



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:55 AM UTC

PDB ID : 2DOJ / pdb_00002doj
Title : Crystal structure of the complex of C-terminal lobe of bovine lactoferrin with adenosine at 2.4 Å resolution
Authors : Singh, N.; Jain, R.; Sharma, S.; Singh, T.P.
Deposited on : 2006-04-30
Resolution : 2.40 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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

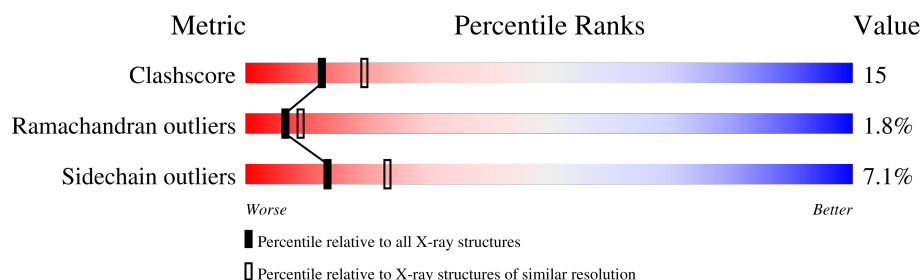
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	 69% 24% 6%
2	B	2	 50% 50%
3	C	4	 100%
4	D	5	 40% 60%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3005 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
			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	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

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



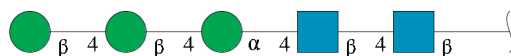
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



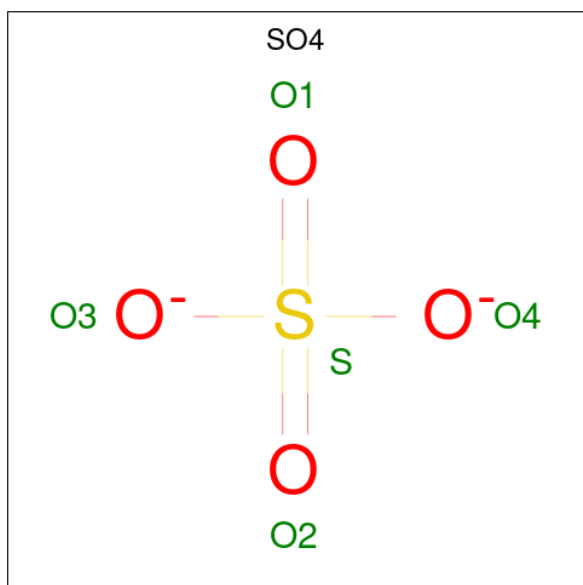
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

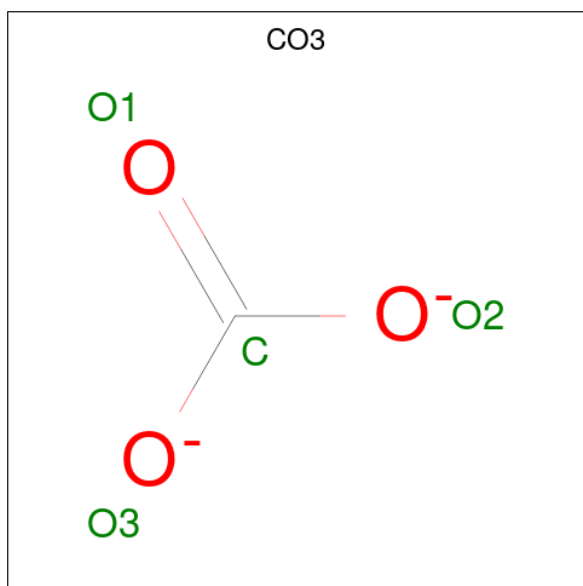
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

