



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 03:48 PM BST

PDB ID : 5W6D
Title : Crystal structure of BG505-SOSIP.v4.1-GT1-N137A in complex with Fabs 35022 and 9H/109L
Authors : Garces, F.; Stanfield, R.L.; Wilson, I.A.
Deposited on : 2017-06-16
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

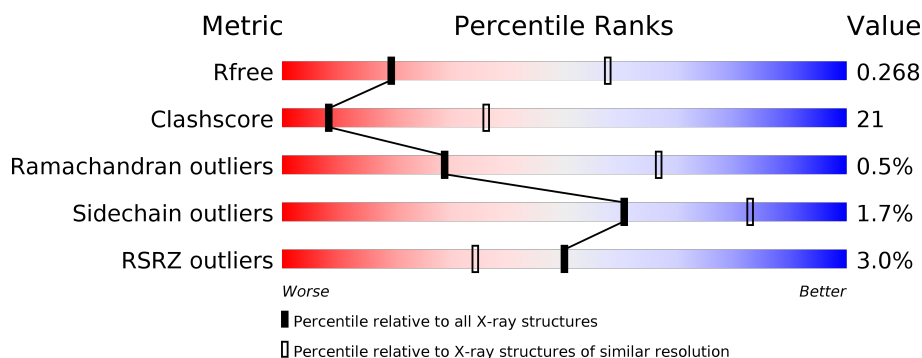
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	G	474	<div> <div>8%</div> <div>51%</div> <div>42%</div> <div>6%</div> </div>
2	B	153	<div> <div>56%</div> <div>28%</div> <div>16%</div> </div>
3	L	218	<div> <div>68%</div> <div>28%</div> </div>
4	H	236	<div> <div>55%</div> <div>40%</div> </div>
5	D	240	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>7%</div> </div>
6	E	216	<div> <div>9%</div> <div>76%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
7	A	10	
8	C	7	
9	F	8	
10	I	4	
11	J	2	
11	K	2	
11	N	2	
12	M	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BMA	I	3	-	-	-	X
10	MAN	I	4	-	-	-	X
7	NAG	A	1	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 11729 atoms, of which 1 is hydrogen 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 BG505-SOSIP.v4.1-GT1-N137A gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	447	Total	C	N	O	S	0	0	0
			3523	2218	622	656	27			

- Molecule 2 is a protein called BG505-SOSIP.v4.1-GT1-N137A gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			1030	655	176	193	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called 109L FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1603	1007	276	315	5			

- Molecule 4 is a protein called 9H FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	231	Total	C	N	O	S	0	0	0
			1744	1106	290	343	5			

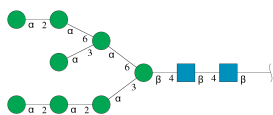
- Molecule 5 is a protein called 35022 FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	223	Total	C	N	O	S	0	0	0
			1691	1078	283	323	7			

- Molecule 6 is a protein called 35022 FAB light chain.

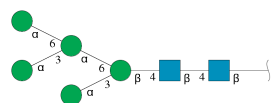
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



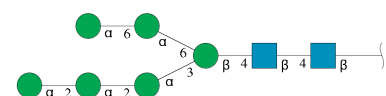
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	10	Total	C	N	O		0	0	0
			116	64	2	50				

- Molecule 8 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
8	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



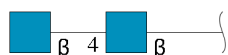
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 10 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.



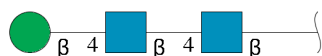
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	4	Total	C	H	N	O	0	0	0
			51	28	1	2	20			

- Molecule 11 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
11	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
11	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
11	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

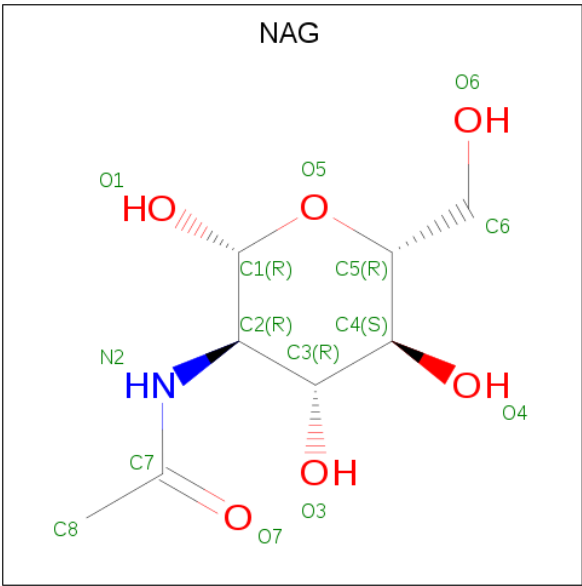
- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: C₈H₁₅NO₆).

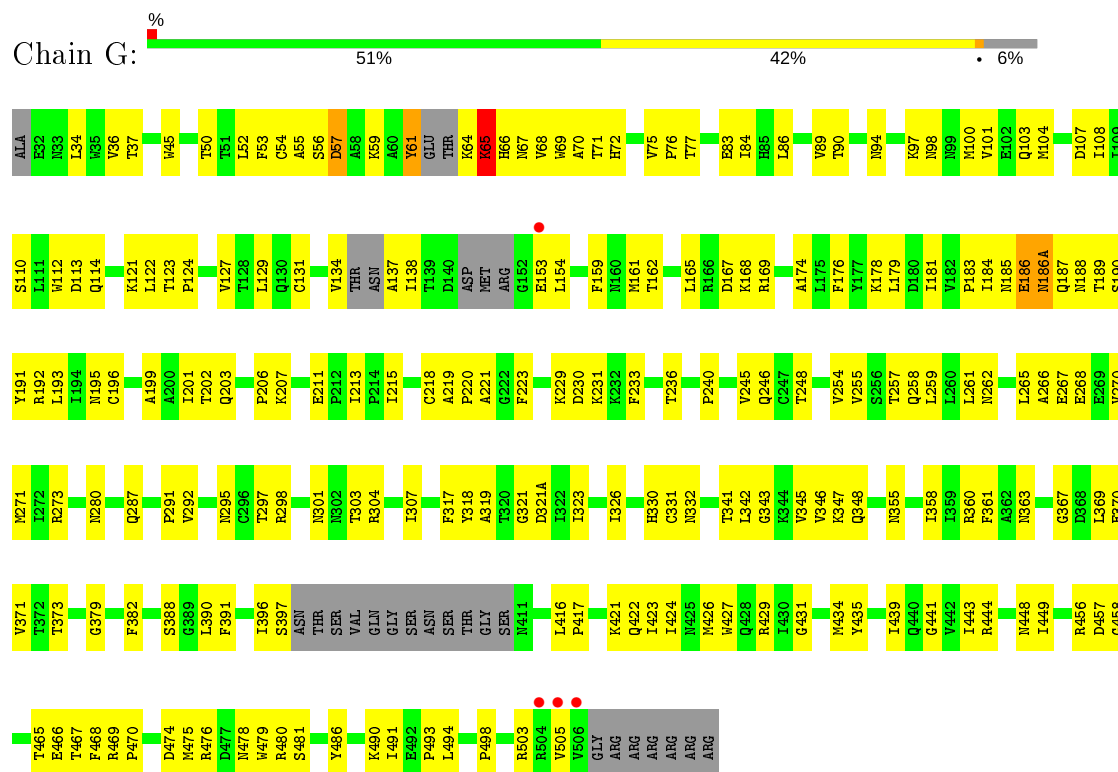


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	G	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		

