Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:46 PM BST

PDB ID	:	5WL1
Title	:	Crystal Structure of Human CD1b in Complex with PG
Authors	:	Shahine, A.; Gras, S.; Rossjohn, J.
Deposited on	:	2017-07-25
Resolution	:	1.38 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 following versions of software and data (see references ⓘ) were used in the production of this report:

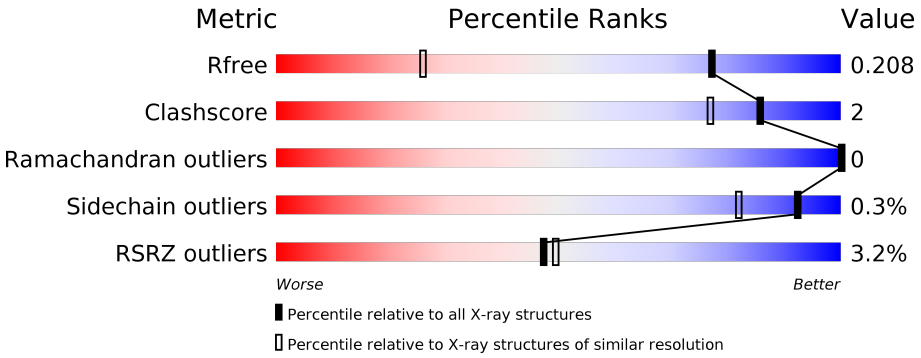
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 on 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	3%, 90%, 7%
2	B	99	4%, 97%
3	C	4	25%, 75%
4	D	5	100%
5	E	7	86%, 14%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7131 atoms, of which 3120 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	H	N	O	S			
1	A	280	4323	1434	2074	385	420	10	0	21	0

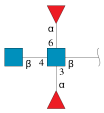
There are 23 discrepancies between the modelled and reference sequences:

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.

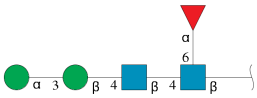
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	98	1545	519	729	139	156	2	0	4	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



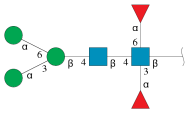
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	C	4	95	28	47	2	18	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



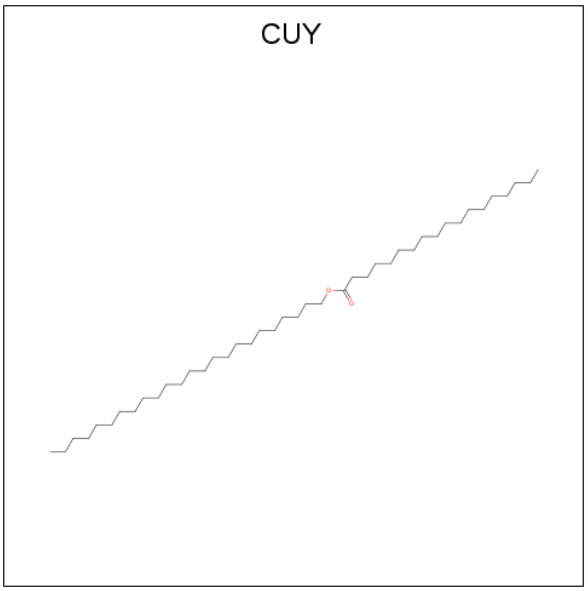
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	D	5	114	34	54	2	24	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	7	156	46	75	2	33	0	0	0

- Molecule 6 is tetracosyl octadecanoate (three-letter code: CUY) (formula: $C_{42}H_{84}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 87 33 52 2	0	0

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total I 1 1	0	0

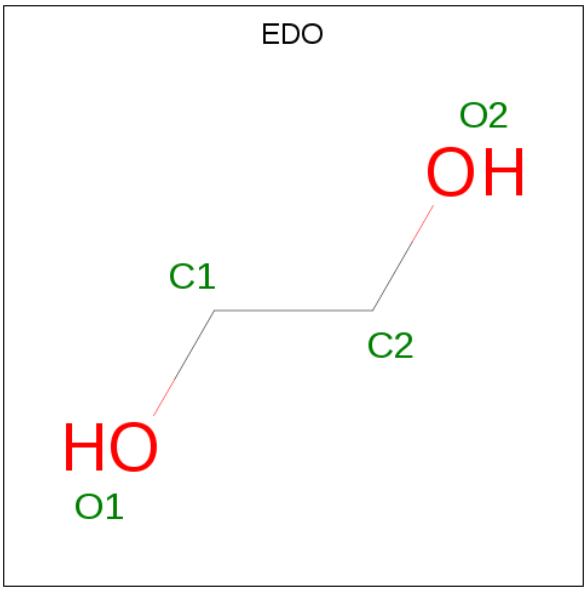
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

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

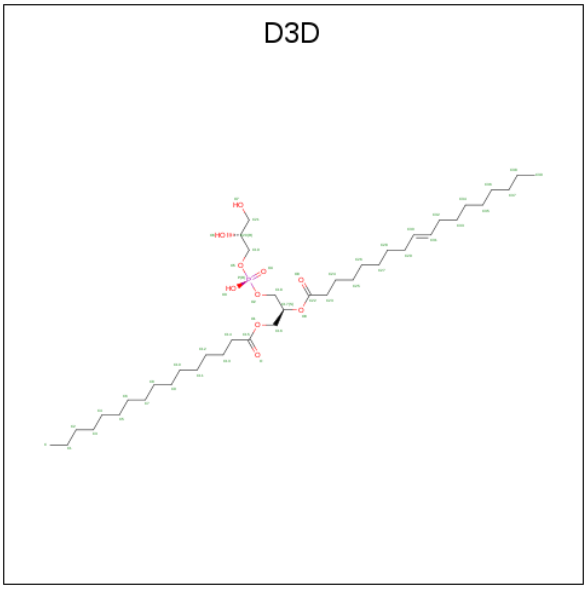
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0
9	A	1	Total Na 1 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is (19S,22R,25R)-22,25,26-trihydroxy-16,22-dioxo-17,21,23-trioxa-22lambda 5 -phosphahexacosan-19-yl (9E)-octadec-9-enoate (three-letter code: D3D) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	H	O	P	0	0
			120	38	71	10	1		

- Molecule 12 is water.

