



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:34 PM UTC

PDB ID : 4NED / pdb_00004ned
Title : Crystal STRUCTURE OF C-LOBE OF BOVINE LACTOFERRIN COM-
PLEXED WITH FENOPROFEN AT 2.1 ANGSTROM RESOLUTION
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Deposited on : 2013-10-29
Resolution : 2.10 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

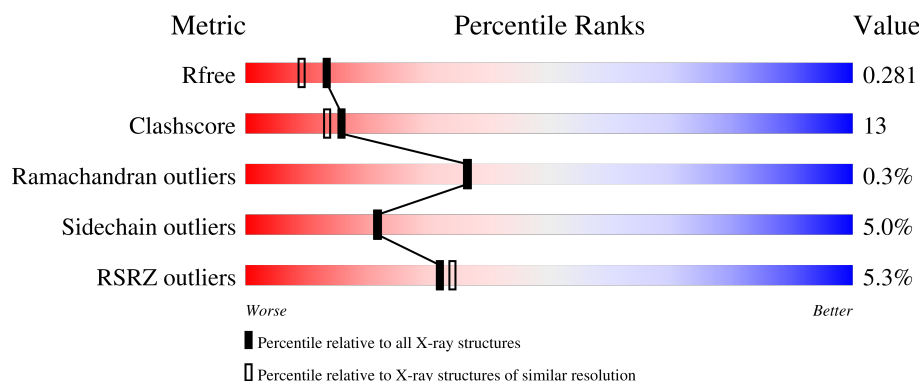
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	345	5% 70% 27% ..
2	B	2	50% 50%

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
8	PFN	A	709	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 2894 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			

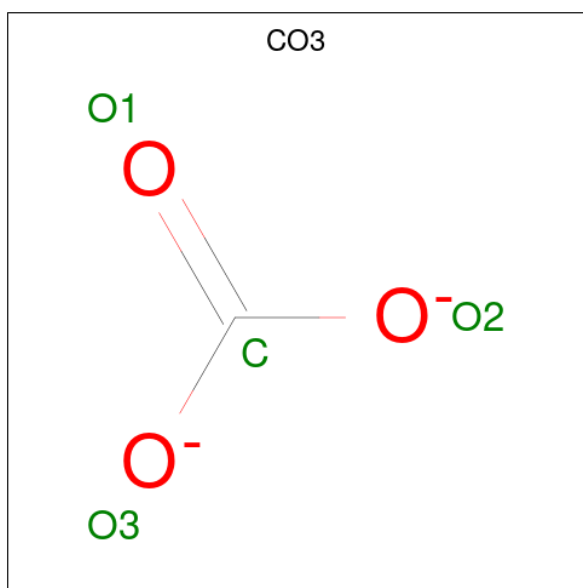
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

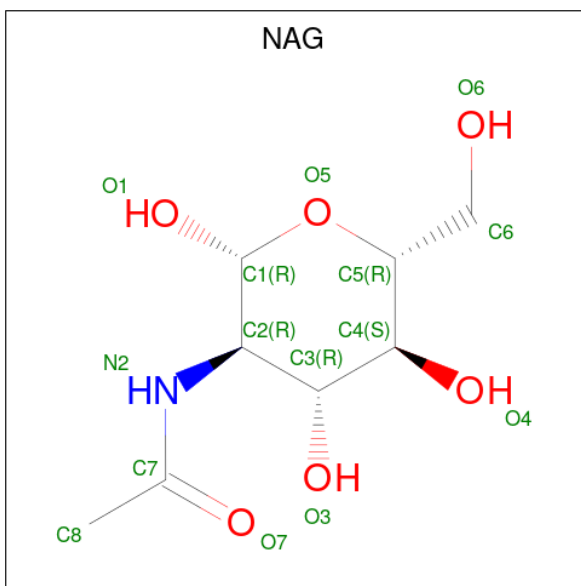
- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

