Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 02:00 AM EDT

PDB ID	:	3UET
Title	:	Crystal structure of alpha-1,3/4-fucosidase from Bifidobacterium longum subsp. infantis D172A/E217A mutant complexed with lacto-N-fucopentaose II
Authors	:	Sakurama, H.; Fushinobu, S.; Yoshida, E.; Honda, Y.; Hidaka, M.; Ashida, H.; Kitaoka, M.; Katayama, T.; Yamamoto, K.; Kumagai, H.
Deposited on	:	2011-10-31
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

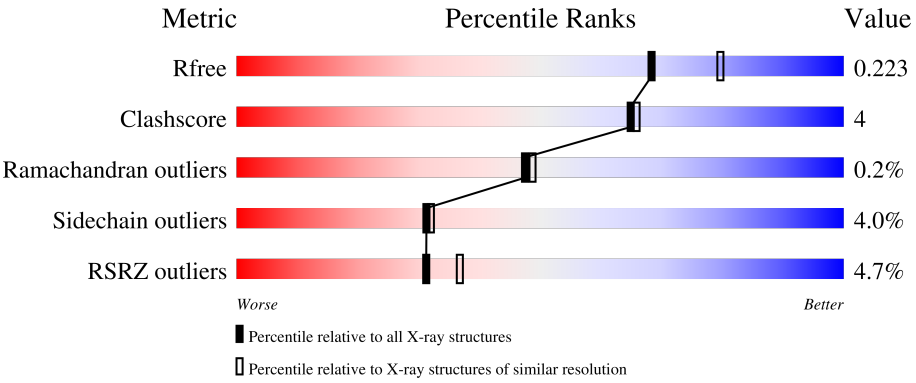
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	478	6% 82% 12% • 5%
1	B	478	3% 83% 10% • 5%
2	C	3	100%
2	D	3	33% 67%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7683 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.

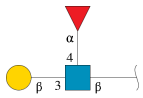
- Molecule 1 is a protein called Alpha-1,3/4-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3569	2234	644	678	13			
1	B	456	Total	C	N	O	S	0	0	0
			3569	2234	644	678	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	ALA	ASP	engineered mutation	UNP B7GNN8
A	217	ALA	GLU	engineered mutation	UNP B7GNN8
B	172	ALA	ASP	engineered mutation	UNP B7GNN8
B	217	ALA	GLU	engineered mutation	UNP B7GNN8

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	D	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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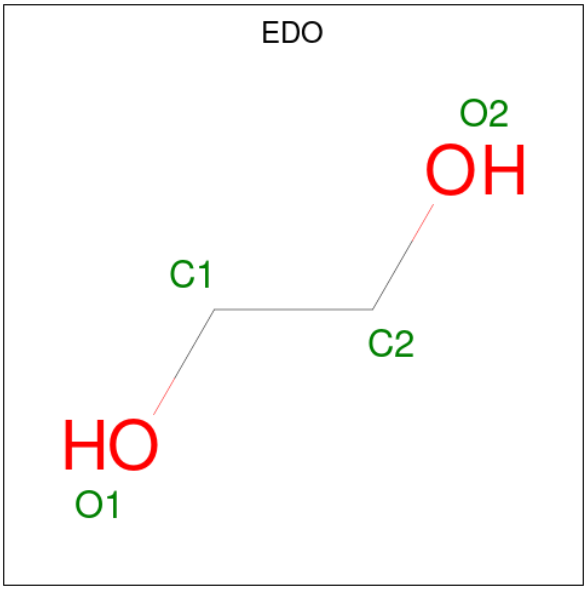
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

