



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 01:10 pm BST

PDB ID : 9GHI / pdb_00009ghi
Title : Machupo virus GP1-GP2 heterodimer in complex with Fab of MAC1
Authors : Bowden, T.A.; Paesen, G.C.
Deposited on : 2024-08-15
Resolution : 2.41 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
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) : 2.43.1

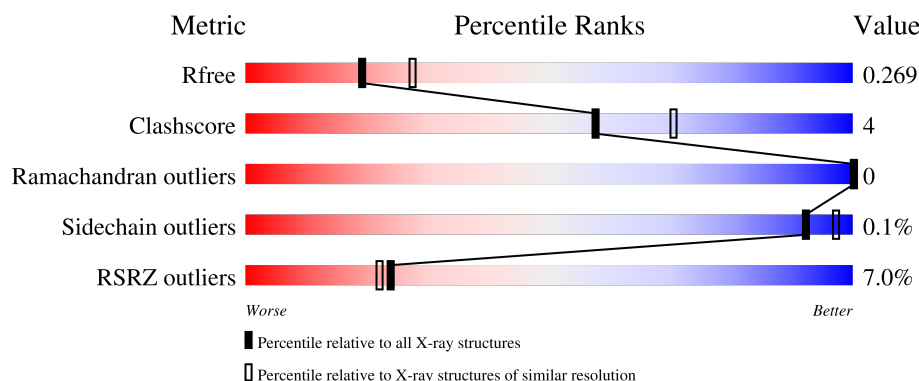
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	204	<div> <div>9%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
2	B	204	<div> <div>10%</div> <div>61%</div> <div>9%</div> <div>30%</div> </div>
3	H	234	<div> <div>4%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
4	L	217	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
5	C	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	2	 50%50%
6	E	5	 20%20%60%
7	F	4	 25%75%
8	G	3	 33%67%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12240 atoms, of which 5818 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 Pre-glycoprotein polypeptide GP complex.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	192	Total	C	H	N	O	S	0	0	0
			3001	968	1463	270	284	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	CYS	LEU	engineered mutation	UNP Q8AZ57
A	138	ALA	LYS	conflict	UNP Q8AZ57
A	227	GLU	ASP	conflict	UNP Q8AZ57
A	258	SER	GLU	engineered mutation	UNP Q8AZ57
A	260	ARG	SER	engineered mutation	UNP Q8AZ57
A	261	LYS	LEU	engineered mutation	UNP Q8AZ57
A	262	ARG	LYS	engineered mutation	UNP Q8AZ57

- Molecule 2 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	143	Total	C	H	N	O	S	0	0	0
			2300	750	1120	197	220	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	263	SER	ALA	engineered mutation	UNP Q6IUF7
B	307	ASP	ASN	conflict	UNP Q6IUF7
B	332	PRO	GLU	engineered mutation	UNP Q6IUF7
B	340	CYS	LEU	engineered mutation	UNP Q6IUF7
B	429	SER	-	expression tag	UNP Q6IUF7
B	430	GLY	-	expression tag	UNP Q6IUF7
B	431	ASP	-	expression tag	UNP Q6IUF7
B	432	ASP	-	expression tag	UNP Q6IUF7
B	433	ASP	-	expression tag	UNP Q6IUF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	434	ASP	-	expression tag	UNP Q6IUF7
B	435	LYS	-	expression tag	UNP Q6IUF7
B	436	GLY	-	expression tag	UNP Q6IUF7
B	437	SER	-	expression tag	UNP Q6IUF7
B	438	GLY	-	expression tag	UNP Q6IUF7
B	439	TRP	-	expression tag	UNP Q6IUF7
B	440	SER	-	expression tag	UNP Q6IUF7
B	441	HIS	-	expression tag	UNP Q6IUF7
B	442	PRO	-	expression tag	UNP Q6IUF7
B	443	GLN	-	expression tag	UNP Q6IUF7
B	444	PHE	-	expression tag	UNP Q6IUF7
B	445	GLU	-	expression tag	UNP Q6IUF7
B	446	LYS	-	expression tag	UNP Q6IUF7
B	447	GLY	-	expression tag	UNP Q6IUF7
B	448	GLY	-	expression tag	UNP Q6IUF7
B	449	GLY	-	expression tag	UNP Q6IUF7
B	450	SER	-	expression tag	UNP Q6IUF7
B	451	GLY	-	expression tag	UNP Q6IUF7
B	452	GLY	-	expression tag	UNP Q6IUF7
B	453	GLY	-	expression tag	UNP Q6IUF7
B	454	SER	-	expression tag	UNP Q6IUF7
B	455	GLY	-	expression tag	UNP Q6IUF7
B	456	GLY	-	expression tag	UNP Q6IUF7
B	457	SER	-	expression tag	UNP Q6IUF7
B	458	ALA	-	expression tag	UNP Q6IUF7
B	459	TRP	-	expression tag	UNP Q6IUF7
B	460	SER	-	expression tag	UNP Q6IUF7
B	461	HIS	-	expression tag	UNP Q6IUF7
B	462	PRO	-	expression tag	UNP Q6IUF7
B	463	GLN	-	expression tag	UNP Q6IUF7
B	464	PHE	-	expression tag	UNP Q6IUF7
B	465	GLU	-	expression tag	UNP Q6IUF7
B	466	LYS	-	expression tag	UNP Q6IUF7

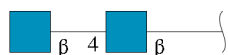
- Molecule 3 is a protein called MAC1 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	221	Total	C	H	N	O	S	0	0	0
			3278	1058	1607	276	330	7			

- Molecule 4 is a protein called MAC1 light chain.

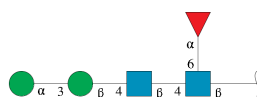
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	215	Total	C	H	N	O	S	0	2	0
			3313	1044	1628	289	345	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



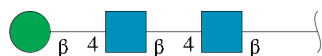
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



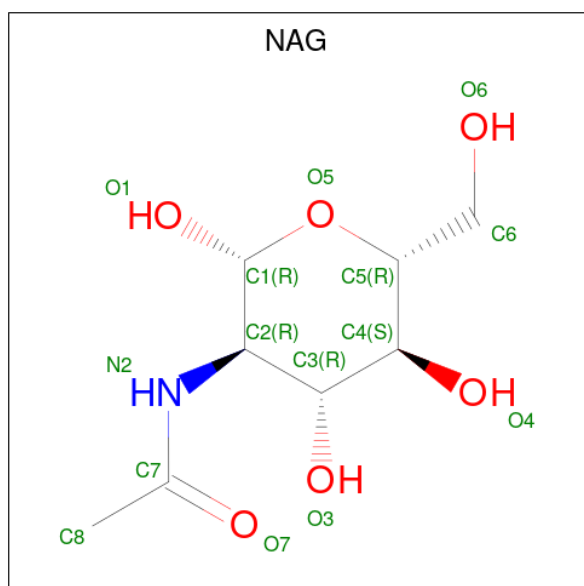
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called 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
8	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

