



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2FA7  
Title : Crystal structure of the complex of bovine lactoferrin C-lobe with a pentasaccharide at 2.38 Å resolution  
Authors : Singh, N.; Jain, R.; Jabeen, T.; Sharma, S.; Bhushan, A.; Singh, T.P.  
Deposited on : 2005-12-07  
Resolution : 2.38 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

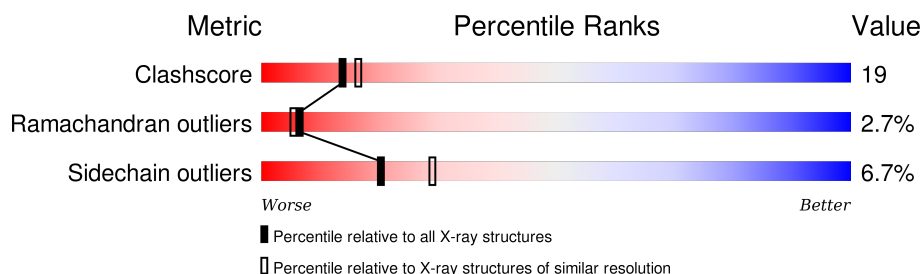
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	

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
5	NAG	A	690	-	-	X	-
5	NDG	A	691	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3123 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
1	A	341	Total	C	N	O	S	0	0	0
			2604	1622	454	507	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 (2-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

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

- 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		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	5	Total	C	N	O	0	0
			70	40	5	25		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Zn	0	0
			3	3		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 10 is water.

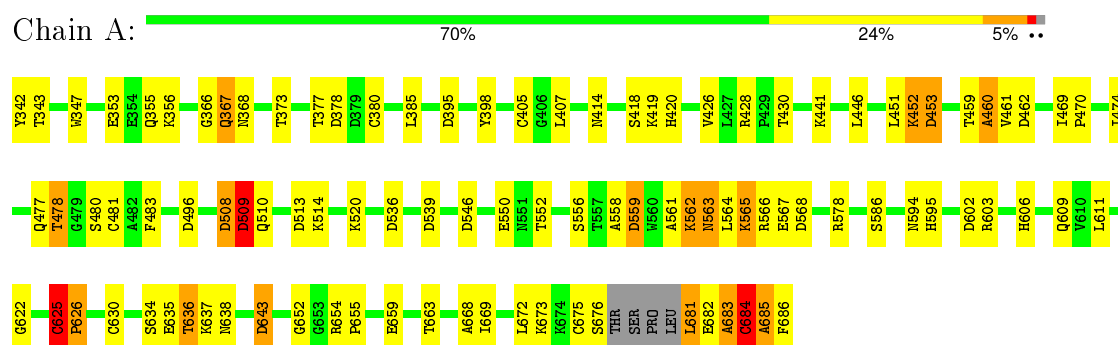
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	275	Total	O	0	0
			275	275		

### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	62.96 Å   50.50 Å   65.86 Å 90.00°   107.50°   90.00°	Depositor
Resolution (Å)	62.02 – 2.38	Depositor
% Data completeness (in resolution range)	96.5 (62.02-2.38)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.198 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: ZN, BMA, NAG, CO3, NDG, 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	0.54	0/2652	0.94	14/3591 (0.4%)

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
1	A	1	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	CYS	N-CA-C	11.65	142.47	111.00
1	A	685	ALA	N-CA-CB	11.25	125.85	110.10
1	A	684	CYS	C-N-CA	8.80	143.69	121.70
1	A	536	ASP	CB-CG-OD2	7.84	125.36	118.30
1	A	453	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	509	ASP	CB-CA-C	-6.13	98.14	110.40
1	A	513	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	378	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	602	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	508	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	643	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	568	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	496	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	539	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	A	625	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	CYS	Peptide

## 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	2604	0	2518	80	0
2	A	28	0	25	1	0
3	A	61	0	52	7	0
4	A	72	0	61	7	0
5	A	70	0	61	14	0
6	A	5	0	0	1	0
7	A	3	0	0	0	0
8	A	1	0	0	0	0
9	A	4	0	0	0	0
10	A	275	0	0	13	0
All	All	3123	0	2717	103	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 19.

