



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:43 AM UTC

PDB ID : 3AMQ / pdb_00003amq
Title : E134C-Cellobiose co-crystal of cellulase 12A from thermotoga maritima
Authors : Cheng, Y.-S.; Ko, T.-P.; Liu, J.-R.; Guo, R.-T.
Deposited on : 2010-08-20
Resolution : 1.80 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

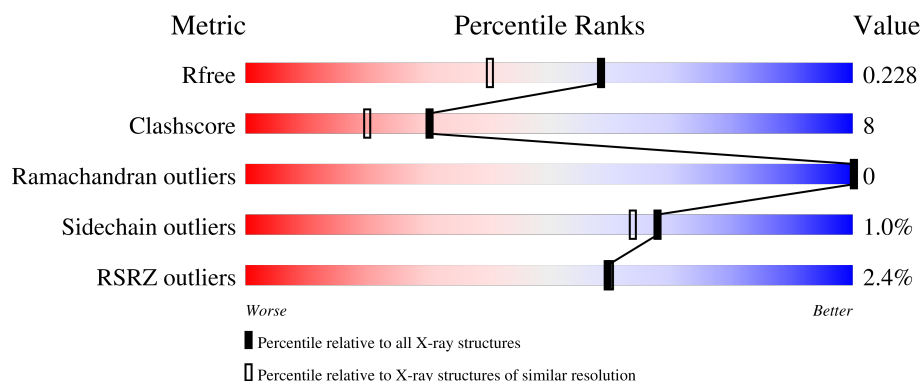
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	265	 80% 16% ..
1	B	265	 86% 9% ..
1	C	265	 2% 75% 18% . .
1	D	265	 7% 70% 23% . .
2	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 50%50%
2	H	2	 50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9533 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 Endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2105	1375	328	394	8			
1	B	256	Total	C	N	O	S	0	0	0
			2095	1370	327	390	8			
1	C	256	Total	C	N	O	S	0	0	0
			2095	1370	327	390	8			
1	D	256	Total	C	N	O	S	0	0	0
			2095	1370	327	390	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q60032
A	-6	GLY	-	expression tag	UNP Q60032
A	-5	HIS	-	expression tag	UNP Q60032
A	-4	HIS	-	expression tag	UNP Q60032
A	-3	HIS	-	expression tag	UNP Q60032
A	-2	HIS	-	expression tag	UNP Q60032
A	-1	HIS	-	expression tag	UNP Q60032
A	0	HIS	-	expression tag	UNP Q60032
A	134	CYS	GLU	engineered mutation	UNP Q60032
B	-7	MET	-	expression tag	UNP Q60032
B	-6	GLY	-	expression tag	UNP Q60032
B	-5	HIS	-	expression tag	UNP Q60032
B	-4	HIS	-	expression tag	UNP Q60032
B	-3	HIS	-	expression tag	UNP Q60032
B	-2	HIS	-	expression tag	UNP Q60032
B	-1	HIS	-	expression tag	UNP Q60032
B	0	HIS	-	expression tag	UNP Q60032
B	134	CYS	GLU	engineered mutation	UNP Q60032
C	-7	MET	-	expression tag	UNP Q60032
C	-6	GLY	-	expression tag	UNP Q60032
C	-5	HIS	-	expression tag	UNP Q60032

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q60032
C	-3	HIS	-	expression tag	UNP Q60032
C	-2	HIS	-	expression tag	UNP Q60032
C	-1	HIS	-	expression tag	UNP Q60032
C	0	HIS	-	expression tag	UNP Q60032
C	134	CYS	GLU	engineered mutation	UNP Q60032
D	-7	MET	-	expression tag	UNP Q60032
D	-6	GLY	-	expression tag	UNP Q60032
D	-5	HIS	-	expression tag	UNP Q60032
D	-4	HIS	-	expression tag	UNP Q60032
D	-3	HIS	-	expression tag	UNP Q60032
D	-2	HIS	-	expression tag	UNP Q60032
D	-1	HIS	-	expression tag	UNP Q60032
D	0	HIS	-	expression tag	UNP Q60032
D	134	CYS	GLU	engineered mutation	UNP Q60032

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

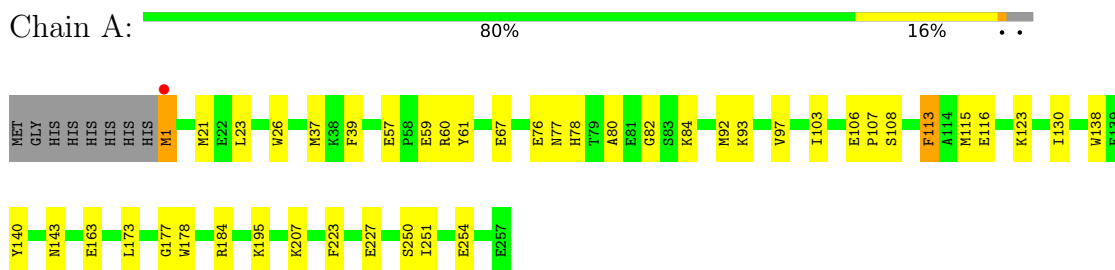
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		
4	B	345	Total	O	0	0
			345	345		
4	C	192	Total	O	0	0
			192	192		
4	D	208	Total	O	0	0
			208	208		

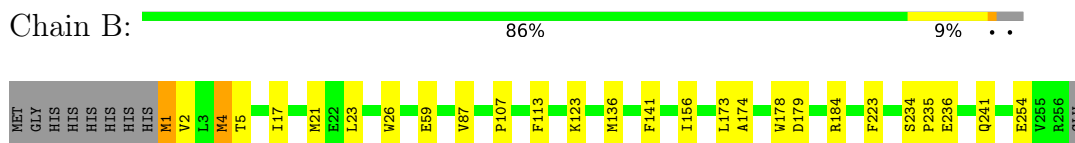
3 Residue-property plots

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.

