



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:36 AM UTC

PDB ID : 2ALU / pdb_00002alu
Title : Detection of new binding site in the C-terminal lobe of lactoferrin:Crystal structure of the complex formed between bovine lactoferrin and a tetrasaccharide at 2.1Å resolution
Authors : Singh, N.; Jabeen, T.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2005-08-08
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

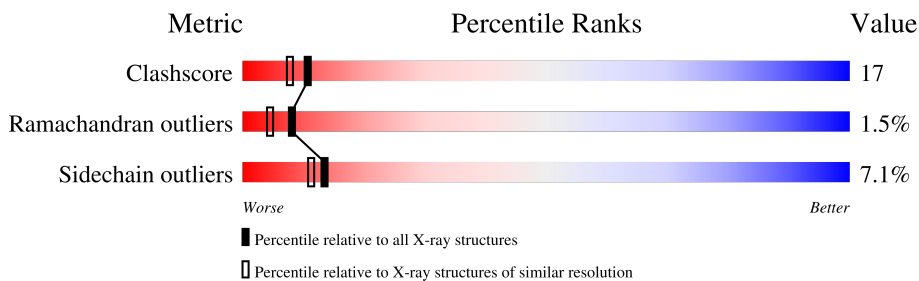
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	 71% 22% . . .
2	B	3	 67% 33%
3	C	6	 33% 67%
4	D	4	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3067 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.

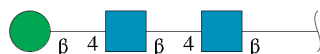
- Molecule 1 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2593	1613	453	506	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 beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



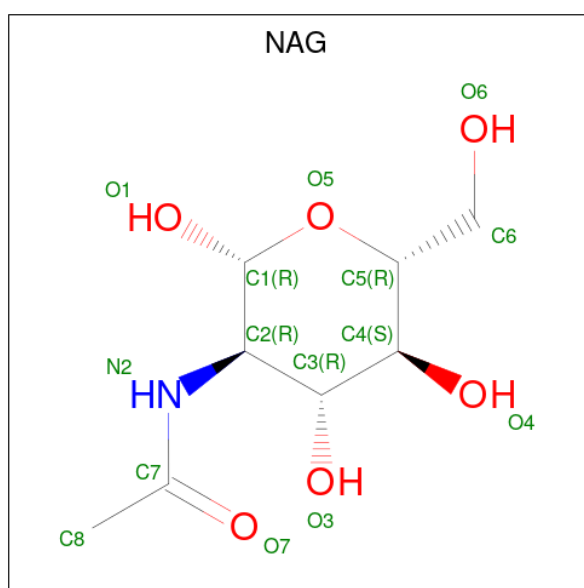
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	72	40	2	30	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			56	32	4	20			

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



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

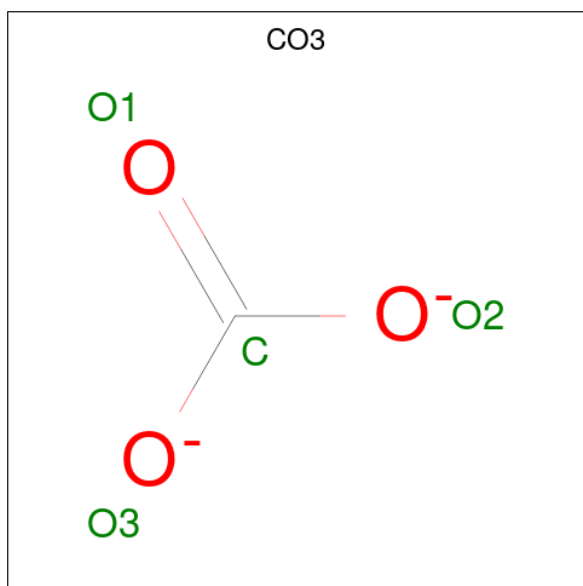
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	281	Total	O	0	0
			281	281		

