



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 AM UTC

PDB ID : 2R9J / pdb_00002r9j
Title : Ligand recognition in C-lobe: The crystal structure of the complex of lactoferrin C-lobe with nicotinamide at 2.5 Å resolution
Authors : Mir, R.; Vikram, G.; Singh, N.; Kumar, S.; Sinha, M.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on : 2007-09-13
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

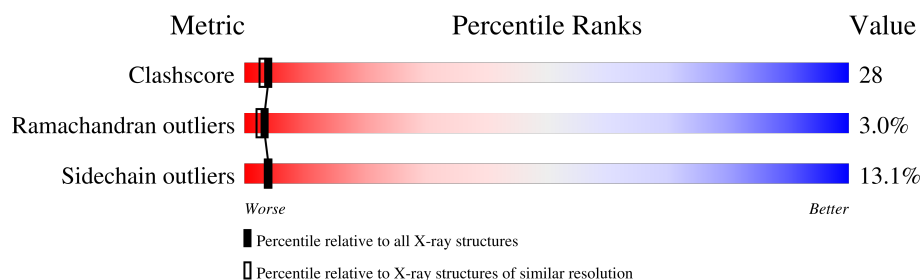
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

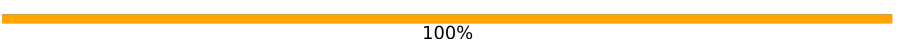
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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	
2	B	2	
2	C	2	

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	2	X	-	-	-
2	NAG	C	1	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 2867 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:

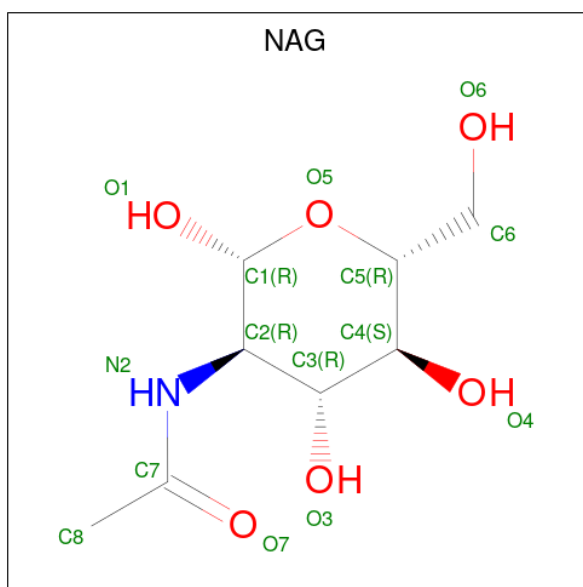
Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

- 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			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

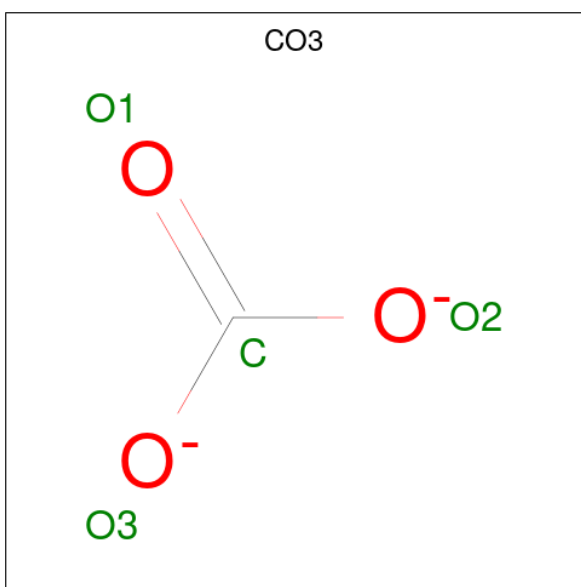
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

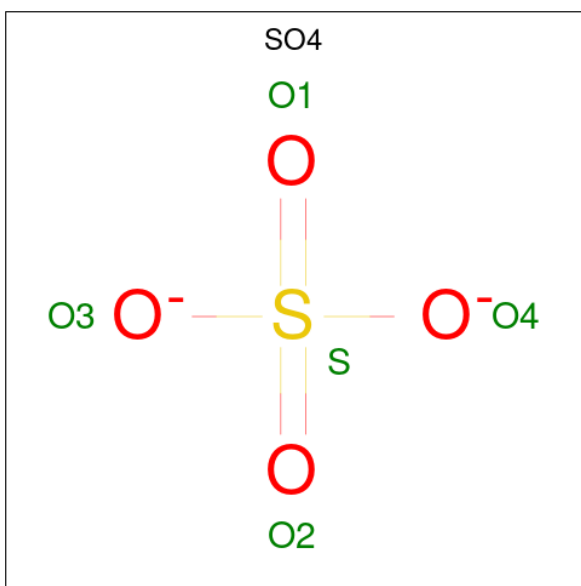
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



