



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:29 AM UTC

PDB ID : 5TJ2 / pdb_00005tj2
Title : Gasdermin-B C-terminal domain containing the polymorphism residues
Gly299:Ser306 fused to maltose binding protein
Authors : Chao, L.K.; Herzberg, O.
Deposited on : 2016-10-03
Resolution : 2.80 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:

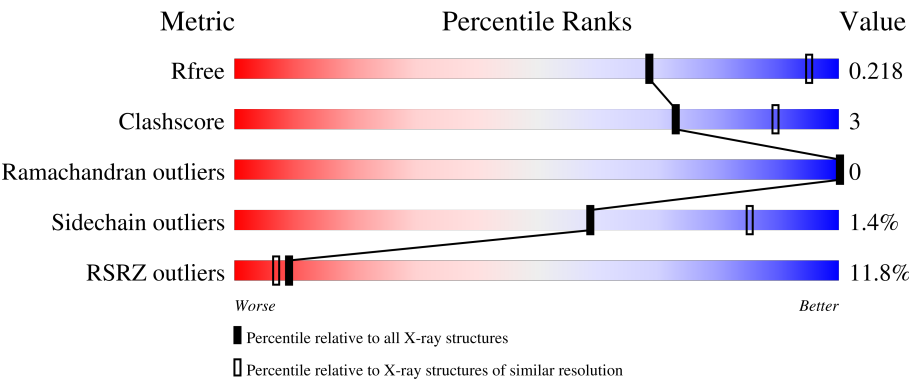
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.



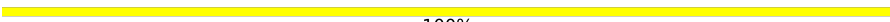
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	553	3% 92%
1	B	553	% 91% 6%
1	C	553	9% 87% 8%
1	D	553	32% 89% 6% 5%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15875 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 Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4029	2579	659	778	13			
1	B	536	Total	C	N	O	S	0	0	0
			4053	2598	663	779	13			
1	C	529	Total	C	N	O	S	0	0	0
			3854	2480	624	738	12			
1	D	528	Total	C	N	O	S	0	0	0
			3810	2447	623	728	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	conflict	UNP A0A178SBV6
A	83	ALA	LYS	conflict	UNP A0A178SBV6
A	172	ALA	GLU	conflict	UNP A0A178SBV6
A	173	ALA	ASN	conflict	UNP A0A178SBV6
A	239	ALA	LYS	conflict	UNP A0A178SBV6
A	362	ALA	LYS	conflict	UNP A0A178SBV6
A	363	ALA	ASP	conflict	UNP A0A178SBV6
A	367	ASN	-	linker	UNP A0A178SBV6
A	368	ALA	-	linker	UNP A0A178SBV6
A	369	ALA	-	linker	UNP A0A178SBV6
A	370	ALA	-	linker	UNP A0A178SBV6
A	1306	SER	PRO	engineered mutation	UNP Q8TAX9
A	?	-	ASP	deletion	UNP Q8TAX9
A	?	-	MET	deletion	UNP Q8TAX9
A	?	-	ASP	deletion	UNP Q8TAX9
A	?	-	TYR	deletion	UNP Q8TAX9
B	82	ALA	ASP	conflict	UNP A0A178SBV6
B	83	ALA	LYS	conflict	UNP A0A178SBV6
B	172	ALA	GLU	conflict	UNP A0A178SBV6
B	173	ALA	ASN	conflict	UNP A0A178SBV6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	239	ALA	LYS	conflict	UNP A0A178SBV6
B	362	ALA	LYS	conflict	UNP A0A178SBV6
B	363	ALA	ASP	conflict	UNP A0A178SBV6
B	367	ASN	-	linker	UNP A0A178SBV6
B	368	ALA	-	linker	UNP A0A178SBV6
B	369	ALA	-	linker	UNP A0A178SBV6
B	370	ALA	-	linker	UNP A0A178SBV6
B	1306	SER	PRO	engineered mutation	UNP Q8TAX9
B	?	-	ASP	deletion	UNP Q8TAX9
B	?	-	MET	deletion	UNP Q8TAX9
B	?	-	ASP	deletion	UNP Q8TAX9
B	?	-	TYR	deletion	UNP Q8TAX9
C	82	ALA	ASP	conflict	UNP A0A178SBV6
C	83	ALA	LYS	conflict	UNP A0A178SBV6
C	172	ALA	GLU	conflict	UNP A0A178SBV6
C	173	ALA	ASN	conflict	UNP A0A178SBV6
C	239	ALA	LYS	conflict	UNP A0A178SBV6
C	362	ALA	LYS	conflict	UNP A0A178SBV6
C	363	ALA	ASP	conflict	UNP A0A178SBV6
C	367	ASN	-	linker	UNP A0A178SBV6
C	368	ALA	-	linker	UNP A0A178SBV6
C	369	ALA	-	linker	UNP A0A178SBV6
C	370	ALA	-	linker	UNP A0A178SBV6
C	1306	SER	PRO	engineered mutation	UNP Q8TAX9
C	?	-	ASP	deletion	UNP Q8TAX9
C	?	-	MET	deletion	UNP Q8TAX9
C	?	-	ASP	deletion	UNP Q8TAX9
C	?	-	TYR	deletion	UNP Q8TAX9
D	82	ALA	ASP	conflict	UNP A0A178SBV6
D	83	ALA	LYS	conflict	UNP A0A178SBV6
D	172	ALA	GLU	conflict	UNP A0A178SBV6
D	173	ALA	ASN	conflict	UNP A0A178SBV6
D	239	ALA	LYS	conflict	UNP A0A178SBV6
D	362	ALA	LYS	conflict	UNP A0A178SBV6
D	363	ALA	ASP	conflict	UNP A0A178SBV6
D	367	ASN	-	linker	UNP A0A178SBV6
D	368	ALA	-	linker	UNP A0A178SBV6
D	369	ALA	-	linker	UNP A0A178SBV6
D	370	ALA	-	linker	UNP A0A178SBV6
D	1306	SER	PRO	engineered mutation	UNP Q8TAX9
D	?	-	ASP	deletion	UNP Q8TAX9
D	?	-	MET	deletion	UNP Q8TAX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP Q8TAX9
D	?	-	TYR	deletion	UNP Q8TAX9

- Molecule 2 is an oligosaccharide called alpha-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			

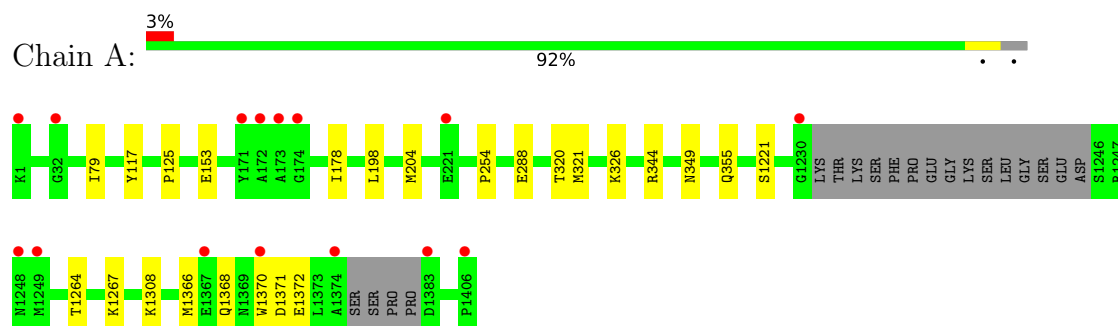
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	12	Total	O	0	0
			12	12		
3	C	3	Total	O	0	0
			3	3		
3	D	1	Total	O	0	0
			1	1		

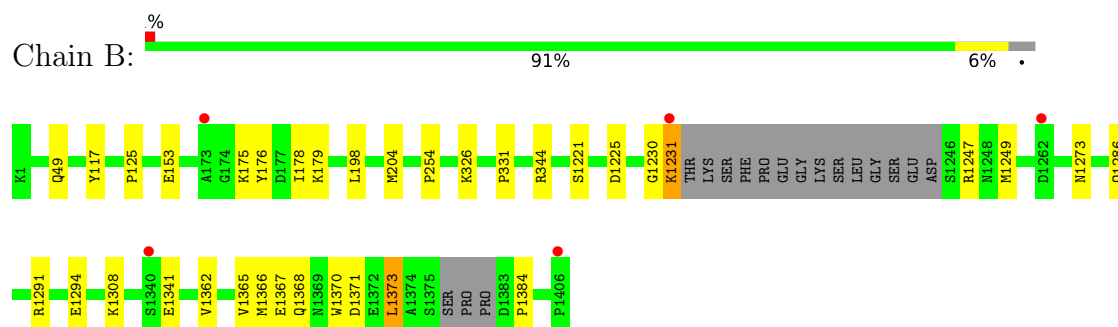
3 Residue-property plots [i](#)

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.

