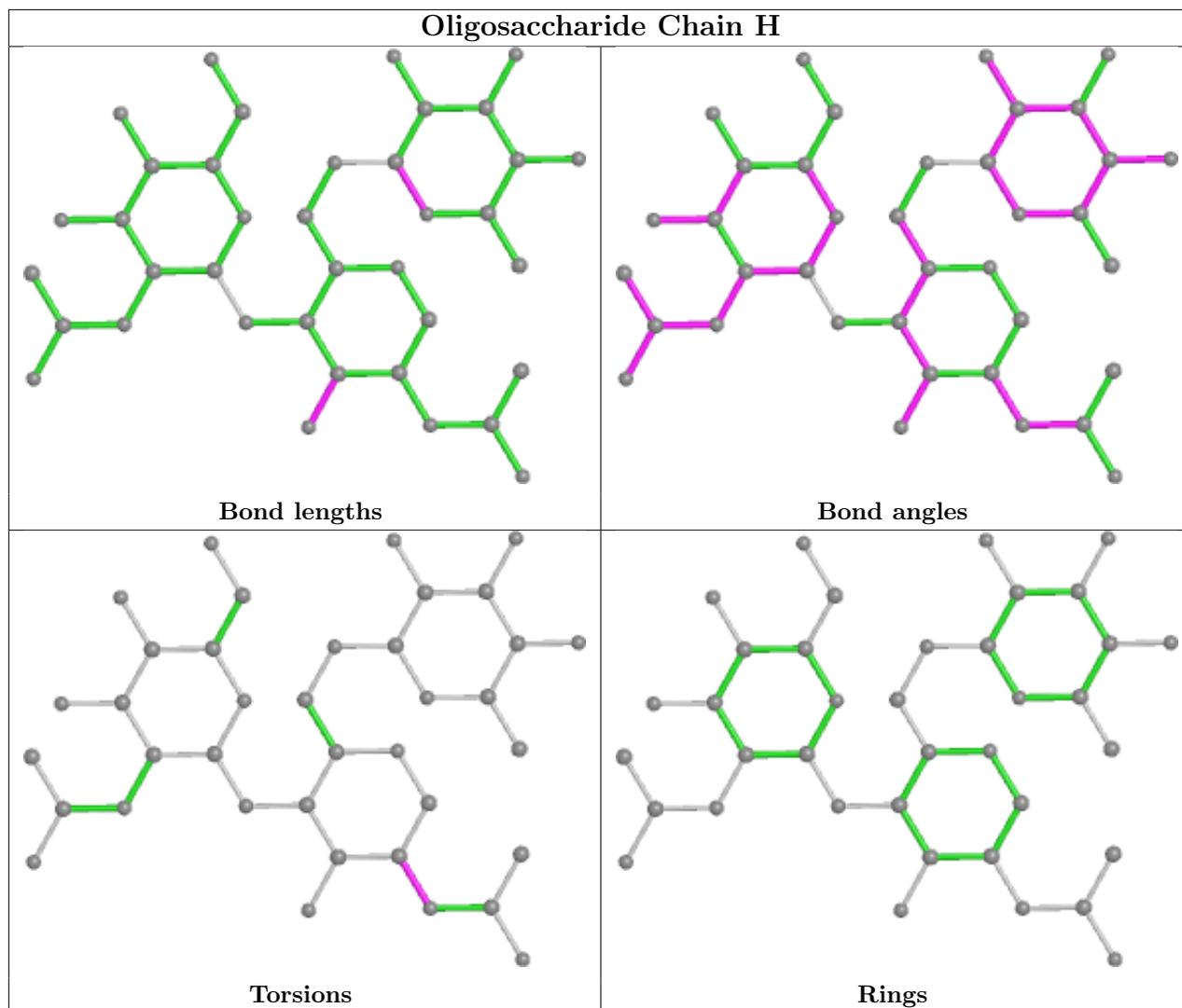
5.6 Ligand geometry ⓘ

13 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	#$|Z| > 2$
7	ACT	A	303	-	3,3,3	0.79	0	3,3,3	1.67	1 (33%)
10	GOL	B	100	-	5,5,5	0.44	0	5,5,5	0.77	0
6	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	SO4	C	303	-	4,4,4	0.53	0	6,6,6	0.25	0
10	GOL	B	101	-	5,5,5	0.81	0	5,5,5	1.57	2 (40%)
6	SO4	D	100	-	4,4,4	0.80	0	6,6,6	0.61	0
9	ULI	A	305	-	39,39,39	0.61	1 (2%)	38,38,38	1.15	2 (5%)
9	ULI	C	305	-	38,38,39	0.55	0	37,37,38	1.07	3 (8%)
6	SO4	D	101	-	4,4,4	0.40	0	6,6,6	0.78	0
6	SO4	A	302	-	4,4,4	0.54	0	6,6,6	0.55	0
10	GOL	D	102	-	5,5,5	0.70	0	5,5,5	1.63	2 (40%)
8	T8X	C	304	-	29,29,74	0.56	0	27,27,94	0.56	0
8	T8X	A	304	-	74,74,74	1.69	9 (12%)	88,94,94	1.83	15 (17%)