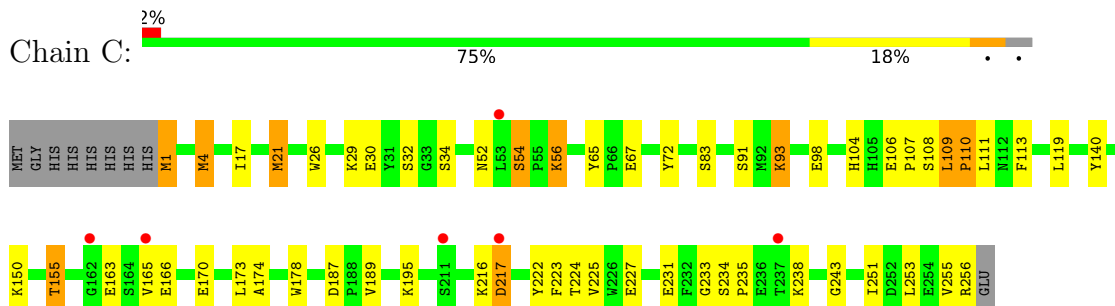
- Molecule 1: Endo-1,4-beta-glucanase



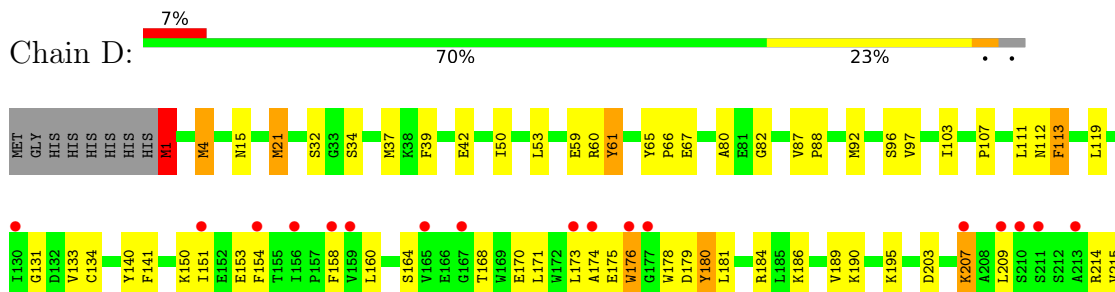
- Molecule 1: Endo-1,4-beta-glucanase



- Molecule 1: Endo-1,4-beta-glucanase



- Molecule 1: Endo-1,4-beta-glucanase





- Molecule 2: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E: 50% 50%



- Molecule 2: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F: 50% 50%



- Molecule 2: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G: 50% 50%



- Molecule 2: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.90Å 46.91Å 116.41Å 90.00° 114.19° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80 25.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-1.80) 94.2 (25.00-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.94 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.230 0.188 , 0.228	Depositor DCC
R_{free} test set	5060 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9533	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: BGC, GLC

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	3/2174 (0.1%)	1.19	14/2950 (0.5%)
1	B	1.12	5/2164 (0.2%)	1.20	10/2938 (0.3%)
1	C	1.01	4/2164 (0.2%)	1.25	19/2938 (0.6%)
1	D	1.06	4/2164 (0.2%)	1.20	12/2938 (0.4%)
All	All	1.06	16/8666 (0.2%)	1.21	55/11764 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	21	MET	SD-CE	-8.09	1.59	1.79
1	D	4	MET	SD-CE	-7.92	1.59	1.79
1	C	21	MET	SD-CE	-7.14	1.61	1.79
1	D	37	MET	SD-CE	-6.91	1.62	1.79
1	B	87	VAL	C-O	-6.79	1.19	1.24
1	B	4	MET	SD-CE	-6.56	1.63	1.79
1	C	4	MET	SD-CE	-6.53	1.63	1.79
1	A	1	MET	SD-CE	5.86	1.94	1.79
1	B	17	ILE	N-CA	5.52	1.51	1.46
1	A	115	MET	SD-CE	5.46	1.93	1.79
1	B	136	MET	SD-CE	5.29	1.92	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	MET	SD-CE	5.26	1.92	1.79
1	C	21	MET	CG-SD	5.25	1.93	1.80
1	A	92	MET	SD-CE	5.17	1.92	1.79
1	B	1	MET	SD-CE	5.17	1.92	1.79
1	D	1	MET	SD-CE	5.13	1.92	1.79

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	PHE	N-CA-C	-8.14	95.25	108.52
1	C	109	LEU	CA-C-N	8.07	129.34	119.98
1	C	109	LEU	C-N-CA	8.07	129.34	119.98
1	C	113	PHE	N-CA-C	-7.91	94.17	108.02
1	D	224	THR	N-CA-C	7.60	121.81	112.23
1	B	107	PRO	N-CA-C	7.48	123.75	113.65
1	D	225	VAL	CB-CA-C	-7.06	105.11	111.74
1	C	106	GLU	N-CA-C	-7.02	100.08	109.84
1	A	107	PRO	N-CA-C	6.96	123.91	113.81
1	C	110	PRO	N-CA-C	-6.94	99.71	110.95
1	C	233	GLY	N-CA-C	6.86	121.32	112.68
1	A	223	PHE	N-CA-C	-6.72	97.59	108.41
1	A	78	HIS	N-CA-C	6.57	120.23	109.06
1	A	80	ALA	N-CA-C	-6.56	102.07	110.53
1	D	87	VAL	CA-C-N	-6.49	113.29	119.85
1	D	87	VAL	C-N-CA	-6.49	113.29	119.85
1	B	223	PHE	N-CA-C	-6.44	98.04	108.41
1	A	113	PHE	N-CA-C	-6.42	96.58	108.02
1	A	106	GLU	N-CA-C	-6.40	101.51	109.64
1	B	26	TRP	N-CA-C	6.37	119.04	111.33
1	B	234	SER	N-CA-C	-6.23	102.53	108.07
1	C	32	SER	N-CA-C	-6.21	99.89	109.14
1	A	178	TRP	N-CA-C	-5.95	99.91	108.60
1	B	113	PHE	N-CA-C	-5.89	97.71	108.02
1	B	23	LEU	N-CA-C	-5.88	96.92	107.98
1	B	123	LYS	N-CA-C	5.86	117.67	111.28
1	A	23	LEU	N-CA-C	-5.82	98.43	108.56
1	C	34	SER	N-CA-C	5.78	118.82	109.40
1	A	123	LYS	N-CA-C	5.72	117.52	111.28
1	D	92	MET	N-CA-C	5.71	117.61	108.41
1	B	178	TRP	N-CA-C	-5.71	100.86	108.74
1	A	26	TRP	N-CA-C	5.66	119.00	111.75
1	D	219	GLU	N-CA-C	5.61	119.23	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	LYS	N-CA-C	5.57	120.23	113.38
1	A	163	GLU	N-CA-C	5.57	118.03	109.07
1	A	82	GLY	N-CA-C	5.49	123.17	115.43
1	B	156	ILE	CA-C-N	5.44	125.34	119.85
1	B	156	ILE	C-N-CA	5.44	125.34	119.85
1	C	56	LYS	N-CA-C	-5.42	104.24	111.24
1	C	231	GLU	N-CA-C	-5.40	102.48	110.48
1	D	80	ALA	N-CA-C	-5.39	103.27	110.55
1	C	107	PRO	N-CA-C	5.37	121.60	113.81
1	C	178	TRP	N-CA-C	-5.37	101.29	108.86
1	C	26	TRP	N-CA-C	5.34	118.59	111.75
1	C	234	SER	N-CA-C	-5.30	102.04	108.14
1	D	32	SER	N-CA-C	-5.24	101.39	109.52
1	D	168	THR	N-CA-C	-5.21	100.68	109.07
1	D	107	PRO	N-CA-C	5.17	123.11	112.47
1	C	17	ILE	N-CA-C	5.14	112.24	107.56
1	A	116	GLU	N-CA-C	5.13	116.64	108.79
1	C	93	LYS	N-CA-C	-5.13	105.14	111.40
1	C	224	THR	N-CA-C	5.11	119.60	112.90
1	D	131	GLY	N-CA-C	-5.08	107.96	114.37
1	A	177	GLY	N-CA-C	-5.08	109.08	114.67
1	C	223	PHE	N-CA-C	-5.03	100.31	108.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	TYR	Sidechain
1	C	65	TYR	Sidechain
1	D	180	TYR	Sidechain
1	D	61	TYR	Sidechain

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	2105	0	2007	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2095	0	2001	12	0
1	C	2095	0	2001	44	1
1	D	2095	0	2001	64	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	12	0	12	0	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
4	A	270	0	0	5	0
4	B	345	0	0	5	2
4	C	192	0	0	10	0
4	D	208	0	0	9	0
All	All	9533	0	8130	140	2

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.

