



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 PM UTC

PDB ID : 6LGE / pdb_00006lge
Title : Bombyx mori GH13 sucrose hydrolase complexed with acarbose
Authors : Miyazaki, T.
Deposited on : 2019-12-05
Resolution : 1.75 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

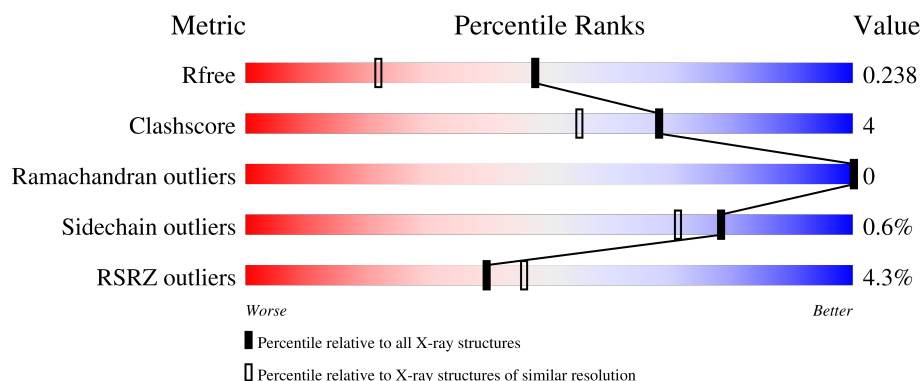
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	598	2% 86% 9% 5%
1	B	598	6% 84% 11% 5%
2	C	3	100%
2	D	3	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10008 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 Sucrose hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4651	2982	769	886	14			
1	B	569	Total	C	N	O	S	0	1	0
			4653	2982	769	888	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP A0A077JI83
A	10	GLY	-	expression tag	UNP A0A077JI83
A	11	SER	-	expression tag	UNP A0A077JI83
A	12	SER	-	expression tag	UNP A0A077JI83
A	13	HIS	-	expression tag	UNP A0A077JI83
A	14	HIS	-	expression tag	UNP A0A077JI83
A	15	HIS	-	expression tag	UNP A0A077JI83
A	16	HIS	-	expression tag	UNP A0A077JI83
A	17	HIS	-	expression tag	UNP A0A077JI83
A	18	HIS	-	expression tag	UNP A0A077JI83
A	19	SER	-	expression tag	UNP A0A077JI83
A	20	SER	-	expression tag	UNP A0A077JI83
A	21	GLY	-	expression tag	UNP A0A077JI83
A	22	LEU	-	expression tag	UNP A0A077JI83
A	23	VAL	-	expression tag	UNP A0A077JI83
A	24	PRO	-	expression tag	UNP A0A077JI83
A	25	ARG	-	expression tag	UNP A0A077JI83
A	26	GLY	-	expression tag	UNP A0A077JI83
A	27	SER	-	expression tag	UNP A0A077JI83
A	28	HIS	-	expression tag	UNP A0A077JI83
A	29	MET	-	expression tag	UNP A0A077JI83
B	9	MET	-	expression tag	UNP A0A077JI83
B	10	GLY	-	expression tag	UNP A0A077JI83
B	11	SER	-	expression tag	UNP A0A077JI83
B	12	SER	-	expression tag	UNP A0A077JI83

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Chain	Residue	Modelled	Actual	Comment	Reference
B	13	HIS	-	expression tag	UNP A0A077JI83
B	14	HIS	-	expression tag	UNP A0A077JI83
B	15	HIS	-	expression tag	UNP A0A077JI83
B	16	HIS	-	expression tag	UNP A0A077JI83
B	17	HIS	-	expression tag	UNP A0A077JI83
B	18	HIS	-	expression tag	UNP A0A077JI83
B	19	SER	-	expression tag	UNP A0A077JI83
B	20	SER	-	expression tag	UNP A0A077JI83
B	21	GLY	-	expression tag	UNP A0A077JI83
B	22	LEU	-	expression tag	UNP A0A077JI83
B	23	VAL	-	expression tag	UNP A0A077JI83
B	24	PRO	-	expression tag	UNP A0A077JI83
B	25	ARG	-	expression tag	UNP A0A077JI83
B	26	GLY	-	expression tag	UNP A0A077JI83
B	27	SER	-	expression tag	UNP A0A077JI83
B	28	HIS	-	expression tag	UNP A0A077JI83
B	29	MET	-	expression tag	UNP A0A077JI83

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0

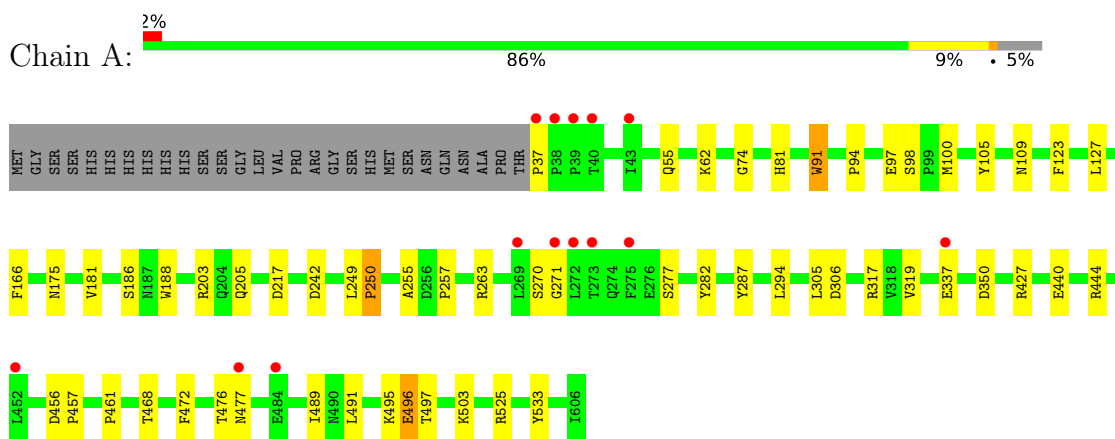
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total 303	O 303	0	0
5	B	307	Total 307	O 307	0	0

