



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 09:32 PM EDT

PDB ID : 2Q8J
Title : Crystal Structure of the complex of C-lobe of bovine lactoferrin with Mannitol and Mannose at 2.7 Å resolution
Authors : Mir, R.; Jain, R.; Sinha, M.; Singh, N.; Sharma, S.; Kaur, P.; Bhushan, A.; Singh, T.P.
Deposited on : 2007-06-11
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
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) : 2.35

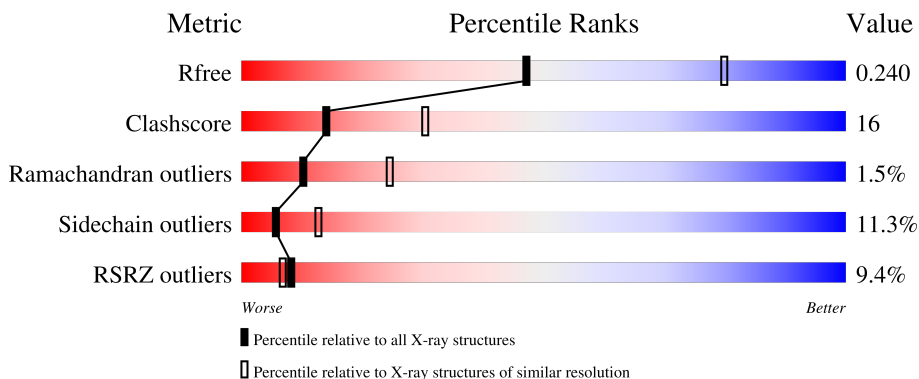
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	348	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">9% 64% 29% 5%</p>
2	B	3	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center; margin-top: 5px;">100%</p>
3	C	2	<div style="width: 100%; height: 10px; background-color: orange;"></div> <p style="text-align: center; margin-top: 5px;">100%</p>

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	M2P	A	707	-	-	-	X
2	MAN	B	3	-	-	-	X
4	NAG	A	701	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 2877 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.

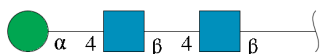
- Molecule 1 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2604	1622	454	507	21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	conflict	UNP P24627
A	608	GLU	LYS	conflict	UNP P24627

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



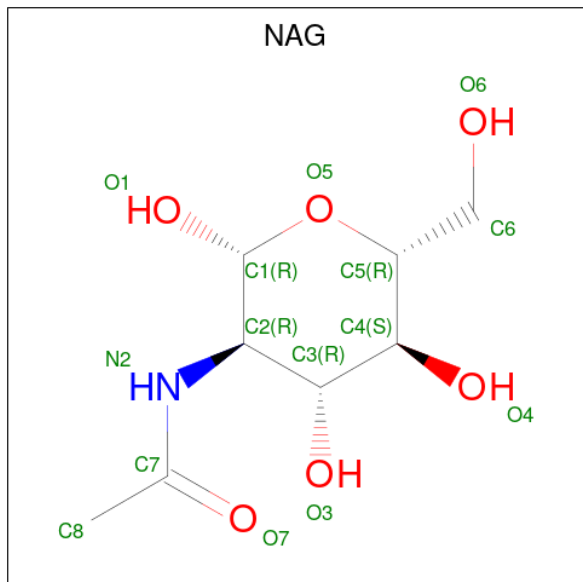
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

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



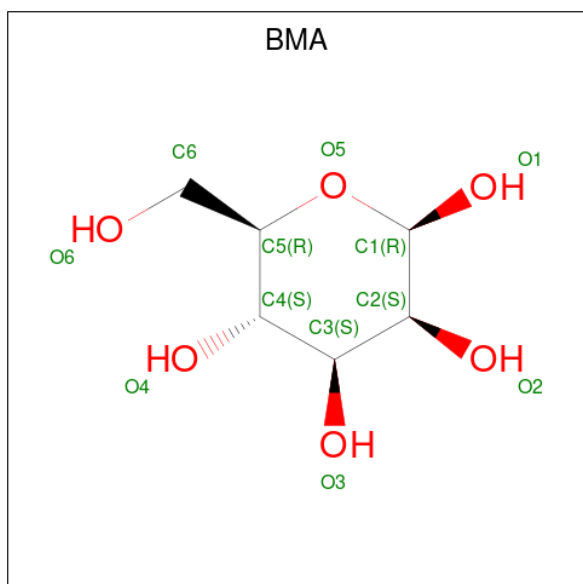
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 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		
4	A	1	14	8	1	5	0	0

- Molecule 5 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

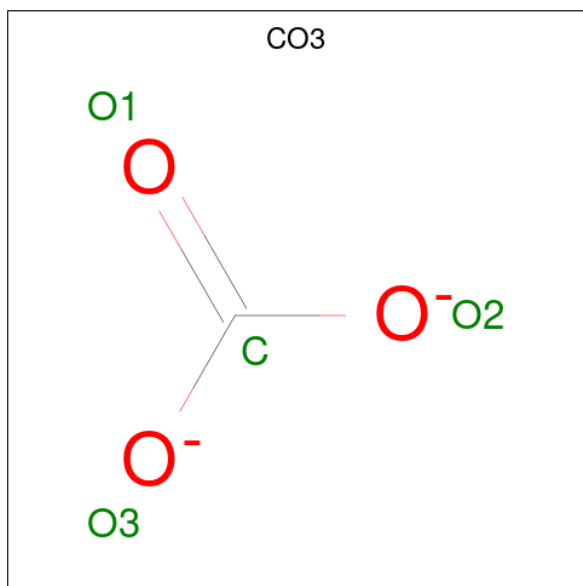


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	12	6	6	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe 1 1	0	0

