



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:02 PM UTC

PDB ID : 1VPS / pdb_00001vps
Title : POLYOMAVIRUS VP1 PENTAMER COMPLEXED WITH A DISIALYLATED HEXASACCHARIDE
Authors : Stehle, T.; Harrison, S.C.
Deposited on : 1997-03-07
Resolution : 1.90 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

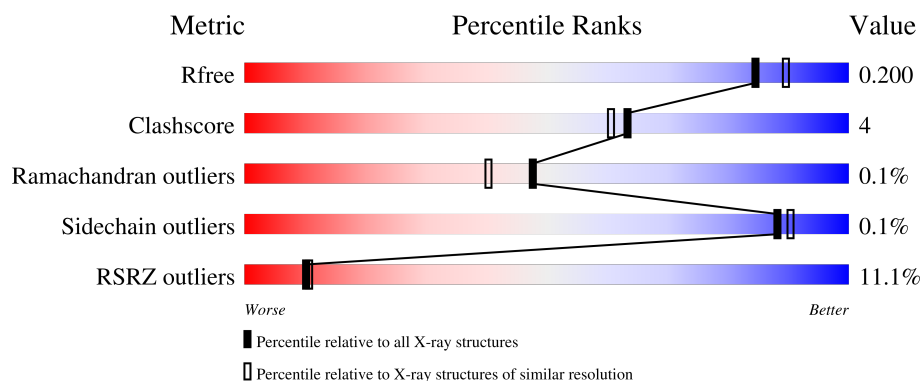
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



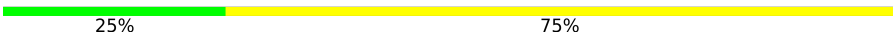
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	289	12% 88% 11% .
1	B	289	11% 87% 13% .
1	C	289	10% 88% 10% .
1	D	289	11% 87% 11% .
1	E	289	10% 89% 9% .

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Mol	Chain	Length	Quality of chain
2	F	4	 25% 75%
2	G	4	 50% 25% 25%
2	H	4	 25% 75%
2	I	4	 50% 25% 25%
2	J	4	 25% 75%

2 Entry composition [i](#)

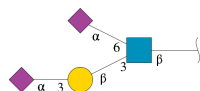
There are 3 unique types of molecules in this entry. The entry contains 13591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 POLYOMAVIRUS VP1 PENTAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2220	1404	373	432	11			
1	B	289	Total	C	N	O	S	0	0	0
			2254	1427	378	438	11			
1	C	285	Total	C	N	O	S	0	0	0
			2220	1404	373	432	11			
1	D	285	Total	C	N	O	S	0	0	0
			2220	1404	373	432	11			
1	E	285	Total	C	N	O	S	0	0	0
			2220	1404	373	432	11			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	G	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	H	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	I	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	J	4	Total	C	N	O	0	0	0
			66	36	3	27			

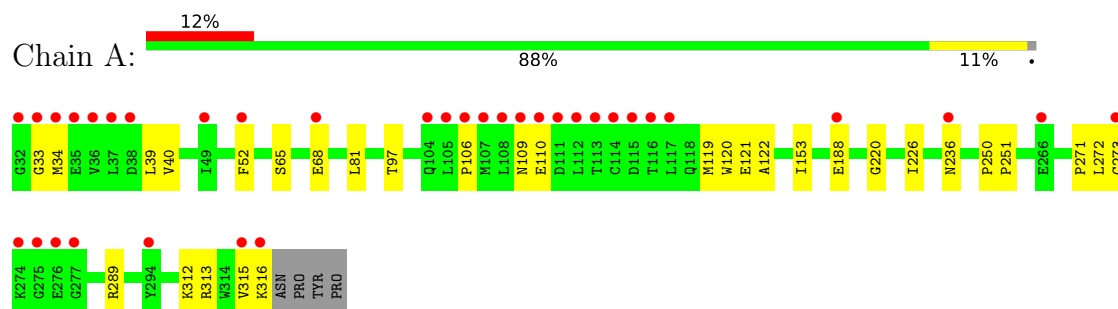
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	391	Total 391	O 391	0	0
3	B	444	Total 444	O 444	0	0
3	C	452	Total 452	O 452	0	0
3	D	436	Total 436	O 436	0	0
3	E	404	Total 404	O 404	0	0

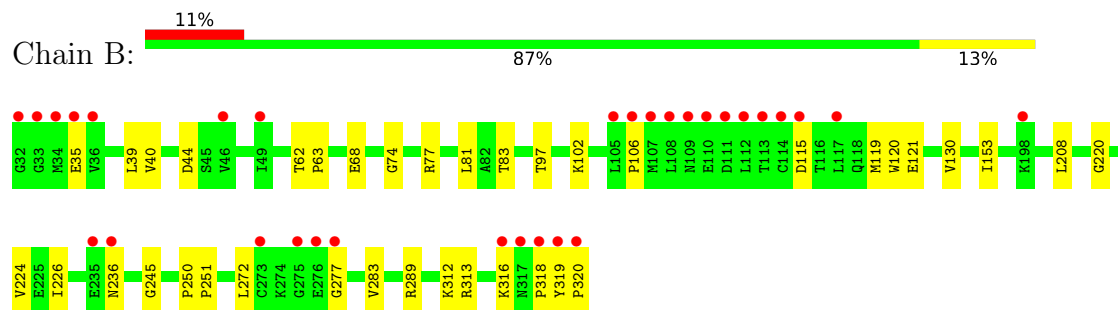
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

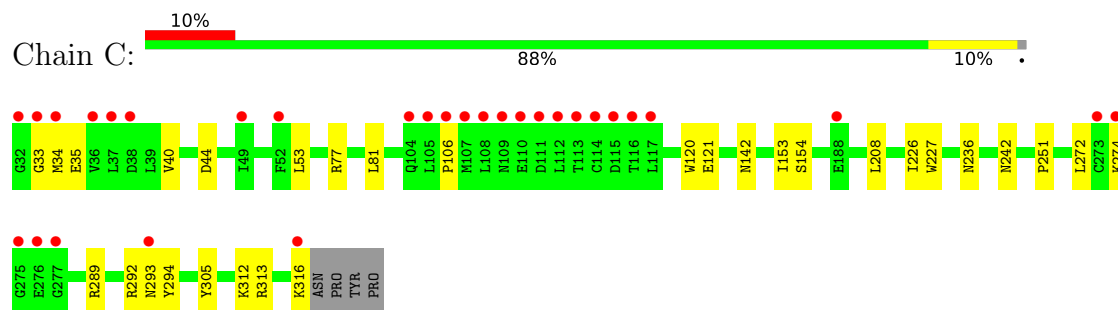
• Molecule 1: POLYOMAVIRUS VP1 PENTAMER



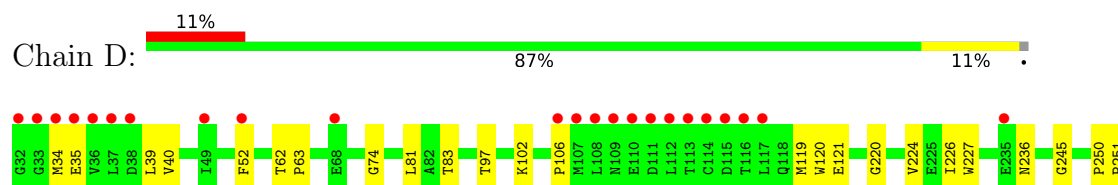
• Molecule 1: POLYOMAVIRUS VP1 PENTAMER

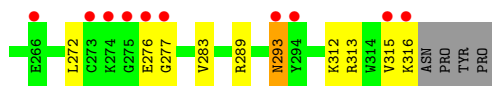


• Molecule 1: POLYOMAVIRUS VP1 PENTAMER

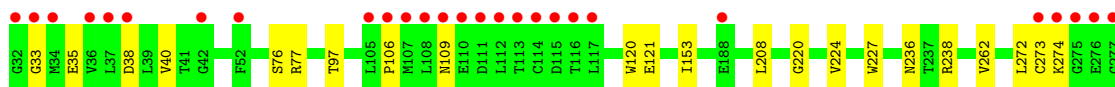
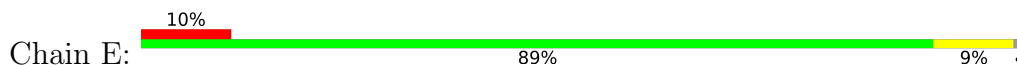


