



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:32 AM GMT

PDB ID : 2DVC  
Title : Structure of the bovine lactoferrin C-lobe complex with sucrose at 3.0 Å resolution  
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Deposited on : 2006-07-31  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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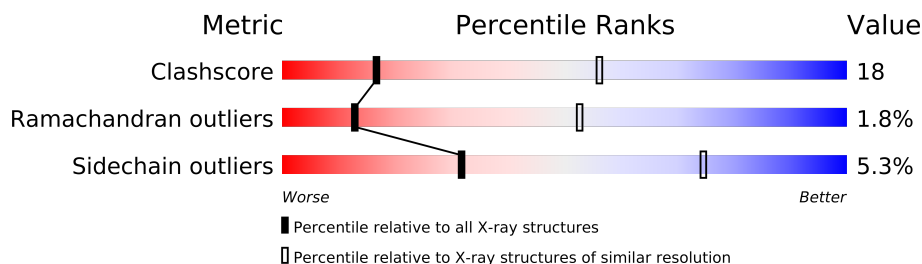
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 2986 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	341	Total	C	N	O	S	0	0	0
			2605	1622	454	508	21			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

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

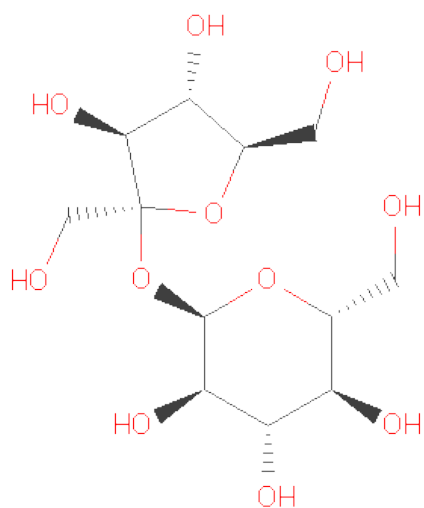
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is SUGAR (SUCROSE) (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).

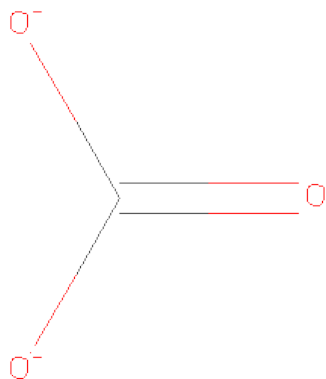


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	12	11		

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

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

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula:  $CO_3$ ).

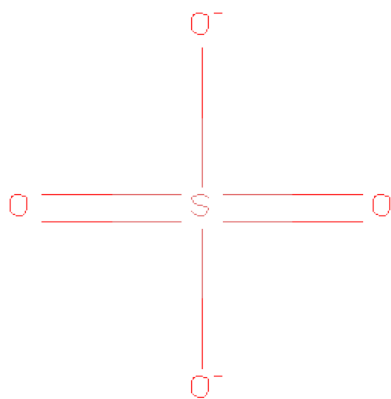


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		

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

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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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	185	Total	O	0	0
			185	185		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: Lactotransferrin



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.46Å 50.40Å 65.92Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	19.84 – 3.00	Depositor
% Data completeness (in resolution range)	87.7 (19.84-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, BMA, SUC, NAG, ZN, SO4, MAN, FE

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	0.39	0/2653	0.69	3/3591 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	ALA	N-CA-C	9.11	135.60	111.00
1	A	683	ALA	CB-CA-C	-7.16	99.36	110.10
1	A	343	THR	N-CA-C	5.29	125.29	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	4	MAN	C1

