



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:26 AM UTC

PDB ID : 2DSF / pdb_00002dsf
Title : Structure of the complex of C-terminal lobe of bovine lactoferrin with xylose at 2.8Å resolution
Authors : Mir, R.; Singh, N.; Sinha, M.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2006-06-29
Resolution : 2.80 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)
Xtrriage (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

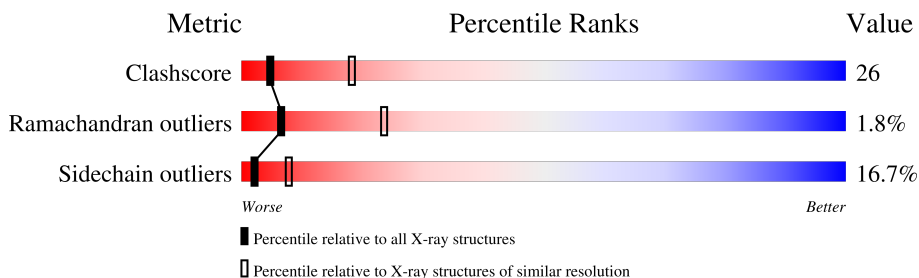
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	345	49% 36% 12% ..
2	B	3	33% 67%
3	C	4	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	X	-	-	-
5	LXC	A	3937	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 2921 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.

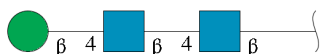
- Molecule 1 is a protein called Lactotransferrin.

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	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	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.



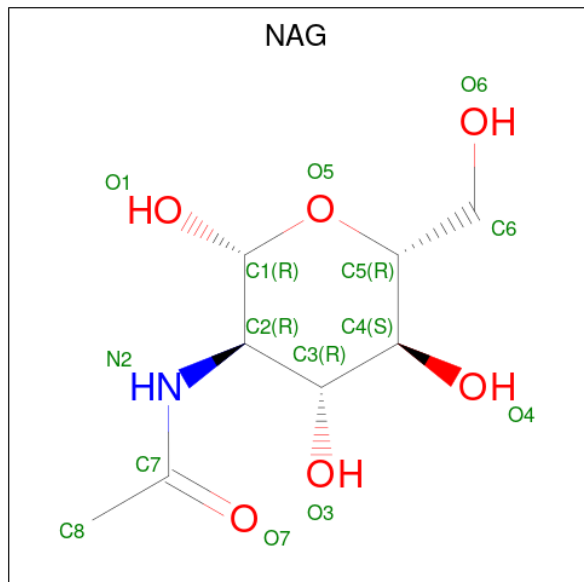
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

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



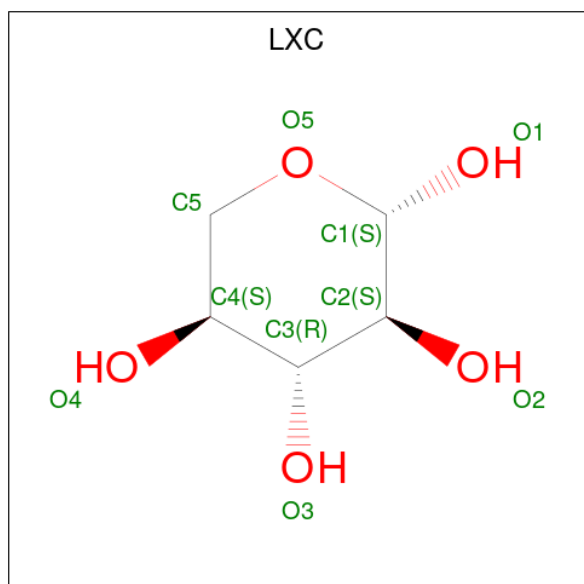
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	50	28	2	20	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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-L-xylopyranose (CCD ID: LXC) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	5	5	0	0