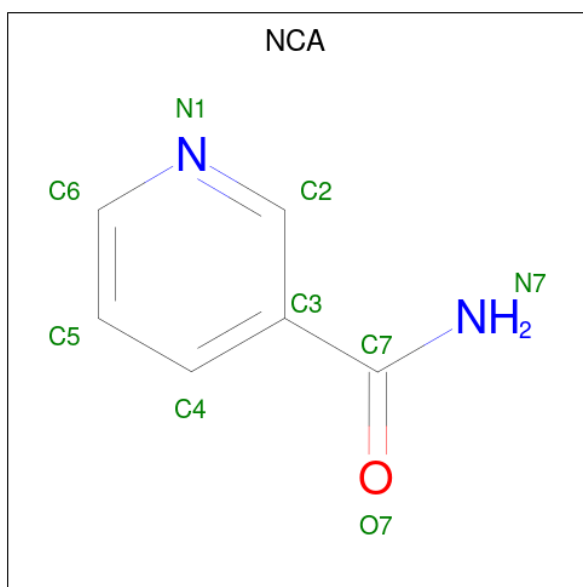
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is NICOTINAMIDE (CCD ID: NCA) (formula: C₆H₆N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 9 is water.

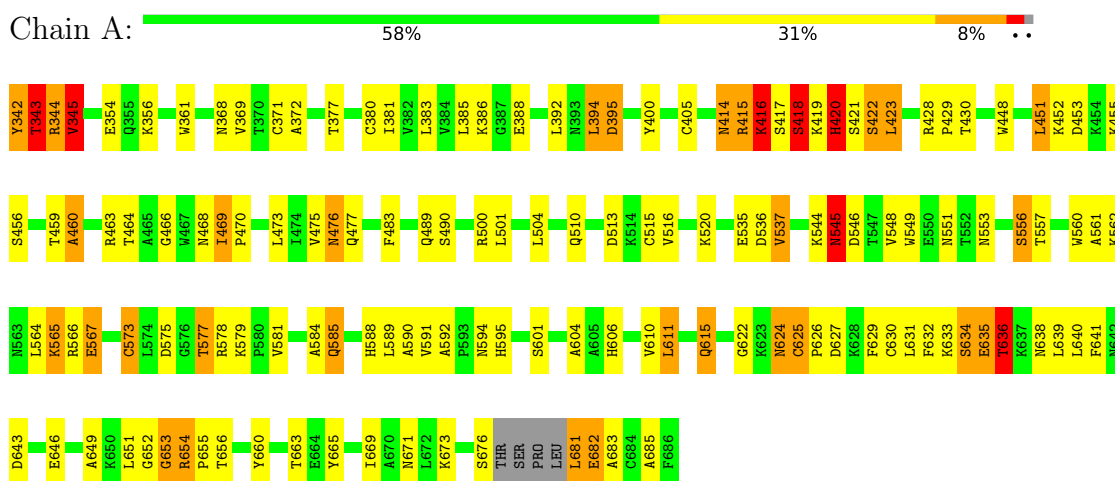
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	172	Total	O	0	0
			172	172		

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.

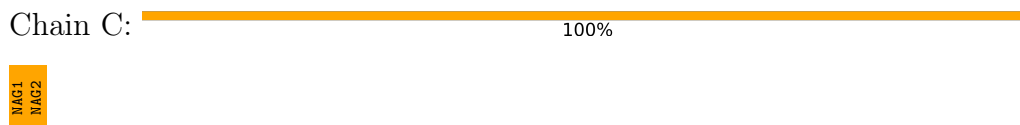
- Molecule 1: Lactotransferrin'



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



- Molecule 2: 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	63.33Å 50.34Å 65.91Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	85.7 (20.00-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2867	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: NAG, FE, CO3, SO4, NCA, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	5/2652 (0.2%)	1.26	32/3591 (0.9%)