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
10	GOL	B	101	-	-	2/4/4/4	-
9	ULI	C	305	-	-	18/36/36/37	-
9	ULI	A	305	-	-	17/37/37/37	-
8	T8X	A	304	-	-	43/68/108/108	0/2/2/2
10	GOL	D	102	-	-	3/4/4/4	-
8	T8X	C	304	-	-	12/25/25/108	-
10	GOL	B	100	-	-	1/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	304	T8X	O8-C40	6.95	1.36	1.21
8	A	304	T8X	C38-C39	6.21	1.41	1.33
8	A	304	T8X	O3-C3	-3.71	1.39	1.44
8	A	304	T8X	O9-S1	-3.70	1.46	1.57
8	A	304	T8X	C40-C39	-3.58	1.38	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	304	T8X	C1-C2-C3	-6.43	97.90	110.75
8	A	304	T8X	C41-O1-C1	6.04	125.20	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	304	T8X	O2-C2-C3	4.72	117.70	108.25
8	A	304	T8X	O1-C1-O5	4.15	122.27	110.67
8	A	304	T8X	O5-C5-C6	4.03	116.44	106.44

There are no chirality outliers.

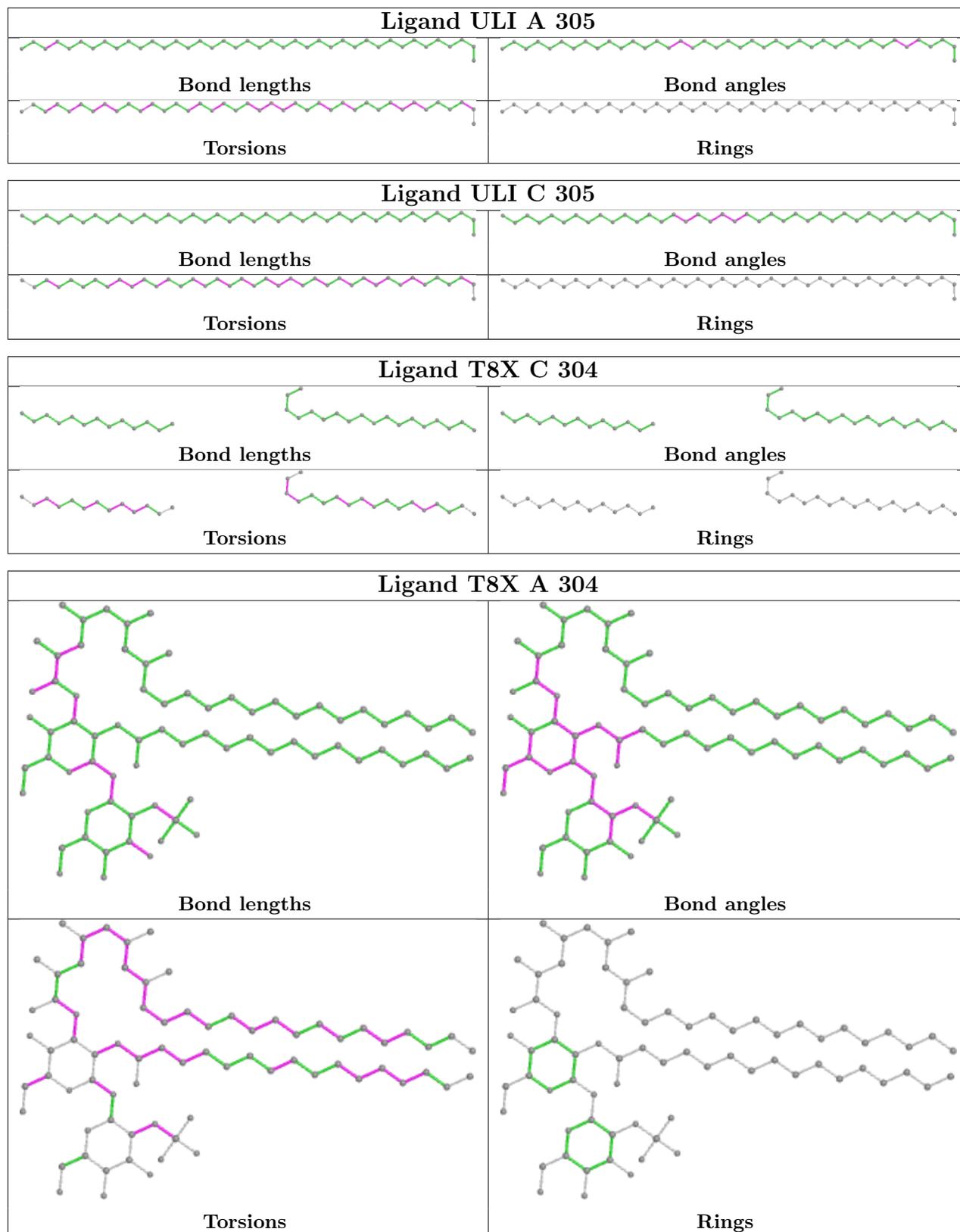5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	304	T8X	C21-C22-O2-C2
8	A	304	T8X	C4-C3-O3-C40
8	A	304	T8X	C32-C33-C34-C35
8	A	304	T8X	C34-C35-C36-C37
8	A	304	T8X	C35-C36-C37-C48