• Molecule 1: POLYOMAVIRUS VP1 PENTAMER

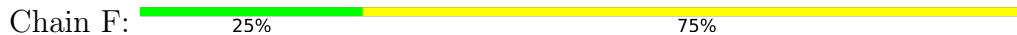




• Molecule 1: POLYOMAVIRUS VP1 PENTAMER



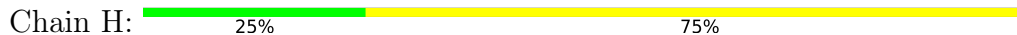
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



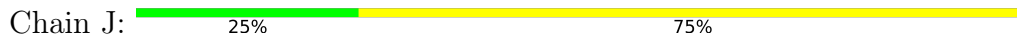
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.50Å 221.50Å 99.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	85.6 (20.00-1.90) 88.6 (20.00-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.92Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.205 0.174 , 0.200	Depositor DCC
R_{free} test set	7533 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13591	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/2273	0.83	4/3098 (0.1%)
1	B	0.47	0/2310	0.86	5/3151 (0.2%)
1	C	0.51	2/2273 (0.1%)	0.86	5/3098 (0.2%)
1	D	0.53	1/2273 (0.0%)	0.84	4/3098 (0.1%)
1	E	0.45	0/2273	0.85	5/3098 (0.2%)
All	All	0.48	3/11402 (0.0%)	0.85	23/15543 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	293	ASN	C-N	-9.32	1.20	1.33
1	C	293	ASN	C-N	6.68	1.43	1.33
1	C	292	ARG	C-N	5.66	1.43	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	ARG	N-CA-C	-6.84	99.07	109.95
1	A	289	ARG	N-CA-C	-6.65	99.38	109.95
1	C	289	ARG	N-CA-C	-6.57	99.51	109.95
1	E	289	ARG	N-CA-C	-6.20	100.09	109.95
1	E	109	ASN	N-CA-C	6.18	118.68	109.59
1	D	226	ILE	CB-CA-C	-6.03	105.68	111.05
1	B	289	ARG	N-CA-C	-6.02	100.38	109.95
1	C	226	ILE	CB-CA-C	-5.87	105.83	111.05
1	C	77	ARG	N-CA-C	-5.86	102.97	110.53
1	A	226	ILE	CB-CA-C	-5.76	105.92	111.05
1	C	293	ASN	O-C-N	-5.62	115.95	122.87
1	A	109	ASN	N-CA-C	5.43	118.48	109.46
1	E	227	TRP	N-CA-C	5.34	117.44	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	N-CA-C	-5.29	102.92	110.59
1	D	227	TRP	N-CA-C	5.21	117.22	108.73
1	E	77	ARG	N-CA-C	-5.20	103.05	110.59
1	D	74	GLY	N-CA-C	-5.19	108.18	114.92
1	B	130	VAL	N-CA-C	5.07	116.26	108.71
1	C	227	TRP	N-CA-C	5.04	116.94	108.73
1	B	226	ILE	CB-CA-C	-5.03	106.58	111.05
1	B	74	GLY	N-CA-C	-5.02	107.61	114.64
1	A	110	GLU	N-CA-C	-5.02	104.89	111.96
1	E	76	SER	N-CA-C	-5.01	103.05	110.46

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	2220	0	2187	16	0
1	B	2254	0	2216	22	0
1	C	2220	0	2187	21	0
1	D	2220	0	2187	21	0
1	E	2220	0	2187	16	0
2	F	66	0	56	0	0
2	G	66	0	56	1	0
2	H	66	0	56	0	0
2	I	66	0	56	1	0
2	J	66	0	56	0	0
3	A	391	0	0	3	0
3	B	444	0	0	6	0
3	C	452	0	0	3	0
3	D	436	0	0	2	0
3	E	404	0	0	6	0
All	All	13591	0	11244	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:CYS:SG	3:A:651:HOH:O	2.50	0.69
1:C:35:GLU:HB3	1:C:316:LYS:HB2	1.75	0.68
1:D:35:GLU:HB3	1:D:316:LYS:HB2	1.75	0.66
1:E:273:CYS:SG	3:E:705:HOH:O	2.50	0.64
1:B:119:MET:HE1	1:B:318:PRO:HG3	1.84	0.59
1:B:35:GLU:HB3	1:B:316:LYS:HB2	1.85	0.57
1:A:33:GLY:O	1:A:316:LYS:HB3	2.04	0.57
1:E:35:GLU:HB3	1:E:316:LYS:HB2	1.87	0.57
1:C:106:PRO:HG2	1:C:120:TRP:CZ2	2.41	0.56
1:D:102:LYS:NZ	1:D:277:GLY:HA3	2.20	0.56
1:E:262:VAL:HG13	3:E:692:HOH:O	2.06	0.56
1:B:153:ILE:HA	1:C:81:LEU:HD21	1.87	0.56
1:C:305:TYR:HE1	3:C:502:HOH:O	1.88	0.56
1:D:102:LYS:HZ1	1:D:277:GLY:HA3	1.71	0.55
1:D:39:LEU:HD23	1:D:313:ARG:HD2	1.89	0.55
1:C:305:TYR:HD2	3:C:717:HOH:O	1.90	0.55
1:B:224:VAL:HG11	1:B:283:VAL:HG21	1.90	0.54
3:B:626:HOH:O	1:C:294:TYR:HA	2.07	0.54
1:D:119:MET:HE3	1:D:315:VAL:HG21	1.90	0.53
1:A:81:LEU:HD21	1:E:153:ILE:HA	1.90	0.53
1:C:34:MET:HE3	1:C:34:MET:HA	1.89	0.53
1:D:121:GLU:OE1	1:D:313:ARG:HD3	2.09	0.53
1:B:115:ASP:HB2	3:B:651:HOH:O	2.08	0.52
1:C:153:ILE:HA	1:D:81:LEU:HD21	1.91	0.52
1:B:106:PRO:HG2	1:B:120:TRP:CZ2	2.44	0.52
1:A:121:GLU:OE1	1:A:313:ARG:HD3	2.10	0.51
3:B:749:HOH:O	1:C:242:ASN:HB2	2.09	0.51
1:C:121:GLU:OE1	1:C:313:ARG:HD3	2.10	0.51
1:C:236:ASN:ND2	1:C:272:LEU:O	2.44	0.51
1:D:34:MET:HE1	1:D:119:MET:SD	2.52	0.50
1:B:102:LYS:NZ	1:B:277:GLY:HA3	2.27	0.49
1:E:208:LEU:HD13	3:E:694:HOH:O	2.12	0.49
1:E:121:GLU:OE1	1:E:313:ARG:HD3	2.13	0.49
1:E:40:VAL:HB	1:E:312:LYS:HB2	1.94	0.49
1:E:238:ARG:HD3	3:E:637:HOH:O	2.13	0.48
1:A:65:SER:HB3	1:A:68:GLU:HB2	1.95	0.48
1:B:236:ASN:ND2	1:B:272:LEU:O	2.46	0.48
1:C:53:LEU:HG	3:C:759:HOH:O	2.13	0.48
1:D:293:ASN:HB3	3:D:733:HOH:O	2.13	0.48
1:D:106:PRO:HG2	1:D:120:TRP:CZ2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD23	1:A:313:ARG:HD2	1.96	0.47
1:A:106:PRO:HG2	1:A:120:TRP:CZ2	2.49	0.47
1:C:236:ASN:ND2	1:C:274:LYS:HE3	2.29	0.47
1:A:119:MET:HE3	1:A:315:VAL:HG21	1.97	0.47
1:C:33:GLY:O	1:C:316:LYS:HB3	2.14	0.47
1:C:236:ASN:HD22	1:C:274:LYS:HE3	1.79	0.47
1:E:236:ASN:ND2	1:E:272:LEU:O	2.48	0.47
1:E:106:PRO:HG2	1:E:120:TRP:CZ2	2.50	0.47
1:E:97:THR:OG1	1:E:220:GLY:HA2	2.15	0.46
1:E:224:VAL:HG11	1:E:283:VAL:HG21	1.97	0.46
1:E:33:GLY:O	1:E:316:LYS:HB3	2.16	0.46
1:D:40:VAL:HB	1:D:312:LYS:HB2	1.97	0.46
1:B:121:GLU:OE1	1:B:313:ARG:HD3	2.16	0.45
1:B:44:ASP:O	1:B:312:LYS:HE3	2.17	0.45
1:A:40:VAL:HB	1:A:312:LYS:HB2	1.99	0.45
3:A:679:HOH:O	1:B:208:LEU:HD13	2.17	0.45
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.80	0.44
3:B:751:HOH:O	1:C:208:LEU:HD13	2.17	0.44
1:E:38:ASP:HB2	3:E:573:HOH:O	2.17	0.44
1:B:83:THR:HG23	2:G:4:SIA:H91	2.00	0.44
1:D:224:VAL:HG11	1:D:283:VAL:HG21	2.00	0.44
1:B:68:GLU:HG2	3:B:752:HOH:O	2.18	0.43
1:D:97:THR:OG1	1:D:220:GLY:HA2	2.18	0.43
1:A:153:ILE:HA	1:B:81:LEU:HD21	2.00	0.43
1:D:52:PHE:HB2	3:E:694:HOH:O	2.18	0.43
1:B:39:LEU:HD23	1:B:313:ARG:HD2	2.01	0.43
1:B:40:VAL:HB	1:B:312:LYS:HB2	2.01	0.43
1:B:251:PRO:HG3	3:B:727:HOH:O	2.19	0.42
1:C:40:VAL:HB	1:C:312:LYS:HB2	1.99	0.42
1:D:236:ASN:ND2	1:D:272:LEU:O	2.50	0.42
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.95	0.42
1:A:122:ALA:HB3	1:A:271:PRO:HD2	2.02	0.42
1:D:83:THR:HG23	2:I:4:SIA:H91	2.02	0.42
1:E:106:PRO:HG2	1:E:120:TRP:HZ2	1.83	0.42
1:D:276:GLU:HB3	3:D:722:HOH:O	2.20	0.41
1:B:62:THR:HA	1:B:63:PRO:C	2.45	0.41
1:C:274:LYS:HE2	1:C:274:LYS:HB3	1.92	0.41
1:A:97:THR:OG1	1:A:220:GLY:HA2	2.19	0.41
1:A:251:PRO:HD2	1:B:245:GLY:HA3	2.02	0.41
1:C:142:ASN:HB2	1:C:154:SER:OG	2.20	0.41
1:D:62:THR:HA	1:D:63:PRO:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:PRO:HG2	1:D:120:TRP:HZ2	1.84	0.41
1:E:274:LYS:HB3	1:E:274:LYS:HE2	1.89	0.41
1:C:251:PRO:HD2	1:D:245:GLY:HA3	2.03	0.40
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.96	0.40
1:A:236:ASN:ND2	1:A:272:LEU:O	2.55	0.40
1:C:44:ASP:O	1:C:312:LYS:HE3	2.21	0.40
1:A:52:PHE:HB3	3:A:656:HOH:O	2.21	0.40
1:B:97:THR:OG1	1:B:220:GLY:HA2	2.21	0.40
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/289 (98%)	273 (96%)	9 (3%)	1 (0%)	30	22
1	B	287/289 (99%)	273 (95%)	14 (5%)	0	100	100
1	C	283/289 (98%)	268 (95%)	15 (5%)	0	100	100
1	D	283/289 (98%)	272 (96%)	11 (4%)	0	100	100
1	E	283/289 (98%)	271 (96%)	12 (4%)	0	100	100
All	All	1419/1445 (98%)	1357 (96%)	61 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	MET