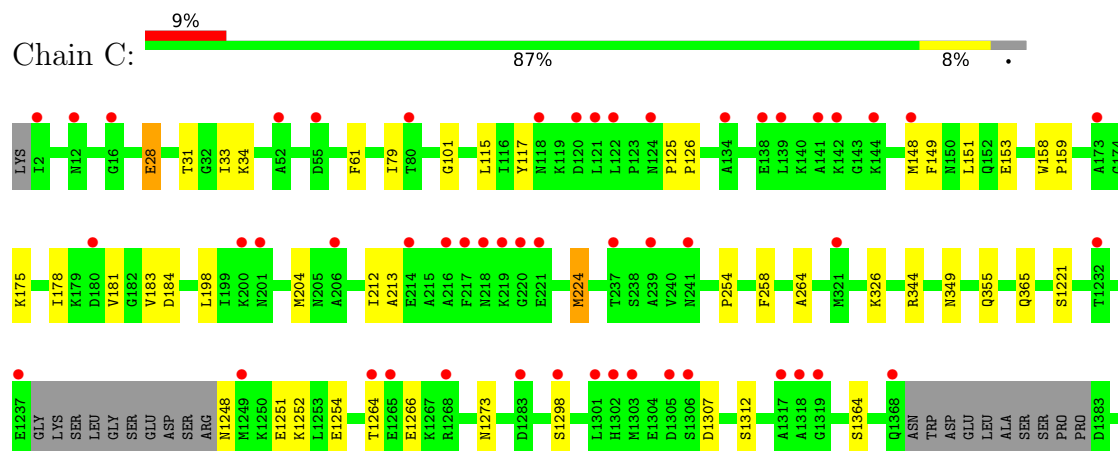
- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein



- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

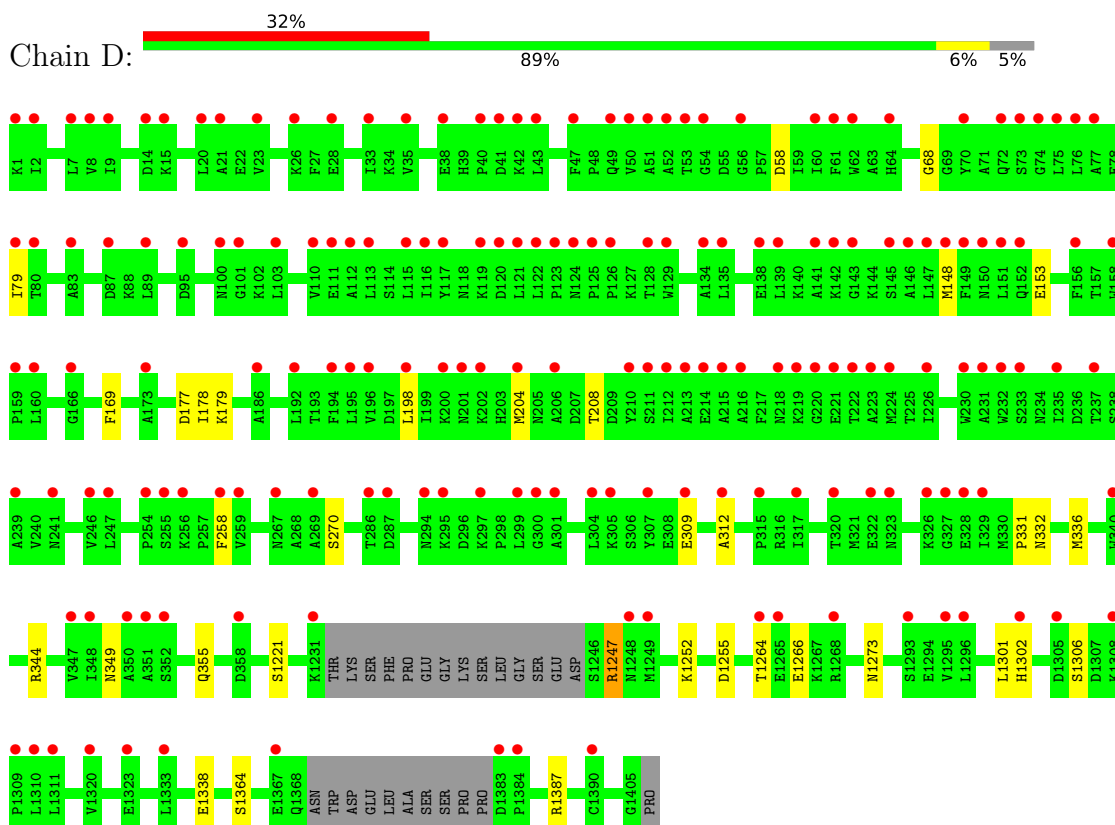


- Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B fusion protein

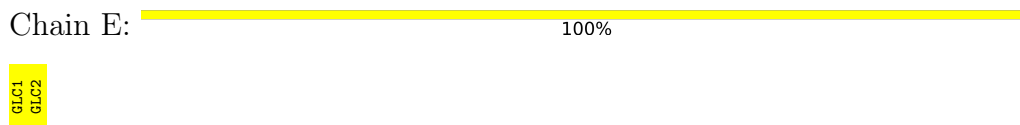




- Molecule 1: Sugar ABC transporter substrate-binding protein, Gasdermin-B fusion protein



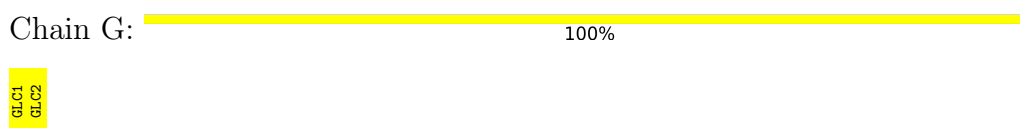
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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



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



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

Chain H:

100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.04Å 152.75Å 255.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.50 – 2.80 42.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.50-2.80) 99.6 (42.50-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.252 0.216 , 0.218	Depositor DCC
R_{free} test set	4823 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15875	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: 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	0.85	2/4109 (0.0%)	0.95	0/5588
1	B	0.83	0/4133	0.94	1/5616 (0.0%)
1	C	0.78	0/3933	0.95	1/5372 (0.0%)
1	D	0.73	0/3887	0.95	3/5316 (0.1%)
All	All	0.80	2/16062 (0.0%)	0.95	5/21892 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1372	GLU	N-CA	5.40	1.53	1.46
1	A	1371	ASP	CA-C	5.06	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1301	LEU	N-CA-C	-7.55	94.63	107.99
1	D	1302	HIS	N-CA-C	-6.28	102.41	110.19
1	D	1252	LYS	N-CA-C	-6.08	104.97	112.38
1	B	175	LYS	N-CA-C	5.99	118.66	108.90
1	C	224	MET	CG-SD-CE	-5.19	89.49	100.90

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	4029	0	3931	13	0
1	B	4053	0	3977	32	0
1	C	3854	0	3623	33	0
1	D	3810	0	3555	26	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	21	0	0	0	0
3	B	12	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
All	All	15875	0	15170	98	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 3.

