



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2021 – 10:19 AM EDT

PDB ID : 3MUG
Title : Crystal structure of human Fab PG16, a broadly reactive and potent HIV-1 neutralizing antibody
Authors : Pejchal, R.; Walker, L.M.; Burton, D.R.; Wilson, I.A.
Deposited on : 2010-05-03
Resolution : 2.49 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 : 2.17.1
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) : 2.17.1

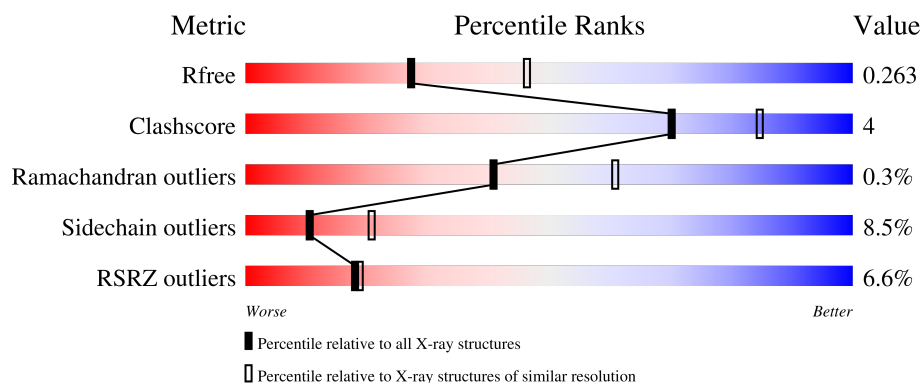
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	216	<div> <div>17%</div> <div>85% 12% ..</div> </div>
1	C	216	<div> <div>4%</div> <div>84% 13% ..</div> </div>
1	E	216	<div> <div>2%</div> <div>88% 9% .</div> </div>
1	G	216	<div> <div>4%</div> <div>87% 11% ..</div> </div>
1	I	216	<div> <div>4%</div> <div>83% 15% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	216	
2	B	241	
2	D	241	
2	F	241	
2	H	241	
2	J	241	
2	L	241	
3	M	2	
3	N	2	

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
2	PCA	D	1	-	-	-	X
2	PCA	J	1	-	-	-	X
3	NAG	M	2	-	-	-	X
4	NAG	A	500	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20630 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 Antibody PG16 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1555	966	263	321	5			
1	C	212	Total	C	N	O	S	0	0	0
			1547	960	261	321	5			
1	E	211	Total	C	N	O	S	0	0	0
			1553	966	263	319	5			
1	G	212	Total	C	N	O	S	0	0	0
			1559	969	264	321	5			
1	I	213	Total	C	N	O	S	0	0	0
			1563	971	264	323	5			
1	K	212	Total	C	N	O	S	0	0	0
			1558	969	264	320	5			

- Molecule 2 is a protein called Antibody PG16 Heavy Chain.

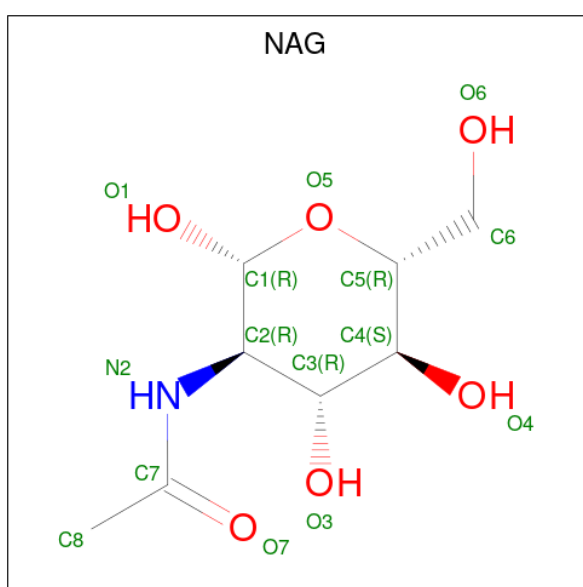
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1795	1129	301	355	10			
2	D	239	Total	C	N	O	S	0	0	0
			1806	1139	302	355	10			
2	F	238	Total	C	N	O	S	0	0	0
			1796	1135	302	349	10			
2	H	239	Total	C	N	O	S	0	0	0
			1799	1132	302	355	10			
2	J	239	Total	C	N	O	S	0	0	0
			1806	1139	302	355	10			
2	L	238	Total	C	N	O	S	0	0	0
			1792	1134	301	347	10			

- 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
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	28	Total	O	0	0
			28	28		
5	C	7	Total	O	0	0
			7	7		
5	D	14	Total	O	0	0
			14	14		

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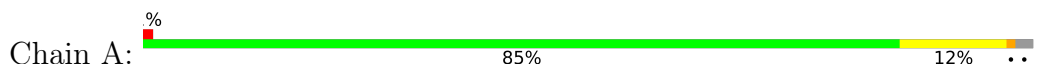
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	53	Total 53	O 53	0	0
5	F	30	Total 30	O 30	0	0
5	G	32	Total 32	O 32	0	0
5	H	39	Total 39	O 39	0	0
5	I	51	Total 51	O 51	0	0
5	J	33	Total 33	O 33	0	0
5	K	64	Total 64	O 64	0	0
5	L	57	Total 57	O 57	0	0