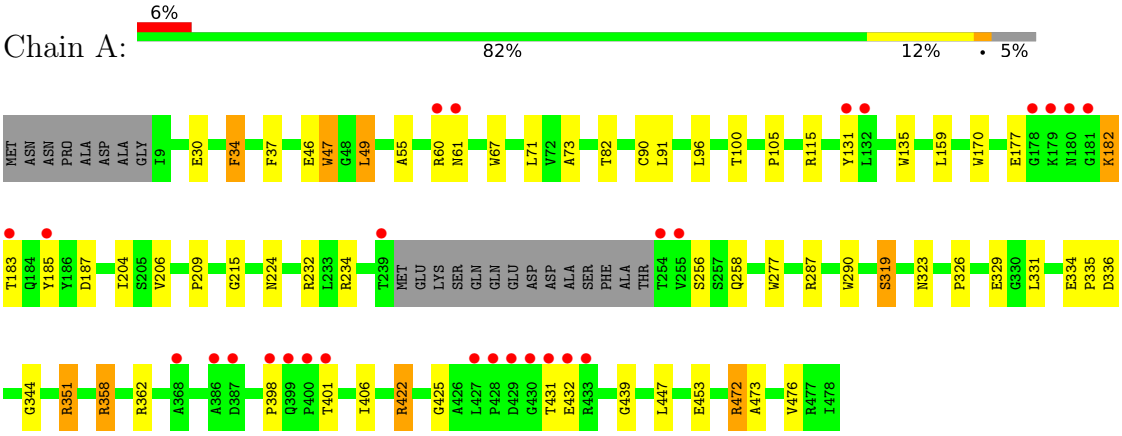
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	218	Total O 218 218	0	0
5	B	245	Total O 245 245	0	0

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.

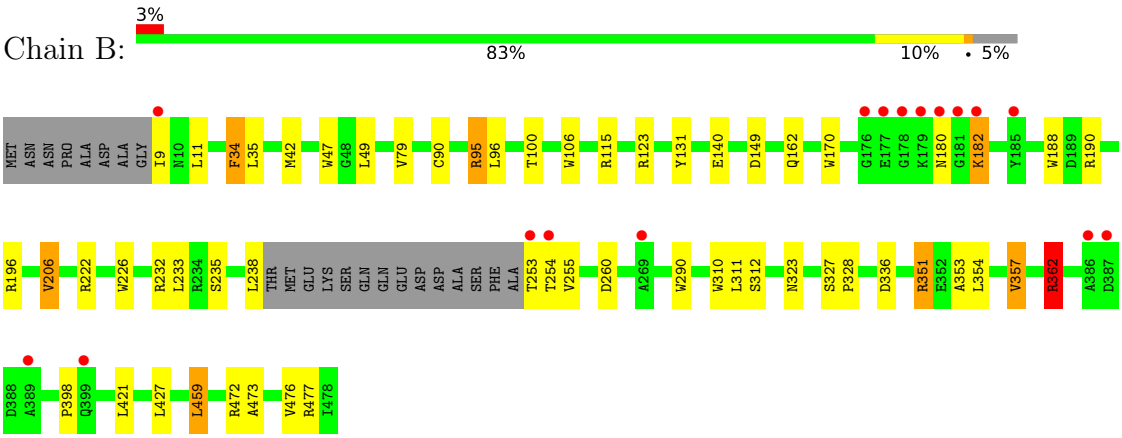
• Molecule 1: Alpha-1,3/4-fucosidase

Chain A:



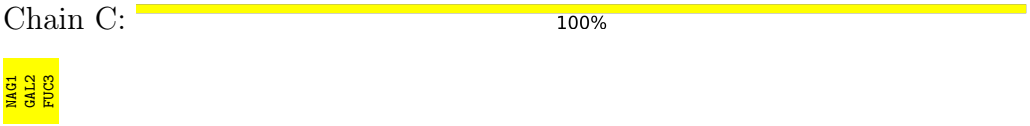
• Molecule 1: Alpha-1,3/4-fucosidase

Chain B:



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

Chain C:



• Molecule 2: beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]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	82.59Å 105.97Å 120.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.05 – 2.10 32.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (32.05-2.10) 96.1 (32.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.173 , 0.223 0.173 , 0.223	Depositor DCC
R_{free} test set	3047 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7683	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: EDO, FUC, NA, NAG, GAL

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	1.04	5/3656 (0.1%)	1.04	11/4974 (0.2%)
1	B	1.09	8/3656 (0.2%)	1.03	10/4974 (0.2%)
All	All	1.07	13/7312 (0.2%)	1.03	21/9948 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	TRP	CD2-CE2	6.83	1.49	1.41
1	B	47	TRP	CG-CD1	6.59	1.46	1.36
1	A	135	TRP	CD2-CE2	6.38	1.49	1.41
1	A	47	TRP	CD2-CE2	6.00	1.48	1.41
1	B	290	TRP	CD2-CE2	5.96	1.48	1.41
1	B	106	TRP	CD2-CE2	5.83	1.48	1.41
1	A	290	TRP	CD2-CE2	5.60	1.48	1.41
1	A	277	TRP	CD2-CE2	5.56	1.48	1.41
1	B	312	SER	CB-OG	-5.37	1.35	1.42
1	B	226	TRP	CD2-CE2	5.08	1.47	1.41
1	A	170	TRP	CD2-CE2	5.06	1.47	1.41
1	B	188	TRP	CD2-CE2	5.01	1.47	1.41
1	B	310	TRP	CD2-CE2	5.00	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	B	149	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	115	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	222	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	351	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	362	ARG	NE-CZ-NH1	6.83	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	B	115	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	190	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	351	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	187	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	319	SER	CB-CA-C	5.74	121.00	110.10
1	A	422	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	123	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	311	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	232	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	234	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	115	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	49	LEU	CB-CG-CD1	5.14	119.73	111.00
1	A	422	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	196	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3569	0	3429	30	0
1	B	3569	0	3430	26	0
2	C	36	0	33	0	0
2	D	36	0	34	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	218	0	0	4	0
5	B	245	0	0	3	0
All	All	7683	0	6938	57	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 4.