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 1 3	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

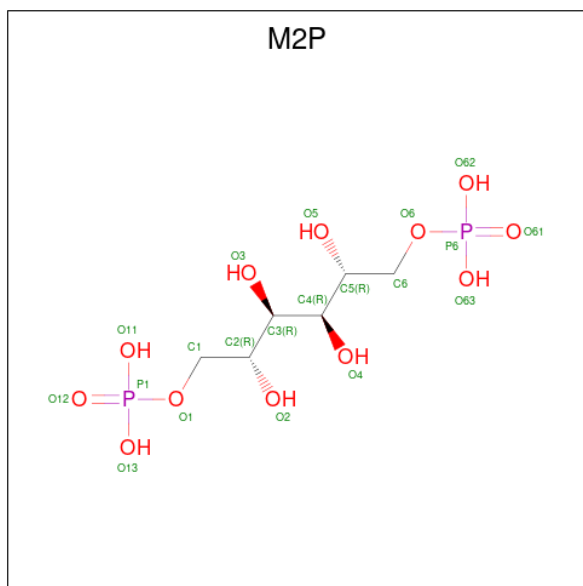
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Zn 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is D-MANNITOL-1,6-DIPHOSPHATE (three-letter code: M2P) (formula: $C_6H_{16}O_{12}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			12	6	6		

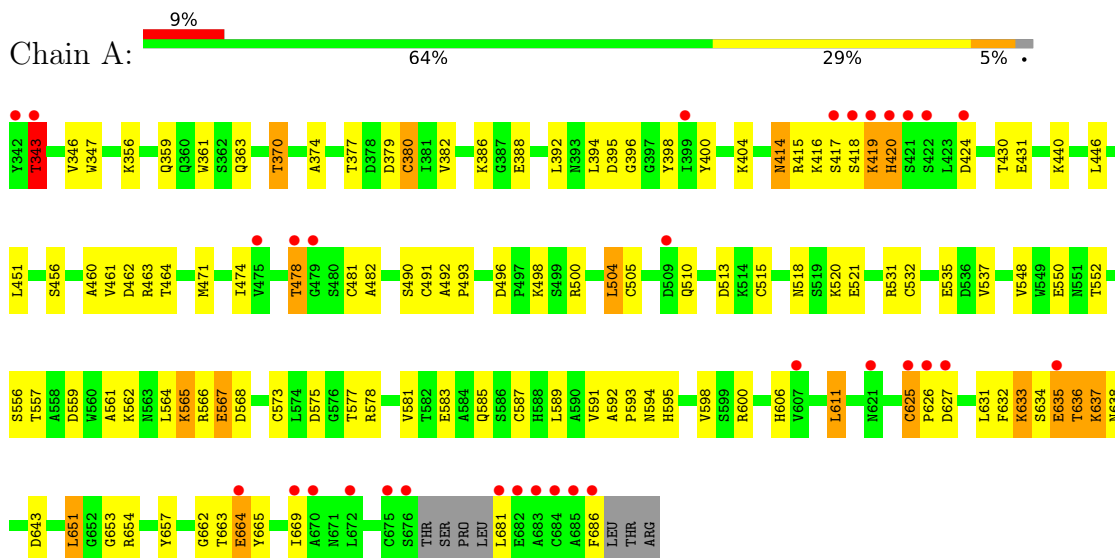
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	156	Total 156	O 156	0	0

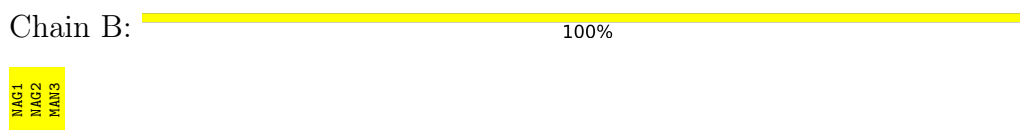
3 Residue-property plots

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.