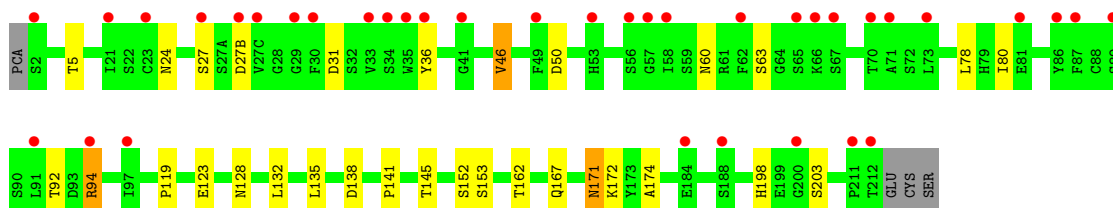
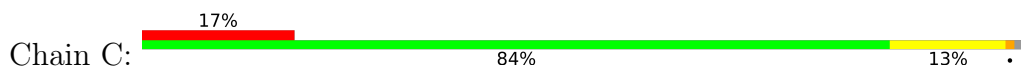
3 Residue-property plots [i](#)

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

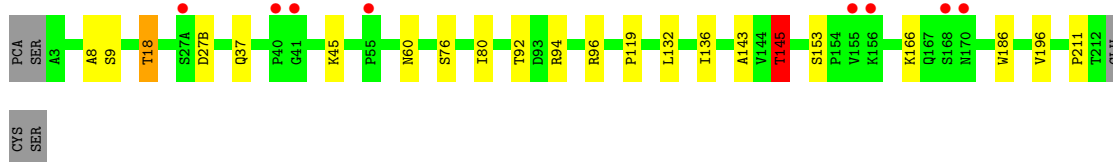
- Molecule 1: Antibody PG16 Light Chain



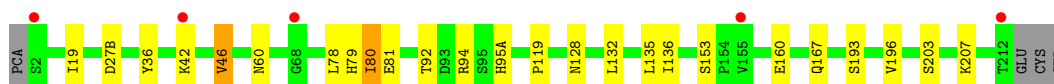
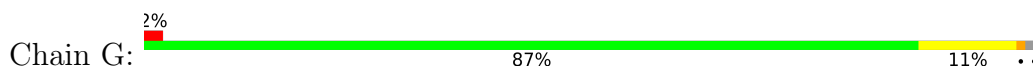
- Molecule 1: Antibody PG16 Light Chain



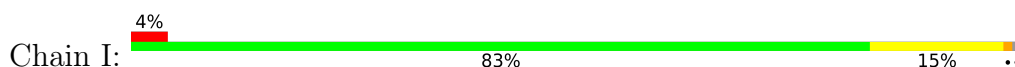
- Molecule 1: Antibody PG16 Light Chain

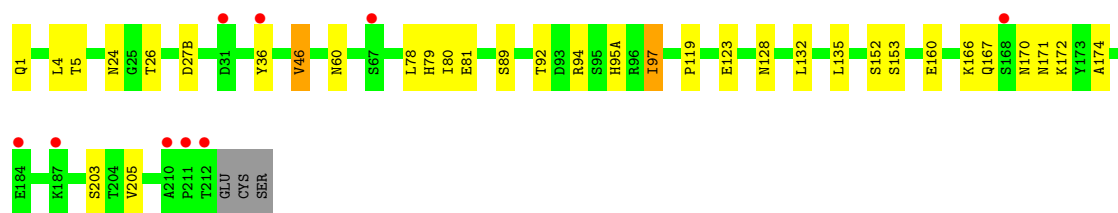


- Molecule 1: Antibody PG16 Light Chain

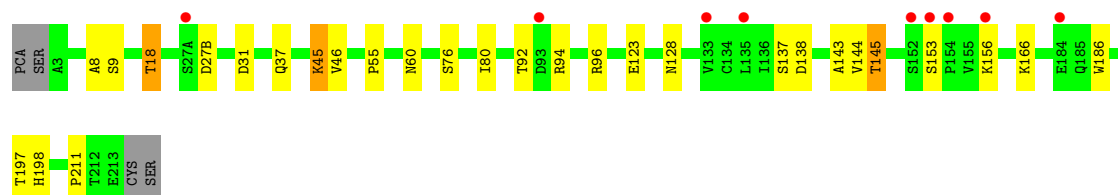
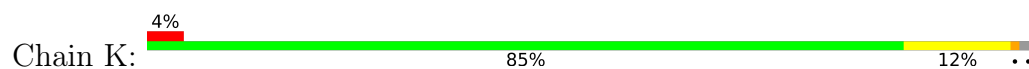