All (57) 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:61:ASN:HB3	5:A:653:HOH:O	1.71	0.89
1:B:362:ARG:HH11	1:B:362:ARG:HG3	1.35	0.88
1:B:232:ARG:HH22	1:B:254:THR:HG22	1.59	0.67
1:B:362:ARG:HG3	1:B:362:ARG:NH1	2.09	0.67
1:B:362:ARG:HH11	1:B:362:ARG:CG	2.09	0.66
1:A:82:THR:HA	1:A:131:TYR:HB3	1.79	0.65
1:B:232:ARG:NH2	1:B:254:THR:HG22	2.13	0.64
1:B:42:MET:HE3	5:B:586:HOH:O	1.97	0.63
1:B:95:ARG:HH22	1:B:162:GLN:HE22	1.45	0.63
1:A:183:THR:CG2	1:A:185:TYR:HE2	2.14	0.61
1:B:233:LEU:HD21	1:B:255:VAL:HG12	1.83	0.58
1:A:183:THR:HG22	1:A:185:TYR:CE2	2.37	0.58
1:A:30:GLU:OE1	1:A:351:ARG:NH2	2.29	0.58
1:A:183:THR:CG2	1:A:185:TYR:CE2	2.87	0.58
1:B:35:LEU:HD11	1:B:79:VAL:HG21	1.84	0.58
1:B:95:ARG:HH22	1:B:162:GLN:NE2	2.02	0.57
1:A:204:ILE:HB	1:A:209:PRO:HD2	1.86	0.56
1:A:351:ARG:NH2	5:A:578:HOH:O	2.37	0.56
1:A:224:ASN:OD1	1:A:439:GLY:HA3	2.06	0.55
1:A:406:ILE:C	1:A:406:ILE:HD12	2.27	0.55
1:A:183:THR:HG21	1:A:185:TYR:HE2	1.71	0.54
1:A:215:GLY:O	1:A:258:GLN:HG3	2.08	0.53
2:D:1:NAG:C4	2:D:3:FUC:C1	2.84	0.52
1:B:35:LEU:CD1	1:B:79:VAL:HG21	2.39	0.52
1:B:90:CYS:HB2	1:B:100:THR:HG22	1.93	0.51
1:B:353:ALA:O	1:B:357:VAL:HG22	2.10	0.51
1:B:353:ALA:HB1	1:B:476:VAL:CG2	2.41	0.50
1:A:472:ARG:HG3	1:A:473:ALA:N	2.27	0.48
1:B:476:VAL:HG22	1:B:477:ARG:N	2.29	0.47
1:A:37:PHE:CD1	1:A:326:PRO:HB2	2.50	0.46
1:B:180:ASN:ND2	1:B:182:LYS:HD3	2.31	0.46
1:B:421:LEU:HD11	1:B:459:LEU:HB3	1.97	0.46
1:B:95:ARG:NH2	5:B:603:HOH:O	2.49	0.45
1:A:67:TRP:O	1:A:71:LEU:HG	2.17	0.45
1:A:60:ARG:HG2	5:A:619:HOH:O	2.17	0.45
1:A:73:ALA:O	1:A:344:GLY:HA3	2.16	0.45
1:A:91:LEU:N	1:A:91:LEU:HD22	2.31	0.45
1:B:351:ARG:NH2	5:B:539:HOH:O	2.49	0.45
1:A:425:GLY:O	1:A:432:GLU:HA	2.17	0.45
1:A:358:ARG:O	1:A:398:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TRP:CZ2	1:B:206:VAL:HG21	2.54	0.43
1:B:34:PHE:HB3	1:B:323:ASN:HB2	2.01	0.43
1:B:472:ARG:HG2	1:B:473:ALA:N	2.34	0.43
1:A:401:THR:O	1:A:453:GLU:HA	2.19	0.43
1:A:334:GLU:N	1:A:335:PRO:CD	2.83	0.42
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.84	0.42
1:A:90:CYS:HB2	1:A:100:THR:HG22	2.02	0.41
1:A:177:GLU:OE1	1:A:182:LYS:N	2.49	0.41
1:B:235:SER:HA	1:B:238:LEU:HG	2.03	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.91	0.41
1:B:327:SER:HB2	1:B:328:PRO:HD2	2.01	0.41
1:A:287:ARG:HD3	5:A:486:HOH:O	2.21	0.41
1:A:329:GLU:OE1	1:A:331:LEU:HD12	2.21	0.41
1:A:55:ALA:HA	1:A:105:PRO:HD3	2.02	0.40
1:A:46:GLU:O	1:A:47:TRP:HD1	2.03	0.40
1:A:34:PHE:HB3	1:A:323:ASN:HB2	2.04	0.40
1:B:9:ILE:HG23	1:B:9:ILE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/478 (95%)	434 (96%)	17 (4%)	1 (0%)	47	49
1	B	452/478 (95%)	437 (97%)	14 (3%)	1 (0%)	47	49
All	All	904/956 (95%)	871 (96%)	31 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	VAL

