Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:02 PM EDT

PDB ID	:	4C53
Title	:	Crystal Structure of Guanarito virus GP2 in the post-fusion conformation
Authors	:	Parsy, M.; Huiskonen, J.T.; Harlos, K.; Bowden, T.A.
Deposited on	:	2013-09-10
Resolution	:	4.14 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 (i) 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 (i)) were used in the production of this report:

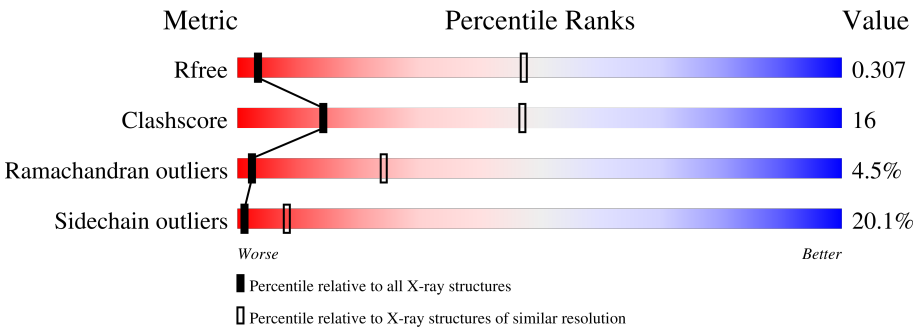
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.14 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}	130704	1018 (4.52-3.76)
Clashscore	141614	1041 (4.50-3.78)
Ramachandran outliers	138981	1036 (4.52-3.76)
Sidechain outliers	138945	1022 (4.52-3.76)

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%

Mol	Chain	Length	Quality of chain
1	A	138	38% 26% 8% • 27%
1	B	138	43% 30% 9% • 17%
1	C	138	43% 26% • 26%
2	D	3	33% 67%
3	E	2	100%
4	F	7	57% 29% 14%
4	G	7	57% 29% 14%

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Mol	Chain	Length	Quality of chain
4	H	7	71% 29%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3007 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 PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	837	533	143	154	7	0	0	0
1	B	115	959	607	164	181	7	0	0	0
1	C	102	853	547	142	157	7	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	THR	-	expression tag	UNP A1A3Z2
A	291	GLY	-	expression tag	UNP A1A3Z2
A	419	GLY	-	expression tag	UNP A1A3Z2
A	420	THR	-	expression tag	UNP A1A3Z2
A	421	LYS	-	expression tag	UNP A1A3Z2
A	422	HIS	-	expression tag	UNP A1A3Z2
A	423	HIS	-	expression tag	UNP A1A3Z2
A	424	HIS	-	expression tag	UNP A1A3Z2
A	425	HIS	-	expression tag	UNP A1A3Z2
A	426	HIS	-	expression tag	UNP A1A3Z2
A	427	HIS	-	expression tag	UNP A1A3Z2
B	290	THR	-	expression tag	UNP A1A3Z2
B	291	GLY	-	expression tag	UNP A1A3Z2
B	419	GLY	-	expression tag	UNP A1A3Z2
B	420	THR	-	expression tag	UNP A1A3Z2
B	421	LYS	-	expression tag	UNP A1A3Z2
B	422	HIS	-	expression tag	UNP A1A3Z2
B	423	HIS	-	expression tag	UNP A1A3Z2
B	424	HIS	-	expression tag	UNP A1A3Z2
B	425	HIS	-	expression tag	UNP A1A3Z2
B	426	HIS	-	expression tag	UNP A1A3Z2
B	427	HIS	-	expression tag	UNP A1A3Z2
C	290	THR	-	expression tag	UNP A1A3Z2

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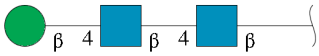
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	GLY	-	expression tag	UNP A1A3Z2
C	419	GLY	-	expression tag	UNP A1A3Z2
C	420	THR	-	expression tag	UNP A1A3Z2
C	421	LYS	-	expression tag	UNP A1A3Z2
C	422	HIS	-	expression tag	UNP A1A3Z2
C	423	HIS	-	expression tag	UNP A1A3Z2
C	424	HIS	-	expression tag	UNP A1A3Z2
C	425	HIS	-	expression tag	UNP A1A3Z2
C	426	HIS	-	expression tag	UNP A1A3Z2
C	427	HIS	-	expression tag	UNP A1A3Z2

- Molecule 2 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.

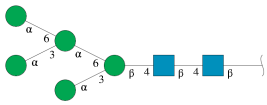


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	39	22	2	15	0	0	0

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

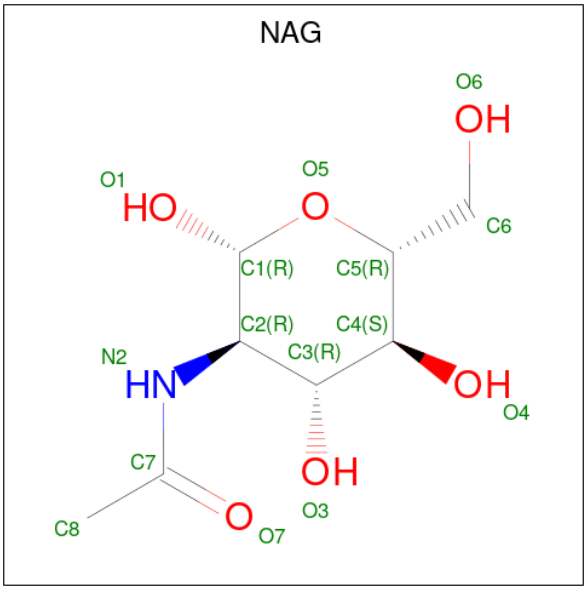
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
			Total	C	N	O			
4	F	7	83	46	2	35	0	0	0
			Total	C	N	O			
4	G	7	83	46	2	35	0	0	0
			Total	C	N	O			
4	H	7	83	46	2	35	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



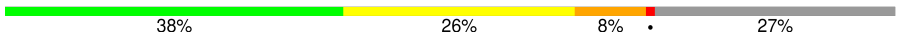
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

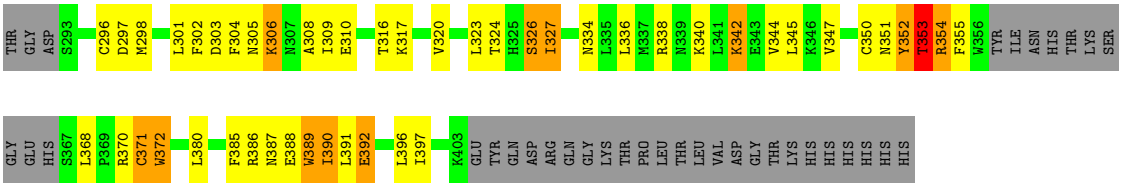
3 Residue-property plots (i)