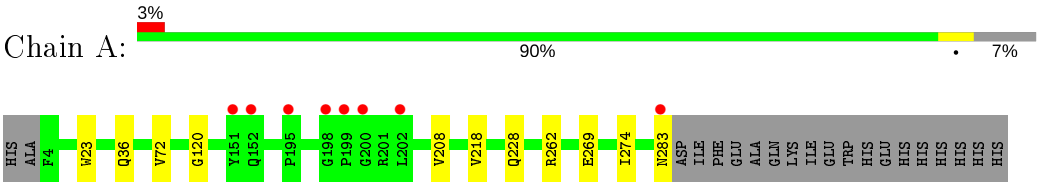
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	496	Total	O	0	0
			496	496		
12	B	161	Total	O	0	0
			161	161		

3 Residue-property plots (i)

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

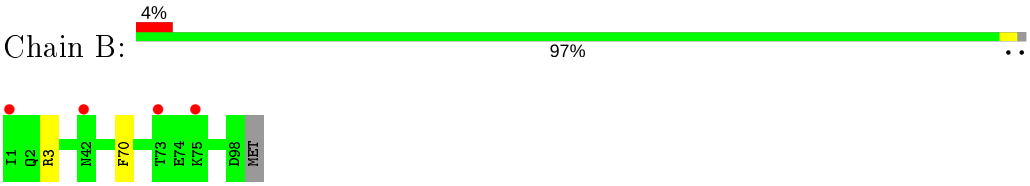
• Molecule 1: T-cell surface glycoprotein CD1b

Chain A:



• Molecule 2: Beta-2-microglobulin

Chain B:

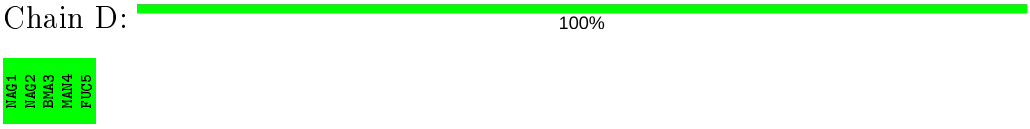


• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

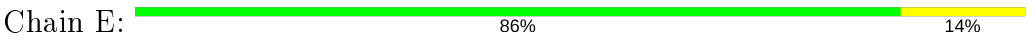
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 5: 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 E:




NAG1
NAG2
BMA3
MAN4
MAN5
FUC6
FUC7

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.89Å 80.28Å 92.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.34 – 1.38 27.63 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.34-1.38) 98.2 (27.63-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.38Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.188 , 0.206 0.194 , 0.208	Depositor DCC
R_{free} test set	4336 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	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	7131	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, NA, EDO, CUY, FUC, D3D, IOD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/2375	0.66	0/3224
2	B	0.43	0/860	0.60	0/1167
All	All	0.48	0/3235	0.64	0/4391

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	2249	2074	2091	10	0
2	B	816	729	743	1	0
3	C	48	47	43	2	0
4	D	60	54	52	0	0
5	E	81	75	70	0	0
6	A	35	52	0	1	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	4	6	0	0	0
11	A	49	71	0	4	0
12	A	496	0	0	7	0
12	B	161	0	0	0	0
All	All	4011	3120	3011	14	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 (14) 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:283:ASN:C	12:A:502:HOH:O	2.18	0.82
1:A:228:GLN:HG3	12:A:804:HOH:O	1.79	0.81
11:A:423:D3D:C16	12:A:501:HOH:O	2.29	0.79
1:A:269:GLU:HG3	12:A:503:HOH:O	1.95	0.67
11:A:423:D3D:O2	12:A:501:HOH:O	2.15	0.63
1:A:208:VAL:HG21	1:A:218[B]:VAL:HG11	1.83	0.60
3:C:1:NAG:H62	3:C:4:FUC:O2	2.02	0.60
6:A:401:CUY:C2	11:A:423:D3D:C37	2.84	0.56
1:A:23:TRP:CZ2	3:C:3:NAG:H82	2.44	0.52
1:A:228:GLN:CG	12:A:804:HOH:O	2.47	0.50
1:A:72:VAL:HG21	11:A:423:D3D:C21	2.45	0.46
1:A:36:GLN:NE2	12:A:504:HOH:O	2.51	0.43
1:A:120:GLY:O	2:B:3:ARG:NH2	2.48	0.42
1:A:262[B]:ARG:CZ	1:A:274:ILE:HD11	2.49	0.42

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	299/300 (100%)	297 (99%)	2 (1%)	0	100	100
2	B	100/99 (101%)	100 (100%)	0	0	100	100
All	All	399/399 (100%)	397 (100%)	2 (0%)	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	242/247 (98%)	242 (100%)	0	100	100
2	B	93/94 (99%)	92 (99%)	1 (1%)	73	48
All	All	335/341 (98%)	334 (100%)	1 (0%)	92	82

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

Mol	Chain	Res	Type
2	B	70	PHE

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

Mol	Chain	Res	Type
1	A	36	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)

16 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	0.56	0	17,19,21	2.63	5 (29%)
3	FUC	C	2	3	10,10,11	0.27	0	14,14,16	0.41	0
3	NAG	C	3	3	14,14,15	0.37	0	17,19,21	1.13	1 (5%)
3	FUC	C	4	3	10,10,11	0.59	0	14,14,16	1.03	2 (14%)
4	NAG	D	1	1,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	D	2	4	14,14,15	0.34	0	17,19,21	0.84	0
4	BMA	D	3	4	11,11,12	0.22	0	15,15,17	0.76	0
4	MAN	D	4	4	11,11,12	0.25	0	15,15,17	0.52	0
4	FUC	D	5	4	10,10,11	0.29	0	14,14,16	0.83	0
5	NAG	E	1	1,5	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.70	0
5	BMA	E	3	5	11,11,12	0.22	0	15,15,17	0.83	0
5	MAN	E	4	5	11,11,12	0.25	0	15,15,17	0.61	0
5	MAN	E	5	5	11,11,12	0.25	0	15,15,17	0.70	0
5	FUC	E	6	5	10,10,11	0.25	0	14,14,16	0.32	0
5	FUC	E	7	5	10,10,11	0.32	0	14,14,16	0.42	0

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

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C1-O5-C5	8.62	123.88	112.19
3	C	3	NAG	O5-C1-C2	-4.03	104.92	111.29
3	C	1	NAG	O5-C1-C2	-3.89	105.14	111.29
3	C	4	FUC	C1-C2-C3	2.81	113.12	109.67
3	C	1	NAG	O5-C5-C6	-2.80	102.82	107.20
3	C	1	NAG	C1-C2-N2	-2.64	105.98	110.49
5	E	1	NAG	O5-C1-C2	-2.40	107.50	111.29
3	C	1	NAG	O5-C5-C4	2.17	116.11	110.83
3	C	4	FUC	O2-C2-C1	2.04	113.32	109.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	3	NAG	C4-C5-C6-O6
3	C	3	NAG	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