All (98) 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:126:PRO:HD2	1:C:224:MET:HE1	1.50	0.93
1:B:1231:LYS:HE2	1:B:1231:LYS:HA	1.50	0.91
1:C:184:ASP:HB3	1:C:365:GLN:OE1	1.72	0.89
1:C:126:PRO:HD2	1:C:224:MET:CE	2.06	0.85
1:D:1247:ARG:NH2	1:D:1255:ASP:OD2	2.15	0.78
1:D:169:PHE:CE2	1:D:336:MET:HE2	2.19	0.78
1:B:1291:ARG:NH1	1:B:1294:GLU:OE1	2.22	0.72
1:A:320:THR:HG22	1:A:321:MET:HE2	1.70	0.72
1:D:169:PHE:HE2	1:D:336:MET:HE2	1.54	0.72
1:B:1231:LYS:HE2	1:B:1231:LYS:CA	2.16	0.71
1:B:1230:GLY:O	1:B:1231:LYS:HG2	1.91	0.71
1:A:320:THR:HG22	1:A:321:MET:CE	2.23	0.67
1:B:1366:MET:HE2	1:B:1373:LEU:HD13	1.76	0.67
1:B:1384:PRO:HB3	1:C:101:GLY:HA3	1.77	0.67
1:B:1231:LYS:HA	1:B:1231:LYS:CE	2.23	0.67
1:C:178:ILE:HG23	1:C:1221:SER:HB3	1.77	0.66
1:A:178:ILE:HG23	1:A:1221:SER:HB3	1.79	0.64
1:C:1251:GLU:HA	1:C:1254:GLU:HB2	1.80	0.64
1:D:331:PRO:HB2	1:D:336:MET:HE3	1.78	0.63
1:C:126:PRO:CD	1:C:224:MET:HE1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ILE:HG23	1:D:1221:SER:HB3	1.80	0.62
1:B:178:ILE:HG23	1:B:1221:SER:HB3	1.81	0.61
1:B:198:LEU:HD13	1:B:204:MET:HE2	1.82	0.61
1:C:198:LEU:HD13	1:C:204:MET:HE2	1.84	0.59
1:A:198:LEU:HD13	1:A:204:MET:HE2	1.84	0.59
1:D:198:LEU:HD13	1:D:204:MET:HE2	1.84	0.58
1:C:148:MET:HE3	1:C:212:ILE:HG22	1.85	0.58
1:B:1362:VAL:O	1:B:1365:VAL:CG2	2.52	0.57
1:C:1307:ASP:HA	1:D:312:ALA:HB1	1.87	0.57
1:A:1366:MET:HE1	1:A:1370:TRP:HE3	1.70	0.57
1:B:1366:MET:HE1	1:B:1370:TRP:CE3	2.41	0.56
1:B:1362:VAL:O	1:B:1365:VAL:HG22	2.06	0.55
1:D:169:PHE:CD2	1:D:336:MET:CE	2.90	0.55
1:C:31:THR:CB	1:C:33:ILE:HD12	2.36	0.55
1:C:148:MET:CE	1:C:212:ILE:HG22	2.38	0.54
1:B:1366:MET:HE1	1:B:1370:TRP:HE3	1.71	0.54
1:B:1373:LEU:O	1:B:1373:LEU:HD23	2.08	0.54
1:D:331:PRO:HG2	1:D:336:MET:HE3	1.90	0.53
1:A:1366:MET:O	1:A:1368:GLN:N	2.43	0.52
1:C:148:MET:HE2	1:C:213:ALA:HA	1.92	0.51
1:D:331:PRO:CB	1:D:336:MET:HE3	2.40	0.51
1:C:115:LEU:HD21	1:C:224:MET:CE	2.41	0.50
1:D:177:ASP:OD1	1:D:179:LYS:HB2	2.11	0.50
1:C:184:ASP:HB3	1:C:365:GLN:CD	2.34	0.50
1:C:254:PRO:HB3	1:C:326:LYS:HD3	1.94	0.49
1:D:169:PHE:CE2	1:D:336:MET:CE	2.93	0.49
1:D:169:PHE:CD2	1:D:336:MET:HE2	2.47	0.49
1:B:1225:ASP:OD2	1:C:175:LYS:HE2	2.12	0.49
1:C:115:LEU:HD21	1:C:224:MET:HE2	1.94	0.49
1:B:1366:MET:O	1:B:1368:GLN:N	2.46	0.48
1:D:148:MET:SD	1:D:208:THR:HG21	2.54	0.48
1:B:179:LYS:NZ	1:B:1341:GLU:OE2	2.46	0.47
1:A:254:PRO:HB3	1:A:326:LYS:HD3	1.96	0.47
1:C:1251:GLU:O	1:C:1252:LYS:C	2.57	0.47
1:B:1230:GLY:C	1:B:1231:LYS:HG2	2.40	0.46
1:D:331:PRO:CG	1:D:336:MET:HE3	2.45	0.46
1:B:254:PRO:HB3	1:B:326:LYS:HD3	1.98	0.46
1:B:1362:VAL:C	1:B:1365:VAL:HG22	2.41	0.46
1:B:1362:VAL:HA	1:B:1365:VAL:HG22	1.97	0.46
1:B:1362:VAL:HA	1:B:1365:VAL:CG2	2.46	0.46
1:C:1312:SER:CB	1:D:309:GLU:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:HG12	1:C:183:VAL:HG22	1.98	0.45
1:B:179:LYS:CE	1:B:1341:GLU:OE2	2.65	0.45
1:C:149:PHE:CE1	1:C:151:LEU:HD23	2.51	0.45
1:B:176:TYR:CE1	1:B:331:PRO:HG3	2.51	0.45
1:C:28:GLU:HG3	1:C:34:LYS:HA	1.99	0.45
1:A:288:GLU:CD	1:A:288:GLU:H	2.25	0.44
1:D:331:PRO:HG2	1:D:336:MET:CE	2.48	0.44
1:B:153:GLU:OE1	1:B:344:ARG:NH1	2.52	0.43
1:D:1338:GLU:OE1	1:D:1387:ARG:HB3	2.17	0.43
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.54	0.43
1:C:254:PRO:CB	1:C:326:LYS:HD3	2.47	0.43
1:C:158:TRP:N	1:C:159:PRO:CD	2.80	0.43
1:C:1264:THR:HG22	1:C:1266:GLU:H	1.83	0.43
1:B:1366:MET:CE	1:B:1373:LEU:HD13	2.47	0.43
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.50	0.42
1:D:153:GLU:OE1	1:D:344:ARG:NH1	2.53	0.42
1:D:169:PHE:HD2	1:D:336:MET:CE	2.30	0.42
1:A:254:PRO:CB	1:A:326:LYS:HD3	2.50	0.42
1:D:169:PHE:CD2	1:D:336:MET:HE1	2.54	0.42
1:B:1362:VAL:O	1:B:1365:VAL:HG23	2.18	0.42
1:C:153:GLU:OE1	1:C:344:ARG:NH1	2.52	0.42
1:B:1366:MET:HB3	1:B:1373:LEU:HD13	2.01	0.42
1:C:349:ASN:HB3	1:C:355:GLN:HB2	2.02	0.42
1:A:349:ASN:HB3	1:A:355:GLN:HB2	2.01	0.41
1:B:117:TYR:CZ	1:B:125:PRO:HG3	2.55	0.41
1:B:1384:PRO:CB	1:C:101:GLY:HA3	2.48	0.41
1:A:1264:THR:HG22	1:A:1267:LYS:HD2	2.02	0.41
1:B:254:PRO:CB	1:B:326:LYS:HD3	2.51	0.41
1:D:68:GLY:HA3	1:D:332:ASN:O	2.21	0.41
1:D:1264:THR:HG22	1:D:1266:GLU:H	1.86	0.41
1:C:117:TYR:CZ	1:C:125:PRO:HG3	2.56	0.41
1:B:49:GLN:HG3	1:B:1367:GLU:O	2.21	0.40
1:C:1312:SER:HB2	1:D:309:GLU:HG3	2.03	0.40
1:D:58:ASP:OD1	1:D:270:SER:OG	2.37	0.40
1:A:117:TYR:CZ	1:A:125:PRO:HG3	2.57	0.40
1:D:349:ASN:HB3	1:D:355:GLN:HB2	2.03	0.40
1:C:1248:ASN:C	1:C:1248:ASN:OD1	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/553 (96%)	513 (97%)	15 (3%)	0	100	100
1	B	530/553 (96%)	516 (97%)	14 (3%)	0	100	100
1	C	523/553 (95%)	509 (97%)	14 (3%)	0	100	100
1	D	522/553 (94%)	508 (97%)	14 (3%)	0	100	100
All	All	2103/2212 (95%)	2046 (97%)	57 (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	404/446 (91%)	402 (100%)	2 (0%)	81	93
1	B	407/446 (91%)	399 (98%)	8 (2%)	48	80
1	C	359/446 (80%)	353 (98%)	6 (2%)	53	83
1	D	349/446 (78%)	343 (98%)	6 (2%)	53	83
All	All	1519/1784 (85%)	1497 (99%)	22 (1%)	59	85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	1308	LYS