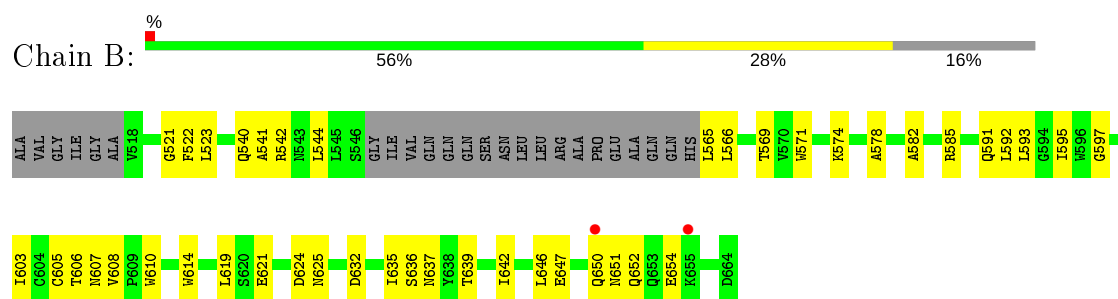
3 Residue-property plots

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: BG505-SOSIP.v4.1-GT1-N137A gp120

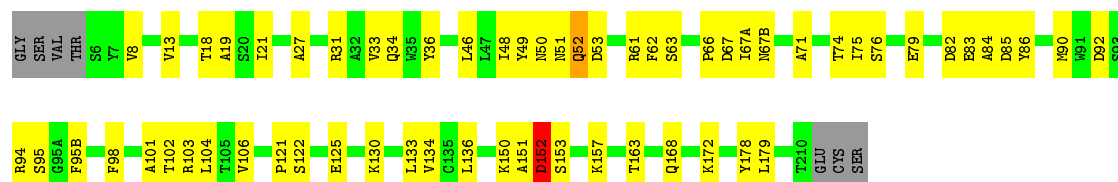


- Molecule 2: BG505-SOSIP.v4.1-GT1-N137A gp41



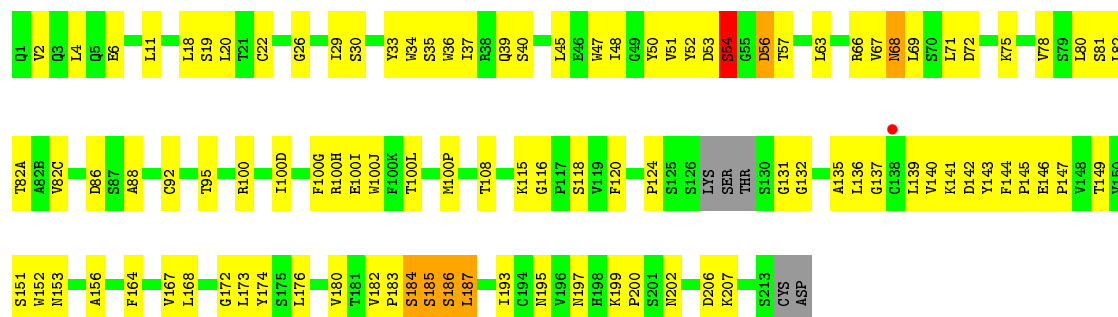
- Molecule 3: 109L FAB light chain





• Molecule 4: 9H FAB heavy chain

Chain H: 55% 40%



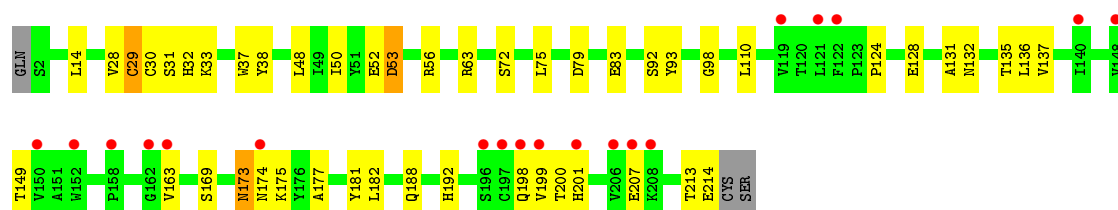
• Molecule 5: 35022 FAB heavy chain

Chain D: 8% 71% 22% 7%



• Molecule 6: 35022 FAB light chain

Chain E: 9% 76% 21%



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  60% 40%




- Molecule 8: 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 C:  14% 71% 14%



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  13% 63% 25%



- Molecule 10: 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 I:  50% 25% 25%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%


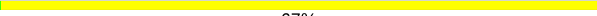


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33%  67%

MAG1
MAG2
BOL3

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	126.95Å 126.95Å 315.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.43 – 3.20 49.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.43-3.20) 100.0 (49.43-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.242 , 0.267 0.242 , 0.268	Depositor DCC
R_{free} test set	2417 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.074 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11729	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: BMA, NAG, 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	G	0.31	0/3598	0.47	0/4885
2	B	0.23	0/1048	0.41	0/1421
3	L	0.34	0/1646	0.47	0/2247
4	H	0.32	0/1790	0.52	1/2447 (0.0%)
5	D	0.25	0/1736	0.45	0/2366
6	E	0.30	0/1659	0.50	1/2269 (0.0%)
All	All	0.30	0/11477	0.47	2/15635 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	54	SER	N-CA-C	7.55	131.40	111.00
6	E	29	CYS	CA-CB-SG	-6.01	103.19	114.00

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	G	3523	0	3466	219	0
2	B	1030	0	1020	59	2
3	L	1603	0	1541	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1744	0	1691	108	0
5	D	1691	0	1661	37	0
6	E	1615	0	1544	38	0
7	A	116	0	97	14	0
8	C	83	0	70	6	0
9	F	94	0	79	5	0
10	I	50	1	43	6	0
11	J	28	0	25	2	0
11	K	28	0	25	0	0
11	N	28	0	25	0	0
12	M	39	0	34	1	0
13	B	14	0	13	6	0
13	G	42	0	39	1	0
All	All	11728	1	11373	488	2

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 21.