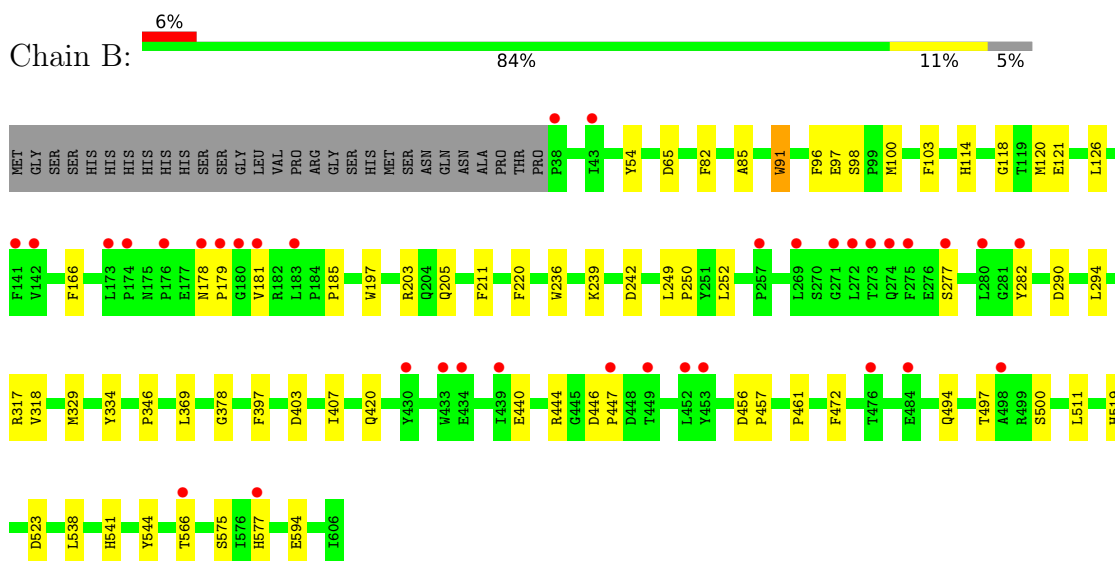
3 Residue-property plots

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.

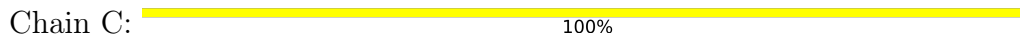
- Molecule 1: Sucrose hydrolase



- Molecule 1: Sucrose hydrolase



- Molecule 2: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



BGC1
GLC2
AC13

- Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D:

100%

BGC1
GLC2
AC13

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.25Å 145.79Å 152.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 1.75 48.66 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.66-1.75) 99.9 (48.66-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.229 0.209 , 0.238	Depositor DCC
R_{free} test set	7296 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, AC1, GLC, BGC, MG

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	1.11	3/4795 (0.1%)	1.32	3/6530 (0.0%)
1	B	1.13	6/4796 (0.1%)	1.34	18/6530 (0.3%)
All	All	1.12	9/9591 (0.1%)	1.33	21/13060 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	GLY	C-O	7.37	1.28	1.23
1	A	250	PRO	C-O	-5.82	1.16	1.24
1	B	523	ASP	C-O	5.57	1.30	1.23
1	B	85	ALA	C-O	5.46	1.30	1.24
1	B	369	LEU	C-O	-5.46	1.17	1.24
1	A	81	HIS	CE1-NE2	5.40	1.38	1.32
1	B	252	LEU	C-O	-5.28	1.18	1.24
1	B	397	PHE	N-CA	5.18	1.49	1.46
1	A	55	GLN	C-O	5.12	1.30	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	HIS	CA-C-N	7.20	126.94	120.10
1	B	519	HIS	C-N-CA	7.20	126.94	120.10
1	A	37	PRO	CA-N-CD	-6.84	102.43	112.00
1	B	220	PHE	CA-CB-CG	-6.76	107.04	113.80
1	B	497	THR	CA-CB-OG1	-6.69	99.56	109.60
1	B	577	HIS	CA-CB-CG	-6.48	107.32	113.80
1	B	566	THR	CA-CB-OG1	-6.28	100.17	109.60
1	B	397	PHE	N-CA-C	-6.14	103.75	108.78
1	B	318	VAL	O-C-N	5.74	129.50	123.02
1	A	306	ASP	CA-CB-CG	5.70	118.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	PHE	CA-CB-CG	-5.51	108.29	113.80
1	B	179	PRO	CA-C-N	5.45	126.03	119.98
1	B	179	PRO	C-N-CA	5.45	126.03	119.98
1	B	121	GLU	CB-CG-CD	5.36	121.71	112.60
1	A	350	ASP	CA-C-O	-5.33	114.90	120.55
1	B	397	PHE	O-C-N	5.23	125.39	121.47
1	B	65	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	211	PHE	CB-CA-C	5.14	120.66	110.42
1	B	82	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	378	GLY	CA-C-N	5.04	124.89	120.10
1	B	378	GLY	C-N-CA	5.04	124.89	120.10