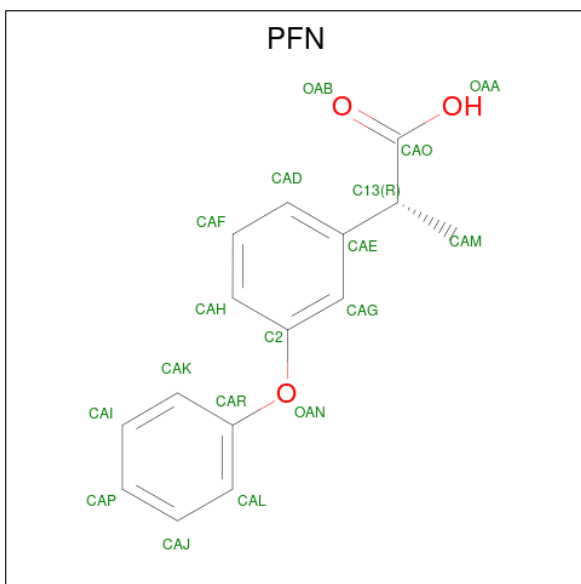
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

- Molecule 8 is FENOPROFEN (CCD ID: PFN) (formula: C₁₅H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			18	15	3		

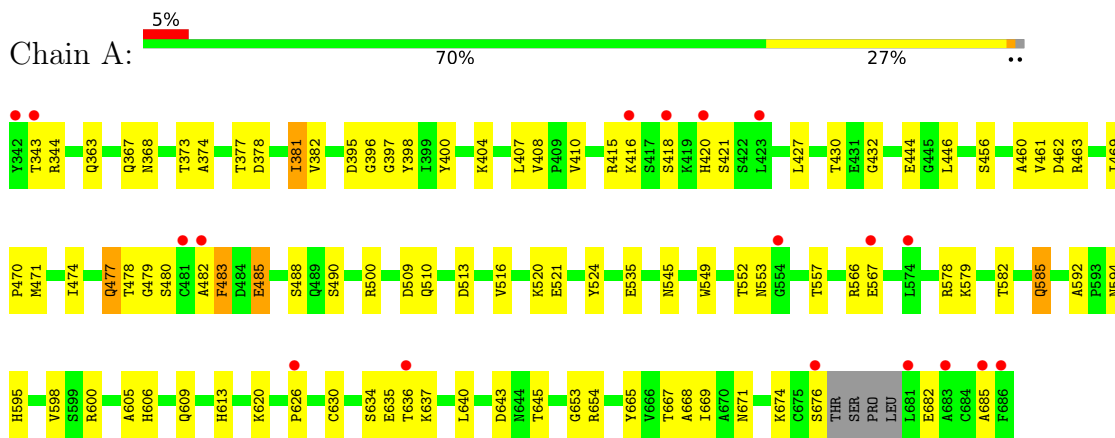
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	204	Total 204	O 204	0	0

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 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.

• Molecule 1: Lactotransferrin



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.47Å 50.07Å 65.49Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	37.89 – 2.10 37.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.89-2.10) 98.0 (37.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.10Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.223 , 0.252 0.215 , 0.281	Depositor DCC
R_{free} test set	1149 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2894	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.25	6/2652 (0.2%)	1.19	4/3591 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	605	ALA	CA-CB	6.22	1.63	1.53
1	A	598	VAL	N-CA	-5.94	1.39	1.46
1	A	382	VAL	CA-CB	5.88	1.61	1.54
1	A	381	ILE	CA-CB	5.81	1.61	1.54
1	A	408	VAL	CA-CB	5.70	1.61	1.54
1	A	645	THR	CA-CB	5.18	1.60	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	GLU	N-CA-C	-7.81	103.65	113.02
1	A	396	GLY	N-CA-C	6.57	120.84	112.83
1	A	640	LEU	CB-CA-C	-5.79	98.90	110.42
1	A	410	VAL	CB-CA-C	-5.50	106.16	111.05

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	2520	67	0
2	B	28	0	25	1	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	4	0	0	0	0
6	A	5	0	0	0	0
7	A	28	0	26	5	0
8	A	18	0	13	9	0
9	A	204	0	0	7	0
All	All	2894	0	2584	70	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 13.