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	249/253 (98%)	248 (100%)	1 (0%)	84	87
1	B	253/253 (100%)	253 (100%)	0	100	100
1	C	249/253 (98%)	249 (100%)	0	100	100
1	D	249/253 (98%)	249 (100%)	0	100	100
1	E	249/253 (98%)	249 (100%)	0	100	100
All	All	1249/1265 (99%)	1248 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLU

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

Mol	Chain	Res	Type
1	A	104	GLN
1	A	242	ASN
1	B	93	ASN
1	B	104	GLN
1	B	242	ASN
1	B	293	ASN
1	D	92	ASN
1	D	93	ASN
1	D	242	ASN
1	E	242	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 ⓘ

20 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	F	1	2	15,15,15	0.86	1 (6%)	21,21,21	1.31	5 (23%)
2	GAL	F	2	2	11,11,12	0.47	0	15,15,17	0.50	0
2	SIA	F	3	2	20,20,21	0.80	0	21,28,31	0.92	2 (9%)
2	SIA	F	4	2	20,20,21	1.51	4 (20%)	21,28,31	1.04	2 (9%)
2	NAG	G	1	2	15,15,15	0.48	0	21,21,21	0.54	0
2	GAL	G	2	2	11,11,12	0.41	0	15,15,17	0.59	0
2	SIA	G	3	2	20,20,21	0.82	1 (5%)	21,28,31	0.92	1 (4%)
2	SIA	G	4	2	20,20,21	0.97	1 (5%)	21,28,31	1.04	2 (9%)
2	NAG	H	1	2	15,15,15	0.93	1 (6%)	21,21,21	1.14	1 (4%)
2	GAL	H	2	2	11,11,12	0.72	0	15,15,17	0.63	0
2	SIA	H	3	2	20,20,21	0.74	0	21,28,31	0.95	1 (4%)
2	SIA	H	4	2	20,20,21	1.32	2 (10%)	21,28,31	1.04	2 (9%)
2	NAG	I	1	2	15,15,15	0.53	0	21,21,21	0.83	0
2	GAL	I	2	2	11,11,12	0.42	0	15,15,17	0.54	0
2	SIA	I	3	2	20,20,21	0.72	0	21,28,31	0.90	1 (4%)
2	SIA	I	4	2	20,20,21	1.24	1 (5%)	21,28,31	1.03	1 (4%)
2	NAG	J	1	2	15,15,15	0.76	0	21,21,21	0.91	1 (4%)
2	GAL	J	2	2	11,11,12	0.61	0	15,15,17	0.51	0
2	SIA	J	3	2	20,20,21	0.79	0	21,28,31	0.92	1 (4%)
2	SIA	J	4	2	20,20,21	1.13	2 (10%)	21,28,31	1.11	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	SIA	F	3	2	-	1/18/34/38	0/1/1/1
2	SIA	F	4	2	-	0/18/34/38	0/1/1/1
2	NAG	G	1	2	-	0/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	1/18/34/38	0/1/1/1
2	SIA	G	4	2	-	0/18/34/38	0/1/1/1
2	NAG	H	1	2	-	0/6/26/26	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	5/18/34/38	0/1/1/1
2	SIA	H	4	2	-	0/18/34/38	0/1/1/1
2	NAG	I	1	2	-	0/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	4/18/34/38	0/1/1/1
2	SIA	I	4	2	-	0/18/34/38	0/1/1/1
2	NAG	J	1	2	-	0/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	2/18/34/38	0/1/1/1
2	SIA	J	4	2	-	0/18/34/38	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	SIA	C2-C1	3.70	1.56	1.52
2	H	4	SIA	C2-C1	3.30	1.56	1.52
2	F	4	SIA	C4-C5	3.15	1.56	1.53
2	F	4	SIA	C2-C1	3.09	1.56	1.52
2	J	4	SIA	C2-C1	3.03	1.55	1.52
2	F	4	SIA	C3-C4	3.01	1.58	1.52
2	H	4	SIA	C4-C5	2.86	1.55	1.53
2	J	4	SIA	C4-C5	2.32	1.55	1.53
2	G	4	SIA	C2-C1	2.24	1.55	1.52
2	F	1	NAG	C1-C2	2.24	1.55	1.52
2	F	4	SIA	C6-C5	2.15	1.56	1.53
2	H	1	NAG	C1-C2	2.11	1.55	1.52
2	G	3	SIA	C2-C1	2.09	1.54	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	4	SIA	C8-C7-C6	-3.05	107.33	113.05
2	F	4	SIA	C8-C7-C6	-2.91	107.59	113.05
2	F	1	NAG	O5-C1-C2	2.88	112.41	109.52
2	H	1	NAG	C1-C2-N2	-2.76	107.53	110.73
2	G	4	SIA	C8-C7-C6	-2.70	107.99	113.05
2	H	4	SIA	O1B-C1-C2	2.60	119.48	112.71
2	I	4	SIA	O1B-C1-C2	2.57	119.40	112.71
2	J	4	SIA	O1B-C1-C2	2.48	119.17	112.71
2	H	3	SIA	O1B-C1-C2	2.48	119.16	112.71
2	I	3	SIA	O1B-C1-C2	2.46	119.11	112.71
2	G	4	SIA	O1B-C1-C2	2.46	119.11	112.71
2	G	3	SIA	O1B-C1-C2	2.44	119.05	112.71
2	J	3	SIA	O1B-C1-C2	2.44	119.04	112.71
2	F	4	SIA	O1B-C1-C2	2.35	118.83	112.71
2	F	3	SIA	O1B-C1-C2	2.33	118.78	112.71
2	F	1	NAG	C1-C2-C3	2.33	113.72	110.54
2	H	4	SIA	C8-C7-C6	-2.32	108.70	113.05
2	F	1	NAG	C3-C4-C5	-2.20	106.24	110.23
2	F	3	SIA	C8-C7-C6	-2.18	108.96	113.05
2	F	1	NAG	C6-C5-C4	2.14	118.28	113.02
2	J	1	NAG	C6-C5-C4	2.09	118.14	113.02
2	F	1	NAG	C1-C2-N2	-2.06	108.34	110.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