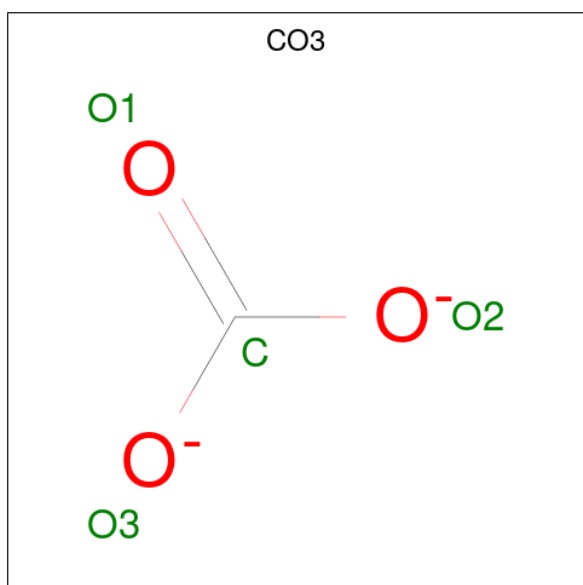
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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: CO₃).



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: O₄S).



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

- Molecule 10 is water.

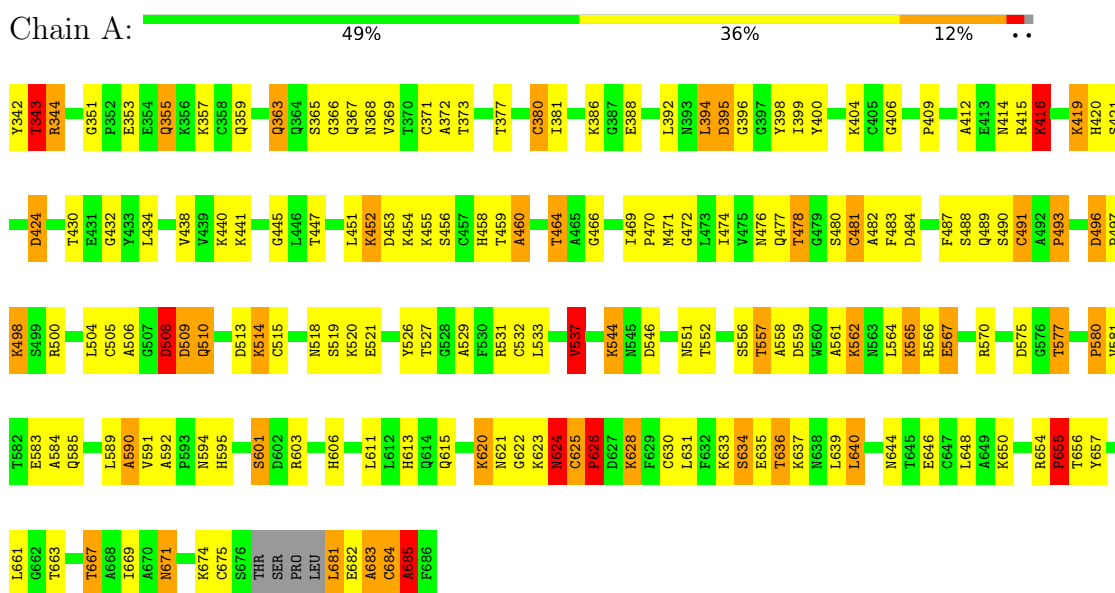
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	192	Total	O	0	0
			192	192		

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.