- Molecule 1: Antibody PG16 Light Chain

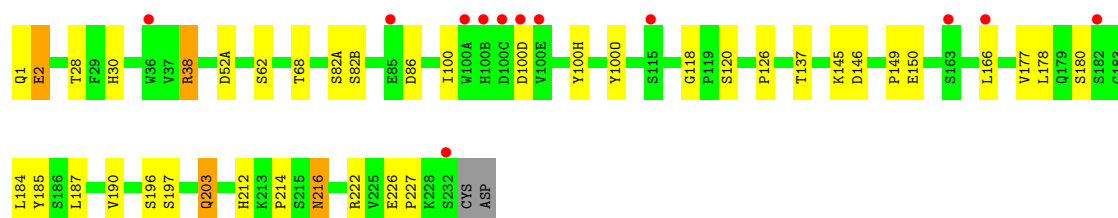
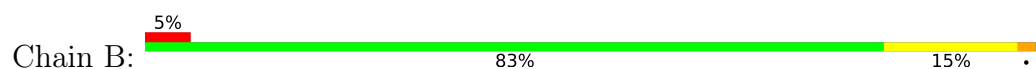




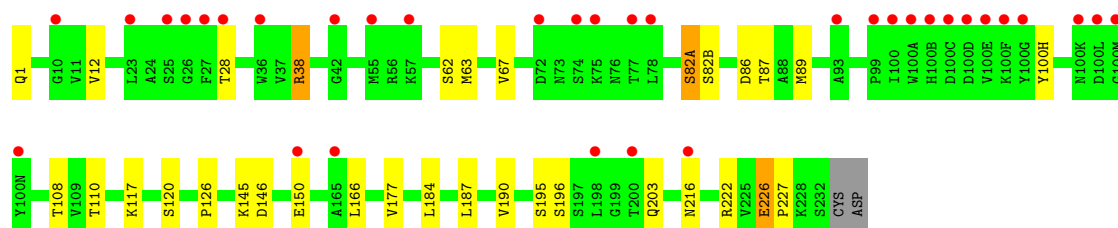
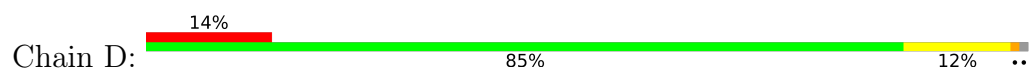
• Molecule 1: Antibody PG16 Light Chain



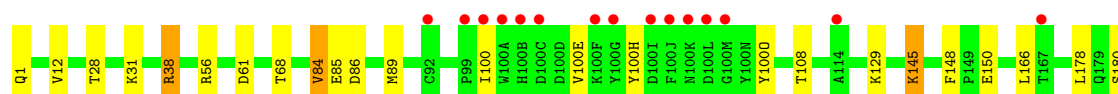
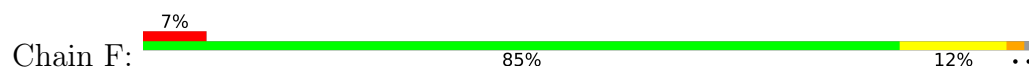
• Molecule 2: Antibody PG16 Heavy Chain

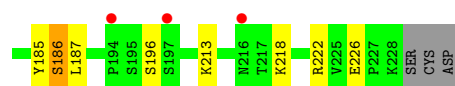


• Molecule 2: Antibody PG16 Heavy Chain

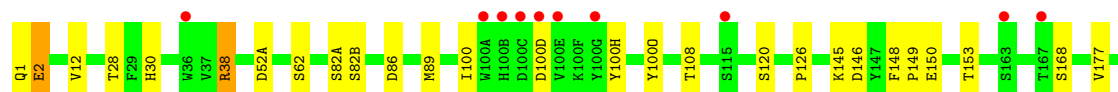
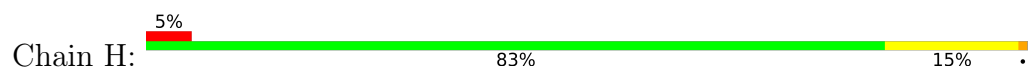


• Molecule 2: Antibody PG16 Heavy Chain

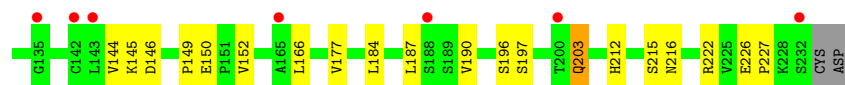
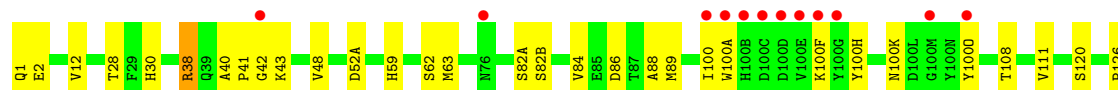
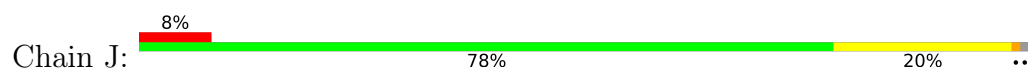




