W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2024 – 12:10 PM EDT

PDB ID	:	5HJ3
Title	:	Crystal structure of host-primed Ebola virus GP, GPcl.
Authors	:	Bornholdt, Z.A.; Fusco, M.L.; Saphire, E.O.
Deposited on	:	2016-01-12
Resolution	:	3.30 Å(reported)

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

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

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

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

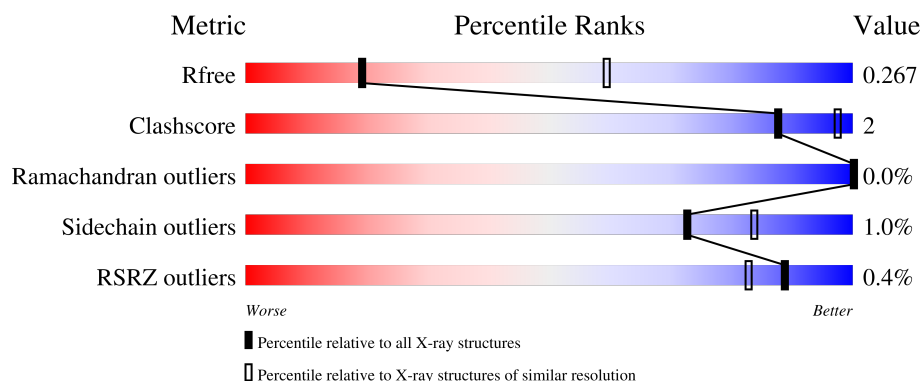|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.30 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		1.0%
RSRZ outliers		0.4%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▊ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	C	179	82% 7% 11%
1	G	179	84% • 12%
1	K	179	84% • 12%
1	O	179	81% 6% • 12%
2	D	136	% 72% 8% • 19%

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Mol	Chain	Length	Quality of chain
2	H	136	76% · · 19%
2	L	136	74% 7% · 19%
2	P	136	74% 6% · 19%
3	A	226	85% · 12%
3	E	226	87% · 10%
3	I	226	85% · 12%
3	M	226	85% 5% 10%
4	B	217	88% 6% 6%
4	F	217	84% · 13%
4	J	217	93% · ·
4	N	217	90% · 6%
5	Q	7	43% 29% 29%
5	R	7	43% 57%
5	S	7	43% 57%
5	T	7	43% 29% 29%

2 Entity composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 41146 atoms, of which 20270 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	159	Total	C	H	N	O	S	0	0	0
			2410	770	1195	215	225	5			
1	G	158	Total	C	H	N	O	S	0	0	0
			2400	767	1190	214	224	5			
1	K	157	Total	C	H	N	O	S	0	0	0
			2376	761	1177	210	223	5			
1	O	157	Total	C	H	N	O	S	0	0	0
			2376	761	1177	210	223	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	TYR	-	expression tag	UNP Q05320
C	17	PRO	-	expression tag	UNP Q05320
C	18	TYR	-	expression tag	UNP Q05320
C	19	ASP	-	expression tag	UNP Q05320
C	20	VAL	-	expression tag	UNP Q05320
C	21	PRO	-	expression tag	UNP Q05320
C	22	ASP	-	expression tag	UNP Q05320
C	23	TYR	-	expression tag	UNP Q05320
C	24	ALA	-	expression tag	UNP Q05320
C	25	ILE	-	expression tag	UNP Q05320
C	26	GLU	-	expression tag	UNP Q05320
C	27	GLY	-	expression tag	UNP Q05320
C	28	ARG	-	expression tag	UNP Q05320
C	29	GLY	-	expression tag	UNP Q05320
C	30	ALA	-	expression tag	UNP Q05320
C	31	ARG	-	expression tag	UNP Q05320
G	16	TYR	-	expression tag	UNP Q05320
G	17	PRO	-	expression tag	UNP Q05320
G	18	TYR	-	expression tag	UNP Q05320
G	19	ASP	-	expression tag	UNP Q05320
G	20	VAL	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
G	21	PRO	-	expression tag	UNP Q05320
G	22	ASP	-	expression tag	UNP Q05320
G	23	TYR	-	expression tag	UNP Q05320
G	24	ALA	-	expression tag	UNP Q05320
G	25	ILE	-	expression tag	UNP Q05320
G	26	GLU	-	expression tag	UNP Q05320
G	27	GLY	-	expression tag	UNP Q05320
G	28	ARG	-	expression tag	UNP Q05320
G	29	GLY	-	expression tag	UNP Q05320
G	30	ALA	-	expression tag	UNP Q05320
G	31	ARG	-	expression tag	UNP Q05320
K	16	TYR	-	expression tag	UNP Q05320
K	17	PRO	-	expression tag	UNP Q05320
K	18	TYR	-	expression tag	UNP Q05320
K	19	ASP	-	expression tag	UNP Q05320
K	20	VAL	-	expression tag	UNP Q05320
K	21	PRO	-	expression tag	UNP Q05320
K	22	ASP	-	expression tag	UNP Q05320
K	23	TYR	-	expression tag	UNP Q05320
K	24	ALA	-	expression tag	UNP Q05320
K	25	ILE	-	expression tag	UNP Q05320
K	26	GLU	-	expression tag	UNP Q05320
K	27	GLY	-	expression tag	UNP Q05320
K	28	ARG	-	expression tag	UNP Q05320
K	29	GLY	-	expression tag	UNP Q05320
K	30	ALA	-	expression tag	UNP Q05320
K	31	ARG	-	expression tag	UNP Q05320
O	16	TYR	-	expression tag	UNP Q05320
O	17	PRO	-	expression tag	UNP Q05320
O	18	TYR	-	expression tag	UNP Q05320
O	19	ASP	-	expression tag	UNP Q05320
O	20	VAL	-	expression tag	UNP Q05320
O	21	PRO	-	expression tag	UNP Q05320
O	22	ASP	-	expression tag	UNP Q05320
O	23	TYR	-	expression tag	UNP Q05320
O	24	ALA	-	expression tag	UNP Q05320
O	25	ILE	-	expression tag	UNP Q05320
O	26	GLU	-	expression tag	UNP Q05320
O	27	GLY	-	expression tag	UNP Q05320
O	28	ARG	-	expression tag	UNP Q05320
O	29	GLY	-	expression tag	UNP Q05320
O	30	ALA	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
O	31	ARG	-	expression tag	UNP Q05320