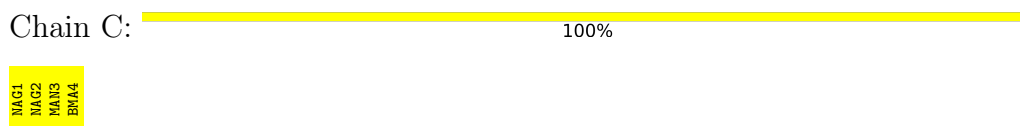
- Molecule 1: Lactotransferrin



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



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



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	63.45Å 50.44Å 65.87Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	19.94 – 2.80	Depositor
% Data completeness (in resolution range)	92.9 (19.94-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.201 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2921	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: SO4, NAG, LXC, FE, CO3, ZN, MAN, 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	0.75	6/2652 (0.2%)	1.65	57/3591 (1.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	ALA	CA-CB	-7.51	1.40	1.53
1	A	510	GLN	CA-CB	-7.02	1.43	1.53
1	A	510	GLN	CA-C	-6.33	1.44	1.52
1	A	508	ASP	CA-C	5.89	1.60	1.52
1	A	685	ALA	C-N	5.26	1.40	1.33
1	A	683	ALA	C-O	5.10	1.30	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	CYS	CA-C-N	30.25	157.66	119.84
1	A	625	CYS	C-N-CA	30.25	157.66	119.84
1	A	683	ALA	N-CA-C	16.73	146.44	110.80
1	A	656	THR	N-CA-C	-13.68	88.20	109.95
1	A	625	CYS	C-N-CD	-12.89	72.15	125.00
1	A	343	THR	N-CA-C	-12.06	97.88	112.59
1	A	537	VAL	N-CA-C	-11.68	100.59	111.45
1	A	625	CYS	N-CA-C	-10.72	95.51	110.31
1	A	510	GLN	OE1-CD-NE2	-10.20	112.40	122.60
1	A	464	THR	N-CA-C	10.19	122.15	111.14
1	A	355	GLN	OE1-CD-NE2	-10.14	112.46	122.60
1	A	368	ASN	N-CA-C	-10.12	100.96	113.20
1	A	419	LYS	N-CA-C	-8.07	97.12	109.95
1	A	684	CYS	N-CA-C	-7.87	94.04	110.80
1	A	624	ASN	N-CA-C	7.85	122.98	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	CYS	N-CA-C	-7.80	102.79	114.64
1	A	372	ALA	N-CA-C	-7.60	97.56	109.72
1	A	416	LYS	N-CA-C	7.45	120.74	110.24
1	A	406	GLY	N-CA-C	7.33	125.10	115.36
1	A	628	LYS	N-CA-C	7.22	122.28	112.68
1	A	682	GLU	CA-C-N	-7.12	107.94	121.54
1	A	682	GLU	C-N-CA	-7.12	107.94	121.54
1	A	409	PRO	CB-CA-C	7.05	120.51	111.56
1	A	626	PRO	CA-N-CD	-7.01	102.18	112.00
1	A	682	GLU	N-CA-CB	7.01	122.45	110.68
1	A	558	ALA	N-CA-C	-7.00	100.11	110.48
1	A	510	GLN	CB-CG-CD	-6.98	100.73	112.60
1	A	395	ASP	N-CA-C	-6.94	100.71	110.50
1	A	371	CYS	N-CA-C	6.86	120.64	109.59
1	A	682	GLU	CA-CB-CG	-6.63	100.84	114.10
1	A	622	GLY	N-CA-C	6.62	121.96	112.82
1	A	394	LEU	N-CA-C	6.61	119.94	109.50
1	A	681	LEU	CA-C-N	-6.52	113.79	122.99
1	A	681	LEU	C-N-CA	-6.52	113.79	122.99
1	A	510	GLN	CG-CD-NE2	6.48	126.12	116.40
1	A	351	GLY	CA-C-N	6.41	126.17	119.05
1	A	351	GLY	C-N-CA	6.41	126.17	119.05
1	A	519	SER	N-CA-C	6.38	120.63	112.34
1	A	650	LYS	N-CA-C	-6.33	102.01	110.55
1	A	509	ASP	CA-C-N	-6.29	112.68	122.37
1	A	509	ASP	C-N-CA	-6.29	112.68	122.37
1	A	355	GLN	CG-CD-NE2	6.24	125.76	116.40
1	A	620	LYS	N-CA-C	6.02	118.62	111.33
1	A	456	SER	N-CA-C	5.87	119.28	109.95
1	A	366	GLY	N-CA-C	-5.86	105.88	114.61
1	A	464	THR	CB-CA-C	-5.84	101.67	110.90
1	A	646	GLU	N-CA-C	-5.81	104.31	111.40
1	A	531	ARG	N-CA-C	-5.80	105.03	111.36
1	A	655	PRO	N-CA-C	5.75	120.26	111.11
1	A	496	ASP	CA-C-N	5.57	125.03	119.24
1	A	496	ASP	C-N-CA	5.57	125.03	119.24
1	A	491	CYS	N-CA-C	-5.52	99.29	108.34
1	A	438	VAL	N-CA-C	5.30	116.94	108.89
1	A	683	ALA	N-CA-CB	-5.24	101.63	110.49
1	A	675	CYS	N-CA-C	-5.23	106.73	113.01
1	A	484	ASP	N-CA-C	-5.18	106.93	113.20
1	A	477	GLN	N-CA-C	-5.03	107.54	113.97

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	2518	136	0
2	B	39	0	34	2	0
3	C	50	0	43	2	0
4	A	14	0	13	0	0
5	A	10	0	7	0	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	192	0	0	22	0
All	All	2921	0	2615	137	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 26.