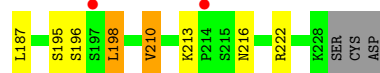
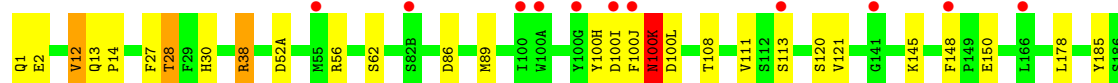
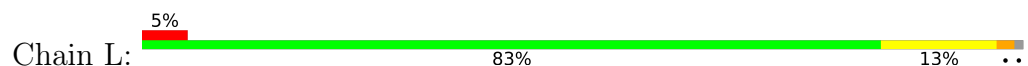
• Molecule 2: Antibody PG16 Heavy Chain



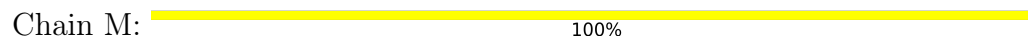
• Molecule 2: Antibody PG16 Heavy Chain



• Molecule 2: Antibody PG16 Heavy Chain



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



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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.77Å 66.25Å 198.70Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.49 24.97 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.97-2.49) 94.6 (24.97-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.207 , 0.248 0.221 , 0.263	Depositor DCC
R_{free} test set	5547 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1728e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/1592	0.69	0/2171
1	C	0.46	0/1584	0.68	0/2163
1	E	0.54	0/1590	0.75	1/2167 (0.0%)
1	G	0.49	0/1596	0.70	0/2175
1	I	0.50	0/1593	0.72	0/2174
1	K	0.55	0/1595	0.75	0/2174
2	B	0.50	0/1819	0.75	0/2480
2	D	0.47	0/1832	0.75	1/2499 (0.0%)
2	F	0.52	0/1820	0.79	0/2480
2	H	0.50	0/1823	0.74	0/2484
2	J	0.50	0/1832	0.75	0/2499
2	L	0.57	0/1816	0.84	0/2474
All	All	0.51	0/20492	0.75	2/27940 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	82(A)	SER	N-CA-C	-5.50	96.15	111.00
1	E	145	THR	N-CA-CB	5.30	120.38	110.30

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	1555	0	1490	17	0
1	C	1547	0	1468	14	0
1	E	1553	0	1497	11	0
1	G	1559	0	1502	10	0
1	I	1563	0	1497	16	0
1	K	1558	0	1499	10	0
2	B	1795	0	1665	17	0
2	D	1806	0	1679	10	0
2	F	1796	0	1682	12	0
2	H	1799	0	1676	13	0
2	J	1806	0	1680	22	0
2	L	1792	0	1681	11	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
4	A	14	0	13	0	0
5	A	23	0	0	0	0
5	B	28	0	0	0	0
5	C	7	0	0	0	0
5	D	14	0	0	0	0
5	E	53	0	0	1	0
5	F	30	0	0	0	0
5	G	32	0	0	0	0
5	H	39	0	0	0	0
5	I	51	0	0	0	0
5	J	33	0	0	1	0
5	K	64	0	0	0	0
5	L	57	0	0	0	0
All	All	20630	0	19079	140	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.

The worst 5 of 140 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:97:ILE:CD1	1:A:97:ILE:CG1	1.74	1.61
1:A:135:LEU:HD13	2:B:190:VAL:HG11	1.49	0.95
1:I:135:LEU:HD13	2:J:190:VAL:HG11	1.50	0.90
1:E:8:ALA:HB2	1:E:145:THR:HG22	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD13	2:D:190:VAL:HG11	1.60	0.84

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	210/216 (97%)	200 (95%)	10 (5%)	0	100	100
1	C	210/216 (97%)	194 (92%)	15 (7%)	1 (0%)	29	48
1	E	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
1	G	210/216 (97%)	201 (96%)	9 (4%)	0	100	100
1	I	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	29	48
1	K	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
2	B	236/241 (98%)	226 (96%)	9 (4%)	1 (0%)	34	54
2	D	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	34	54
2	F	235/241 (98%)	222 (94%)	12 (5%)	1 (0%)	34	54
2	H	236/241 (98%)	228 (97%)	7 (3%)	1 (0%)	34	54
2	J	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	34	54
2	L	235/241 (98%)	221 (94%)	12 (5%)	2 (1%)	17	31
All	All	2674/2742 (98%)	2556 (96%)	109 (4%)	9 (0%)	41	61

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	171	ASN
2	L	100(K)	ASN
2	D	82(B)	SER
2	B	82(B)	SER

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Mol	Chain	Res	Type
2	H	82(B)	SER