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	100	GOL	3	0
10	B	101	GOL	1	0
9	A	305	ULI	16	0
9	C	305	ULI	8	0
8	C	304	T8X	4	0
8	A	304	T8X	33	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 ULI A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand ULI C 305

Bond lengths

Bond angles

Torsions

Rings

Ligand T8X C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand T8X A 304

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	275/301 (91%)	-0.19	9 (3%)	46	49	19, 32, 56, 77	0
1	C	277/301 (92%)	-0.18	9 (3%)	47	50	25, 36, 56, 74	0
2	B	99/99 (100%)	-0.27	2 (2%)	65	68	19, 32, 53, 62	0
2	D	99/99 (100%)	-0.08	3 (3%)	50	53	26, 41, 61, 72	0
All	All	750/800 (93%)	-0.18	23 (3%)	49	51	19, 35, 57, 77	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	SER	4.4
1	C	195	PRO	4.2
1	C	198	GLY	3.8
1	C	281	ILE	3.3
1	A	257	ALA	3.2

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.
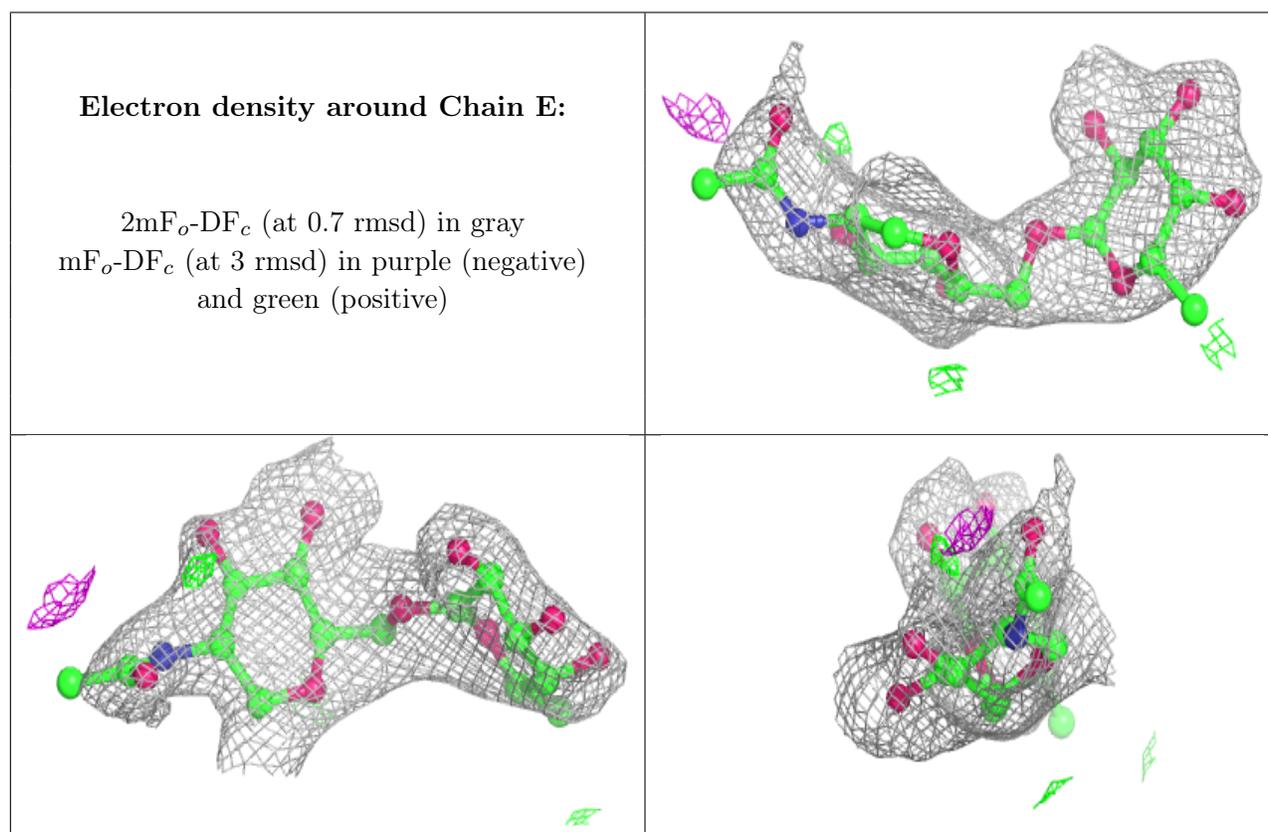
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	F	4	11/12	0.78	0.36	73,90,95,96	0
4	BMA	F	3	11/12	0.82	0.34	62,75,95,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	G	1	14/15	0.86	0.24	57,69,75,84	0