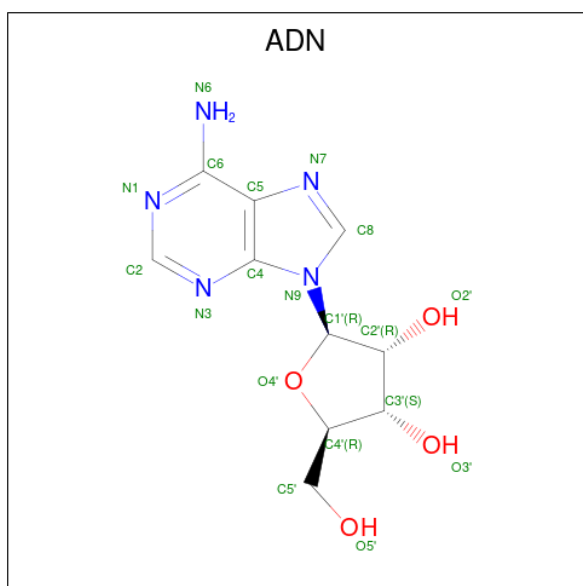
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		

- 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 ADENOSINE (CCD ID: ADN) (formula: $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 10 is water.

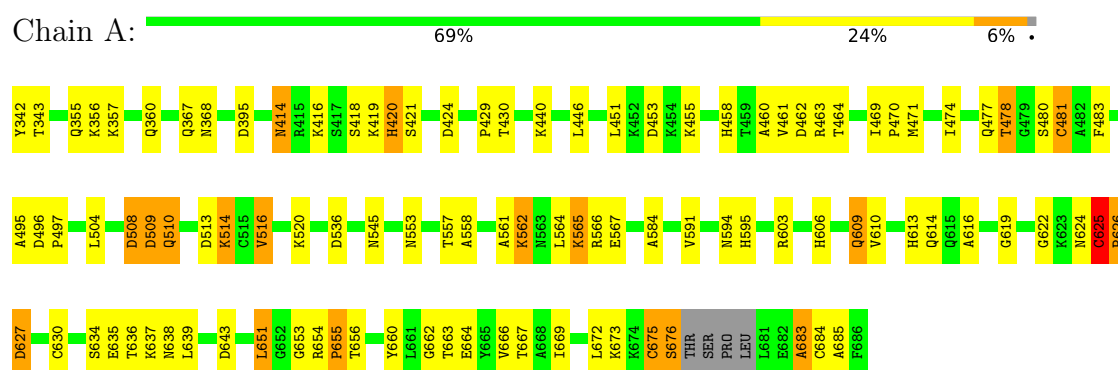
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	230	Total	O	0	0
			230	230		

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.

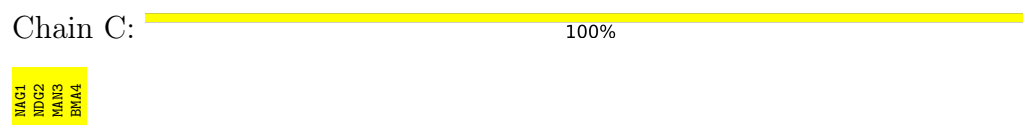
- Molecule 1: Lactotransferrin



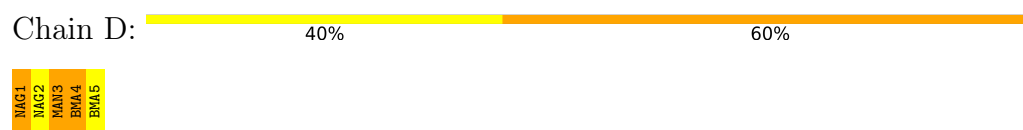
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-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	63.32Å 50.47Å 65.92Å 90.00° 107.66° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.4 (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.192 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3005	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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, MAN, FE, ZN, ADN, NDG, NAG, BMA, SO4