All (70) 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:368:ASN:HD21	7:A:705:NAG:H2	1.26	0.98
1:A:471:MET:HE3	1:A:483:PHE:HB2	1.54	0.89
1:A:685:ALA:CB	8:A:709:PFN:HAP	2.04	0.87
1:A:609:GLN:HG3	9:A:876:HOH:O	1.71	0.87
8:A:709:PFN:CAG	8:A:709:PFN:HAL	2.09	0.83
8:A:709:PFN:CAG	8:A:709:PFN:CAL	2.56	0.79
1:A:482:ALA:HB1	1:A:485:GLU:HG3	1.71	0.72
1:A:368:ASN:ND2	7:A:705:NAG:H2	2.06	0.67
1:A:636:THR:HA	1:A:643:ASP:OD2	1.95	0.66
1:A:509:ASP:HB3	9:A:933:HOH:O	1.96	0.66
1:A:415:ARG:HG3	1:A:416:LYS:N	2.13	0.64
1:A:400:TYR:CZ	1:A:404:LYS:HE3	2.33	0.62
1:A:430:THR:HB	1:A:594:ASN:ND2	2.14	0.62
1:A:553:ASN:OD1	1:A:566:ARG:HG3	2.00	0.62
1:A:685:ALA:HB1	8:A:709:PFN:HAP	1.80	0.61
1:A:676:SER:HB3	8:A:709:PFN:HAM3	1.84	0.59
1:A:585:GLN:HB2	9:A:835:HOH:O	2.03	0.58
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.38	0.58
1:A:344:ARG:HD3	1:A:367:GLN:O	2.04	0.58
1:A:368:ASN:HD21	7:A:705:NAG:C2	2.11	0.55
1:A:668:ALA:HB1	7:A:706:NAG:H83	1.88	0.55
1:A:421:SER:HB2	9:A:870:HOH:O	2.07	0.54
1:A:600:ARG:HB2	9:A:873:HOH:O	2.08	0.53
1:A:553:ASN:CG	1:A:566:ARG:HG3	2.34	0.53
1:A:474:ILE:O	1:A:478:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PHE:CD2	1:A:483:PHE:C	2.87	0.53
1:A:626:PRO:HA	1:A:630:CYS:SG	2.49	0.53
1:A:685:ALA:HB2	8:A:709:PFN:HAP	1.90	0.52
1:A:416:LYS:HE3	1:A:620:LYS:HE3	1.92	0.52
1:A:377:THR:O	1:A:381:ILE:HG12	2.12	0.50
1:A:415:ARG:CG	1:A:416:LYS:N	2.73	0.50
8:A:709:PFN:CAL	8:A:709:PFN:HAG	2.41	0.50
1:A:462:ASP:OD1	8:A:709:PFN:HAH	2.13	0.49
1:A:653:GLY:O	1:A:654:ARG:C	2.56	0.48
1:A:513:ASP:O	1:A:516:VAL:HG22	2.13	0.48
1:A:509:ASP:OD1	1:A:510:GLN:N	2.46	0.48
1:A:446:LEU:O	1:A:578:ARG:NH1	2.45	0.47
1:A:469:ILE:HB	1:A:470:PRO:HD3	1.96	0.47
1:A:471:MET:CE	1:A:483:PHE:HB2	2.36	0.47
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.50	0.47
1:A:671:ASN:HA	1:A:674:LYS:HD2	1.98	0.46
1:A:483:PHE:C	1:A:483:PHE:HD2	2.23	0.46
1:A:671:ASN:ND2	7:A:706:NAG:H5	2.32	0.45
1:A:567:GLU:HA	1:A:567:GLU:OE1	2.16	0.45
1:A:456:SER:O	1:A:490:SER:HA	2.16	0.45
1:A:549:TRP:HB2	2:B:1:NAG:H62	1.99	0.45
1:A:415:ARG:HG3	1:A:416:LYS:H	1.82	0.44
1:A:579:LYS:NZ	9:A:959:HOH:O	2.50	0.44
1:A:520:LYS:HA	1:A:520:LYS:HD2	1.85	0.44
1:A:432:GLY:HA2	1:A:592:ALA:O	2.17	0.44
1:A:674:LYS:C	1:A:676:SER:H	2.25	0.43
1:A:378:ASP:OD2	8:A:709:PFN:HAK	2.18	0.43
1:A:460:ALA:HB3	1:A:463:ARG:HD3	2.00	0.43
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.54	0.43
1:A:415:ARG:NH2	1:A:432:GLY:O	2.46	0.43
1:A:635:GLU:CD	1:A:637:LYS:HZ3	2.27	0.43
1:A:477:GLN:NE2	9:A:817:HOH:O	2.53	0.42
1:A:343:THR:HG22	1:A:606:HIS:HB3	2.00	0.42
1:A:549:TRP:CH2	1:A:582:THR:HG22	2.53	0.42
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.54	0.42
1:A:521:GLU:HB3	1:A:524:TYR:HB2	2.03	0.41
1:A:488:SER:O	1:A:500:ARG:HD3	2.21	0.41
1:A:373:THR:HG22	1:A:374:ALA:N	2.36	0.41
1:A:469:ILE:HB	1:A:470:PRO:CD	2.51	0.41
1:A:397:GLY:HA3	1:A:462:ASP:O	2.21	0.41
1:A:461:VAL:O	1:A:462:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:C	1:A:480:SER:N	2.78	0.41
1:A:407:LEU:CD2	1:A:600:ARG:HG3	2.51	0.41
1:A:634:SER:O	1:A:637:LYS:HE2	2.21	0.41
1:A:552:THR:OG1	1:A:566:ARG:HG2	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%)	310 (92%)	26 (8%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	GLY