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	110	Total 1697	C 549	H 835	N 151	O 156	S 6	0	0	0
2	H	110	Total 1698	C 549	H 836	N 151	O 156	S 6	0	0	0
2	L	110	Total 1698	C 549	H 836	N 151	O 156	S 6	0	0	0
2	P	110	Total 1697	C 549	H 835	N 151	O 156	S 6	0	0	0

- Molecule 3 is a protein called KZ52 Antibody Fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	204	Total 3025	C 962	H 1495	N 260	O 300	S 8	0	0	0
3	I	199	Total 2973	C 948	H 1470	N 256	O 291	S 8	0	0	0
3	M	203	Total 3021	C 960	H 1495	N 260	O 298	S 8	0	0	0
3	A	199	Total 2982	C 950	H 1476	N 256	O 292	S 8	0	0	0

- Molecule 4 is a protein called KZ52 Antibody Fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	189	Total 2891	C 927	H 1423	N 242	O 295	S 4	0	0	0
4	J	209	Total 3172	C 1007	H 1566	N 266	O 328	S 5	0	0	0
4	N	203	Total 3066	C 989	H 1495	N 258	O 319	S 5	0	0	0
4	B	203	Total 3052	C 975	H 1489	N 263	O 320	S 5	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
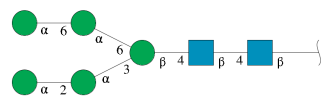
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			
5	R	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			
5	S	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			
5	T	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			

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: Envelope glycoprotein

Chain C:
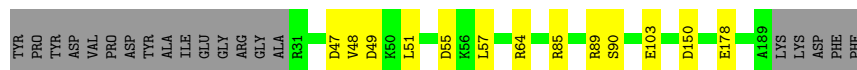
- Molecule 1: Envelope glycoprotein

Chain G:
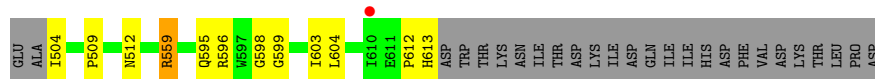

- Molecule 1: Envelope glycoprotein

Chain K:

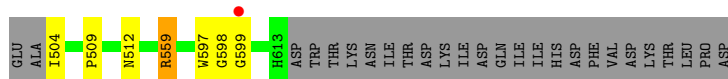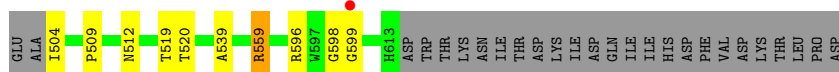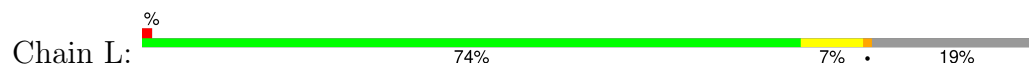- Molecule 1: Envelope glycoprotein

Chain O:

- Molecule 2: Envelope glycoprotein

Chain D:

- Molecule 2: Envelope glycoprotein

Chain H:

GLU ALA I504 P509 N512 R559 W597 G598 G599 H613 ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP LYS THR LEU PRO ASP

• Molecule 2: Envelope glycoprotein

Chain L:

74%   7% •   19%

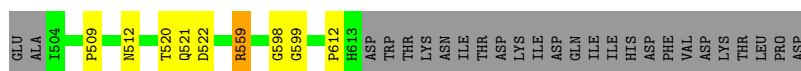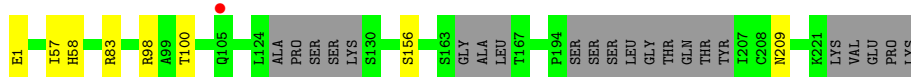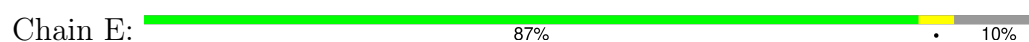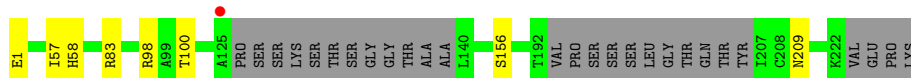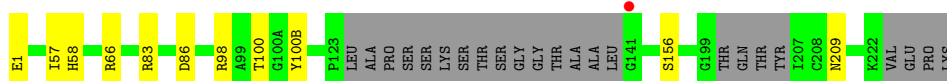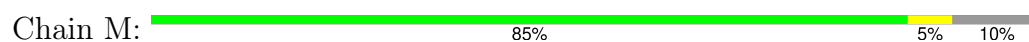GLU ALA I504 P509 N512 T519 T520 A539 R559 R596 W597 G598 G599 H613 ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP LYS THR LEU PRO ASP

• Molecule 2: Envelope glycoprotein

Chain P:

74%   6% •   19%

GLU ALA I504 P509 N512 T520 Q521 D522 R559 G598 G599 P612 H613 ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP LYS THR LEU PRO ASP

• Molecule 3: KZ52 Antibody Fragment

Chain E:

87%   •   10%

E1 I57 H58 R83 R98 A99 T100 Q105 L124 ALA PRO SER SER LYS S130 S156 S163 GLY ALA LEU T167 P194 SER SER LEU GLY THR GLN THR TYR I207 C208 N209 K221 LYS VAL GLU PRO LYS

• Molecule 3: KZ52 Antibody Fragment

Chain I:

85%   •   12%

E1 I57 H58 R83 R98 A99 T100 A125 PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA L140 S156 T192 VAL PRO SER SER LEU GLY THR GLN THR TYR I207 C208 N209 K222 VAL GLU PRO LYS

• Molecule 3: KZ52 Antibody Fragment

Chain M:

85%   5% 10%

E1 I57 H58 R66 R83 D86 R98 A99 T100 G100A Y100B P123 LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU G141 S156 G199 THR GLN THR TYR I207 C208 N209 K222 VAL GLU PRO LYS

• Molecule 3: KZ52 Antibody Fragment

Chain A:

85%   •   12%

E1 I57 H58 R71 D72 N73 R83 R98 A99 T100 L124 ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU G141 V191 THR VAL PRO SER SER LEU GLY THR GLN THR TYR I207 P227 LYS

• Molecule 4: KZ52 Antibody Fragment
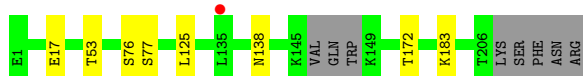
Chain F:

• Molecule 4: KZ52 Antibody Fragment

Chain J:

• Molecule 4: KZ52 Antibody Fragment

Chain N:

• Molecule 4: KZ52 Antibody Fragment

Chain B:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

43%   57%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

43%   29%   29%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	193.10Å 193.10Å 350.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 – 3.30 48.28 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.28-3.30) 99.9 (48.28-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.258 0.238 , 0.267	Depositor DCC
R_{free} test set	3692 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	124.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 96.1	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41146	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG

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	C	0.26	0/1244	0.40	0/1689
1	G	0.24	0/1239	0.39	0/1682
1	K	0.24	0/1228	0.39	0/1668
1	O	0.26	0/1228	0.40	0/1668
2	D	0.25	0/884	0.43	0/1205
2	H	0.23	0/884	0.42	0/1205
2	L	0.24	0/884	0.40	0/1205
2	P	0.24	0/884	0.41	0/1205
3	A	0.25	0/1539	0.38	0/2089
3	E	0.23	0/1562	0.38	0/2121
3	I	0.30	0/1535	0.40	0/2083
3	M	0.23	0/1559	0.38	0/2116
4	B	0.25	0/1591	0.39	0/2150
4	F	0.23	0/1498	0.38	0/2028
4	J	0.25	0/1639	0.39	0/2226
4	N	0.23	0/1603	0.40	1/2171 (0.0%)
All	All	0.24	0/21001	0.40	1/28511 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	204	PRO	N-CA-CB	5.91	110.39	103.30

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	C	1215	1195	1195	6	0
1	G	1210	1190	1190	4	0
1	K	1199	1177	1177	4	0
1	O	1199	1177	1177	7	0
2	D	862	835	835	8	0
2	H	862	836	835	5	0
2	L	862	836	835	8	0
2	P	862	835	835	9	0
3	A	1506	1476	1476	4	0
3	E	1530	1495	1495	4	0
3	I	1503	1470	1477	4	0
3	M	1526	1495	1495	6	0
4	B	1563	1489	1509	8	1
4	F	1468	1423	1430	5	0
4	J	1606	1566	1566	4	1
4	N	1571	1495	1503	3	0
5	Q	83	70	70	2	0
5	R	83	70	70	0	0
5	S	83	70	70	0	0
5	T	83	70	70	1	0
All	All	20876	20270	20310	78	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 78 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)
2:D:512:ASN:O	2:D:559:ARG:NH1	2.06	0.89
2:P:512:ASN:O	2:P:559:ARG:NH1	2.10	0.85
2:H:512:ASN:O	2:H:559:ARG:NH1	2.14	0.81
2:L:512:ASN:O	2:L:559:ARG:NH1	2.15	0.80
2:D:598:GLY:N	2:D:599:GLY:HA3	2.11	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:17:GLU:OE1	4:B:7:SER:OG[9_664]	2.08	0.12

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	C	157/179 (88%)	150 (96%)	7 (4%)	0	100	100
1	G	156/179 (87%)	149 (96%)	7 (4%)	0	100	100
1	K	155/179 (87%)	146 (94%)	9 (6%)	0	100	100
1	O	155/179 (87%)	149 (96%)	6 (4%)	0	100	100
2	D	108/136 (79%)	102 (94%)	6 (6%)	0	100	100
2	H	108/136 (79%)	102 (94%)	6 (6%)	0	100	100
2	L	108/136 (79%)	101 (94%)	7 (6%)	0	100	100
2	P	108/136 (79%)	97 (90%)	10 (9%)	1 (1%)	14	44
3	A	193/226 (85%)	185 (96%)	8 (4%)	0	100	100
3	E	196/226 (87%)	191 (97%)	5 (3%)	0	100	100
3	I	193/226 (85%)	186 (96%)	7 (4%)	0	100	100
3	M	197/226 (87%)	190 (96%)	7 (4%)	0	100	100
4	B	193/217 (89%)	185 (96%)	8 (4%)	0	100	100
4	F	179/217 (82%)	169 (94%)	10 (6%)	0	100	100
4	J	205/217 (94%)	197 (96%)	8 (4%)	0	100	100
4	N	193/217 (89%)	185 (96%)	8 (4%)	0	100	100
All	All	2604/3032 (86%)	2484 (95%)	119 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	612	PRO

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	C	130/146 (89%)	126 (97%)	4 (3%)	35	61
1	G	130/146 (89%)	129 (99%)	1 (1%)	79	87
1	K	129/146 (88%)	128 (99%)	1 (1%)	79	87
1	O	129/146 (88%)	126 (98%)	3 (2%)	45	68
2	D	90/115 (78%)	88 (98%)	2 (2%)	47	69
2	H	90/115 (78%)	88 (98%)	2 (2%)	47	69
2	L	90/115 (78%)	88 (98%)	2 (2%)	47	69
2	P	90/115 (78%)	89 (99%)	1 (1%)	70	82
3	A	169/190 (89%)	167 (99%)	2 (1%)	67	80
3	E	172/190 (90%)	170 (99%)	2 (1%)	67	80
3	I	168/190 (88%)	166 (99%)	2 (1%)	67	80
3	M	172/190 (90%)	171 (99%)	1 (1%)	84	90
4	B	176/191 (92%)	176 (100%)	0	100	100
4	F	167/191 (87%)	167 (100%)	0	100	100
4	J	183/191 (96%)	183 (100%)	0	100	100
4	N	177/191 (93%)	177 (100%)	0	100	100
All	All	2262/2568 (88%)	2239 (99%)	23 (1%)	73	84

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	504	ILE
1	O	57	LEU
3	M	83	ARG
1	O	64	ARG
3	E	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	F	189	HIS
4	J	28	ASN
4	N	28	ASN
4	N	89	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 ⓘ