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Mol	Chain	Res	Type
1	B	206	VAL

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	374/391 (96%)	360 (96%)	14 (4%)	34	35
1	B	374/391 (96%)	358 (96%)	16 (4%)	29	29
All	All	748/782 (96%)	718 (96%)	30 (4%)	31	32

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	PHE
1	A	49	LEU
1	A	96	LEU
1	A	182	LYS
1	A	256	SER
1	A	319	SER
1	A	336	ASP
1	A	358	ARG
1	A	362	ARG
1	A	422	ARG
1	A	431	THR
1	A	447	LEU
1	A	472	ARG
1	A	476	VAL
1	B	11	LEU
1	B	34	PHE
1	B	49	LEU
1	B	95	ARG
1	B	96	LEU
1	B	131	TYR
1	B	140	GLU
1	B	182	LYS

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Mol	Chain	Res	Type
1	B	253	THR
1	B	260	ASP
1	B	336	ASP
1	B	357	VAL
1	B	362	ARG
1	B	398	PRO
1	B	427	LEU
1	B	459	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	ASN
1	B	162	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)

6 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	$\#\|Z\| > 2$
2	NAG	C	1	2	15,15,15	1.29	1 (6%)	21,21,21	1.85	5 (23%)
2	GAL	C	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.48	3 (20%)
2	FUC	C	3	2	10,10,11	1.32	1 (10%)	14,14,16	1.25	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	1	2	15,15,15	1.05	1 (6%)	21,21,21	1.98	5 (23%)
2	GAL	D	2	2	11,11,12	0.82	1 (9%)	15,15,17	1.90	3 (20%)
2	FUC	D	3	2	10,10,11	0.85	0	14,14,16	2.03	2 (14%)

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
2	NAG	C	1	2	-	4/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	NAG	D	1	2	-	4/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	3.49	1.57	1.52
2	C	3	FUC	C2-C3	3.19	1.57	1.52
2	D	1	NAG	C1-C2	2.80	1.56	1.52
2	C	2	GAL	O5-C1	-2.26	1.40	1.43
2	D	2	GAL	O5-C1	-2.25	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	FUC	C1-O5-C5	6.47	127.44	112.78
2	D	1	NAG	O1-C1-C2	5.38	120.39	109.22
2	C	1	NAG	O1-C1-C2	4.67	118.93	109.22
2	D	2	GAL	C1-C2-C3	-4.39	104.27	109.67
2	D	2	GAL	C1-O5-C5	-3.99	106.78	112.19
2	C	2	GAL	O2-C2-C1	-3.82	101.33	109.15
2	D	1	NAG	C1-C2-N2	3.65	114.96	110.73
2	D	1	NAG	C1-C2-C3	-3.38	105.94	110.54
2	D	1	NAG	O6-C6-C5	-3.26	100.11	111.29
2	C	1	NAG	O6-C6-C5	-3.21	100.29	111.29
2	C	1	NAG	O3-C3-C2	3.12	115.97	109.66
2	C	1	NAG	C1-C2-C3	-2.52	107.11	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	FUC	O5-C5-C4	2.42	113.86	109.52
2	C	1	NAG	C2-N2-C7	2.39	129.00	123.18
2	D	1	NAG	O7-C7-C8	-2.38	117.64	122.06
2	C	2	GAL	O5-C1-C2	2.34	114.38	110.77
2	D	3	FUC	O3-C3-C2	-2.14	105.90	109.99
2	C	2	GAL	C1-C2-C3	-2.13	107.04	109.67
2	D	2	GAL	O3-C3-C2	2.10	114.02	109.99
2	C	3	FUC	C1-O5-C5	2.06	117.44	112.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7
2	D	2	GAL	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	D	2	GAL	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7