The worst 5 of 488 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:G:61:TYR:CD1	1:G:65:LYS:HB3	1.85	1.11
4:H:132:GLY:C	4:H:184:SER:HG	1.57	1.08
4:H:132:GLY:O	4:H:184:SER:OG	1.72	1.04
4:H:132:GLY:O	4:H:184:SER:N	1.89	1.04
4:H:132:GLY:CA	4:H:184:SER:OG	2.08	1.02

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:541:ALA:O	2:B:591:GLN:NE2[2_655]	2.09	0.11
2:B:542:ARG:NH1	2:B:647:GLU:OE1[2_655]	2.12	0.08

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	G	437/474 (92%)	398 (91%)	37 (8%)	2 (0%)	29	67
2	B	125/153 (82%)	118 (94%)	7 (6%)	0	100	100
3	L	209/218 (96%)	198 (95%)	9 (4%)	2 (1%)	15	54
4	H	227/236 (96%)	213 (94%)	12 (5%)	2 (1%)	17	56
5	D	219/240 (91%)	217 (99%)	2 (1%)	0	100	100
6	E	211/216 (98%)	205 (97%)	5 (2%)	1 (0%)	29	67
All	All	1428/1537 (93%)	1349 (94%)	72 (5%)	7 (0%)	29	67

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	65	LYS
3	L	84	ALA
3	L	152	ASP
4	H	185	SER
4	H	186	SER

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	G	398/421 (94%)	390 (98%)	8 (2%)	55	80
2	B	112/129 (87%)	111 (99%)	1 (1%)	78	91
3	L	175/181 (97%)	172 (98%)	3 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	197/204 (97%)	190 (96%)	7 (4%)	35	69
5	D	187/203 (92%)	186 (100%)	1 (0%)	88	95
6	E	186/189 (98%)	185 (100%)	1 (0%)	88	95
All	All	1255/1327 (95%)	1234 (98%)	21 (2%)	60	83

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	52	GLN
3	L	152	ASP
4	H	187	LEU
2	B	603	ILE
4	H	202	ASN

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

Mol	Chain	Res	Type
1	G	67	ASN
1	G	185	ASN
3	L	52	GLN
5	D	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

38 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	$\# Z > 2$
7	NAG	A	1	1,7	14,14,15	0.28	0	17,19,21	1.48	3 (17%)
7	MAN	A	10	7	11,11,12	0.77	0	15,15,17	0.99	1 (6%)
7	NAG	A	2	7	14,14,15	0.56	0	17,19,21	0.52	0
7	BMA	A	3	7	11,11,12	0.50	0	15,15,17	1.09	1 (6%)
7	MAN	A	4	7	11,11,12	0.61	0	15,15,17	1.13	2 (13%)
7	MAN	A	5	7	11,11,12	0.69	0	15,15,17	0.91	0
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	0.95	2 (13%)
7	MAN	A	7	7	11,11,12	0.71	0	15,15,17	0.95	2 (13%)
7	MAN	A	8	7	11,11,12	0.88	1 (9%)	15,15,17	1.02	1 (6%)
7	MAN	A	9	7	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
8	NAG	C	1	1,8	14,14,15	0.28	0	17,19,21	0.41	0
8	NAG	C	2	8	14,14,15	0.18	0	17,19,21	0.64	0
8	BMA	C	3	8	11,11,12	0.68	0	15,15,17	0.71	0
8	MAN	C	4	8	11,11,12	1.16	1 (9%)	15,15,17	1.82	4 (26%)
8	MAN	C	5	8	11,11,12	0.81	1 (9%)	15,15,17	1.33	2 (13%)
8	MAN	C	6	8	11,11,12	0.89	1 (9%)	15,15,17	1.25	3 (20%)
8	MAN	C	7	8	11,11,12	0.65	0	15,15,17	1.08	2 (13%)
9	NAG	F	1	1,9	14,14,15	0.24	0	17,19,21	0.41	0
9	NAG	F	2	9	14,14,15	0.23	0	17,19,21	0.50	0
9	BMA	F	3	9	11,11,12	0.58	0	15,15,17	0.70	0
9	MAN	F	4	9	11,11,12	0.55	0	15,15,17	1.14	2 (13%)
9	MAN	F	5	9	11,11,12	0.55	0	15,15,17	1.06	2 (13%)
9	MAN	F	6	9	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
9	MAN	F	7	9	11,11,12	0.73	1 (9%)	15,15,17	1.23	2 (13%)
9	MAN	F	8	9	11,11,12	0.74	0	15,15,17	0.87	1 (6%)
10	NAG	I	1	1,10	14,14,15	0.41	0	17,19,21	0.79	1 (5%)
10	NAG	I	2	10	14,14,15	0.18	0	17,19,21	0.35	0
10	BMA	I	3	10	11,11,12	0.98	0	15,15,17	1.02	2 (13%)
10	MAN	I	4	10	11,11,12	0.27	0	15,15,17	0.64	0
11	NAG	J	1	1,11	14,14,15	0.22	0	17,19,21	0.43	0
11	NAG	J	2	11	14,14,15	0.20	0	17,19,21	0.38	0
11	NAG	K	1	1,11	14,14,15	0.16	0	17,19,21	0.45	0
11	NAG	K	2	11	14,14,15	0.22	0	17,19,21	0.42	0
12	NAG	M	1	1,12	14,14,15	0.19	0	17,19,21	0.43	0
12	NAG	M	2	12	14,14,15	0.43	0	17,19,21	0.50	0
12	BMA	M	3	12	11,11,12	0.52	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	N	1	1,11	14,14,15	0.23	0	17,19,21	0.40	0
11	NAG	N	2	11	14,14,15	0.19	0	17,19,21	0.39	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
7	NAG	A	1	1,7	-	3/6/23/26	0/1/1/1
7	MAN	A	10	7	-	0/2/19/22	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
7	MAN	A	6	7	-	2/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
7	MAN	A	8	7	-	2/2/19/22	0/1/1/1
7	MAN	A	9	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	5/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	MAN	C	5	8	-	0/2/19/22	0/1/1/1
8	MAN	C	6	8	-	0/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
9	BMA	F	3	9	-	0/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	2/2/19/22	0/1/1/1
9	MAN	F	6	9	-	0/2/19/22	0/1/1/1
9	MAN	F	7	9	-	2/2/19/22	0/1/1/1
9	MAN	F	8	9	-	1/2/19/22	0/1/1/1
10	NAG	I	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	0/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	1,11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	NAG	K	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	2/6/23/26	0/1/1/1
12	NAG	M	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	M	2	12	-	2/6/23/26	0/1/1/1
12	BMA	M	3	12	-	1/2/19/22	0/1/1/1
11	NAG	N	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	4	MAN	C1-C2	2.76	1.58	1.52
8	C	6	MAN	C1-C2	2.64	1.58	1.52
9	F	7	MAN	C1-C2	2.23	1.57	1.52
8	C	5	MAN	C1-C2	2.15	1.57	1.52
7	A	8	MAN	C1-C2	2.14	1.57	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	4	MAN	C1-O5-C5	5.50	119.65	112.19
8	C	5	MAN	C1-O5-C5	3.81	117.36	112.19
7	A	1	NAG	C2-N2-C7	3.73	128.22	122.90
9	F	4	MAN	C1-O5-C5	3.45	116.86	112.19
9	F	7	MAN	C1-O5-C5	3.38	116.77	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