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	0.84	3/2653 (0.1%)	1.29	28/3591 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	ASN	CA-C	7.28	1.63	1.52
1	A	625	CYS	N-CA	6.17	1.54	1.46
1	A	626	PRO	CA-C	5.70	1.61	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	ASP	CA-CB-CG	10.33	122.93	112.60
1	A	510	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	A	477	GLN	OE1-CD-NE2	-8.94	113.66	122.60
1	A	624	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	421	SER	N-CA-C	8.43	121.41	111.71
1	A	656	THR	N-CA-C	-7.75	100.53	110.53
1	A	651	LEU	CA-C-N	-7.63	114.95	122.20
1	A	651	LEU	C-N-CA	-7.63	114.95	122.20
1	A	453	ASP	CA-CB-CG	7.24	119.83	112.60
1	A	509	ASP	CB-CA-C	-7.20	98.78	110.74
1	A	477	GLN	CG-CD-NE2	6.85	126.67	116.40
1	A	626	PRO	N-CA-C	6.32	122.98	113.81
1	A	510	GLN	CG-CD-NE2	6.25	125.77	116.40
1	A	624	ASN	CA-C-O	-6.06	115.57	121.02
1	A	464	THR	N-CA-C	6.04	117.55	110.97
1	A	675	CYS	N-CA-C	6.02	117.64	111.14
1	A	655	PRO	N-CA-C	5.97	120.58	111.15
1	A	558	ALA	N-CA-C	-5.75	101.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	VAL	N-CA-CB	5.53	115.68	109.99
1	A	653	GLY	N-CA-C	-5.41	107.32	114.95
1	A	496	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	627	ASP	N-CA-C	5.24	116.80	111.14
1	A	508	ASP	N-CA-C	5.20	116.69	109.31
1	A	368	ASN	N-CA-C	-5.14	105.86	111.82
1	A	508	ASP	O-C-N	5.09	128.45	121.78
1	A	683	ALA	N-CA-C	5.07	121.60	110.80
1	A	481	CYS	N-CA-C	-5.05	107.14	113.15
1	A	624	ASN	N-CA-CB	-5.04	105.74	111.79

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	2605	0	2519	80	0
2	B	28	0	25	2	0
3	C	50	0	42	0	0
4	D	61	0	52	3	0
5	A	5	0	0	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	19	0	13	1	0
10	A	230	0	0	17	0
All	All	3005	0	2651	83	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 15.