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Mol	Chain	Res	Type
1	B	1231	LYS
1	B	1247	ARG
1	B	1249	MET
1	B	1273	ASN
1	B	1286	GLN
1	B	1308	LYS
1	B	1371	ASP
1	B	1373	LEU
1	C	28	GLU
1	C	79	ILE
1	C	258	PHE
1	C	1273	ASN
1	C	1298	SER
1	C	1364	SER
1	D	79	ILE
1	D	258	PHE
1	D	1247	ARG
1	D	1273	ASN
1	D	1306	SER
1	D	1364	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	241	ASN
1	A	325	GLN
1	A	349	ASN
1	B	72	GLN
1	B	152	GLN
1	B	241	ASN
1	B	325	GLN
1	C	152	GLN
1	C	325	GLN
1	C	1273	ASN
1	D	152	GLN
1	D	282	ASN
1	D	325	GLN
1	D	349	ASN
1	D	1273	ASN

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 ⓘ

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	0.68	0	17,17,17	1.39	3 (17%)
2	GLC	E	2	2	11,11,12	0.84	0	15,15,17	1.56	2 (13%)
2	GLC	F	1	2	12,12,12	0.75	0	17,17,17	0.83	0
2	GLC	F	2	2	11,11,12	0.71	0	15,15,17	1.70	1 (6%)
2	GLC	G	1	2	12,12,12	0.81	0	17,17,17	1.02	2 (11%)
2	GLC	G	2	2	11,11,12	0.61	0	15,15,17	1.58	1 (6%)
2	GLC	H	1	2	12,12,12	0.99	0	17,17,17	1.67	3 (17%)
2	GLC	H	2	2	11,11,12	0.38	0	15,15,17	1.55	3 (20%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	1/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-O5-C5	5.21	119.17	112.19
2	G	2	GLC	C1-O5-C5	4.86	118.70	112.19
2	E	2	GLC	C1-O5-C5	4.73	118.53	112.19
2	H	1	GLC	C3-C4-C5	3.85	117.22	110.23
2	H	1	GLC	C4-C3-C2	3.51	116.99	110.83
2	H	2	GLC	C1-O5-C5	3.36	116.69	112.19
2	H	1	GLC	O4-C4-C5	-2.78	102.48	109.32
2	G	1	GLC	C3-C4-C5	2.59	114.94	110.23
2	E	1	GLC	O2-C2-C3	-2.54	104.38	110.38
2	H	2	GLC	C1-C2-C3	2.40	113.13	109.64
2	E	1	GLC	C1-C2-C3	2.38	115.21	110.36
2	H	2	GLC	C3-C4-C5	2.13	114.10	110.23
2	E	2	GLC	O4-C4-C3	2.12	115.38	110.38
2	E	1	GLC	O3-C3-C2	-2.05	105.54	110.38
2	G	1	GLC	C4-C3-C2	2.03	114.40	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

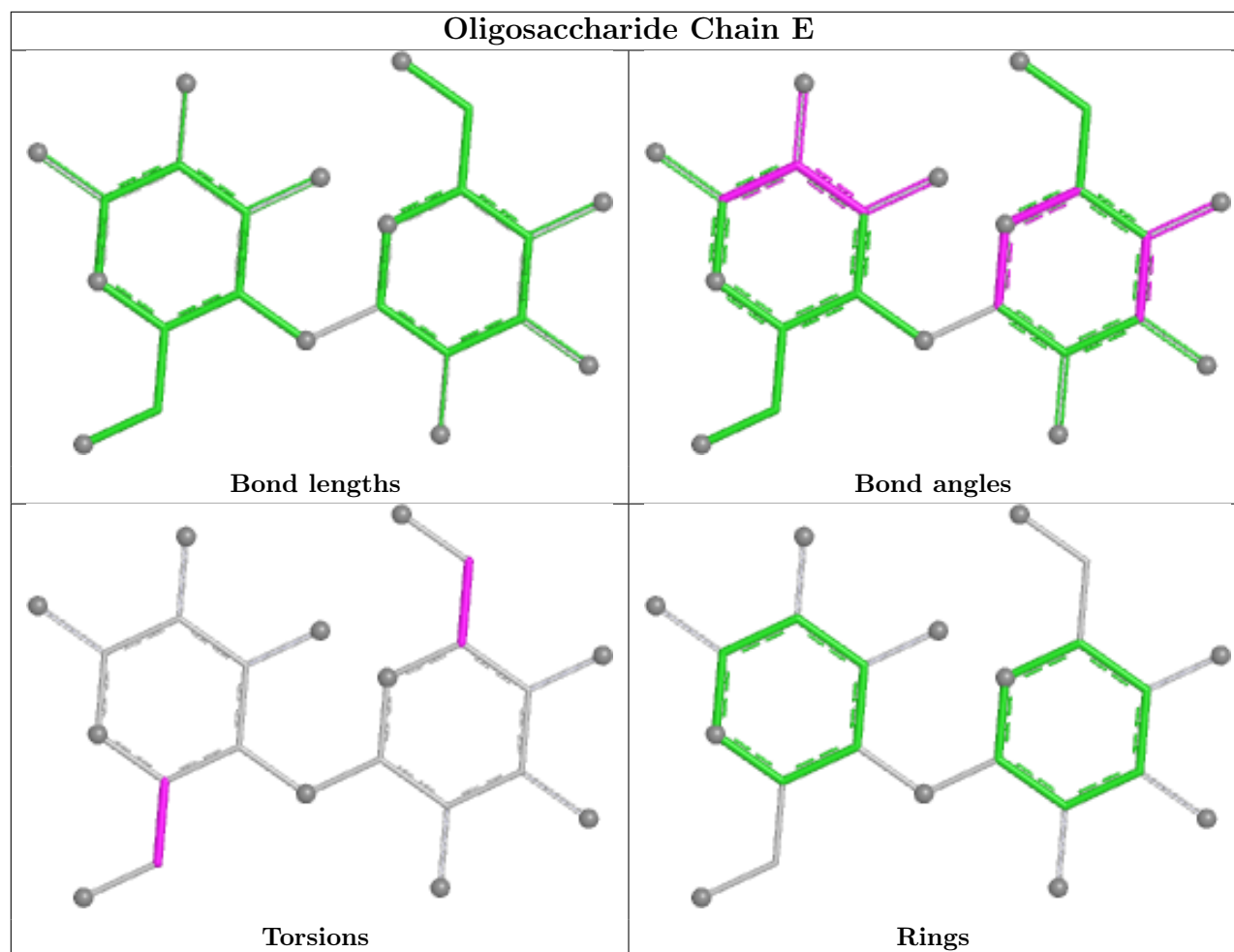
Mol	Chain	Res	Type	Atoms
2	G	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6