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	4651	0	4371	34	0
1	B	4653	0	4369	32	0
2	C	44	0	30	0	0
2	D	44	0	30	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	303	0	0	5	0
5	B	307	0	0	5	0
All	All	10008	0	8800	66	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 (66) 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:203:ARG:HE	1:A:205:GLN:HE21	1.31	0.76
1:A:477:ASN:HB2	5:A:1048:HOH:O	1.90	0.70
1:A:203:ARG:HE	1:A:205:GLN:NE2	1.91	0.68
1:B:203:ARG:HH21	1:B:205:GLN:HE22	1.40	0.68
1:B:290:ASP:HB3	1:B:329:MET:HE2	1.75	0.67
1:B:594:GLU:HG3	5:B:806:HOH:O	1.94	0.66
1:B:203:ARG:HE	1:B:205:GLN:HE21	1.44	0.63
1:B:277:SER:HA	1:B:282:TYR:CD2	2.35	0.61
1:A:271:GLY:N	5:A:801:HOH:O	2.33	0.60
1:B:203:ARG:HE	1:B:205:GLN:NE2	2.04	0.56
1:A:277:SER:HA	1:A:282:TYR:CD2	2.42	0.55
1:A:496:GLU:HB3	5:A:807:HOH:O	2.06	0.55
1:A:186:SER:HG	1:A:188:TRP:CG	2.24	0.54
1:A:270:SER:C	5:A:801:HOH:O	2.50	0.54
1:B:100:MET:HE3	1:B:114:HIS:CD2	2.43	0.54
1:B:178:ASN:CB	1:B:181:VAL:HG12	2.38	0.53
1:A:440:GLU:OE2	1:A:444:ARG:NH1	2.41	0.53
1:A:337:GLU:HG3	5:B:1069:HOH:O	2.08	0.53
1:A:271:GLY:CA	5:A:801:HOH:O	2.56	0.52
1:B:178:ASN:HB3	1:B:181:VAL:HG12	1.91	0.52
1:A:427:ARG:CZ	1:A:489:ILE:HD11	2.40	0.51
1:A:461:PRO:HB3	1:A:472:PHE:CG	2.45	0.51
1:B:242:ASP:O	1:B:317:ARG:HA	2.11	0.50
1:A:123:PHE:CE2	1:A:127:LEU:HD22	2.47	0.50
1:A:337:GLU:CB	5:B:1069:HOH:O	2.61	0.49
1:A:91:TRP:C	1:A:91:TRP:CD1	2.90	0.48
1:B:538:LEU:HD23	1:B:541:HIS:CD2	2.48	0.48
1:B:440:GLU:OE2	1:B:444:ARG:NH1	2.46	0.48
1:B:446:ASP:HB2	1:B:447:PRO:CD	2.43	0.48
1:A:249:LEU:N	1:A:250:PRO:CD	2.77	0.48
1:A:203:ARG:HH21	1:A:205:GLN:HE22	1.61	0.47
1:B:461:PRO:HB3	1:B:472:PHE:CG	2.50	0.46
1:A:175:ASN:ND2	1:A:181:VAL:HB	2.31	0.46
1:B:277:SER:HA	1:B:282:TYR:CG	2.51	0.46
1:B:290:ASP:HB3	1:B:329:MET:CE	2.44	0.46
1:A:497:THR:O	1:A:503:LYS:HE2	2.15	0.45
1:A:255:ALA:HB2	1:A:287:TYR:HB3	1.99	0.45
1:B:126:LEU:C	1:B:126:LEU:HD23	2.41	0.45
1:B:456:ASP:N	1:B:457:PRO:CD	2.79	0.45
1:A:525:ARG:HB2	1:A:533:TYR:CZ	2.52	0.44
1:B:91:TRP:CD1	1:B:91:TRP:C	2.95	0.44
1:B:294:LEU:C	1:B:294:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HD3	1:A:105:TYR:CZ	2.53	0.44
1:A:97:GLU:HB2	1:A:109:ASN:HB3	1.99	0.44
1:B:403:ASP:O	1:B:407:ILE:HG13	2.19	0.43
1:A:468:THR:HG23	1:A:476:THR:HG22	2.01	0.42
1:B:98:SER:HB3	1:B:100:MET:HE2	2.01	0.42
1:A:305:LEU:HD22	1:A:319:VAL:HG13	2.00	0.42
1:A:98:SER:HB3	1:A:100:MET:HE2	2.00	0.42
1:B:96:PHE:CE1	1:B:236:TRP:CZ2	3.08	0.42
1:A:294:LEU:HD12	1:A:294:LEU:C	2.45	0.42
1:B:120:MET:SD	1:B:239:LYS:HE3	2.59	0.42
1:A:456:ASP:N	1:A:457:PRO:CD	2.83	0.42
1:B:494:GLN:HB3	1:B:500:SER:HB2	2.02	0.42
1:A:491:LEU:HG	1:A:495:LYS:HE3	2.02	0.41
1:B:185:PRO:HD2	1:B:197:TRP:CG	2.55	0.41
1:A:62:LYS:O	1:A:74:GLY:HA3	2.19	0.41
1:A:257:PRO:HA	1:A:263:ARG:O	2.21	0.41
1:B:97:GLU:CG	5:B:884:HOH:O	2.68	0.41
1:B:511:LEU:HD11	1:B:544:TYR:CE1	2.56	0.41
1:B:249:LEU:N	1:B:250:PRO:CD	2.84	0.40
1:A:497:THR:O	1:A:503:LYS:CE	2.69	0.40
1:B:54:TYR:CZ	1:B:420:GLN:HA	2.56	0.40
1:A:242:ASP:O	1:A:317:ARG:HA	2.21	0.40
1:B:334:TYR:CZ	1:B:346:PRO:HD2	2.57	0.40
1:B:575:SER:HB3	5:B:1011:HOH: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	568/598 (95%)	552 (97%)	16 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	568/598 (95%)	552 (97%)	16 (3%)	0	100	100
All	All	1136/1196 (95%)	1104 (97%)	32 (3%)	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	500/524 (95%)	496 (99%)	4 (1%)	73	64
1	B	500/524 (95%)	498 (100%)	2 (0%)	84	80
All	All	1000/1048 (95%)	994 (99%)	6 (1%)	78	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	TRP
1	A	166	PHE
1	A	217	ASP
1	A	496	GLU
1	B	91	TRP
1	B	166	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	205	GLN
1	A	227	GLN
1	A	514	GLN
1	B	55	GLN
1	B	165	ASN
1	B	191	GLN

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Mol	Chain	Res	Type
1	B	205	GLN
1	B	391	ASN
1	B	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	BGC	C	1	2	12,12,12	0.64	0	17,17,17	1.35	1 (5%)
2	GLC	C	2	2	11,11,12	0.71	0	15,15,17	1.57	2 (13%)
2	AC1	C	3	2	21,22,23	1.26	2 (9%)	22,32,34	1.88	8 (36%)
2	BGC	D	1	2	12,12,12	0.79	0	17,17,17	0.94	1 (5%)
2	GLC	D	2	2	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
2	AC1	D	3	2	21,22,23	1.58	5 (23%)	22,32,34	1.81	6 (27%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	AC1	C	3	2	-	3/6/43/46	0/2/2/2
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	3/6/43/46	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	C4A-C5B	3.68	1.54	1.51
2	D	3	AC1	O4-C4A	2.94	1.47	1.42
2	D	3	AC1	C1B-C7B	2.72	1.54	1.50
2	D	3	AC1	C7B-C5B	2.24	1.36	1.32
2	C	3	AC1	O6B-C6B	2.18	1.48	1.41
2	C	3	AC1	O4-C4A	-2.09	1.38	1.42
2	D	3	AC1	C1B-N4A	2.00	1.50	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	AC1	O3-C3-C2	-5.17	99.51	110.05
2	C	3	AC1	C1-C2-C3	4.41	116.06	109.64
2	C	2	GLC	O2-C2-C3	-3.45	103.01	110.15
2	C	1	BGC	O5-C1-C2	-3.26	104.56	110.30
2	D	3	AC1	C7B-C1B-N4A	3.03	115.14	110.68
2	D	3	AC1	O6B-C6B-C5B	-2.98	103.37	112.74
2	C	3	AC1	O6B-C6B-C5B	-2.78	103.99	112.74
2	C	2	GLC	C1-O5-C5	2.73	115.85	112.19
2	C	3	AC1	O3B-C3B-C2B	2.69	116.73	110.38
2	C	3	AC1	O5-C5-C6	-2.68	101.58	107.40
2	C	3	AC1	O4-C4A-C5B	2.57	115.65	110.75
2	D	2	GLC	O5-C5-C4	-2.54	104.64	110.83
2	C	3	AC1	O3-C3-C4	2.42	114.39	109.58
2	D	3	AC1	C1-O5-C5	2.32	118.43	112.97
2	D	3	AC1	C6-C5-C4	2.29	117.76	113.57
2	C	3	AC1	C2B-C3B-C4A	-2.23	106.69	110.22
2	D	3	AC1	O2B-C2B-C3B	2.22	115.62	110.38
2	D	2	GLC	C3-C4-C5	-2.18	106.28	110.23
2	C	3	AC1	O3B-C3B-C4A	-2.16	105.36	109.64
2	D	1	BGC	O5-C5-C4	2.04	113.38	109.70

There are no chirality outliers.