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. 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. 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

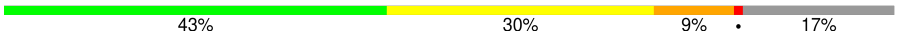
Chain A:

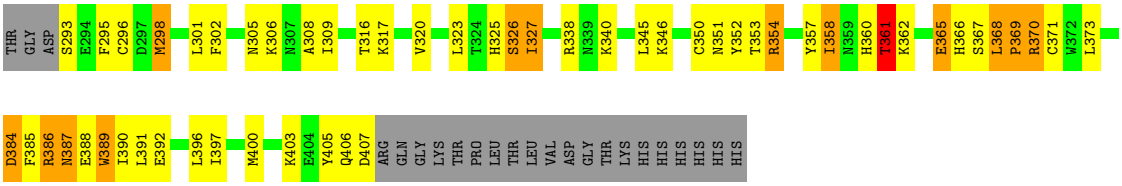




• Molecule 1: PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX

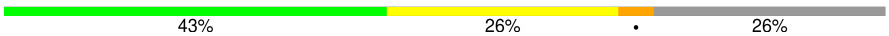
Chain B:

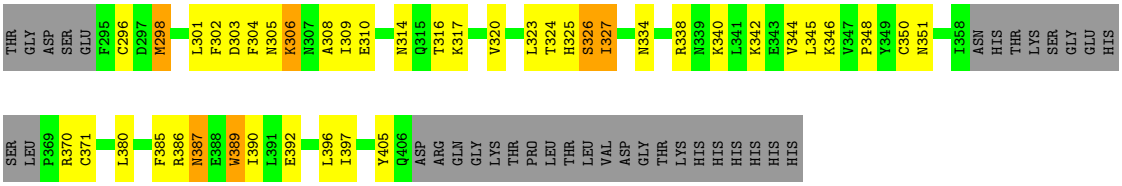




• Molecule 1: PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX

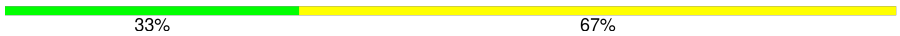
Chain C:





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

Chain D:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1
NAG2

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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: 57% 29% 14%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 G: 57% 29% 14%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 H: 71% 29%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	98.50Å 98.50Å 78.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.44 – 4.14 38.44 – 4.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.44-4.14) 99.6 (38.44-4.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 4.13Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.255 , 0.276 0.281 , 0.307	Depositor DCC
R_{free} test set	259 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å^2)	192.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 179.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.061 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3007	wwPDB-VP
Average B, all atoms (Å^2)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.50	0/853	0.81	1/1150 (0.1%)
1	B	0.53	0/980	0.85	0/1323
1	C	0.50	0/871	0.77	0/1175
All	All	0.51	0/2704	0.81	1/3648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	ASN	C-N-CA	5.12	134.50	121.70

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	837	0	823	35	0
1	B	959	0	928	36	0
1	C	853	0	833	34	0
2	D	39	0	34	0	0
3	E	28	0	25	0	0
4	F	83	0	70	2	0
4	G	83	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	83	0	70	8	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
All	All	3007	0	2892	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 16.