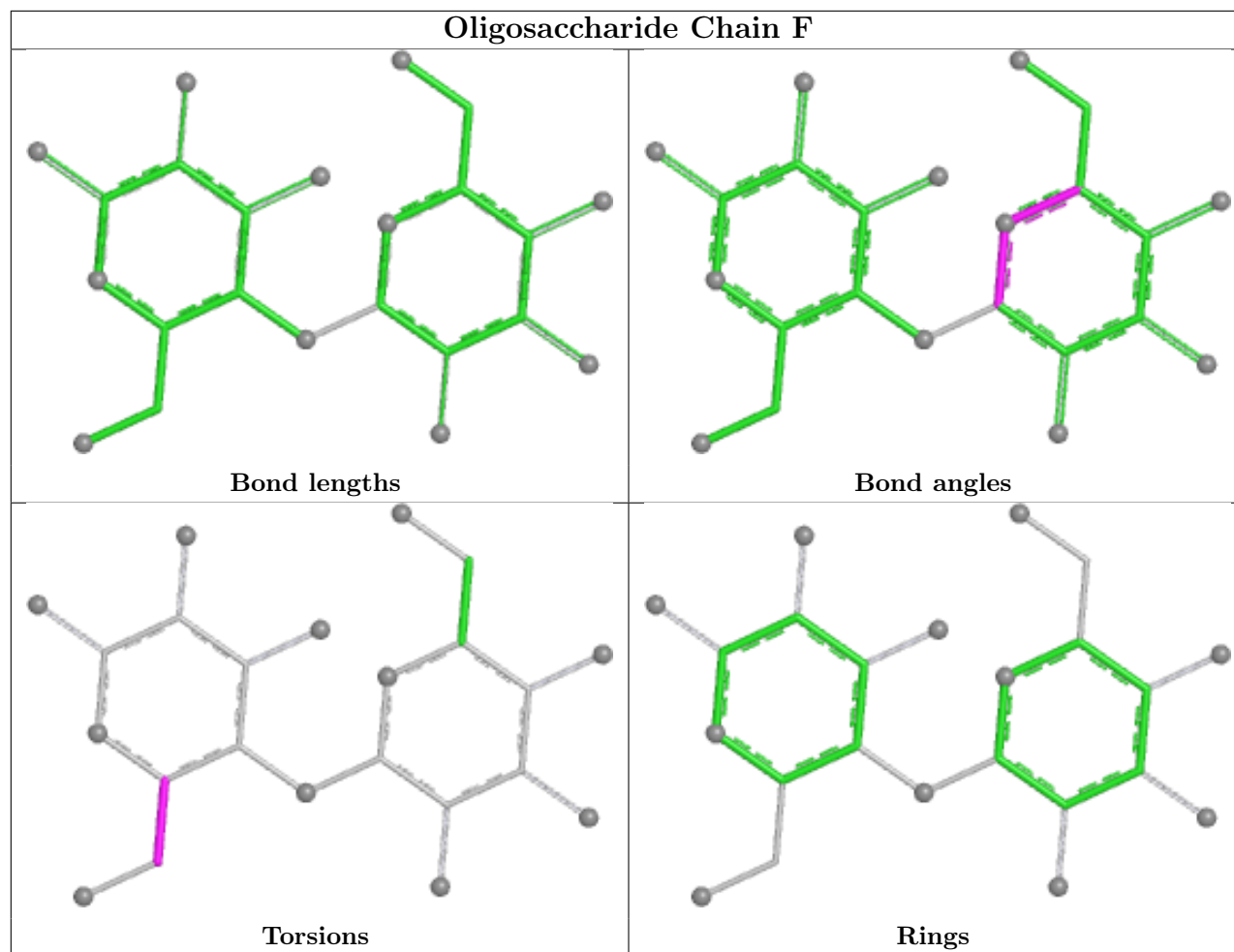
There are no ring outliers.

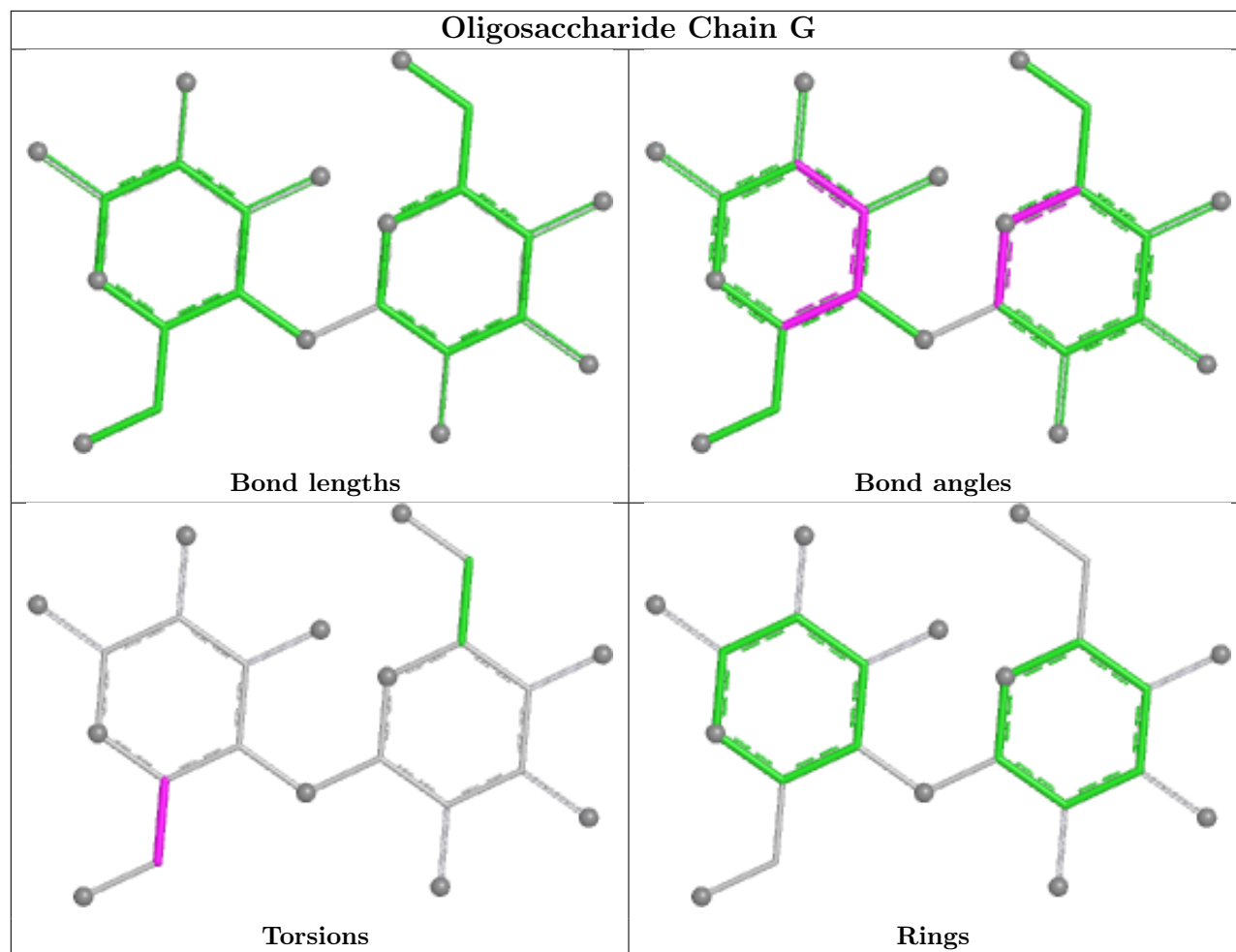
No monomer is involved in short contacts.