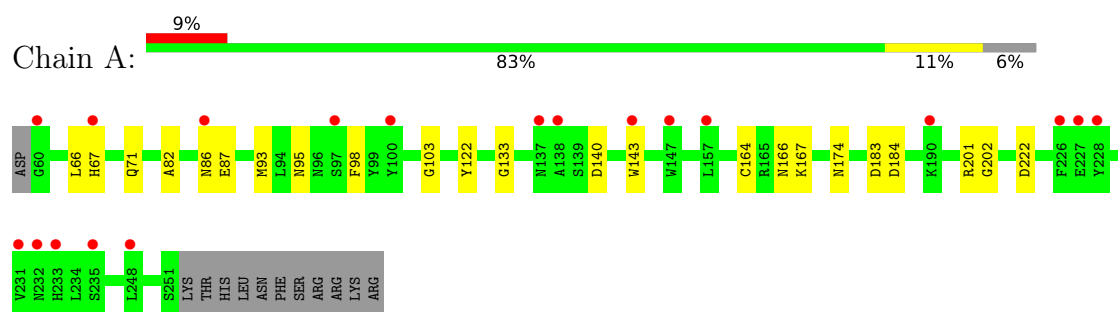
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	10	Total	O	0	0
			10	10		
10	B	4	Total	O	0	0
			4	4		
10	H	36	Total	O	0	0
			36	36		
10	L	65	Total	O	0	0
			65	65		

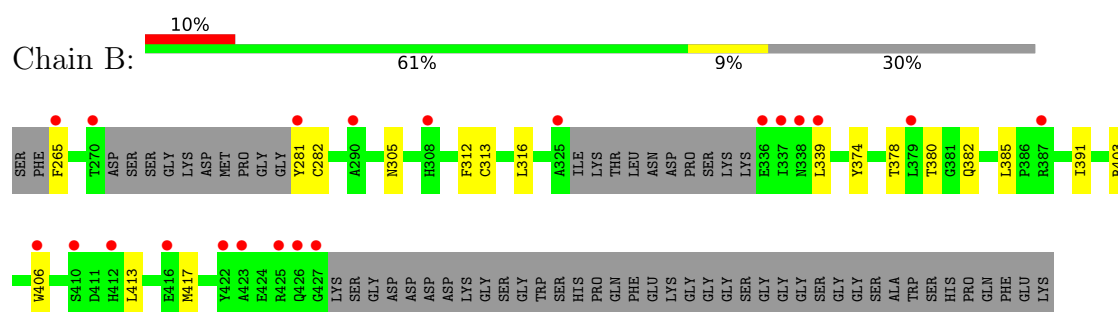
3 Residue-property plots

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.

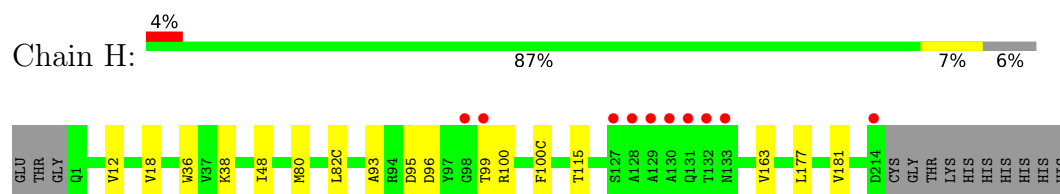
- Molecule 1: Pre-glycoprotein polyprotein GP complex



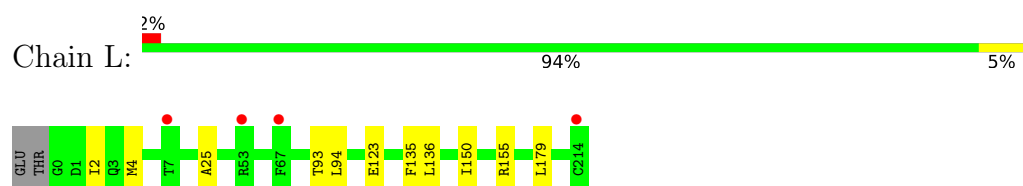
- Molecule 2: Glycoprotein G2



- Molecule 3: MAC1 heavy chain



- Molecule 4: MAC1 light chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

NAG1
NAG2

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

Chain E:  20% 20% 60%

NAG1
NAG2
BMA3
MAN4
FUC5

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 75%

NAG1
NAG2
BMA3
MAN4

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.68Å 73.58Å 184.96Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.41 47.25 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.25-2.41) 99.9 (47.25-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.230 , 0.268 0.231 , 0.269	Depositor DCC
R_{free} test set	2454 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12240	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: FUC, MAN, NAG, BMA

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	0.11	0/1576	0.28	0/2127
2	B	0.11	0/1206	0.27	0/1627
3	H	0.14	0/1717	0.29	0/2343
4	L	0.11	0/1724	0.27	0/2337
All	All	0.12	0/6223	0.28	0/8434