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	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	ASN	CA-CB	-6.77	1.42	1.53
1	A	476	ASN	CB-CG	-5.80	1.37	1.52
1	A	636	THR	CA-CB	5.10	1.61	1.53
1	A	545	ASN	N-CA	-5.07	1.39	1.46
1	A	545	ASN	CA-C	5.04	1.59	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	SER	N-CA-C	13.53	129.92	113.41
1	A	556	SER	N-CA-C	7.77	123.07	112.90
1	A	476	ASN	N-CA-C	7.44	120.04	111.11
1	A	604	ALA	N-CA-C	7.31	119.88	111.11
1	A	343	THR	N-CA-C	7.02	125.75	110.80
1	A	656	THR	N-CA-C	-6.97	100.73	110.35
1	A	372	ALA	N-CA-C	-6.91	98.66	109.72
1	A	420	HIS	N-CA-C	-6.82	96.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	VAL	N-CA-C	-6.68	104.00	110.42
1	A	622	GLY	N-CA-C	6.65	119.57	111.93
1	A	651	LEU	N-CA-C	6.64	119.86	111.69
1	A	354	GLU	N-CA-C	-6.45	104.33	111.36
1	A	371	CYS	N-CA-C	6.39	119.88	109.59
1	A	345	VAL	N-CA-C	6.33	117.03	108.17
1	A	510	GLN	N-CA-C	6.24	120.59	112.92
1	A	395	ASP	N-CA-C	-6.08	101.93	110.50
1	A	624	ASN	N-CA-C	5.83	120.52	113.17
1	A	456	SER	N-CA-C	5.83	119.04	109.72
1	A	544	LYS	CA-C-N	-5.75	111.57	120.31
1	A	544	LYS	C-N-CA	-5.75	111.57	120.31
1	A	468	ASN	N-CA-C	5.65	118.17	111.33
1	A	653	GLY	N-CA-C	-5.59	105.92	115.08
1	A	419	LYS	CA-C-N	5.59	132.21	121.54
1	A	419	LYS	C-N-CA	5.59	132.21	121.54
1	A	636	THR	N-CA-C	5.51	119.24	111.52
1	A	545	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	537	VAL	N-CA-C	-5.32	104.31	111.44
1	A	394	LEU	N-CA-C	5.12	117.91	109.72
1	A	476	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	422	SER	N-CA-C	-5.04	104.78	112.04
1	A	510	GLN	CB-CA-C	-5.01	102.10	110.56
1	A	649	ALA	N-CA-C	5.00	117.73	109.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	660	TYR	Sidechain

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	2519	149	0
2	B	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	19	0
3	A	14	0	13	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	0	0	0
7	A	5	0	0	0	0
8	A	9	0	6	0	0
9	A	172	0	0	30	0
All	All	2867	0	2588	149	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 28.