All (83) 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:430:THR:HB	1:A:594:ASN:HD22	1.34	0.91
1:A:478:THR:HG22	1:A:480:SER:H	1.39	0.86
1:A:625:CYS:SG	1:A:626:PRO:HD3	2.15	0.85
1:A:430:THR:HB	1:A:594:ASN:ND2	1.91	0.85
1:A:625:CYS:HB3	1:A:626:PRO:HD2	1.61	0.83
1:A:625:CYS:C	1:A:630:CYS:SG	2.64	0.81
1:A:355:GLN:HG3	10:A:2178:HOH:O	1.81	0.81
1:A:478:THR:CG2	1:A:480:SER:H	1.96	0.79
1:A:635:GLU:O	1:A:636:THR:HG22	1.82	0.79
1:A:474:ILE:O	1:A:478:THR:HB	1.83	0.78
1:A:676:SER:HA	10:A:2107:HOH:O	1.85	0.77
1:A:478:THR:HG22	1:A:480:SER:N	2.02	0.74
1:A:613:HIS:HD2	10:A:2143:HOH:O	1.71	0.73
1:A:638:ASN:HD22	1:A:643:ASP:H	1.38	0.70
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.22	0.70
1:A:565:LYS:HD3	1:A:567:GLU:H	1.55	0.69
1:A:625:CYS:CB	1:A:626:PRO:CD	2.72	0.68
1:A:478:THR:HG21	10:A:2077:HOH:O	1.92	0.67
4:D:3:MAN:H5	4:D:4:BMA:H2	1.78	0.66
1:A:419:LYS:O	1:A:420:HIS:HB2	1.97	0.65
1:A:662:GLY:O	1:A:666:VAL:HG23	1.98	0.64
1:A:606:HIS:HB2	10:A:2134:HOH:O	1.99	0.63
1:A:638:ASN:ND2	1:A:643:ASP:H	1.96	0.63
1:A:626:PRO:HD3	1:A:630:CYS:SG	2.38	0.63
1:A:660:TYR:O	9:A:2001:ADN:H5'1	2.00	0.61
1:A:565:LYS:CD	1:A:567:GLU:H	2.14	0.61
1:A:606:HIS:HD2	10:A:2180:HOH:O	1.84	0.60
1:A:565:LYS:HD3	1:A:567:GLU:N	2.16	0.60
1:A:562:LYS:NZ	10:A:2167:HOH:O	2.34	0.59
1:A:639:LEU:HD22	10:A:2138:HOH:O	2.03	0.58
1:A:625:CYS:SG	1:A:626:PRO:CD	2.89	0.58
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.39	0.57
1:A:565:LYS:HZ3	1:A:567:GLU:N	2.02	0.57
1:A:634:SER:O	1:A:637:LYS:HG3	2.06	0.56
1:A:416:LYS:H	1:A:416:LYS:HD3	1.71	0.56
1:A:446:LEU:HD11	1:A:451:LEU:HD23	1.88	0.55
1:A:565:LYS:CE	1:A:567:GLU:H	2.20	0.55
2:B:1:NAG:H5	2:B:2:NAG:HN2	1.72	0.55
1:A:565:LYS:HZ3	1:A:567:GLU:H	1.54	0.54
1:A:429:PRO:HD3	10:A:2198:HOH:O	2.07	0.54
1:A:469:ILE:N	1:A:470:PRO:HD2	2.23	0.53
1:A:342:TYR:HD1	1:A:343:THR:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:CB	1:A:594:ASN:HD22	2.15	0.52
1:A:565:LYS:NZ	1:A:567:GLU:H	2.08	0.52
1:A:513:ASP:O	1:A:516:VAL:HG22	2.09	0.52
1:A:419:LYS:HG2	10:A:2083:HOH:O	2.09	0.51
1:A:565:LYS:HZ2	1:A:567:GLU:HB2	1.77	0.50
1:A:654:ARG:N	1:A:655:PRO:CD	2.75	0.49
1:A:672:LEU:O	1:A:675:CYS:HB2	2.13	0.49
1:A:520:LYS:HG3	10:A:2064:HOH:O	2.12	0.49
1:A:654:ARG:N	1:A:655:PRO:HD3	2.27	0.49
1:A:495:ALA:O	1:A:497:PRO:HD3	2.12	0.49
1:A:613:HIS:CD2	10:A:2143:HOH:O	2.56	0.49
1:A:440:LYS:NZ	1:A:536:ASP:OD1	2.46	0.48
4:D:3:MAN:C5	4:D:4:BMA:H2	2.43	0.48
1:A:520:LYS:HA	1:A:520:LYS:HD2	1.56	0.47
1:A:610:VAL:O	1:A:614:GLN:HG2	2.13	0.47
1:A:424:ASP:HB2	10:A:2132:HOH:O	2.14	0.47
1:A:461:VAL:O	1:A:462:ASP:HB2	2.16	0.46
1:A:478:THR:C	1:A:480:SER:H	2.24	0.46
1:A:603:ARG:HH22	1:A:606:HIS:CE1	2.34	0.46
1:A:357:LYS:HA	1:A:360:GLN:HE21	1.81	0.46
1:A:616:ALA:O	1:A:622:GLY:HA2	2.16	0.45
1:A:613:HIS:CD2	2:B:1:NAG:H62	2.52	0.44
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.99	0.43
1:A:606:HIS:CD2	10:A:2180:HOH:O	2.66	0.43
1:A:553:ASN:OD1	1:A:565:LYS:HA	2.18	0.43
1:A:609:GLN:HB2	10:A:2203:HOH:O	2.17	0.43
1:A:508:ASP:HB2	1:A:509:ASP:H	1.46	0.43
1:A:469:ILE:HD13	1:A:469:ILE:HA	1.87	0.43
1:A:458:HIS:CE1	1:A:471:MET:HE2	2.54	0.42
1:A:565:LYS:NZ	1:A:567:GLU:HB2	2.34	0.42
1:A:514:LYS:HE3	1:A:514:LYS:HB2	1.81	0.42
1:A:662:GLY:HA2	10:A:2135:HOH:O	2.20	0.42
1:A:553:ASN:CG	1:A:566:ARG:HG3	2.45	0.42
1:A:584:ALA:HB3	4:D:1:NAG:H82	2.01	0.41
1:A:455:LYS:HB3	1:A:504:LEU:HD11	2.02	0.41
1:A:669:ILE:CG2	1:A:673:LYS:HE2	2.50	0.41
1:A:414:ASN:HD22	1:A:414:ASN:HA	1.57	0.41
1:A:458:HIS:HE1	1:A:471:MET:HE2	1.87	0.40
1:A:561:ALA:HA	1:A:564:LEU:HG	2.04	0.40
1:A:565:LYS:CE	10:A:2078:HOH:O	2.69	0.40
1:A:619:GLY:O	1:A:625:CYS:HB2	2.22	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%)	319 (95%)	12 (4%)	6 (2%)	6 9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	CYS
1	A	483	PHE
1	A	685	ALA
1	A	684	CYS
1	A	683	ALA
1	A	420	HIS