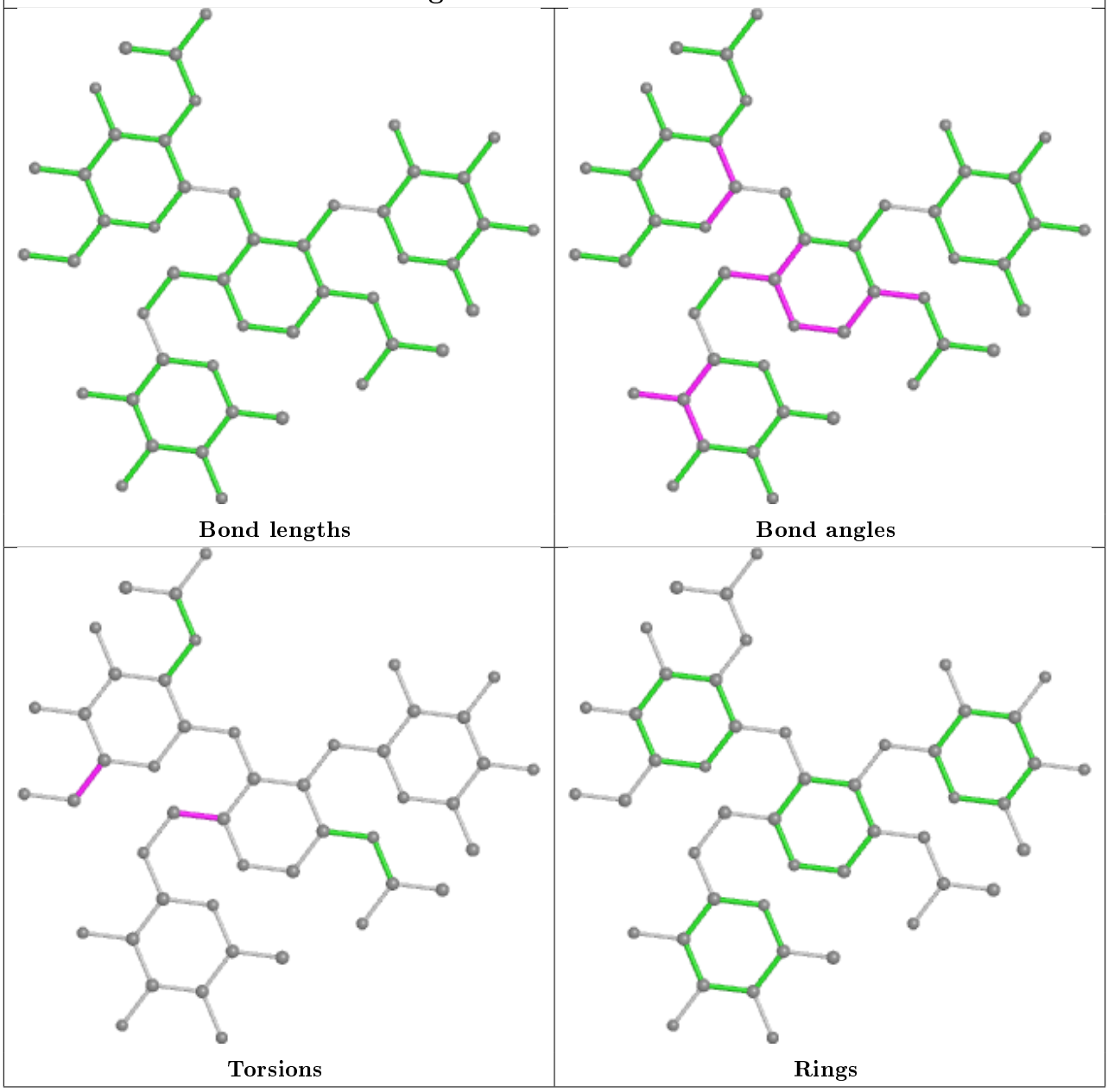
There are no ring outliers.

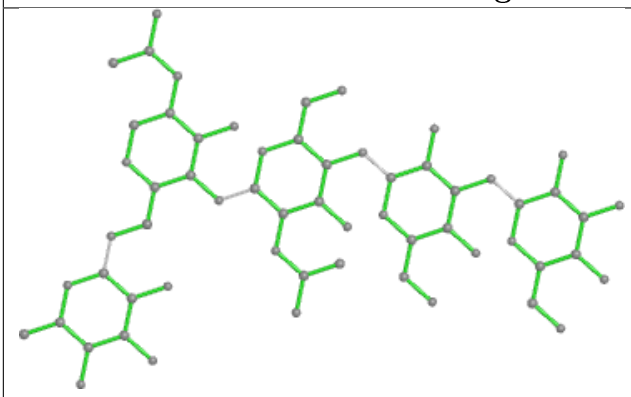
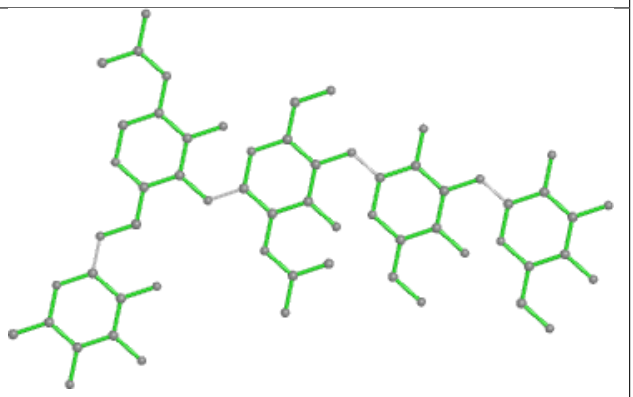
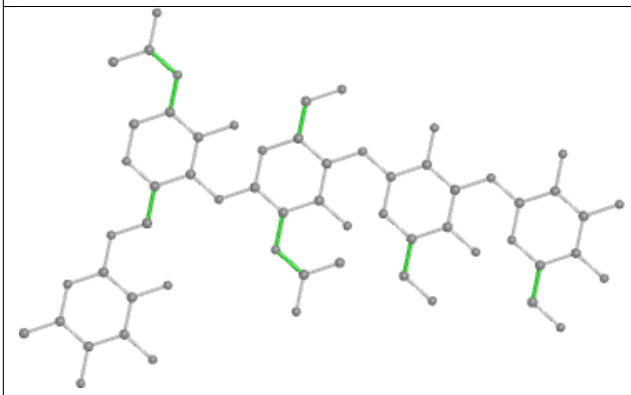
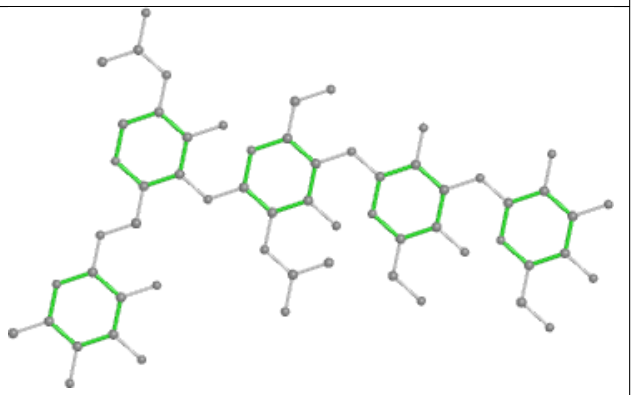
3 monomers are involved in 2 short contacts:

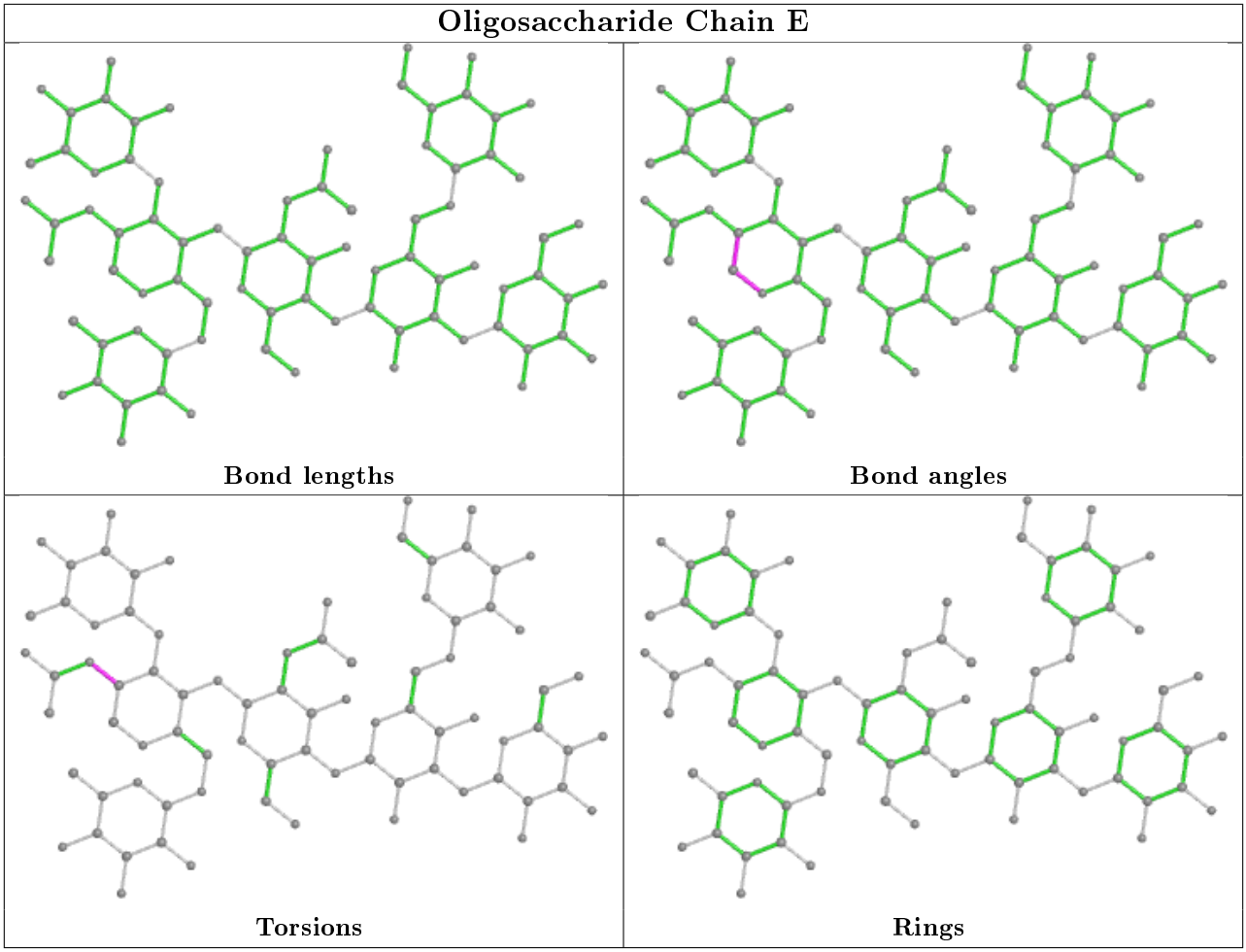
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	NAG	1	0
3	C	4	FUC	1	0
3	C	1	NAG	1	0

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



Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
10	EDO	A	421	-	3,3,3	0.67	0	2,2,2	0.30	0
6	CUY	A	401	-	34,34,43	0.69	1 (2%)	34,34,43	0.84	1 (2%)
11	D3D	A	423	-	48,48,50	0.96	3 (6%)	51,54,56	1.16	3 (5%)
10	EDO	B	101	-	3,3,3	3.56	2 (66%)	2,2,2	0.76	0
10	EDO	A	422	-	3,3,3	0.57	0	2,2,2	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	A	421	-	-	1/1/1/1	-
6	CUY	A	401	-	-	10/33/33/42	-
11	D3D	A	423	-	-	13/53/53/55	-
10	EDO	B	101	-	-	0/1/1/1	-
10	EDO	A	422	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	101	EDO	C2-C1	-4.32	1.18	1.48
10	B	101	EDO	O1-C1	-4.20	1.20	1.42
6	A	401	CUY	OAQ-CAP	2.80	1.41	1.33
11	A	423	D3D	O8-C22	2.71	1.42	1.34
11	A	423	D3D	O1-C16	-2.68	1.39	1.45
11	A	423	D3D	O1-C15	2.26	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	423	D3D	C18-C17-C16	-4.84	100.35	111.79
11	A	423	D3D	O1-C16-C17	2.69	116.25	108.43
6	A	401	CUY	OAQ-CAP-CAO	2.66	120.24	111.91
11	A	423	D3D	O8-C22-C23	2.58	117.07	111.50

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	423	D3D	C7-C8-C9-C10
6	A	401	CUY	CAF-CAG-CAH-CAI
11	A	423	D3D	C23-C24-C25-C26
6	A	401	CUY	CAG-CAH-CAI-CAJ
11	A	423	D3D	C25-C26-C27-C28
10	A	422	EDO	O1-C1-C2-O2
11	A	423	D3D	C9-C10-C11-C12
6	A	401	CUY	CAS-CAT-CAU-CAV
11	A	423	D3D	C4-C5-C6-C7