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2605	0	2519	88	0
2	A	61	0	52	5	0
3	A	28	0	25	0	0
4	A	72	0	61	8	0
5	A	23	0	21	6	0
6	A	1	0	0	0	0
7	A	4	0	0	0	0
8	A	2	0	0	0	0
9	A	5	0	0	0	0
10	A	185	0	0	9	0
All	All	2986	0	2678	98	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:2:NAG:O3	2:A:3:BMA:H2	1.44	1.16
1:A:662:GLY:HA2	5:A:1001:SUC:H61	1.23	1.09
1:A:343:THR:HA	1:A:606:HIS:NE2	1.76	0.99
1:A:662:GLY:CA	5:A:1001:SUC:H61	1.97	0.94
1:A:430:THR:HB	1:A:594:ASN:HD22	1.38	0.89
1:A:549:TRP:HB3	4:A:690:NAG:H82	1.56	0.86
1:A:625:CYS:HA	1:A:629:PHE:O	1.75	0.86
1:A:430:THR:HB	1:A:594:ASN:ND2	1.98	0.77
4:A:691:BMA:H5	4:A:692:BMA:O2	1.85	0.77
1:A:662:GLY:HA2	5:A:1001:SUC:C6	2.13	0.72
1:A:565:LYS:HD3	1:A:566:ARG:N	2.07	0.70
2:A:2:NAG:C3	2:A:3:BMA:H2	2.24	0.68
1:A:402:ALA:HB1	1:A:407:LEU:HD12	1.78	0.65
1:A:478:THR:HG22	1:A:480:SER:HB3	1.79	0.65
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.31	0.64
1:A:343:THR:CA	1:A:606:HIS:NE2	2.56	0.63
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.80	0.63
1:A:625:CYS:C	1:A:630:CYS:SG	2.77	0.63
1:A:682:GLU:HG3	1:A:682:GLU:O	1.97	0.63
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.80	0.63
1:A:663:THR:H	5:A:1001:SUC:C6	2.12	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:692:BMA:O3	4:A:693:MAN:H2	1.99	0.62
1:A:638:ASN:HD22	1:A:643:ASP:H	1.46	0.62
1:A:464:THR:HG21	1:A:592:ALA:CB	2.29	0.62
1:A:565:LYS:CD	1:A:567:GLU:H	2.13	0.61
2:A:2:NAG:HO3	2:A:3:BMA:H2	1.58	0.61
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.85	0.59
1:A:577:THR:CG2	1:A:578:ARG:N	2.66	0.58
4:A:689:NAG:H61	4:A:690:NAG:HN2	1.70	0.57
1:A:663:THR:H	5:A:1001:SUC:H61	1.69	0.56
1:A:452:LYS:O	1:A:453:ASP:HB2	2.06	0.56
4:A:691:BMA:H3	4:A:692:BMA:O2	2.06	0.56
1:A:625:CYS:CB	1:A:626:PRO:HD3	2.36	0.55
1:A:410:VAL:HG12	1:A:411:LEU:HG	1.89	0.54
1:A:343:THR:O	1:A:343:THR:HG23	2.06	0.54
1:A:638:ASN:ND2	1:A:643:ASP:H	2.05	0.54
1:A:565:LYS:HD2	1:A:567:GLU:H	1.73	0.54
1:A:460:ALA:HA	1:A:493:PRO:HD2	1.90	0.54
1:A:343:THR:N	1:A:606:HIS:NE2	2.57	0.52
1:A:663:THR:N	5:A:1001:SUC:H61	2.25	0.52
4:A:689:NAG:H61	4:A:690:NAG:N2	2.25	0.52
1:A:577:THR:HG22	1:A:578:ARG:N	2.24	0.51
1:A:392:LEU:HD11	1:A:394:LEU:HD21	1.92	0.51
1:A:662:GLY:O	1:A:666:VAL:HG23	2.10	0.51
1:A:478:THR:CG2	1:A:480:SER:HB3	2.40	0.51
1:A:475:VAL:HG13	1:A:480:SER:O	2.11	0.51
1:A:621:ASN:HB2	10:A:1155:HOH:O	2.09	0.51
1:A:440:LYS:HB2	10:A:1028:HOH:O	2.11	0.50
1:A:625:CYS:O	1:A:630:CYS:SG	2.69	0.50
1:A:548:VAL:HG11	1:A:581:VAL:HG11	1.93	0.50