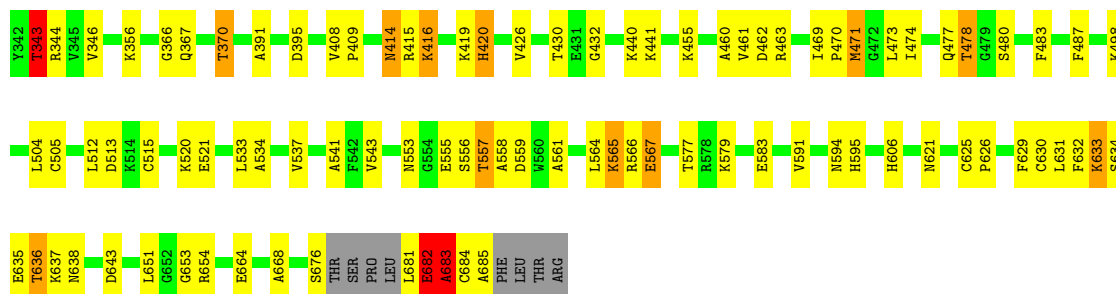
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Lactotransferrin

Chain A: 



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

Chain B: 



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

Chain C: 



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

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.51Å 50.52Å 66.11Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	63.25 – 2.09	Depositor
% Data completeness (in resolution range)	91.5 (63.25-2.09)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.198 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3067	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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, NDG, FE, SO4, BMA, MAN, CO3, ZN

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	0.88	1/2640 (0.0%)	1.16	7/3575 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	MET	SD-CE	-8.01	1.59	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	ALA	N-CA-C	-7.23	95.41	110.80
1	A	537	VAL	CA-C-N	-6.61	116.58	122.47
1	A	537	VAL	C-N-CA	-6.61	116.58	122.47
1	A	391	ALA	N-CA-C	5.89	117.20	108.60
1	A	651	LEU	N-CA-C	5.85	118.54	111.40
1	A	537	VAL	N-CA-C	-5.52	105.73	111.58
1	A	343	THR	N-CA-C	-5.13	107.19	112.93

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	2593	0	2510	80	0
2	B	39	0	34	1	0
3	C	72	0	61	10	0
4	D	56	0	48	4	0
5	A	14	0	13	1	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0
9	A	5	0	0	0	0
10	A	281	0	0	9	0
All	All	3067	0	2666	91	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 17.