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	177/182 (97%)	166 (94%)	11 (6%)	18	35
1	C	175/182 (96%)	159 (91%)	16 (9%)	9	18
1	E	177/182 (97%)	167 (94%)	10 (6%)	21	40
1	G	178/182 (98%)	165 (93%)	13 (7%)	14	27
1	I	177/182 (97%)	164 (93%)	13 (7%)	14	27
1	K	177/182 (97%)	163 (92%)	14 (8%)	12	24
2	B	191/203 (94%)	173 (91%)	18 (9%)	8	17
2	D	193/203 (95%)	175 (91%)	18 (9%)	9	17
2	F	190/203 (94%)	173 (91%)	17 (9%)	9	19
2	H	192/203 (95%)	171 (89%)	21 (11%)	6	12
2	J	193/203 (95%)	176 (91%)	17 (9%)	10	19
2	L	189/203 (93%)	169 (89%)	20 (11%)	6	13
All	All	2209/2310 (96%)	2021 (92%)	188 (8%)	10	21

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	153	THR
2	J	89	MET
2	H	196	SER
1	I	97	ILE
2	J	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	189	HIS
2	J	212	HIS
2	L	30	HIS
1	K	108	GLN
1	E	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

13 non-standard protein/DNA/RNA residues 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	PCA	F	1	2	7,8,9	1.02	1 (14%)	9,10,12	0.84	0
2	PCA	D	1	2	7,8,9	0.90	0	9,10,12	1.82	2 (22%)
2	PCA	H	1	2	7,8,9	0.83	0	9,10,12	1.52	2 (22%)
2	TYS	H	100(H)	2	15,16,17	1.13	2 (13%)	18,22,24	1.65	4 (22%)
2	TYS	J	100(H)	2	15,16,17	1.72	2 (13%)	18,22,24	1.59	4 (22%)
2	TYS	D	100(H)	2	15,16,17	1.54	1 (6%)	18,22,24	1.75	5 (27%)
2	PCA	B	1	2	7,8,9	0.81	0	9,10,12	1.67	3 (33%)
1	PCA	I	1	1	7,8,9	1.23	1 (14%)	9,10,12	1.15	0
2	TYS	F	100(H)	2	15,16,17	1.79	1 (6%)	18,22,24	1.23	1 (5%)
2	TYS	L	100(H)	2	15,16,17	2.33	4 (26%)	18,22,24	1.71	5 (27%)
2	PCA	J	1	2	7,8,9	1.01	0	9,10,12	1.60	2 (22%)
2	PCA	L	1	2	7,8,9	0.81	0	9,10,12	1.46	1 (11%)
2	TYS	B	100(H)	2	15,16,17	1.20	1 (6%)	18,22,24	1.62	3 (16%)

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	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	TYS	H	100(H)	2	-	0/10/11/13	0/1/1/1
2	TYS	J	100(H)	2	-	0/10/11/13	0/1/1/1
2	TYS	D	100(H)	2	-	0/10/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
1	PCA	I	1	1	-	0/0/11/13	0/1/1/1
2	TYS	F	100(H)	2	-	0/10/11/13	0/1/1/1
2	TYS	L	100(H)	2	-	0/10/11/13	0/1/1/1
2	PCA	J	1	2	-	0/0/11/13	0/1/1/1
2	PCA	L	1	2	-	0/0/11/13	0/1/1/1
2	TYS	B	100(H)	2	-	0/10/11/13	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	100(H)	TYS	OH-S	-7.12	1.47	1.58
2	F	100(H)	TYS	OH-S	-5.70	1.49	1.58
2	J	100(H)	TYS	OH-S	-5.67	1.49	1.58
2	D	100(H)	TYS	OH-S	-4.50	1.51	1.58
2	L	100(H)	TYS	CE1-CZ	2.97	1.44	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100(H)	TYS	CG-CB-CA	-3.99	106.03	114.10
2	D	1	PCA	CB-CA-C	3.99	118.19	112.70
2	H	100(H)	TYS	O2-S-O1	3.91	127.91	112.22
2	J	100(H)	TYS	O2-S-O1	3.47	126.16	112.22
2	B	100(H)	TYS	O2-S-O1	3.42	125.94	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

4 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
3	NAG	M	1	1,3	14,14,15	2.10	5 (35%)	17,19,21	1.77	3 (17%)
3	NAG	M	2	3	14,14,15	2.93	7 (50%)	17,19,21	2.81	5 (29%)
3	NAG	N	1	1,3	14,14,15	2.01	3 (21%)	17,19,21	1.92	5 (29%)
3	NAG	N	2	3	14,14,15	2.94	8 (57%)	17,19,21	3.52	10 (58%)

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
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O3-C3	4.91	1.54	1.43
3	M	2	NAG	C3-C2	4.87	1.62	1.52
3	N	2	NAG	C3-C2	4.87	1.62	1.52
3	M	2	NAG	O5-C5	4.74	1.53	1.43
3	M	2	NAG	O5-C1	4.51	1.50	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	O5-C5-C6	9.40	121.93	107.20
3	N	2	NAG	O5-C5-C6	8.97	121.27	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	2	NAG	C2-N2-C7	6.02	131.48	122.90
3	N	2	NAG	C4-C3-C2	4.53	117.65	111.02
3	M	2	NAG	C4-C3-C2	4.32	117.35	111.02

There are no chirality outliers.