All (140) 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:C:4:MET:HE2	1:C:21:MET:HE2	1.36	1.05
1:A:195:LYS:HE2	4:A:979:HOH:O	1.54	1.05
1:C:93:LYS:HD2	1:C:256:ARG:HD2	1.46	0.95
1:C:256:ARG:HB2	4:C:444:HOH:O	1.70	0.89
1:D:164:SER:HB3	4:D:541:HOH:O	1.71	0.89
1:D:173:LEU:HD12	1:D:174:ALA:H	1.44	0.83
1:C:173:LEU:HD23	4:C:940:HOH:O	1.77	0.82
1:C:4:MET:HE2	1:C:21:MET:CE	2.13	0.79
1:D:173:LEU:HD12	1:D:174:ALA:N	1.98	0.79
1:D:174:ALA:HB1	1:D:176:TRP:HE1	1.50	0.76
1:C:52:ASN:HB3	4:C:1023:HOH:O	1.85	0.76
1:C:30:GLU:HG3	4:C:410:HOH:O	1.88	0.74
1:D:151:ILE:HD13	1:D:173:LEU:HB3	1.68	0.73
1:D:174:ALA:HB1	1:D:176:TRP:NE1	2.04	0.73
1:D:103:ILE:HD13	1:D:113:PHE:HB2	1.72	0.71
4:B:316:HOH:O	1:D:1:MET:HE2	1.91	0.69
1:D:103:ILE:CD1	1:D:113:PHE:HB2	2.22	0.69
1:C:253:LEU:HG	1:C:255:VAL:HG23	1.74	0.68
1:D:158:PHE:HE1	1:D:160:LEU:HB2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD13	1:A:113:PHE:HB2	1.76	0.68
1:C:235:PRO:HB3	4:C:703:HOH:O	1.93	0.68
1:C:4:MET:CE	1:C:21:MET:HE2	2.20	0.67
1:C:187:ASP:OD1	4:C:964:HOH:O	2.13	0.66
1:B:4:MET:HE2	1:B:21:MET:HG3	1.79	0.65
1:C:52:ASN:O	4:C:410:HOH:O	2.15	0.64
1:A:93:LYS:HD3	1:A:254:GLU:OE2	1.98	0.64
1:D:175:GLU:HB3	1:D:214:ARG:CZ	2.28	0.63
1:A:250:SER:HB2	4:A:279:HOH:O	1.98	0.62
1:D:140:TYR:HB2	1:D:189:VAL:O	1.99	0.62
1:D:42:GLU:HG3	4:D:320:HOH:O	2.01	0.61
1:B:59:GLU:HG2	4:B:305:HOH:O	2.00	0.61
1:D:174:ALA:CB	1:D:176:TRP:HE1	2.13	0.60
1:A:103:ILE:CD1	1:A:113:PHE:HB2	2.32	0.60
1:D:158:PHE:CE1	1:D:160:LEU:HB2	2.35	0.60
1:A:21:MET:HG2	1:A:37:MET:SD	2.42	0.58
1:C:29:LYS:HE3	1:C:56:LYS:HA	1.84	0.58
1:D:1:MET:N	4:D:323:HOH:O	2.36	0.58
1:D:151:ILE:HD13	1:D:173:LEU:CB	2.34	0.58
1:C:150:LYS:HE3	1:C:170:GLU:HG2	1.85	0.57
1:D:4:MET:CE	1:D:21:MET:HG3	2.35	0.57
1:C:163:GLU:O	1:C:165:VAL:HG13	2.05	0.56
1:D:15:ASN:ND2	4:D:708:HOH:O	2.25	0.56
1:A:93:LYS:HD3	1:A:254:GLU:CD	2.31	0.56
1:A:130:ILE:N	1:A:130:ILE:HD12	2.20	0.56
1:C:109:LEU:HD12	1:C:110:PRO:HD2	1.87	0.56
1:C:256:ARG:C	4:C:444:HOH:O	2.49	0.55
1:D:60:ARG:HH21	1:D:176:TRP:HZ3	1.52	0.55
1:D:59:GLU:HG3	4:D:823:HOH:O	2.06	0.55
1:C:173:LEU:HG	1:C:174:ALA:N	2.21	0.55
1:D:203:ASP:O	1:D:207:LYS:HG2	2.06	0.55
1:D:179:ASP:OD1	1:D:214:ARG:NH2	2.39	0.55
1:D:4:MET:HE1	1:D:21:MET:HG3	1.89	0.54
1:D:1:MET:CB	4:D:322:HOH:O	2.56	0.54
1:A:59:GLU:HG2	4:A:302:HOH:O	2.07	0.54
1:D:174:ALA:CB	1:D:176:TRP:NE1	2.70	0.54
1:A:21:MET:CG	1:A:37:MET:SD	2.96	0.53
1:D:150:LYS:NZ	1:D:170:GLU:HG2	2.23	0.53
1:D:1:MET:HB2	4:D:322:HOH:O	2.09	0.53
1:D:190:LYS:NZ	4:D:428:HOH:O	2.41	0.53
1:A:108:SER:HB2	4:A:355:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:CG	1:C:255:VAL:HG23	2.39	0.53
1:D:96:SER:OG	1:D:195:LYS:NZ	2.27	0.53
1:D:174:ALA:HB1	1:D:176:TRP:CD1	2.44	0.53
1:D:150:LYS:NZ	1:D:153:GLU:OE2	2.40	0.52
1:D:111:LEU:C	1:D:111:LEU:HD23	2.34	0.52
1:C:4:MET:CE	1:C:21:MET:CE	2.85	0.51
1:C:140:TYR:HB2	1:C:189:VAL:O	2.10	0.51
1:B:235:PRO:HB2	1:B:236:GLU:OE2	2.10	0.51
1:D:153:GLU:OE2	1:D:186:LYS:NZ	2.43	0.51
1:B:4:MET:HE2	1:B:21:MET:SD	2.51	0.50
1:A:76:GLU:O	1:A:77:ASN:C	2.55	0.50
1:C:163:GLU:HG3	1:C:165:VAL:HG13	1.93	0.50
1:D:154:PHE:HE2	1:D:171:LEU:HD22	1.76	0.50
1:B:1:MET:HG2	1:B:2:VAL:N	2.25	0.50
1:D:203:ASP:O	1:D:207:LYS:HD3	2.12	0.49
1:A:130:ILE:HD12	1:A:130:ILE:H	1.77	0.49
1:B:4:MET:HE2	1:B:21:MET:CG	2.42	0.49
1:C:98:GLU:OE1	1:C:195:LYS:NZ	2.44	0.49
1:C:83:SER:HB3	4:C:678:HOH:O	2.13	0.48
1:D:209:LEU:HD13	1:D:215:VAL:HG21	1.95	0.48
1:D:133:VAL:HG12	1:D:134:CYS:N	2.28	0.48
3:B:902:BGC:O1	4:B:426:HOH:O	2.20	0.48
1:A:173:LEU:C	1:A:173:LEU:HD23	2.39	0.48
1:C:155:THR:HG23	1:C:166:GLU:OE2	2.14	0.48
1:B:241:GLN:HG2	4:B:584:HOH:O	2.13	0.47
1:C:93:LYS:HB2	1:C:256:ARG:HG3	1.96	0.47
1:C:163:GLU:HG3	1:C:165:VAL:CG1	2.45	0.47
1:D:61:TYR:CZ	1:D:234:SER:HB2	2.50	0.47
1:D:153:GLU:CD	1:D:186:LYS:NZ	2.72	0.46
1:D:176:TRP:HE3	4:D:512:HOH:O	1.98	0.46
1:D:180:TYR:C	1:D:181:LEU:HD12	2.41	0.46
1:C:163:GLU:O	1:C:163:GLU:HG3	2.16	0.46
1:D:150:LYS:HE3	1:D:170:GLU:HG2	1.97	0.46
1:D:88:PRO:HG3	1:D:222:TYR:CE1	2.51	0.46
1:C:4:MET:HE2	1:C:21:MET:HG3	1.98	0.45
1:D:4:MET:HE2	1:D:21:MET:SD	2.56	0.45
1:C:72:TYR:O	1:C:225:VAL:HB	2.17	0.45
1:A:1:MET:HA	1:A:39:PHE:O	2.16	0.45
1:D:150:LYS:CE	1:D:170:GLU:HG2	2.46	0.45
1:D:141:PHE:CD2	1:D:184:ARG:HD2	2.52	0.44
1:D:119:LEU:HA	1:D:222:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:MET:HE1	1:D:39:PHE:HB2	2.00	0.44
1:C:238:LYS:HA	1:C:238:LYS:HD3	1.72	0.43
1:C:111:LEU:C	1:C:111:LEU:HD23	2.43	0.43
1:A:207:LYS:HE3	4:A:788:HOH:O	2.18	0.43
1:A:97:VAL:HG22	1:A:251:ILE:HG22	2.00	0.43
1:C:91:SER:HB3	1:C:255:VAL:HG13	2.01	0.43
1:C:98:GLU:HB2	1:C:195:LYS:HG3	2.01	0.43
1:D:1:MET:HE3	1:D:1:MET:HB3	1.78	0.42
1:B:254:GLU:HG3	4:B:341:HOH:O	2.19	0.42
1:D:50:ILE:HD12	1:D:53:LEU:HD21	2.00	0.42
1:D:67:GLU:OE1	1:D:227:GLU:OE2	2.37	0.42
1:D:203:ASP:O	1:D:207:LYS:CD	2.67	0.42
1:A:67:GLU:OE1	1:A:227:GLU:OE2	2.38	0.42
1:A:113:PHE:HB3	1:A:140:TYR:HB3	2.00	0.42
1:C:109:LEU:HA	1:C:110:PRO:HD3	1.83	0.42
1:C:108:SER:O	1:C:110:PRO:HD3	2.19	0.41
1:C:54:SER:HB3	4:C:410:HOH:O	2.21	0.41
1:C:251:ILE:C	1:C:251:ILE:HD12	2.46	0.41
1:D:154:PHE:HE2	1:D:171:LEU:CD2	2.33	0.41
1:D:97:VAL:O	1:D:195:LYS:HA	2.21	0.41
1:D:153:GLU:OE1	1:D:186:LYS:NZ	2.53	0.41
1:D:4:MET:HE2	1:D:21:MET:HG3	2.03	0.41
1:D:154:PHE:CE2	1:D:171:LEU:HD22	2.55	0.41
1:C:93:LYS:HD2	1:C:256:ARG:CD	2.34	0.41
1:A:57:GLU:HB2	1:A:60:ARG:HG2	2.03	0.41
1:A:138:TRP:HB2	1:A:184:ARG:HA	2.03	0.41
1:C:4:MET:CE	1:C:21:MET:HG3	2.50	0.41
1:C:104:HIS:CE1	1:C:243:GLY:HA3	2.55	0.41
1:D:65:TYR:O	1:D:66:PRO:C	2.63	0.41
1:C:119:LEU:HA	1:C:222:TYR:O	2.20	0.41
1:C:67:GLU:OE1	1:C:227:GLU:OE2	2.38	0.41
1:B:173:LEU:HG	1:B:174:ALA:N	2.35	0.41
1:B:141:PHE:CD2	1:B:184:ARG:HD2	2.57	0.40
1:D:178:TRP:HD1	1:D:179:ASP:O	2.04	0.40
1:A:84:LYS:O	1:D:82:GLY:HA2	2.22	0.40
1:B:4:MET:CE	1:B:21:MET:HG3	2.50	0.40
1:C:238:LYS:HG2	1:D:236:GLU:HG3	2.03	0.40
1:B:5:THR:HG23	1:D:34:SER:HB3	2.03	0.40
1:D:111:LEU:HD23	1:D:112:ASN:N	2.37	0.40