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%)	262 (93%)	20 (7%)	13 23

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

Mol	Chain	Res	Type
1	A	356	LYS
1	A	367	GLN

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Mol	Chain	Res	Type
1	A	414	ASN
1	A	418	SER
1	A	478	THR
1	A	481	CYS
1	A	510	GLN
1	A	514	LYS
1	A	545	ASN
1	A	557	THR
1	A	562	LYS
1	A	565	LYS
1	A	591	VAL
1	A	609	GLN
1	A	627	ASP
1	A	651	LEU
1	A	663	THR
1	A	664	GLU
1	A	667	THR
1	A	676	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	360	GLN
1	A	414	ASN
1	A	420	HIS
1	A	551	ASN
1	A	594	ASN
1	A	613	HIS
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 ⓘ

11 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	0.49	0	17,19,21	2.05	3 (17%)
2	NAG	B	2	2	14,14,15	0.42	0	17,19,21	1.06	0
3	NAG	C	1	3,1	14,14,15	0.47	0	17,19,21	2.04	2 (11%)
3	NDG	C	2	3	14,14,15	0.64	0	17,19,21	1.09	1 (5%)
3	MAN	C	3	3	11,11,12	0.53	0	15,15,17	1.05	2 (13%)
3	BMA	C	4	3	11,11,12	0.57	0	15,15,17	0.91	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.78	1 (7%)	17,19,21	1.71	4 (23%)
4	NAG	D	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.34	1 (5%)
4	MAN	D	3	4	11,11,12	0.45	0	15,15,17	1.90	3 (20%)
4	BMA	D	4	4	11,11,12	0.74	0	15,15,17	2.03	4 (26%)
4	BMA	D	5	4	11,11,12	0.61	0	15,15,17	0.98	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	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NDG	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	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	D	4	4	-	2/2/19/22	0/1/1/1
4	BMA	D	5	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	2.34	1.55	1.52
4	D	2	NAG	C1-C2	2.29	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	7.11	121.72	112.19
3	C	1	NAG	C1-O5-C5	6.96	121.51	112.19
4	D	3	MAN	C1-O5-C5	5.90	120.09	112.19
4	D	2	NAG	C3-C4-C5	-4.48	102.10	110.23
4	D	4	BMA	C1-O5-C5	4.31	117.96	112.19
4	D	1	NAG	C1-O5-C5	4.25	117.88	112.19
4	D	4	BMA	C3-C4-C5	3.85	117.21	110.23
4	D	4	BMA	C2-C3-C4	3.63	117.25	110.86
4	D	3	MAN	O4-C4-C5	3.22	117.26	109.32
3	C	2	NDG	C1-O5-C5	3.22	116.50	112.19
4	D	1	NAG	C2-N2-C7	3.19	127.18	122.90
4	D	5	BMA	C1-C2-C3	2.83	113.77	109.64
2	B	1	NAG	O5-C5-C4	2.82	117.69	110.83
3	C	1	NAG	O5-C5-C4	2.74	117.50	110.83
4	D	1	NAG	O5-C1-C2	-2.61	107.25	111.29
3	C	3	MAN	C1-C2-C3	2.49	113.27	109.64
2	B	1	NAG	C3-C4-C5	2.48	114.74	110.23
4	D	4	BMA	C1-C2-C3	2.48	113.26	109.64
3	C	4	BMA	C1-C2-C3	2.40	113.14	109.64
4	D	3	MAN	O5-C5-C6	2.24	112.02	107.66
4	D	1	NAG	C4-C3-C2	2.06	114.04	111.02
3	C	3	MAN	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