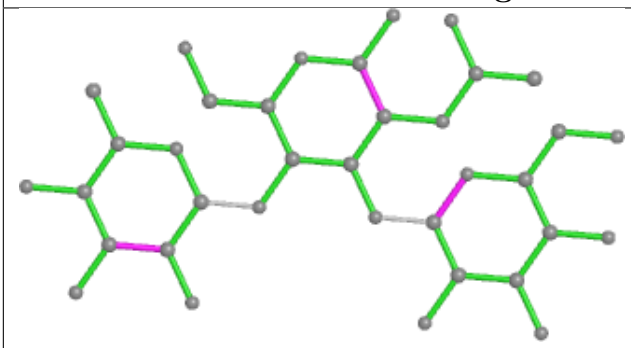
There are no ring outliers.

2 monomers are involved in 1 short contact:

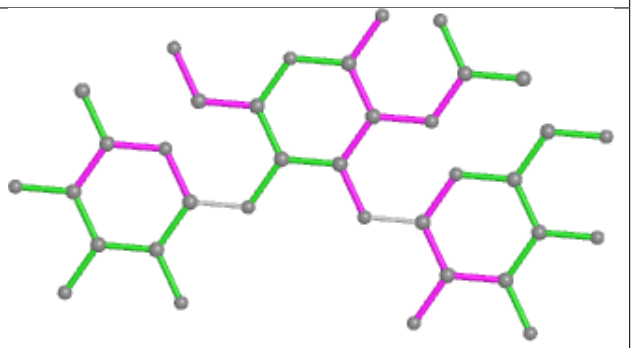
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	FUC	1	0
2	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