All (2) 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)
4:B:374:HOH:O	4:B:374:HOH:O[2_555]	1.98	0.22
1:C:217:ASP:OD2	4:B:1003:HOH:O[2_545]	2.12	0.08

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	255/265 (96%)	247 (97%)	8 (3%)	0	100	100
1	B	254/265 (96%)	246 (97%)	8 (3%)	0	100	100
1	C	254/265 (96%)	245 (96%)	9 (4%)	0	100	100
1	D	254/265 (96%)	244 (96%)	10 (4%)	0	100	100
All	All	1017/1060 (96%)	982 (97%)	35 (3%)	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	227/234 (97%)	226 (100%)	1 (0%)	84	83
1	B	226/234 (97%)	225 (100%)	1 (0%)	84	83
1	C	226/234 (97%)	222 (98%)	4 (2%)	51	43
1	D	226/234 (97%)	223 (99%)	3 (1%)	61	54
All	All	905/936 (97%)	896 (99%)	9 (1%)	68	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	B	179	ASP
1	C	1	MET
1	C	54	SER
1	C	155	THR
1	C	217	ASP
1	D	1	MET
1	D	176	TRP
1	D	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	B	77	ASN
1	B	241	GLN
1	C	77	ASN
1	C	104	HIS
1	C	161	ASN
1	D	77	ASN
1	D	161	ASN
1	D	241	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](#)

8 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	GLC	E	1	2	12,12,12	0.51	0	17,17,17	0.87	1 (5%)
2	BGC	E	2	2	11,11,12	0.41	0	15,15,17	0.87	0
2	GLC	F	1	2	12,12,12	0.48	0	17,17,17	0.90	1 (5%)
2	BGC	F	2	2	11,11,12	0.42	0	15,15,17	0.86	0
2	GLC	G	1	2	12,12,12	0.52	0	17,17,17	0.86	1 (5%)
2	BGC	G	2	2	11,11,12	0.37	0	15,15,17	0.74	0
2	GLC	H	1	2	12,12,12	0.50	0	17,17,17	0.73	0
2	BGC	H	2	2	11,11,12	0.42	0	15,15,17	0.95	1 (6%)

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	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	1/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLC	O5-C5-C4	2.48	114.17	109.70
2	H	2	BGC	C6-C5-C4	-2.40	107.13	113.02
2	E	1	GLC	O5-C5-C4	2.33	113.90	109.70
2	F	1	GLC	O5-C5-C4	2.30	113.84	109.70

There are no chirality outliers.