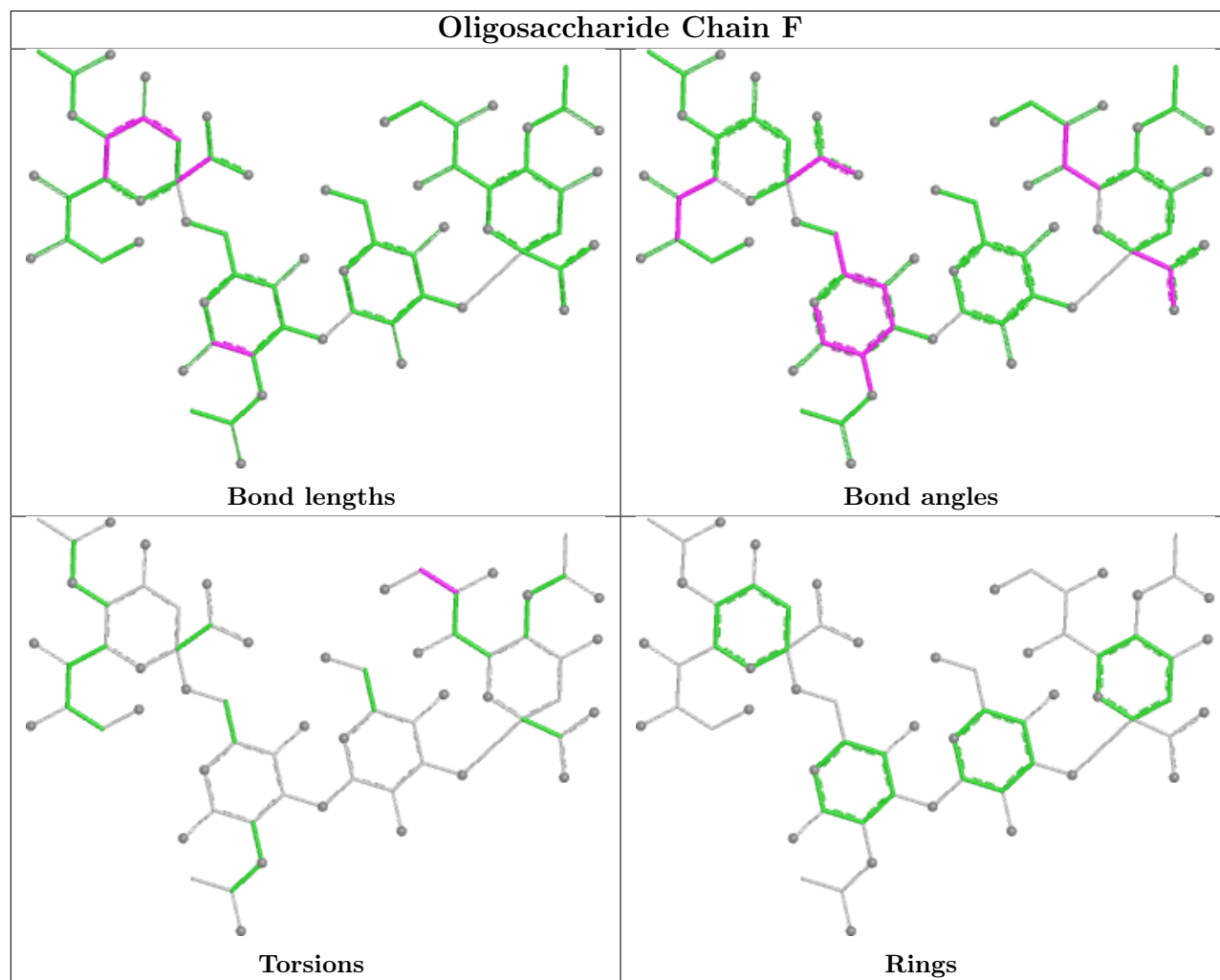
Mol	Chain	Res	Type	Atoms
2	H	3	SIA	C7-C8-C9-O9
2	H	3	SIA	O8-C8-C9-O9
2	J	3	SIA	O8-C8-C9-O9
2	J	3	SIA	C7-C8-C9-O9
2	I	3	SIA	C6-C7-C8-O8
2	I	3	SIA	O7-C7-C8-C9
2	I	3	SIA	O7-C7-C8-O8
2	F	3	SIA	O8-C8-C9-O9
2	H	3	SIA	C6-C7-C8-O8
2	H	3	SIA	O7-C7-C8-C9
2	H	3	SIA	O7-C7-C8-O8
2	I	3	SIA	C6-C7-C8-C9
2	G	3	SIA	O8-C8-C9-O9