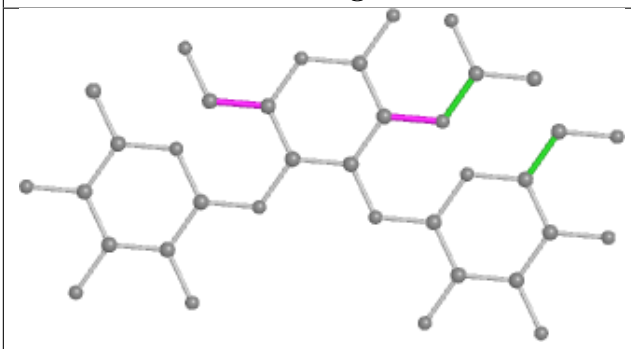
Oligosaccharide Chain C



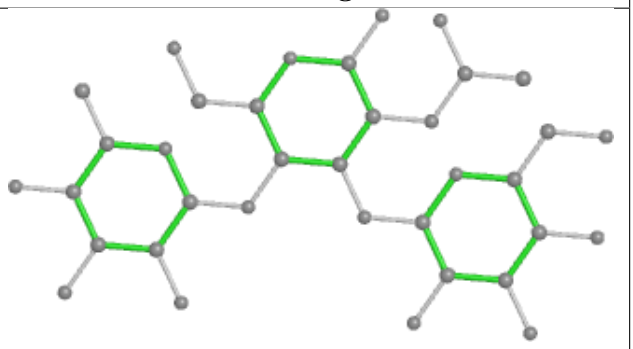
Bond lengths



Bond angles

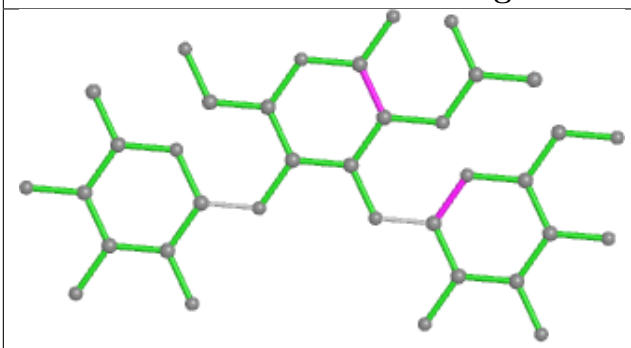


Torsions

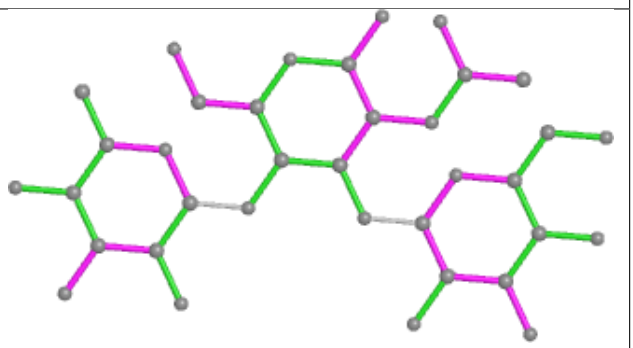


Rings

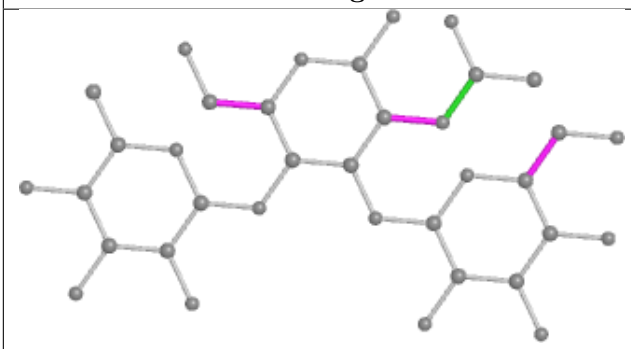
Oligosaccharide Chain D



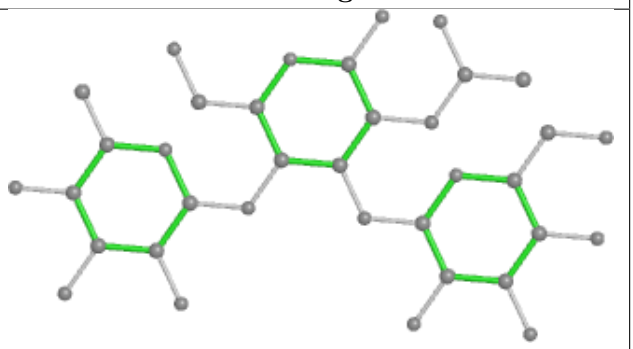
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	EDO	B	505	-	3,3,3	0.22	0	2,2,2	0.58	0
4	EDO	A	505	-	3,3,3	0.37	0	2,2,2	0.31	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
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	EDO	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	456/478 (95%)	0.11	27 (5%)	22	27	18, 27, 53, 83	0
1	B	456/478 (95%)	0.01	16 (3%)	44	50	17, 26, 47, 98	0
All	All	912/956 (95%)	0.06	43 (4%)	31	37	17, 27, 50, 98	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	THR	10.9
1	A	178	GLY	5.2
1	B	181	GLY	5.1
1	A	254	THR	5.0
1	A	399	GLN	5.0
1	A	239	THR	4.9
1	B	269	ALA	4.3
1	A	398	PRO	4.2
1	A	179	LYS	4.2
1	A	428	PRO	4.0
1	B	182	LYS	3.9
1	B	178	GLY	3.9
1	B	179	LYS	3.8
1	A	185	TYR	3.8
1	A	430	GLY	3.7
1	B	254	THR	3.6
1	B	180	ASN	3.6
1	A	60	ARG	3.5
1	A	386	ALA	3.5
1	A	180	ASN	3.4
1	A	387	ASP	3.2
1	A	433	ARG	3.2
1	A	429	ASP	3.0
1	A	431	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	389	ALA	2.8
1	B	9	ILE	2.7
1	A	427	LEU	2.7
1	B	176	GLY	2.7
1	A	255	VAL	2.7
1	B	386	ALA	2.6
1	A	181	GLY	2.6
1	B	185	TYR	2.6
1	A	131	TYR	2.5
1	B	177	GLU	2.5
1	A	183	THR	2.4
1	A	368	ALA	2.3
1	A	132	LEU	2.3
1	A	61	ASN	2.3
1	A	401	THR	2.2
1	A	400	PRO	2.2
1	B	399	GLN	2.2
1	A	432	GLU	2.0
1	B	387	ASP	2.0