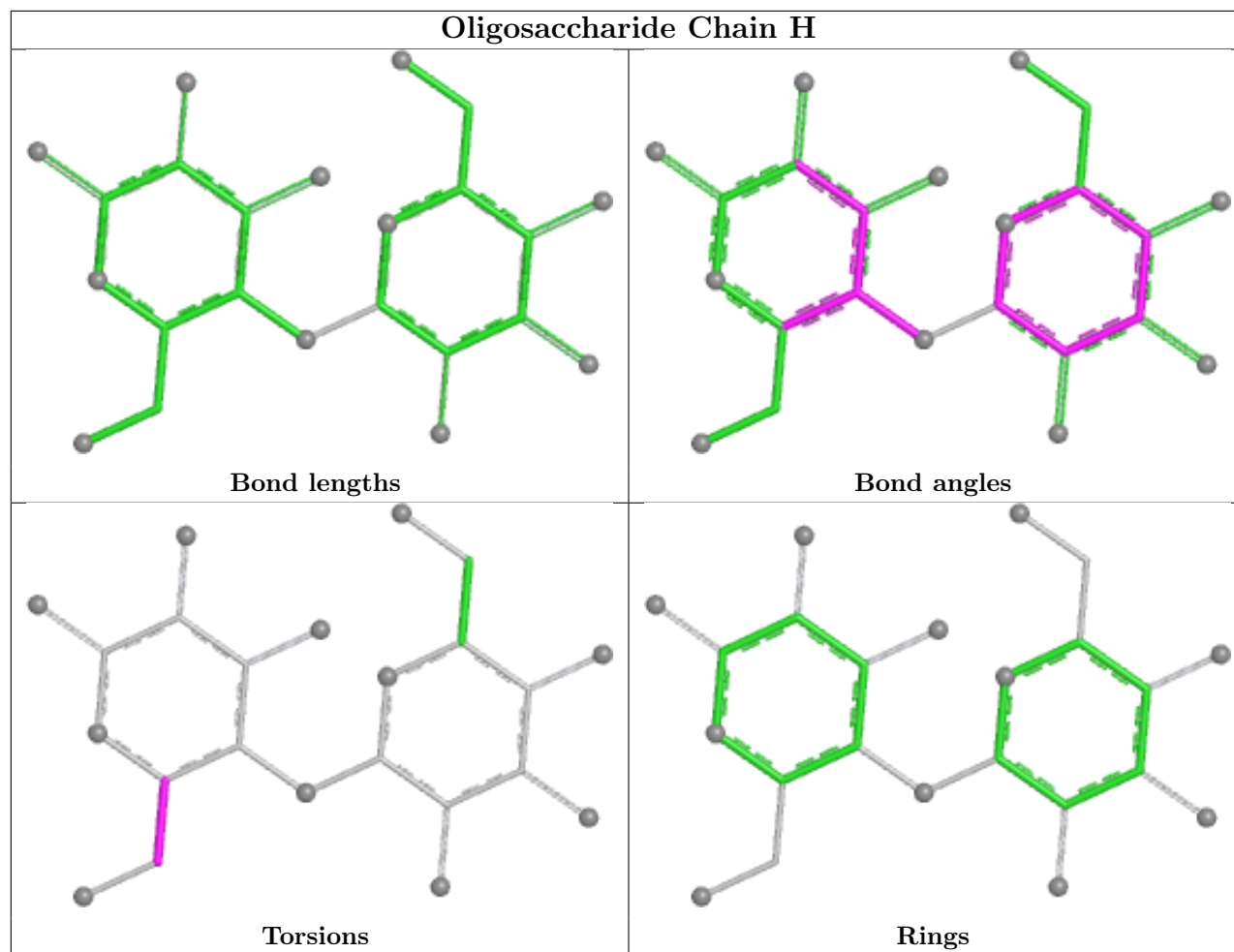
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	534/553 (96%)	-0.22	15 (2%) 55 45	23, 39, 71, 120	0
1	B	536/553 (96%)	-0.23	5 (0%) 81 74	22, 40, 72, 124	0
1	C	529/553 (95%)	0.69	51 (9%) 13 10	33, 74, 112, 133	0
1	D	528/553 (95%)	1.56	179 (33%) 1 1	41, 107, 158, 215	0
All	All	2127/2212 (96%)	0.45	250 (11%) 9 7	22, 58, 132, 215	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ILE	6.0
1	D	141	ALA	5.7
1	D	75	LEU	5.5
1	D	214	GLU	5.5
1	D	220	GLY	5.3
1	C	1265	GLU	5.2
1	D	351	ALA	5.0
1	A	173	ALA	4.8
1	D	221	GLU	4.7
1	A	1249	MET	4.5
1	B	1406	PRO	4.5
1	D	226	ILE	4.2
1	D	323	ASN	4.1
1	D	116	ILE	4.1
1	D	148	MET	3.7
1	D	255	SER	3.7
1	A	172	ALA	3.7
1	D	121	LEU	3.7
1	D	231	ALA	3.7
1	D	233	SER	3.7
1	D	1320	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	76	LEU	3.6
1	D	115	LEU	3.6
1	D	315	PRO	3.6
1	D	149	PHE	3.6
1	D	8	VAL	3.6
1	D	112	ALA	3.5
1	C	321	MET	3.5
1	D	147	LEU	3.5
1	D	1248	ASN	3.5
1	C	121	LEU	3.5
1	C	201	ASN	3.4
1	D	1309	PRO	3.4
1	D	224	MET	3.4
1	D	47	PHE	3.4
1	D	347	VAL	3.3
1	D	160	LEU	3.3
1	D	50	VAL	3.3
1	C	218	ASN	3.3
1	D	56	GLY	3.3
1	D	173	ALA	3.3
1	C	141	ALA	3.3
1	D	259	VAL	3.3
1	D	1293	SER	3.3
1	D	145	SER	3.2
1	D	120	ASP	3.2
1	D	40	PRO	3.2
1	D	134	ALA	3.2
1	C	217	PHE	3.2
1	C	1237	GLU	3.2
1	D	216	ALA	3.2
1	A	174	GLY	3.2
1	A	1406	PRO	3.2
1	C	206	ALA	3.1
1	D	200	LYS	3.1
1	D	43	LEU	3.1
1	C	241	ASN	3.1
1	D	218	ASN	3.1
1	D	72	GLN	3.1
1	D	1265	GLU	3.1
1	D	124	ASN	3.1
1	A	1367	GLU	3.1
1	C	237	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	210	TYR	3.0
1	C	118	ASN	3.0
1	D	38	GLU	3.0
1	C	1305	ASP	3.0
1	D	254	PRO	3.0
1	C	80	THR	3.0
1	D	246	VAL	3.0
1	D	198	LEU	3.0
1	D	223	ALA	3.0
1	D	212	ILE	3.0
1	D	235	ILE	3.0
1	D	287	ASP	3.0
1	D	1390	CYS	3.0
1	C	219	LYS	2.9
1	D	1231	LYS	2.9
1	D	151	LEU	2.9
1	D	111	GLU	2.9
1	D	51	ALA	2.9
1	D	135	LEU	2.9
1	C	1301	LEU	2.9
1	C	52	ALA	2.9
1	D	269	ALA	2.9
1	D	1249	MET	2.9
1	D	79	ILE	2.9
1	C	214	GLU	2.8
1	C	1264	THR	2.8
1	D	62	TRP	2.8
1	D	142	LYS	2.8
1	D	215	ALA	2.8
1	D	1268	ARG	2.8
1	D	247	LEU	2.8
1	C	1232	THR	2.8
1	D	320	THR	2.8
1	D	33	ILE	2.8
1	D	267	ASN	2.8
1	D	297	LYS	2.8
1	D	1383	ASP	2.8
1	D	202	LYS	2.8
1	C	216	ALA	2.7
1	C	200	LYS	2.7
1	C	1298	SER	2.7
1	C	221	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	134	ALA	2.7
1	D	186	ALA	2.7
1	D	138	GLU	2.7
1	D	1295	VAL	2.7
1	C	1317	ALA	2.7
1	D	7	LEU	2.7
1	D	206	ALA	2.7
1	C	120	ASP	2.7
1	D	9	ILE	2.7
1	D	329	ILE	2.7
1	D	117	TYR	2.7
1	C	1319	GLY	2.7
1	D	113	LEU	2.7
1	D	195	LEU	2.7
1	C	148	MET	2.6
1	D	307	TYR	2.6
1	D	100	ASN	2.6
1	D	23	VAL	2.6
1	D	294	ASN	2.6
1	D	49	GLN	2.6
1	A	1370	TRP	2.6
1	D	158	TRP	2.6
1	D	309	GLU	2.6
1	A	1374	ALA	2.6
1	C	173	ALA	2.6
1	D	21	ALA	2.6
1	D	87	ASP	2.6
1	C	139	LEU	2.6
1	D	146	ALA	2.6
1	D	350	ALA	2.6
1	D	73	SER	2.5
1	D	219	LYS	2.5
1	D	340	TRP	2.5
1	D	194	PHE	2.5
1	D	1302	HIS	2.5
1	C	144	LYS	2.5
1	A	32	GLY	2.5
1	D	299	LEU	2.5
1	D	301	ALA	2.5
1	D	41	ASP	2.5
1	D	95	ASP	2.5
1	D	328	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	80	THR	2.5
1	D	83	ALA	2.5
1	D	239	ALA	2.5
1	D	150	ASN	2.5
1	C	220	GLY	2.5
1	D	1264	THR	2.5
1	A	1383	ASP	2.4
1	D	143	GLY	2.4
1	D	286	THR	2.4
1	D	101	GLY	2.4
1	D	300	GLY	2.4
1	D	42	LYS	2.4
1	D	119	LYS	2.4
1	D	295	LYS	2.4
1	D	305	LYS	2.4
1	D	61	PHE	2.4
1	B	173	ALA	2.4
1	D	230	TRP	2.4
1	D	312	ALA	2.4
1	C	1249	MET	2.4
1	C	1303	MET	2.4
1	D	126	PRO	2.4
1	C	1318	ALA	2.4
1	D	139	LEU	2.4
1	D	14	ASP	2.3
1	D	152	GLN	2.3
1	D	129	TRP	2.3
1	D	204	MET	2.3
1	D	128	THR	2.3
1	D	222	THR	2.3
1	D	60	ILE	2.3
1	C	12	ASN	2.3
1	D	213	ALA	2.3
1	D	232	TRP	2.3
1	A	171	TYR	2.3
1	D	1	LYS	2.3
1	A	1230	GLY	2.3
1	D	241	ASN	2.3
1	D	1311	LEU	2.3
1	D	1333	LEU	2.3
1	C	1302	HIS	2.3
1	D	326	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	352	SER	2.3
1	D	125	PRO	2.3
1	D	15	LYS	2.3
1	D	1308	LYS	2.3
1	C	16	GLY	2.3
1	D	201	ASN	2.2
1	A	1	LYS	2.2
1	B	1231	LYS	2.2
1	D	26	LYS	2.2
1	D	2	ILE	2.2
1	D	35	VAL	2.2
1	D	20	LEU	2.2
1	D	348	ILE	2.2
1	C	55	ASP	2.2
1	D	53	THR	2.2
1	D	123	PRO	2.2
1	B	1340	SER	2.2
1	D	258	PHE	2.2
1	D	122	LEU	2.2
1	D	304	LEU	2.2
1	D	1323	GLU	2.2
1	D	70	TYR	2.2
1	D	166	GLY	2.2
1	C	124	ASN	2.2
1	B	1262	ASP	2.2
1	D	89	LEU	2.2
1	D	28	GLU	2.2
1	D	64	HIS	2.1
1	C	1283	ASP	2.1
1	D	1305	ASP	2.1
1	D	237	THR	2.1
1	D	103	LEU	2.1
1	D	1367	GLU	2.1
1	C	1368	GLN	2.1
1	D	110	VAL	2.1
1	D	54	GLY	2.1
1	D	156	PHE	2.1
1	A	221	GLU	2.1
1	C	142	LYS	2.1
1	D	1384	PRO	2.1
1	C	122	LEU	2.1
1	C	180	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	192	LEU	2.1
1	D	1296	LEU	2.1
1	C	1268	ARG	2.1
1	C	239	ALA	2.1
1	D	77	ALA	2.1
1	C	138	GLU	2.1
1	D	256	LYS	2.1
1	D	52	ALA	2.1
1	D	317	ILE	2.1
1	D	322	GLU	2.1
1	C	1306	SER	2.0
1	D	211	SER	2.0
1	D	196	VAL	2.0
1	D	159	PRO	2.0
1	A	1248	ASN	2.0
1	D	1310	LEU	2.0
1	D	327	GLY	2.0
1	D	74	GLY	2.0
1	D	358	ASP	2.0