All (149) 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:545:ASN:C	1:A:545:ASN:ND2	1.91	1.23
1:A:545:ASN:HD22	1:A:546:ASP:N	1.49	1.11
1:A:535:GLU:HB2	9:A:817:HOH:O	1.60	1.02
1:A:545:ASN:C	1:A:545:ASN:HD22	1.59	1.00
1:A:546:ASP:HA	2:C:1:NAG:O5	1.64	0.97
1:A:546:ASP:HB3	2:C:1:NAG:O6	1.64	0.97
1:A:546:ASP:CB	2:C:1:NAG:O6	2.12	0.97
1:A:549:TRP:HB2	2:C:1:NAG:H62	1.48	0.93
1:A:549:TRP:CD1	2:C:1:NAG:H5	2.03	0.93
1:A:546:ASP:CA	2:C:1:NAG:O6	2.16	0.93
1:A:546:ASP:HA	2:C:1:NAG:C6	1.99	0.92
1:A:584:ALA:HB3	2:C:1:NAG:H82	1.55	0.89
1:A:546:ASP:HA	2:C:1:NAG:O6	1.74	0.87
1:A:636:THR:O	1:A:636:THR:HG23	1.74	0.87
1:A:415:ARG:HG3	1:A:416:LYS:H	1.38	0.86
1:A:549:TRP:CG	2:C:1:NAG:H5	2.13	0.84
1:A:343:THR:O	1:A:344:ARG:HD3	1.79	0.83
1:A:386:LYS:HB2	9:A:832:HOH:O	1.78	0.83
1:A:549:TRP:HB2	2:C:1:NAG:C6	2.08	0.83
1:A:343:THR:HA	1:A:606:HIS:NE2	1.94	0.83
1:A:638:ASN:HD22	1:A:643:ASP:H	1.27	0.82
1:A:520:LYS:HB3	9:A:823:HOH:O	1.79	0.82
1:A:545:ASN:ND2	1:A:546:ASP:N	2.17	0.81
1:A:453:ASP:HB3	9:A:771:HOH:O	1.80	0.81
1:A:383:LEU:HA	9:A:832:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LYS:HZ3	1:A:567:GLU:H	1.31	0.79
1:A:638:ASN:ND2	1:A:643:ASP:H	1.82	0.76
1:A:546:ASP:HA	2:C:1:NAG:C5	2.14	0.76
1:A:560:TRP:HB2	9:A:846:HOH:O	1.86	0.76
1:A:473:LEU:HD23	2:B:1:NAG:H82	1.68	0.76
1:A:685:ALA:HB3	9:A:813:HOH:O	1.85	0.75
1:A:681:LEU:O	1:A:682:GLU:HB3	1.87	0.75
1:A:636:THR:O	1:A:636:THR:CG2	2.37	0.73
1:A:625:CYS:HA	1:A:629:PHE:O	1.89	0.73
1:A:415:ARG:CG	1:A:416:LYS:H	2.04	0.70
1:A:473:LEU:CD2	2:B:1:NAG:H82	2.23	0.69
1:A:430:THR:HB	1:A:594:ASN:ND2	2.08	0.68
1:A:386:LYS:HE3	9:A:832:HOH:O	1.93	0.68
1:A:415:ARG:HG3	1:A:416:LYS:N	2.07	0.68
1:A:565:LYS:HZ2	1:A:567:GLU:HB2	1.59	0.68
1:A:565:LYS:HZ3	1:A:567:GLU:N	1.90	0.67
1:A:565:LYS:NZ	1:A:567:GLU:H	1.92	0.66
1:A:343:THR:O	1:A:343:THR:HG23	1.95	0.66
1:A:513:ASP:HB2	9:A:823:HOH:O	1.95	0.66
1:A:575:ASP:OD1	1:A:577:THR:HB	1.95	0.66
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.31	0.66
1:A:546:ASP:CA	2:C:1:NAG:O5	2.43	0.65
1:A:545:ASN:ND2	1:A:545:ASN:O	2.29	0.65
1:A:546:ASP:O	2:C:1:NAG:H62	1.98	0.64
1:A:513:ASP:O	1:A:516:VAL:HG22	1.98	0.64
1:A:459:THR:OG1	1:A:466:GLY:HA3	1.98	0.63