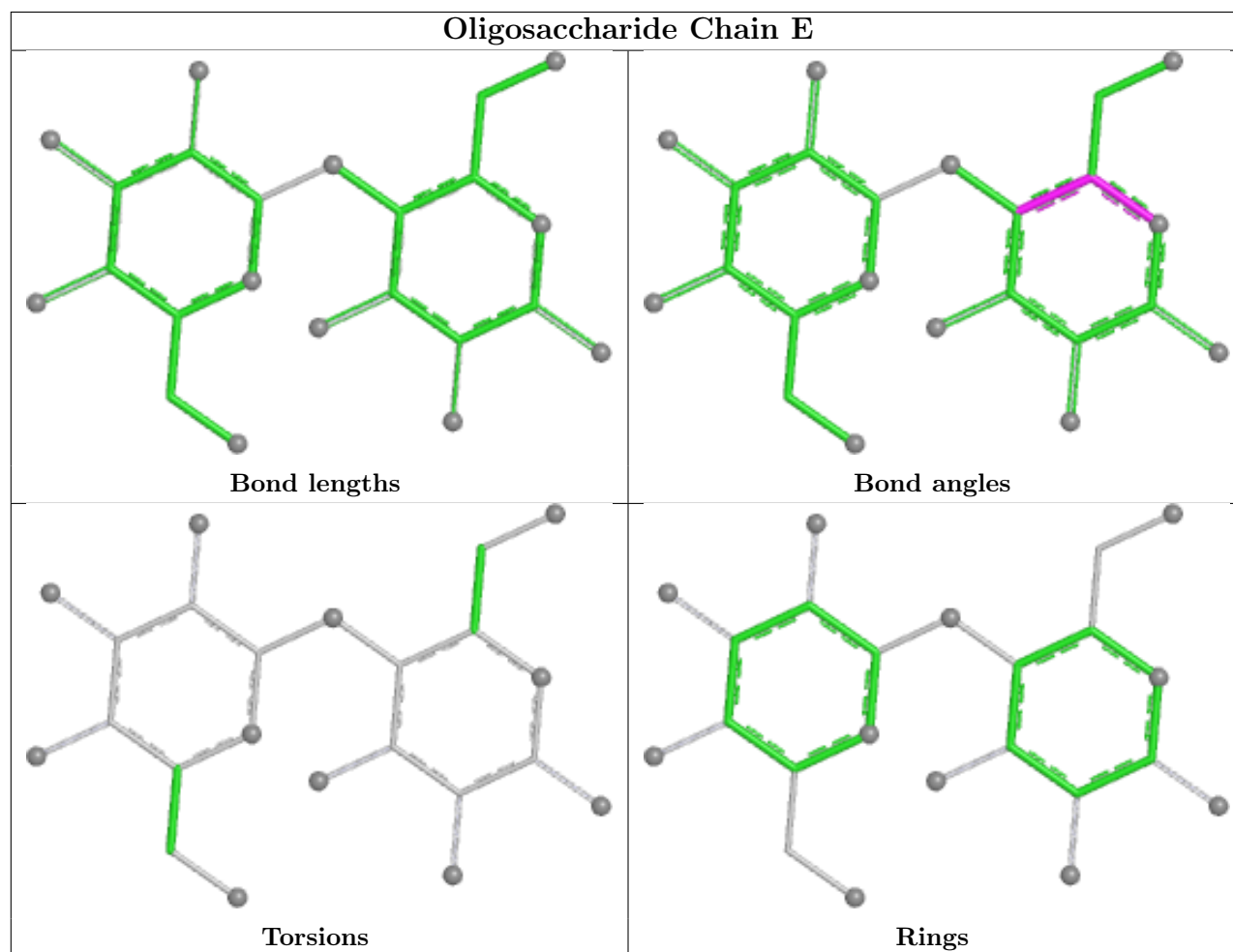
All (1) torsion outliers are listed below:

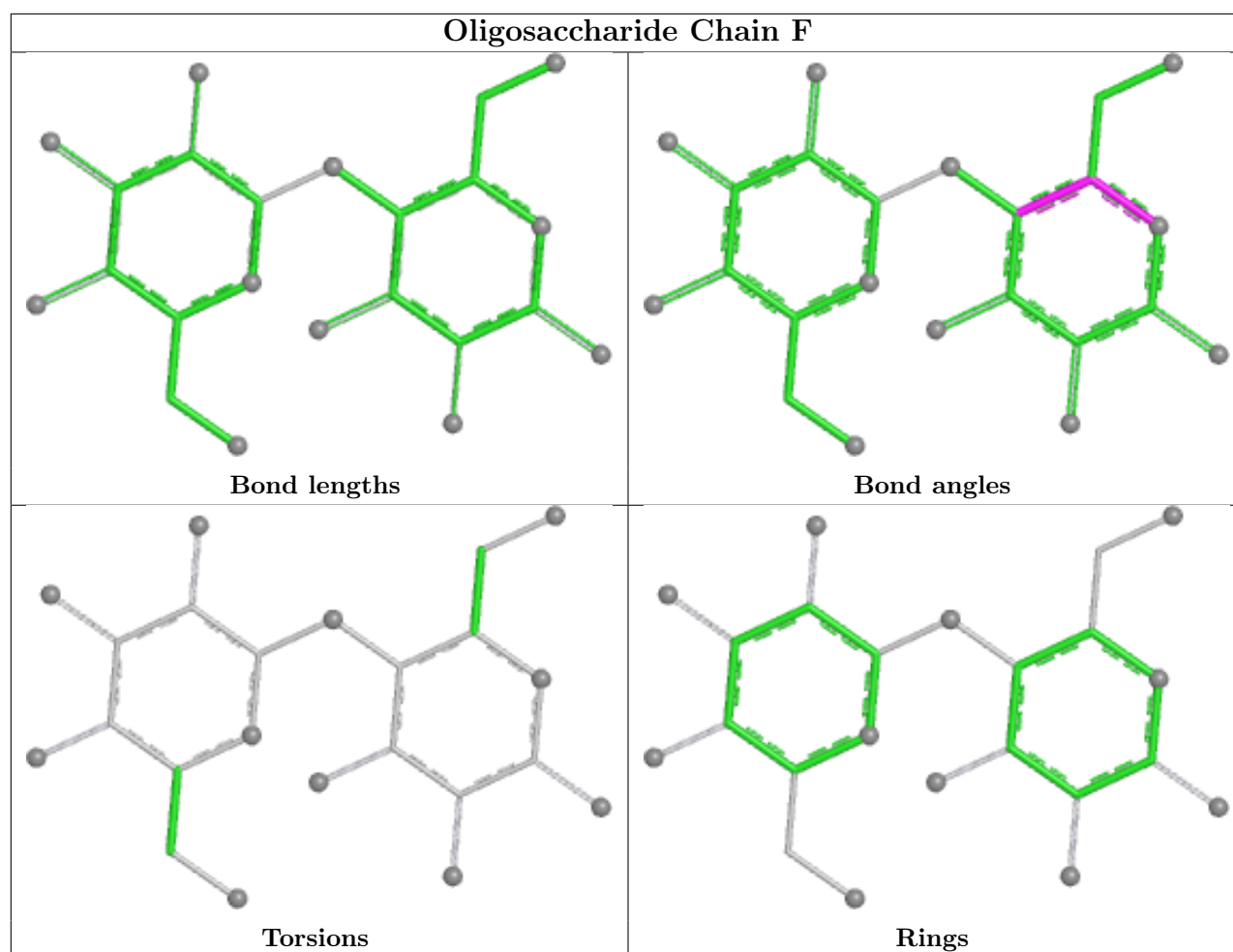
Mol	Chain	Res	Type	Atoms
2	G	1	GLC	C4-C5-C6-O6