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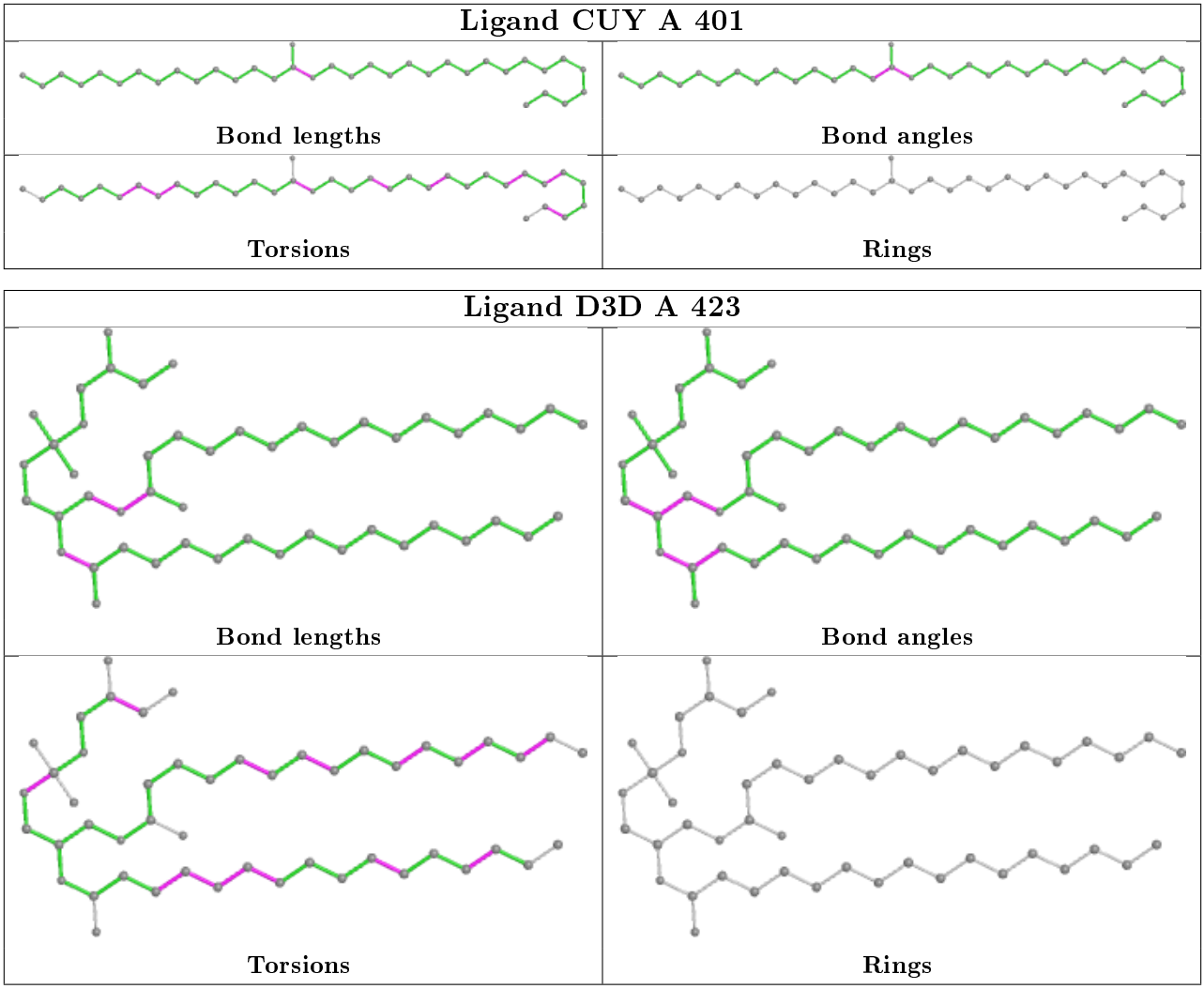
Mol	Chain	Res	Type	Atoms
10	A	421	EDO	O1-C1-C2-O2
11	A	423	D3D	C26-C27-C28-C29
11	A	423	D3D	C-C1-C2-C3
6	A	401	CUY	CAV-CAW-CBM-CBL
6	A	401	CUY	CBF-CBG-CBH-CBI
6	A	401	CUY	CAO-CAP-OAQ-CAR
6	A	401	CUY	OBO-CAP-OAQ-CAR
11	A	423	D3D	C18-O2-P-O5
11	A	423	D3D	C30-C31-C32-C33
11	A	423	D3D	C24-C25-C26-C27
11	A	423	D3D	C33-C34-C35-C36
6	A	401	CUY	CAH-CAI-CAJ-CAK
11	A	423	D3D	C2-C3-C4-C5
11	A	423	D3D	O6-C20-C21-O7
6	A	401	CUY	CBH-CBI-CBJ-CBK
6	A	401	CUY	C2-C1-CBD-CBE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	CUY	1	0
11	A	423	D3D	4	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.



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, 95^{th} 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%)	0.04	8 (2%) 51 54	9, 17, 35, 61	0
2	B	98/99 (98%)	0.24	4 (4%) 37 39	10, 21, 45, 48	0
All	All	378/399 (94%)	0.09	12 (3%) 47 49	9, 17, 40, 61	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLN	6.0
1	A	151	TYR	4.4
2	B	1	ILE	3.8
1	A	200	GLY	2.7
1	A	195	PRO	2.6
2	B	75	LYS	2.6
1	A	199	PRO	2.5
2	B	42	ASN	2.5
2	B	73	THR	2.3
1	A	198	GLY	2.2
1	A	202	LEU	2.1
1	A	283	ASN	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