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

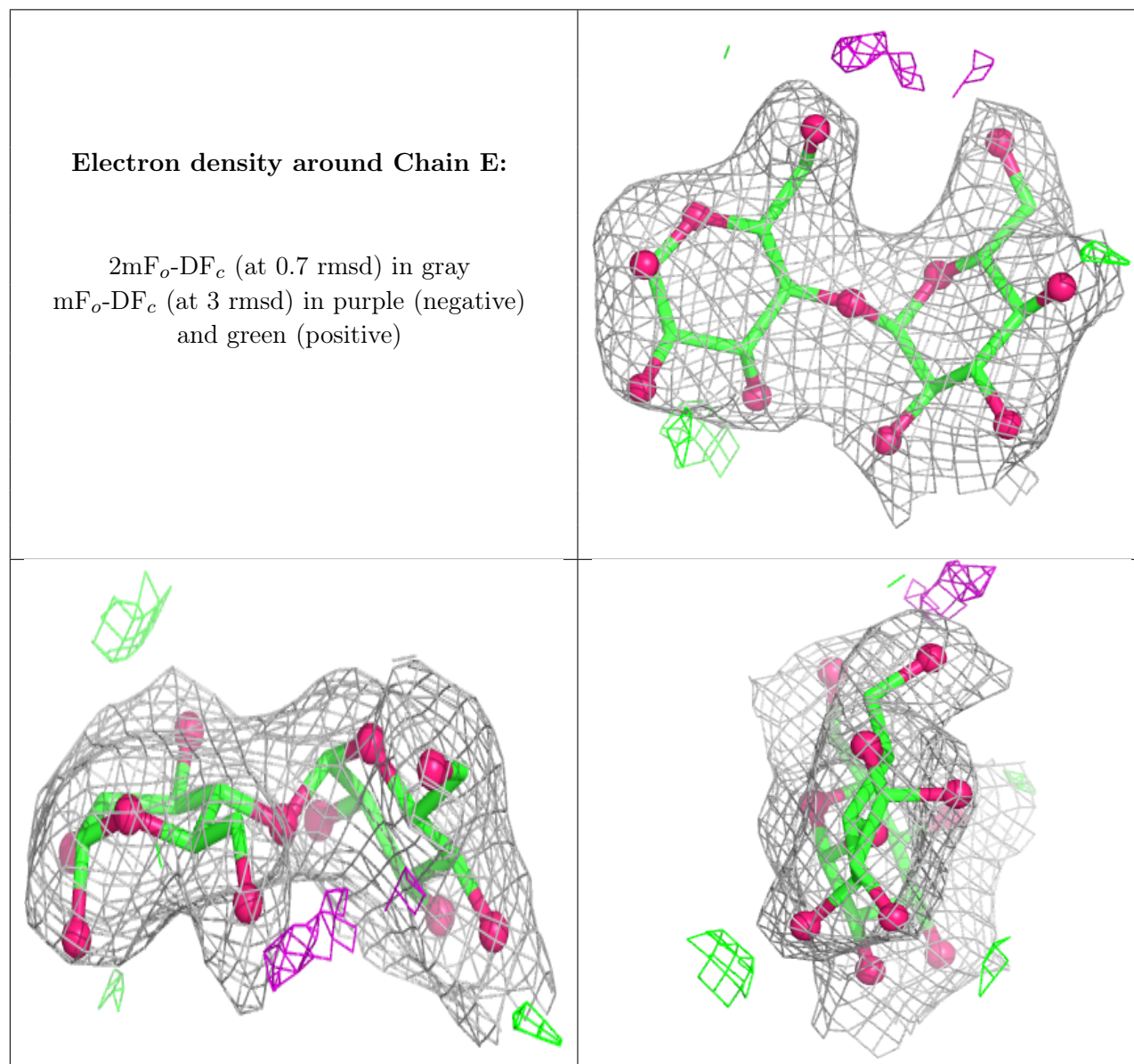
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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.