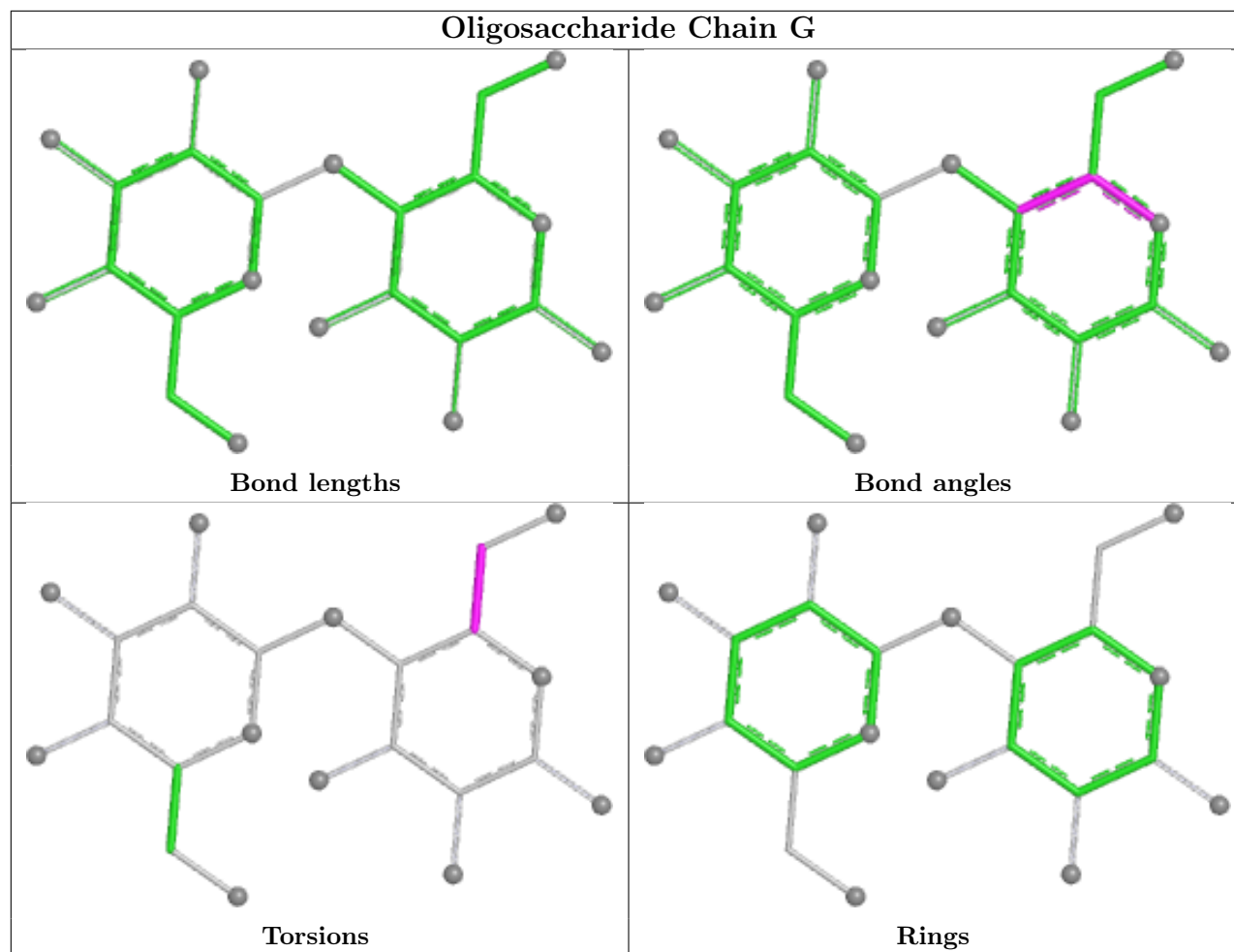
There are no ring outliers.

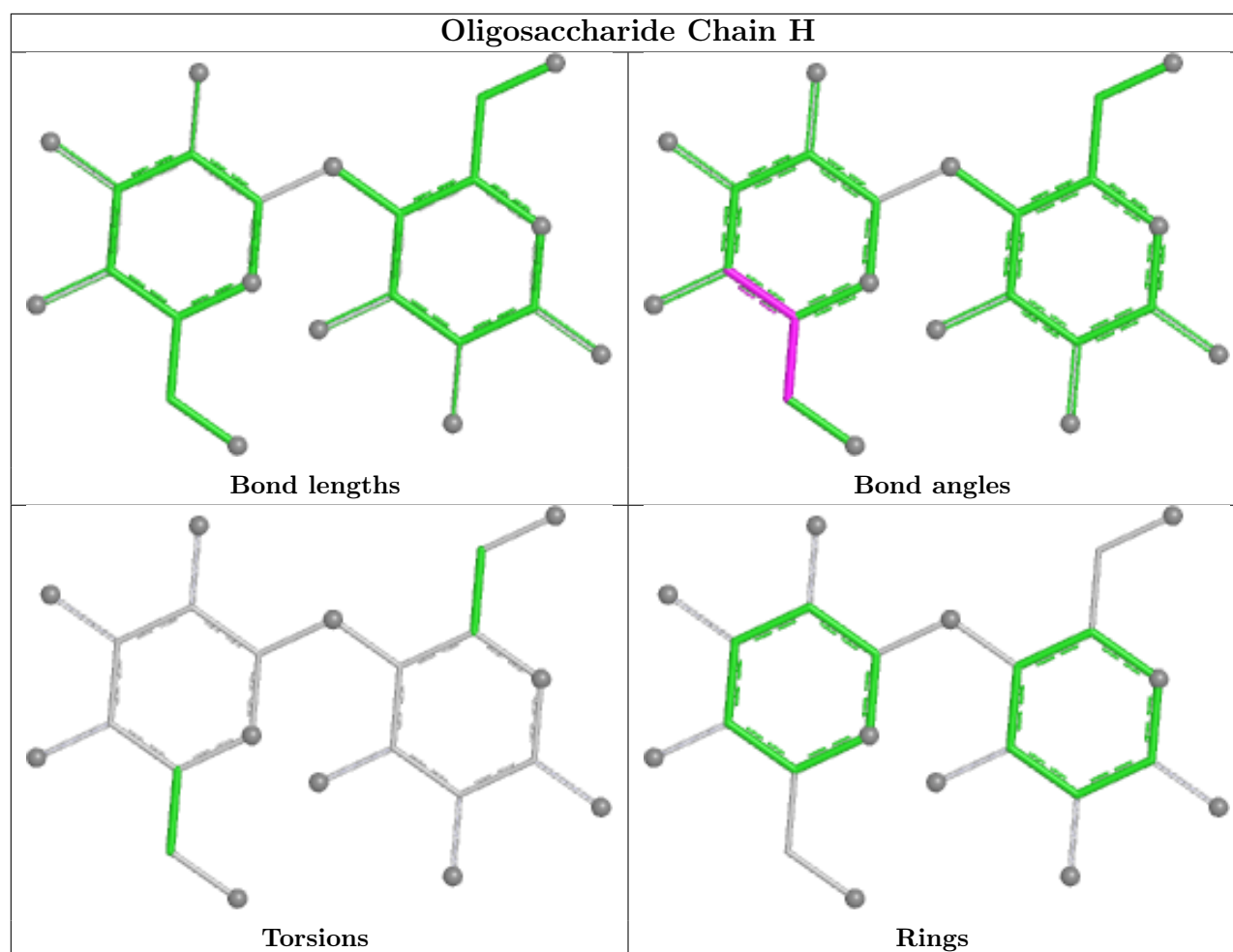
No monomer is involved in short contacts.