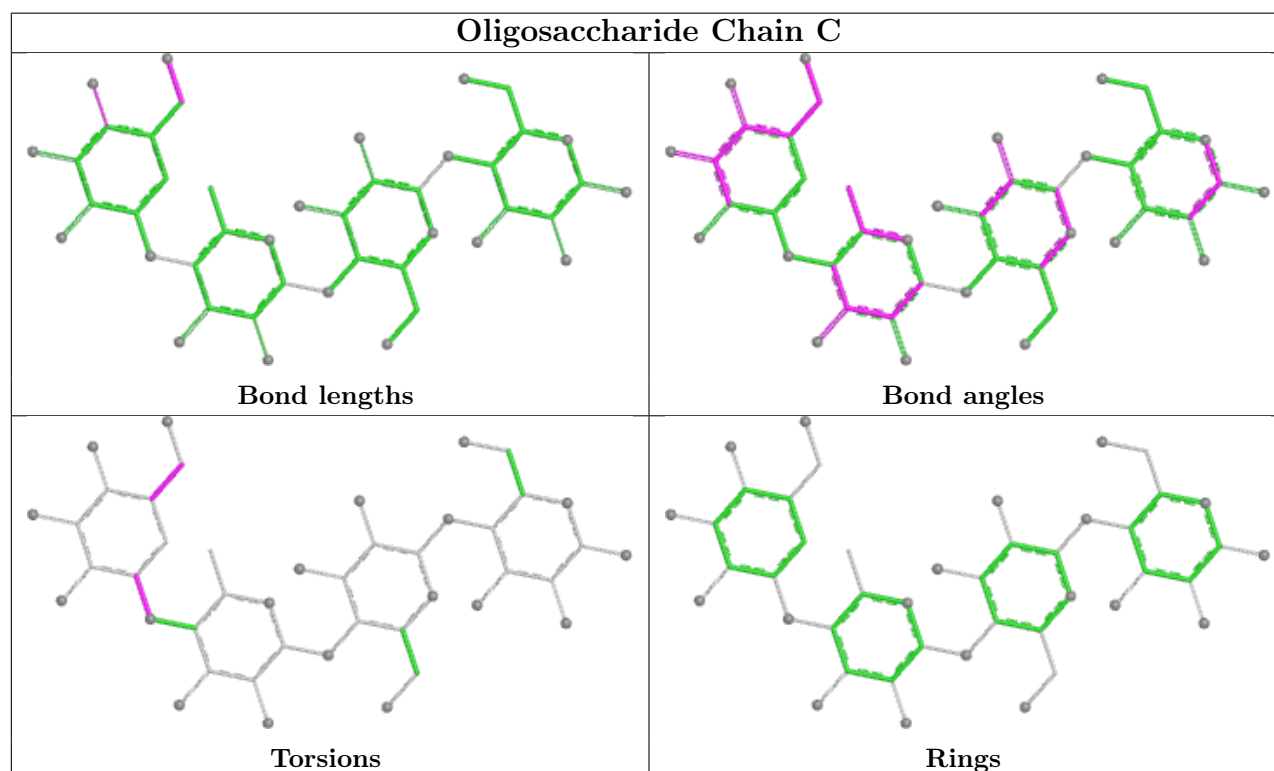
All (6) torsion outliers are listed below:

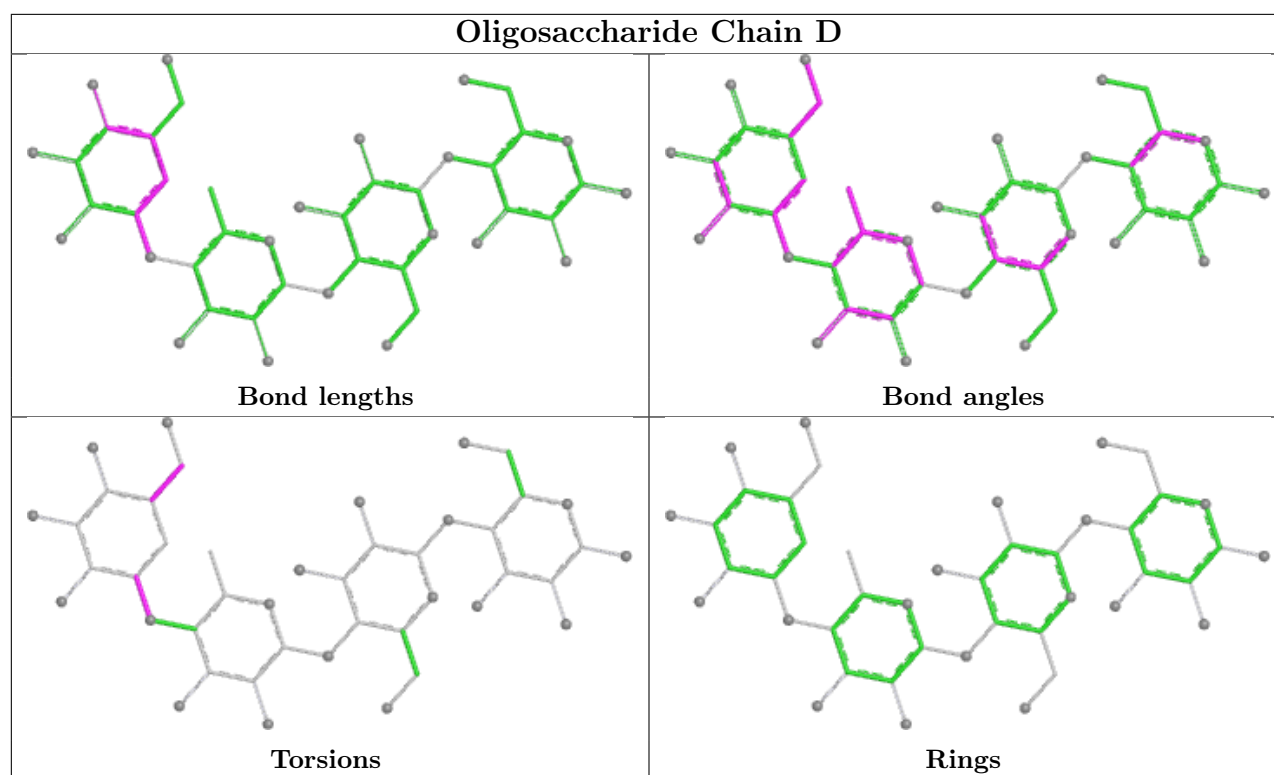
Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C1B-N4A-C4
2	C	3	AC1	C4A-C5B-C6B-O6B
2	C	3	AC1	C7B-C5B-C6B-O6B
2	D	3	AC1	C7B-C1B-N4A-C4
2	D	3	AC1	C7B-C5B-C6B-O6B
2	D	3	AC1	C4A-C5B-C6B-O6B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	570/598 (95%)	0.47	14 (2%) 58 64	20, 30, 48, 88	0
1	B	569/598 (95%)	0.48	35 (6%) 26 30	15, 28, 55, 101	1 (0%)
All	All	1139/1196 (95%)	0.48	49 (4%) 40 46	15, 30, 53, 101	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	6.4
1	A	37	PRO	6.2
1	A	38	PRO	4.9
1	B	272	LEU	4.6
1	B	173	LEU	4.4
1	B	275	PHE	4.4
1	B	181	VAL	4.2
1	B	176	PRO	4.2
1	A	273	THR	3.9
1	B	38	PRO	3.9
1	B	183	LEU	3.7
1	B	282	TYR	3.7
1	B	269	LEU	3.6
1	B	452	LEU	3.6
1	A	275	PHE	3.5
1	A	452	LEU	3.5
1	B	273	THR	3.4
1	B	433	TRP	3.4
1	B	180	GLY	3.2
1	B	141	PHE	3.2
1	B	277	SER	3.1
1	B	447	PRO	3.1
1	B	271	GLY	3.1
1	A	43	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	449	THR	2.8
1	B	174	PRO	2.8
1	A	269	LEU	2.7
1	B	453	TYR	2.7
1	B	577	HIS	2.7
1	A	477	ASN	2.6
1	A	337	GLU	2.6
1	B	274	GLN	2.5
1	A	40	THR	2.5
1	B	566	THR	2.4
1	B	179	PRO	2.3
1	B	280	LEU	2.3
1	B	434	GLU	2.3
1	B	178	ASN	2.3
1	A	39	PRO	2.2
1	B	476	THR	2.2
1	A	271	GLY	2.2
1	B	257	PRO	2.2
1	A	484	GLU	2.1
1	B	484	GLU	2.1
1	B	498	ALA	2.1
1	B	439	ILE	2.1
1	B	142	VAL	2.1
1	B	43	ILE	2.0
1	B	430	TYR	2.0

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.