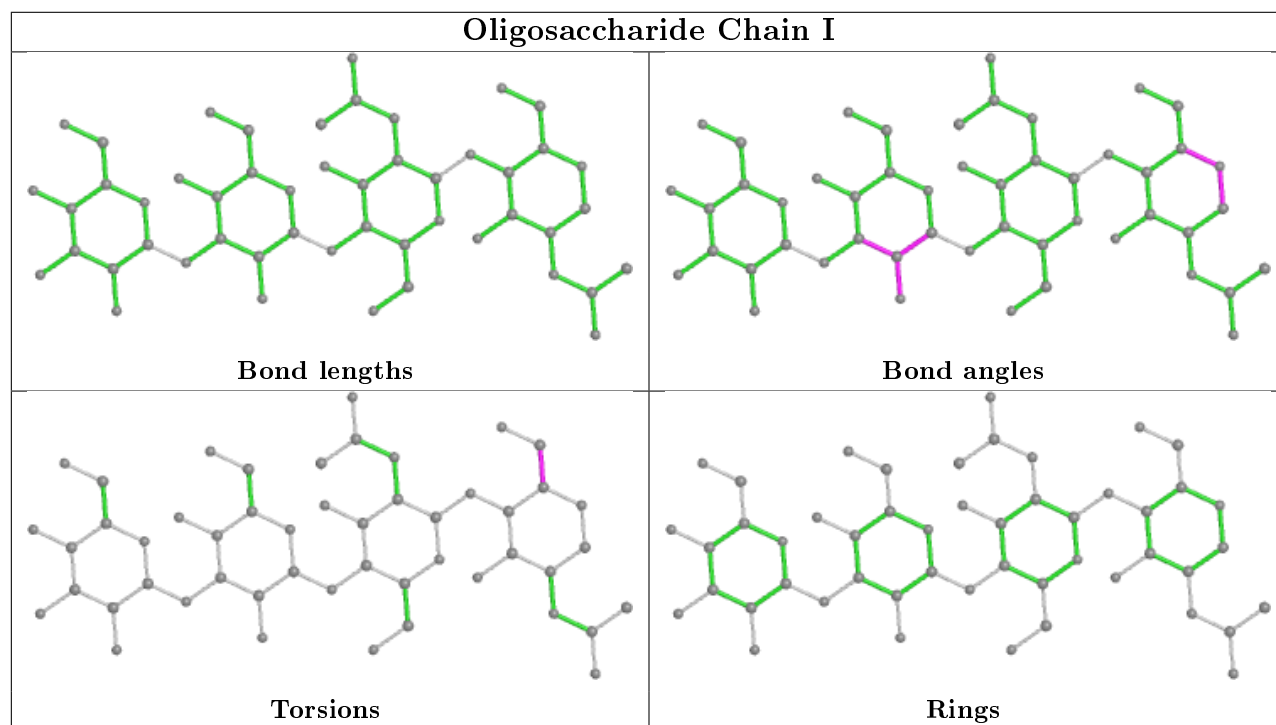
Mol	Chain	Res	Type	Atoms
11	J	1	NAG	O5-C5-C6-O6
11	K	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C1-C2-N2-C7
7	A	6	MAN	O5-C5-C6-O6
9	F	7	MAN	O5-C5-C6-O6

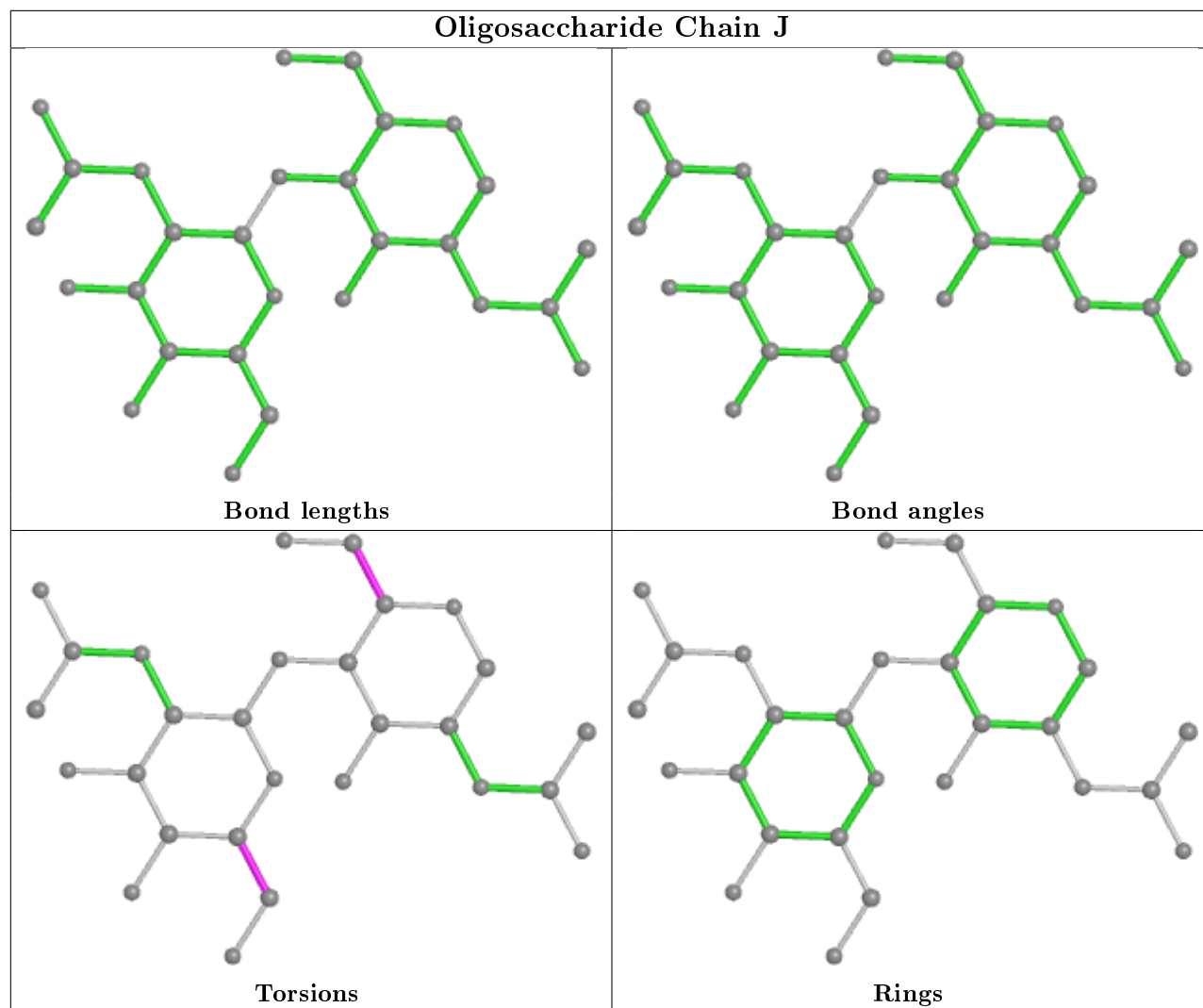
There are no ring outliers.