4	NAG	F	2	14/15	0.86	0.16	40,45,52,56	0
5	FUC	H	3	10/11	0.88	0.24	45,56,61,74	0
5	NAG	H	2	14/15	0.89	0.25	44,54,67,75	0
3	NAG	E	1	14/15	0.90	0.16	58,64,74,77	0
3	FUC	E	2	10/11	0.90	0.30	60,69,74,75	0
4	FUC	F	5	10/11	0.93	0.18	46,49,52,59	0
3	FUC	G	2	10/11	0.94	0.28	68,72,76,83	0
4	NAG	F	1	14/15	0.98	0.05	30,36,42,45	0
5	NAG	H	1	14/15	0.98	0.11	39,44,50,53	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.
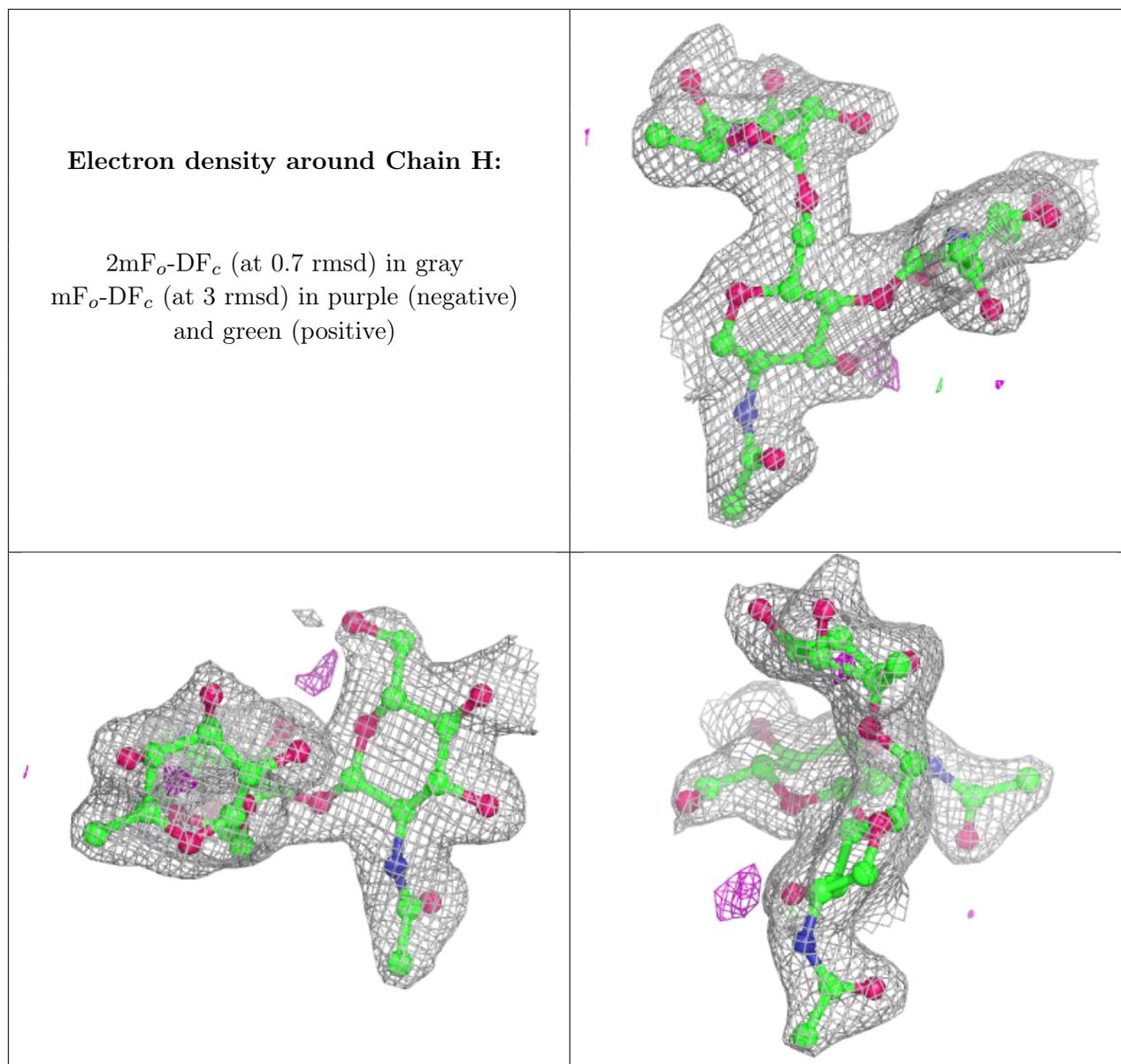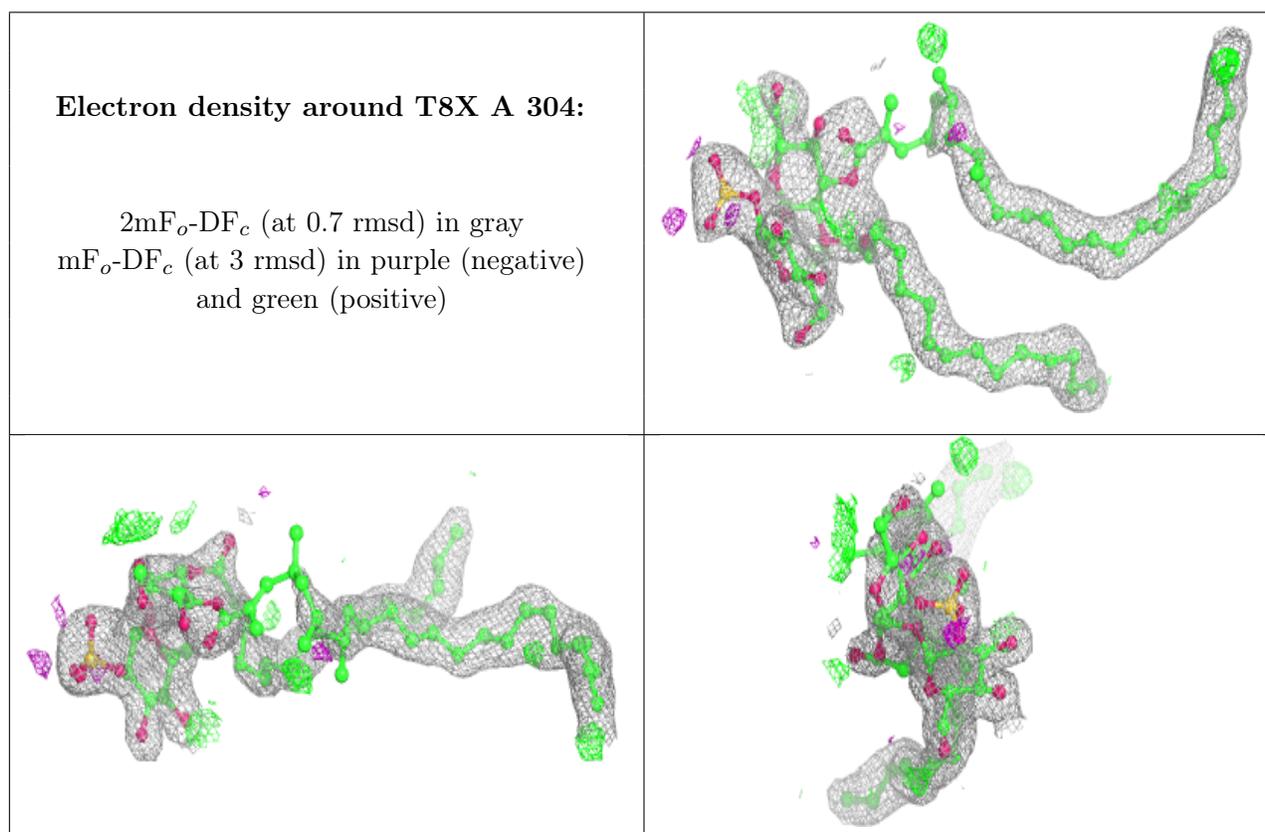