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:B:323:LEU:O	1:B:327:ILE:HG22	1.75	0.86
1:C:323:LEU:O	1:C:327:ILE:HG22	1.79	0.82
1:A:323:LEU:O	1:A:327:ILE:HG22	1.79	0.80
1:C:350:CYS:HG	1:C:371:CYS:HG	0.81	0.80
1:A:303:ASP:HA	1:A:306:LYS:HG2	1.69	0.74
1:A:308:ALA:HB2	1:B:389:TRP:HB3	1.70	0.73
1:B:301:LEU:HD23	1:C:396:LEU:HD23	1.70	0.72
1:A:327:ILE:HD11	1:C:326:SER:HB3	1.70	0.72
1:B:350:CYS:HG	1:B:371:CYS:HG	0.74	0.72
1:C:387:ASN:HA	1:C:390:ILE:HD13	1.72	0.72
1:B:326:SER:HB3	1:C:327:ILE:HD11	1.73	0.71
1:A:301:LEU:HD23	1:B:396:LEU:HD23	1.74	0.70
1:A:326:SER:HB3	1:B:327:ILE:HD11	1.72	0.70
1:A:389:TRP:HB3	1:C:308:ALA:HB2	1.75	0.69
1:B:358:ILE:HG21	1:B:373:LEU:HD13	1.75	0.68
1:A:310:GLU:HG2	1:A:390:ILE:HG13	1.76	0.66
4:H:4:MAN:O4	4:H:6:MAN:H5	1.98	0.63
1:A:396:LEU:HD23	1:C:301:LEU:HD23	1.80	0.63
1:B:351:ASN:O	1:B:353:THR:N	2.31	0.62
1:A:302:PHE:CD2	1:C:301:LEU:HB3	2.35	0.61
4:H:3:BMA:H2	4:H:7:MAN:H5	1.82	0.61
1:A:327:ILE:CD1	1:C:326:SER:HB3	2.31	0.61
1:B:301:LEU:HB3	1:C:302:PHE:CD2	2.37	0.60
1:B:302:PHE:HE1	1:B:397:ILE:HD11	1.66	0.60
4:G:2:NAG:H62	4:G:3:BMA:C1	2.32	0.60
1:B:308:ALA:HB2	1:C:389:TRP:HB3	1.85	0.59
1:A:302:PHE:HE1	1:A:397:ILE:HD11	1.68	0.58
1:C:338:ARG:HG2	1:C:345:LEU:HD21	1.85	0.58
4:F:2:NAG:H62	4:F:3:BMA:C1	2.33	0.57
1:B:316:THR:O	1:B:320:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HG21	1:B:373:LEU:CD1	2.34	0.57
1:C:302:PHE:HE1	1:C:397:ILE:HD11	1.69	0.57
1:A:350:CYS:HG	1:A:371:CYS:CB	2.18	0.56
1:B:298:MET:SD	1:C:298:MET:HB3	2.46	0.55
1:C:324:THR:HG23	1:C:380:LEU:HB2	1.88	0.55
1:A:347:VAL:HG11	1:A:372:TRP:CZ3	2.42	0.55
1:C:316:THR:O	1:C:320:VAL:HG23	2.05	0.54
1:B:305:ASN:O	1:B:309:ILE:HG13	2.08	0.54
1:B:338:ARG:HG2	1:B:345:LEU:HD21	1.89	0.54
1:A:301:LEU:HD11	1:B:400:MET:HG3	1.90	0.53
1:A:316:THR:O	1:A:320:VAL:HG23	2.08	0.53
1:C:314:ASN:OD1	4:H:1:NAG:H83	2.08	0.53
1:B:370:ARG:HG3	1:B:371:CYS:SG	2.49	0.53
1:A:305:ASN:O	1:A:309:ILE:HG13	2.09	0.52
1:C:306:LYS:O	1:C:310:GLU:HG3	2.09	0.52
1:C:303:ASP:HA	1:C:306:LYS:HG2	1.91	0.52
1:A:323:LEU:HD11	1:B:320:VAL:HG13	1.92	0.52
1:A:388:GLU:O	1:A:391:LEU:HG	2.10	0.51
1:A:303:ASP:O	1:A:306:LYS:HG3	2.11	0.51
1:B:293:SER:C	1:B:295:PHE:H	2.13	0.51
1:B:317:LYS:HE3	1:B:385:PHE:H	1.76	0.51
1:C:305:ASN:O	1:C:309:ILE:HG13	2.11	0.50
1:B:357:TYR:O	1:B:361:THR:HG22	2.11	0.50
1:A:301:LEU:HB3	1:B:302:PHE:CD2	2.47	0.49
1:A:387:ASN:HB3	1:A:390:ILE:HD12	1.93	0.49
1:A:324:THR:HG23	1:A:380:LEU:HB2	1.94	0.49
1:B:354:ARG:HH21	1:B:370:ARG:CZ	2.26	0.49
1:A:338:ARG:HD3	1:A:372:TRP:CE2	2.48	0.48
1:A:297:ASP:HB3	1:B:400:MET:SD	2.53	0.48
1:A:320:VAL:HG13	1:C:323:LEU:HD11	1.96	0.48
1:B:350:CYS:HB3	1:B:354:ARG:HB3	1.96	0.47
1:B:301:LEU:CD2	1:C:396:LEU:HD23	2.41	0.47
4:H:4:MAN:O4	4:H:5:MAN:H3	2.15	0.46
1:A:396:LEU:HD23	1:C:301:LEU:CD2	2.45	0.46
1:A:326:SER:HB3	1:B:327:ILE:CD1	2.43	0.46
1:B:386:ARG:C	1:B:388:GLU:H	2.18	0.46
1:C:350:CYS:HG	1:C:371:CYS:CB	2.27	0.46
4:H:4:MAN:H3	4:H:5:MAN:H2	1.65	0.46
1:B:326:SER:HB3	1:C:327:ILE:CD1	2.43	0.45
1:C:317:LYS:HG3	1:C:385:PHE:HD1	1.80	0.45
1:C:317:LYS:HE3	1:C:385:PHE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLU:HG2	1:C:390:ILE:CG2	2.46	0.45
1:A:392:GLU:HB3	1:C:304:PHE:CE2	2.51	0.45
4:H:3:BMA:H4	4:H:5:MAN:H2	1.98	0.45
1:A:304:PHE:CE2	1:B:392:GLU:HB3	2.51	0.45
1:A:353:THR:HG22	1:A:354:ARG:HD2	1.98	0.45
1:C:303:ASP:O	1:C:306:LYS:HG3	2.17	0.45
1:C:348:PRO:HG2	1:C:370:ARG:HH21	1.81	0.44
4:H:4:MAN:O4	4:H:6:MAN:H3	2.18	0.44
1:B:317:LYS:HE3	1:B:384:ASP:HA	2.00	0.43
4:G:2:NAG:C6	4:G:3:BMA:C1	2.96	0.43
4:F:2:NAG:C6	4:F:3:BMA:C1	2.97	0.42
1:A:306:LYS:HD2	1:A:397:ILE:HD11	2.01	0.42
1:A:342:LYS:O	1:A:342:LYS:HG3	2.19	0.41
1:A:336:LEU:HD13	1:B:369:PRO:HB3	2.02	0.41
1:A:317:LYS:HE3	1:A:385:PHE:H	1.85	0.41
4:H:1:NAG:O3	4:H:2:NAG:C1	2.68	0.41
1:B:350:CYS:HG	1:B:371:CYS:CB	2.27	0.41
1:C:310:GLU:HG2	1:C:390:ILE:HG23	2.03	0.41
1:B:323:LEU:HD11	1:C:320:VAL:HG13	2.03	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	97/138 (70%)	91 (94%)	3 (3%)	3 (3%)	4 31
1	B	113/138 (82%)	98 (87%)	5 (4%)	10 (9%)	1 12
1	C	98/138 (71%)	92 (94%)	5 (5%)	1 (1%)	15 53
All	All	308/414 (74%)	281 (91%)	13 (4%)	14 (4%)	2 24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	THR
1	A	371	CYS
1	B	352	TYR
1	B	365	GLU
1	B	367	SER
1	B	369	PRO
1	B	405	TYR
1	B	406	GLN
1	A	352	TYR
1	B	361	THR
1	B	362	LYS
1	B	387	ASN
1	C	351	ASN
1	B	368	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	96/130 (74%)	75 (78%)	21 (22%)	1 6
1	B	110/130 (85%)	86 (78%)	24 (22%)	1 6
1	C	97/130 (75%)	81 (84%)	16 (16%)	2 14
All	All	303/390 (78%)	242 (80%)	61 (20%)	1 8

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	CYS
1	A	298	MET
1	A	306	LYS
1	A	326	SER
1	A	327	ILE
1	A	334	ASN
1	A	340	LYS
1	A	342	LYS
1	A	344	VAL

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Mol	Chain	Res	Type
1	A	345	LEU
1	A	352	TYR
1	A	353	THR
1	A	354	ARG
1	A	355	PHE
1	A	368	LEU
1	A	370	ARG
1	A	372	TRP
1	A	386	ARG
1	A	389	TRP
1	A	390	ILE
1	A	392	GLU
1	B	296	CYS
1	B	298	MET
1	B	306	LYS
1	B	325	HIS
1	B	326	SER
1	B	327	ILE
1	B	340	LYS
1	B	346	LYS
1	B	354	ARG
1	B	358	ILE
1	B	360	HIS
1	B	361	THR
1	B	365	GLU
1	B	366	HIS
1	B	368	LEU
1	B	370	ARG
1	B	384	ASP
1	B	386	ARG
1	B	387	ASN
1	B	389	TRP
1	B	390	ILE
1	B	391	LEU
1	B	403	LYS
1	B	407	ASP
1	C	296	CYS
1	C	298	MET
1	C	306	LYS
1	C	325	HIS
1	C	326	SER
1	C	327	ILE

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Mol	Chain	Res	Type
1	C	334	ASN
1	C	340	LYS
1	C	342	LYS
1	C	344	VAL
1	C	346	LYS
1	C	386	ARG
1	C	387	ASN
1	C	389	TRP
1	C	392	GLU
1	C	405	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	C	339	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