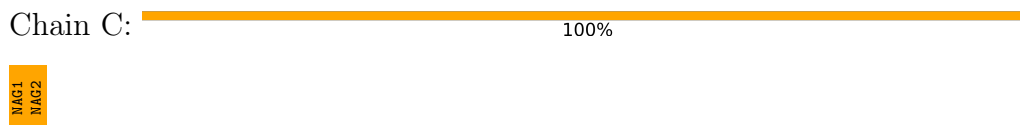
- Molecule 1: Lactotransferrin



- Molecule 2: alpha-D-mannopyranose-(1-4)-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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 50.30Å 65.90Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.71 14.79 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.71) 93.1 (14.79-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.240 0.192 , 0.240	Depositor DCC
R_{free} test set	492 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.031 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2877	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.74% 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: ZN, CO3, FE, NAG, MAN, M2P, SO4, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.18	7/2652 (0.3%)	1.08	8/3591 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	CYS	CB-SG	-7.99	1.68	1.82
1	A	481	CYS	CB-SG	-7.03	1.70	1.82
1	A	567	GLU	CG-CD	5.80	1.60	1.51
1	A	491	CYS	CB-SG	-5.62	1.72	1.81
1	A	346	VAL	CB-CG2	-5.42	1.41	1.52
1	A	657	TYR	CB-CG	-5.23	1.43	1.51
1	A	532	CYS	CB-SG	-5.01	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	343	THR	N-CA-C	6.15	127.61	111.00
1	A	568	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	651	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	A	681	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	496	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	415	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	531	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2519	83	0
2	B	39	0	34	0	0
3	C	28	0	25	2	0
4	A	14	0	13	0	0
5	A	12	0	12	1	0
6	A	1	0	0	0	0
7	A	4	0	0	1	0
8	A	2	0	0	0	0
9	A	5	0	0	0	0
10	A	12	0	12	1	0
11	A	156	0	0	14	0
All	All	2877	0	2615	84	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 (84) 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:664:GLU:OE2	1:A:664:GLU:HA	1.45	1.14
1:A:638:ASN:ND2	1:A:643:ASP:H	1.62	0.97
1:A:414:ASN:HD21	1:A:430:THR:HA	1.32	0.94
1:A:359:GLN:HG2	11:A:110:HOH:O	1.69	0.92
1:A:638:ASN:HD22	1:A:643:ASP:H	1.15	0.86
1:A:664:GLU:HG3	11:A:122:HOH:O	1.78	0.83
1:A:585:GLN:HG2	11:A:14:HOH:O	1.79	0.82
1:A:343:THR:HA	1:A:606:HIS:NE2	1.97	0.80
1:A:513:ASP:OD2	1:A:520:LYS:HE2	1.81	0.80
1:A:474:ILE:O	1:A:478:THR:HB	1.83	0.79
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.65	0.78
1:A:370:THR:HG21	11:A:71:HOH:O	1.85	0.75
1:A:343:THR:N	1:A:606:HIS:NE2	2.34	0.75
1:A:626:PRO:HD3	11:A:40:HOH:O	1.89	0.72
1:A:347:TRP:CZ3	1:A:611:LEU:HD11	2.25	0.72
1:A:430:THR:HB	1:A:594:ASN:ND2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:GLU:OE2	1:A:664:GLU:CA	2.32	0.71
1:A:593:PRO:HB3	5:A:708:BMA:O4	1.89	0.71
1:A:575:ASP:OD1	1:A:577:THR:HB	1.91	0.71
1:A:638:ASN:HD22	1:A:643:ASP:N	1.92	0.67
1:A:414:ASN:ND2	1:A:430:THR:HA	2.10	0.65
1:A:400:TYR:CZ	1:A:404:LYS:HE2	2.34	0.63
1:A:343:THR:CA	1:A:606:HIS:NE2	2.62	0.63
1:A:513:ASP:OD2	1:A:520:LYS:CE	2.47	0.62
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.36	0.61
1:A:370:THR:CG2	11:A:71:HOH:O	2.46	0.60
1:A:430:THR:HB	1:A:594:ASN:HD22	1.68	0.59
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.36	0.59
1:A:548:VAL:HG11	1:A:581:VAL:HG11	1.87	0.57
1:A:347:TRP:HZ3	1:A:611:LEU:HD11	1.70	0.56
11:A:115:HOH:O	3:C:2:NAG:H82	2.05	0.56
1:A:577:THR:CG2	1:A:578:ARG:N	2.69	0.55
1:A:638:ASN:ND2	1:A:643:ASP:N	2.45	0.55
1:A:552:THR:OG1	1:A:566:ARG:HG2	2.06	0.55
1:A:585:GLN:NE2	3:C:1:NAG:H81	2.21	0.54
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.43	0.54
1:A:380:CYS:HB3	1:A:392:LEU:HD13	1.89	0.54
1:A:567:GLU:H	1:A:567:GLU:CD	2.09	0.54
1:A:626:PRO:CG	11:A:40:HOH:O	2.56	0.52
1:A:577:THR:HG23	1:A:578:ARG:H	1.75	0.52
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.89	0.52
1:A:626:PRO:CD	11:A:40:HOH:O	2.53	0.51
1:A:417:SER:HB2	1:A:431:GLU:OE2	2.11	0.50
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.47	0.50
1:A:461:VAL:O	1:A:462:ASP:HB2	2.12	0.49
1:A:626:PRO:HG3	11:A:40:HOH:O	2.12	0.49
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.94	0.49
1:A:635:GLU:OE2	1:A:637:LYS:HD2	2.14	0.48
1:A:662:GLY:HA2	10:A:707:M2P:O5	2.13	0.48
1:A:394:LEU:HD12	1:A:598:VAL:HG21	1.93	0.48
1:A:446:LEU:HD11	1:A:451:LEU:HD23	1.95	0.48
1:A:394:LEU:CD1	1:A:598:VAL:HG21	2.44	0.48
1:A:464:THR:HG21	1:A:592:ALA:CB	2.44	0.48
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.42	0.48
1:A:382:VAL:HG12	1:A:386:LYS:HD3	1.95	0.48
1:A:505:CYS:HB3	1:A:521:GLU:OE1	2.13	0.48
1:A:518:ASN:OD1	1:A:520:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ALA:HA	1:A:564:LEU:HG	1.96	0.47
1:A:653:GLY:O	1:A:654:ARG:C	2.52	0.47
1:A:456:SER:O	1:A:490:SER:HA	2.14	0.47
1:A:535:GLU:HG2	11:A:34:HOH:O	2.14	0.47
1:A:394:LEU:HD12	1:A:598:VAL:CG2	2.44	0.47
1:A:632:PHE:O	1:A:633:LYS:HE3	2.14	0.47
1:A:556:SER:O	1:A:557:THR:OG1	2.19	0.46
1:A:463:ARG:HB3	7:A:802:CO3:O3	2.16	0.45
1:A:446:LEU:O	1:A:578:ARG:NH1	2.39	0.44
1:A:635:GLU:O	1:A:636:THR:HG22	2.17	0.44
1:A:386:LYS:HE3	1:A:388:GLU:OE1	2.17	0.44
1:A:395:ASP:O	1:A:396:GLY:C	2.55	0.44
1:A:636:THR:HG21	11:A:29:HOH:O	2.17	0.44
1:A:361:TRP:CE2	1:A:631:LEU:HD21	2.52	0.44
1:A:417:SER:CB	1:A:431:GLU:OE2	2.65	0.43
1:A:419:LYS:O	1:A:420:HIS:HB2	2.18	0.43
1:A:504:LEU:HG	1:A:537:VAL:CG1	2.48	0.43
1:A:585:GLN:CG	11:A:14:HOH:O	2.53	0.43
1:A:374:ALA:HB1	1:A:379:ASP:HB2	1.99	0.43
1:A:492:ALA:O	1:A:493:PRO:C	2.57	0.43
1:A:498:LYS:HE2	1:A:498:LYS:HB2	1.82	0.43
1:A:589:LEU:N	1:A:589:LEU:HD23	2.34	0.42
1:A:651:LEU:HA	1:A:651:LEU:HD23	1.70	0.42
1:A:565:LYS:HD3	1:A:567:GLU:OE2	2.19	0.42
1:A:550:GLU:HA	11:A:115:HOH:O	2.21	0.41
1:A:561:ALA:HA	1:A:564:LEU:CD1	2.49	0.41
1:A:471:MET:HE2	1:A:474:ILE:HD12	2.03	0.41