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

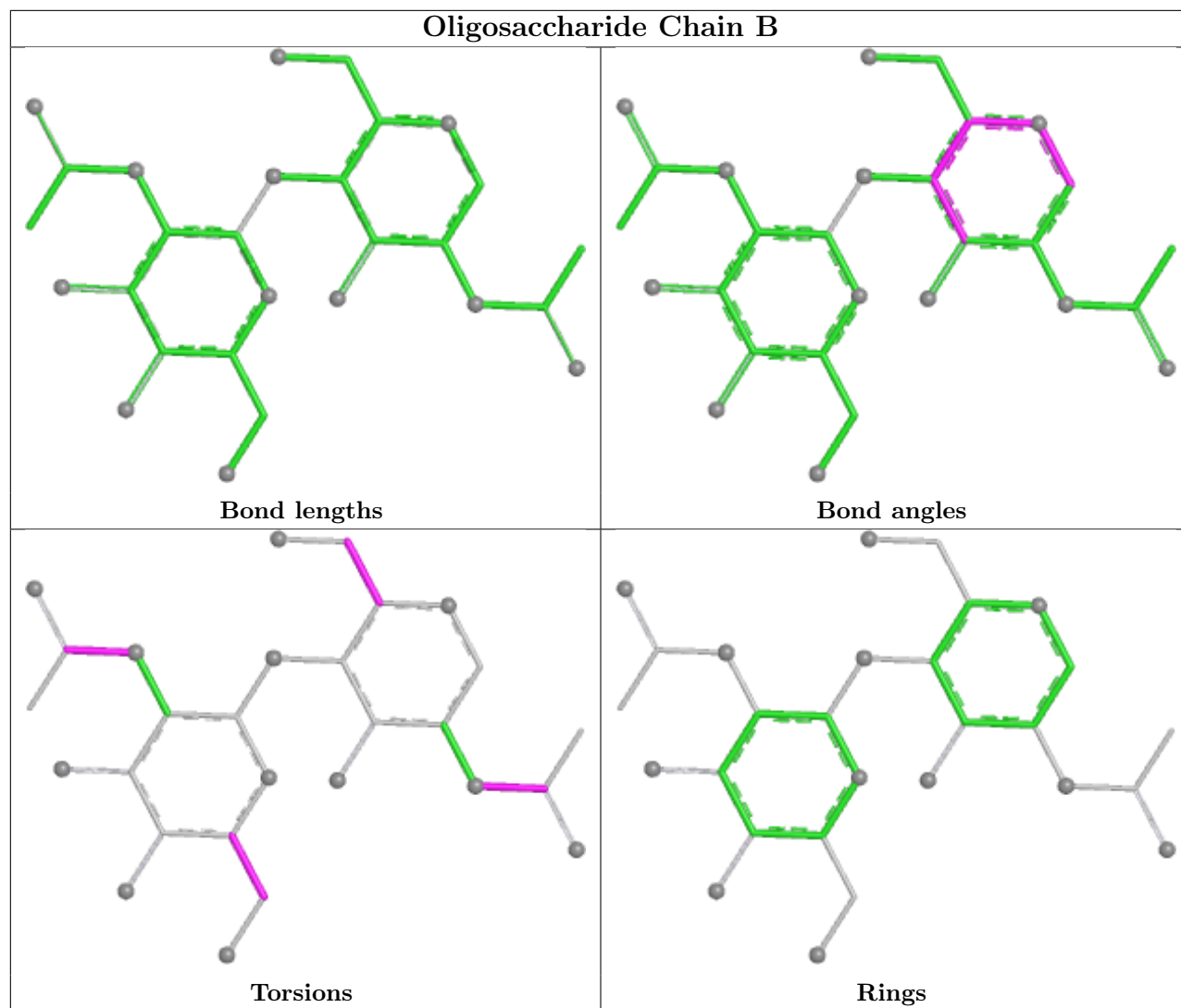
All (1) ring outliers are listed below:

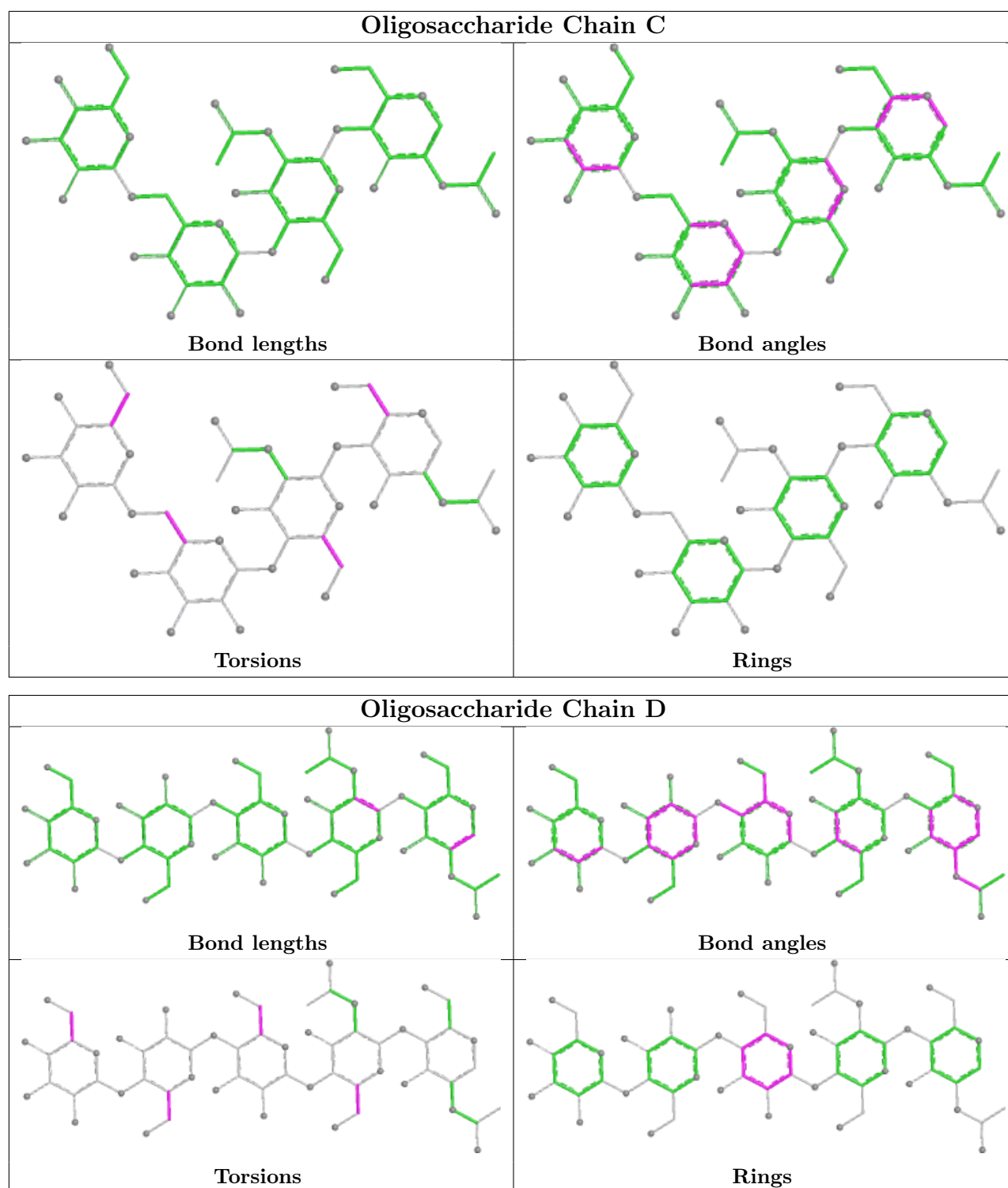
Mol	Chain	Res	Type	Atoms
4	D	3	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	BMA	2	0
2	B	2	NAG	1	0
2	B	1	NAG	2	0
4	D	1	NAG	1	0
4	D	3	MAN	2	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
8	CO3	A	688	7	3,3,3	0.45	0	2,3,3	0.97	0
9	ADN	A	2001	-	21,21,21	1.50	4 (19%)	31,31,31	2.13	5 (16%)
5	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.26	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
9	ADN	A	2001	-	-	0/6/22/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2001	ADN	C5-C4	4.24	1.46	1.39
9	A	2001	ADN	C5-N7	-2.88	1.33	1.39
9	A	2001	ADN	C5-C6	2.78	1.48	1.41
9	A	2001	ADN	C8-N7	2.15	1.35	1.31