1:A:635:GLU:O	1:A:636:THR:HG22	2.12	0.50
1:A:653:GLY:O	1:A:654:ARG:C	2.50	0.50
1:A:375:SER:O	1:A:376:THR:CG2	2.60	0.49
1:A:356:LYS:HG3	1:A:357:LYS:N	2.27	0.49
1:A:342:TYR:O	1:A:344:ARG:N	2.46	0.49
1:A:419:LYS:HG2	1:A:420:HIS:N	2.27	0.49
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.48	0.49
1:A:585:GLN:HG2	10:A:1091:HOH:O	2.12	0.48
1:A:355:GLN:O	1:A:359:GLN:HG3	2.14	0.47
1:A:565:LYS:HD3	1:A:567:GLU:H	1.79	0.47
1:A:512:LEU:O	1:A:513:ASP:HB2	2.13	0.47
1:A:471:MET:HE1	1:A:487:PHE:HE2	1.79	0.47
1:A:636:THR:HG23	1:A:636:THR:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:561:ALA:HA	1:A:564:LEU:HG	1.98	0.47
1:A:473:LEU:O	1:A:477:GLN:HG3	2.15	0.46
1:A:518:ASN:O	1:A:520:LYS:N	2.49	0.46
1:A:342:TYR:C	1:A:606:HIS:NE2	2.69	0.46
1:A:376:THR:HG22	1:A:517:PRO:HG2	1.98	0.45
1:A:669:ILE:O	1:A:673:LYS:HG2	2.15	0.45
1:A:681:LEU:HD12	10:A:1078:HOH:O	2.15	0.45
1:A:549:TRP:HB3	4:A:690:NAG:C8	2.37	0.45
1:A:575:ASP:OD1	1:A:577:THR:HB	2.17	0.44
1:A:345:VAL:HG23	1:A:610:VAL:HG21	1.98	0.44
1:A:668:ALA:HB1	2:A:1:NAG:H83	1.99	0.44
1:A:631:LEU:HD22	1:A:641:PHE:CE2	2.53	0.44
1:A:353:GLU:HB2	10:A:1010:HOH:O	2.17	0.43
1:A:565:LYS:C	1:A:565:LYS:HD3	2.39	0.43
1:A:513:ASP:OD2	1:A:520:LYS:HD3	2.18	0.43
1:A:583:GLU:HG3	10:A:1065:HOH:O	2.19	0.43
1:A:464:THR:HG21	1:A:592:ALA:HB2	2.00	0.43
2:A:2:NAG:O3	2:A:3:BMA:C2	2.38	0.42
1:A:543:VAL:HG23	1:A:544:LYS:N	2.34	0.42
1:A:683:ALA:HA	10:A:1063:HOH:O	2.19	0.42
1:A:458:HIS:HB3	1:A:466:GLY:O	2.20	0.42
1:A:342:TYR:O	1:A:606:HIS:CE1	2.73	0.42
1:A:375:SER:C	1:A:376:THR:HG23	2.40	0.42
1:A:459:THR:O	1:A:460:ALA:HB2	2.20	0.41
1:A:684:CYS:O	1:A:686:PHE:N	2.53	0.41
1:A:673:LYS:HA	1:A:673:LYS:HD3	1.92	0.41
1:A:514:LYS:HB2	1:A:514:LYS:HE3	1.81	0.41
1:A:652:GLY:N	10:A:1049:HOH:O	2.50	0.40
1:A:433:TYR:CE1	1:A:592:ALA:HB3	2.56	0.40
1:A:428:ARG:HA	1:A:429:PRO:HD3	1.92	0.40
4:A:691:BMA:C5	4:A:692:BMA:O2	2.63	0.40
1:A:380:CYS:HB3	1:A:392:LEU:HD13	2.03	0.40
1:A:416:LYS:HB3	10:A:1094:HOH:O	2.21	0.40
1:A:474:ILE:HD13	1:A:486:PHE:CD2	2.56	0.40
1:A:474:ILE:HD13	1:A:486:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	337/345 (98%)	315 (94%)	16 (5%)	6 (2%)	13 53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	519	SER
1	A	685	ALA
1	A	559	ASP
1	A	652	GLY
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	282/286 (99%)	267 (95%)	15 (5%)	32 74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	356	LYS
1	A	414	ASN
1	A	490	SER
1	A	500	ARG
1	A	515	CYS
1	A	546	ASP
1	A	559	ASP