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

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

6.3 Carbohydrates (i)

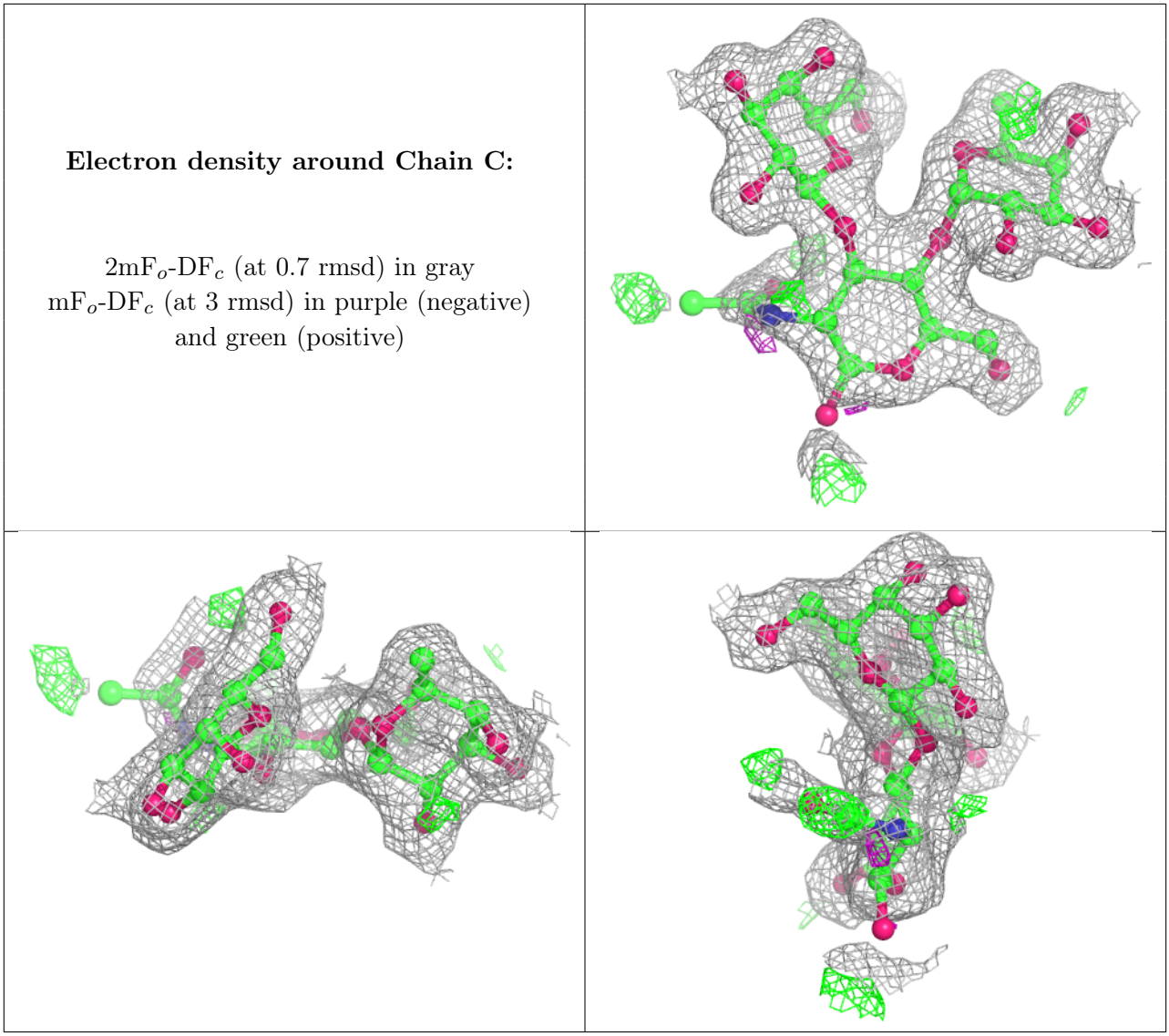
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	C	1	15/15	0.86	0.16	25,33,58,60	0
2	NAG	D	1	15/15	0.89	0.17	27,37,52,58	0
2	FUC	C	3	10/11	0.96	0.13	20,25,28,29	0
2	GAL	D	2	11/12	0.96	0.10	26,29,33,36	0
2	FUC	D	3	10/11	0.97	0.11	21,24,25,27	0
2	GAL	C	2	11/12	0.98	0.10	22,25,28,29	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.