28 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	$\#|Z| > 2$
5	NAG	Q	1	5,2	14,14,15	0.40	0	17,19,21	0.44	0
5	NAG	Q	2	5	14,14,15	0.24	0	17,19,21	0.57	0
5	BMA	Q	3	5	11,11,12	0.59	0	15,15,17	0.74	0
5	MAN	Q	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.16	2 (13%)
5	MAN	Q	5	5	11,11,12	0.77	0	15,15,17	0.82	1 (6%)
5	MAN	Q	6	5	11,11,12	0.83	0	15,15,17	1.07	2 (13%)
5	MAN	Q	7	5	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
5	NAG	R	1	5,2	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	R	2	5	14,14,15	0.16	0	17,19,21	0.56	0
5	BMA	R	3	5	11,11,12	0.63	0	15,15,17	0.73	0
5	MAN	R	4	5	11,11,12	0.81	1 (9%)	15,15,17	1.15	2 (13%)
5	MAN	R	5	5	11,11,12	0.82	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	MAN	R	6	5	11,11,12	0.87	0	15,15,17	1.06	2 (13%)
5	MAN	R	7	5	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
5	NAG	S	1	5,2	14,14,15	0.32	0	17,19,21	0.43	0
5	NAG	S	2	5	14,14,15	0.24	0	17,19,21	0.52	0
5	BMA	S	3	5	11,11,12	0.66	0	15,15,17	0.81	0
5	MAN	S	4	5	11,11,12	0.86	1 (9%)	15,15,17	1.12	1 (6%)
5	MAN	S	5	5	11,11,12	0.80	0	15,15,17	0.82	1 (6%)
5	MAN	S	6	5	11,11,12	0.89	0	15,15,17	1.04	2 (13%)
5	MAN	S	7	5	11,11,12	0.70	0	15,15,17	1.04	2 (13%)
5	NAG	T	1	5,2	14,14,15	0.29	0	17,19,21	0.44	0
5	NAG	T	2	5	14,14,15	0.18	0	17,19,21	0.57	0
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	0.72	0
5	MAN	T	4	5	11,11,12	0.79	1 (9%)	15,15,17	1.14	2 (13%)
5	MAN	T	5	5	11,11,12	0.80	0	15,15,17	0.81	1 (6%)
5	MAN	T	6	5	11,11,12	0.84	0	15,15,17	1.06	2 (13%)
5	MAN	T	7	5	11,11,12	0.71	0	15,15,17	1.04	2 (13%)

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
5	NAG	Q	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	5	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	6	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	7	5	-	0/2/19/22	1/1/1/1
5	NAG	R	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	4/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
5	MAN	R	5	5	-	1/2/19/22	0/1/1/1
5	MAN	R	6	5	-	2/2/19/22	0/1/1/1
5	MAN	R	7	5	-	0/2/19/22	1/1/1/1
5	NAG	S	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	4/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	4	MAN	O5-C1	-2.43	1.39	1.43
5	Q	4	MAN	O5-C1	-2.34	1.39	1.43
5	R	4	MAN	O5-C1	-2.30	1.39	1.43
5	T	4	MAN	O5-C1	-2.26	1.39	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	4	MAN	O2-C2-C3	-3.07	103.80	110.15
5	T	4	MAN	O2-C2-C3	-3.00	103.94	110.15
5	S	4	MAN	O2-C2-C3	-2.98	103.99	110.15
5	R	4	MAN	O2-C2-C3	-2.94	104.06	110.15
5	T	6	MAN	C1-O5-C5	2.84	116.00	112.19

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	6	MAN	O5-C5-C6-O6
5	R	6	MAN	O5-C5-C6-O6
5	S	6	MAN	O5-C5-C6-O6
5	T	6	MAN	O5-C5-C6-O6
5	S	6	MAN	C4-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	7	MAN	C1-C2-C3-C4-C5-O5
5	R	7	MAN	C1-C2-C3-C4-C5-O5
5	T	7	MAN	C1-C2-C3-C4-C5-O5
5	S	7	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	7	MAN	1	0
5	Q	7	MAN	2	0
5	Q	6	MAN	1	0
5	T	6	MAN	1	0