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1538	1463	1462	19	0
2	B	1180	1120	1126	12	0
3	H	1671	1607	1614	10	0
4	L	1685	1628	1631	7	0
5	C	28	0	25	2	0
5	D	28	0	25	1	0
6	E	60	0	52	6	0
7	F	50	0	43	2	0
8	G	39	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	14	0	13	2	0
9	B	14	0	13	2	0
10	A	10	0	0	0	0
10	B	4	0	0	0	0
10	H	36	0	0	0	0
10	L	65	0	0	1	0
All	All	6422	5818	6038	54	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 (54) 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:86:ASN:ND2	1:A:103:GLY:O	2.19	0.76
1:A:87:GLU:N	1:A:87:GLU:OE2	2.23	0.70
8:G:2:NAG:H83	8:G:2:NAG:H3	1.72	0.69
2:B:339:LEU:HD23	2:B:339:LEU:O	1.92	0.69
5:C:1:NAG:H61	5:C:2:NAG:C7	2.30	0.61
2:B:374:TYR:OH	9:B:501:NAG:H81	2.00	0.61
1:A:201:ARG:HH12	8:G:1:NAG:H83	1.66	0.61
6:E:3:BMA:H2	6:E:4:MAN:H2	1.83	0.61
4:L:2:ILE:HD12	4:L:2:ILE:N	2.22	0.55
1:A:166:ASN:HD22	6:E:1:NAG:H83	1.75	0.52
4:L:135:PHE:C	4:L:136:LEU:HD12	2.35	0.51
4:L:93:THR:HG22	4:L:94:LEU:O	2.11	0.51
3:H:99:THR:O	3:H:99:THR:HG22	2.10	0.51
3:H:95:ASP:OD1	3:H:96:ASP:N	2.45	0.50
1:A:222:ASP:OD1	5:D:1:NAG:H3	2.11	0.49
2:B:265:PHE:CD2	2:B:265:PHE:N	2.80	0.49
3:H:18:VAL:HG12	3:H:82(C):LEU:HD11	1.94	0.49
4:L:150:ILE:HD11	4:L:179:LEU:HD21	1.95	0.48
1:A:66:LEU:HD23	1:A:66:LEU:O	2.13	0.48
4:L:155:ARG:NH2	10:L:304:HOH:O	2.46	0.48
3:H:177:LEU:C	3:H:177:LEU:HD12	2.39	0.47
1:A:71:GLN:OE1	9:B:501:NAG:H83	2.14	0.47
2:B:403:ARG:HA	2:B:406:TRP:CE2	2.50	0.47
1:A:98:PHE:HE2	9:A:301:NAG:H5	1.80	0.47
3:H:163:VAL:HG22	3:H:181:VAL:HG23	1.96	0.47
1:A:82:ALA:HB3	5:C:1:NAG:H83	1.97	0.47
1:A:183:ASP:OD2	7:F:2:NAG:H3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:3:BMA:H3	7:F:4:MAN:C5	2.45	0.47
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	1.97	0.46
1:A:86:ASN:OD1	1:A:140:ASP:OD2	2.33	0.46
2:B:305:ASN:O	2:B:305:ASN:ND2	2.49	0.46
1:A:184:ASP:OD2	1:A:184:ASP:N	2.49	0.46
4:L:123:GLU:OE1	4:L:123:GLU:N	2.44	0.46
6:E:1:NAG:O4	6:E:2:NAG:H83	2.16	0.46
1:A:133:GLY:O	1:A:167:LYS:NZ	2.41	0.45
2:B:391:ILE:HG21	8:G:1:NAG:H62	1.98	0.45
6:E:3:BMA:O2	6:E:4:MAN:C1	2.63	0.45
1:A:164:CYS:HA	1:A:174:ASN:O	2.16	0.45
6:E:3:BMA:O2	6:E:3:BMA:H61	2.16	0.45
2:B:312:PHE:CE2	2:B:316:LEU:HD11	2.53	0.44
4:L:4:MET:HE1	4:L:25:ALA:HB2	1.98	0.44
1:A:95:ASN:CG	9:A:301:NAG:H83	2.42	0.44
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.99	0.43
3:H:93:ALA:HB1	3:H:100(C):PHE:HB3	1.99	0.43
1:A:93:MET:HE1	1:A:202:GLY:O	2.18	0.43
2:B:313:CYS:SG	2:B:385:LEU:HD21	2.59	0.43
3:H:36:TRP:CE3	3:H:80:MET:HE2	2.54	0.42
2:B:413:LEU:O	2:B:417:MET:HG3	2.19	0.42
1:A:122:TYR:CG	3:H:100:ARG:HD3	2.54	0.42
2:B:380:THR:HG22	2:B:382:GLN:H	1.85	0.42
2:B:281:TYR:HD1	2:B:282:CYS:N	2.18	0.41
6:E:3:BMA:H2	6:E:4:MAN:C2	2.46	0.41
1:A:67:HIS:O	2:B:378:THR:OG1	2.33	0.41
1:A:143:TRP:HA	1:A:143:TRP:CE3	2.56	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	190/204 (93%)	175 (92%)	15 (8%)	0	100	100
2	B	137/204 (67%)	131 (96%)	6 (4%)	0	100	100
3	H	219/234 (94%)	214 (98%)	5 (2%)	0	100	100
4	L	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
All	All	761/859 (89%)	730 (96%)	31 (4%)	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	173/185 (94%)	173 (100%)	0	100	100
2	B	132/178 (74%)	132 (100%)	0	100	100
3	H	185/196 (94%)	184 (100%)	1 (0%)	86	94
4	L	195/195 (100%)	195 (100%)	0	100	100
All	All	685/754 (91%)	684 (100%)	1 (0%)	92	97

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

Mol	Chain	Res	Type
3	H	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	106	ASN
1	A	146	HIS
1	A	219	GLN
1	A	233	HIS
1	A	246	HIS

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Mol	Chain	Res	Type
2	B	305	ASN
2	B	398	ASN
2	B	426	GLN
3	H	3	GLN
3	H	50	GLN
3	H	133	ASN
3	H	171	GLN
3	H	191	GLN
4	L	77	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 ⓘ

16 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	C	1	1,5	14,14,15	0.75	0	17,19,21	0.91	0
5	NAG	C	2	5	14,14,15	0.70	0	17,19,21	0.90	0
5	NAG	D	1	1,5	14,14,15	0.74	0	17,19,21	1.41	2 (11%)
5	NAG	D	2	5	14,14,15	0.72	0	17,19,21	0.90	0
6	NAG	E	1	1,6	14,14,15	0.71	0	17,19,21	1.15	1 (5%)
6	NAG	E	2	6	14,14,15	0.76	0	17,19,21	0.78	0
6	BMA	E	3	6	11,11,12	0.89	1 (9%)	15,15,17	2.25	4 (26%)
6	MAN	E	4	6	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
6	FUC	E	5	6	10,10,11	0.85	0	14,14,16	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	F	1	1,7	14,14,15	0.74	0	17,19,21	0.90	0
7	NAG	F	2	7	14,14,15	0.73	0	17,19,21	0.86	1 (5%)
7	BMA	F	3	7	11,11,12	0.81	0	15,15,17	2.34	3 (20%)
7	MAN	F	4	7	11,11,12	0.64	0	15,15,17	1.44	1 (6%)
8	NAG	G	1	2,8	14,14,15	0.74	0	17,19,21	0.86	1 (5%)
8	NAG	G	2	8	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
8	BMA	G	3	8	11,11,12	0.83	0	15,15,17	2.03	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
5	NAG	C	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
6	MAN	E	4	6	-	2/2/19/22	0/1/1/1
6	FUC	E	5	6	-	-	0/1/1/1
7	NAG	F	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
7	MAN	F	4	7	-	0/2/19/22	0/1/1/1
8	NAG	G	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	G	2	8	-	3/6/23/26	0/1/1/1
8	BMA	G	3	8	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3	BMA	C2-C3	2.12	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3	BMA	C1-O5-C5	7.16	121.90	112.19
6	E	3	BMA	C1-O5-C5	6.43	120.90	112.19
8	G	3	BMA	C1-O5-C5	5.79	120.03	112.19
7	F	4	MAN	C1-O5-C5	4.57	118.39	112.19
5	D	1	NAG	C1-O5-C5	4.31	118.03	112.19
8	G	2	NAG	C2-N2-C7	3.36	127.68	122.90
6	E	1	NAG	C1-O5-C5	3.21	116.54	112.19
6	E	3	BMA	O2-C2-C3	3.06	116.27	110.14
6	E	4	MAN	C1-O5-C5	2.83	116.03	112.19
7	F	3	BMA	C3-C4-C5	2.69	115.03	110.24
8	G	3	BMA	C3-C4-C5	2.69	115.03	110.24
7	F	2	NAG	O5-C1-C2	-2.56	107.24	111.29
8	G	1	NAG	O5-C1-C2	-2.35	107.57	111.29
5	D	1	NAG	C3-C4-C5	-2.29	106.15	110.24
6	E	3	BMA	C3-C4-C5	2.28	114.30	110.24
8	G	3	BMA	O4-C4-C3	-2.14	105.41	110.35
7	F	3	BMA	O4-C4-C3	-2.08	105.55	110.35
6	E	3	BMA	O4-C4-C3	-2.01	105.69	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