26 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	D	1	1,2	14,14,15	0.69	0	17,19,21	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	2	2	14,14,15	0.88	0	17,19,21	1.01	2 (11%)
2	BMA	D	3	2	11,11,12	0.72	0	15,15,17	0.74	0
3	NAG	E	1	1,3	14,14,15	0.81	0	17,19,21	1.26	3 (17%)
3	NAG	E	2	3	14,14,15	0.68	0	17,19,21	1.01	2 (11%)
4	NAG	F	1	1,4	14,14,15	0.69	0	17,19,21	1.29	2 (11%)
4	NAG	F	2	4	14,14,15	0.76	0	17,19,21	1.07	1 (5%)
4	BMA	F	3	4	11,11,12	0.55	0	15,15,17	0.72	0
4	MAN	F	4	4	11,11,12	0.71	0	15,15,17	0.70	0
4	MAN	F	5	4	11,11,12	0.59	0	15,15,17	0.74	0
4	MAN	F	6	4	11,11,12	0.65	0	15,15,17	0.68	0
4	MAN	F	7	4	11,11,12	0.51	0	15,15,17	0.73	0
4	NAG	G	1	1,4	14,14,15	0.77	0	17,19,21	1.34	2 (11%)
4	NAG	G	2	4	14,14,15	0.79	0	17,19,21	1.10	1 (5%)
4	BMA	G	3	4	11,11,12	0.55	0	15,15,17	0.79	0
4	MAN	G	4	4	11,11,12	0.65	0	15,15,17	0.82	0
4	MAN	G	5	4	11,11,12	0.60	0	15,15,17	0.73	0
4	MAN	G	6	4	11,11,12	0.67	0	15,15,17	0.70	0
4	MAN	G	7	4	11,11,12	0.50	0	15,15,17	0.72	0
4	NAG	H	1	1,4	14,14,15	0.77	0	17,19,21	1.34	2 (11%)
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	1.09	3 (17%)
4	BMA	H	3	4	11,11,12	0.77	0	15,15,17	0.63	0
4	MAN	H	4	4	11,11,12	0.72	0	15,15,17	0.83	0
4	MAN	H	5	4	11,11,12	0.72	0	15,15,17	0.57	0
4	MAN	H	6	4	11,11,12	0.73	0	15,15,17	0.64	0
4	MAN	H	7	4	11,11,12	0.55	0	15,15,17	0.65	0

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	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	NAG	C8-C7-N2	3.36	121.69	116.12
3	E	1	NAG	C8-C7-N2	3.11	121.27	116.12
4	G	1	NAG	C8-C7-N2	2.95	121.01	116.12
4	F	1	NAG	C8-C7-N2	2.81	120.78	116.12
2	D	1	NAG	C8-C7-N2	2.80	120.77	116.12
4	H	1	NAG	C4-C3-C2	-2.73	107.02	111.02
4	F	1	NAG	C4-C3-C2	-2.55	107.29	111.02
3	E	1	NAG	C1-O5-C5	-2.46	108.89	112.19
4	H	2	NAG	C4-C3-C2	-2.36	107.56	111.02
2	D	2	NAG	C8-C7-N2	2.33	119.99	116.12
4	G	1	NAG	C4-C3-C2	-2.30	107.64	111.02
4	G	2	NAG	C8-C7-N2	2.26	119.86	116.12
4	F	2	NAG	C8-C7-N2	2.25	119.85	116.12
4	H	2	NAG	C8-C7-N2	2.16	119.70	116.12
3	E	2	NAG	C8-C7-N2	2.16	119.69	116.12
3	E	2	NAG	C4-C3-C2	-2.13	107.89	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C1-O5-C5	-2.11	109.36	112.19
2	D	2	NAG	C4-C3-C2	-2.09	107.95	111.02
3	E	1	NAG	C4-C3-C2	-2.05	108.02	111.02

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
4	H	5	MAN	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	5	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C1-C2-N2-C7

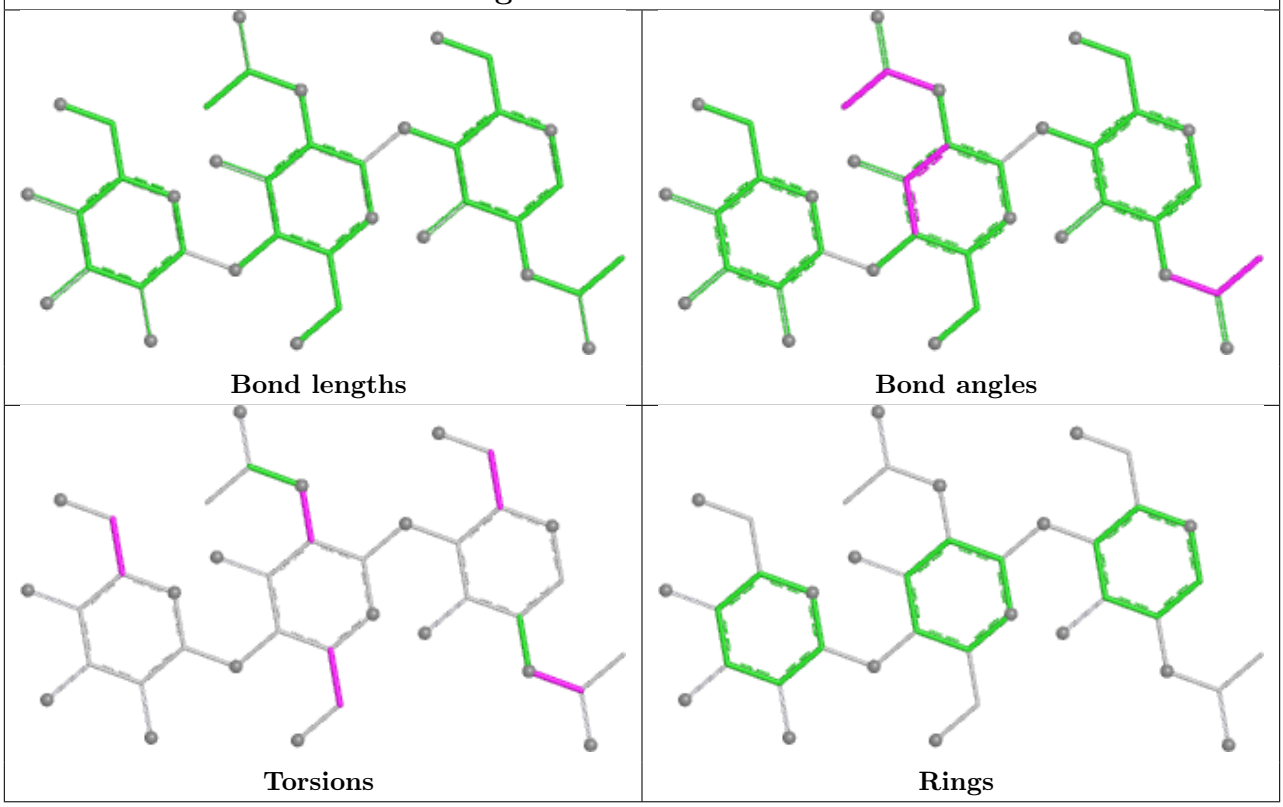
There are no ring outliers.