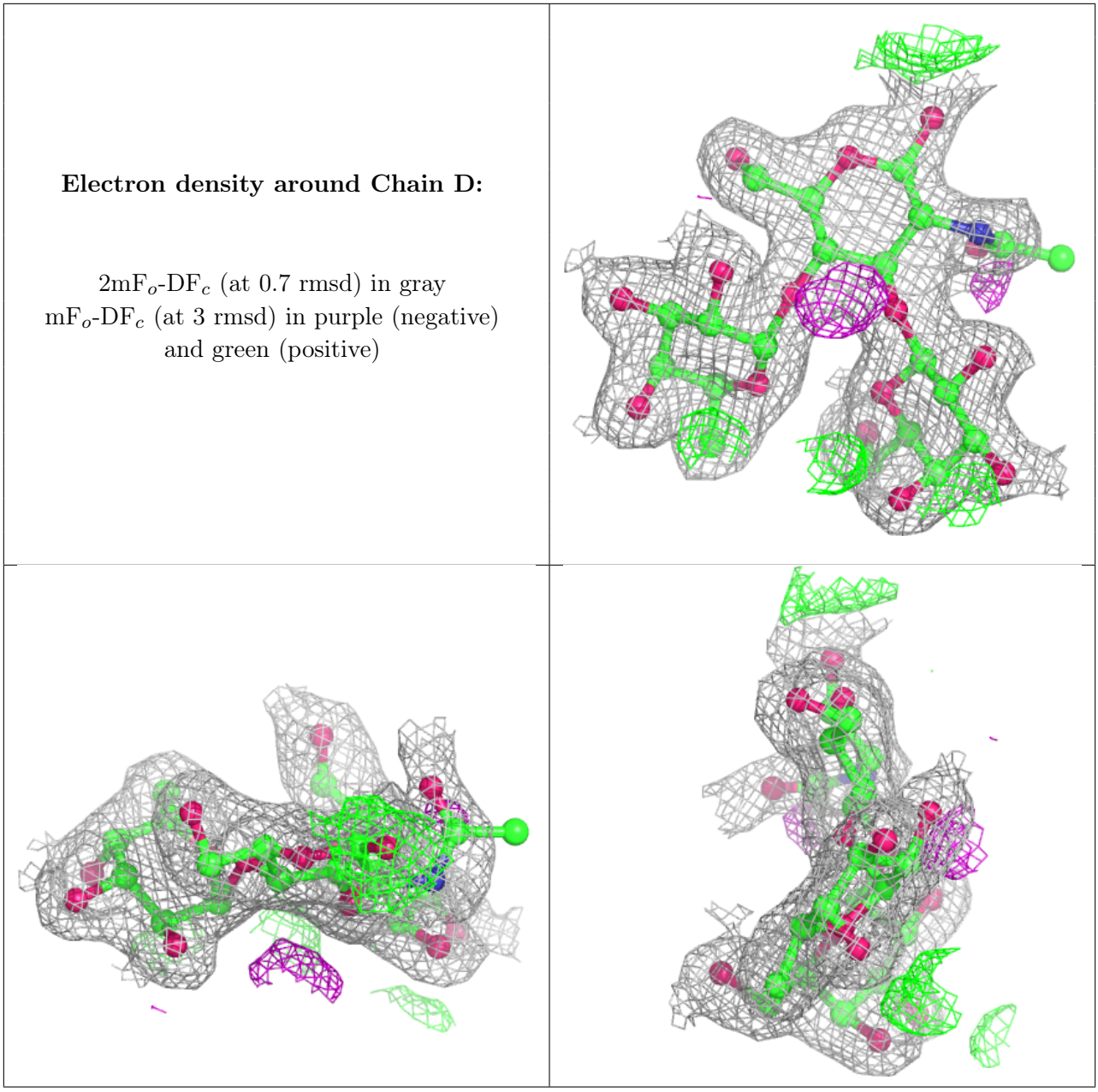
Electron density around Chain C:

$2mF_o$-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
4	EDO	B	505	4/4	0.95	0.12	31,32,33,36	0
4	EDO	A	505	4/4	0.96	0.14	33,36,40,42	0
3	NA	A	501	1/1	0.98	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	B	501	1/1	0.99	0.08	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.