All (103) 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:342:TYR:HD1	1:A:343:THR:N	1.28	1.28
1:A:342:TYR:CD1	1:A:343:THR:N	2.07	1.14
5:A:687:NAG:H3	5:A:688:NAG:O5	1.51	1.07
4:A:10:MAN:H3	4:A:11:BMA:H2	1.38	1.06
3:A:4:NDG:O3	3:A:5:MAN:H2	1.58	1.03
5:A:690:NAG:HN2	5:A:691:NDG:H8C1	1.30	0.94
4:A:10:MAN:H3	4:A:11:BMA:C2	1.98	0.94
1:A:659:GLU:HB3	5:A:689:NAG:H62	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:690:NAG:H3	5:A:691:NDG:N2	1.88	0.88
3:A:4:NDG:O3	3:A:5:MAN:C2	2.22	0.87
1:A:478:THR:HG22	1:A:480:SER:H	1.40	0.86
5:A:688:NAG:H62	10:A:968:HOH:O	1.79	0.81
1:A:668:ALA:HB1	3:A:3:NAG:H83	1.63	0.81
1:A:638:ASN:HD22	1:A:643:ASP:H	1.29	0.80
1:A:638:ASN:ND2	1:A:643:ASP:H	1.80	0.80
1:A:606:HIS:CD2	10:A:923:HOH:O	2.33	0.80
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.64	0.79
1:A:430:THR:HB	1:A:594:ASN:ND2	1.97	0.79
1:A:565:LYS:CD	1:A:567:GLU:H	1.96	0.78
5:A:690:NAG:N2	5:A:691:NDG:H8C1	1.98	0.77
1:A:683:ALA:O	1:A:684:CYS:HB3	1.83	0.76
1:A:559:ASP:N	1:A:559:ASP:OD1	2.15	0.76
5:A:687:NAG:C3	5:A:688:NAG:O5	2.33	0.73
1:A:635:GLU:O	1:A:636:THR:HG22	1.89	0.72
4:A:12:BMA:H4	4:A:13:MAN:H5	1.72	0.71
1:A:565:LYS:HD3	1:A:567:GLU:H	1.53	0.71
1:A:430:THR:HB	1:A:594:ASN:HD22	1.57	0.69
1:A:478:THR:CG2	1:A:480:SER:H	2.06	0.68
1:A:654:ARG:N	1:A:655:PRO:HD3	2.09	0.67
1:A:565:LYS:HD3	1:A:567:GLU:N	2.10	0.66
1:A:342:TYR:HD1	1:A:343:THR:CA	2.07	0.66
4:A:10:MAN:C3	4:A:11:BMA:H2	2.19	0.65
5:A:690:NAG:H3	5:A:691:NDG:HA	1.58	0.65
1:A:565:LYS:C	1:A:565:LYS:HD3	2.18	0.63
1:A:461:VAL:O	1:A:462:ASP:HB2	1.98	0.63
1:A:685:ALA:N	10:A:951:HOH:O	2.31	0.63
5:A:690:NAG:H83	5:A:691:NDG:H8C3	1.81	0.62
1:A:606:HIS:HD2	10:A:923:HOH:O	1.74	0.62
1:A:668:ALA:CB	3:A:3:NAG:H83	2.30	0.61
5:A:690:NAG:H83	5:A:691:NDG:C8	2.31	0.61
1:A:565:LYS:HD3	1:A:566:ARG:N	2.15	0.61
1:A:634:SER:O	1:A:637:LYS:HG3	2.00	0.60
1:A:385:LEU:HD23	1:A:407:LEU:HD21	1.84	0.60
1:A:682:GLU:O	1:A:683:ALA:HB2	2.02	0.59
3:A:4:NDG:HB	3:A:5:MAN:H2	1.67	0.59
1:A:683:ALA:O	1:A:684:CYS:CB	2.50	0.59
1:A:565:LYS:CD	1:A:567:GLU:N	2.65	0.59
1:A:684:CYS:C	1:A:686:PHE:H	2.06	0.58
1:A:606:HIS:HB2	10:A:923:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ASN:ND2	10:A:915:HOH:O	2.37	0.57
1:A:659:GLU:O	5:A:689:NAG:H5	2.06	0.56