All (137) 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:625:CYS:SG	1:A:626:PRO:HD3	1.71	1.28
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.00	0.96
1:A:625:CYS:SG	1:A:626:PRO:CD	2.62	0.88
1:A:685:ALA:HB2	10:A:4026:HOH:O	1.75	0.85
1:A:474:ILE:O	1:A:478:THR:HB	1.76	0.85
1:A:620:LYS:C	1:A:621:ASN:HD22	1.86	0.82
1:A:419:LYS:HZ2	1:A:420:HIS:CE1	2.00	0.80
1:A:355:GLN:HG3	1:A:373:THR:OG1	1.87	0.74
1:A:635:GLU:O	1:A:637:LYS:HG3	1.89	0.73
1:A:419:LYS:NZ	1:A:420:HIS:NE2	2.36	0.71
1:A:404:LYS:HD3	1:A:683:ALA:HB3	1.72	0.71
1:A:552:THR:OG1	1:A:566:ARG:HG2	1.90	0.71
1:A:472:GLY:O	1:A:476:ASN:HB2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:HG22	1:A:480:SER:H	1.57	0.69
1:A:342:TYR:O	1:A:606:HIS:NE2	2.28	0.67
1:A:565:LYS:NZ	1:A:567:GLU:HB2	2.09	0.67
1:A:424:ASP:HB2	10:A:4020:HOH:O	1.94	0.66
1:A:343:THR:HA	1:A:606:HIS:NE2	2.11	0.66
1:A:458:HIS:HE1	1:A:471:MET:HE3	1.58	0.66
1:A:584:ALA:HB3	3:C:1:NAG:H82	1.76	0.66
1:A:603:ARG:NH2	10:A:4036:HOH:O	2.27	0.66
1:A:685:ALA:CB	10:A:4026:HOH:O	2.38	0.66
1:A:585:GLN:HG2	10:A:3958:HOH:O	1.98	0.64
1:A:601:SER:C	1:A:603:ARG:H	2.04	0.64
1:A:606:HIS:HD2	10:A:4036:HOH:O	1.82	0.63
1:A:357:LYS:HG3	10:A:4022:HOH:O	1.99	0.62
1:A:478:THR:CG2	1:A:480:SER:H	2.12	0.62
1:A:478:THR:CG2	1:A:480:SER:HB3	2.30	0.61
1:A:404:LYS:HB3	1:A:684:CYS:H	1.64	0.60
1:A:380:CYS:HB3	1:A:392:LEU:HD13	1.83	0.60
1:A:363:GLN:HA	10:A:4068:HOH:O	2.00	0.60
10:A:4085:HOH:O	2:B:3:BMA:H4	2.01	0.60
1:A:626:PRO:HD3	1:A:630:CYS:SG	2.42	0.59
1:A:488:SER:HA	1:A:500:ARG:NH2	2.19	0.58
1:A:529:ALA:O	1:A:532:CYS:HB3	2.03	0.58
1:A:565:LYS:HZ2	1:A:567:GLU:HB2	1.68	0.58
1:A:654:ARG:N	1:A:655:PRO:HD3	2.19	0.57
1:A:489:GLN:HB3	1:A:504:LEU:HD13	1.85	0.57
1:A:513:ASP:OD2	1:A:520:LYS:HD3	2.04	0.57
1:A:518:ASN:OD1	1:A:520:LYS:HB2	2.04	0.57
1:A:399:ILE:CG2	1:A:661:LEU:HD11	2.35	0.56
1:A:556:SER:C	1:A:557:THR:HG23	2.30	0.56
1:A:685:ALA:HA	10:A:4080:HOH:O	2.06	0.56
1:A:430:THR:HB	1:A:594:ASN:ND2	2.19	0.56
1:A:654:ARG:NH2	10:A:4042:HOH:O	2.39	0.56
1:A:399:ILE:HG22	1:A:661:LEU:HD11	1.87	0.55
1:A:575:ASP:OD1	1:A:577:THR:HB	2.06	0.55
1:A:357:LYS:HD3	1:A:640:LEU:HG	1.88	0.55
1:A:532:CYS:O	1:A:537:VAL:HB	2.07	0.54
1:A:452:LYS:O	1:A:453:ASP:HB2	2.07	0.54
1:A:565:LYS:HZ3	1:A:567:GLU:H	1.56	0.54
1:A:601:SER:C	1:A:603:ARG:N	2.66	0.53
1:A:589:LEU:O	1:A:590:ALA:HB2	2.09	0.53
1:A:394:LEU:O	1:A:595:HIS:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:SER:C	1:A:504:LEU:HB2	2.34	0.52
1:A:445:GLY:O	1:A:447:THR:HG23	2.10	0.52
1:A:469:ILE:N	1:A:470:PRO:HD2	2.25	0.52
1:A:478:THR:HG23	1:A:480:SER:HB3	1.91	0.52
1:A:496:ASP:OD1	1:A:498:LYS:HD3	2.09	0.52
1:A:483:PHE:CD2	1:A:483:PHE:C	2.88	0.51
1:A:357:LYS:HG2	1:A:357:LYS:O	2.10	0.51
1:A:654:ARG:N	1:A:655:PRO:CD	2.74	0.51
1:A:634:SER:C	1:A:635:GLU:HG3	2.36	0.51
1:A:464:THR:HG21	1:A:592:ALA:CB	2.41	0.51
1:A:459:THR:OG1	1:A:466:GLY:HA3	2.12	0.50
1:A:634:SER:OG	1:A:639:LEU:HG	2.10	0.50
1:A:526:TYR:CE2	1:A:544:LYS:HE2	2.45	0.50
1:A:419:LYS:HZ2	1:A:420:HIS:CD2	2.23	0.50
1:A:455:LYS:HB3	1:A:504:LEU:HD21	1.95	0.49
1:A:570:ARG:NH1	1:A:580:PRO:HA	2.27	0.49
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.94	0.49