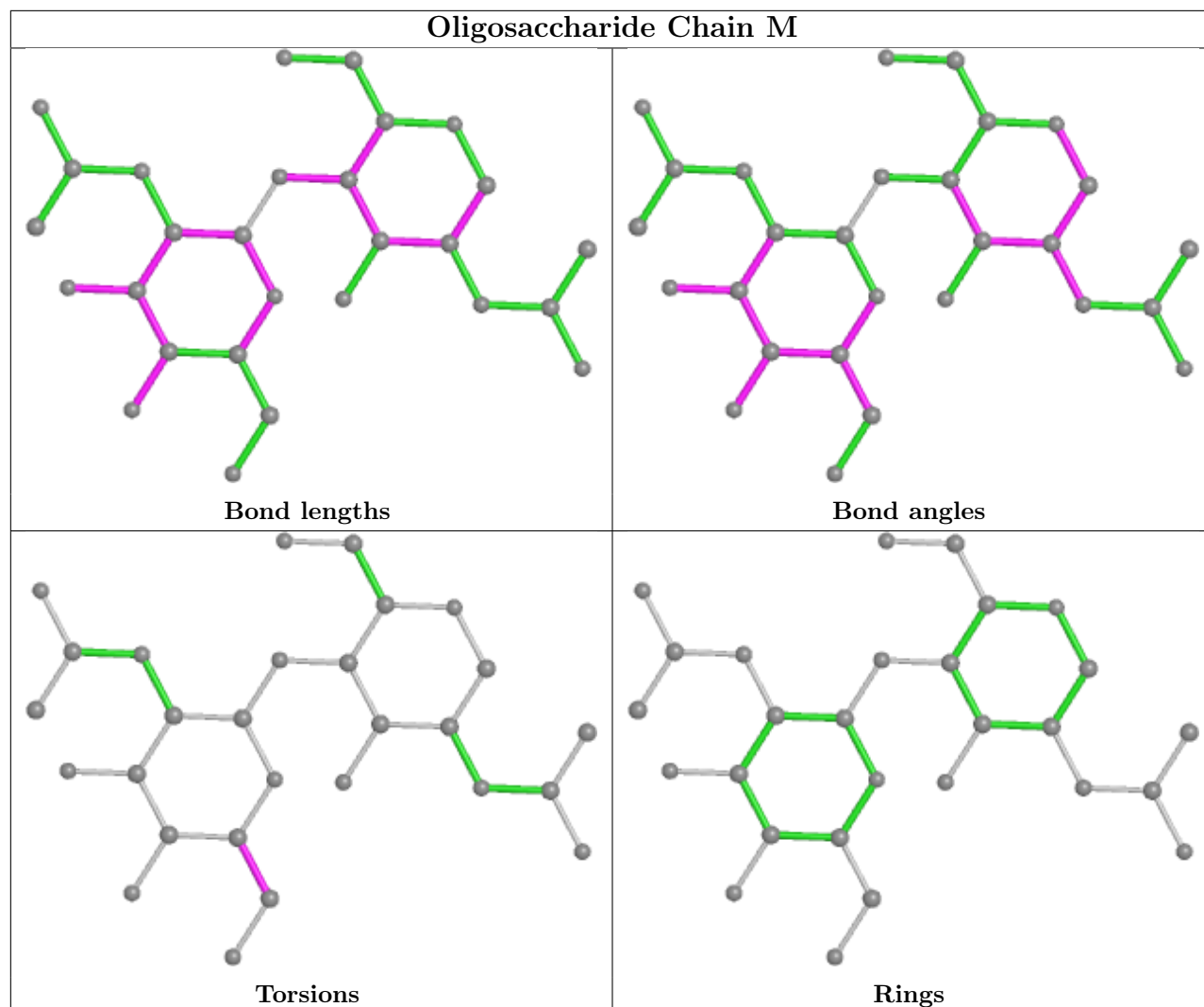
All (2) torsion outliers are listed below:

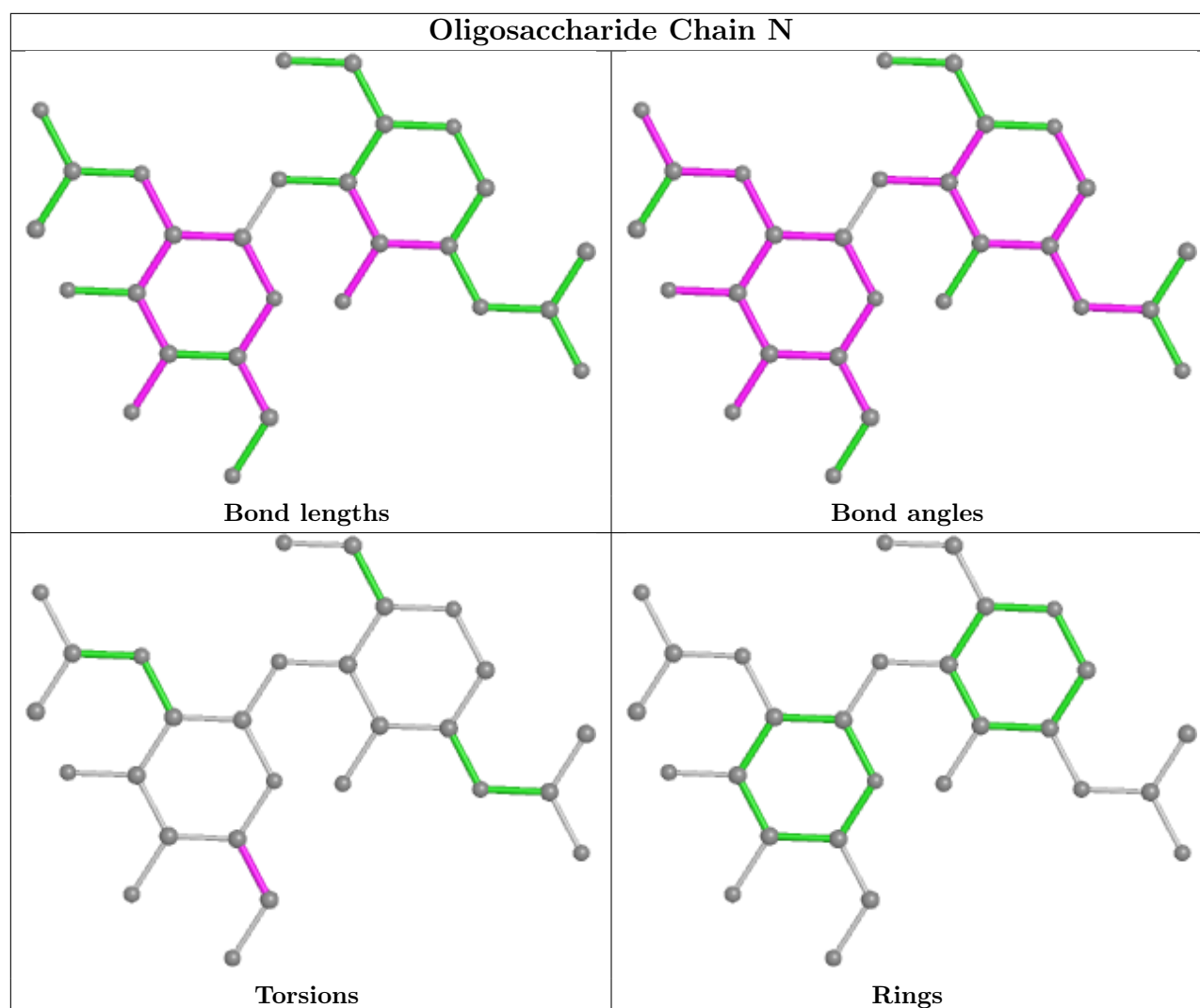
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

1 ligand is 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	$\# Z > 2$
4	NAG	A	500	1	14,14,15	1.61	3 (21%)	17,19,21	1.58	5 (29%)

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
4	NAG	A	500	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	NAG	C4-C3	2.88	1.59	1.52
4	A	500	NAG	C3-C2	2.77	1.58	1.52
4	A	500	NAG	C4-C5	2.04	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	NAG	O5-C1-C2	3.24	116.40	111.29
4	A	500	NAG	C4-C3-C2	2.77	115.08	111.02
4	A	500	NAG	C1-C2-N2	-2.44	106.32	110.49
4	A	500	NAG	O4-C4-C3	2.28	115.62	110.35
4	A	500	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	NAG	O5-C5-C6-O6
4	A	500	NAG	C4-C5-C6-O6

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](#)

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	212/216 (98%)	0.04	3 (1%) 75 77	31, 56, 80, 99	0
1	C	212/216 (98%)	0.76	37 (17%) 1 1	36, 74, 112, 129	0
1	E	211/216 (97%)	0.07	8 (3%) 40 43	38, 53, 81, 89	0
1	G	212/216 (98%)	-0.01	5 (2%) 59 62	31, 50, 71, 81	0
1	I	212/216 (98%)	0.06	9 (4%) 36 39	29, 47, 78, 105	0
1	K	212/216 (98%)	-0.04	9 (4%) 36 39	35, 47, 77, 89	0
2	B	237/241 (98%)	0.17	12 (5%) 28 29	25, 58, 87, 122	0
2	D	237/241 (98%)	0.68	34 (14%) 2 2	42, 67, 122, 186	0
2	F	236/241 (97%)	0.45	18 (7%) 13 14	45, 67, 100, 128	0
2	H	237/241 (98%)	0.15	11 (4%) 32 34	25, 51, 83, 120	0
2	J	237/241 (98%)	0.37	19 (8%) 12 12	37, 59, 89, 154	0
2	L	236/241 (97%)	0.10	13 (5%) 25 26	39, 56, 78, 99	0
All	All	2691/2742 (98%)	0.24	178 (6%) 18 19	25, 57, 93, 186	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	100(A)	TRP	9.4
2	F	100(A)	TRP	8.9
2	D	100(M)	GLY	8.1
2	J	100(G)	TYR	7.2
2	F	100	ILE	7.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	D	1	8/9	0.63	0.51	111,118,125,129	0
2	PCA	J	1	8/9	0.65	0.45	88,92,95,98	0
1	PCA	I	1	8/9	0.80	0.38	83,86,87,88	0
2	TYS	J	100(H)	16/17	0.81	0.30	94,108,128,131	0
2	PCA	F	1	8/9	0.83	0.22	76,79,80,80	0
2	TYS	D	100(H)	16/17	0.83	0.24	134,143,157,162	0
2	TYS	F	100(H)	16/17	0.84	0.23	114,120,128,130	0
2	PCA	L	1	8/9	0.91	0.22	59,62,65,69	0
2	TYS	L	100(H)	16/17	0.91	0.17	68,76,93,94	0
2	TYS	B	100(H)	16/17	0.93	0.12	53,65,84,84	0
2	PCA	H	1	8/9	0.95	0.19	63,69,74,75	0
2	PCA	B	1	8/9	0.95	0.16	60,65,69,70	0
2	TYS	H	100(H)	16/17	0.96	0.11	46,58,78,79	0