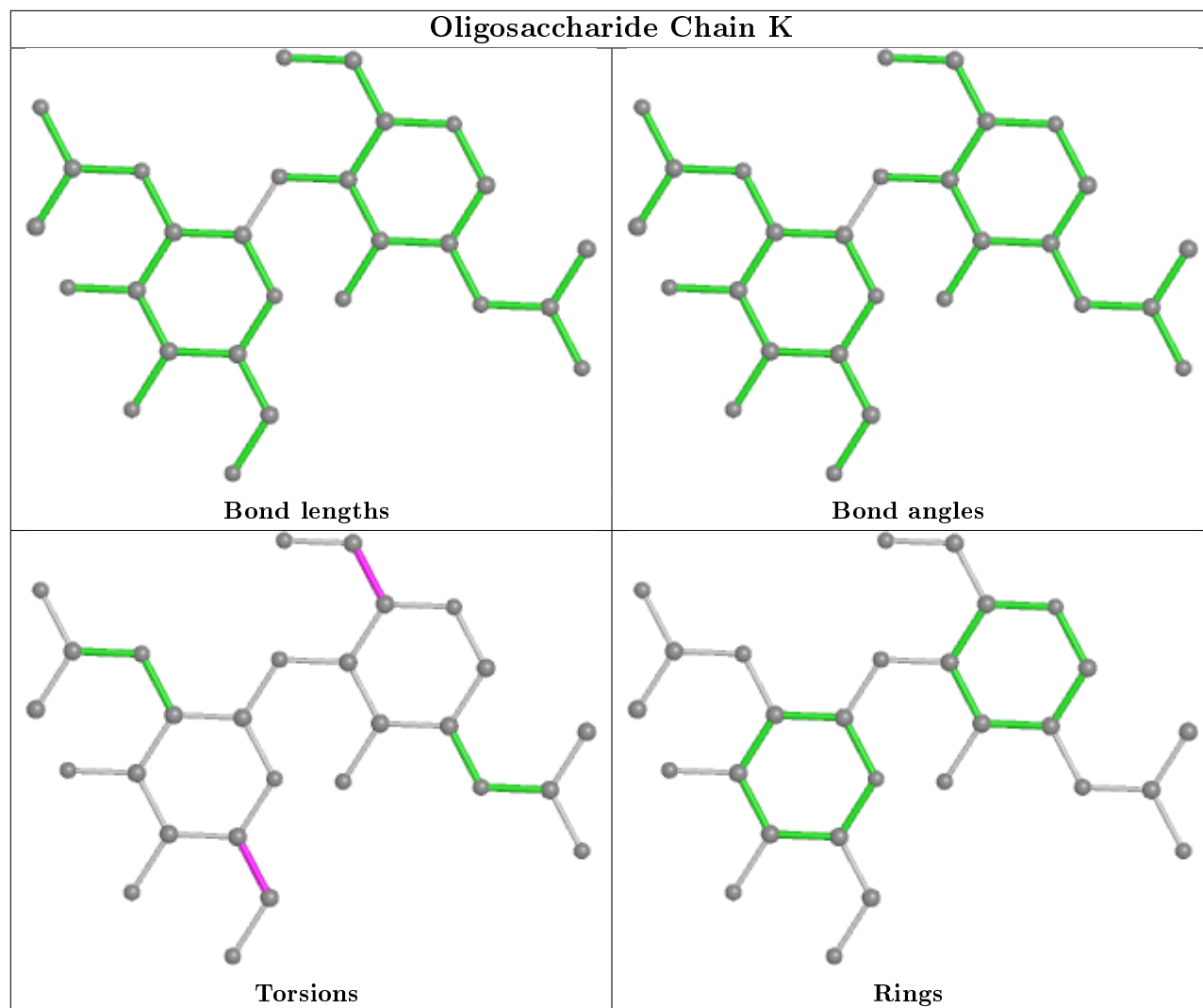
17 monomers are involved in 32 short contacts:

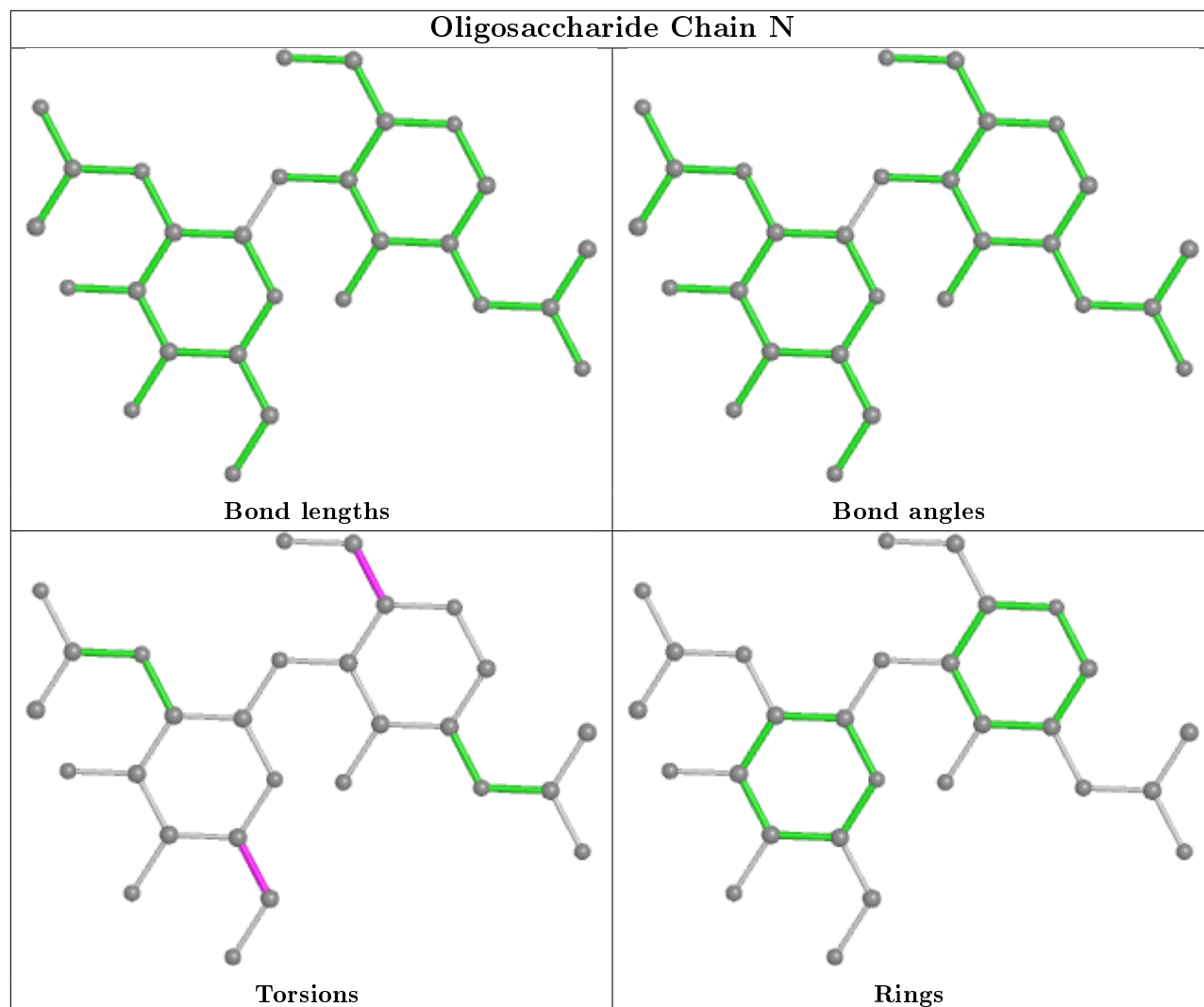
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	3	BMA	1	0
10	I	1	NAG	6	0
9	F	2	NAG	1	0
8	C	2	NAG	5	0
8	C	4	MAN	1	0
7	A	7	MAN	3	0
11	J	1	NAG	2	0
7	A	5	MAN	2	0
9	F	7	MAN	2	0
9	F	1	NAG	2	0
7	A	3	BMA	2	0
8	C	3	BMA	1	0
9	F	8	MAN	2	0
7	A	2	NAG	1	0
12	M	2	NAG	1	0
7	A	1	NAG	8	0
7	A	10	MAN	1	0

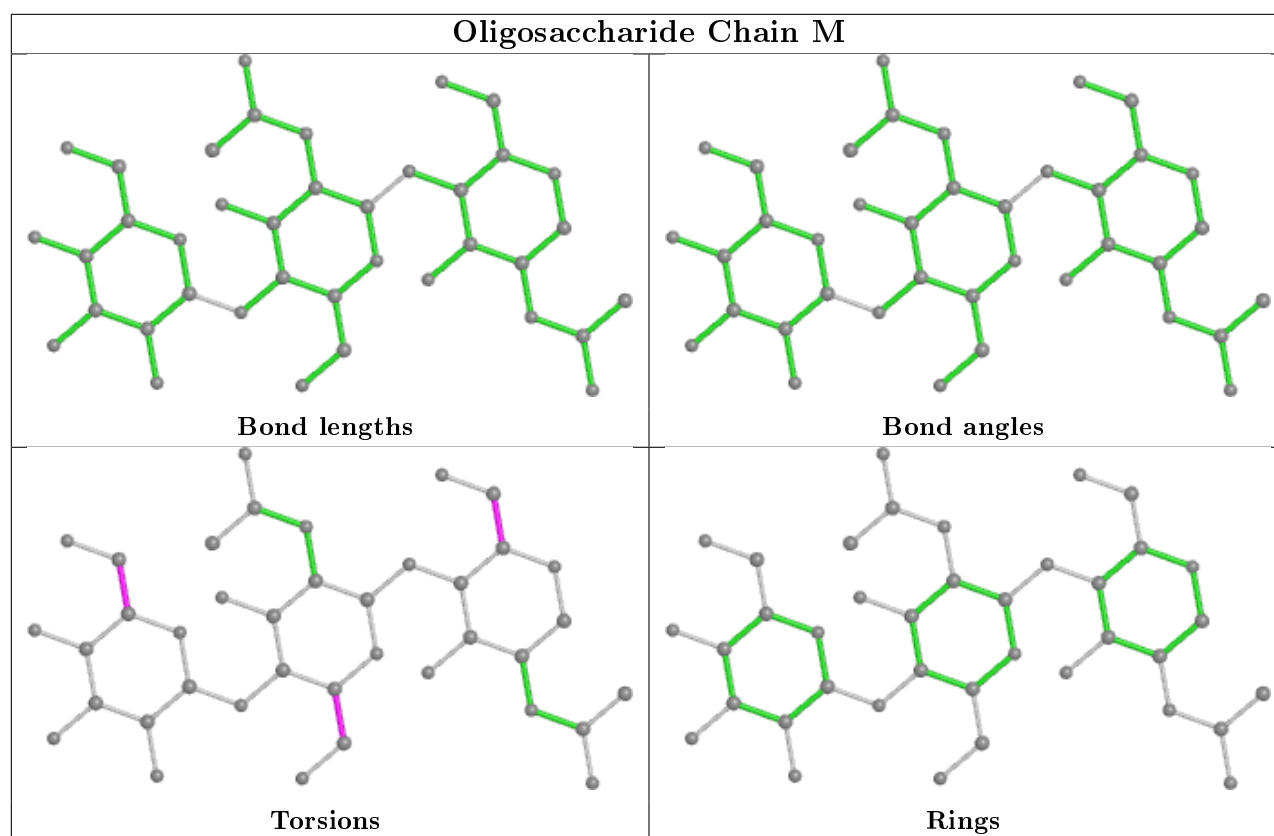
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
13	NAG	B	701	2	14,14,15	0.28	0	17,19,21	0.62	0
13	NAG	G	602	1	14,14,15	0.49	0	17,19,21	0.77	0
13	NAG	G	601	1	14,14,15	0.56	0	17,19,21	0.79	1 (5%)
13	NAG	G	634	1	14,14,15	0.51	0	17,19,21	0.66	1 (5%)

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
13	NAG	B	701	2	-	2/6/23/26	0/1/1/1
13	NAG	G	602	1	-	0/6/23/26	0/1/1/1
13	NAG	G	601	1	-	2/6/23/26	0/1/1/1
13	NAG	G	634	1	-	2/6/23/26	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(°)
13	G	601	NAG	C1-O5-C5	2.65	115.78	112.19
13	G	634	NAG	C1-O5-C5	2.20	115.18	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	701	NAG	C8-C7-N2-C2
13	B	701	NAG	O7-C7-N2-C2
13	G	634	NAG	C4-C5-C6-O6
13	G	634	NAG	O5-C5-C6-O6
13	G	601	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	701	NAG	6	0
13	G	602	NAG	1	0