1:A:565:LYS:NZ	1:A:567:GLU:HB2	2.12	0.63
1:A:626:PRO:HD3	9:A:835:HOH:O	1.98	0.63
1:A:536:ASP:HA	9:A:698:HOH:O	1.99	0.62
1:A:653:GLY:O	1:A:654:ARG:C	2.41	0.62
1:A:626:PRO:HG2	9:A:860:HOH:O	1.98	0.62
1:A:584:ALA:HB3	2:C:1:NAG:C8	2.29	0.61
1:A:388:GLU:HB2	9:A:832:HOH:O	1.99	0.61
1:A:343:THR:O	1:A:343:THR:CG2	2.47	0.61
1:A:343:THR:N	1:A:606:HIS:NE2	2.49	0.61
1:A:549:TRP:HB3	2:C:2:NAG:H82	1.83	0.61
1:A:632:PHE:HE2	9:A:724:HOH:O	1.84	0.61
1:A:342:TYR:C	1:A:606:HIS:NE2	2.60	0.60
1:A:415:ARG:O	1:A:646:GLU:HB2	2.01	0.60
1:A:625:CYS:SG	1:A:626:PRO:N	2.75	0.60
1:A:634:SER:C	1:A:635:GLU:HG3	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:GLU:HG2	9:A:759:HOH:O	2.04	0.58
1:A:343:THR:O	1:A:344:ARG:CD	2.49	0.57
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.86	0.56
1:A:344:ARG:H	1:A:606:HIS:HE1	1.55	0.55
1:A:565:LYS:CE	1:A:567:GLU:H	2.19	0.55
1:A:343:THR:CA	1:A:606:HIS:NE2	2.67	0.55
1:A:369:VAL:HG23	9:A:791:HOH:O	2.06	0.55
1:A:361:TRP:HB2	1:A:629:PHE:CZ	2.42	0.54
1:A:565:LYS:HE2	1:A:566:ARG:N	2.23	0.53
1:A:414:ASN:HD21	1:A:430:THR:HA	1.73	0.53
1:A:577:THR:HG23	1:A:578:ARG:N	2.22	0.53
1:A:625:CYS:O	1:A:626:PRO:C	2.51	0.53
1:A:400:TYR:HE2	9:A:852:HOH:O	1.91	0.53
1:A:577:THR:CG2	1:A:578:ARG:N	2.73	0.51
1:A:638:ASN:HD22	1:A:643:ASP:N	2.03	0.51
1:A:464:THR:HG21	1:A:592:ALA:HB1	1.92	0.51
1:A:415:ARG:CG	1:A:416:LYS:N	2.67	0.51
1:A:459:THR:O	1:A:460:ALA:HB2	2.11	0.50
1:A:415:ARG:O	1:A:416:LYS:HB3	2.11	0.50
1:A:537:VAL:HG23	9:A:817:HOH:O	2.11	0.50
1:A:551:ASN:HA	1:A:556:SER:HB2	1.95	0.49
1:A:343:THR:HA	1:A:606:HIS:CE1	2.47	0.49
1:A:625:CYS:C	1:A:630:CYS:SG	2.96	0.49
1:A:513:ASP:CB	9:A:823:HOH:O	2.57	0.48
1:A:566:ARG:NH2	2:C:2:NAG:H81	2.28	0.48
1:A:420:HIS:CE1	1:A:429:PRO:HD2	2.48	0.48
1:A:639:LEU:O	1:A:640:LEU:HB2	2.13	0.48
1:A:606:HIS:HB3	9:A:834:HOH:O	2.13	0.47
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.50	0.47
1:A:573:CYS:SG	1:A:579:LYS:HD2	2.55	0.47
1:A:590:ALA:HA	9:A:741:HOH:O	2.14	0.47
1:A:625:CYS:SG	1:A:626:PRO:HD3	2.55	0.47
1:A:625:CYS:CB	1:A:626:PRO:CD	2.93	0.46
1:A:682:GLU:O	1:A:682:GLU:HG3	2.16	0.46
1:A:537:VAL:CG2	9:A:817:HOH:O	2.63	0.46
1:A:345:VAL:O	1:A:369:VAL:HA	2.16	0.46
1:A:368:ASN:CB	9:A:791:HOH:O	2.64	0.46