1:A:367:GLN:HB2	10:A:4056:HOH:O	2.13	0.49
1:A:639:LEU:O	1:A:640:LEU:HB2	2.13	0.49
1:A:657:TYR:O	1:A:661:LEU:HD12	2.13	0.48
1:A:419:LYS:HD3	1:A:420:HIS:N	2.28	0.48
1:A:482:ALA:HA	10:A:4097:HOH:O	2.13	0.48
1:A:342:TYR:O	1:A:606:HIS:CD2	2.66	0.48
1:A:544:LYS:HG3	1:A:546:ASP:H	1.79	0.48
1:A:667:THR:O	1:A:671:ASN:ND2	2.47	0.48
1:A:415:ARG:HG2	1:A:415:ARG:HH11	1.78	0.47
1:A:551:ASN:HA	1:A:556:SER:HB2	1.96	0.47
1:A:565:LYS:C	1:A:565:LYS:HD3	2.39	0.47
1:A:481:CYS:C	1:A:483:PHE:H	2.23	0.47
1:A:620:LYS:O	1:A:621:ASN:ND2	2.41	0.47
1:A:505:CYS:HB3	1:A:521:GLU:OE1	2.15	0.47
1:A:559:ASP:HB3	10:A:3962:HOH:O	2.14	0.47
1:A:344:ARG:HB2	10:A:4032:HOH:O	2.13	0.47
1:A:506:ALA:HA	1:A:514:LYS:HE2	1.96	0.47
1:A:367:GLN:C	1:A:369:VAL:H	2.20	0.47
1:A:434:LEU:HD12	1:A:584:ALA:HB1	1.96	0.46
1:A:518:ASN:OD1	1:A:518:ASN:C	2.59	0.46
1:A:471:MET:HE2	1:A:474:ILE:HD12	1.98	0.46
1:A:505:CYS:O	1:A:514:LYS:HE2	2.14	0.46
1:A:546:ASP:HA	3:C:1:NAG:H62	1.96	0.46
1:A:353:GLU:OE1	1:A:637:LYS:HE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:HB2	1:A:498:LYS:HE2	1.63	0.46
1:A:671:ASN:ND2	2:B:1:NAG:H3	2.31	0.46
1:A:459:THR:O	1:A:460:ALA:HB2	2.15	0.46
1:A:365:SER:C	1:A:367:GLN:N	2.71	0.45
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.52	0.45
1:A:419:LYS:O	1:A:420:HIS:HB2	2.14	0.45
1:A:377:THR:O	1:A:381:ILE:HG12	2.16	0.45
1:A:505:CYS:HB3	1:A:521:GLU:CD	2.41	0.45
1:A:416:LYS:H	1:A:416:LYS:HG2	1.47	0.45
1:A:487:PHE:O	1:A:488:SER:C	2.60	0.45
1:A:559:ASP:HA	1:A:562:LYS:HG3	1.99	0.45
1:A:624:ASN:HB3	1:A:628:LYS:HB2	1.98	0.45
1:A:671:ASN:HB3	10:A:4019:HOH:O	2.16	0.45
1:A:355:GLN:HE21	1:A:359:GLN:CD	2.25	0.45
1:A:633:LYS:HD3	1:A:633:LYS:HA	1.88	0.44
1:A:561:ALA:HA	1:A:564:LEU:HG	1.98	0.44
1:A:623:LYS:C	1:A:624:ASN:ND2	2.75	0.44
1:A:367:GLN:C	1:A:369:VAL:N	2.71	0.44
1:A:396:GLY:HA2	1:A:399:ILE:HD12	2.00	0.44
1:A:400:TYR:CD2	1:A:669:ILE:HG21	2.53	0.43
1:A:451:LEU:HD12	10:A:3994:HOH:O	2.18	0.43
1:A:464:THR:O	1:A:469:ILE:HG12	2.18	0.43
1:A:395:ASP:HA	1:A:595:HIS:CG	2.52	0.43
1:A:685:ALA:CB	10:A:4080:HOH:O	2.65	0.43
1:A:636:THR:HG22	10:A:3971:HOH:O	2.18	0.42
1:A:613:HIS:HD2	10:A:4015:HOH:O	2.01	0.42
1:A:491:CYS:SG	1:A:493:PRO:HD3	2.59	0.42
1:A:623:LYS:C	1:A:624:ASN:HD22	2.27	0.42
1:A:483:PHE:C	1:A:483:PHE:HD2	2.27	0.42
1:A:565:LYS:HZ3	1:A:567:GLU:HB2	1.83	0.41
1:A:469:ILE:H	1:A:470:PRO:HD2	1.85	0.41
1:A:412:ALA:O	1:A:648:LEU:HA	2.20	0.41
1:A:556:SER:C	1:A:557:THR:CG2	2.93	0.41
1:A:480:SER:OG	1:A:481:CYS:N	2.53	0.41
1:A:526:TYR:CZ	1:A:544:LYS:HE2	2.56	0.41
1:A:386:LYS:HD2	1:A:388:GLU:OE1	2.19	0.41
1:A:683:ALA:HB1	1:A:684:CYS:O	2.21	0.41
1:A:415:ARG:NH2	1:A:432:GLY:O	2.48	0.41
1:A:644:ASN:N	10:A:3952:HOH:O	2.53	0.40
1:A:508:ASP:OD1	1:A:508:ASP:N	2.53	0.40
1:A:606:HIS:CD2	10:A:4036:HOH:O	2.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HD2	1:A:546:ASP:OD1	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	337/345 (98%)	302 (90%)	29 (9%)	6 (2%)	6 23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	ASP
1	A	626	PRO
1	A	685	ALA
1	A	590	ALA
1	A	636	THR
1	A	460	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	282/286 (99%)	235 (83%)	47 (17%)	2 8