11 monomers are involved in 12 short contacts:

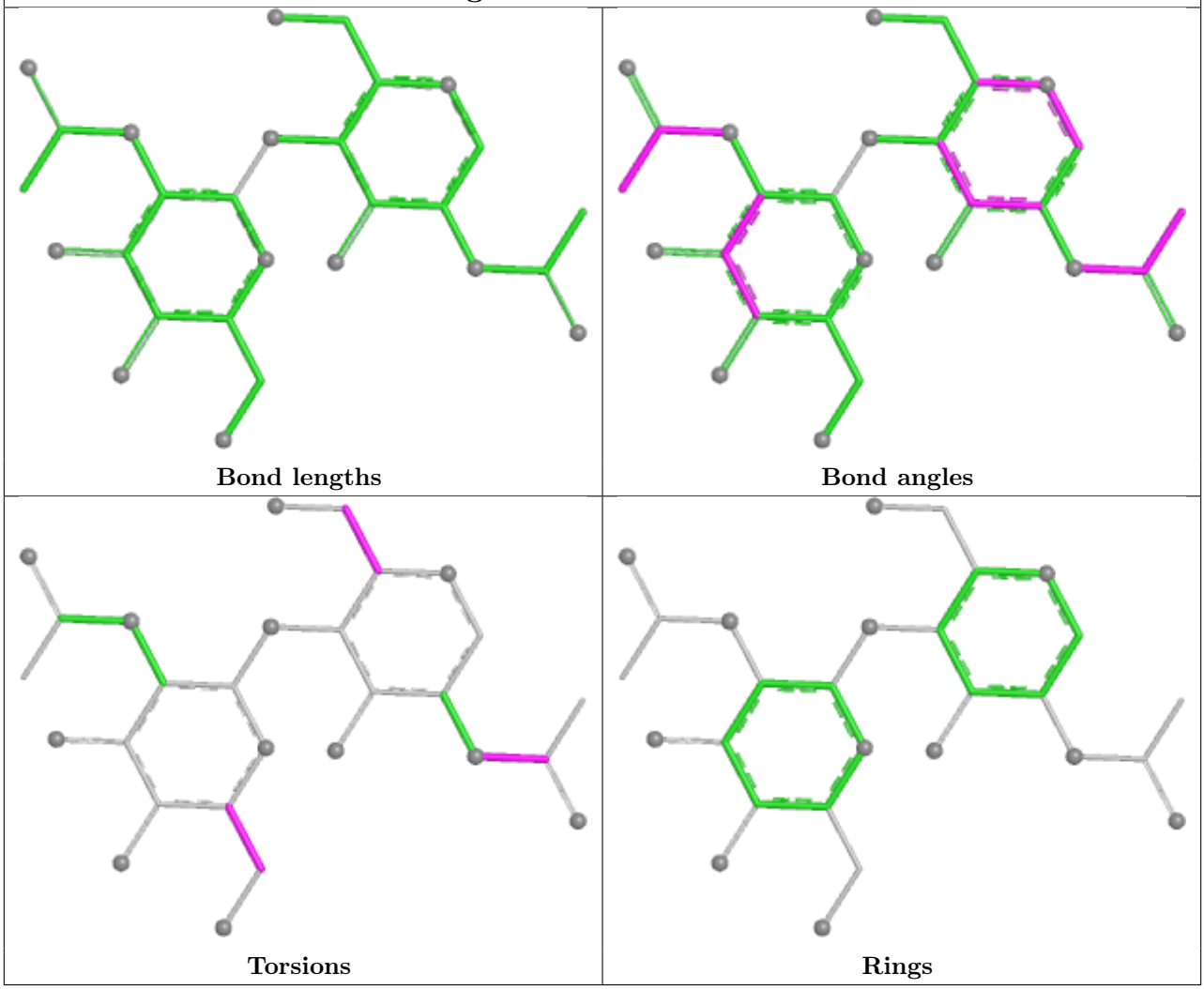
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
4	H	4	MAN	4	0
4	H	1	NAG	2	0
4	H	6	MAN	2	0
4	G	3	BMA	2	0
4	H	5	MAN	3	0
4	H	7	MAN	1	0
4	H	3	BMA	2	0
4	F	3	BMA	2	0
4	F	2	NAG	2	0
4	H	2	NAG	1	0