1:A:452:LYS:O	1:A:453:ASP:HB2	2.07	0.55
1:A:654:ARG:N	1:A:655:PRO:CD	2.70	0.54
1:A:441:LYS:NZ	10:A:878:HOH:O	2.41	0.53
1:A:428:ARG:HD2	10:A:831:HOH:O	2.08	0.52
1:A:561:ALA:HA	1:A:564:LEU:HG	1.91	0.52
1:A:366:GLY:O	1:A:367:GLN:HB2	2.09	0.52
1:A:347:TRP:CZ3	1:A:611:LEU:HD11	2.45	0.51
1:A:654:ARG:NH2	10:A:788:HOH:O	2.43	0.50
1:A:520:LYS:HE2	10:A:715:HOH:O	2.10	0.50
1:A:676:SER:HA	10:A:795:HOH:O	2.12	0.50
1:A:659:GLU:HB3	5:A:689:NAG:C6	2.33	0.49
1:A:546:ASP:O	1:A:550:GLU:HG3	2.12	0.49
1:A:355:GLN:HG3	1:A:373:THR:OG1	2.12	0.49
1:A:558:ALA:O	1:A:562:LYS:HG2	2.12	0.49
1:A:681:LEU:O	1:A:682:GLU:HG3	2.12	0.49
1:A:419:LYS:HZ3	1:A:420:HIS:CD2	2.30	0.49
1:A:578:ARG:NE	6:A:301:SO4:O1	2.39	0.49
1:A:446:LEU:HD11	1:A:451:LEU:HD23	1.95	0.48
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.48	0.48
4:A:12:BMA:H4	4:A:13:MAN:C5	2.43	0.48
3:A:5:MAN:H62	10:A:842:HOH:O	2.12	0.48
1:A:514:LYS:HB2	1:A:514:LYS:HE3	1.70	0.48
4:A:9:NAG:O3	4:A:10:MAN:C1	2.61	0.47
5:A:690:NAG:C8	5:A:691:NDG:H8C1	2.45	0.47
1:A:478:THR:CG2	1:A:480:SER:HB3	2.46	0.46
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.50	0.46
1:A:672:LEU:O	1:A:675:CYS:HB2	2.16	0.46
5:A:690:NAG:C8	5:A:691:NDG:C8	2.93	0.46
1:A:474:ILE:O	1:A:478:THR:HB	2.17	0.45
1:A:561:ALA:O	1:A:563:ASN:N	2.49	0.45
1:A:565:LYS:HD2	1:A:567:GLU:CB	2.41	0.45
1:A:459:THR:O	1:A:460:ALA:HB2	2.17	0.45
1:A:565:LYS:HZ3	1:A:567:GLU:H	1.65	0.45
1:A:368:ASN:ND2	2:A:1:NAG:C7	2.78	0.45
1:A:469:ILE:N	1:A:470:PRO:HD2	2.31	0.45
1:A:510:GLN:NE2	10:A:919:HOH:O	2.38	0.45
1:A:385:LEU:HD11	1:A:405:CYS:HB3	1.99	0.44
1:A:426:VAL:HG12	1:A:426:VAL:O	2.18	0.44
1:A:638:ASN:HD22	1:A:643:ASP:N	2.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TRP:HZ3	1:A:611:LEU:HD11	1.82	0.44
1:A:353:GLU:OE2	1:A:637:LYS:NZ	2.50	0.43
1:A:520:LYS:HA	1:A:520:LYS:HD2	1.60	0.43
1:A:478:THR:HG22	1:A:480:SER:N	2.20	0.43
1:A:552:THR:OG1	1:A:566:ARG:HG2	2.19	0.43
4:A:10:MAN:H3	4:A:11:BMA:O2	2.19	0.42
1:A:565:LYS:NZ	1:A:567:GLU:HB2	2.35	0.42
3:A:4:NDG:O3	3:A:5:MAN:O2	2.37	0.41
1:A:603:ARG:HD2	1:A:603:ARG:HA	1.93	0.41
1:A:508:ASP:O	1:A:509:ASP:C	2.59	0.41
1:A:626:PRO:HA	1:A:630:CYS:SG	2.61	0.41
1:A:561:ALA:O	1:A:562:LYS:C	2.59	0.41
1:A:669:ILE:O	1:A:673:LYS:HG2	2.21	0.41