All (91) 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:555:GLU:OE2	3:C:5:MAN:H3	1.59	1.00
1:A:343:THR:HA	1:A:606:HIS:NE2	1.77	0.99
1:A:565:LYS:HD2	1:A:567:GLU:H	1.37	0.90
1:A:638:ASN:HD22	1:A:643:ASP:H	1.25	0.84
1:A:565:LYS:CD	1:A:567:GLU:H	1.95	0.80
5:A:1:NAG:H3	10:A:971:HOH:O	1.84	0.78
1:A:638:ASN:ND2	1:A:643:ASP:H	1.81	0.77
1:A:474:ILE:O	1:A:478:THR:HB	1.88	0.73
1:A:625:CYS:C	1:A:630:CYS:SG	2.71	0.73
1:A:635:GLU:HG3	1:A:637:LYS:HD3	1.74	0.70
1:A:478:THR:HG22	1:A:480:SER:H	1.58	0.69
1:A:636:THR:HA	10:A:857:HOH:O	1.92	0.68
1:A:577:THR:HG21	1:A:579:LYS:NZ	2.08	0.68
1:A:556:SER:C	1:A:558:ALA:H	2.03	0.66
1:A:635:GLU:HB3	10:A:939:HOH:O	1.97	0.64
1:A:565:LYS:HD3	1:A:566:ARG:N	2.12	0.64
1:A:664:GLU:HB2	10:A:877:HOH:O	1.96	0.64
1:A:555:GLU:CD	3:C:5:MAN:H3	2.22	0.64
1:A:632:PHE:O	1:A:633:LYS:HE3	2.00	0.62
1:A:513:ASP:OD2	1:A:520:LYS:NZ	2.31	0.61
1:A:419:LYS:HD3	1:A:420:HIS:N	2.15	0.61
1:A:565:LYS:HD2	1:A:567:GLU:N	2.13	0.60
1:A:635:GLU:HG2	10:A:748:HOH:O	2.01	0.60
3:C:2:NAG:O3	3:C:3:BMA:H5	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLU:O	1:A:636:THR:HG22	2.02	0.59
3:C:2:NAG:O3	3:C:3:BMA:C1	2.50	0.59
1:A:440:LYS:HE3	1:A:534:ALA:HA	1.84	0.58
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.86	0.58
1:A:478:THR:HG23	1:A:480:SER:HB3	1.85	0.58
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.86	0.57
1:A:556:SER:O	1:A:558:ALA:N	2.37	0.57
4:D:1:NAG:H61	4:D:2:NDG:O5	2.04	0.57
1:A:555:GLU:OE2	3:C:5:MAN:O4	2.22	0.57
1:A:625:CYS:O	1:A:630:CYS:SG	2.63	0.57
1:A:625:CYS:CB	1:A:626:PRO:HD3	2.36	0.56
1:A:416:LYS:NZ	1:A:416:LYS:HB3	2.22	0.55
1:A:471:MET:HE1	1:A:487:PHE:HE2	1.71	0.55
1:A:343:THR:HG23	1:A:343:THR:O	2.07	0.55
1:A:478:THR:CG2	1:A:480:SER:H	2.20	0.55
1:A:415:ARG:NH2	1:A:432:GLY:O	2.31	0.55
1:A:653:GLY:O	1:A:654:ARG:C	2.49	0.54
1:A:561:ALA:HA	1:A:564:LEU:HG	1.90	0.54
1:A:344:ARG:NH2	10:A:809:HOH:O	2.40	0.54
4:D:1:NAG:H61	4:D:2:NDG:C1	2.38	0.53
1:A:513:ASP:OD2	1:A:520:LYS:CE	2.56	0.53
1:A:681:LEU:O	1:A:682:GLU:CB	2.57	0.53
3:C:2:NAG:O3	3:C:3:BMA:C5	2.58	0.52