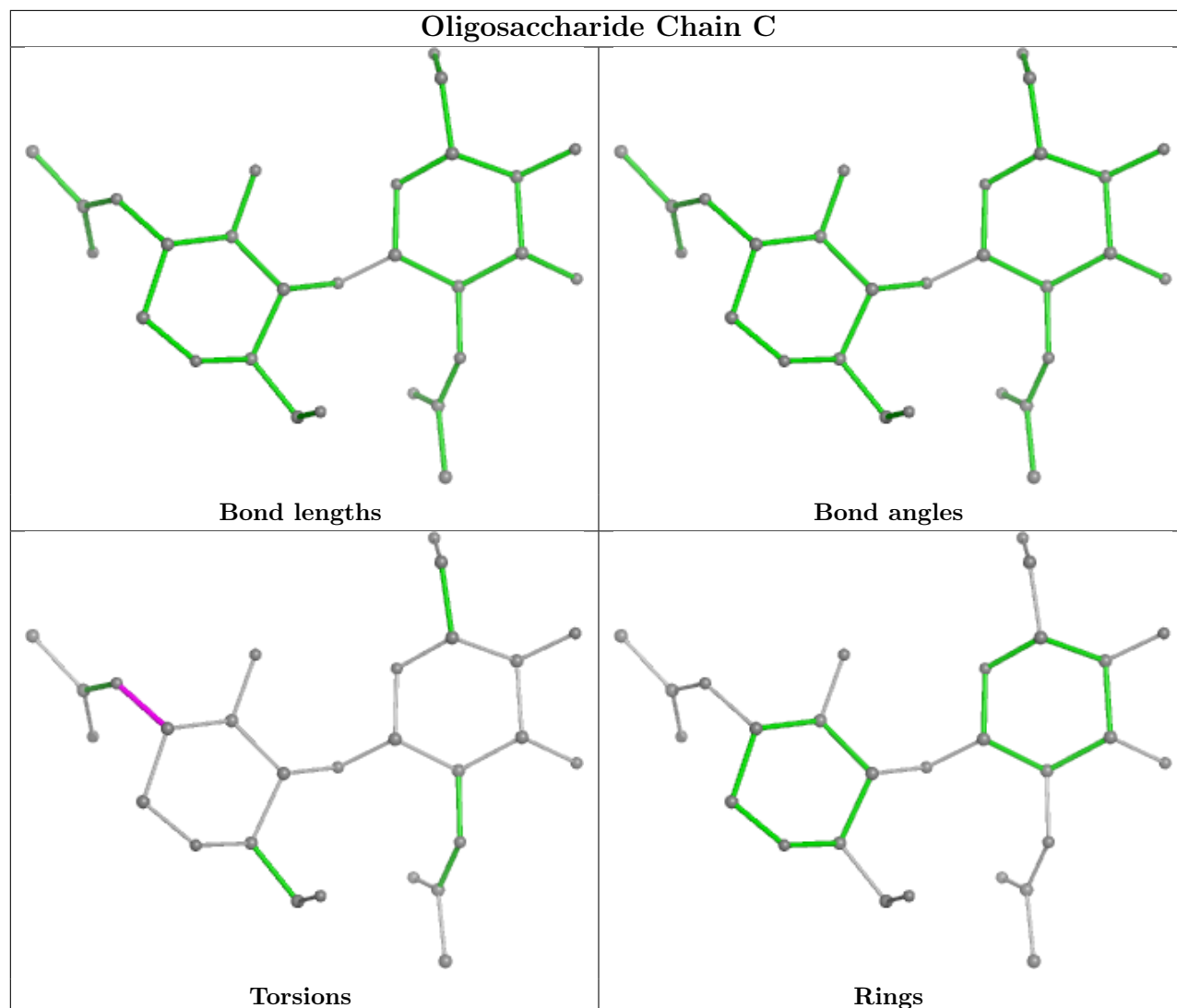
Mol	Chain	Res	Type	Atoms
6	E	4	MAN	O5-C5-C6-O6
6	E	1	NAG	C8-C7-N2-C2
6	E	1	NAG	O7-C7-N2-C2
6	E	2	NAG	C8-C7-N2-C2
6	E	2	NAG	O7-C7-N2-C2
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
8	G	1	NAG	C8-C7-N2-C2
8	G	1	NAG	O7-C7-N2-C2
8	G	2	NAG	C8-C7-N2-C2
8	G	2	NAG	O7-C7-N2-C2
6	E	4	MAN	C4-C5-C6-O6
5	C	1	NAG	C1-C2-N2-C7
8	G	2	NAG	C3-C2-N2-C7
7	F	2	NAG	O5-C5-C6-O6