1:A:553:ASN:OD1	1:A:565:LYS:HA	2.15	0.46
1:A:585:GLN:HB2	9:A:713:HOH:O	2.16	0.46
1:A:342:TYR:N	1:A:342:TYR:CD1	2.84	0.45
1:A:585:GLN:HG2	9:A:851:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:N	1:A:342:TYR:HD1	2.14	0.45
1:A:625:CYS:SG	1:A:626:PRO:CD	3.04	0.45
1:A:448:TRP:HE1	1:A:477:GLN:HE22	1.64	0.45
1:A:546:ASP:CA	2:C:1:NAG:C6	2.77	0.45
1:A:565:LYS:HE2	1:A:566:ARG:H	1.81	0.45
1:A:669:ILE:O	1:A:673:LYS:HG2	2.17	0.44
1:A:671:ASN:HB3	9:A:753:HOH:O	2.17	0.44
1:A:483:PHE:CD2	1:A:483:PHE:C	2.96	0.44
1:A:415:ARG:O	1:A:416:LYS:CB	2.65	0.44
1:A:548:VAL:HG11	1:A:581:VAL:HG11	2.00	0.44
1:A:556:SER:O	1:A:557:THR:OG1	2.20	0.44
1:A:385:LEU:HD11	1:A:405:CYS:HB3	2.00	0.44
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.76	0.43
1:A:423:LEU:HD22	1:A:428:ARG:HA	1.99	0.43
1:A:589:LEU:O	1:A:590:ALA:HB2	2.19	0.43
1:A:392:LEU:HD11	1:A:394:LEU:HD21	2.01	0.43
1:A:676:SER:C	9:A:842:HOH:O	2.62	0.43
1:A:610:VAL:HG21	9:A:798:HOH:O	2.18	0.43
1:A:430:THR:HB	1:A:594:ASN:HD22	1.82	0.42
1:A:490:SER:HB2	1:A:501:LEU:HA	2.00	0.42
1:A:681:LEU:O	1:A:682:GLU:CB	2.62	0.42
1:A:611:LEU:O	1:A:615:GLN:HB3	2.20	0.42
1:A:626:PRO:CG	9:A:860:HOH:O	2.59	0.42
1:A:549:TRP:CD1	2:C:1:NAG:C5	2.90	0.42
1:A:377:THR:O	1:A:381:ILE:HG13	2.19	0.42
1:A:585:GLN:O	1:A:588:HIS:HE1	2.02	0.42
1:A:561:ALA:HA	1:A:564:LEU:CD1	2.50	0.41
1:A:653:GLY:O	1:A:655:PRO:N	2.53	0.41
1:A:464:THR:HG21	1:A:592:ALA:CB	2.50	0.41
1:A:685:ALA:HA	9:A:762:HOH:O	2.20	0.41
1:A:417:SER:O	1:A:418:SER:C	2.63	0.41
1:A:577:THR:HG23	1:A:578:ARG:H	1.85	0.41
1:A:639:LEU:C	1:A:641:PHE:H	2.29	0.41
1:A:344:ARG:H	1:A:606:HIS:CE1	2.36	0.41
1:A:452:LYS:O	1:A:453:ASP:HB2	2.21	0.41
1:A:682:GLU:O	1:A:683:ALA:HB2	2.21	0.41
1:A:414:ASN:HD22	1:A:414:ASN:HA	1.52	0.41
1:A:573:CYS:SG	1:A:577:THR:HG22	2.60	0.41
1:A:469:ILE:N	1:A:470:PRO:HD2	2.35	0.41
1:A:585:GLN:O	1:A:588:HIS:CE1	2.74	0.41
1:A:624:ASN:O	1:A:625:CYS:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:HD3	1:A:489:GLN:HE21	1.86	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%)	306 (91%)	21 (6%)	10 (3%)	3 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	418	SER
1	A	420	HIS
1	A	625	CYS
1	A	416	LYS
1	A	682	GLU
1	A	460	ALA
1	A	634	SER
1	A	652	GLY
1	A	654	ARG