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	344	ARG
1	A	363	GLN
1	A	380	CYS
1	A	414	ASN
1	A	416	LYS
1	A	421	SER
1	A	424	ASP
1	A	440	LYS
1	A	441	LYS
1	A	452	LYS
1	A	454	LYS
1	A	478	THR
1	A	493	PRO
1	A	497	PRO
1	A	498	LYS
1	A	509	ASP
1	A	510	GLN
1	A	514	LYS
1	A	515	CYS
1	A	527	THR
1	A	533	LEU
1	A	537	VAL
1	A	544	LYS
1	A	557	THR
1	A	562	LYS
1	A	565	LYS
1	A	567	GLU
1	A	577	THR
1	A	580	PRO
1	A	581	VAL
1	A	583	GLU
1	A	591	VAL
1	A	601	SER
1	A	611	LEU
1	A	615	GLN
1	A	624	ASN
1	A	626	PRO
1	A	631	LEU
1	A	634	SER
1	A	640	LEU
1	A	655	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	663	THR
1	A	667	THR
1	A	671	ASN
1	A	674	LYS
1	A	681	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	363	GLN
1	A	414	ASN
1	A	443	ASN
1	A	458	HIS
1	A	510	GLN
1	A	621	ASN
1	A	671	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](#)

7 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	1.33	2 (14%)	17,19,21	1.40	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.54	4 (23%)
2	BMA	B	3	2	11,11,12	0.88	1 (9%)	15,15,17	0.83	0
3	NAG	C	1	3,1	14,14,15	0.88	0	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	1.00	0	17,19,21	1.03	1 (5%)
3	MAN	C	3	3	11,11,12	1.08	1 (9%)	15,15,17	1.56	3 (20%)
3	BMA	C	4	3	11,11,12	0.77	0	15,15,17	1.27	1 (6%)