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](#)

3 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	$\# Z > 2$
3	BGC	C	902	-	12,12,12	1.01	0	17,17,17	1.01	1 (5%)
3	BGC	B	902	-	12,12,12	0.55	0	17,17,17	0.96	1 (5%)
3	BGC	A	902	-	12,12,12	0.64	0	17,17,17	0.80	1 (5%)

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	BGC	C	902	-	-	1/2/22/22	0/1/1/1
3	BGC	B	902	-	-	1/2/22/22	0/1/1/1
3	BGC	A	902	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	BGC	C1-O5-C5	-2.43	108.95	113.65
3	A	902	BGC	C3-C4-C5	2.29	114.38	110.23
3	B	902	BGC	C1-O5-C5	-2.25	109.31	113.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	BGC	O5-C5-C6-O6
3	A	902	BGC	O5-C5-C6-O6
3	B	902	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	BGC	1	0

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	257/265 (96%)	-0.22	1 (0%) 88 89	22, 32, 46, 59	0
1	B	256/265 (96%)	-0.47	0 100 100	19, 27, 41, 47	0
1	C	256/265 (96%)	0.21	6 (2%) 61 61	18, 35, 55, 73	0
1	D	256/265 (96%)	0.32	18 (7%) 22 21	19, 34, 57, 68	0
All	All	1025/1060 (96%)	-0.04	25 (2%) 59 60	18, 32, 52, 73	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	TRP	3.5
1	D	213	ALA	2.7
1	C	162	GLY	2.6
1	D	165	VAL	2.6
1	D	159	VAL	2.6
1	D	154	PHE	2.5
1	D	210	SER	2.5
1	C	237	THR	2.4
1	A	1	MET	2.4
1	C	217	ASP	2.3
1	D	173	LEU	2.3
1	D	216	LYS	2.3
1	D	130	ILE	2.3
1	C	211	SER	2.3
1	D	209	LEU	2.2
1	C	165	VAL	2.2
1	C	53	LEU	2.2
1	D	167	GLY	2.1
1	D	207	LYS	2.1
1	D	151	ILE	2.1
1	D	156	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	211	SER	2.0
1	D	174	ALA	2.0
1	D	158	PHE	2.0
1	D	177	GLY	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](#)

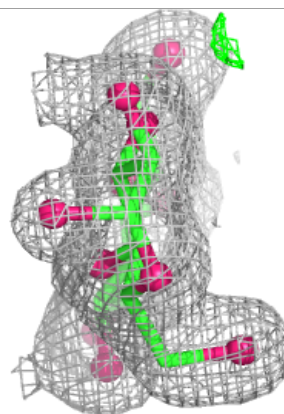
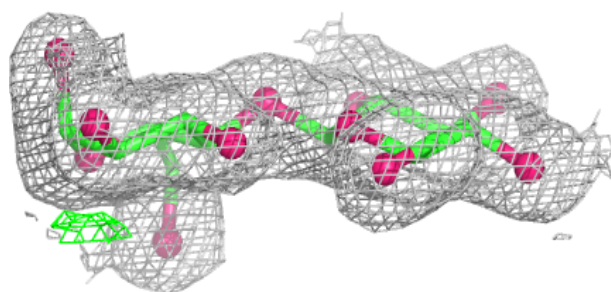
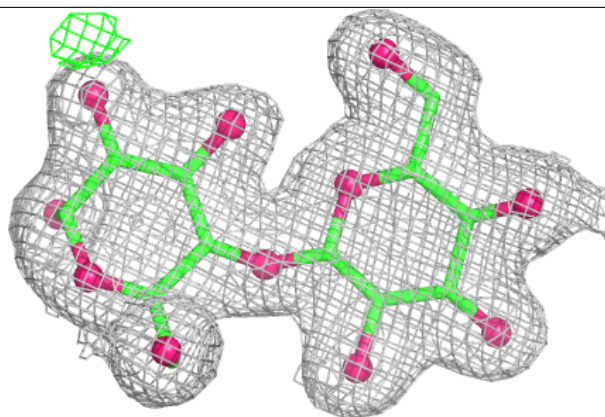
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	H	1	12/12	0.91	0.08	32,37,43,45	0
2	BGC	H	2	11/12	0.94	0.07	26,30,34,41	0
2	GLC	G	1	12/12	0.96	0.06	26,29,33,34	0
2	BGC	G	2	11/12	0.96	0.06	23,27,29,34	0
2	BGC	E	2	11/12	0.97	0.05	25,27,31,34	0
2	GLC	F	1	12/12	0.97	0.05	23,28,33,35	0
2	GLC	E	1	12/12	0.97	0.06	27,29,35,35	0
2	BGC	F	2	11/12	0.98	0.05	21,25,26,27	0