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%)	312 (93%)	16 (5%)	9 (3%)	6 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ASP
1	A	483	PHE
1	A	683	ALA
1	A	626	PRO
1	A	652	GLY
1	A	684	CYS
1	A	460	ALA
1	A	625	CYS

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Mol	Chain	Res	Type
1	A	622	GLY

### 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%)	263 (93%)	19 (7%)	20	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	LYS
1	A	367	GLN
1	A	380	CYS
1	A	414	ASN
1	A	418	SER
1	A	452	LYS
1	A	477	GLN
1	A	478	THR
1	A	481	CYS
1	A	556	SER
1	A	559	ASP
1	A	562	LYS
1	A	563	ASN
1	A	565	LYS
1	A	586	SER
1	A	609	GLN
1	A	636	THR
1	A	663	THR
1	A	681	LEU

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	360	GLN

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Mol	Chain	Res	Type
1	A	414	ASN
1	A	594	ASN
1	A	621	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 ⓘ

18 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	14,14,15	0.55	0	15,19,21	1.03	2 (13%)
4	MAN	A	10	4	11,11,12	0.46	0	14,15,17	3.68	6 (42%)
4	BMA	A	11	4	11,11,12	0.49	0	14,15,17	2.43	3 (21%)
4	BMA	A	12	4	11,11,12	0.60	0	14,15,17	3.62	5 (35%)
4	MAN	A	13	4	11,11,12	0.51	0	14,15,17	1.67	3 (21%)
2	NAG	A	2	2	14,14,15	0.54	0	15,19,21	0.88	0
3	NAG	A	3	1,3	14,14,15	0.67	0	15,19,21	1.49	1 (6%)
3	NDG	A	4	3	14,14,15	0.55	0	15,19,21	1.20	1 (6%)
3	MAN	A	5	3	11,11,12	0.47	0	14,15,17	2.62	5 (35%)
3	BMA	A	6	3	11,11,12	0.61	0	14,15,17	0.98	1 (7%)
5	NAG	A	687	5	14,14,15	0.64	0	15,19,21	1.54	2 (13%)
5	NAG	A	688	5	14,14,15	0.78	0	15,19,21	1.56	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	689	5	14,14,15	0.58	0	15,19,21	1.72	3 (20%)
5	NAG	A	690	5	14,14,15	0.79	0	15,19,21	1.83	4 (26%)
5	NDG	A	691	5	14,14,15	0.56	0	15,19,21	1.57	3 (20%)
3	BMA	A	7	3	11,11,12	0.69	0	14,15,17	1.78	3 (21%)
4	NAG	A	8	1,4	14,14,15	0.76	1 (7%)	15,19,21	1.11	2 (13%)
4	NAG	A	9	4	14,14,15	0.50	0	15,19,21	1.93	5 (33%)