1:A:556:SER:C	1:A:558:ALA:N	2.68	0.51
1:A:555:GLU:OE2	3:C:5:MAN:C3	2.45	0.50
1:A:430:THR:HB	1:A:594:ASN:HD22	1.74	0.50
1:A:638:ASN:HD22	1:A:643:ASP:N	2.03	0.50
1:A:625:CYS:HA	1:A:629:PHE:O	2.12	0.50
1:A:556:SER:C	1:A:557:THR:HG23	2.36	0.49
1:A:441:LYS:HD3	10:A:819:HOH:O	2.13	0.49
3:C:2:NAG:C3	3:C:3:BMA:O5	2.60	0.48
1:A:346:VAL:HG22	1:A:370:THR:HG22	1.96	0.48
1:A:682:GLU:O	1:A:683:ALA:HB2	2.15	0.47
1:A:343:THR:CA	1:A:606:HIS:NE2	2.65	0.47
1:A:505:CYS:HB3	1:A:521:GLU:OE1	2.14	0.47
1:A:577:THR:HG21	1:A:579:LYS:HZ3	1.78	0.46
3:C:2:NAG:O3	3:C:3:BMA:O5	2.33	0.46
1:A:455:LYS:NZ	10:A:791:HOH:O	2.45	0.45
1:A:430:THR:HB	1:A:594:ASN:ND2	2.30	0.45
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.51	0.45
1:A:473:LEU:O	1:A:477:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:O	1:A:426:VAL:HG12	2.16	0.45
1:A:577:THR:HG21	1:A:579:LYS:HZ2	1.79	0.45
1:A:483:PHE:CD2	1:A:483:PHE:C	2.95	0.45
1:A:461:VAL:O	1:A:462:ASP:HB2	2.17	0.44
4:D:2:NDG:H3	4:D:3:NAG:O7	2.17	0.44
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.99	0.44
1:A:637:LYS:HE2	10:A:909:HOH:O	2.18	0.44
4:D:3:NAG:H61	4:D:4:NAG:C1	2.48	0.44
1:A:366:GLY:O	1:A:367:GLN:HB2	2.17	0.43
1:A:668:ALA:HB1	2:B:1:NAG:H83	2.00	0.43
1:A:395:ASP:HB2	1:A:595:HIS:CE1	2.53	0.43
1:A:553:ASN:OD1	1:A:566:ARG:HG3	2.19	0.43
1:A:416:LYS:HB3	1:A:416:LYS:HZ3	1.83	0.43
1:A:414:ASN:HD22	1:A:414:ASN:HA	1.68	0.42
3:C:4:MAN:O3	3:C:5:MAN:H5	2.19	0.42
1:A:533:LEU:HB2	1:A:541:ALA:HB2	2.02	0.42
1:A:498:LYS:HE2	1:A:498:LYS:HB2	1.61	0.42
1:A:513:ASP:OD2	1:A:520:LYS:HE2	2.20	0.42
1:A:634:SER:O	1:A:637:LYS:HB2	2.20	0.41
1:A:683:ALA:O	1:A:685:ALA:N	2.53	0.41
1:A:408:VAL:HA	1:A:409:PRO:HD3	1.85	0.41
1:A:565:LYS:HD3	1:A:565:LYS:C	2.45	0.41
1:A:681:LEU:O	1:A:682:GLU:HB2	2.20	0.41
1:A:469:ILE:HB	1:A:470:PRO:HD3	2.02	0.40
1:A:512:LEU:O	1:A:513:ASP:HB2	2.21	0.40
1:A:636:THR:O	1:A:636:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	336/348 (97%)	318 (95%)	13 (4%)	5 (2%)	8 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ALA
1	A	684	CYS
1	A	682	GLU
1	A	557	THR
1	A	543	VAL