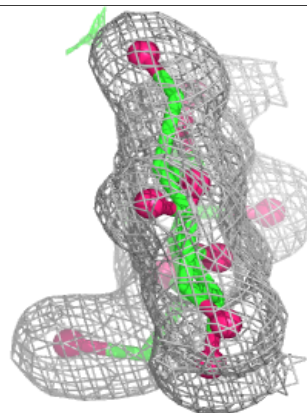
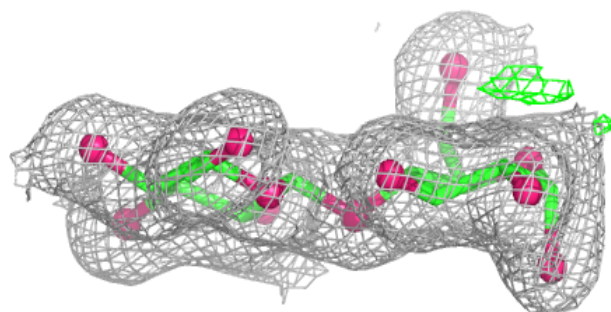
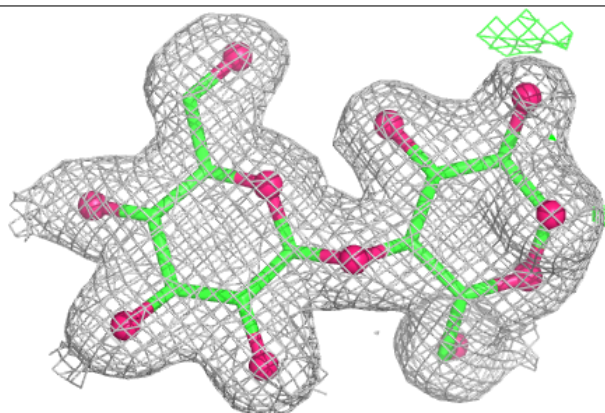
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

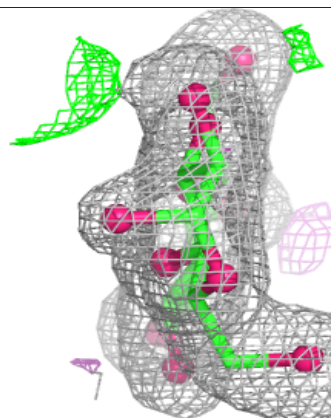
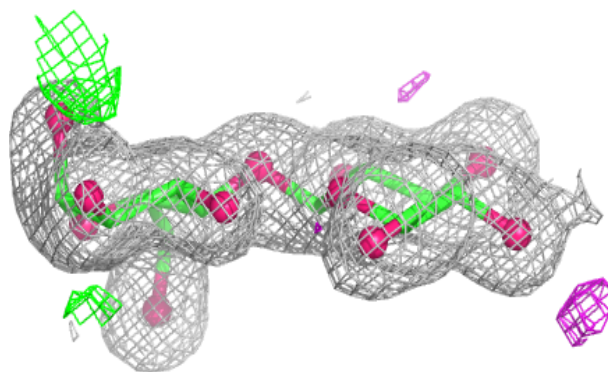
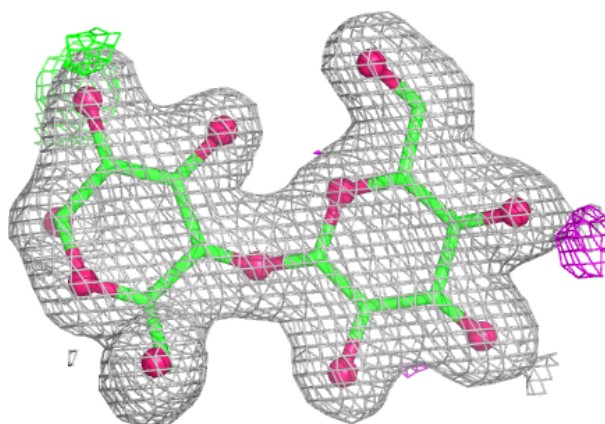
**Electron density around Chain F:**

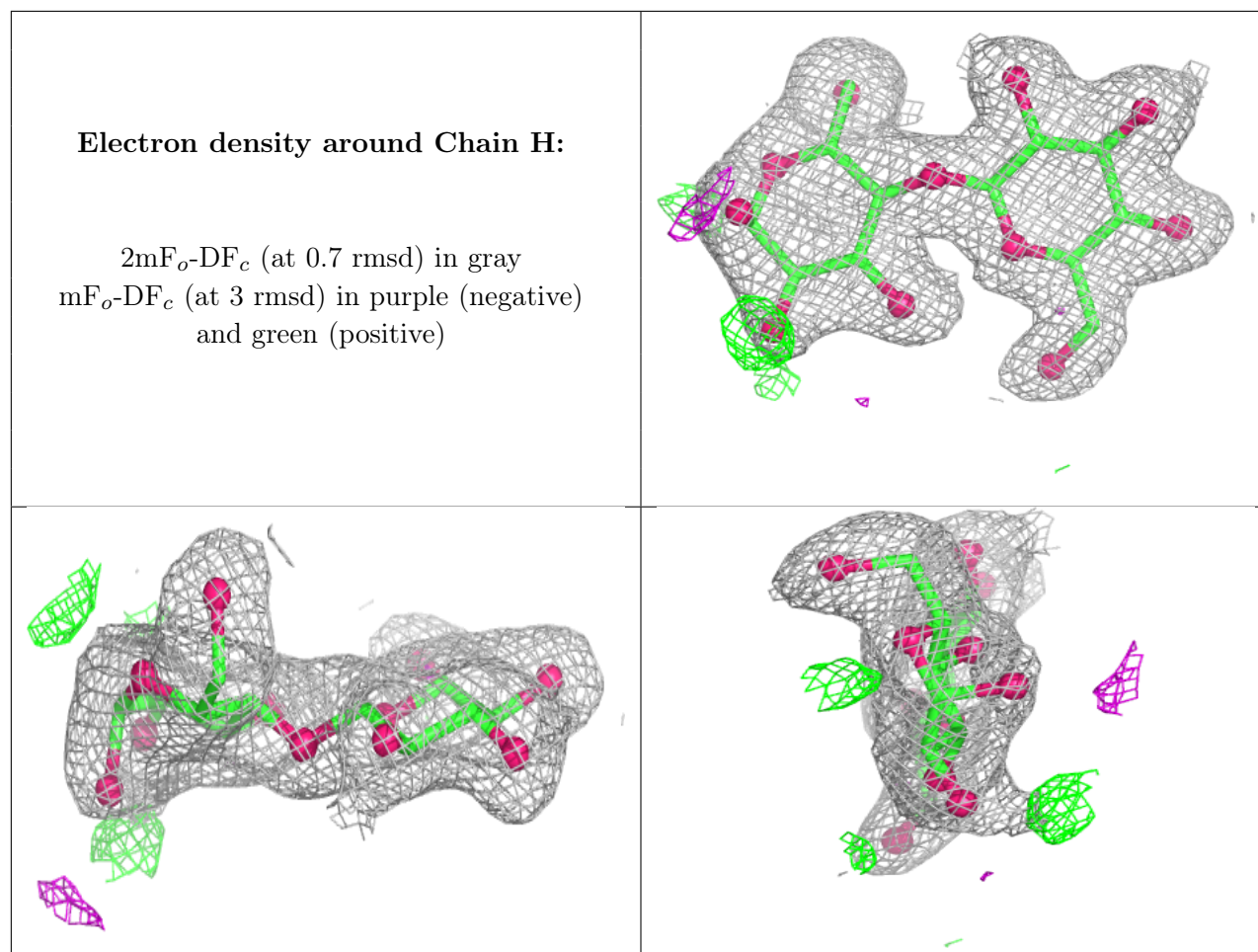
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	BGC	C	902	12/12	0.75	0.15	39,48,50,53	0
3	BGC	B	902	12/12	0.87	0.12	31,45,49,54	0
3	BGC	A	902	12/12	0.89	0.09	33,43,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.