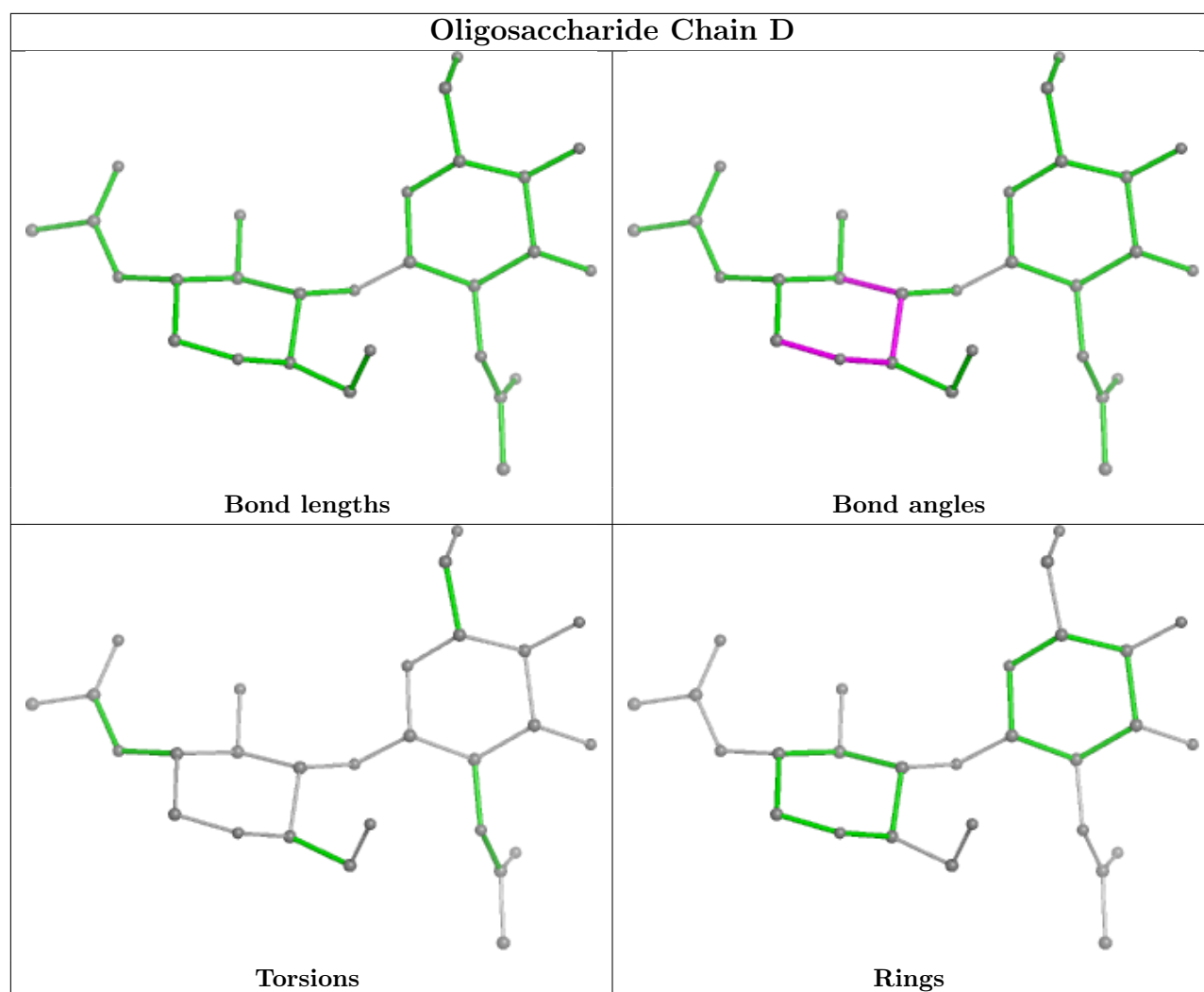
There are no ring outliers.

12 monomers are involved in 14 short contacts:

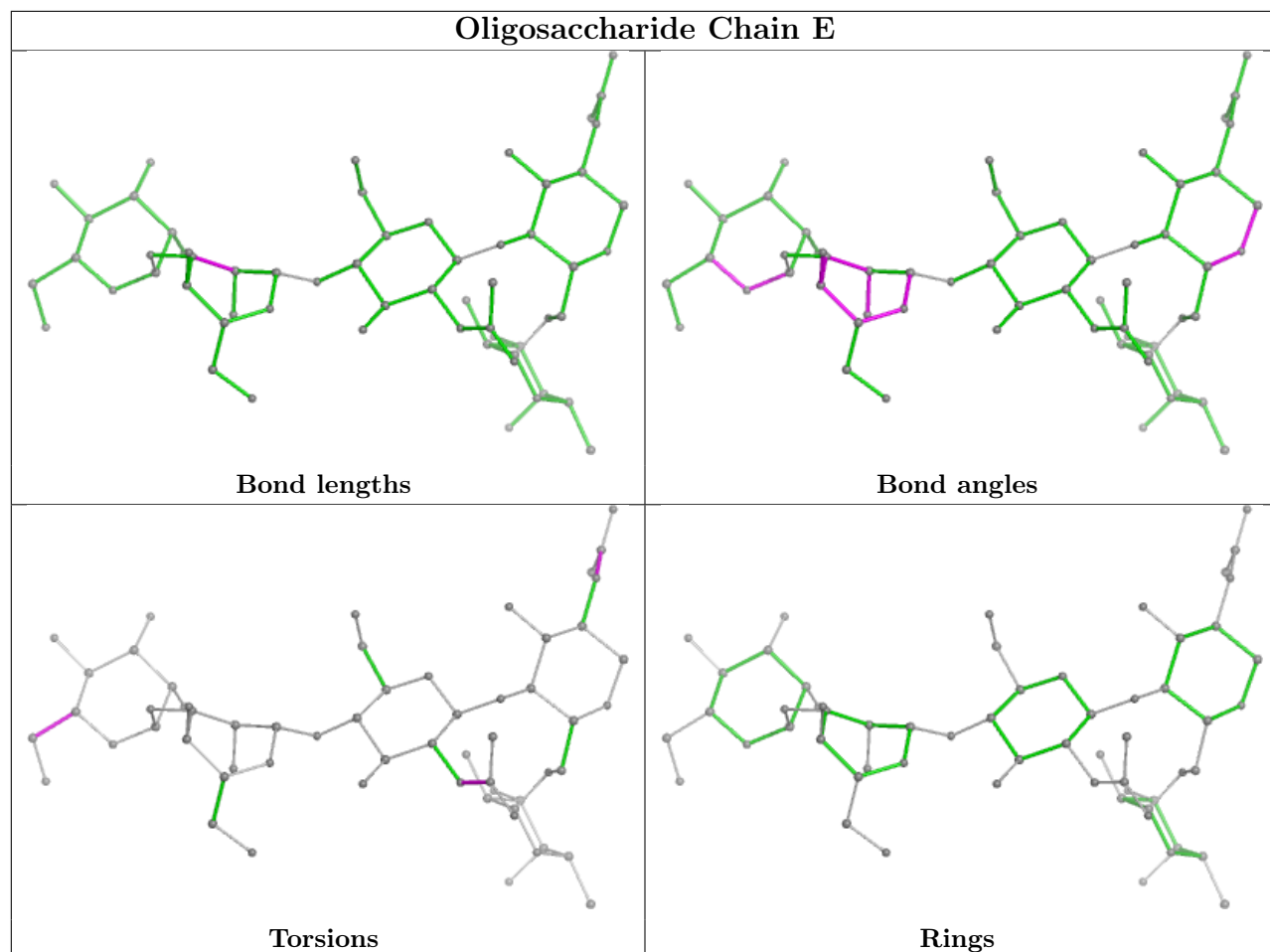
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	4	MAN	3	0
5	C	1	NAG	2	0
8	G	2	NAG	1	0
7	F	2	NAG	1	0
6	E	2	NAG	1	0
7	F	4	MAN	1	0
5	D	1	NAG	1	0
8	G	1	NAG	2	0
7	F	3	BMA	1	0
6	E	1	NAG	2	0
6	E	3	BMA	4	0
5	C	2	NAG	1	0