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	281/289 (97%)	261 (93%)	20 (7%)	13 11

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	356	LYS
1	A	370	THR
1	A	414	ASN
1	A	416	LYS
1	A	420	HIS
1	A	478	THR
1	A	504	LEU
1	A	515	CYS
1	A	559	ASP
1	A	565	LYS
1	A	567	GLU
1	A	583	GLU
1	A	591	VAL
1	A	621	ASN
1	A	631	LEU

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Mol	Chain	Res	Type
1	A	633	LYS
1	A	636	THR
1	A	676	SER
1	A	682	GLU

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	360	GLN
1	A	414	ASN
1	A	594	ASN
1	A	621	ASN
1	A	624	ASN
1	A	638	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	2,1	14,14,15	0.83	0	17,19,21	1.31	2 (11%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	1.74	2 (11%)
2	BMA	B	3	2	11,11,12	0.51	0	15,15,17	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	3,1	14,14,15	1.20	1 (7%)	17,19,21	1.40	4 (23%)
3	NAG	C	2	3	14,14,15	0.69	0	17,19,21	1.64	4 (23%)
3	BMA	C	3	3	11,11,12	0.94	1 (9%)	15,15,17	1.57	4 (26%)
3	MAN	C	4	3	11,11,12	0.47	0	15,15,17	1.45	2 (13%)
3	MAN	C	5	3	11,11,12	0.65	0	15,15,17	1.42	2 (13%)
3	MAN	C	6	3	11,11,12	0.57	0	15,15,17	0.96	2 (13%)
4	NAG	D	1	4	14,14,15	0.65	0	17,19,21	1.60	2 (11%)
4	NDG	D	2	4	14,14,15	1.11	1 (7%)	17,19,21	2.36	4 (23%)
4	NAG	D	3	4	14,14,15	0.91	1 (7%)	17,19,21	1.40	4 (23%)
4	NAG	D	4	4	14,14,15	0.66	0	17,19,21	0.82	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
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	4	-	0/6/23/26	0/1/1/1
4	NDG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	3	4	-	0/6/23/26	0/1/1/1
4	NAG	D	4	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	3.76	1.57	1.52
4	D	3	NAG	C1-C2	2.93	1.56	1.52
4	D	2	NDG	O5-C1	-2.91	1.38	1.43
3	C	3	BMA	O5-C1	-2.32	1.39	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NDG	O5-C1-C2	-5.71	102.45	111.29
2	B	2	NAG	C1-O5-C5	5.21	119.17	112.19
4	D	2	NDG	C1-O5-C5	-4.94	105.56	112.19
4	D	2	NDG	C4-C3-C2	4.78	118.02	111.02
4	D	1	NAG	O4-C4-C3	-4.45	99.89	110.38
4	D	1	NAG	C2-N2-C7	-3.71	117.93	122.90
3	C	2	NAG	C1-O5-C5	-3.67	107.27	112.19
3	C	4	MAN	C1-O5-C5	3.22	116.51	112.19
3	C	3	BMA	C3-C4-C5	3.10	115.85	110.23
3	C	2	NAG	O5-C5-C4	-3.06	103.39	110.83
2	B	1	NAG	C1-O5-C5	3.02	116.23	112.19
4	D	3	NAG	C4-C3-C2	2.98	115.38	111.02
3	C	3	BMA	C2-C3-C4	2.95	116.05	110.86
3	C	5	MAN	O4-C4-C5	2.87	116.39	109.32
3	C	1	NAG	O5-C1-C2	-2.76	107.03	111.29
3	C	2	NAG	C3-C4-C5	-2.74	105.26	110.23
3	C	5	MAN	C1-O5-C5	2.59	115.66	112.19
4	D	3	NAG	C1-C2-N2	2.49	114.36	110.43
3	C	3	BMA	C1-O5-C5	2.41	115.42	112.19
2	B	1	NAG	O4-C4-C5	-2.37	103.50	109.32
2	B	3	BMA	C1-O5-C5	2.35	115.33	112.19
3	C	1	NAG	O4-C4-C3	-2.34	104.86	110.38
4	D	4	NAG	C1-O5-C5	2.33	115.31	112.19
2	B	2	NAG	C6-C5-C4	-2.32	107.32	113.02
4	D	2	NDG	C6-C5-C4	2.32	118.71	113.02
4	D	3	NAG	C3-C4-C5	2.23	114.27	110.23
3	C	3	BMA	O5-C1-C2	-2.22	105.49	110.79
3	C	1	NAG	C1-C2-N2	2.22	113.93	110.43
3	C	6	MAN	O5-C1-C2	-2.21	105.51	110.79
4	D	3	NAG	O5-C1-C2	-2.09	108.06	111.29
3	C	2	NAG	O5-C5-C6	2.06	111.67	107.66
3	C	1	NAG	C1-O5-C5	2.05	114.93	112.19
3	C	6	MAN	C3-C4-C5	2.04	113.94	110.23
3	C	4	MAN	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NDG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