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%)	268 (95%)	14 (5%)	22	22

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	418	SER
1	A	420	HIS
1	A	427	LEU
1	A	444	GLU
1	A	477	GLN
1	A	483	PHE
1	A	485	GLU
1	A	545	ASN
1	A	557	THR
1	A	585	GLN
1	A	613	HIS
1	A	667	THR
1	A	682	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	367	GLN
1	A	368	ASN
1	A	594	ASN
1	A	613	HIS
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](#)

2 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	0.76	1 (7%)	17,19,21	1.61	2 (11%)
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	2.41	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.16	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.30	121.97	112.19
2	B	1	NAG	C1-O5-C5	5.62	119.72	112.19
2	B	2	NAG	O5-C1-C2	3.60	116.86	111.29
2	B	2	NAG	C3-C4-C5	-3.59	103.72	110.23
2	B	1	NAG	C2-N2-C7	2.52	126.28	122.90
2	B	2	NAG	C4-C3-C2	-2.46	107.41	111.02
2	B	2	NAG	O4-C4-C5	2.18	114.68	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

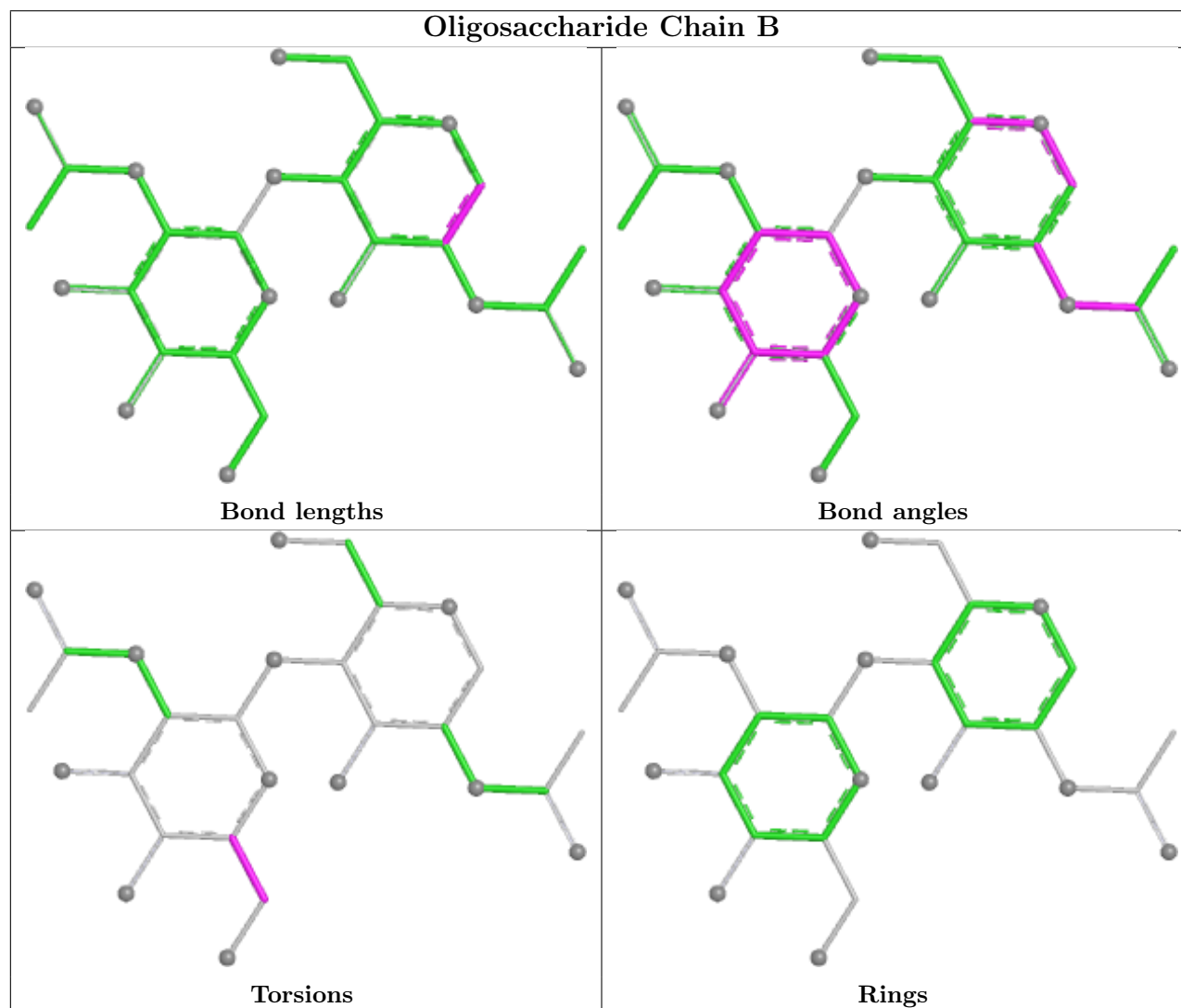
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	PFN	A	709	-	19,19,19	1.27	2 (10%)	25,25,25	1.32	3 (12%)
7	NAG	A	705	-	14,14,15	0.62	0	17,19,21	1.63	3 (17%)
6	SO4	A	704	-	4,4,4	0.23	0	6,6,6	0.37	0
5	CO3	A	703	4	3,3,3	0.89	0	2,3,3	1.31	0
7	NAG	A	706	1	14,14,15	0.63	0	17,19,21	1.58	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