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	337/348 (97%)	307 (91%)	25 (7%)	5 (2%)	10 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	634	SER
1	A	420	HIS
1	A	625	CYS
1	A	482	ALA

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	282/289 (98%)	250 (89%)	32 (11%)	6 13

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	356	LYS
1	A	363	GLN
1	A	370	THR
1	A	380	CYS
1	A	414	ASN
1	A	416	LYS
1	A	418	SER
1	A	419	LYS
1	A	424	ASP
1	A	440	LYS
1	A	478	THR
1	A	500	ARG
1	A	504	LEU
1	A	510	GLN
1	A	515	CYS

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Mol	Chain	Res	Type
1	A	559	ASP
1	A	562	LYS
1	A	565	LYS
1	A	573	CYS
1	A	583	GLU
1	A	591	VAL
1	A	600	ARG
1	A	611	LEU
1	A	627	ASP
1	A	633	LYS
1	A	635	GLU
1	A	636	THR
1	A	637	LYS
1	A	663	THR
1	A	664	GLU
1	A	686	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	414	ASN
1	A	489	GLN
1	A	585	GLN
1	A	621	ASN
1	A	638	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](#)

5 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	B	1	1,2	14,14,15	0.69	0	17,19,21	1.77	4 (23%)
2	NAG	B	2	2	14,14,15	0.88	1 (7%)	17,19,21	2.45	7 (41%)
2	MAN	B	3	2	11,11,12	0.85	0	15,15,17	2.86	6 (40%)
3	NAG	C	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	2.70	7 (41%)
3	NAG	C	2	3	14,14,15	0.92	0	17,19,21	1.60	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
2	NAG	B	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C2-N2	-2.62	1.41	1.46
2	B	2	NAG	C1-C2	2.16	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MAN	C1-O5-C5	7.07	121.78	112.19
3	C	1	NAG	C1-O5-C5	6.84	121.46	112.19
2	B	2	NAG	O3-C3-C2	-4.78	99.57	109.47
2	B	3	MAN	C1-C2-C3	4.50	115.19	109.67
2	B	2	NAG	C1-O5-C5	4.46	118.24	112.19
2	B	3	MAN	O5-C1-C2	4.40	117.56	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C8-C7-N2	4.23	123.27	116.10
3	C	1	NAG	C2-N2-C7	-4.13	117.03	122.90
3	C	1	NAG	O5-C1-C2	-4.07	104.86	111.29
2	B	2	NAG	C1-C2-N2	4.04	117.39	110.49
3	C	1	NAG	C4-C3-C2	3.64	116.35	111.02
2	B	1	NAG	C4-C3-C2	3.54	116.20	111.02
2	B	3	MAN	O5-C5-C6	3.48	112.66	107.20
3	C	2	NAG	C4-C3-C2	3.38	115.97	111.02
2	B	2	NAG	C2-N2-C7	3.08	127.28	122.90
3	C	2	NAG	O4-C4-C5	2.90	116.50	109.30
2	B	2	NAG	C4-C3-C2	2.80	115.13	111.02
3	C	1	NAG	C8-C7-N2	2.79	120.83	116.10
2	B	1	NAG	C1-O5-C5	2.69	115.84	112.19
2	B	3	MAN	C2-C3-C4	-2.64	106.32	110.89
3	C	1	NAG	O5-C5-C6	2.54	111.18	107.20
2	B	3	MAN	C3-C4-C5	-2.43	105.91	110.24
2	B	2	NAG	O7-C7-C8	-2.29	117.81	122.06
2	B	2	NAG	C6-C5-C4	-2.21	107.82	113.00
3	C	1	NAG	O3-C3-C4	-2.08	105.54	110.35
2	B	1	NAG	O7-C7-N2	-2.02	118.25	121.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