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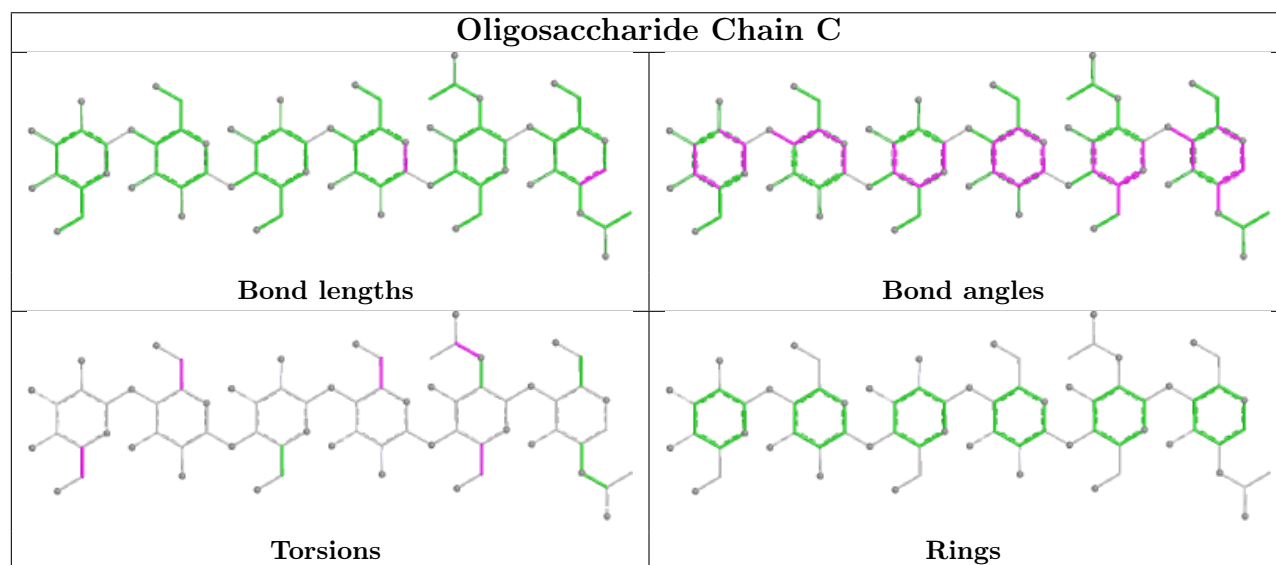
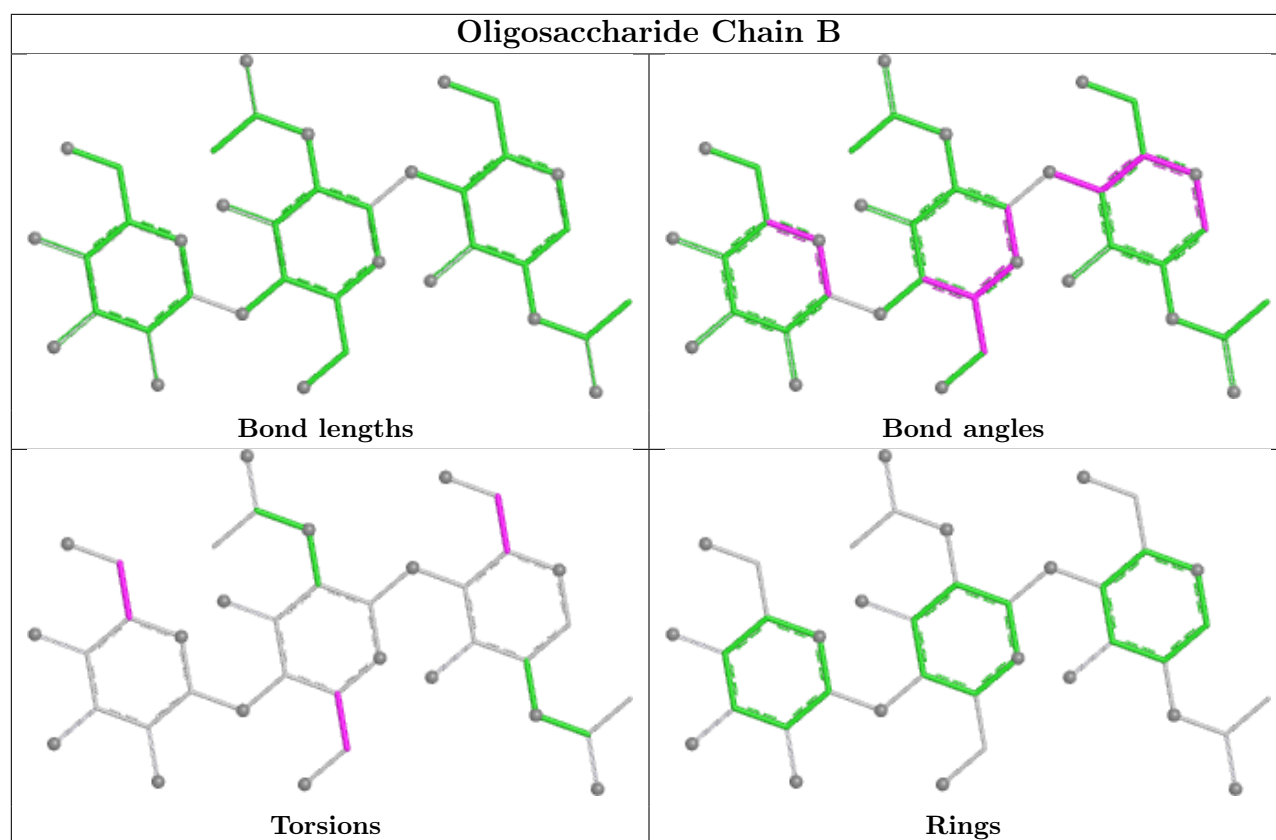
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
4	D	2	NDG	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	6	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