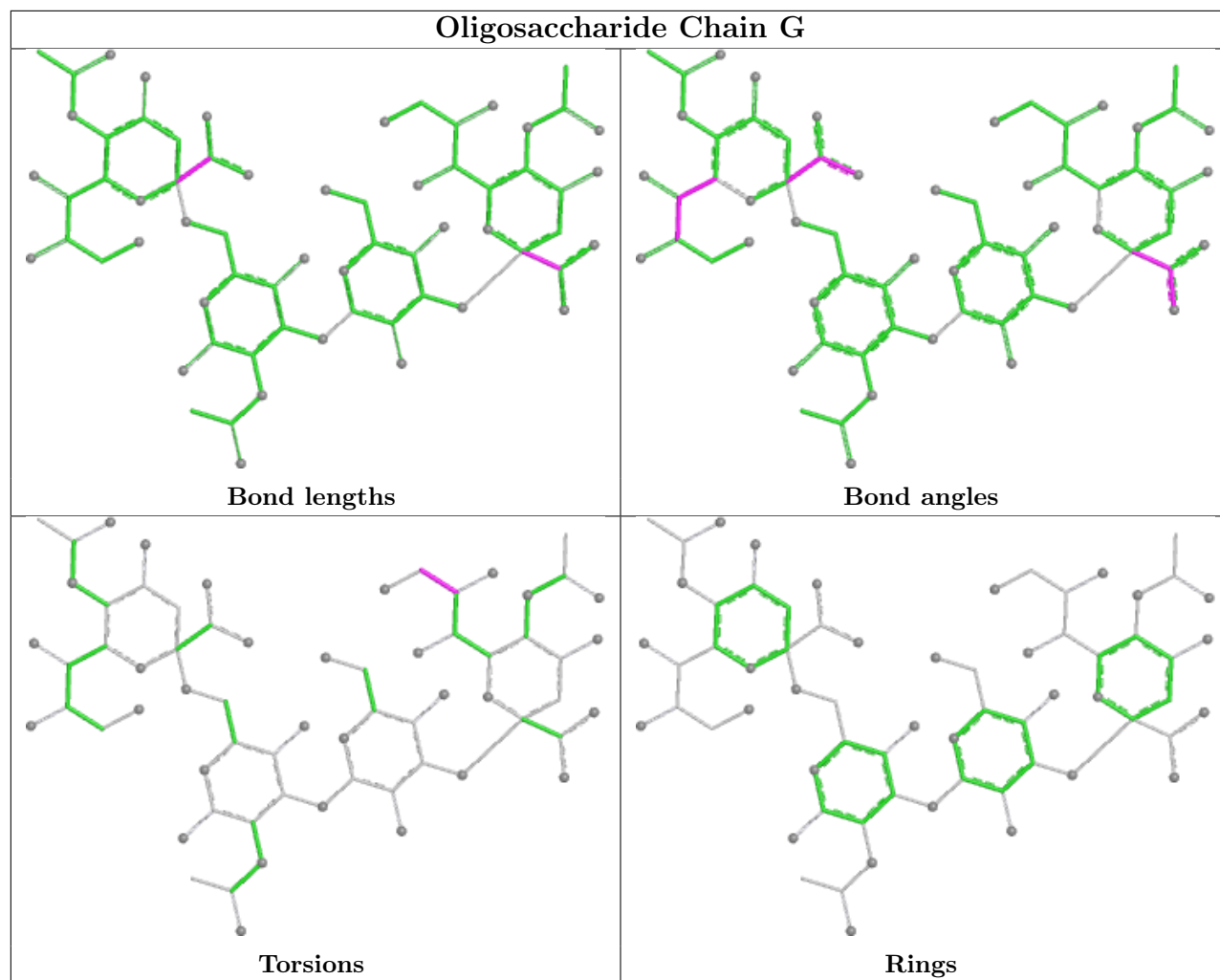
There are no ring outliers.

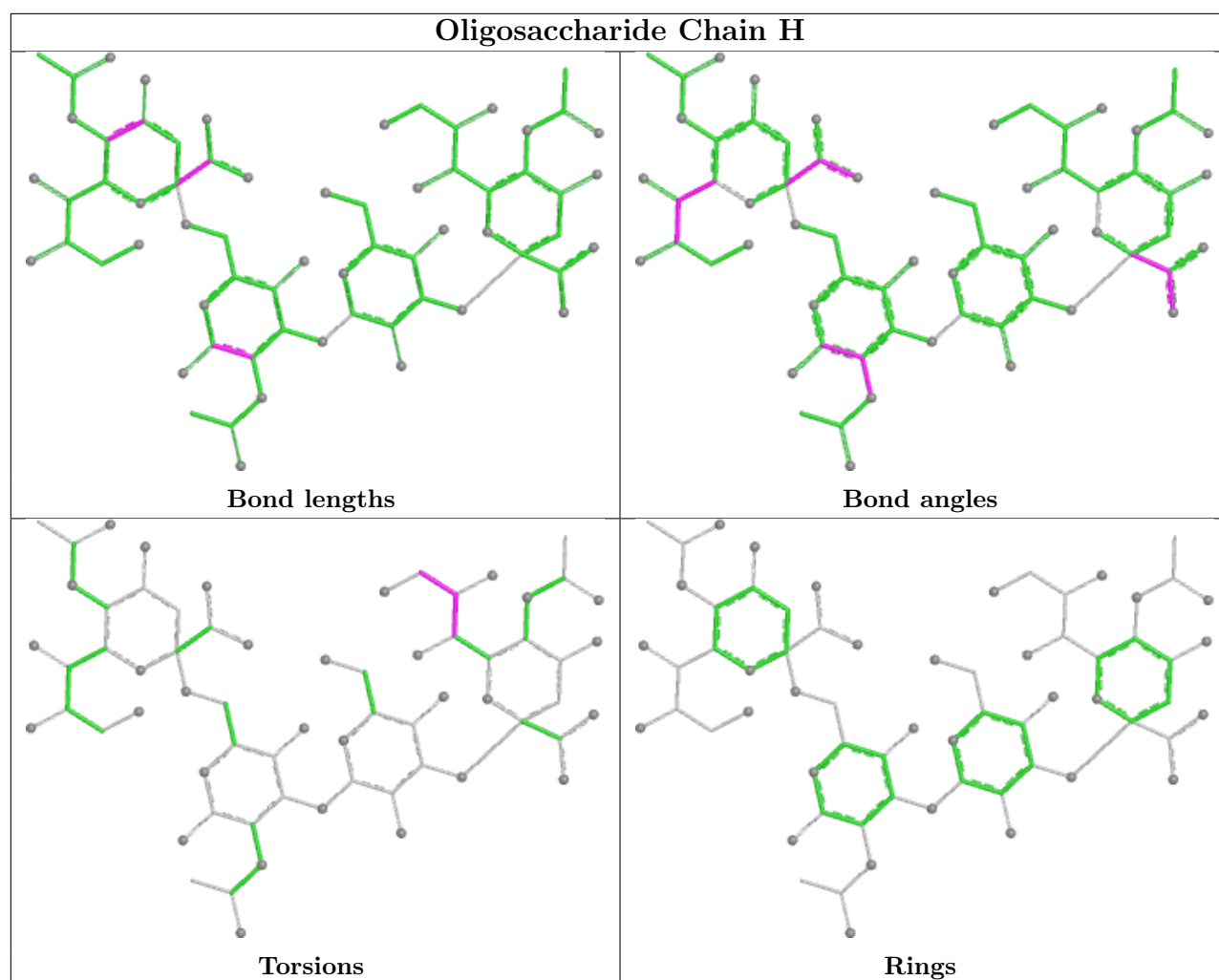
2 monomers are involved in 2 short contacts:

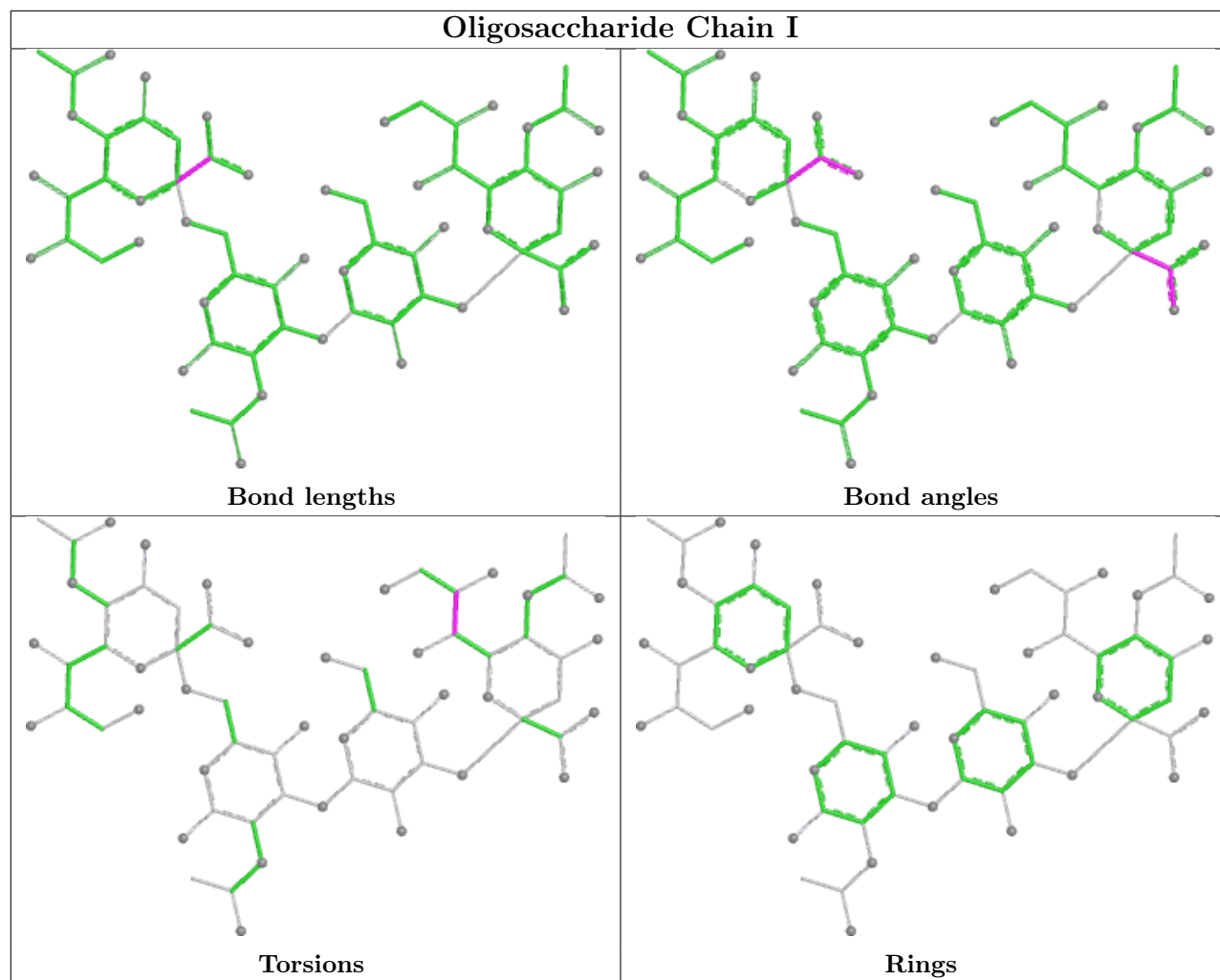
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	4	SIA	1	0
2	I	4	SIA	1	0

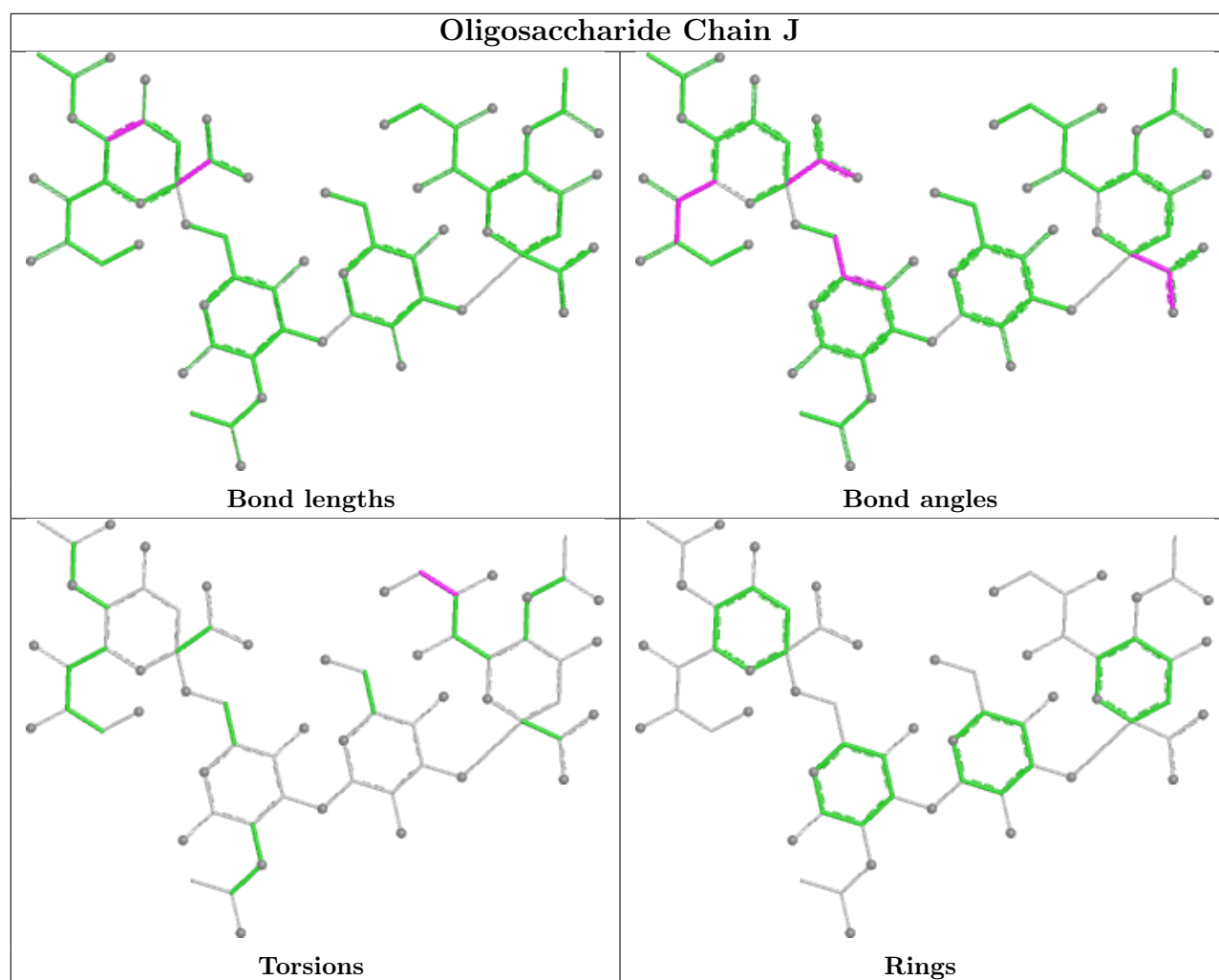
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	285/289 (98%)	0.45	35 (12%) 8 9	16, 25, 59, 95	0
1	B	289/289 (100%)	0.24	31 (10%) 11 11	14, 22, 53, 82	0
1	C	285/289 (98%)	0.18	30 (10%) 11 12	14, 20, 54, 92	0
1	D	285/289 (98%)	0.26	33 (11%) 9 10	13, 20, 57, 92	0
1	E	285/289 (98%)	0.39	30 (10%) 11 12	17, 25, 59, 94	0
All	All	1429/1445 (98%)	0.30	159 (11%) 10 11	13, 22, 58, 95	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	GLY	10.5
1	B	32	GLY	9.0
1	A	33	GLY	8.3
1	C	33	GLY	6.7
1	C	113	THR	6.3
1	C	107	MET	6.2
1	E	34	MET	6.1
1	B	320	PRO	5.8
1	C	112	LEU	5.7
1	A	34	MET	5.6
1	D	112	LEU	5.5
1	D	108	LEU	5.5
1	C	108	LEU	5.4
1	B	33	GLY	5.3
1	E	108	LEU	5.3
1	A	108	LEU	5.2
1	D	109	ASN	5.2
1	D	34	MET	5.2
1	D	107	MET	5.0
1	E	107	MET	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	107	MET	5.0
1	D	114	CYS	4.9
1	A	113	THR	4.8
1	D	113	THR	4.8
1	C	277	GLY	4.8
1	E	114	CYS	4.7
1	C	34	MET	4.7
1	A	294	TYR	4.7
1	A	112	LEU	4.6
1	D	276	GLU	4.6
1	A	276	GLU	4.6
1	A	114	CYS	4.6
1	E	110	GLU	4.5
1	B	276	GLU	4.4
1	E	33	GLY	4.4
1	E	113	THR	4.3
1	E	117	LEU	4.3
1	D	277	GLY	4.3
1	A	109	ASN	4.2
1	C	276	GLU	4.2
1	A	111	ASP	4.1
1	D	32	GLY	4.1
1	E	276	GLU	4.1
1	D	111	ASP	4.0
1	C	117	LEU	4.0
1	C	111	ASP	4.0
1	A	115	ASP	4.0
1	D	117	LEU	4.0
1	E	277	GLY	3.9
1	E	52	PHE	3.9
1	A	117	LEU	3.9
1	C	106	PRO	3.8
1	D	106	PRO	3.8
1	A	32	GLY	3.8
1	B	108	LEU	3.8
1	C	188	GLU	3.7
1	C	293	ASN	3.7
1	B	107	MET	3.7
1	A	49	ILE	3.7
1	A	106	PRO	3.7
1	C	115	ASP	3.6
1	B	317	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	36	VAL	3.6
1	C	316	LYS	3.6
1	C	109	ASN	3.5
1	B	117	LEU	3.5
1	C	32	GLY	3.5
1	E	112	LEU	3.5
1	A	273	CYS	3.5
1	E	105	LEU	3.5
1	E	115	ASP	3.5
1	D	316	LYS	3.4
1	E	109	ASN	3.4
1	E	316	LYS	3.4
1	B	277	GLY	3.4
1	D	36	VAL	3.4
1	E	32	GLY	3.3
1	E	106	PRO	3.3
1	E	111	ASP	3.3
1	D	52	PHE	3.3
1	E	275	GLY	3.3
1	B	106	PRO	3.2
1	E	36	VAL	3.2
1	B	109	ASN	3.2
1	A	275	GLY	3.1
1	E	294	TYR	3.1
1	B	115	ASP	3.1
1	B	273	CYS	3.1
1	B	318	PRO	3.1
1	B	236	ASN	3.0
1	C	116	THR	3.0
1	A	116	THR	3.0
1	B	113	THR	3.0
1	B	275	GLY	3.0
1	C	38	ASP	3.0
1	D	38	ASP	3.0
1	D	273	CYS	3.0
1	C	110	GLU	3.0
1	B	112	LEU	2.9
1	D	116	THR	2.9
1	B	110	GLU	2.9
1	E	116	THR	2.9
1	C	114	CYS	2.9
1	C	275	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	274	LYS	2.8
1	D	115	ASP	2.8
1	C	273	CYS	2.8
1	B	49	ILE	2.8
1	B	111	ASP	2.8
1	C	36	VAL	2.8
1	B	319	TYR	2.7
1	B	105	LEU	2.7
1	A	316	LYS	2.7
1	D	68	GLU	2.7
1	D	315	VAL	2.7
1	A	52	PHE	2.7
1	A	104	GLN	2.7
1	E	274	LYS	2.6
1	D	293	ASN	2.6
1	E	273	CYS	2.6
1	D	37	LEU	2.6
1	E	38	ASP	2.6
1	A	315	VAL	2.5
1	C	104	GLN	2.5
1	B	114	CYS	2.5
1	A	105	LEU	2.5
1	C	49	ILE	2.5
1	E	37	LEU	2.5
1	D	49	ILE	2.5
1	A	37	LEU	2.4
1	C	105	LEU	2.4
1	A	110	GLU	2.4
1	D	235	GLU	2.4
1	B	46	VAL	2.4
1	B	34	MET	2.4
1	B	36	VAL	2.3
1	A	274	LYS	2.3
1	D	275	GLY	2.3
1	E	42	GLY	2.3
1	A	188	GLU	2.3
1	A	266	GLU	2.3
1	A	277	GLY	2.2
1	D	266	GLU	2.2
1	A	236	ASN	2.2
1	C	52	PHE	2.2
1	D	294	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	316	LYS	2.2
1	E	188	GLU	2.2
1	A	68	GLU	2.2
1	E	315	VAL	2.1
1	D	35	GLU	2.1
1	D	110	GLU	2.1
1	A	38	ASP	2.1
1	A	35	GLU	2.0
1	B	198	LYS	2.0
1	C	37	LEU	2.0
1	B	35	GLU	2.0
1	B	235	GLU	2.0
1	C	274	LYS	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.