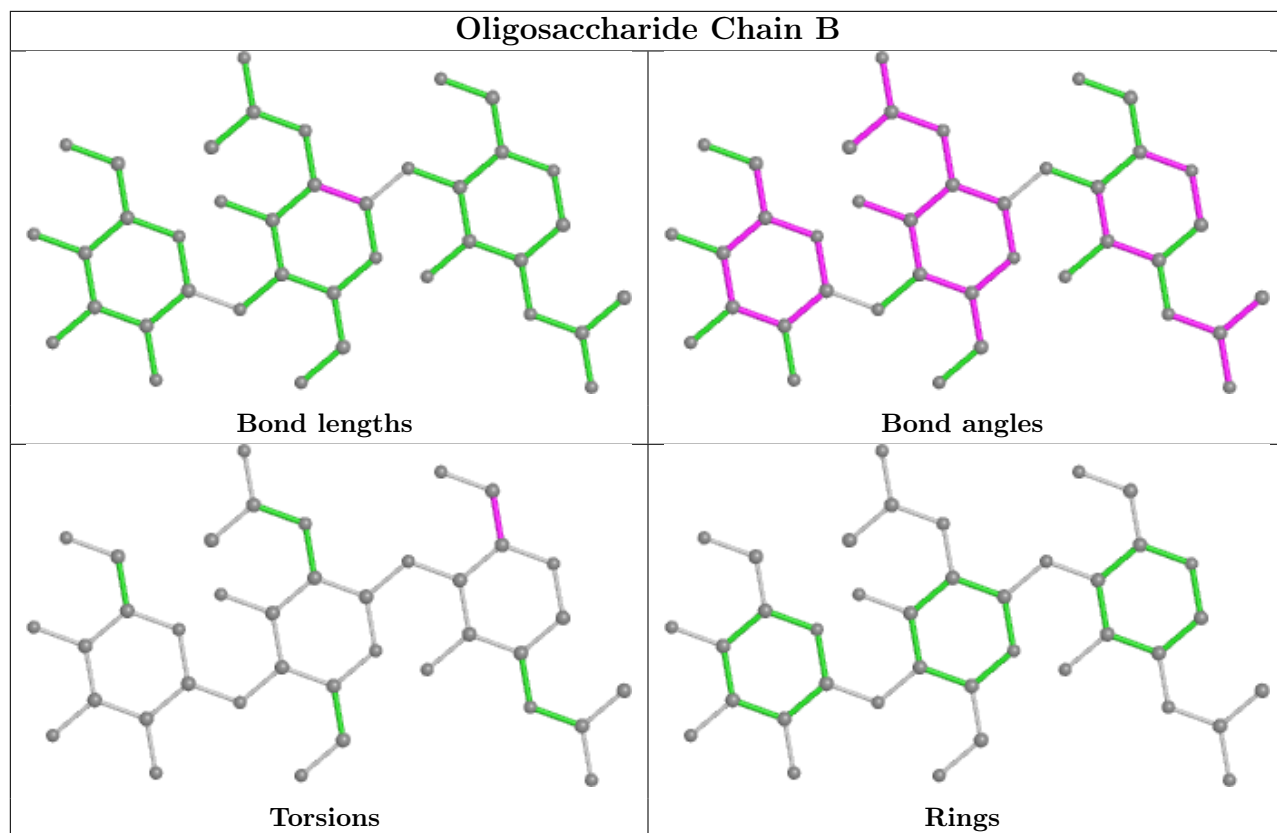
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