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](#)

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	G	447/474 (94%)	0.04	4 (0%) 84 75	54, 98, 190, 518	0
2	B	129/153 (84%)	0.11	2 (1%) 72 59	60, 107, 202, 266	0
3	L	211/218 (96%)	-0.22	0 100 100	69, 113, 162, 209	0
4	H	231/236 (97%)	-0.09	1 (0%) 92 89	81, 126, 190, 227	0
5	D	223/240 (92%)	0.31	18 (8%) 12 6	78, 141, 254, 313	0
6	E	213/216 (98%)	0.49	19 (8%) 9 5	100, 162, 247, 307	0
All	All	1454/1537 (94%)	0.09	44 (3%) 50 34	54, 118, 221, 518	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	E	152	TRP	7.6
5	D	192	GLN	5.5
5	D	194	TYR	5.3
5	D	126	PRO	5.1
1	G	506	VAL	5.1

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](#)

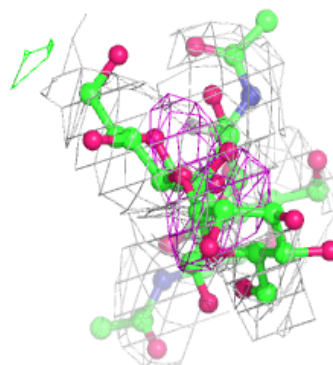
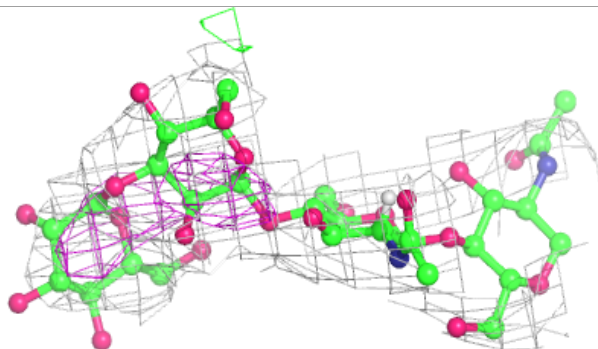
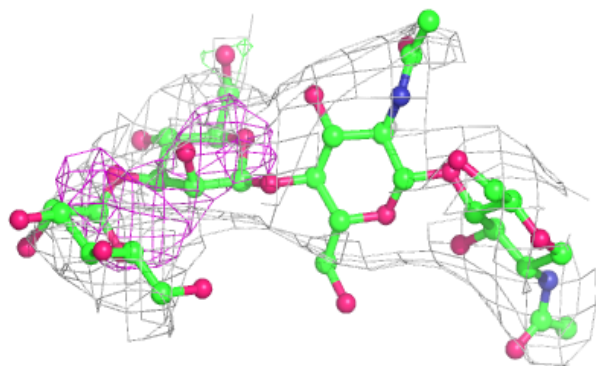
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	MAN	I	4	11/12	0.72	0.55	168,186,189,191	0
9	MAN	F	8	11/12	0.74	0.22	150,164,171,172	0
10	BMA	I	3	11/12	0.74	0.41	175,178,182,185	0
12	BMA	M	3	11/12	0.75	0.26	162,168,174,174	0
9	MAN	F	6	11/12	0.78	0.35	160,168,171,172	0
9	MAN	F	7	11/12	0.78	0.19	154,159,164,165	0
11	NAG	K	2	14/15	0.79	0.34	135,147,151,151	0
8	MAN	C	6	11/12	0.83	0.28	142,152,154,156	0
9	BMA	F	3	11/12	0.83	0.13	142,150,154,158	0
10	NAG	I	2	14/15	0.86	0.22	141,151,172,176	0
8	BMA	C	3	11/12	0.86	0.28	114,129,144,147	0
8	MAN	C	5	11/12	0.86	0.27	142,156,162,163	0
12	NAG	M	2	14/15	0.86	0.26	143,154,163,170	0
8	MAN	C	4	11/12	0.86	0.21	143,145,152,153	0
11	NAG	K	1	14/15	0.86	0.21	122,129,137,145	0
11	NAG	J	2	14/15	0.87	0.18	142,147,156,163	0
9	NAG	F	2	14/15	0.87	0.19	116,127,132,139	0
7	MAN	A	9	11/12	0.88	0.51	142,146,152,155	0
9	MAN	F	5	11/12	0.88	0.16	146,159,163,164	0
7	MAN	A	10	11/12	0.89	0.14	121,126,128,130	0
12	NAG	M	1	14/15	0.90	0.24	117,132,139,141	0
7	NAG	A	1	14/15	0.90	0.22	100,106,115,115	0
9	MAN	F	4	11/12	0.91	0.12	140,157,159,160	0
8	NAG	C	2	14/15	0.91	0.29	101,107,116,131	0
8	MAN	C	7	11/12	0.91	0.34	100,118,125,128	0
11	NAG	N	2	14/15	0.92	0.20	132,141,149,151	0
7	MAN	A	8	11/12	0.92	0.10	119,126,134,141	0
7	MAN	A	7	11/12	0.92	0.12	115,121,124,125	0
8	NAG	C	1	14/15	0.93	0.29	93,101,111,111	0
10	NAG	I	1	14/15	0.93	0.16	112,127,135,143	0
11	NAG	J	1	14/15	0.93	0.27	114,127,137,153	0
9	NAG	F	1	14/15	0.94	0.21	96,100,109,123	0
7	BMA	A	3	11/12	0.94	0.16	111,114,123,127	0
7	MAN	A	4	11/12	0.94	0.15	106,113,126,126	0
11	NAG	N	1	14/15	0.94	0.16	114,121,127,136	0
7	MAN	A	5	11/12	0.95	0.16	106,110,113,113	0
7	NAG	A	2	14/15	0.95	0.18	103,108,116,122	0
7	MAN	A	6	11/12	0.96	0.15	104,111,117,118	0

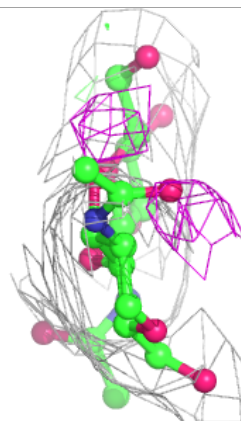
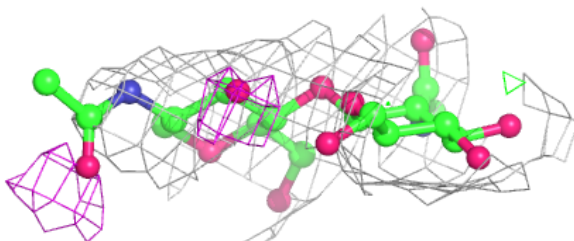
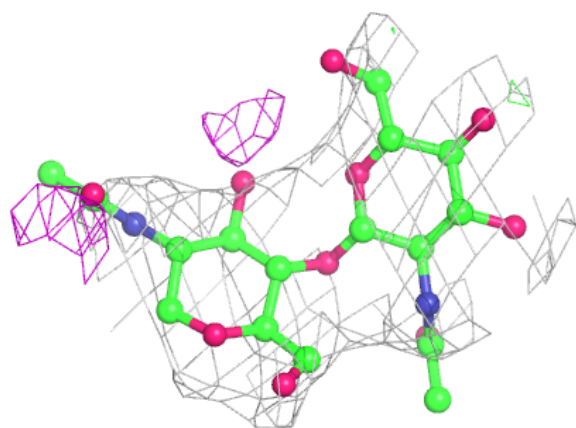
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