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
4	MAN	A	10	4	-	0/2/19/22	0/1/1/1
4	BMA	A	11	4	-	0/2/19/22	0/1/1/1
4	BMA	A	12	4	-	0/2/19/22	0/1/1/1
4	MAN	A	13	4	-	0/2/19/22	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
3	NAG	A	3	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	4	3	-	0/6/23/26	0/1/1/1
3	MAN	A	5	3	-	0/2/19/22	0/1/1/1
3	BMA	A	6	3	-	0/2/19/22	0/1/1/1
5	NAG	A	687	5	-	0/6/23/26	0/1/1/1
5	NAG	A	688	5	-	0/6/23/26	0/1/1/1
5	NAG	A	689	5	-	0/6/23/26	0/1/1/1
5	NAG	A	690	5	-	0/6/23/26	0/1/1/1
5	NDG	A	691	5	-	0/6/23/26	0/1/1/1
3	BMA	A	7	3	-	0/2/19/22	0/1/1/1
4	NAG	A	8	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	9	4	-	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)
4	A	8	NAG	C1-C2	2.35	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5	MAN	C3-C4-C5	-4.45	102.44	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	9	NAG	C4-C3-C2	-4.19	104.71	111.23
3	A	5	MAN	C2-C3-C4	-4.11	104.07	111.04
3	A	3	NAG	C3-C4-C5	-4.06	103.13	110.20
5	A	689	NAG	C2-N2-C7	-3.88	118.06	123.04
3	A	7	BMA	C1-C2-C3	-3.86	104.98	109.54
5	A	691	NDG	C1-O-C5	-3.48	107.84	112.25
5	A	690	NAG	O4-C4-C5	-3.07	101.11	109.24
4	A	9	NAG	C3-C4-C5	-3.06	104.86	110.20
5	A	691	NDG	C2-N2-C7	-2.66	119.62	123.04
4	A	9	NAG	C2-N2-C7	-2.63	119.66	123.04
3	A	6	BMA	O5-C1-C2	-2.36	107.02	110.86
4	A	11	BMA	C1-C2-C3	-2.25	106.87	109.54
3	A	5	MAN	O2-C2-C3	-2.16	105.78	110.12
3	A	7	BMA	C1-O5-C5	-2.16	109.51	112.25
5	A	688	NAG	C1-O5-C5	-2.12	109.55	112.25
4	A	10	MAN	C6-C5-C4	-2.02	108.03	113.02
2	A	1	NAG	C1-O5-C5	2.07	114.87	112.25
4	A	8	NAG	C1-O5-C5	2.16	114.98	112.25
4	A	13	MAN	O5-C1-C2	2.27	114.54	110.86
4	A	8	NAG	C2-N2-C7	2.27	125.96	123.04
2	A	1	NAG	C3-C4-C5	2.33	114.27	110.20
5	A	689	NAG	C3-C4-C5	2.34	114.28	110.20
5	A	687	NAG	C4-C3-C2	2.59	115.25	111.23
4	A	11	BMA	C3-C4-C5	2.69	114.88	110.20
4	A	9	NAG	O5-C5-C6	2.69	113.17	107.35
5	A	690	NAG	O4-C4-C3	2.78	116.60	110.34
5	A	691	NDG	O-C5-C6	2.98	113.80	107.35
4	A	13	MAN	C1-C2-C3	3.16	113.28	109.54
3	A	4	NDG	C1-O-C5	3.19	116.29	112.25
5	A	690	NAG	C4-C3-C2	3.25	116.28	111.23
4	A	9	NAG	O4-C4-C3	3.27	117.70	110.34
4	A	12	BMA	C3-C4-C5	3.28	115.91	110.20
4	A	12	BMA	C2-C3-C4	3.44	116.88	111.04
4	A	10	MAN	C2-C3-C4	3.52	117.01	111.04
5	A	690	NAG	C3-C4-C5	3.54	116.37	110.20
3	A	5	MAN	O4-C4-C5	3.64	118.89	109.24
5	A	687	NAG	C3-C4-C5	3.81	116.84	110.20
5	A	689	NAG	C4-C3-C2	3.87	117.25	111.23
3	A	7	BMA	C3-C4-C5	4.01	117.19	110.20
4	A	13	MAN	C1-O5-C5	4.33	117.75	112.25
4	A	10	MAN	C3-C4-C5	4.34	117.76	110.20
4	A	12	BMA	O5-C1-C2	4.41	118.01	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	10	MAN	O5-C1-C2	4.43	118.05	110.86
5	A	688	NAG	O4-C4-C3	4.61	120.72	110.34
3	A	5	MAN	C1-O5-C5	5.86	119.69	112.25
4	A	10	MAN	C1-C2-C3	6.18	116.85	109.54
4	A	12	BMA	C1-C2-C3	7.79	118.76	109.54
4	A	11	BMA	C1-O5-C5	8.12	122.56	112.25
4	A	12	BMA	C1-O5-C5	8.75	123.35	112.25
4	A	10	MAN	C1-O5-C5	9.65	124.50	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	1	0
4	A	10	MAN	5	0
4	A	11	BMA	4	0
4	A	12	BMA	2	0
4	A	13	MAN	2	0
3	A	3	NAG	2	0
3	A	4	NDG	4	0
3	A	5	MAN	5	0
5	A	687	NAG	2	0
5	A	688	NAG	3	0
5	A	689	NAG	3	0
5	A	690	NAG	8	0
5	A	691	NDG	8	0
4	A	9	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
6	SO4	A	301	-	4,4,4	0.31	0	6,6,6	0.33	0
9	CO3	A	693	8	0,3,3	0.00	-	0,3,3	0.00	-

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
6	SO4	A	301	-	-	0/0/0/0	0/0/0/0
9	CO3	A	693	8	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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
6	A	301	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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