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

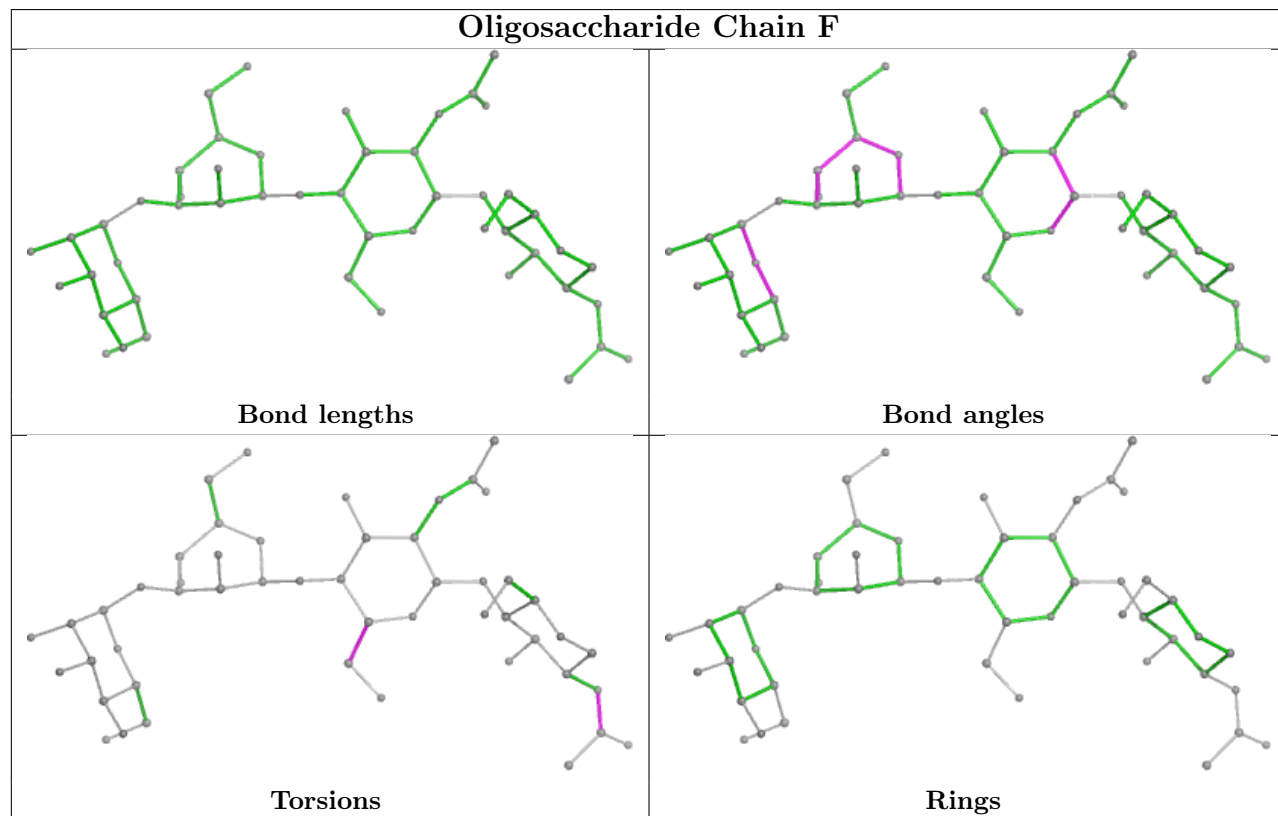


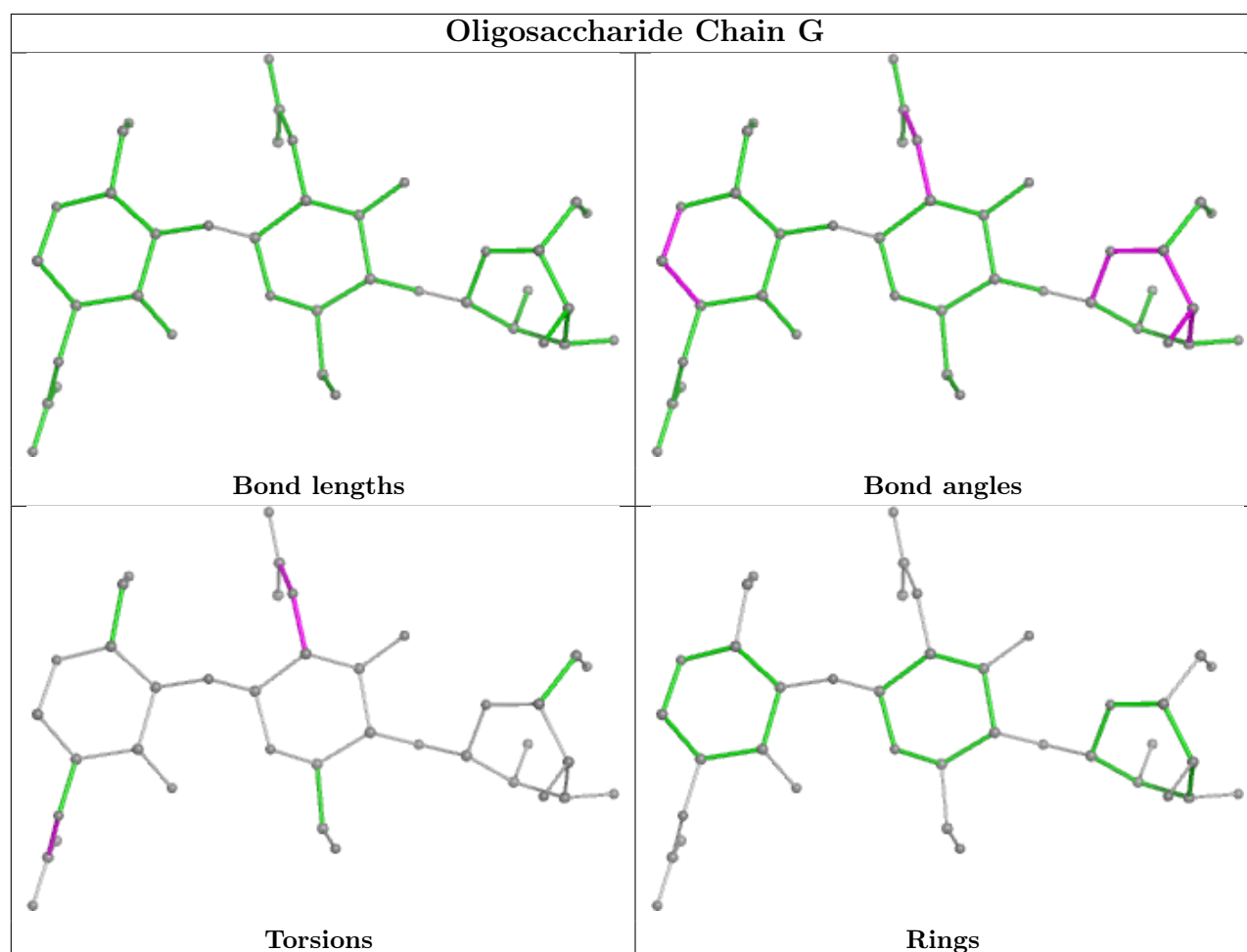


Oligosaccharide Chain E



Oligosaccharide Chain F





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	B	501	2	14,14,15	0.70	0	17,19,21	0.90	0
9	NAG	A	301	1	14,14,15	0.73	0	17,19,21	1.25	2 (11%)

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
9	NAG	B	501	2	-	2/6/23/26	0/1/1/1
9	NAG	A	301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	301	NAG	C1-O5-C5	-3.19	107.87	112.19
9	A	301	NAG	O5-C1-C2	-2.00	108.12	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

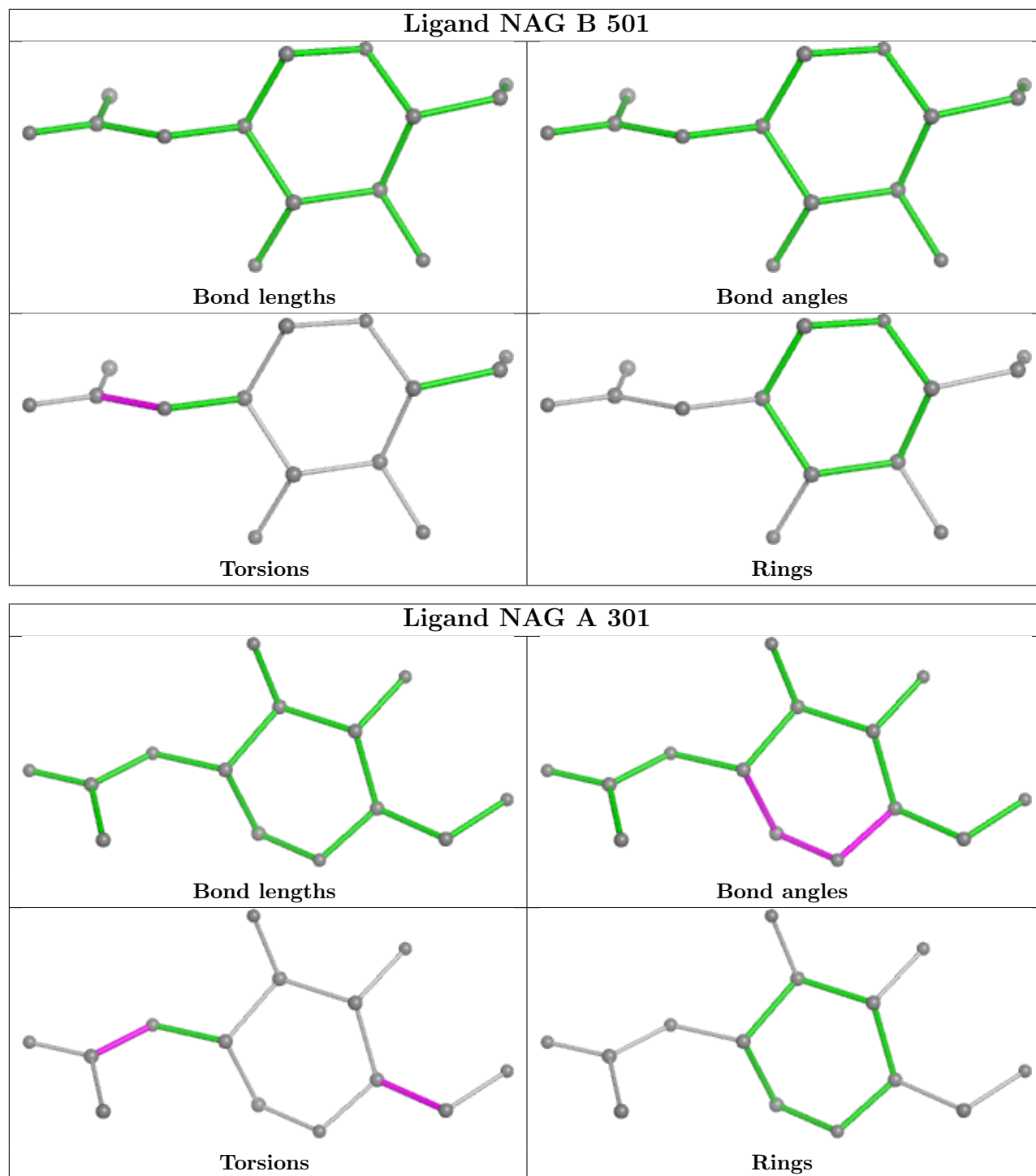
Mol	Chain	Res	Type	Atoms
9	A	301	NAG	C8-C7-N2-C2
9	A	301	NAG	O7-C7-N2-C2
9	B	501	NAG	C8-C7-N2-C2
9	B	501	NAG	O7-C7-N2-C2
9	A	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	NAG	2	0
9	A	301	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	192/204 (94%)	0.75	19 (9%) 14 13	62, 78, 112, 126	0
2	B	143/204 (70%)	0.98	21 (14%) 7 6	65, 89, 123, 157	0
3	H	221/234 (94%)	0.17	10 (4%) 39 36	43, 59, 83, 130	0
4	L	215/217 (99%)	0.04	4 (1%) 66 63	28, 57, 78, 115	2 (0%)