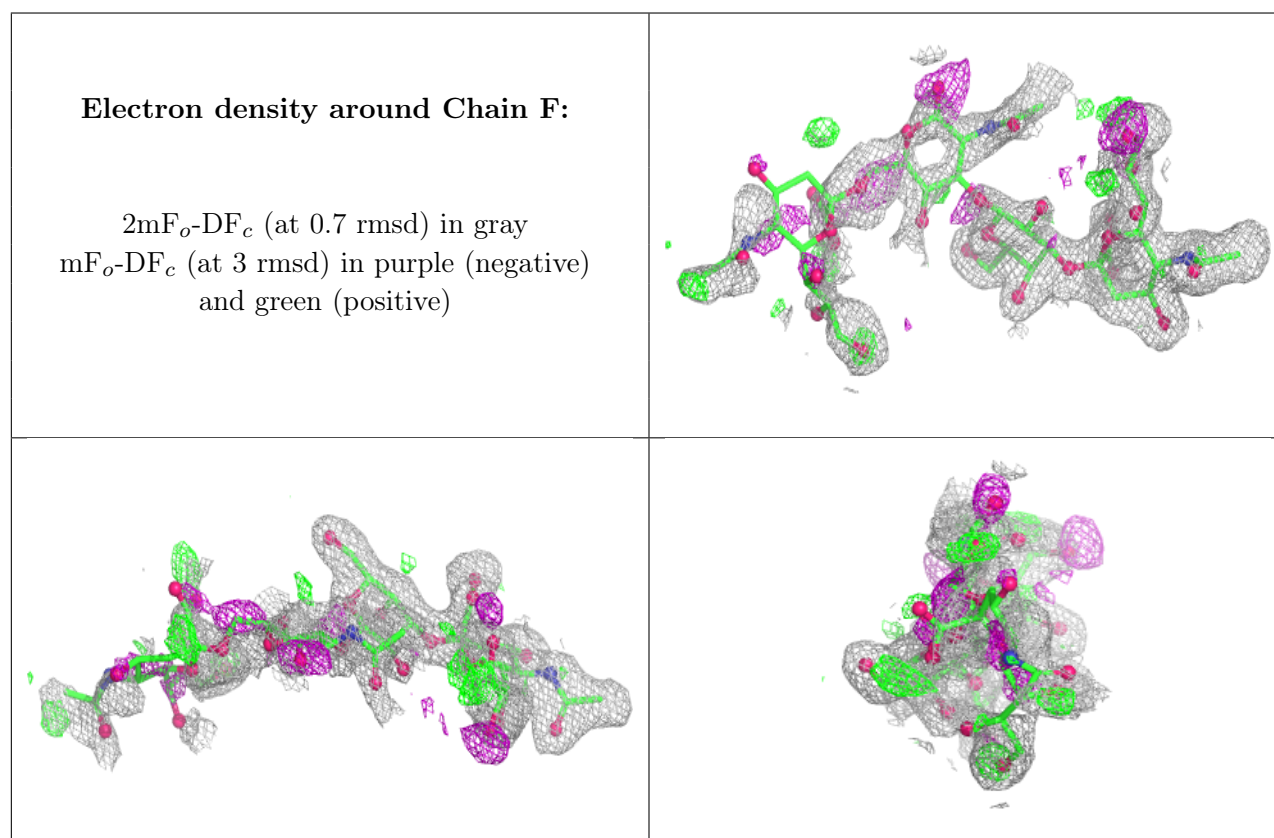
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SIA	F	4	20/21	0.57	0.25	66,71,73,73	0
2	SIA	H	4	20/21	0.59	0.25	67,71,77,77	0
2	NAG	G	1	15/15	0.61	0.26	53,66,72,77	0
2	SIA	J	4	20/21	0.61	0.25	78,81,82,82	0
2	NAG	I	1	15/15	0.65	0.23	41,51,53,54	0
2	NAG	H	1	15/15	0.66	0.23	46,58,63,67	0
2	SIA	G	4	20/21	0.66	0.25	80,82,83,84	0
2	NAG	J	1	15/15	0.67	0.20	59,69,74,78	0
2	NAG	F	1	15/15	0.67	0.21	54,62,66,69	0
2	SIA	I	4	20/21	0.78	0.19	46,56,62,63	0
2	SIA	F	3	20/21	0.87	0.13	28,32,36,40	0
2	SIA	J	3	20/21	0.88	0.13	31,34,37,38	0
2	SIA	G	3	20/21	0.90	0.12	24,27,31,35	0
2	GAL	J	2	11/12	0.90	0.12	40,46,51,53	0
2	SIA	I	3	20/21	0.91	0.11	23,25,29,33	0

