



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:13 AM UTC

PDB ID : 1LXK / pdb_00001lxk
Title : Streptococcus pneumoniae Hyaluronate Lyase in Complex with Tetrasaccharide Hyaluronan Substrate
Authors : Jedrzejewski, M.J.; Mello, L.V.; De Groot, B.L.; Li, S.
Deposited on : 2002-06-05
Resolution : 1.53 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

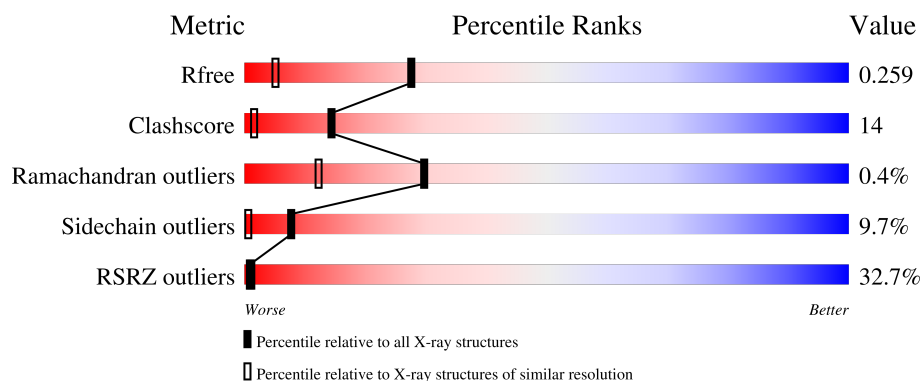
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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 $\leq 5\%$. 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	721	
2	B	4	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6512 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 Hyaluronate Lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5774	3632	966	1154	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	PHE	TYR	engineered mutation	GB 437705
A	731	VAL	GLY	SEE REMARK 999	GB 437705

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			53	28	2	23			

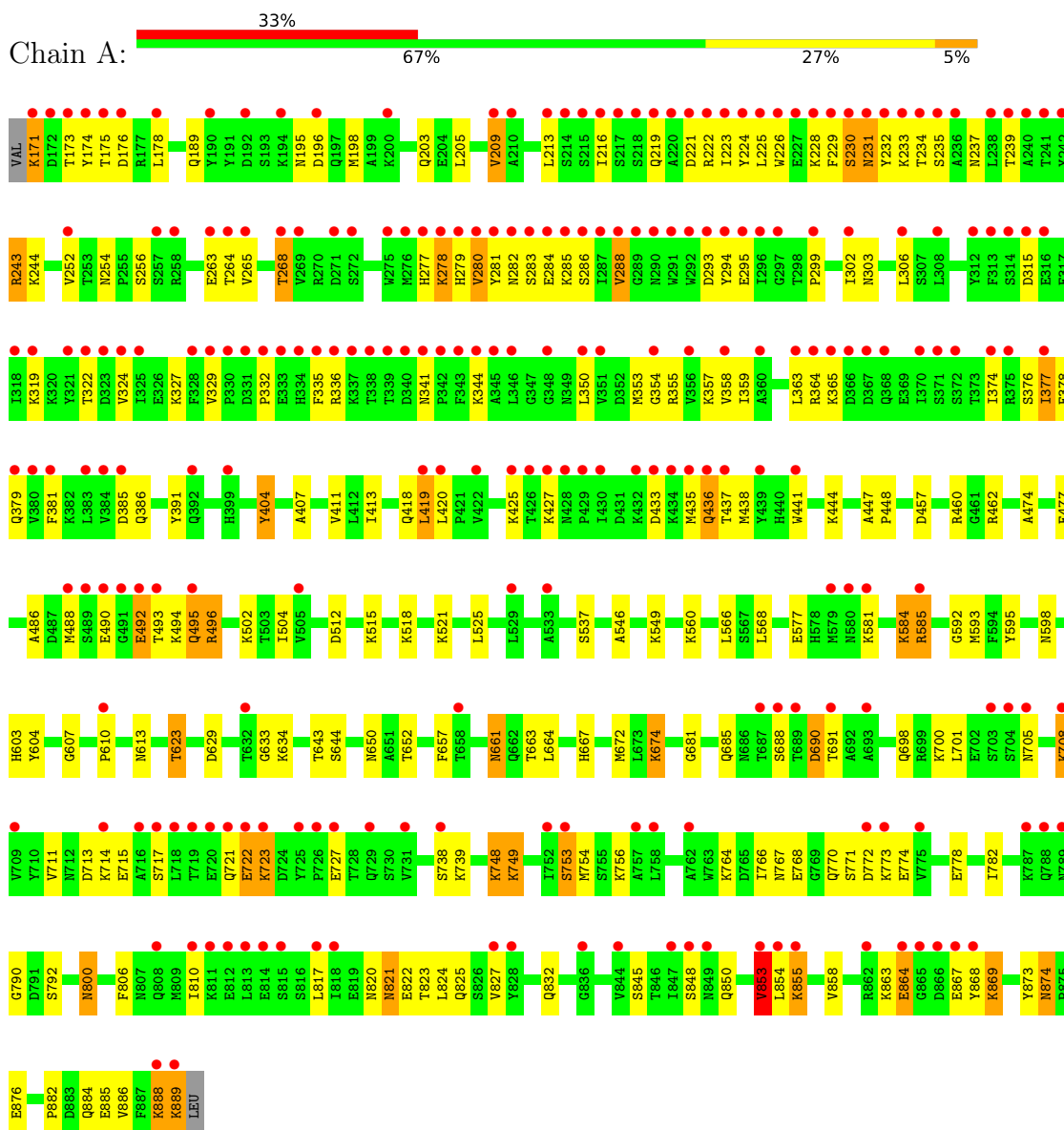
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	685	Total	O	0	0
			685	685		