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

Oligosaccharide Chain Q

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain R

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain S

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

Bond lengths

Bond angles

Torsions

Rings
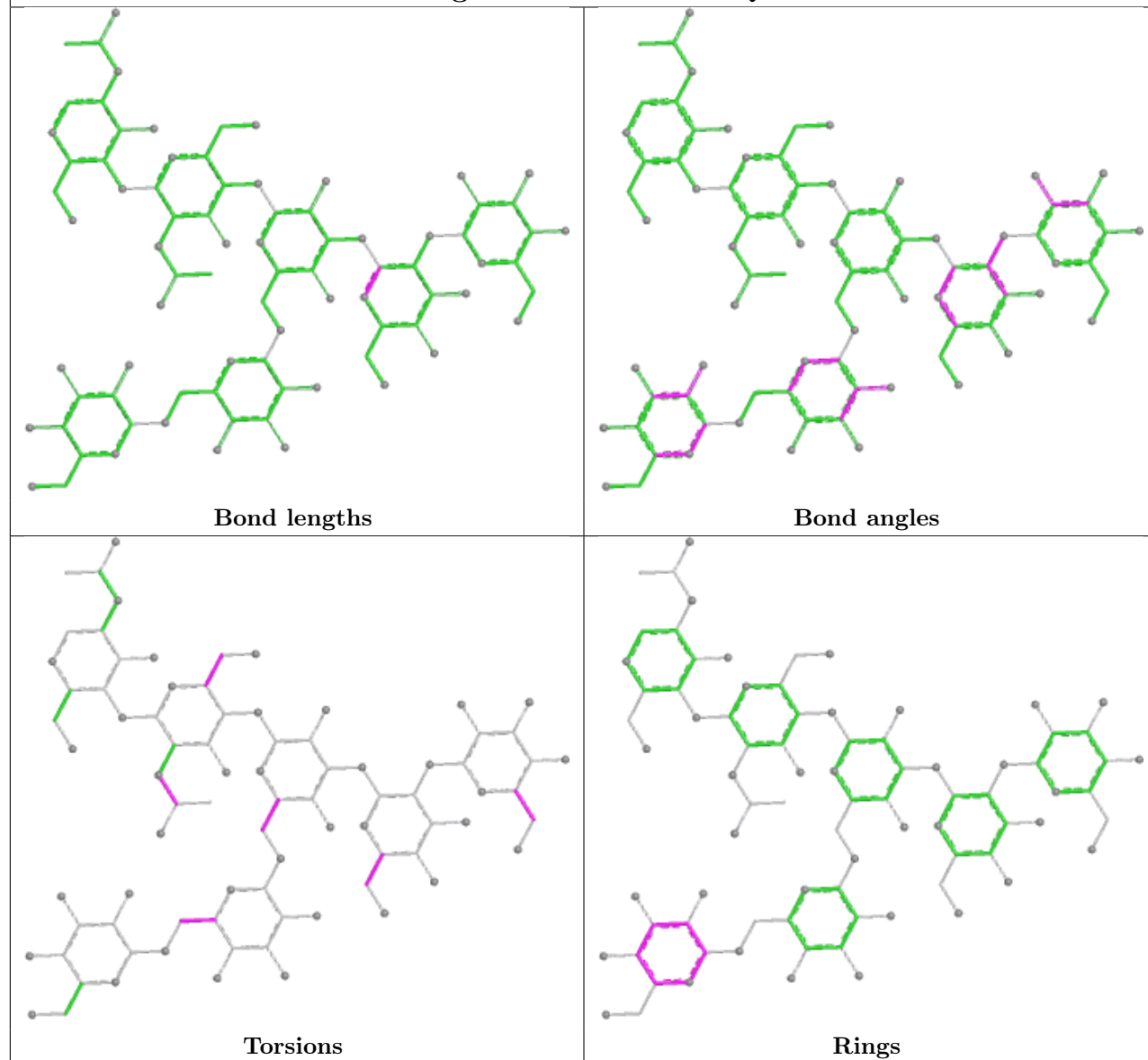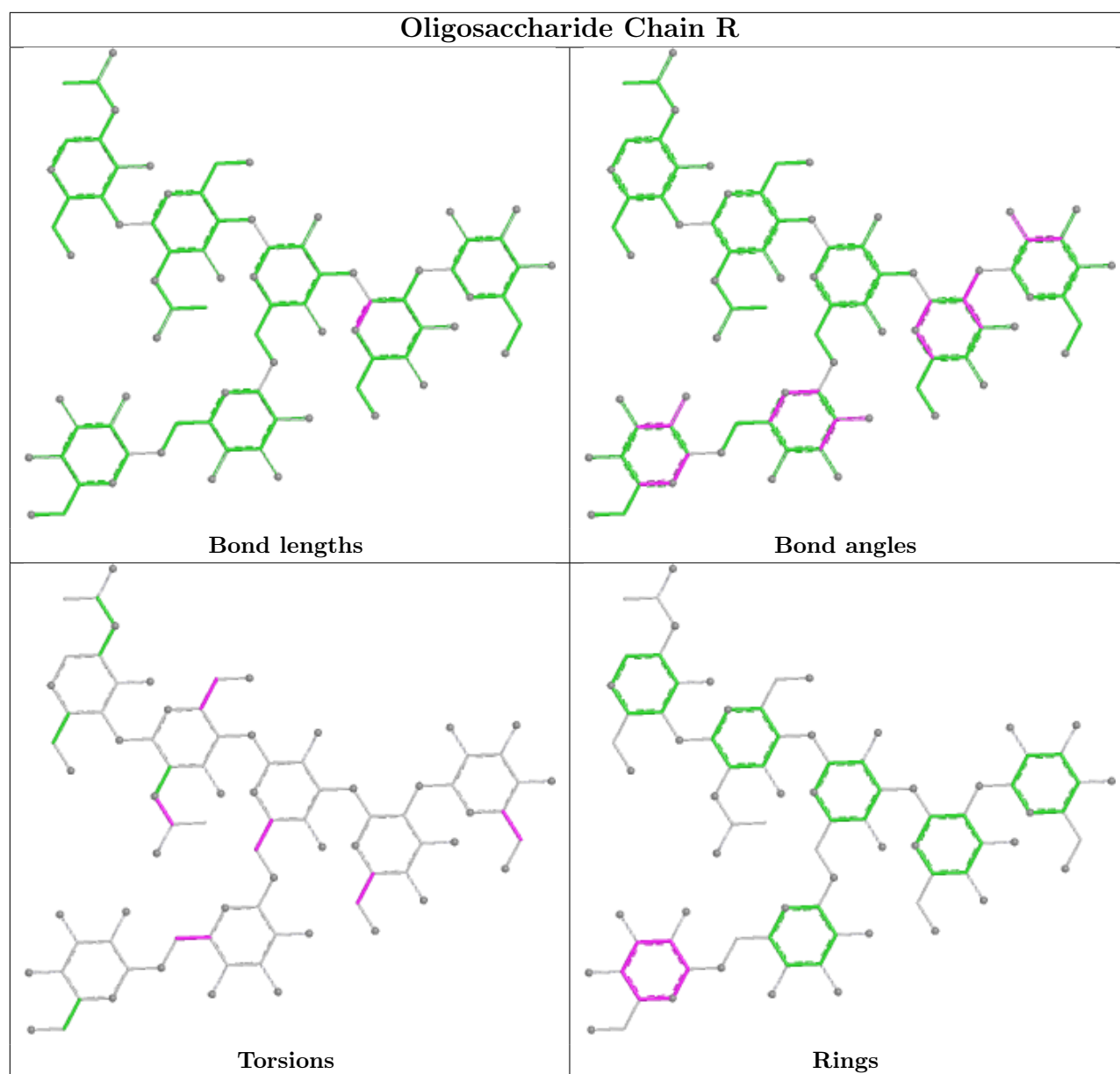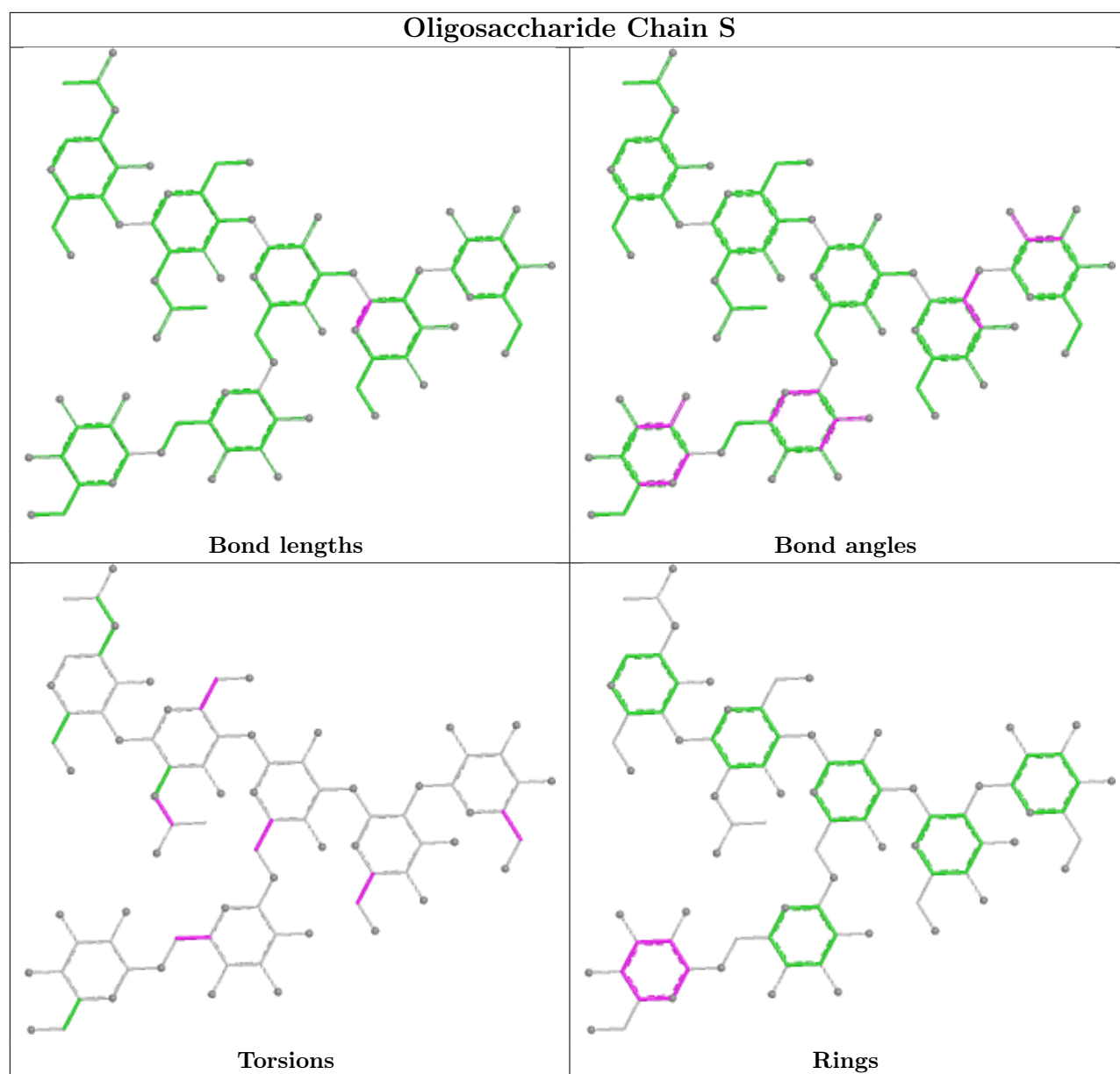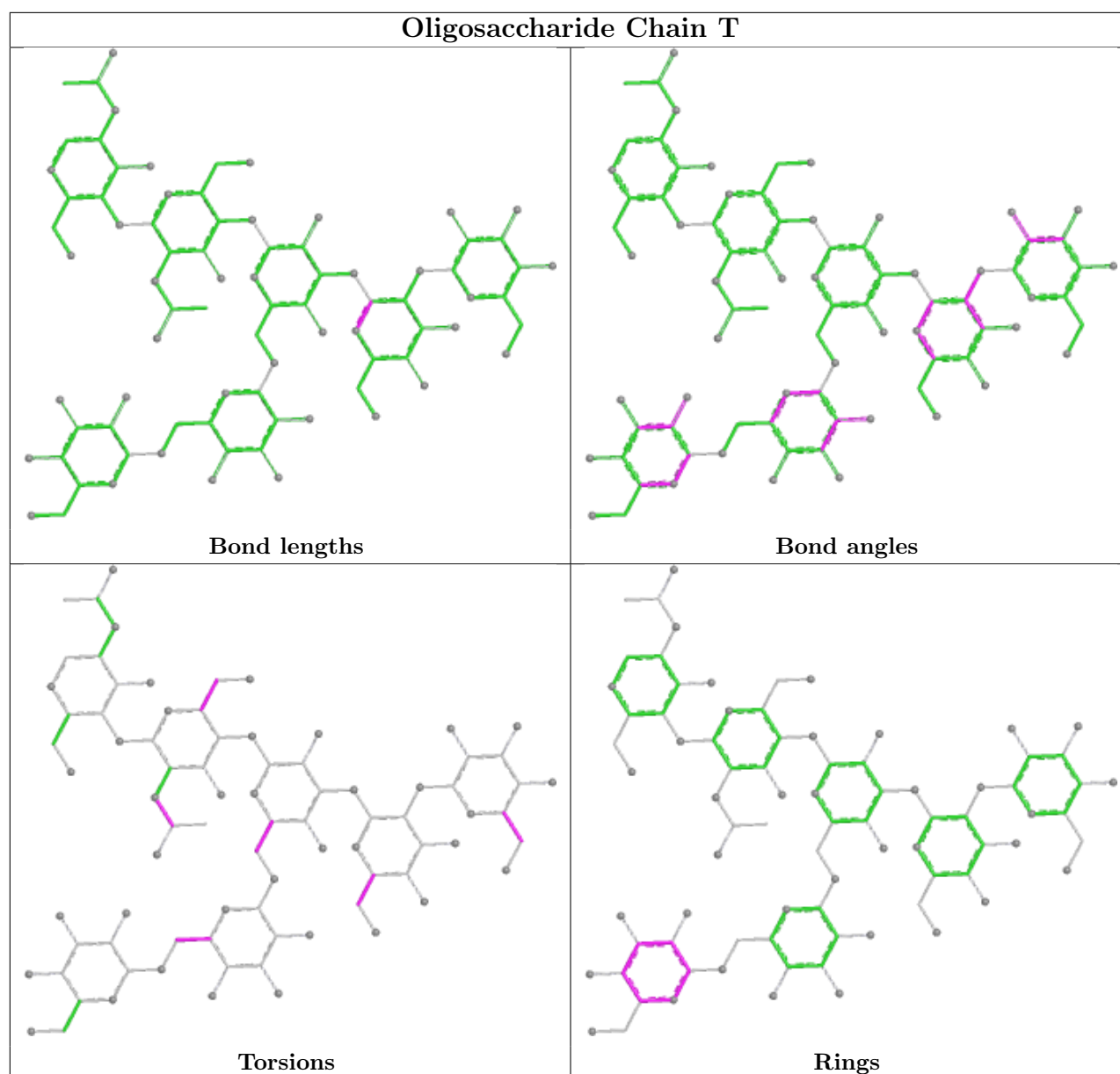
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	C	159/179 (88%)	-0.38	0	100	100	89, 113, 163, 190	0
1	G	158/179 (88%)	-0.29	0	100	100	106, 127, 164, 202	0
1	K	157/179 (87%)	-0.27	0	100	100	102, 128, 173, 188	0
1	O	157/179 (87%)	-0.34	0	100	100	93, 117, 168, 191	0
2	D	110/136 (80%)	-0.14	1 (0%)	81	70	93, 109, 174, 281	0