6.3 Carbohydrates

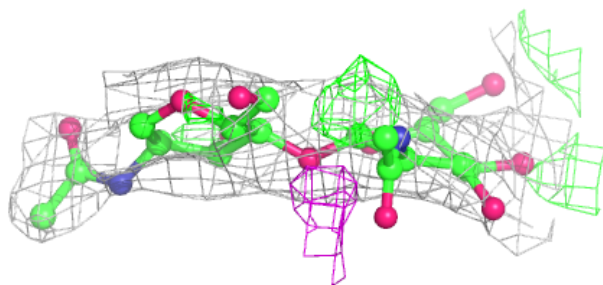
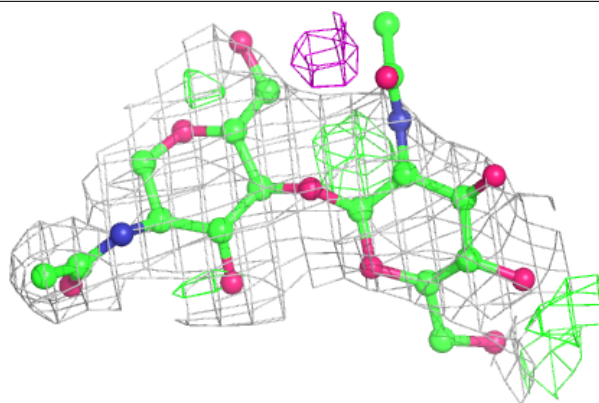
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	M	2	14/15	0.61	0.41	107,115,119,121	0
3	NAG	M	1	14/15	0.78	0.18	88,94,103,106	0
3	NAG	N	2	14/15	0.86	0.29	63,69,72,73	0
3	NAG	N	1	14/15	0.91	0.14	52,55,60,63	0

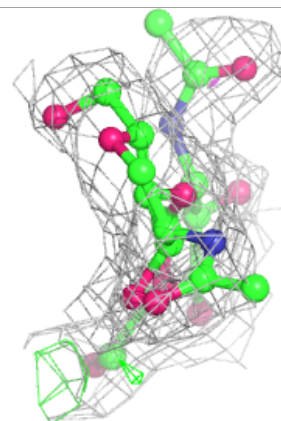
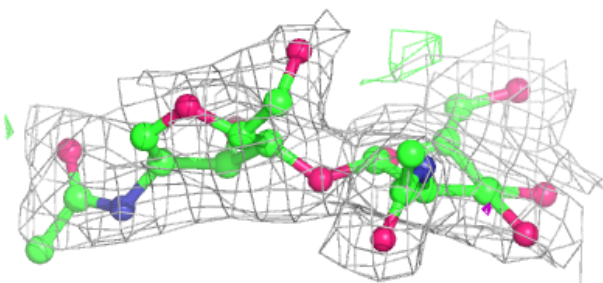
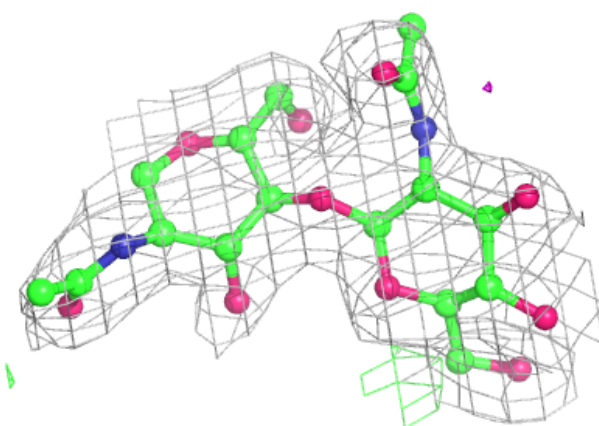
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

$2mF_o-DF_c$ (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)



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(\AA^2)	Q<0.9
4	NAG	A	500	14/15	0.73	0.51	109,113,120,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.