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%)	245 (87%)	37 (13%)	4 4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	TYR
1	A	343	THR
1	A	344	ARG
1	A	345	VAL
1	A	356	LYS
1	A	380	CYS
1	A	414	ASN
1	A	415	ARG
1	A	416	LYS
1	A	418	SER
1	A	420	HIS
1	A	422	SER
1	A	423	LEU
1	A	451	LEU
1	A	469	ILE
1	A	476	ASN
1	A	500	ARG
1	A	504	LEU
1	A	515	CYS
1	A	545	ASN
1	A	562	LYS
1	A	565	LYS
1	A	567	GLU
1	A	573	CYS
1	A	577	THR
1	A	585	GLN
1	A	591	VAL
1	A	601	SER
1	A	611	LEU
1	A	615	GLN
1	A	627	ASP
1	A	631	LEU
1	A	633	LYS
1	A	635	GLU
1	A	636	THR
1	A	663	THR
1	A	681	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	414	ASN
1	A	420	HIS
1	A	489	GLN
1	A	624	ASN
1	A	638	ASN
1	A	671	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 ⓘ

4 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	1.71	4 (28%)	17,19,21	1.84	3 (17%)
2	NAG	B	2	2	14,14,15	0.54	0	17,19,21	0.66	0
2	NAG	C	1	2,1	14,14,15	1.97	2 (14%)	17,19,21	1.99	7 (41%)
2	NAG	C	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.12	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	-4.88	1.45	1.52
2	C	1	NAG	C3-C2	-4.38	1.43	1.52
2	B	1	NAG	C1-C2	2.94	1.56	1.52
2	B	1	NAG	C4-C5	-2.74	1.47	1.53
2	B	1	NAG	O4-C4	-2.70	1.36	1.43
2	C	2	NAG	C4-C3	2.47	1.58	1.52
2	B	1	NAG	O5-C1	2.20	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C4-C3-C2	-6.20	101.93	111.02
2	C	1	NAG	C2-N2-C7	-4.49	116.88	122.90
2	C	1	NAG	O4-C4-C3	-2.86	103.63	110.38
2	C	1	NAG	C4-C3-C2	2.71	114.98	111.02
2	C	1	NAG	O5-C5-C6	2.53	112.59	107.66
2	C	1	NAG	C1-C2-N2	-2.38	106.67	110.43
2	C	2	NAG	C4-C3-C2	2.36	114.47	111.02
2	C	2	NAG	C1-C2-N2	-2.34	106.75	110.43
2	B	1	NAG	O4-C4-C5	-2.21	103.89	109.32
2	C	1	NAG	O4-C4-C5	-2.13	104.08	109.32
2	C	1	NAG	C3-C4-C5	2.03	113.91	110.23
2	B	1	NAG	O5-C5-C4	-2.02	105.91	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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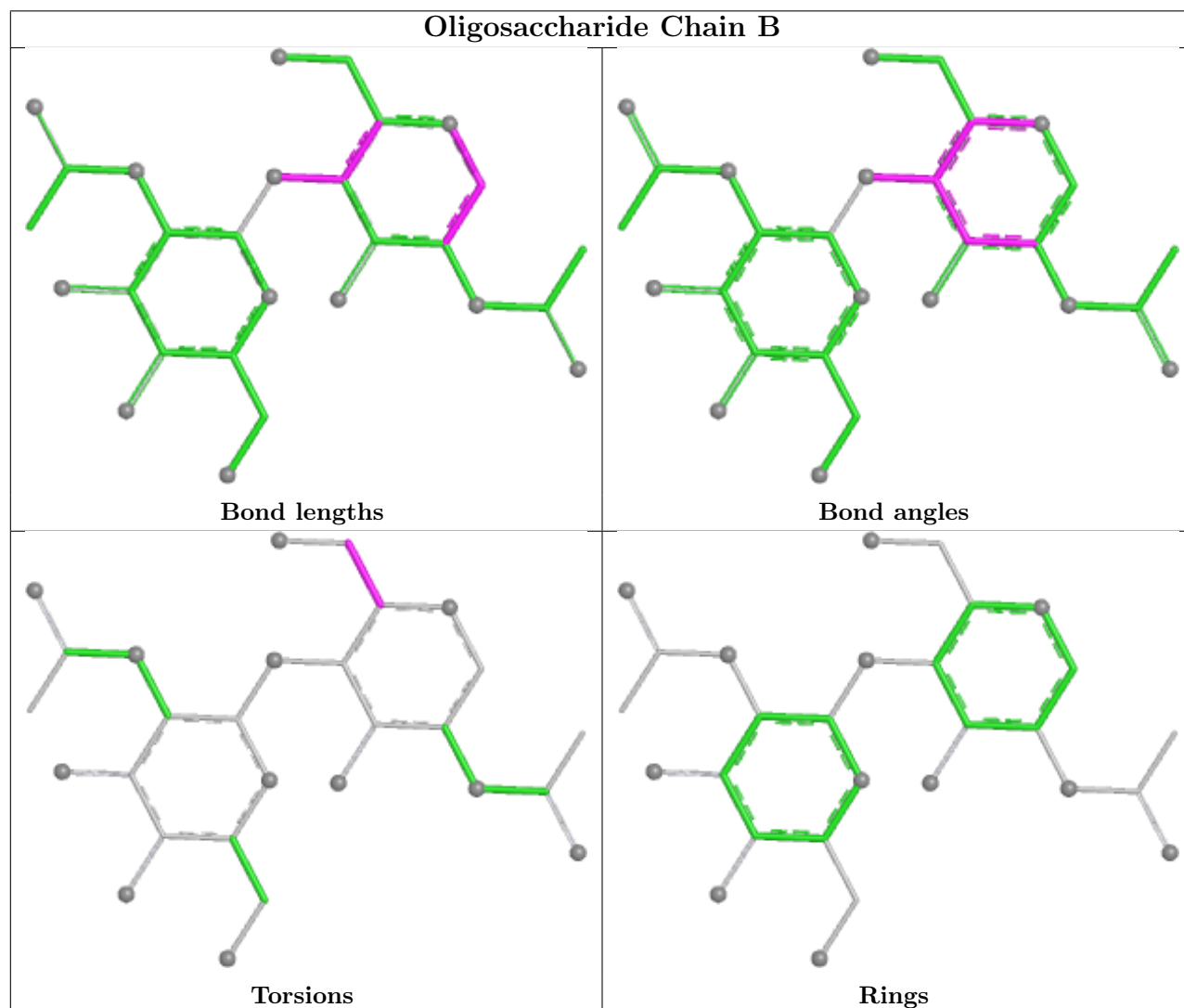
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