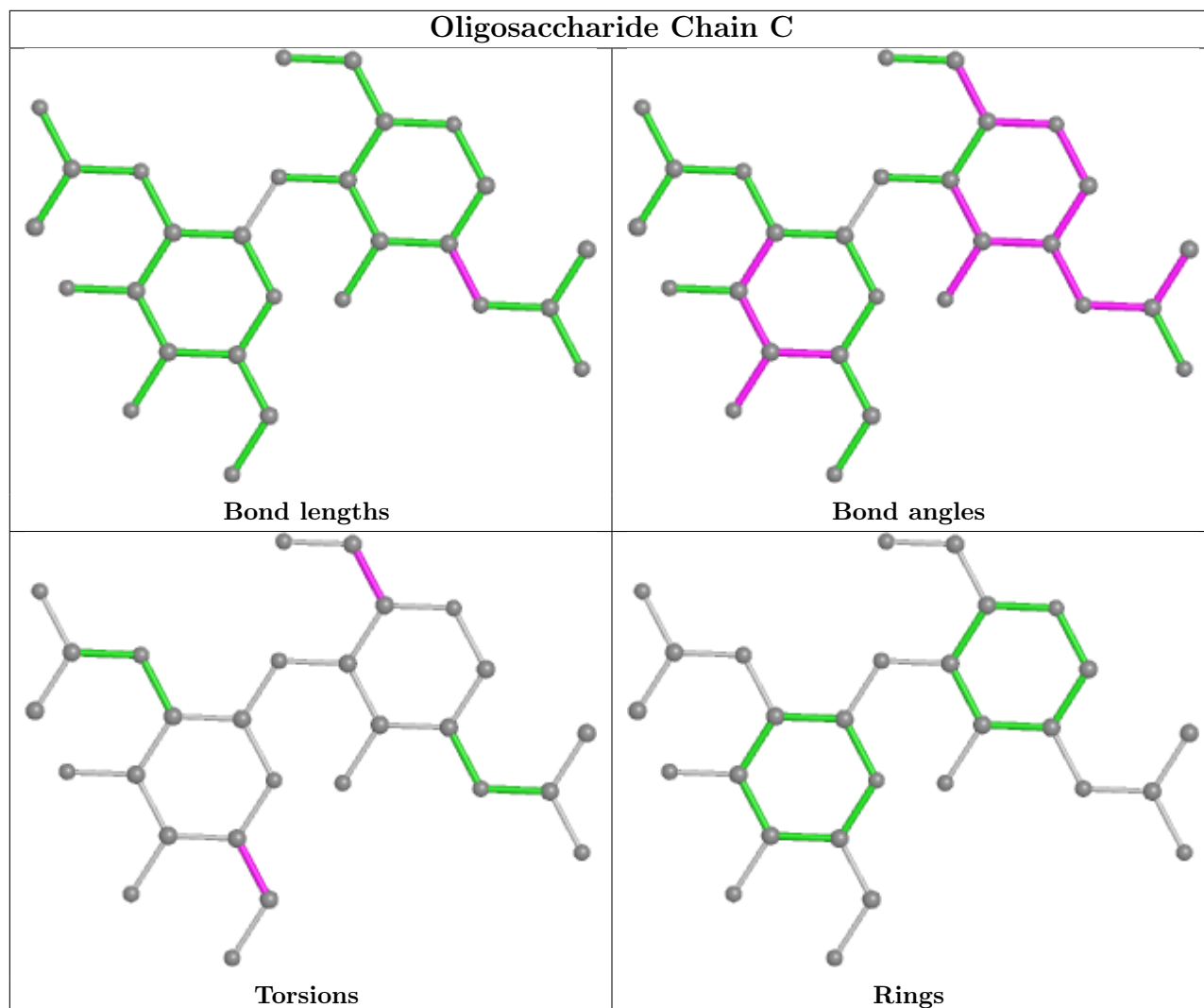
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	CO3	A	802	6	2,3,3	0.21	0	2,3,3	2.12	2 (100%)
10	M2P	A	707	-	11,11,19	0.45	0	14,14,28	1.06	1 (7%)
4	NAG	A	701	1	14,14,15	0.58	0	17,19,21	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	A	708	-	12,12,12	0.61	0	17,17,17	1.08	2 (11%)
9	SO4	A	805	-	4,4,4	0.11	0	6,6,6	0.48	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
5	BMA	A	708	-	-	0/2/22/22	0/1/1/1
10	M2P	A	707	-	-	13/16/16/24	-
4	NAG	A	701	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	NAG	C1-O5-C5	3.60	117.06	112.19
4	A	701	NAG	C1-C2-N2	2.55	114.85	110.49
5	A	708	BMA	O4-C4-C3	-2.50	104.56	110.35
7	A	802	CO3	O3-C-O1	2.17	125.17	119.55
4	A	701	NAG	O3-C3-C2	-2.14	105.03	109.47
7	A	802	CO3	O2-C-O1	-2.07	114.19	119.55
10	A	707	M2P	C6-C5-C4	2.04	116.84	112.41
5	A	708	BMA	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	707	M2P	O1-C1-C2-O2
10	A	707	M2P	C4-C5-C6-O6
10	A	707	M2P	O5-C5-C6-O6
10	A	707	M2P	O4-C4-C5-C6
10	A	707	M2P	C3-C4-C5-O5
10	A	707	M2P	O4-C4-C5-O5
10	A	707	M2P	O2-C2-C3-C4
10	A	707	M2P	O2-C2-C3-O3
10	A	707	M2P	O1-C1-C2-C3
10	A	707	M2P	C1-C2-C3-O3
10	A	707	M2P	C3-C4-C5-C6