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Mol	Chain	Res	Type
1	A	583	GLU
1	A	591	VAL
1	A	625	CYS
1	A	631	LEU
1	A	636	THR
1	A	664	GLU
1	A	674	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	414	ASN
1	A	594	ASN
1	A	621	ASN
1	A	638	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	A	1	1,2	12,14,15	0.72	1 (8%)	15,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	2	2	12,14,15	0.61	0	15,19,21	0.80	0
2	BMA	A	3	2	10,11,12	0.61	0	11,15,17	0.94	0
2	MAN	A	4	2	10,11,12	0.74	0	11,15,17	1.03	1 (9%)
2	MAN	A	5	2	10,11,12	0.65	0	11,15,17	1.09	1 (9%)
3	NAG	A	687	1,3	12,14,15	0.57	0	15,19,21	1.21	0
3	NAG	A	688	3	12,14,15	0.51	0	15,19,21	1.45	3 (20%)
4	NAG	A	689	1,4	12,14,15	0.59	0	15,19,21	0.97	1 (6%)
4	NAG	A	690	4	12,14,15	0.49	0	15,19,21	0.82	0
4	BMA	A	691	4	10,11,12	0.78	0	11,15,17	0.68	0
4	BMA	A	692	4	10,11,12	0.47	0	11,15,17	1.11	1 (9%)
4	MAN	A	693	4	10,11,12	0.53	0	11,15,17	0.33	0
4	BMA	A	694	4	10,11,12	0.59	0	11,15,17	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	A	5	2	-	0/2/19/22	0/1/1/1
3	NAG	A	687	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	688	3	-	0/6/23/26	0/1/1/1
4	NAG	A	689	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	690	4	-	0/6/23/26	0/1/1/1
4	BMA	A	691	4	-	0/2/19/22	0/1/1/1
4	BMA	A	692	4	-	0/2/19/22	0/1/1/1
4	MAN	A	693	4	-	0/2/19/22	0/1/1/1
4	BMA	A	694	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAG	O5-C5	-2.10	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	688	NAG	C2-N2-C7	3.68	129.26	123.09
2	A	5	MAN	O5-C5-C6	3.00	110.13	106.98
2	A	4	MAN	O5-C5-C6	2.70	109.82	106.98
4	A	689	NAG	C2-N2-C7	-2.70	118.56	123.09
4	A	692	BMA	C4-C3-C2	-2.16	107.60	110.50
3	A	688	NAG	C8-C7-N2	2.12	120.25	116.11
3	A	688	NAG	O5-C5-C4	2.03	113.23	110.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	4	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
5	SUC	A	1001	-	24,24,24	1.07	3 (12%)	36,36,36	0.92	1 (2%)
7	CO3	A	1003	6	0,3,3	0.00	-	0,3,3	0.00	-
9	SO4	A	1006	-	4,4,4	0.18	0	6,6,6	0.21	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	SUC	A	1001	-	-	0/12/51/51	0/2/2/2
7	CO3	A	1003	6	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	A	1006	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	SUC	O5-C1	2.70	1.48	1.41
5	A	1001	SUC	O5-C5	2.36	1.50	1.44
5	A	1001	SUC	O1'-C1'	-2.29	1.35	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	SUC	C6-C5-C4	2.85	119.88	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.