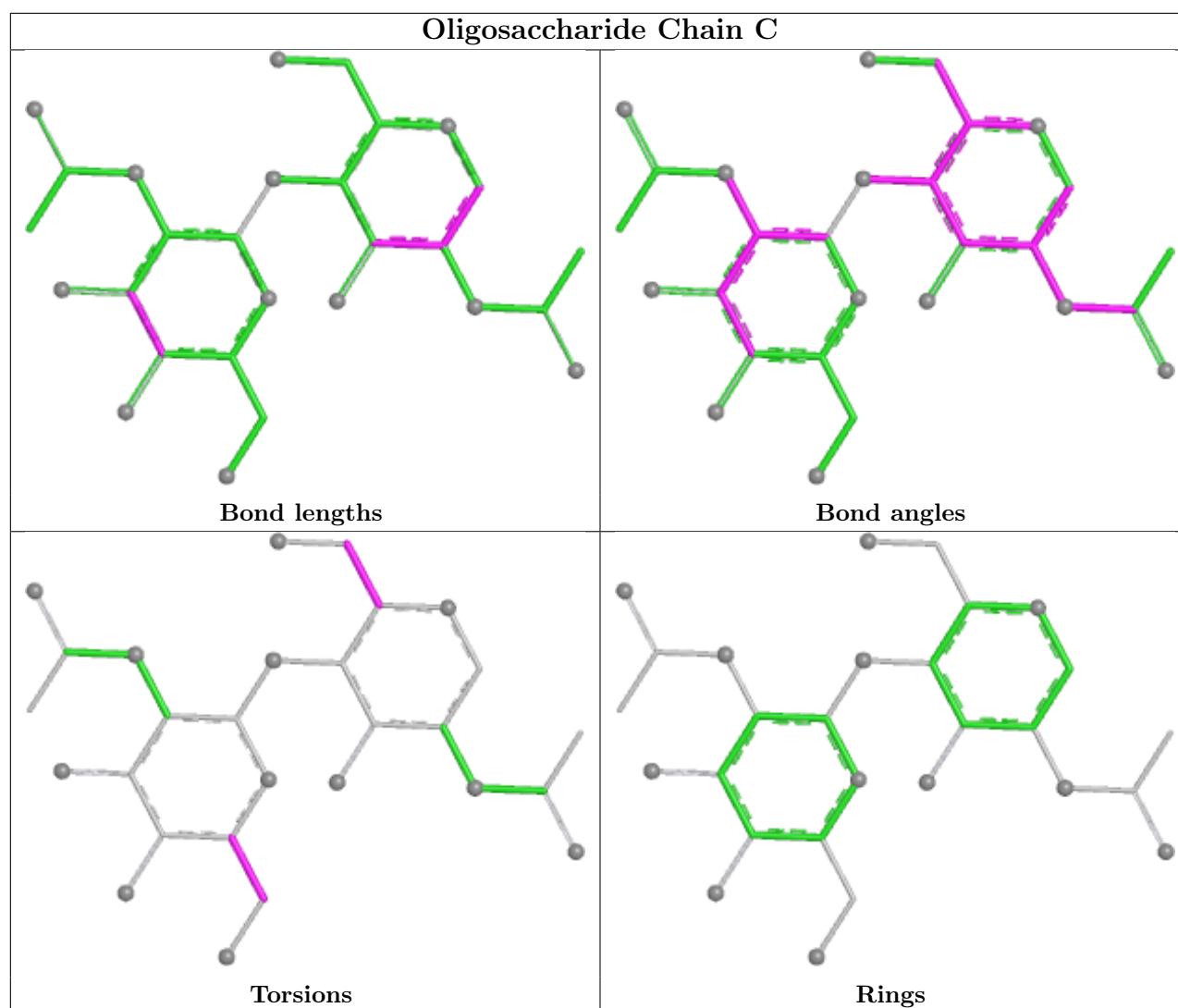
There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
2	C	1	NAG	17	0
2	C	2	NAG	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 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	$\# Z > 2$
7	SO4	A	691	-	4,4,4	0.80	0	6,6,6	0.41	0
6	CO3	A	690	5	3,3,3	0.91	0	2,3,3	0.14	0
3	NAG	A	1	1	14,14,15	0.69	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NCA	A	692	-	9,9,9	1.81	3 (33%)	11,11,11	1.33	1 (9%)

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
3	NAG	A	1	1	-	0/6/23/26	0/1/1/1
8	NCA	A	692	-	-	0/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	692	NCA	C4-C3	3.32	1.44	1.39
8	A	692	NCA	C2-C3	2.82	1.43	1.39
8	A	692	NCA	C7-N7	2.24	1.37	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	692	NCA	C6-N1-C2	2.89	121.91	116.85

There are no chirality outliers.

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.