7	NAG	A	705	-	-	2/6/23/26	0/1/1/1
8	PFN	A	709	-	-	3/12/12/12	0/2/2/2
7	NAG	A	706	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	709	PFN	CAE-C13	-3.40	1.46	1.52
8	A	709	PFN	CAG-CAE	-2.02	1.36	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	706	NAG	C1-O5-C5	4.77	118.58	112.19
7	A	705	NAG	C4-C3-C2	3.75	116.52	111.02
7	A	705	NAG	C3-C4-C5	3.32	116.24	110.23
7	A	705	NAG	O5-C1-C2	-3.01	106.63	111.29
8	A	709	PFN	C2-OAN-CAR	-2.60	112.84	118.78
8	A	709	PFN	CAM-C13-CAE	-2.59	106.44	112.92
8	A	709	PFN	CAG-CAE-C13	-2.10	114.72	120.29
7	A	706	NAG	C2-N2-C7	2.02	125.61	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	705	NAG	O5-C5-C6-O6
7	A	705	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	709	PFN	CAE-C13-CAO-OAA
8	A	709	PFN	CAE-C13-CAO-OAB
8	A	709	PFN	CAM-C13-CAO-OAB

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	709	PFN	9	0
7	A	705	NAG	3	0
7	A	706	NAG	2	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/345 (98%)	0.55	18 (5%) 32 34	24, 41, 73, 93	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	5.6
1	A	554	GLY	4.3
1	A	420	HIS	3.8
1	A	418	SER	3.6
1	A	416	LYS	3.4
1	A	685	ALA	3.4
1	A	683	ALA	3.3
1	A	626	PRO	3.1
1	A	343	THR	2.8
1	A	636	THR	2.8
1	A	676	SER	2.7
1	A	567	GLU	2.6
1	A	686	PHE	2.5
1	A	482	ALA	2.4
1	A	342	TYR	2.3
1	A	681	LEU	2.0
1	A	481	CYS	2.0
1	A	574	LEU	2.0