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

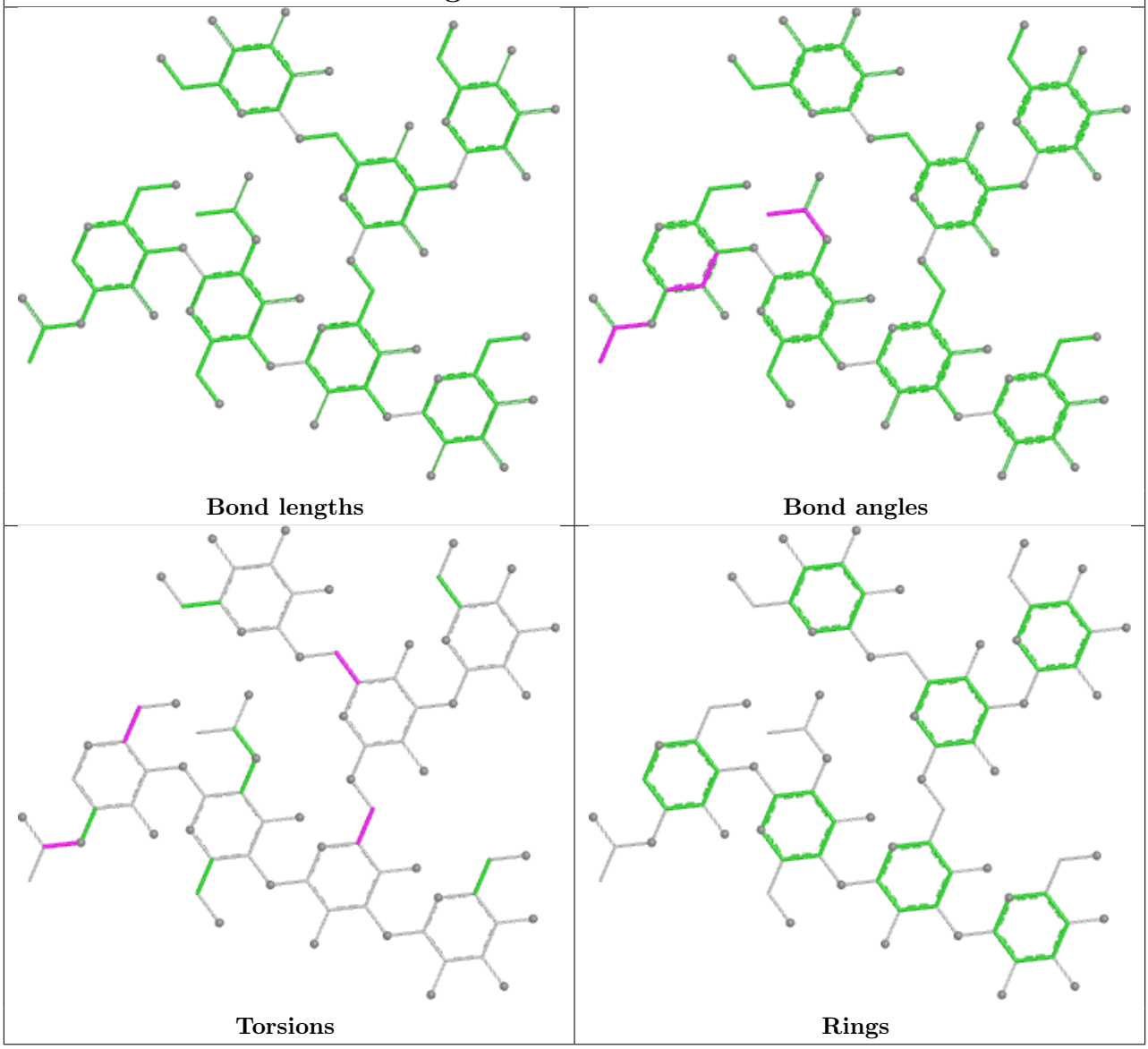
Oligosaccharide Chain D



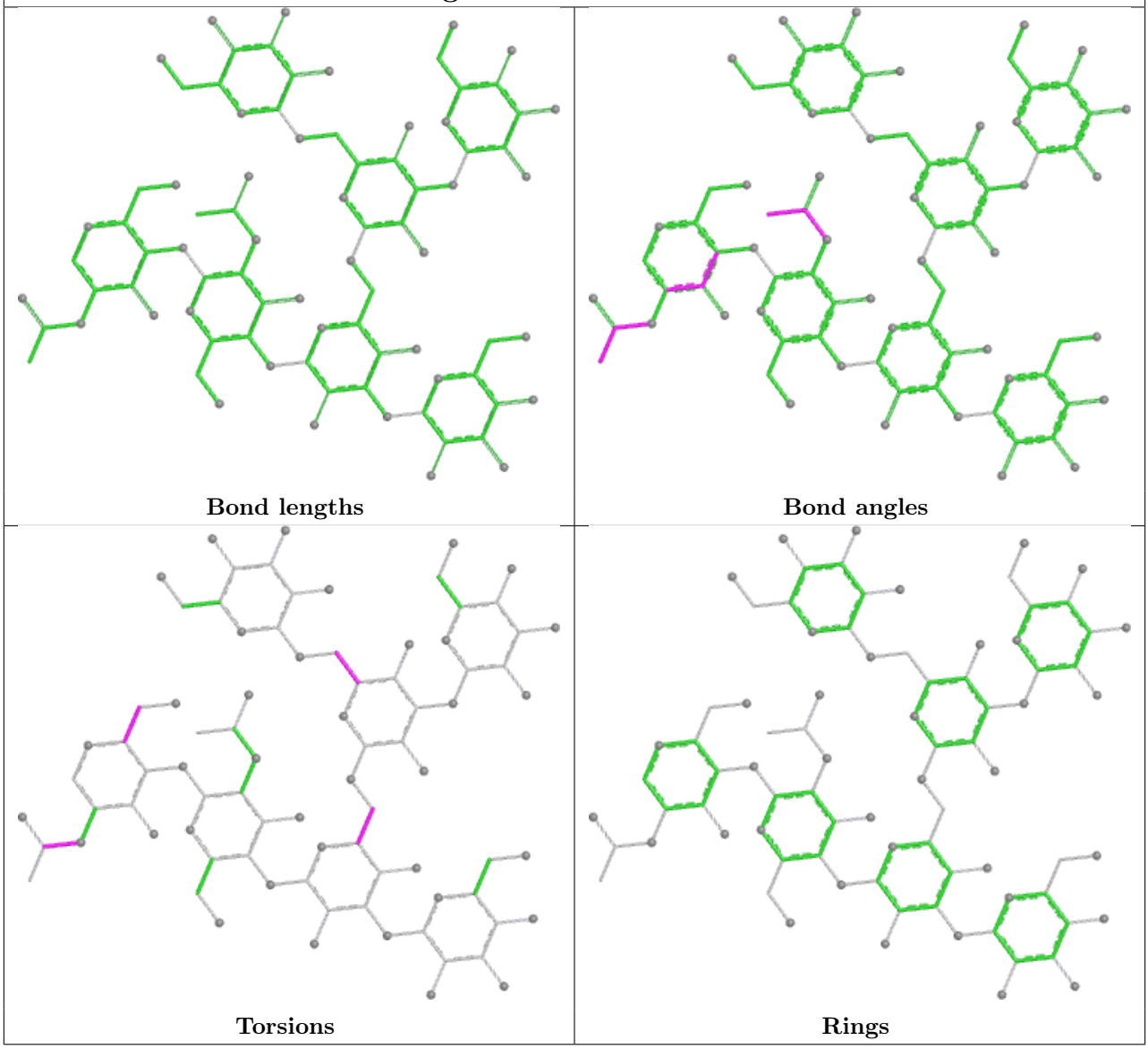
Oligosaccharide Chain E



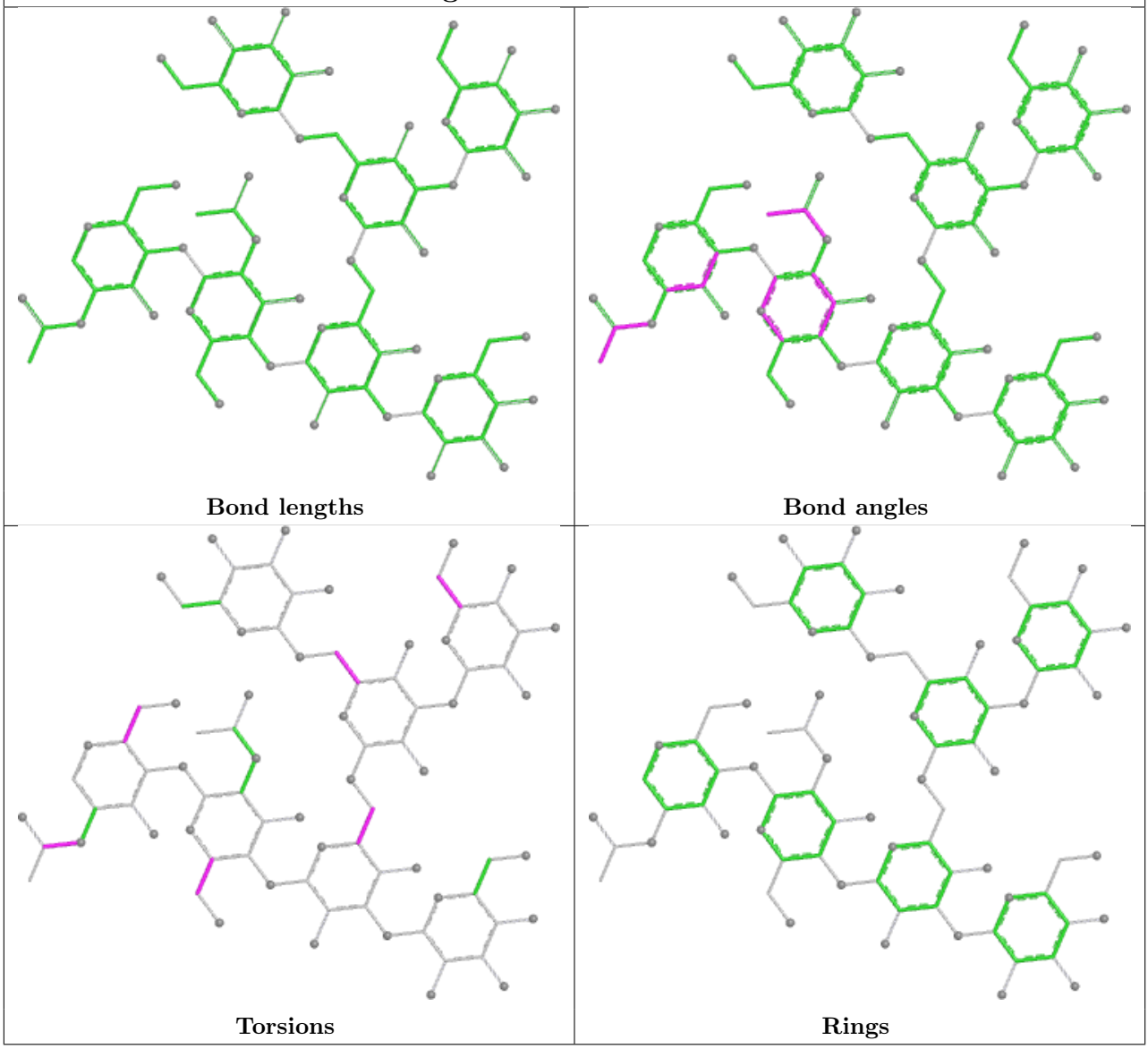
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1407	1	14,14,15	0.81	0	17,19,21	1.18	2 (11%)
5	NAG	A	1408	1	14,14,15	0.69	0	17,19,21	1.32	3 (17%)
5	NAG	B	1417	1	14,14,15	0.79	0	17,19,21	1.19	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
5	NAG	A	1407	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1417	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1417	NAG	C8-C7-N2	2.98	121.07	116.12
5	A	1408	NAG	C8-C7-N2	2.90	120.93	116.12
5	A	1407	NAG	C8-C7-N2	2.86	120.85	116.12
5	A	1408	NAG	C4-C3-C2	-2.41	107.49	111.02
5	B	1417	NAG	C4-C3-C2	-2.37	107.55	111.02