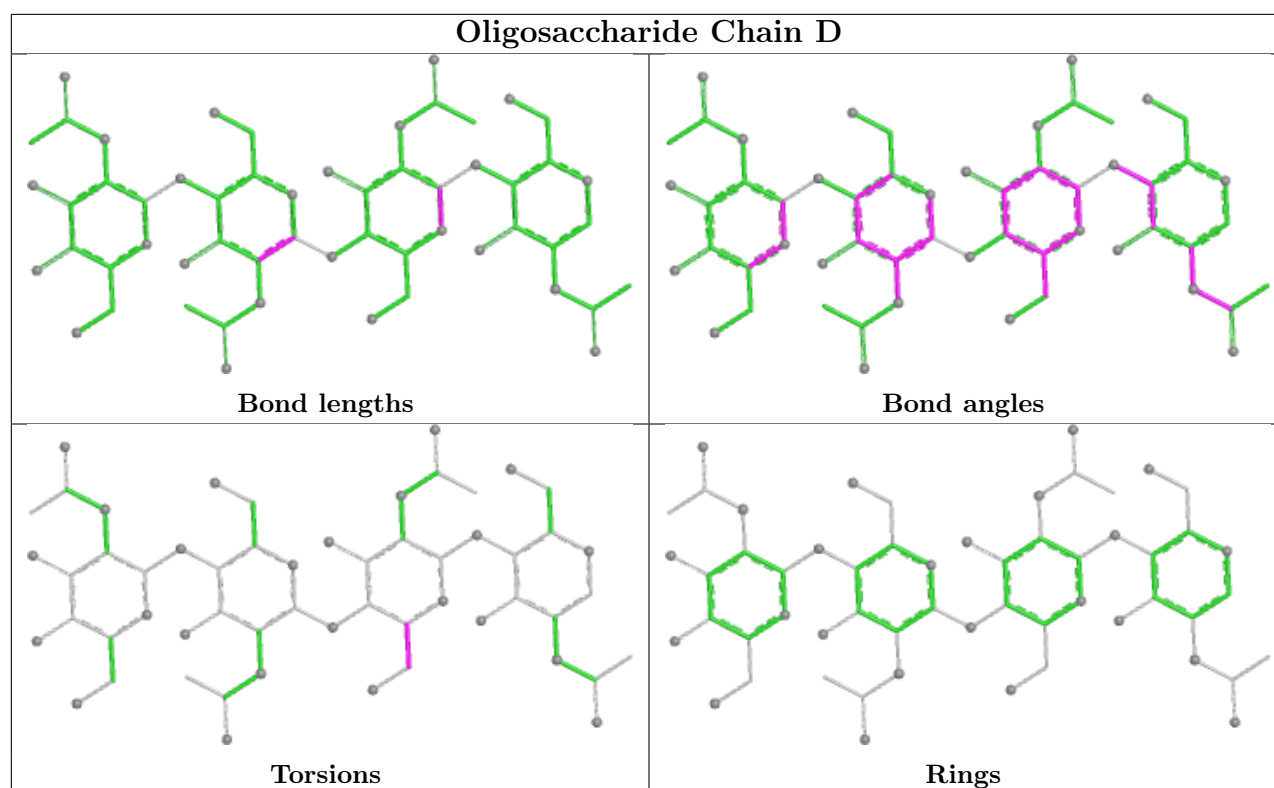
There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NDG	3	0
3	C	4	MAN	1	0
4	D	3	NAG	2	0
2	B	1	NAG	1	0
4	D	1	NAG	2	0
3	C	2	NAG	5	0
4	D	4	NAG	1	0
3	C	5	MAN	5	0
3	C	3	BMA	5	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
9	SO4	A	301	-	4,4,4	0.18	0	6,6,6	0.30	0
8	CO3	A	695	7	3,3,3	0.96	0	2,3,3	0.41	0
5	NAG	A	1	1	14,14,15	0.86	1 (7%)	17,19,21	1.61	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	NAG	O5-C1	-2.21	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	NAG	O5-C1-C2	-4.24	104.73	111.29
5	A	1	NAG	C4-C3-C2	2.59	114.81	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.