2	H	110/136 (80%)	-0.16	1 (0%)	81	70	95, 123, 196, 255	0
2	L	110/136 (80%)	-0.23	1 (0%)	81	70	95, 119, 205, 309	0
2	P	110/136 (80%)	-0.23	0	100	100	97, 117, 192, 298	0
3	A	199/226 (88%)	-0.25	0	100	100	88, 112, 204, 245	0
3	E	204/226 (90%)	-0.25	1 (0%)	87	80	110, 129, 241, 337	0
3	I	199/226 (88%)	-0.26	1 (0%)	87	80	90, 120, 211, 259	0
3	M	203/226 (89%)	-0.21	1 (0%)	87	80	103, 135, 242, 312	0
4	B	203/217 (93%)	-0.16	3 (1%)	71	58	91, 128, 247, 279	0
4	F	189/217 (87%)	-0.10	1 (0%)	87	80	24, 171, 254, 307	0
4	J	209/217 (96%)	-0.17	1 (0%)	87	80	93, 134, 256, 287	0
4	N	203/217 (93%)	-0.09	1 (0%)	87	80	119, 174, 273, 308	0
All	All	2680/3032 (88%)	-0.22	12 (0%)	89	83	24, 128, 237, 337	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	189	HIS	3.9
2	H	599	GLY	3.7
4	B	195	GLU	3.6
3	M	141	GLY	3.1
4	B	135	LEU	3.1