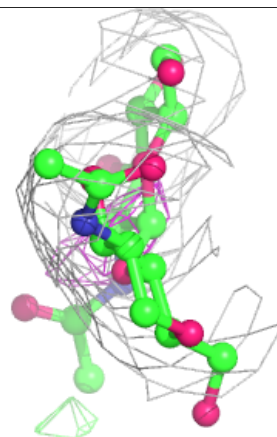
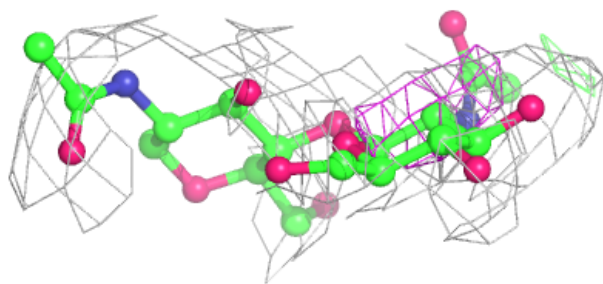
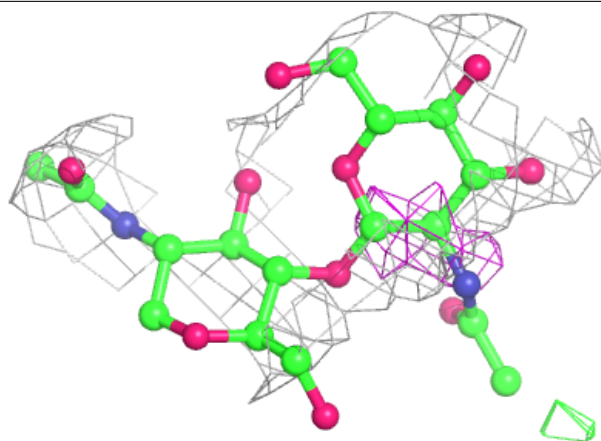
**Electron density around Chain J:**

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



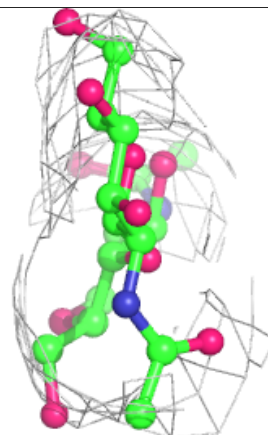
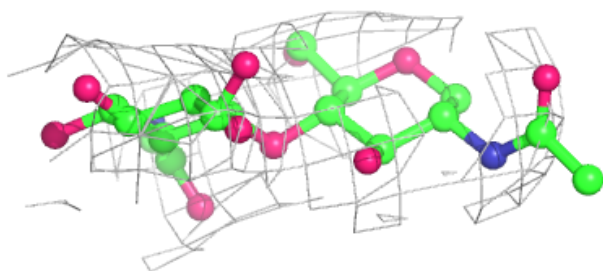
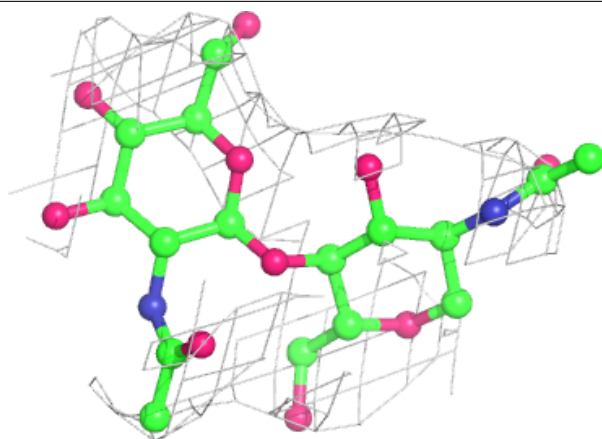
Electron density around Chain K:

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

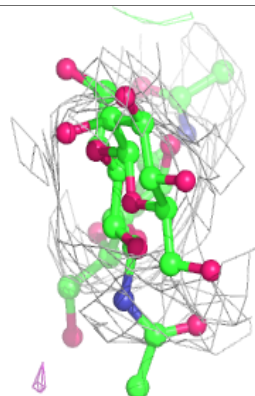
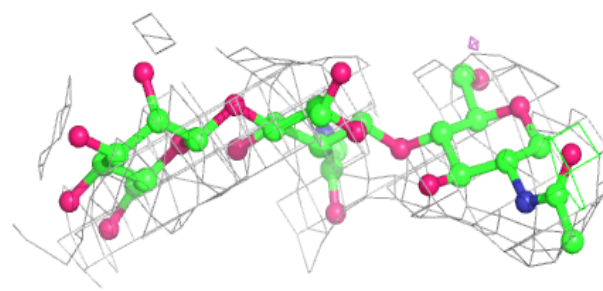
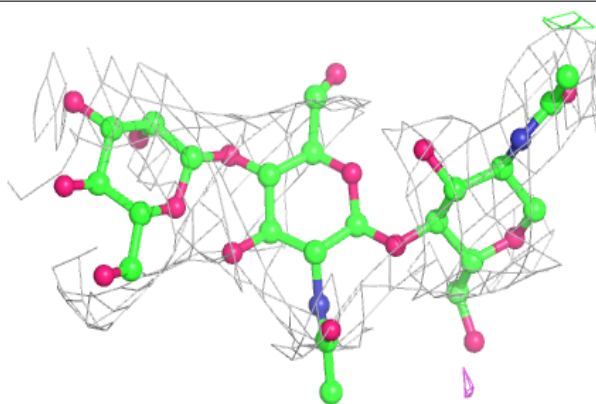


Electron density around Chain N:

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

**Electron density around Chain M:**

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



6.4 Ligands [i](#)

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
13	NAG	G	602	14/15	0.85	0.18	119,130,136,136	0
13	NAG	B	701	14/15	0.89	0.21	134,151,156,158	0
13	NAG	G	601	14/15	0.89	0.20	99,132,146,147	0
13	NAG	G	634	14/15	0.89	0.24	116,131,136,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.