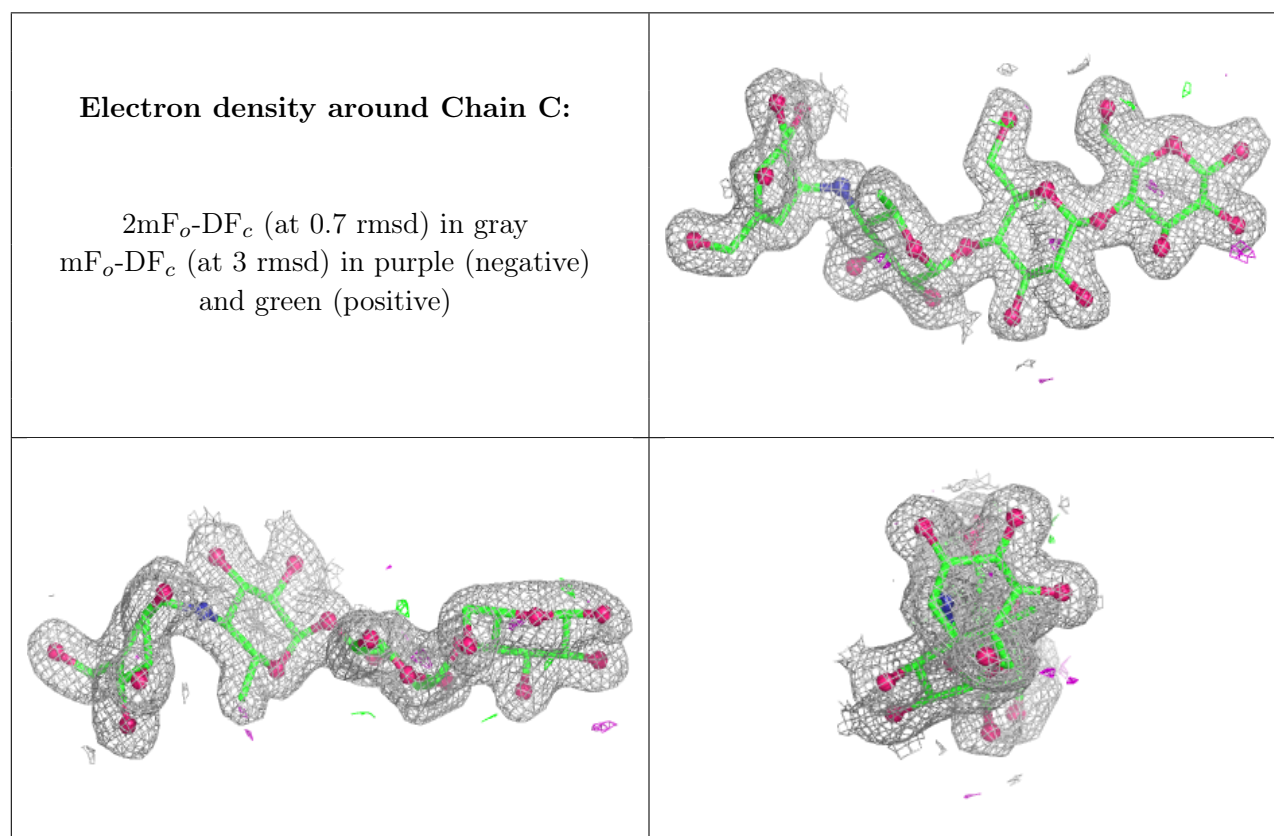
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	D	1	12/12	0.90	0.11	32,35,37,38	0
2	GLC	C	2	11/12	0.92	0.09	27,29,35,36	0
2	GLC	D	2	11/12	0.92	0.10	33,35,41,41	0

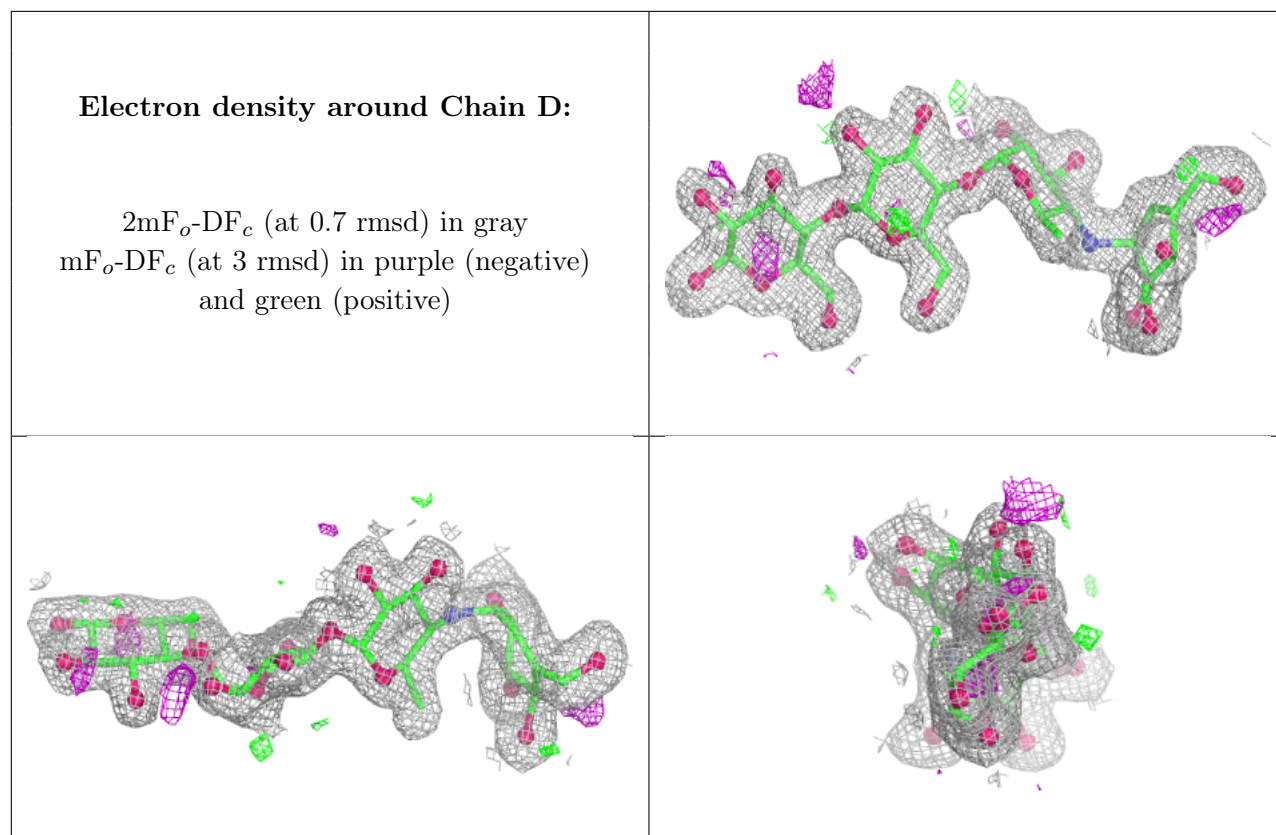
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	C	1	12/12	0.93	0.08	31,34,36,42	0
2	AC1	D	3	21/22	0.95	0.08	23,27,31,34	0
2	AC1	C	3	21/22	0.97	0.07	22,24,28,30	0

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.