All	All	771/859 (89%)	0.43	54 (7%) 24 22	28, 69, 112, 157	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	GLY	5.6
2	B	427	GLY	5.4
2	B	265	PHE	5.1
2	B	270	THR	5.0
4	L	214	CYS	5.0
2	B	325	ALA	4.9
1	A	143	TRP	4.3
2	B	337	ILE	4.0
2	B	379	LEU	4.0
2	B	290	ALA	3.9
3	H	127	SER	3.9
3	H	128	ALA	3.8
1	A	226	PHE	3.7
3	H	130	ALA	3.6
2	B	339	LEU	3.6
4	L	67	PHE	3.6
1	A	86	ASN	3.4
1	A	138	ALA	3.3
2	B	412	HIS	3.2
4	L	7	THR	3.2
3	H	129	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	H	132	THR	3.1
2	B	422	TYR	3.0
1	A	100	TYR	2.9
1	A	248	LEU	2.8
1	A	232	ASN	2.8
4	L	53[A]	ARG	2.8
1	A	157	LEU	2.7
2	B	308	HIS	2.6
2	B	336	GLU	2.6
1	A	137	ASN	2.5
1	A	97	SER	2.5
1	A	190	LYS	2.5
1	A	231	VAL	2.4
1	A	228	TYR	2.4
2	B	410	SER	2.4
2	B	406	TRP	2.3
2	B	416	GLU	2.3
1	A	67	HIS	2.3
3	H	98	GLY	2.3
3	H	214	ASP	2.2
2	B	338	ASN	2.2
2	B	281	TYR	2.2
3	H	131	GLN	2.2
3	H	133	ASN	2.1
1	A	235	SER	2.1
1	A	147	TRP	2.1
2	B	423	ALA	2.1
3	H	99	THR	2.1
2	B	426	GLN	2.1
1	A	233	HIS	2.1
2	B	425	ARG	2.1
1	A	227	GLU	2.1
2	B	387	ARG	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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