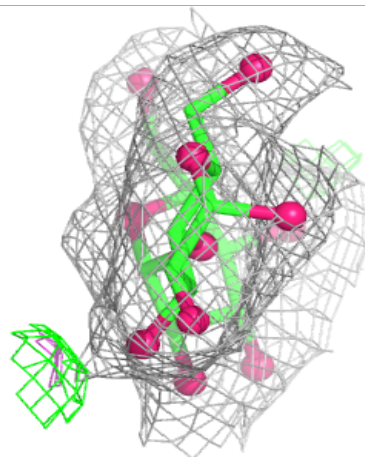
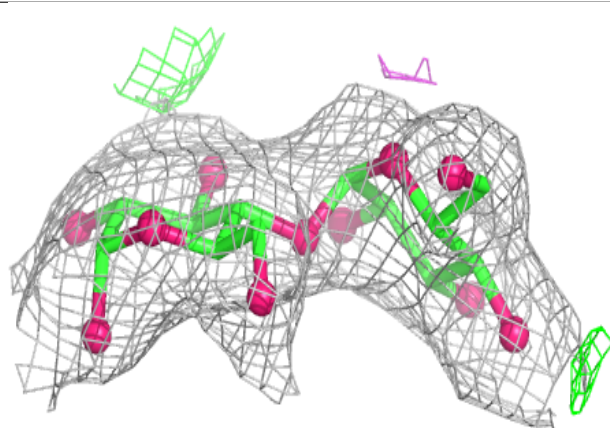
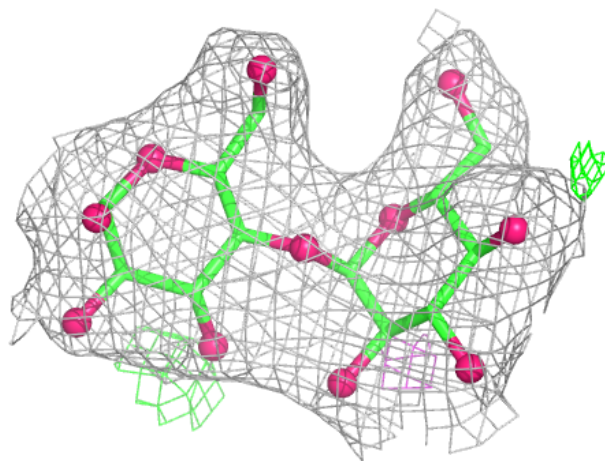
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	H	1	12/12	0.78	0.16	84,103,123,128	0
2	GLC	G	1	12/12	0.92	0.11	52,66,79,79	0
2	GLC	H	2	11/12	0.93	0.11	96,104,108,109	0
2	GLC	E	1	12/12	0.95	0.07	32,35,38,43	0
2	GLC	F	1	12/12	0.96	0.07	27,31,35,36	0
2	GLC	G	2	11/12	0.96	0.06	43,48,53,58	0
2	GLC	E	2	11/12	0.97	0.06	28,30,33,36	0
2	GLC	F	2	11/12	0.97	0.06	24,27,29,32	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.



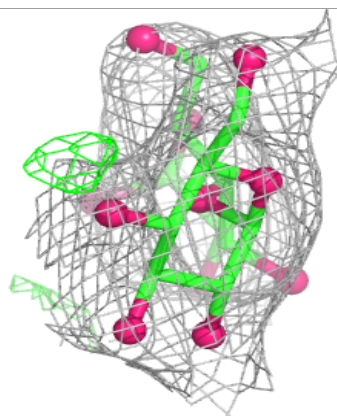
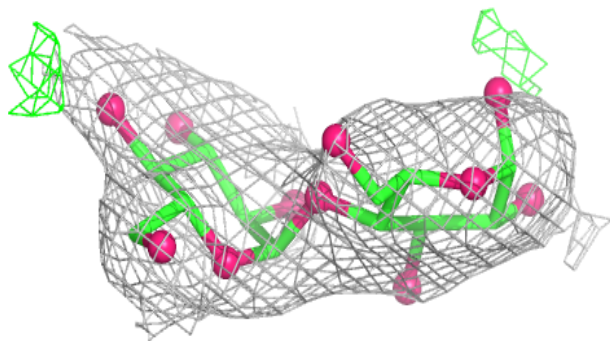
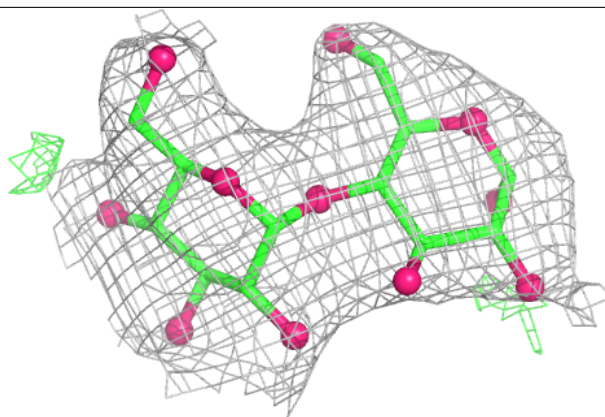
Electron density around Chain F:

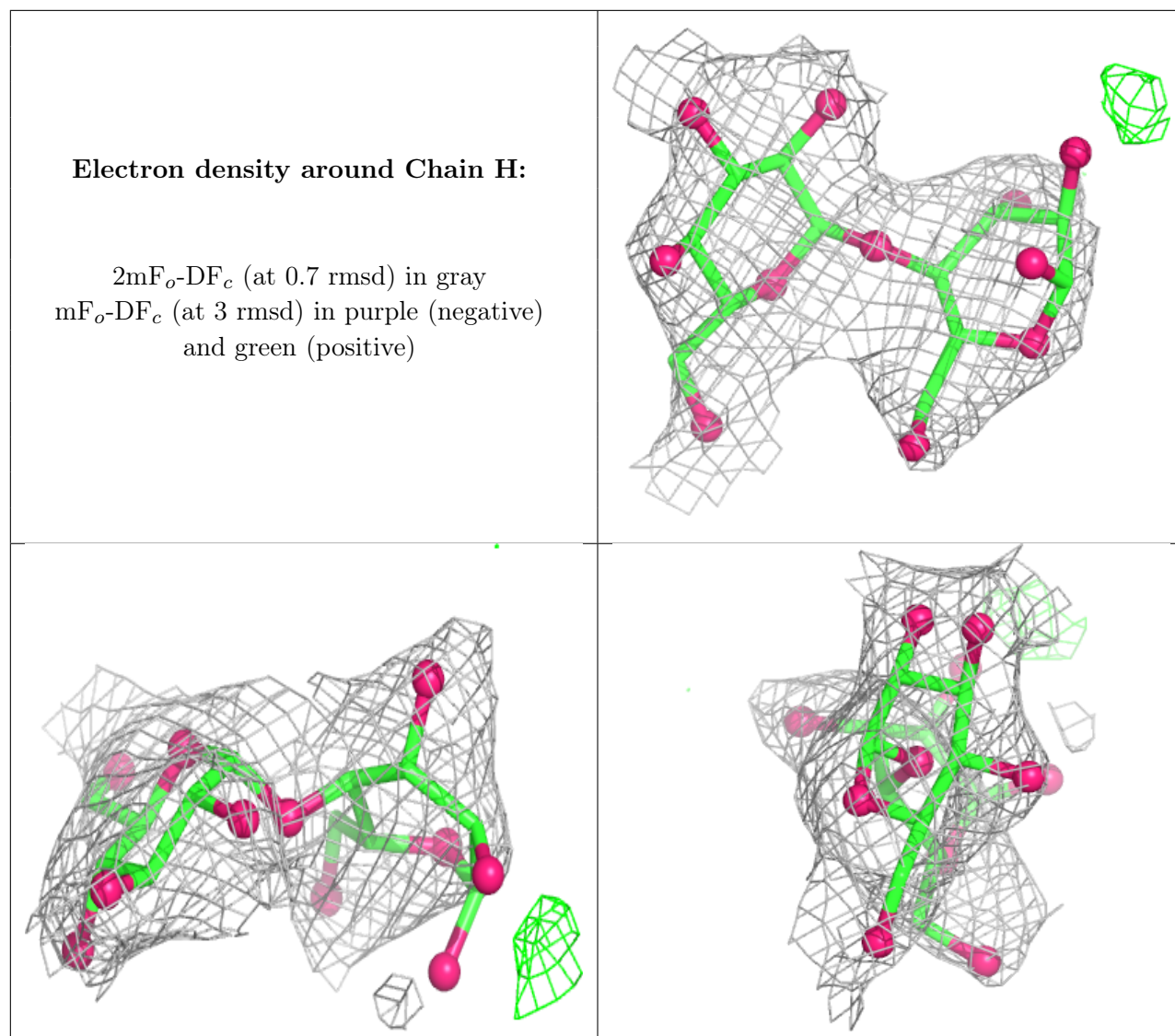
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.