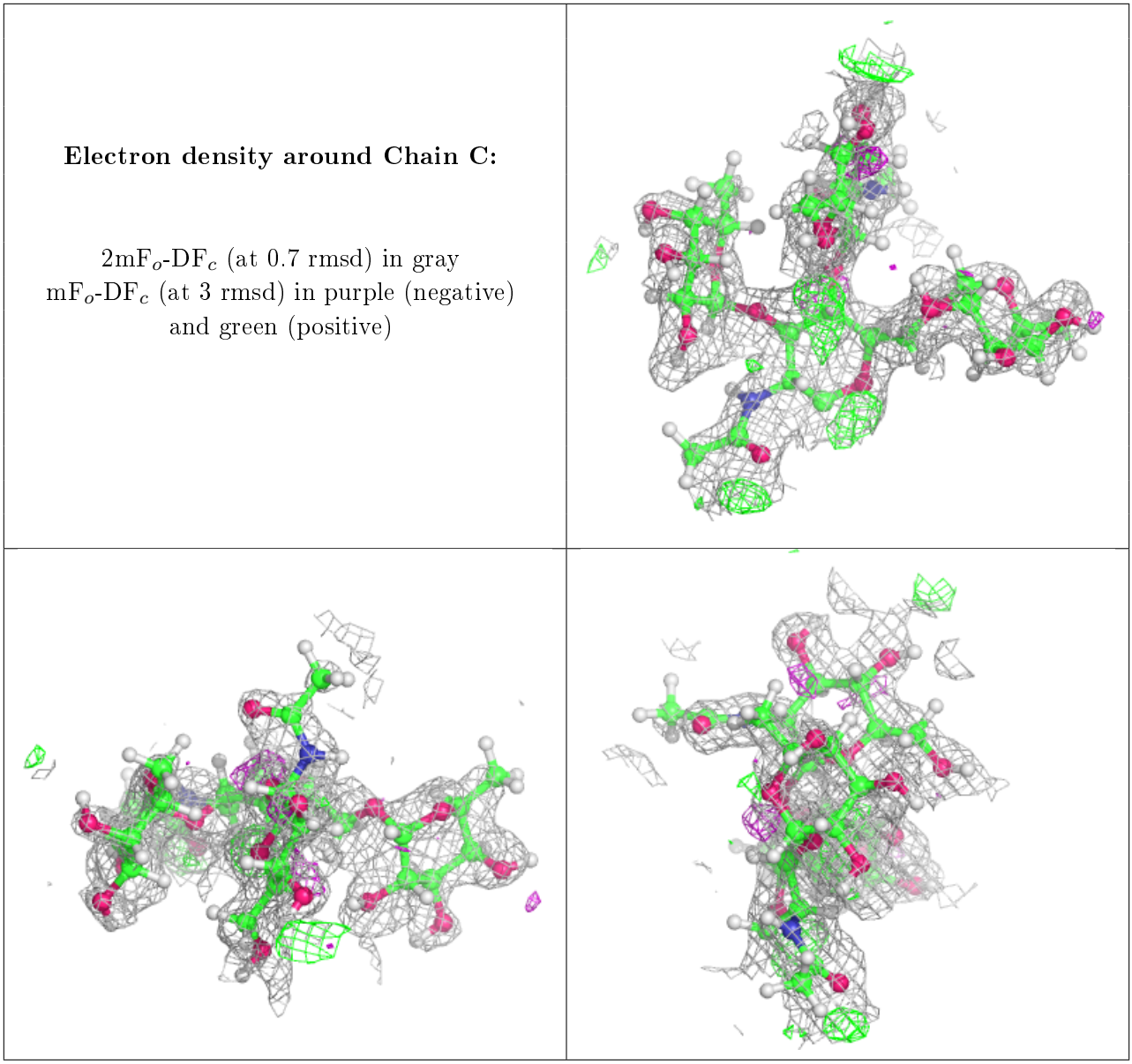
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	C	2	10/11	0.48	0.26	60,65,66,66	0
3	NAG	C	1	14/15	0.61	0.19	42,44,48,55	0
4	NAG	D	2	14/15	0.64	0.30	39,42,45,47	0
4	FUC	D	5	10/11	0.69	0.33	45,48,50,51	0
4	NAG	D	1	14/15	0.69	0.26	39,44,50,50	0
3	NAG	C	3	14/15	0.70	0.27	36,39,41,43	0
3	FUC	C	4	10/11	0.72	0.25	41,42,46,46	0
4	MAN	D	4	11/12	0.72	0.23	33,37,40,41	0
4	BMA	D	3	11/12	0.79	0.33	37,42,47,48	0
5	FUC	E	6	10/11	0.90	0.10	15,20,24,24	0
5	MAN	E	5	11/12	0.93	0.09	12,15,18,19	0
5	MAN	E	4	11/12	0.94	0.09	15,18,20,21	0
5	FUC	E	7	10/11	0.95	0.07	15,18,21,22	0
5	NAG	E	2	14/15	0.97	0.06	7,12,17,23	0
5	BMA	E	3	11/12	0.97	0.07	11,13,16,18	0
5	NAG	E	1	14/15	0.98	0.05	8,12,15,16	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

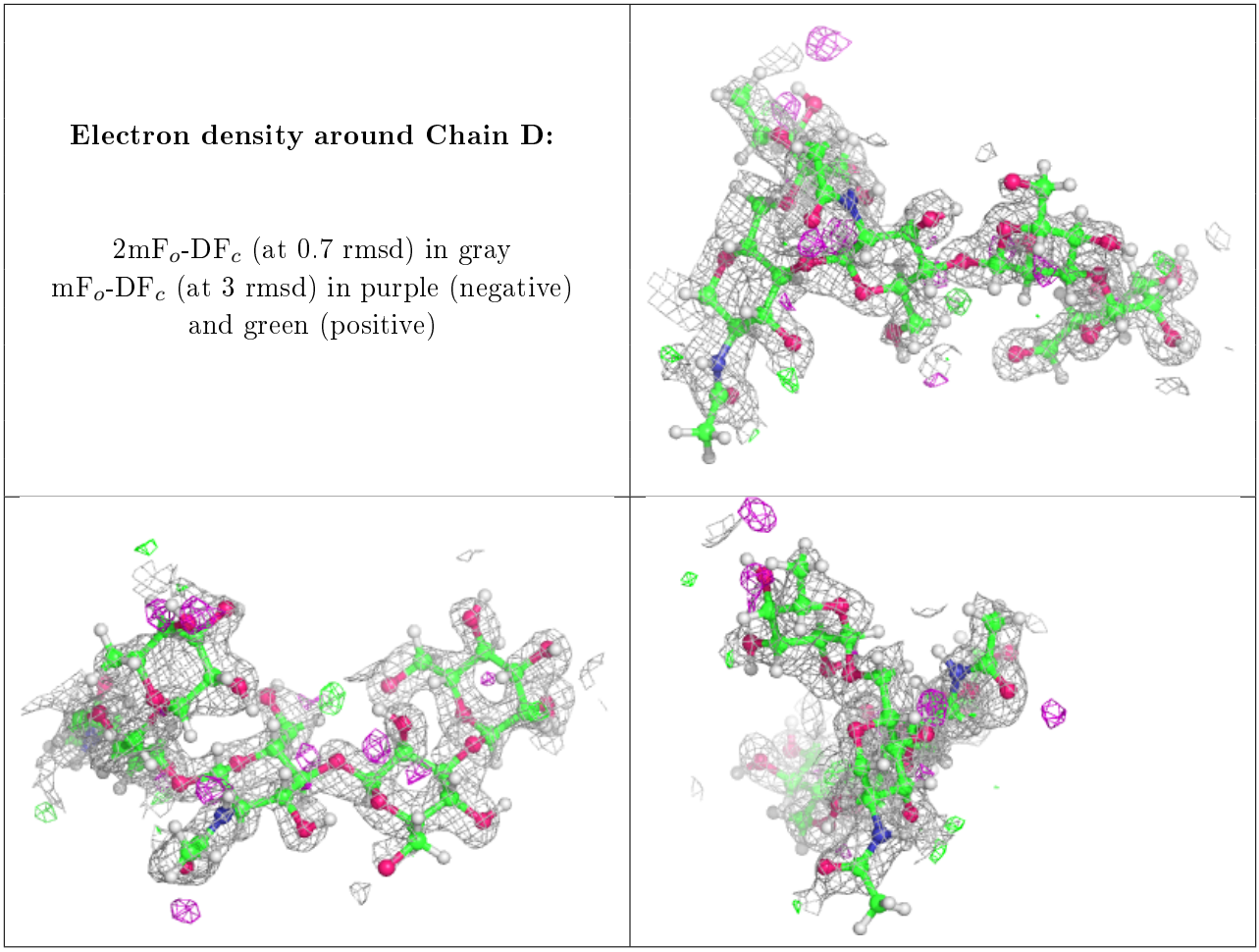
Electron density around Chain C:

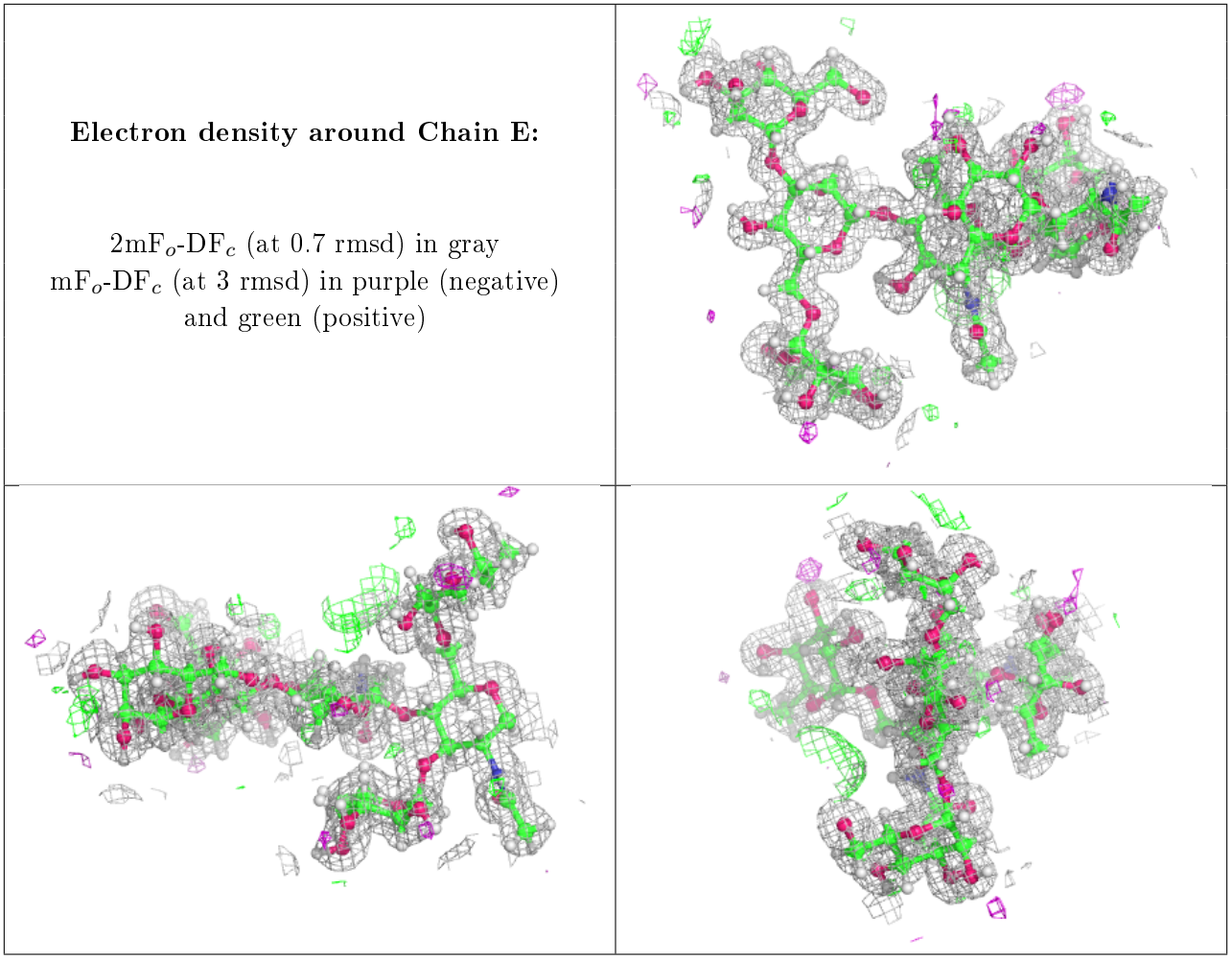
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain D:

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





6.4 Ligands

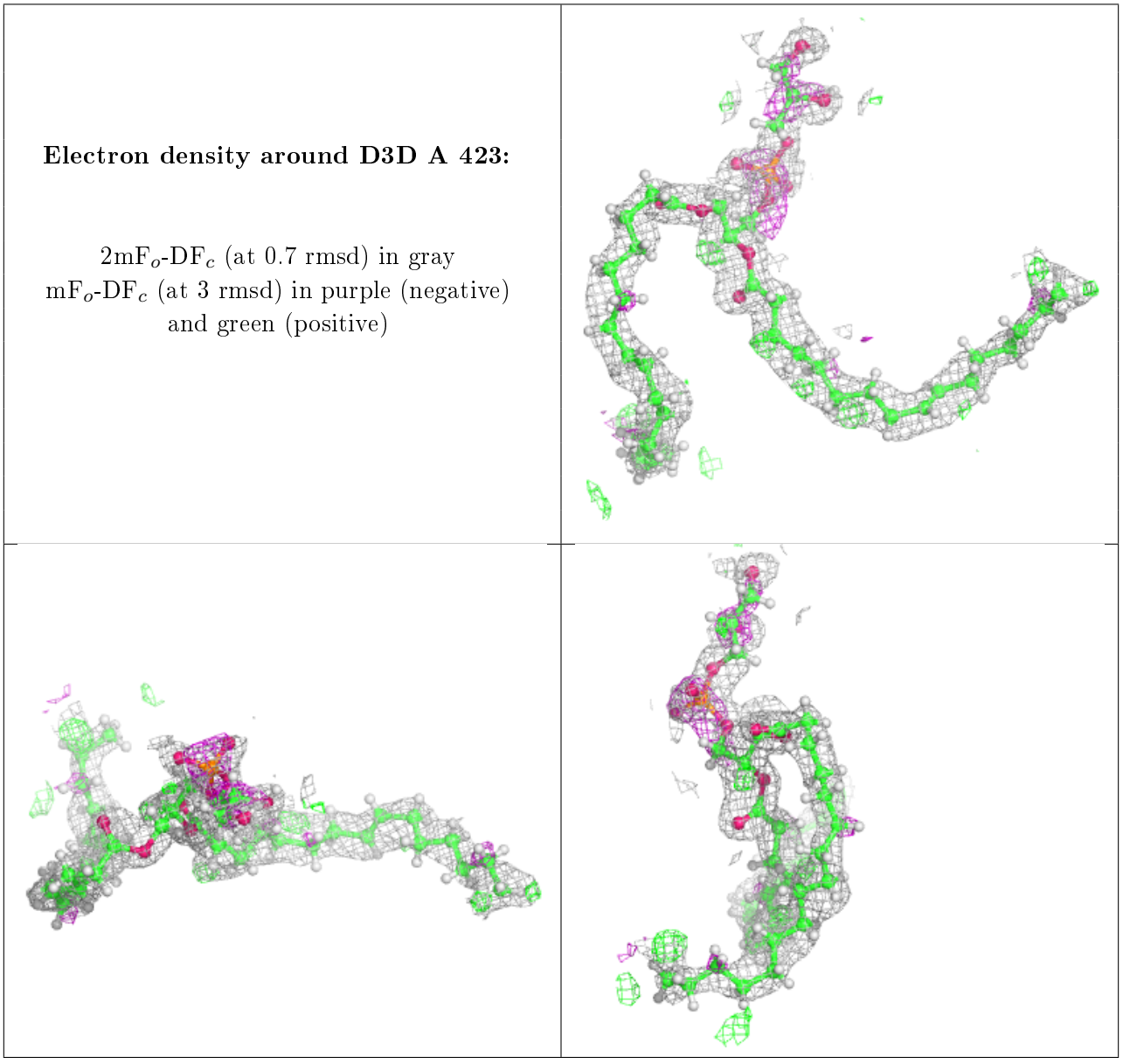
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
10	EDO	A	421	4/4	0.58	0.24	39,40,40,40	0
11	D3D	A	423	49/51	0.59	0.20	29,30,34,38	0
6	CUY	A	401	35/44	0.69	0.16	31,35,38,39	0
10	EDO	A	422	4/4	0.81	0.15	41,43,43,43	0
10	EDO	B	101	4/4	0.93	0.25	3,12,25,26	0
9	NA	A	420	1/1	0.96	0.07	23,23,23,23	0
8	CL	A	419	1/1	0.98	0.08	17,17,17,17	0
9	NA	B	102	1/1	0.99	0.07	16,16,16,16	0
7	IOD	A	402	1/1	0.99	0.22	6,6,6,6	1

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.

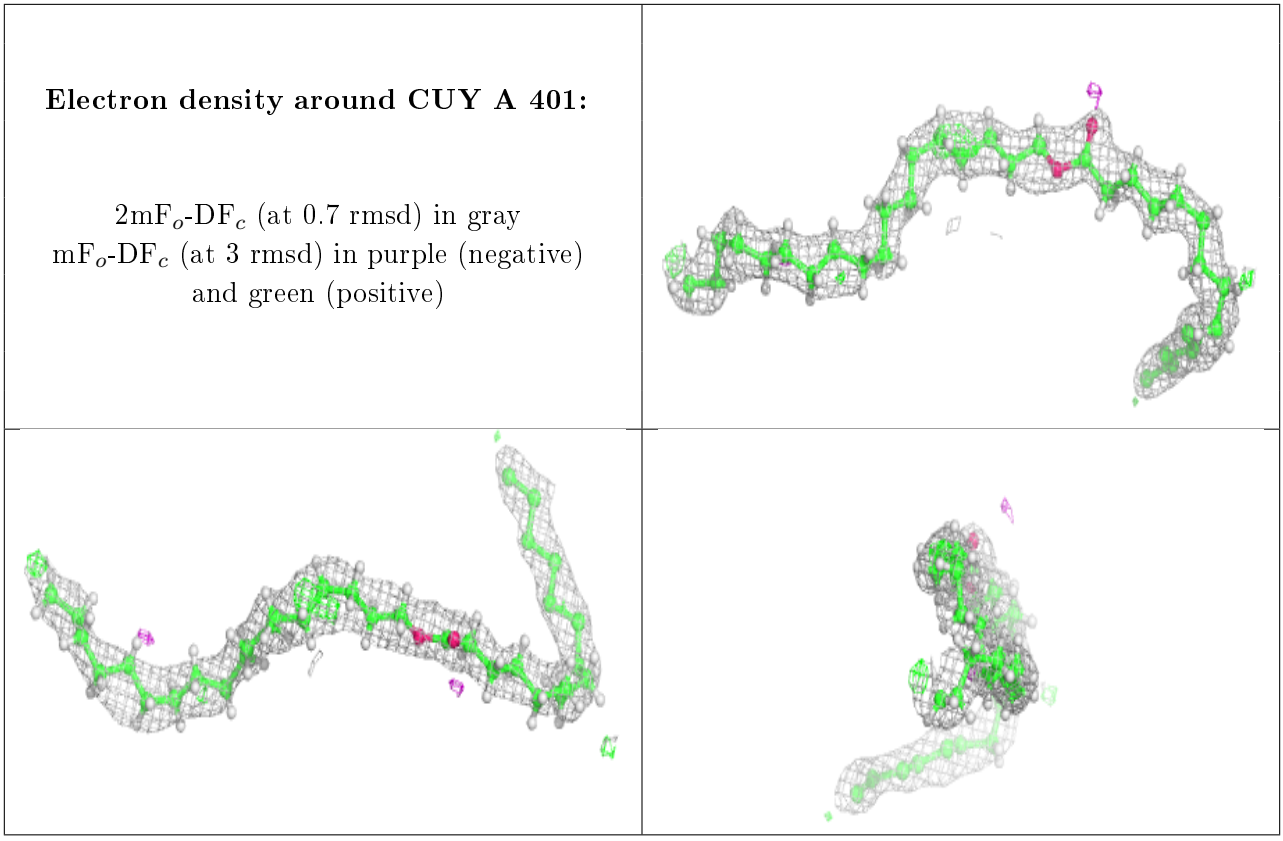
Electron density around D3D A 423:

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



Electron density around CUY A 401:

$2mF_o$-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.