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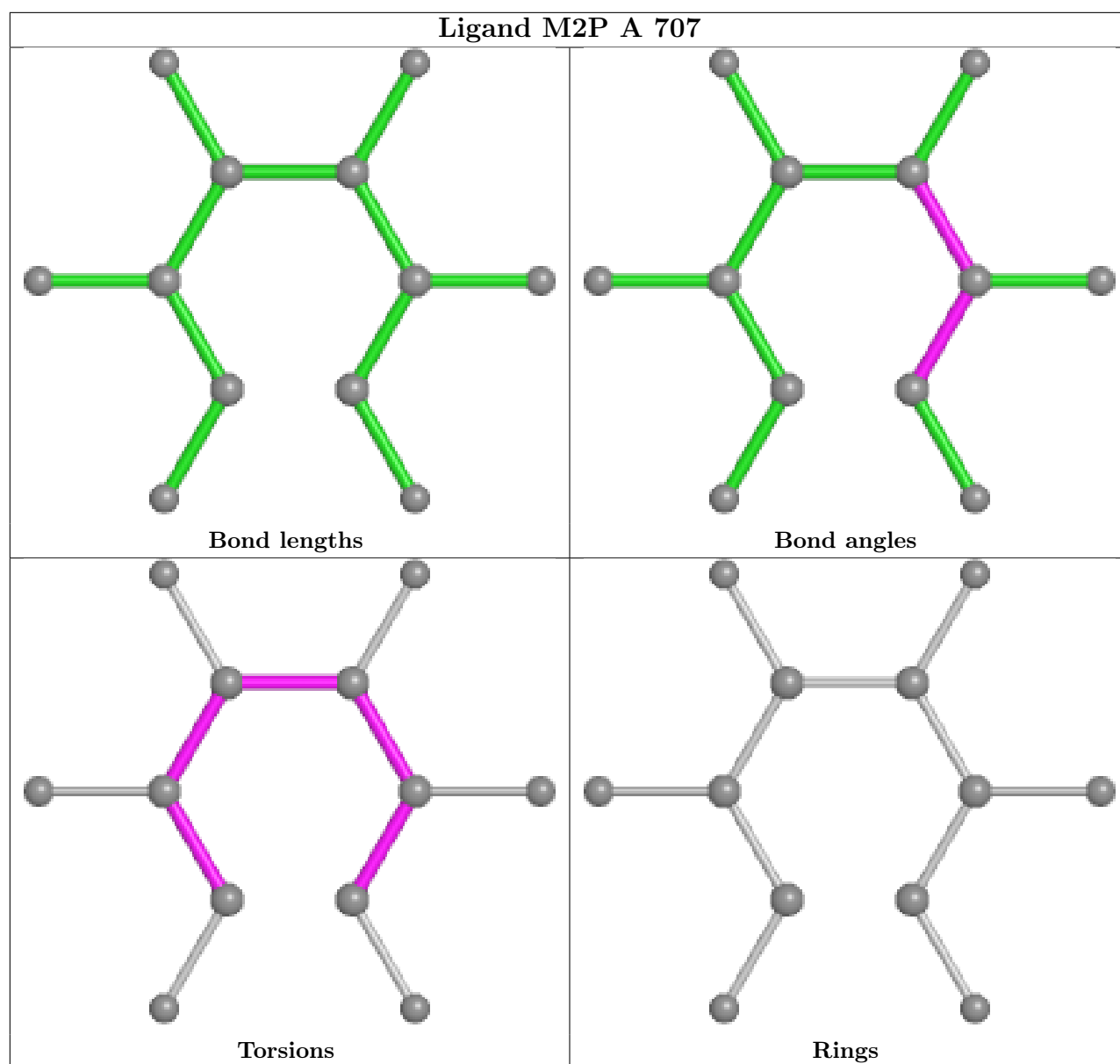
Mol	Chain	Res	Type	Atoms
10	A	707	M2P	C1-C2-C3-C4
4	A	701	NAG	O7-C7-N2-C2
10	A	707	M2P	O3-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	802	CO3	1	0
10	A	707	M2P	1	0
5	A	708	BMA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/348 (97%)	0.40	32 (9%) 8 7	6, 21, 48, 85	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	ALA	7.9
1	A	682	GLU	7.1
1	A	681	LEU	6.8
1	A	421	SER	6.7
1	A	418	SER	6.2
1	A	479	GLY	5.8
1	A	342	TYR	5.5
1	A	684	CYS	5.0
1	A	670	ALA	4.7
1	A	676	SER	4.0
1	A	509	ASP	4.0
1	A	625	CYS	3.7
1	A	420	HIS	3.7
1	A	683	ALA	3.2
1	A	422	SER	3.1
1	A	627	ASP	3.0
1	A	343	THR	2.9
1	A	672	LEU	2.9
1	A	478	THR	2.8
1	A	675	CYS	2.6
1	A	621	ASN	2.5
1	A	626	PRO	2.5
1	A	424	ASP	2.5
1	A	669	ILE	2.5
1	A	419	LYS	2.5
1	A	635	GLU	2.5
1	A	417	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	475	VAL	2.3
1	A	399	ILE	2.2
1	A	607	VAL	2.1
1	A	686	PHE	2.1
1	A	664	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

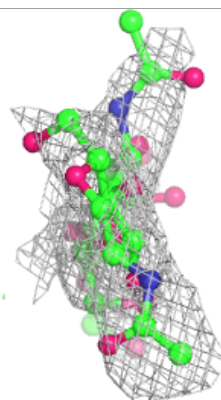
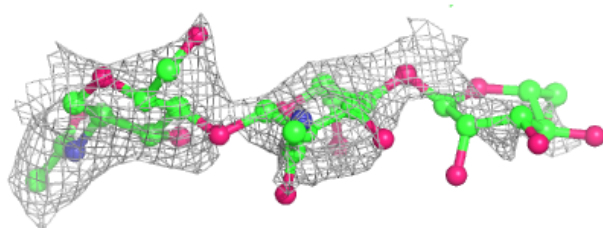
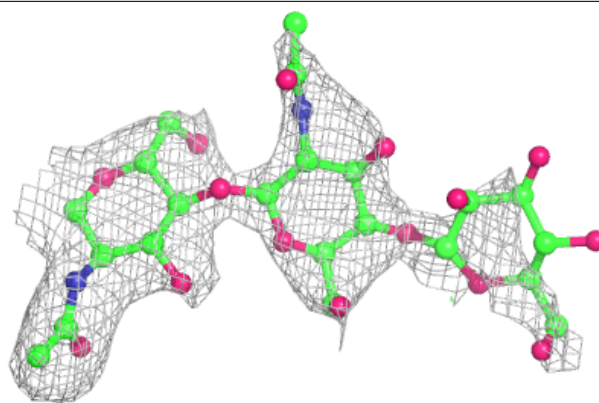
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	3	11/12	0.69	0.59	76,79,82,82	0
3	NAG	C	2	14/15	0.69	0.38	44,48,55,55	0
2	NAG	B	2	14/15	0.83	0.37	59,62,69,70	0
2	NAG	B	1	14/15	0.84	0.28	38,45,49,56	0
3	NAG	C	1	14/15	0.96	0.19	19,24,28,35	0