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	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.77	1.56	1.52
2	B	1	NAG	O5-C5	2.73	1.48	1.43
2	B	3	BMA	C2-C3	2.32	1.56	1.52
3	C	3	MAN	C2-C3	2.22	1.55	1.52
2	B	2	NAG	C1-C2	2.14	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	BMA	C3-C4-C5	3.88	117.26	110.23
3	C	3	MAN	C3-C4-C5	3.74	117.02	110.23
3	C	3	MAN	O5-C1-C2	3.03	118.03	110.79
2	B	2	NAG	C4-C3-C2	-2.95	106.69	111.02
2	B	2	NAG	C2-N2-C7	-2.90	119.02	122.90
2	B	1	NAG	C1-O5-C5	2.68	115.78	112.19
2	B	2	NAG	C1-O5-C5	2.45	115.47	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C6-C5-C4	-2.35	107.25	113.02
2	B	1	NAG	C3-C4-C5	-2.35	105.97	110.23
2	B	1	NAG	C2-N2-C7	-2.24	119.89	122.90
2	B	2	NAG	O5-C1-C2	-2.15	107.97	111.29
3	C	2	NAG	C3-C4-C5	-2.12	106.39	110.23
2	B	1	NAG	O7-C7-C8	-2.03	118.45	122.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (6) torsion outliers are listed below:

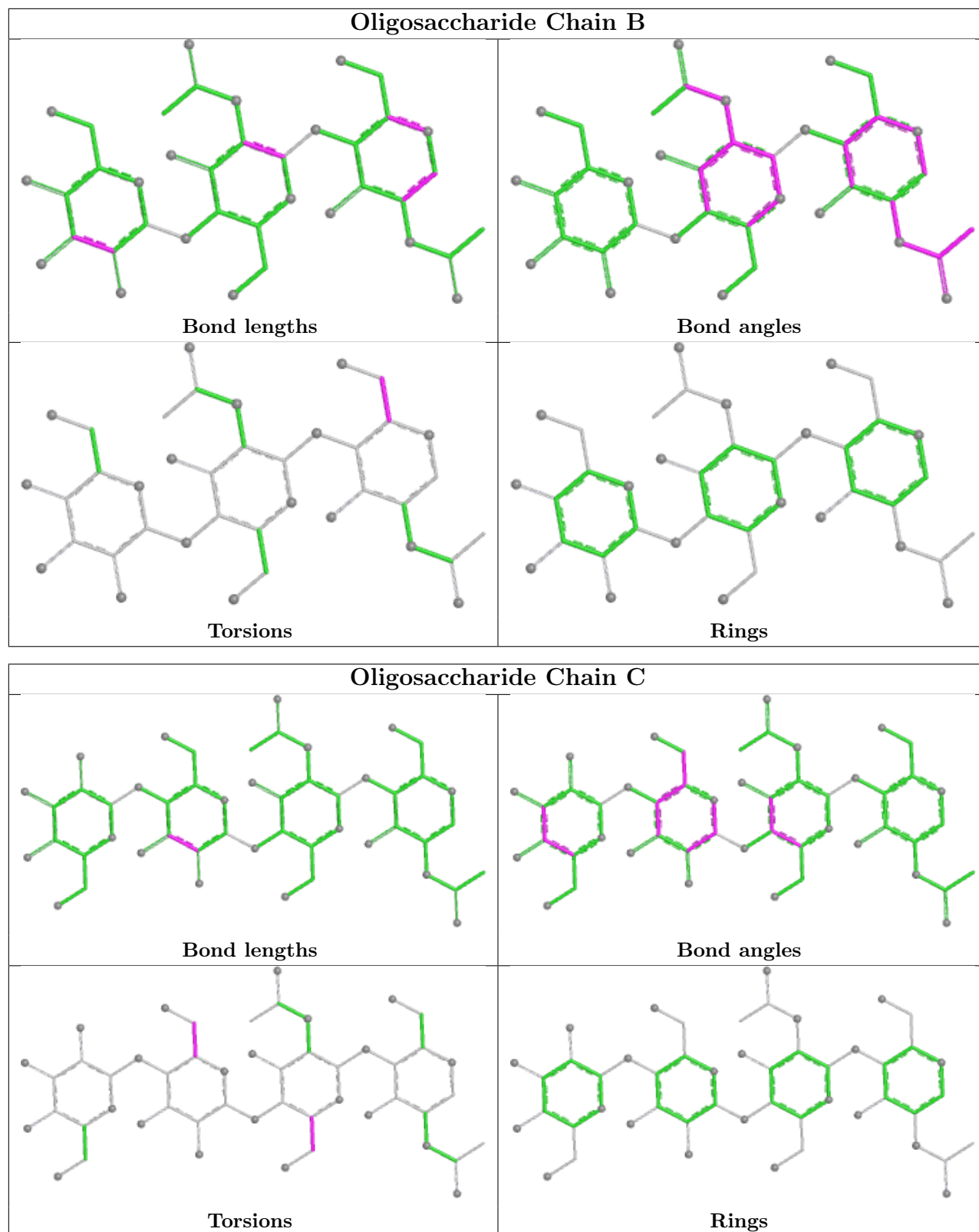
Mol	Chain	Res	Type	Atoms
3	C	3	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	BMA	1	0
3	C	1	NAG	2	0
2	B	1	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	LXC	A	3937	-	10,10,10	1.18	0	14,14,14	4.28	12 (85%)
8	CO3	A	1999	7	3,3,3	1.74	1 (33%)	2,3,3	0.10	0
9	SO4	A	3938	-	4,4,4	0.34	0	6,6,6	0.10	0
4	NAG	A	1001	1	14,14,15	0.65	0	17,19,21	1.89	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LXC	A	3937	-	3/3/4/4	-	0/1/1/1
4	NAG	A	1001	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)
8	A	1999	CO3	O1-C	2.60	1.34	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3937	LXC	O3-C3-C4	6.80	123.94	110.05
5	A	3937	LXC	C5-C4-C3	6.40	118.97	109.64
5	A	3937	LXC	O2-C2-C1	6.31	123.80	109.25
5	A	3937	LXC	O4-C4-C5	4.65	119.87	109.22
5	A	3937	LXC	O1-C1-O5	4.46	121.33	109.91
5	A	3937	LXC	O5-C1-C2	4.14	122.00	109.94
5	A	3937	LXC	O4-C4-C3	4.08	118.60	110.15
4	A	1001	NAG	C3-C4-C5	4.01	117.50	110.23
5	A	3937	LXC	C1-C2-C3	3.84	118.19	110.36
4	A	1001	NAG	C2-N2-C7	-3.41	118.33	122.90
5	A	3937	LXC	O3-C3-C2	3.34	118.25	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C6-C5-C4	-3.28	104.95	113.02
5	A	3937	LXC	O2-C2-C3	3.23	118.00	110.38
5	A	3937	LXC	C4-C3-C2	2.91	115.98	110.86
4	A	1001	NAG	O5-C1-C2	-2.41	107.56	111.29
5	A	3937	LXC	O1-C1-C2	2.39	115.92	108.98
4	A	1001	NAG	C1-O5-C5	2.12	115.03	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3937	LXC	C2
5	A	3937	LXC	C1
5	A	3937	LXC	C3

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.