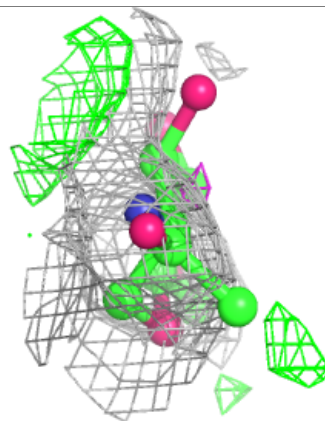
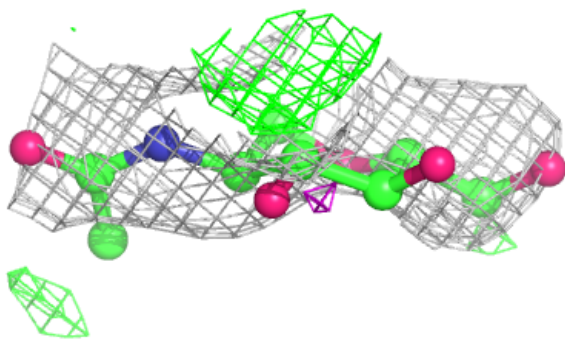
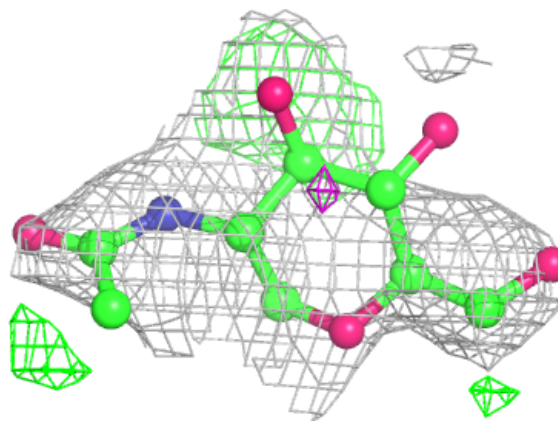
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	301	14/15	0.45	0.25	102,110,115,118	0
9	NAG	B	501	14/15	0.76	0.16	88,101,104,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

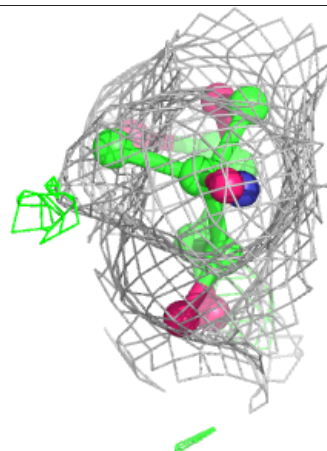
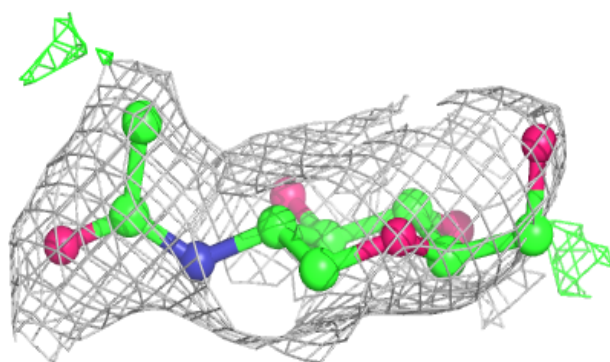
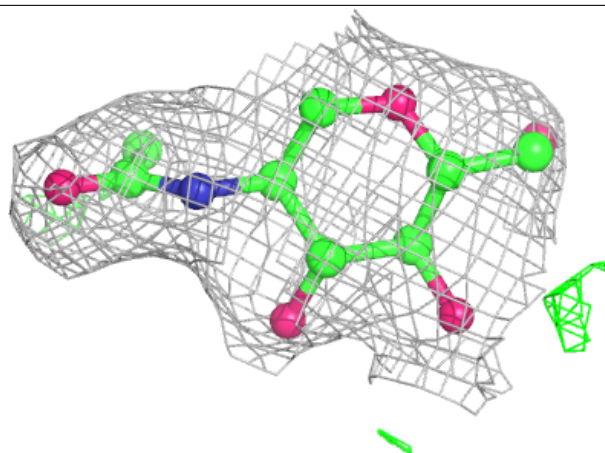
Electron density around NAG A 301:

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 NAG B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.