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	MAN	T	5	11/12	-0.27	0.12	247,276,331,340	0
5	MAN	R	5	11/12	0.04	0.12	247,276,331,341	0
5	MAN	Q	5	11/12	0.28	0.09	247,276,331,340	0
5	MAN	S	5	11/12	0.30	0.12	245,276,331,340	0
5	MAN	S	6	11/12	0.36	0.11	227,276,334,345	0
5	MAN	Q	6	11/12	0.41	0.13	227,276,334,345	0
5	MAN	R	6	11/12	0.48	0.14	226,276,334,345	0
5	BMA	S	3	11/12	0.52	0.09	169,204,288,288	0
5	MAN	T	6	11/12	0.54	0.12	227,276,334,345	0
5	MAN	Q	7	11/12	0.65	0.20	243,287,344,361	0
5	MAN	R	7	11/12	0.67	0.17	243,287,345,361	0
5	BMA	R	3	11/12	0.68	0.09	169,204,288,288	0
5	BMA	T	3	11/12	0.70	0.08	169,204,288,288	0
5	MAN	S	7	11/12	0.72	0.13	243,287,344,361	0
5	MAN	S	4	11/12	0.72	0.14	194,231,267,278	0
5	BMA	Q	3	11/12	0.73	0.09	168,204,288,288	0
5	MAN	T	4	11/12	0.76	0.14	193,231,266,277	0
5	MAN	T	7	11/12	0.81	0.19	243,287,344,361	0
5	MAN	R	4	11/12	0.83	0.13	193,231,266,278	0
5	NAG	R	2	14/15	0.83	0.12	120,144,181,188	0
5	NAG	T	2	14/15	0.88	0.13	119,144,182,189	0
5	NAG	S	2	14/15	0.90	0.09	117,146,181,187	0
5	MAN	Q	4	11/12	0.91	0.11	193,231,267,278	0
5	NAG	Q	2	14/15	0.92	0.11	117,143,180,186	0
5	NAG	Q	1	14/15	0.95	0.11	86,115,155,155	0
5	NAG	S	1	14/15	0.95	0.09	87,117,156,156	0
5	NAG	R	1	14/15	0.96	0.07	86,118,157,157	0
5	NAG	T	1	14/15	0.96	0.11	85,117,155,155	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.
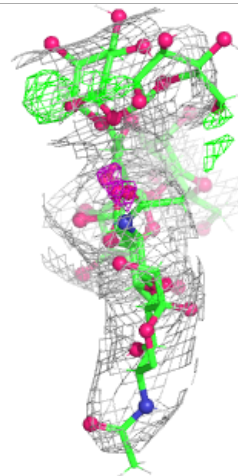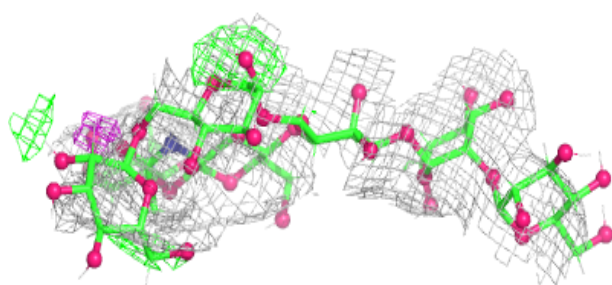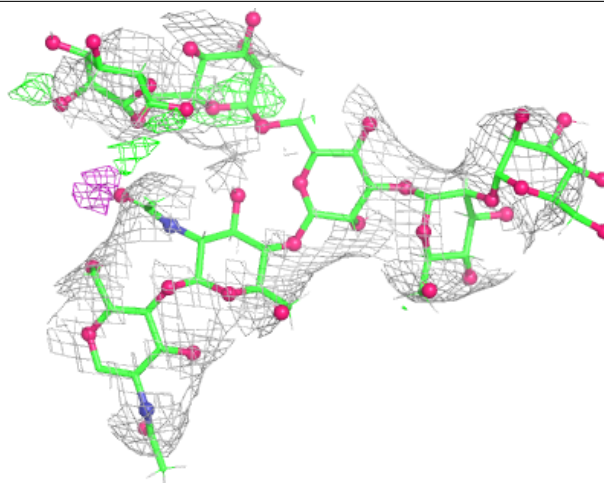
Electron density around Chain Q:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
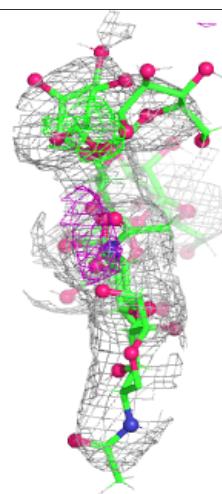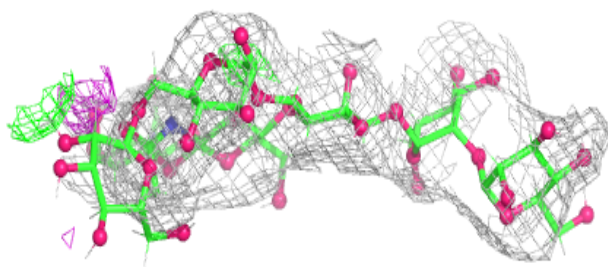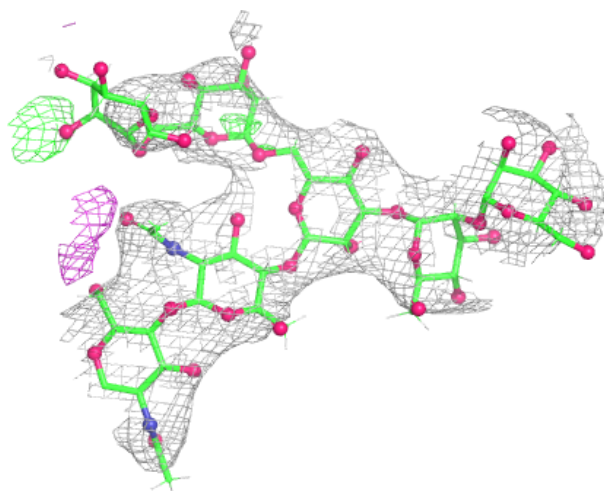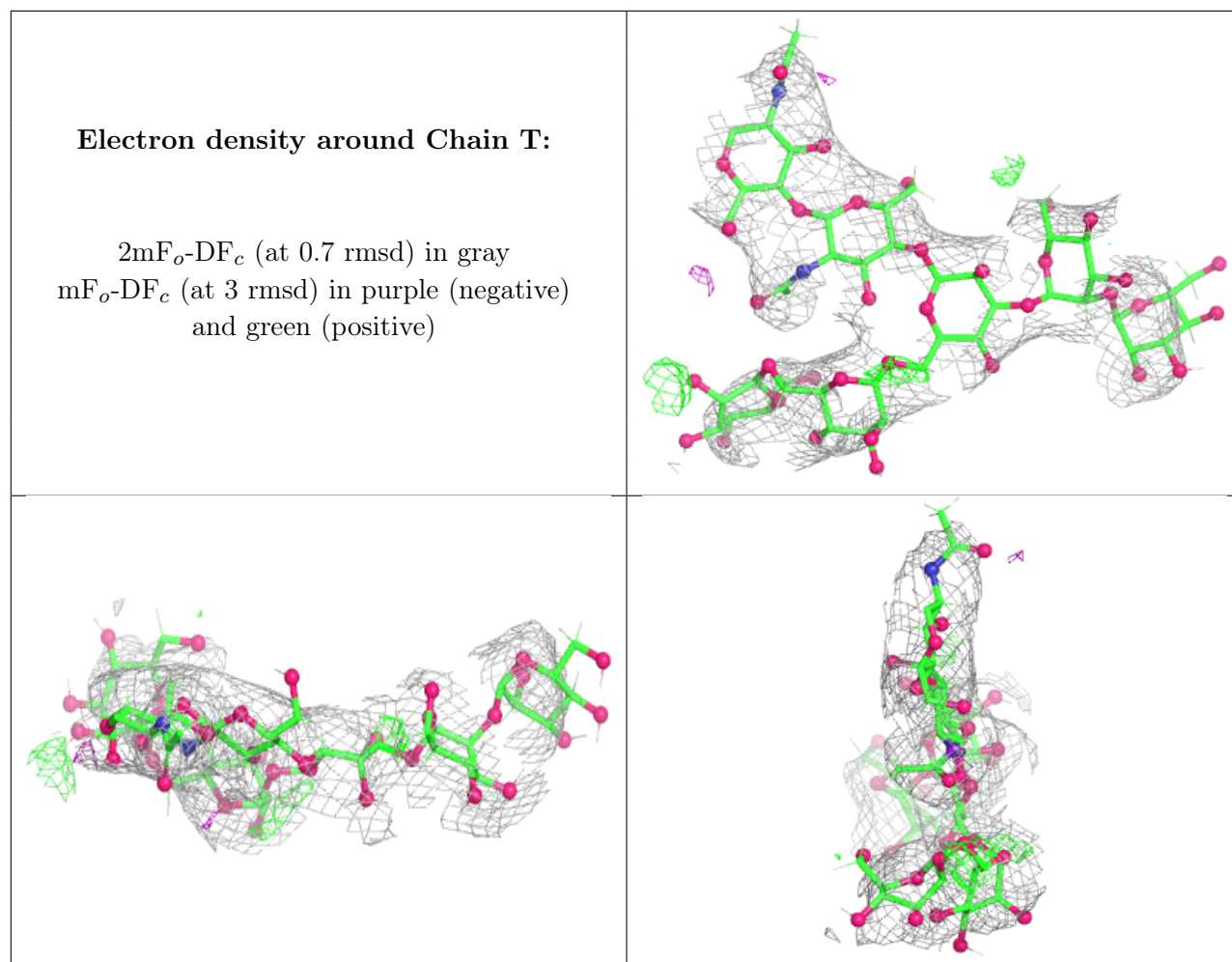
Electron density around Chain R:

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

Electron density around Chain S:

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

Electron density around Chain T:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
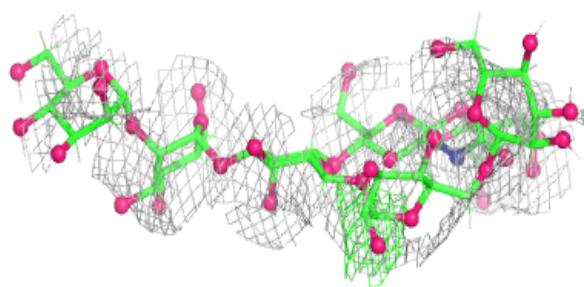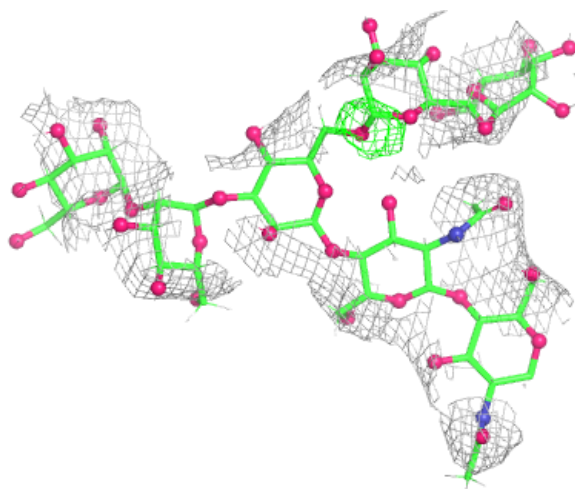
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.