5	A	1407	NAG	C4-C3-C2	-2.34	107.58	111.02
5	A	1408	NAG	C2-N2-C7	-2.24	119.90	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1407	NAG	C4-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1417	NAG	C4-C5-C6-O6
5	A	1407	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1417	NAG	O5-C5-C6-O6
5	A	1407	NAG	C8-C7-N2-C2
5	A	1407	NAG	O7-C7-N2-C2
5	A	1408	NAG	C8-C7-N2-C2
5	A	1408	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	1417	NAG	C8-C7-N2-C2
5	B	1417	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

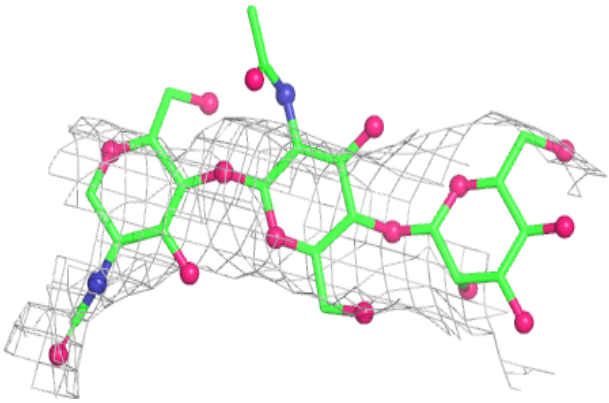
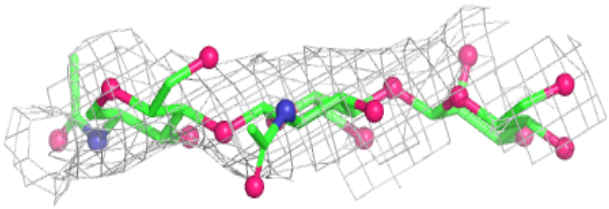
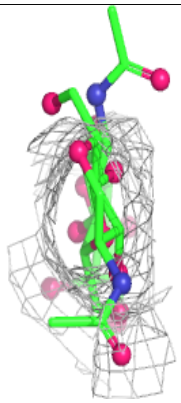
Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

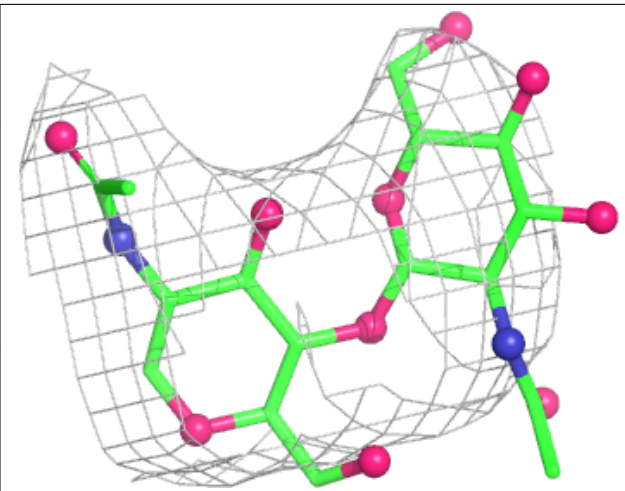
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