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2001	ADN	C5-C4-N3	-6.78	117.38	126.72
9	A	2001	ADN	N3-C4-N9	6.06	137.47	127.17
9	A	2001	ADN	C2-N3-C4	3.56	120.53	111.83
9	A	2001	ADN	N3-C2-N1	-2.66	124.56	128.58
9	A	2001	ADN	C4-N9-C8	2.36	108.22	105.74

There are no chirality outliers.

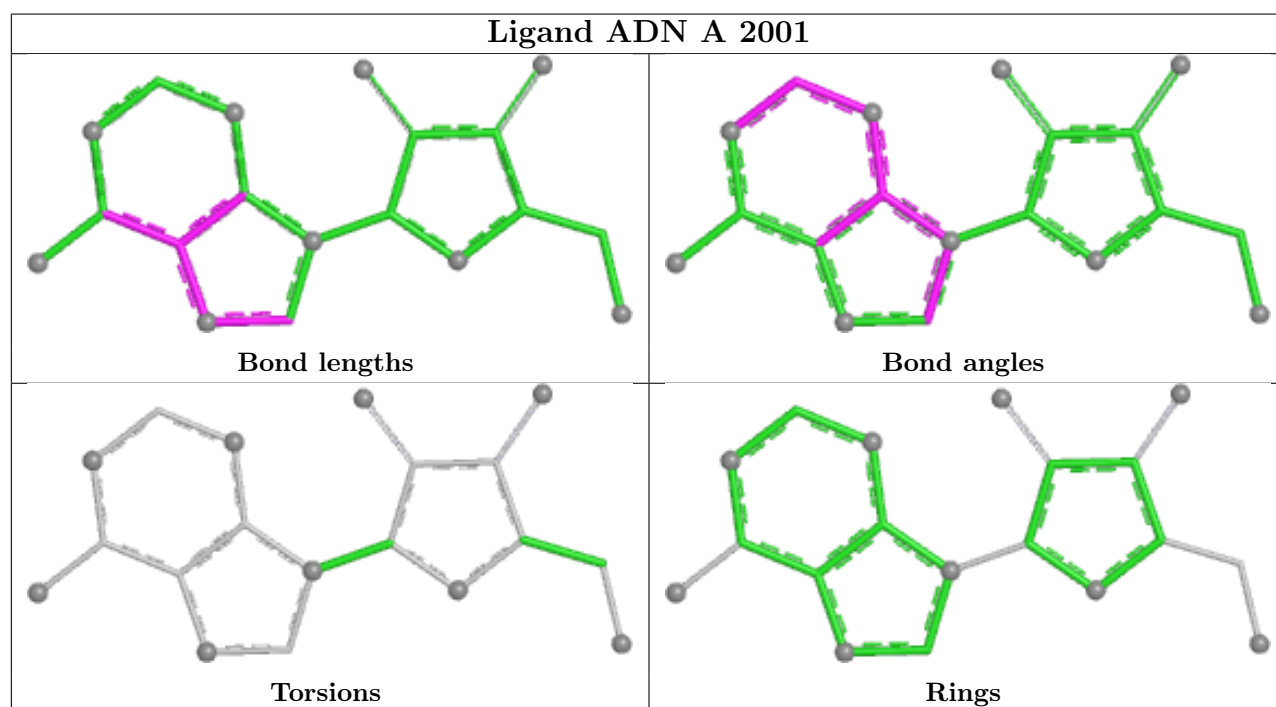
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2001	ADN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.