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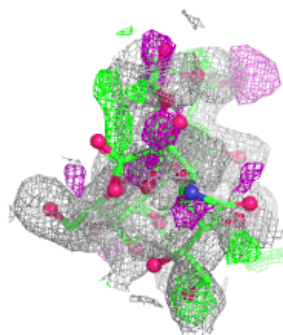
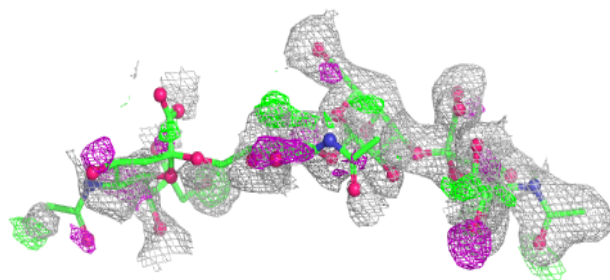
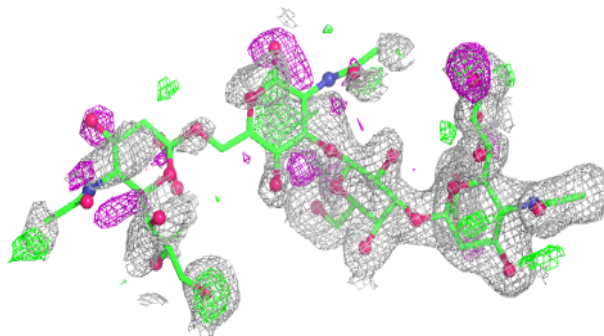
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SIA	H	3	20/21	0.91	0.10	22,24,29,34	0
2	GAL	F	2	11/12	0.92	0.11	37,44,46,48	0
2	GAL	I	2	11/12	0.94	0.09	28,31,33,36	0
2	GAL	G	2	11/12	0.95	0.10	32,37,41,44	0
2	GAL	H	2	11/12	0.95	0.10	28,32,35,38	0

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.

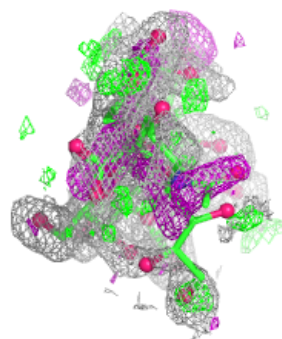
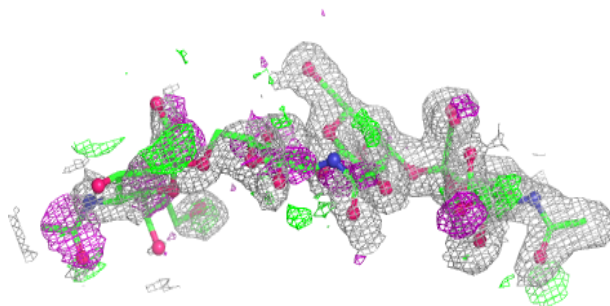
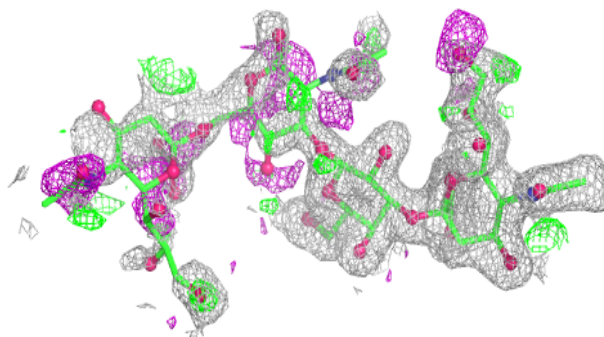


Electron density around Chain G:

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

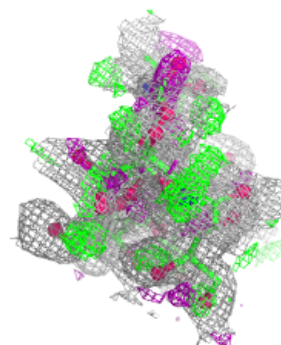
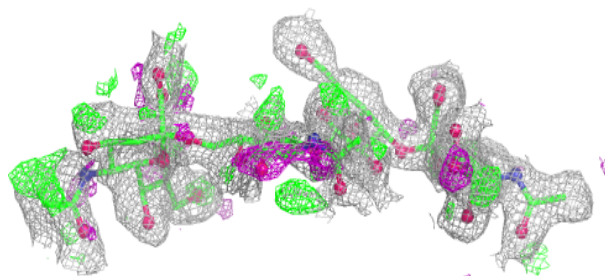
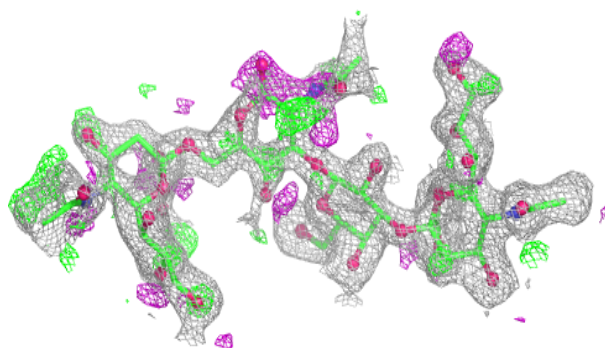
**Electron density around Chain H:**

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

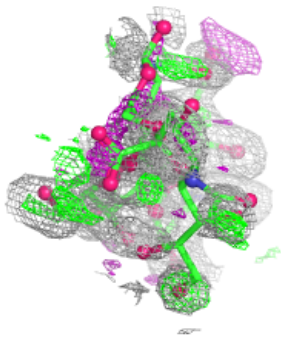
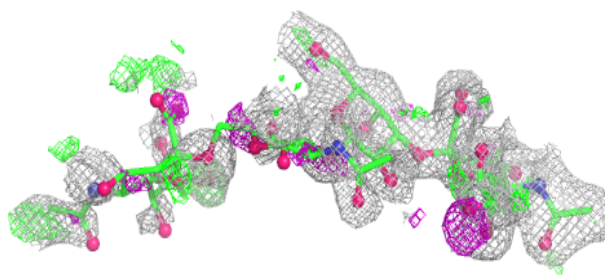
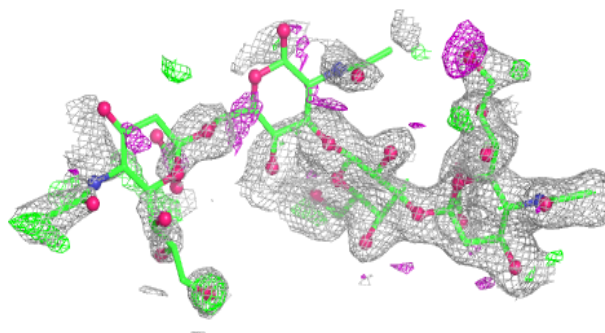


Electron density around Chain I:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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.