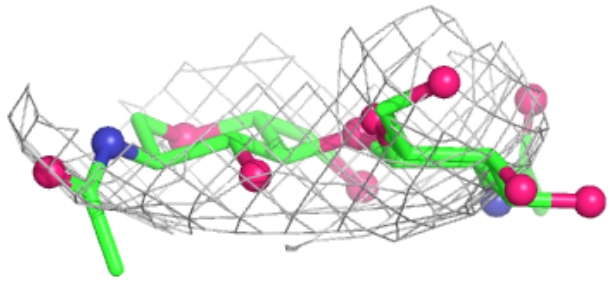
<table>
<tr><td>Electron density around Chain D:

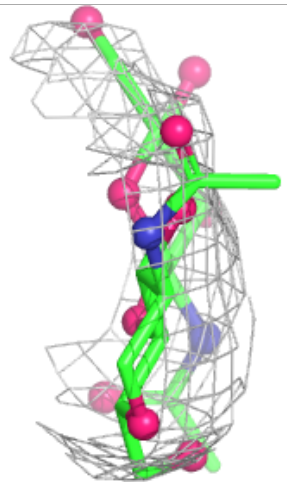
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)</td><td>  </td></tr>
<tr><td>  </td><td>  </td></tr>
</table>

Electron density around Chain E:

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

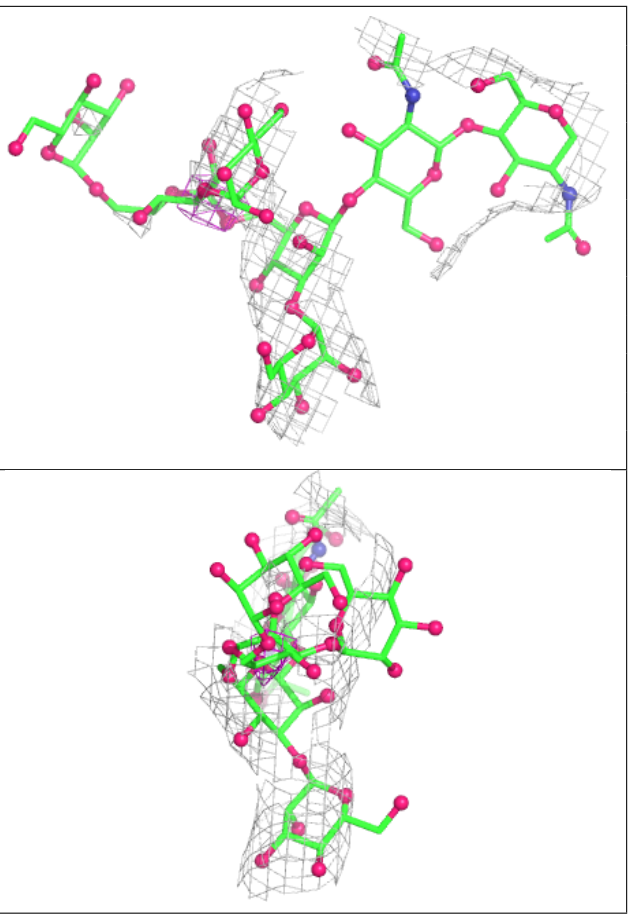






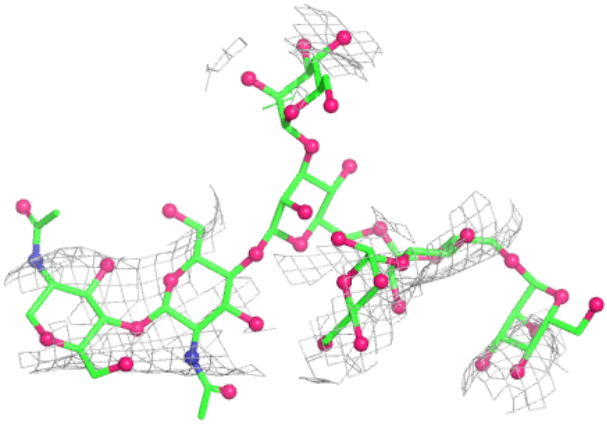
Electron density around Chain F:

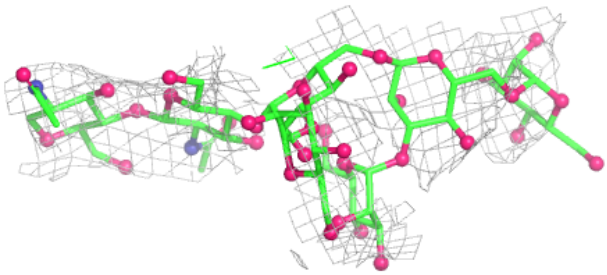
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

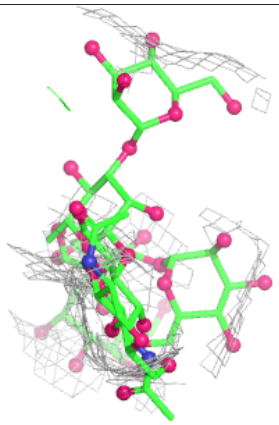


Electron density around Chain G:

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

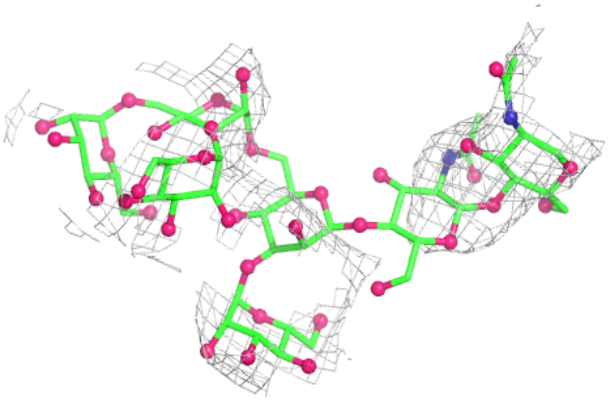


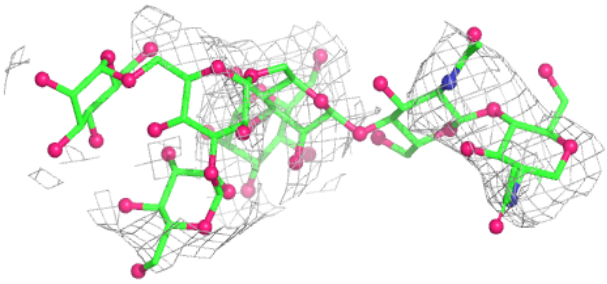


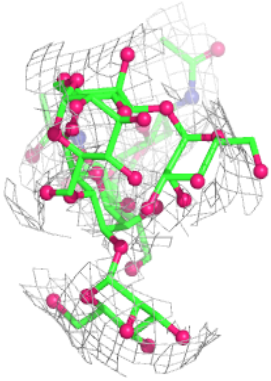


Electron density around Chain H:

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







6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.