6.4 Ligands [i](#)

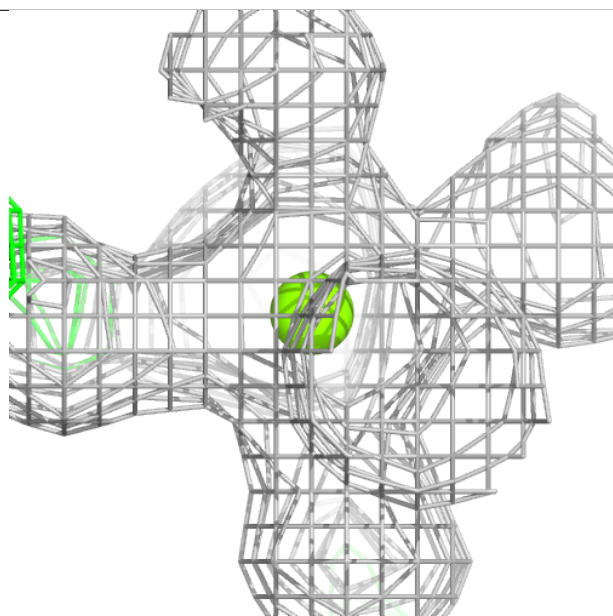
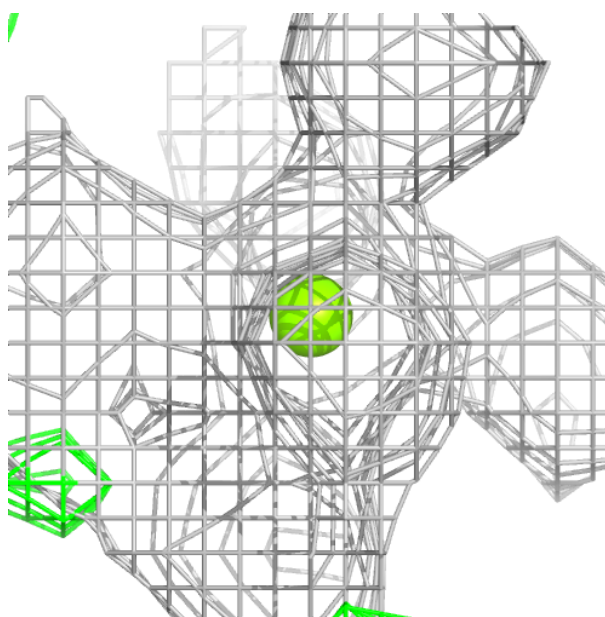
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	703	1/1	0.97	0.17	41,41,41,41	0
3	MG	A	701	1/1	0.98	0.04	27,27,27,27	0
3	MG	A	704	1/1	0.99	0.03	23,23,23,23	0
3	MG	B	701	1/1	0.99	0.02	24,24,24,24	0
4	CA	B	702	1/1	0.99	0.03	26,26,26,26	0
4	CA	A	702	1/1	1.00	0.03	25,25,25,25	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.

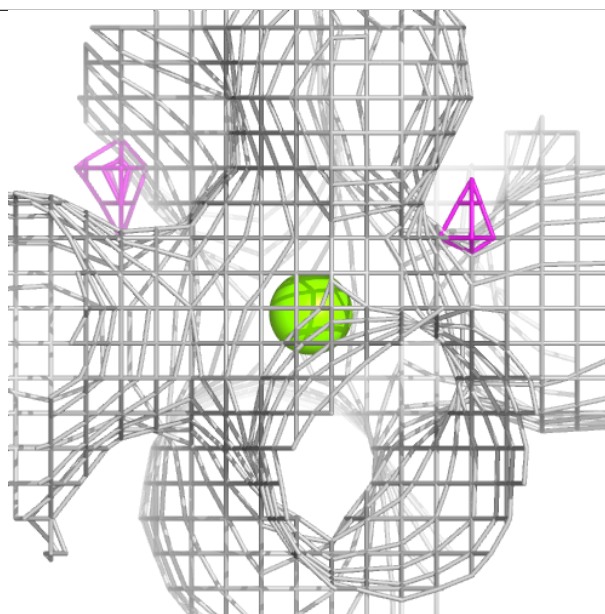
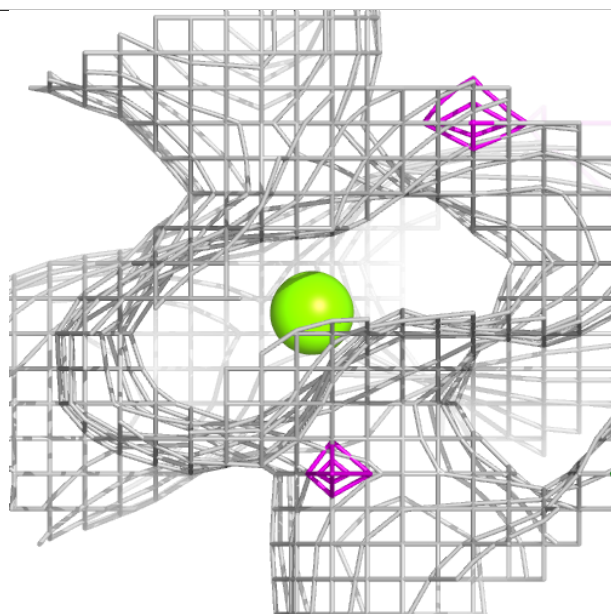
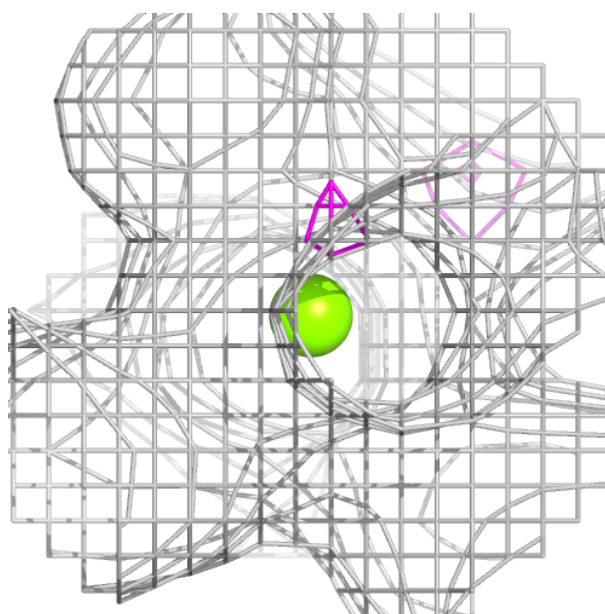
Electron density around MG A 703:

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



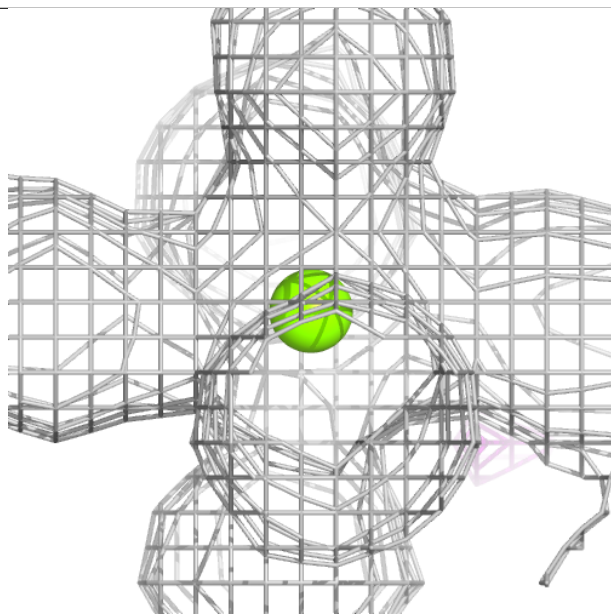
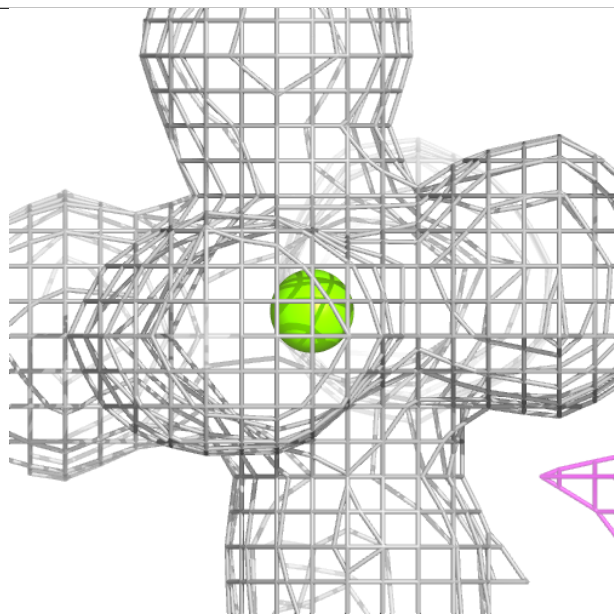
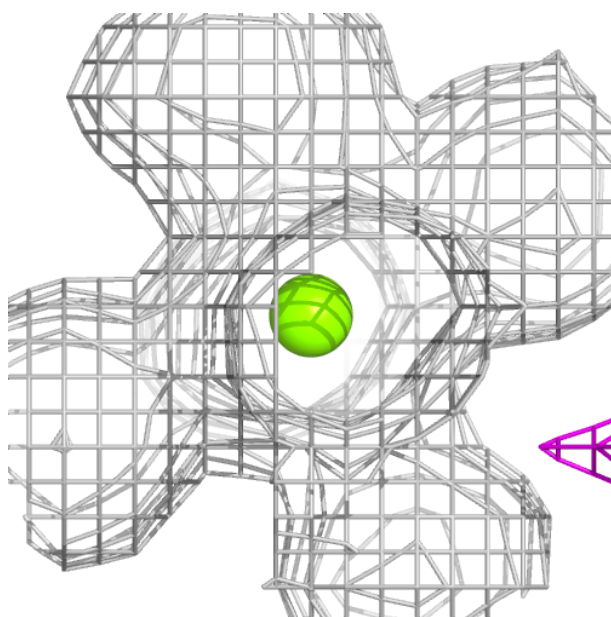
Electron density around MG A 701:

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



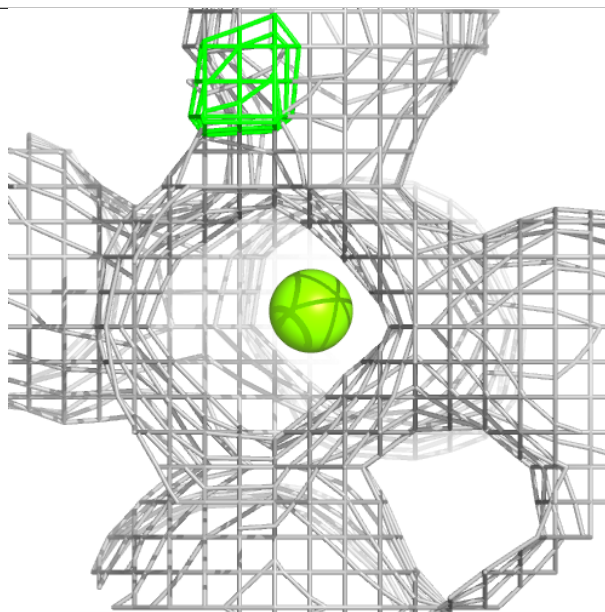
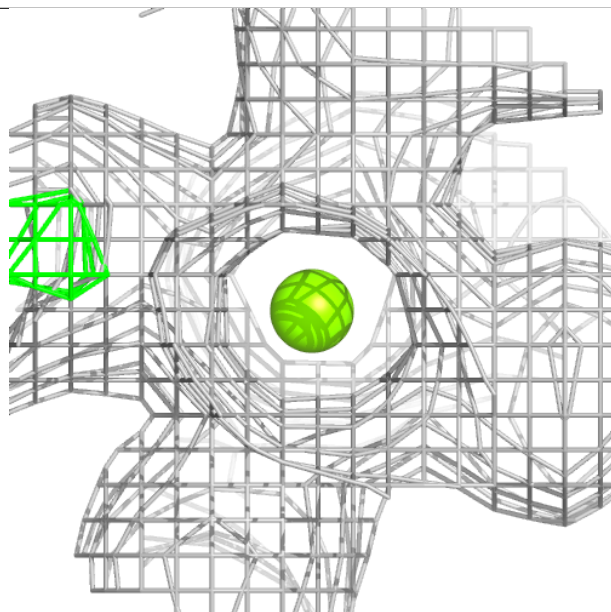
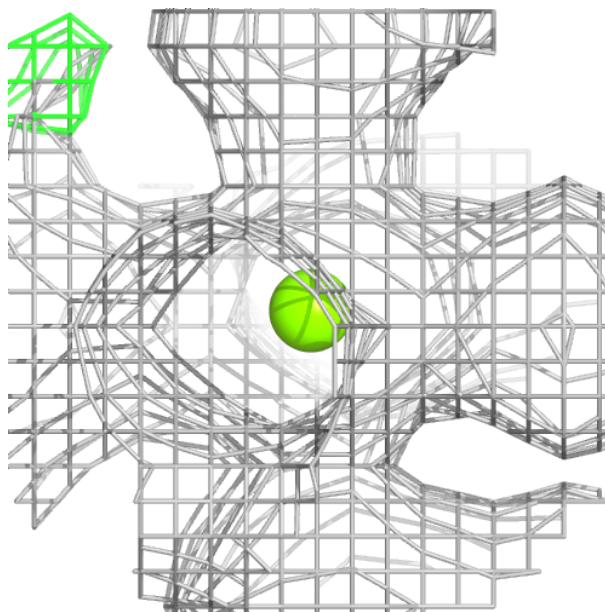
Electron density around MG A 704:

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



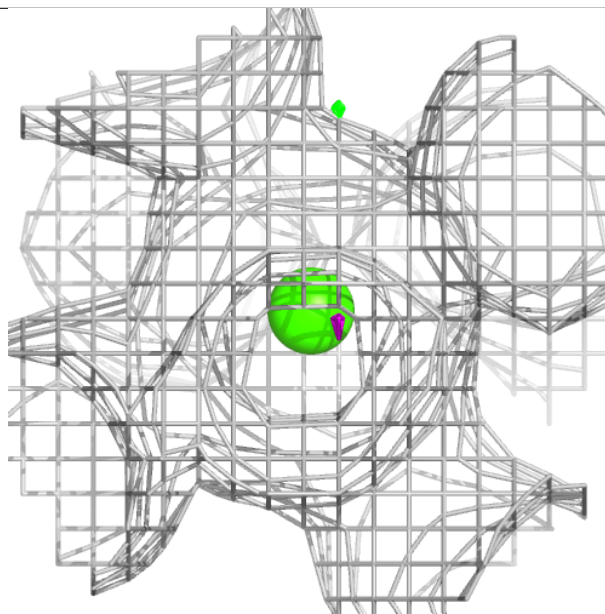
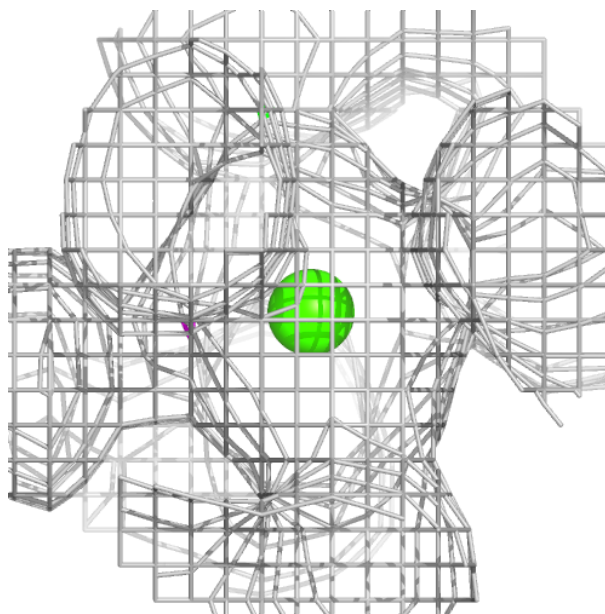
Electron density around MG B 701:

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



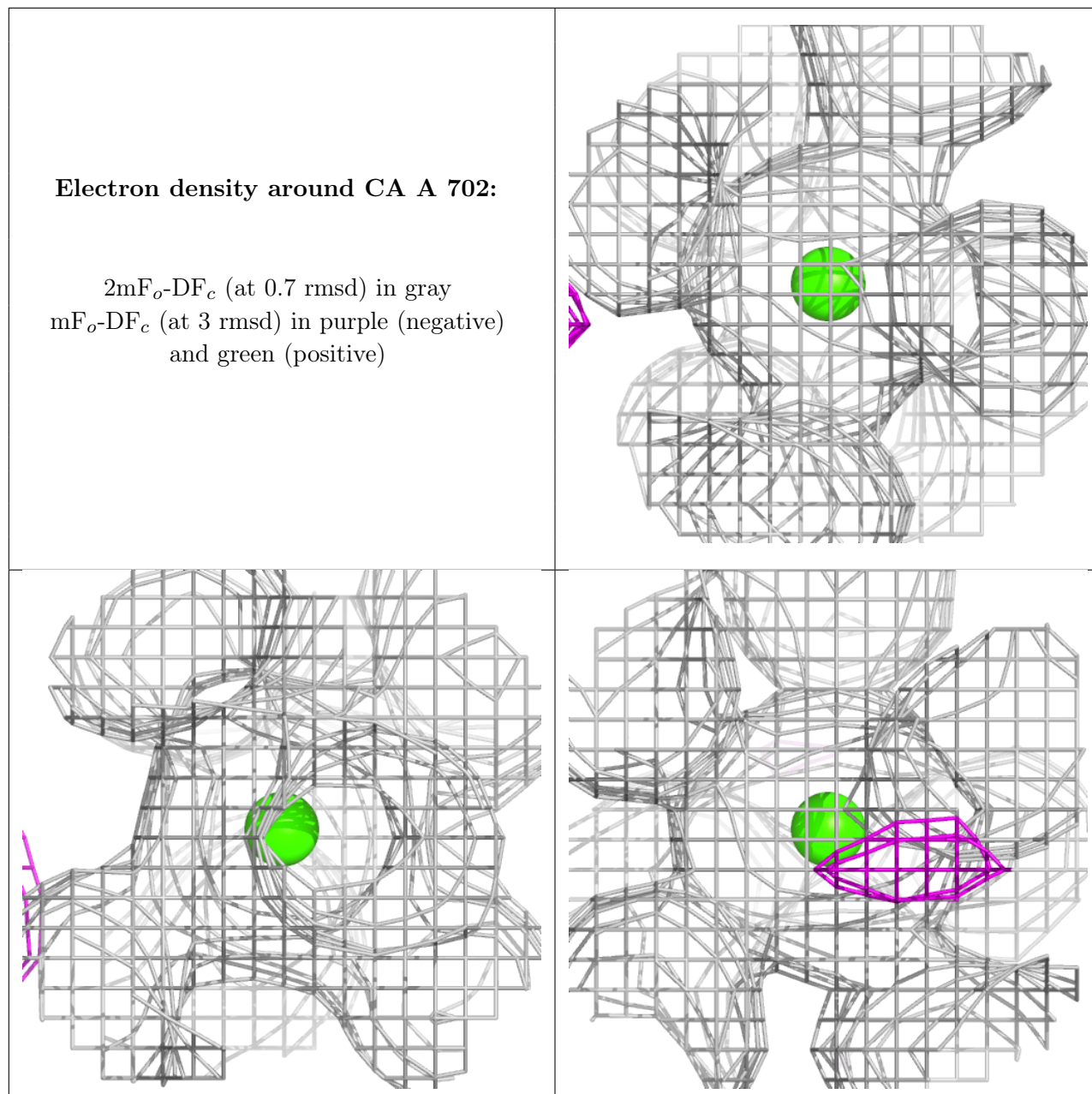
Electron density around CA B 702:

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



Electron density around CA A 702:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.