Electron density around Chain E:

$2mF_o$-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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
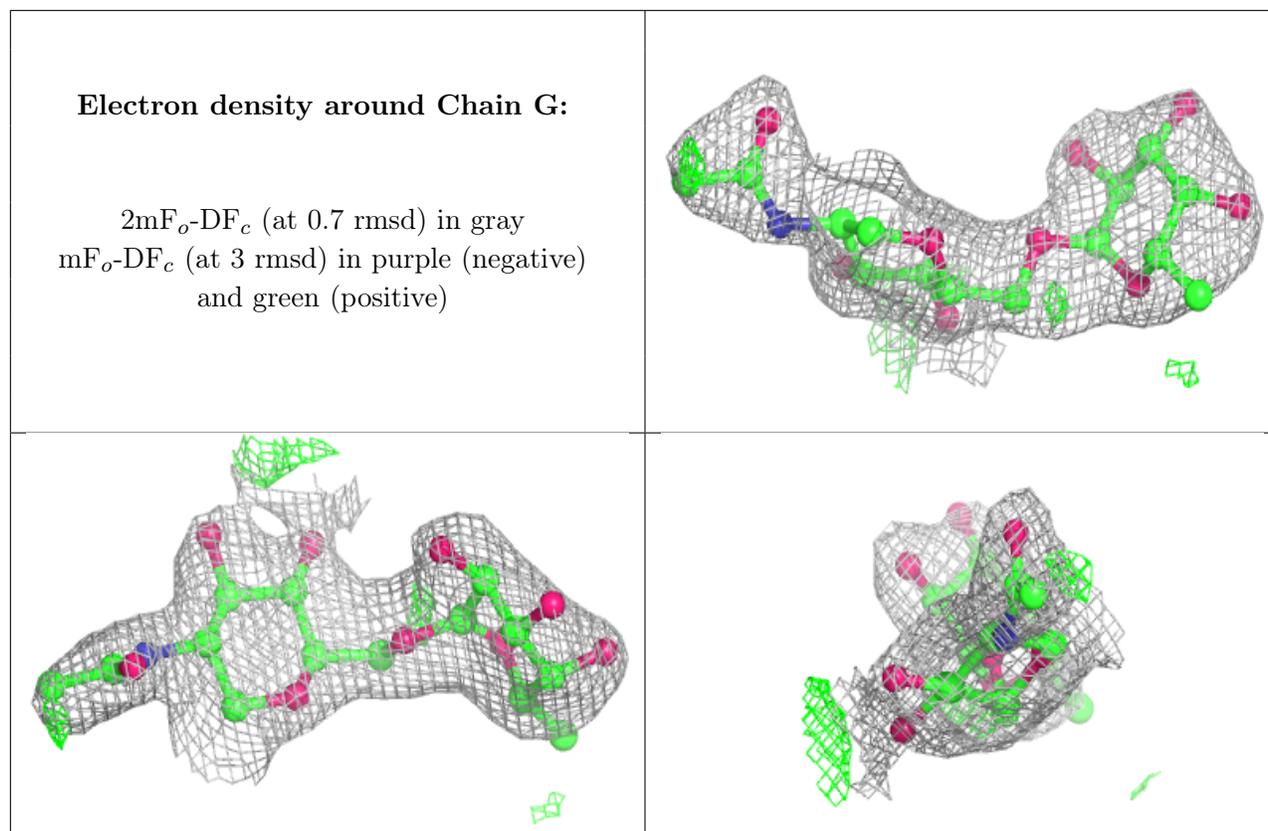
Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
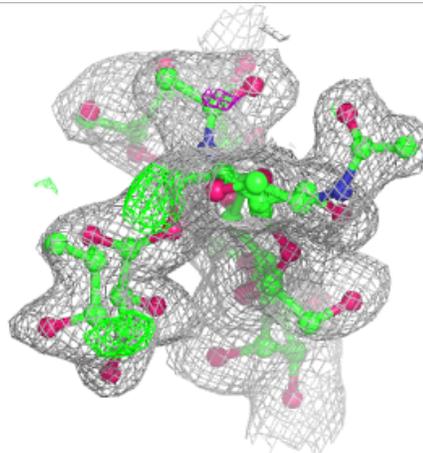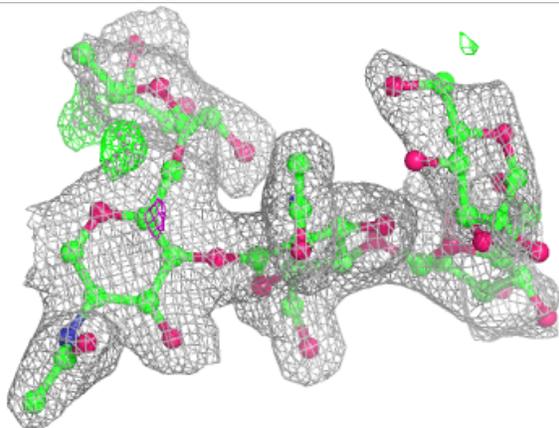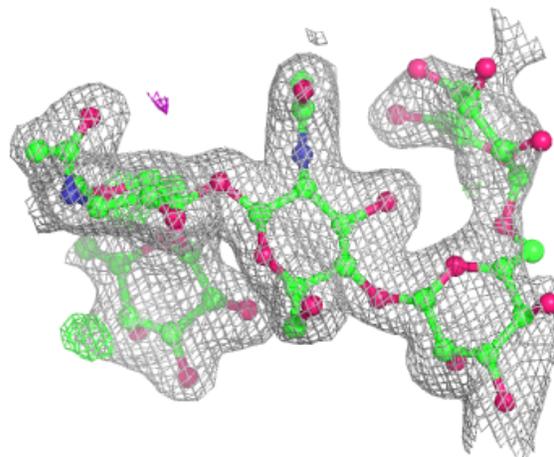
Electron density around Chain H:

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

6.4 Ligands ⓘ

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	ACT	A	303	4/4	0.42	0.29	68,71,76,76	0
10	GOL	B	100	6/6	0.71	0.23	49,63,65,65	0
6	SO4	A	302	5/5	0.73	0.27	84,88,106,107	0
8	T8X	A	304	73/73	0.74	0.22	40,72,112,116	0
8	T8X	C	304	31/73	0.80	0.21	41,58,66,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
9	ULI	C	305	39/40	0.85	0.27	45,57,68,78	0
10	GOL	D	102	6/6	0.88	0.14	52,57,70,77	0
6	SO4	C	303	5/5	0.89	0.20	77,78,104,104	0
10	GOL	B	101	6/6	0.90	0.18	45,53,63,69	0
9	ULI	A	305	40/40	0.93	0.21	31,47,62,78	0
6	SO4	D	101	5/5	0.95	0.10	66,76,84,86	0
6	SO4	D	100	5/5	0.99	0.06	42,46,48,50	0
6	SO4	C	302	5/5	0.99	0.07	43,52,57,62	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.
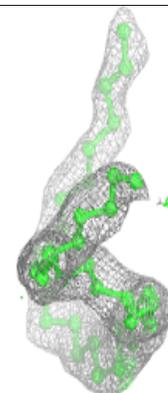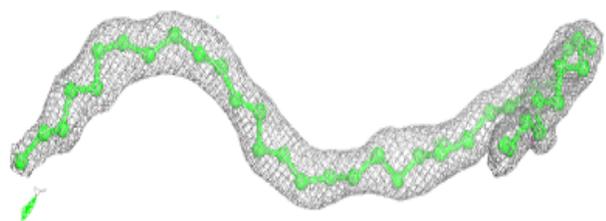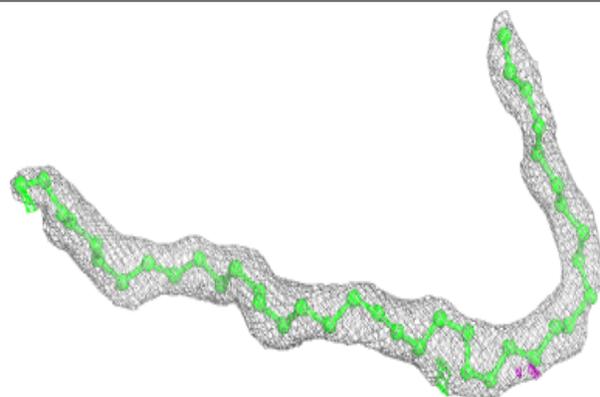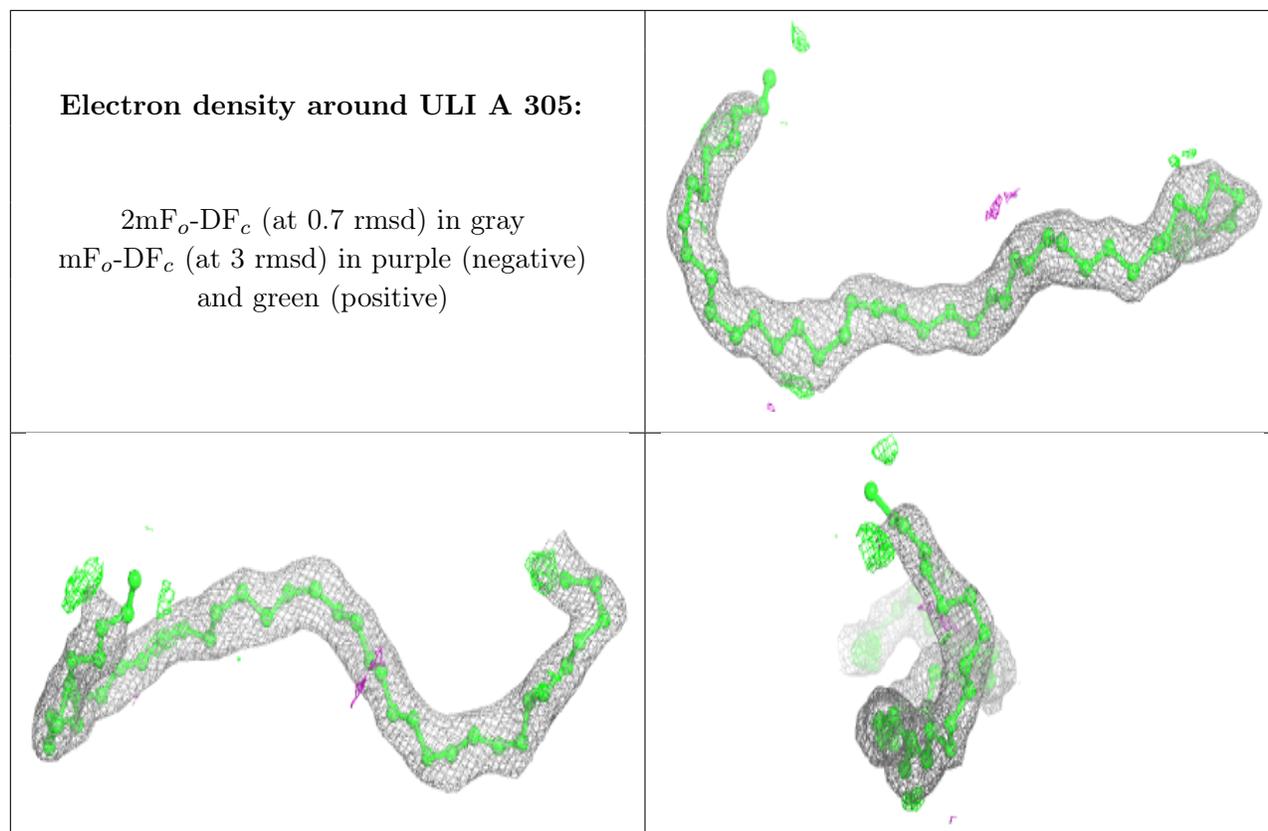
Electron density around T8X A 304:

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

Electron density around T8X C 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
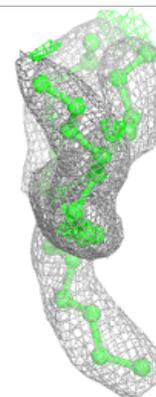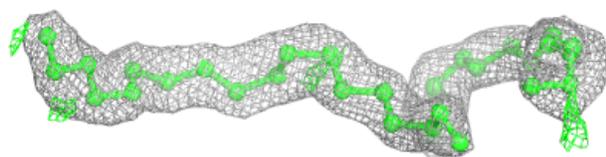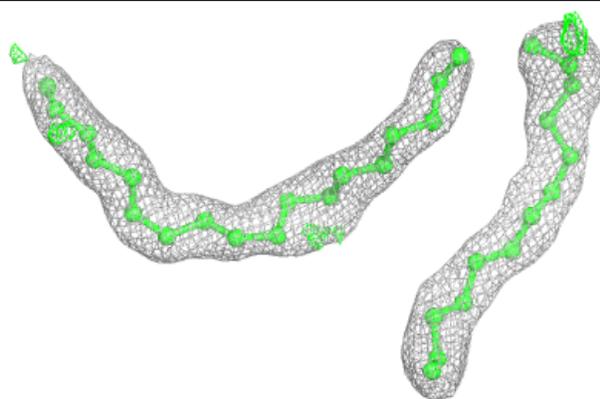
Electron density around ULI C 305:

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

Electron density around ULI A 305:

$2mF_o$-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.