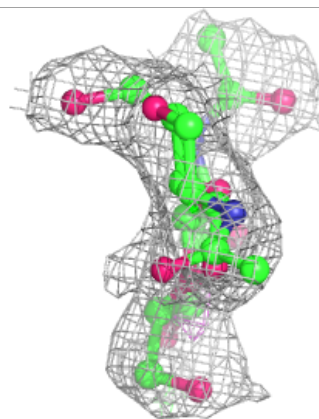
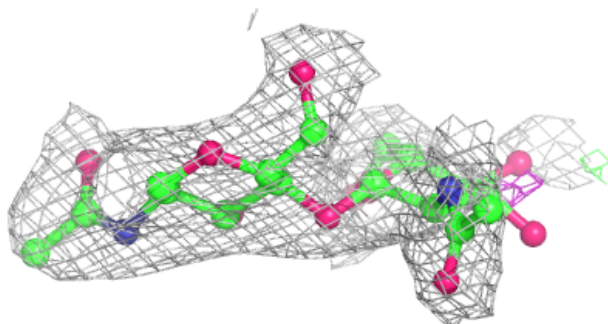
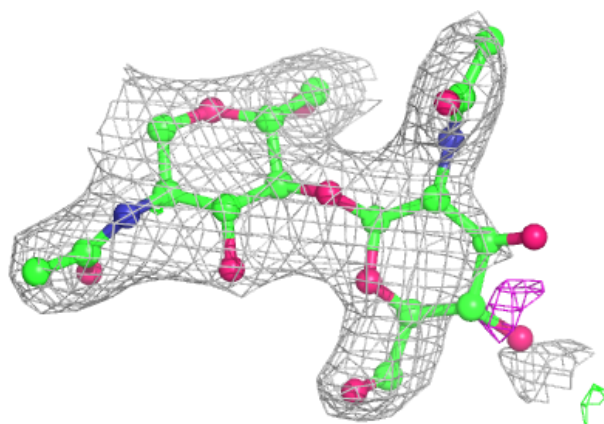
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**Electron density around Chain C:**

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

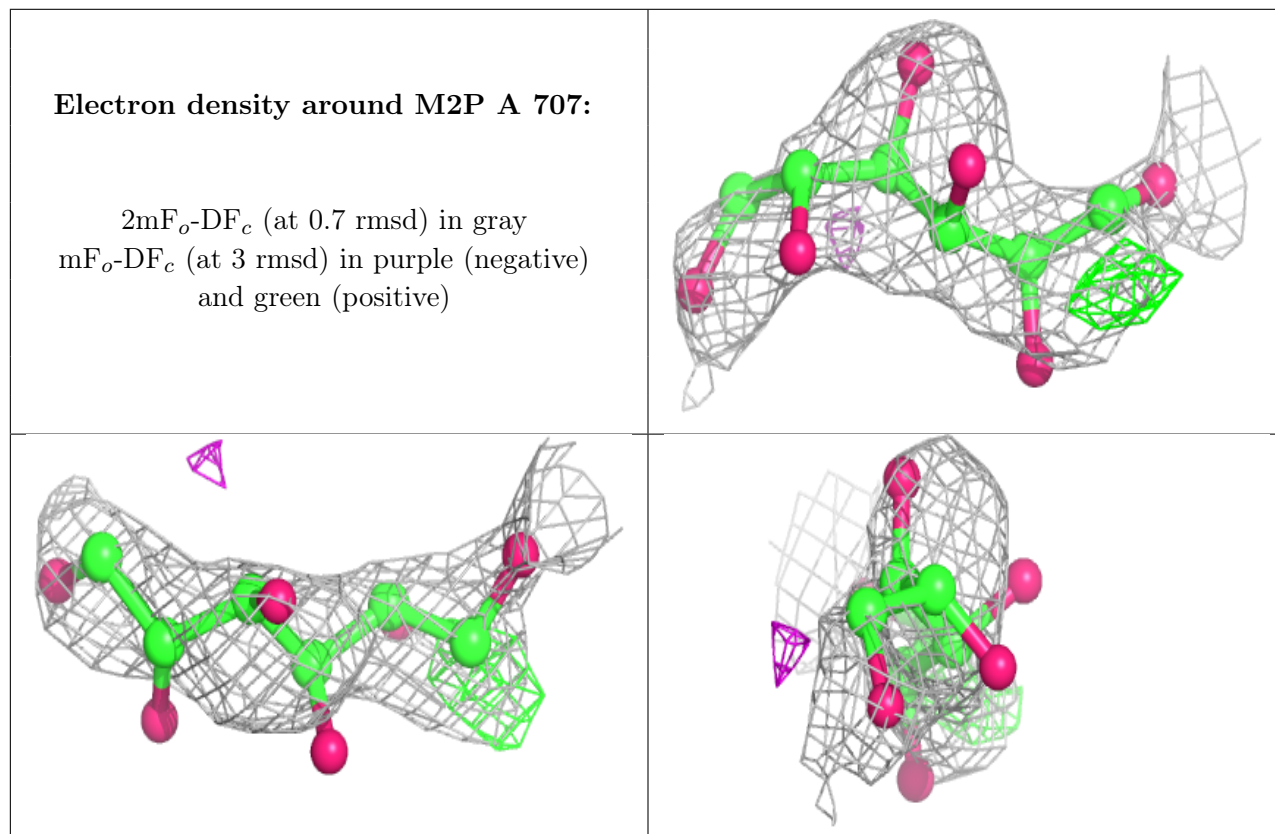


6.4 Ligands [i](#)

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
10	M2P	A	707	12/20	0.70	0.42	60,62,63,63	12
4	NAG	A	701	14/15	0.73	0.44	51,56,62,63	0
5	BMA	A	708	12/12	0.78	0.36	61,64,66,67	12
9	SO4	A	805	5/5	0.95	0.16	26,28,29,29	5
7	CO3	A	802	4/4	0.96	0.19	17,20,20,21	0
6	FE	A	801	1/1	0.99	0.03	22,22,22,22	0
8	ZN	A	803	1/1	0.99	0.03	20,20,20,20	0
8	ZN	A	804	1/1	1.00	0.03	26,26,26,26	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.