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

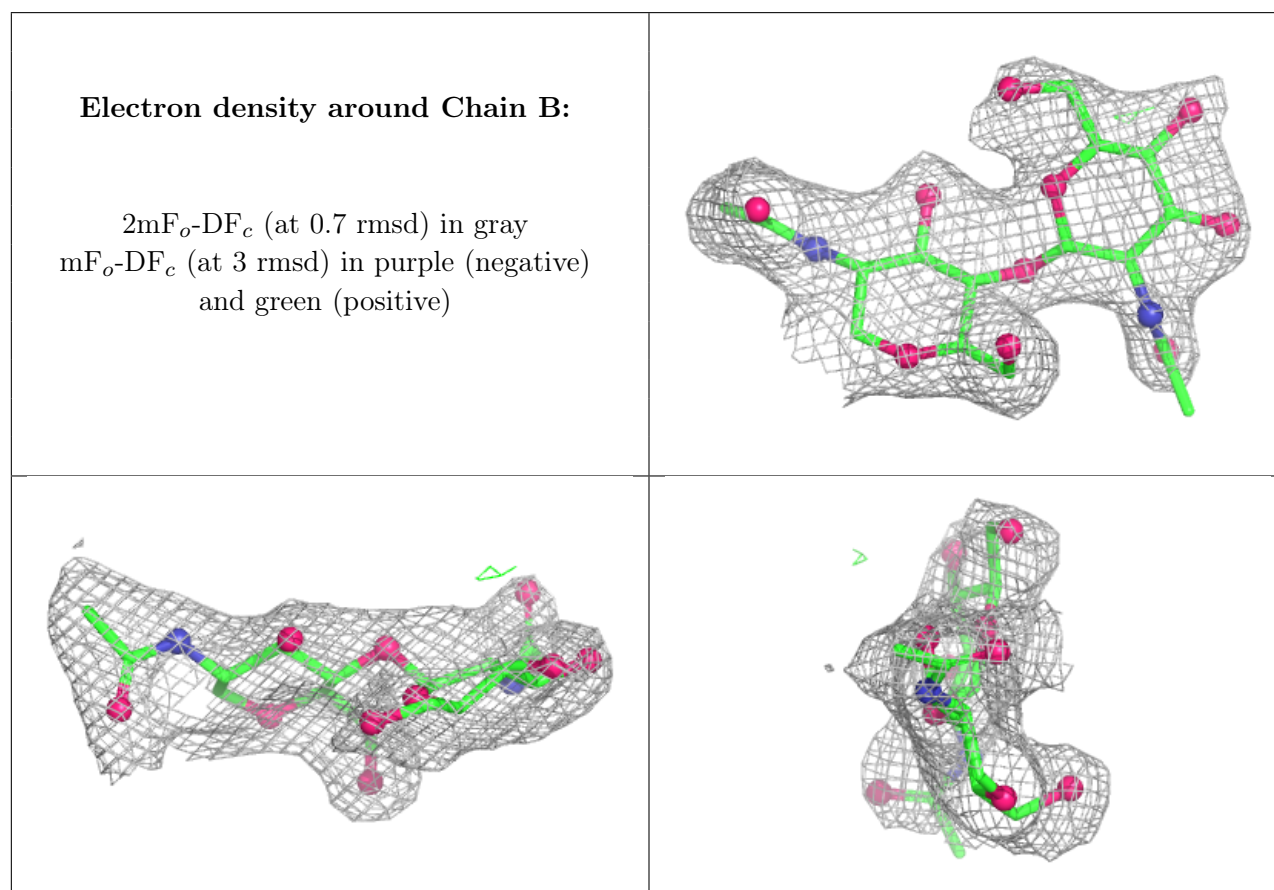
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.81	0.12	74,78,80,81	0
2	NAG	B	1	14/15	0.86	0.10	50,55,61,67	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	PFN	A	709	18/18	0.63	0.17	67,73,78,79	0
7	NAG	A	705	14/15	0.65	0.17	98,100,101,101	0
7	NAG	A	706	14/15	0.77	0.12	70,74,81,82	0
6	SO4	A	704	5/5	0.80	0.12	108,108,109,109	0
3	ZN	A	710	1/1	0.95	0.09	56,56,56,56	0
5	CO3	A	703	4/4	0.95	0.06	21,24,25,26	0
4	FE	A	702	1/1	0.99	0.03	27,27,27,27	0
3	ZN	A	701	1/1	0.99	0.02	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.