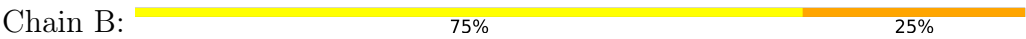
3 Residue-property plots [i](#)

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: Hyaluronate Lyase



- Molecule 2: beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



MA31
BDP2
MA33
BDP4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.74Å 103.82Å 101.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.53 20.00 – 1.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.53) 93.5 (20.00-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.52Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.239 0.226 , 0.259	Depositor DCC
R_{free} test set	1227 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6512	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 3.87% 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, BDP

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	0.39	0/5893	0.87	10/7958 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	ASN	N-CA-C	7.46	121.75	111.90
1	A	518	LYS	N-CA-C	7.43	121.25	112.93
1	A	657	PHE	N-CA-C	6.87	120.45	110.28
1	A	633	GLY	N-CA-C	6.48	119.46	112.33
1	A	233	LYS	N-CA-C	-6.42	105.27	113.23
1	A	623	THR	N-CA-C	-6.20	101.61	110.59
1	A	853	VAL	N-CA-C	-5.71	100.25	108.53
1	A	225	LEU	N-CA-C	-5.48	104.71	111.40
1	A	280	VAL	N-CA-C	5.43	120.64	109.34
1	A	419	LEU	N-CA-C	5.23	116.78	111.14

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	5774	0	5591	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	38	1	0
3	A	685	0	0	30	0
All	All	6512	0	5629	161	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 14.

All (161) 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:613:ASN:H	1:A:698:GLN:HE22	1.08	0.92
1:A:264:THR:O	1:A:268:THR:HG22	1.70	0.91
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.58	0.86
1:A:821:ASN:ND2	1:A:824:LEU:H	1.76	0.82
1:A:821:ASN:HD21	1:A:824:LEU:H	1.32	0.74
1:A:171:LYS:HB2	1:A:175:THR:HG21	1.73	0.70
1:A:644:SER:HB3	3:A:1281:HOH:O	1.93	0.67
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.41	0.67
1:A:754:MET:HG2	1:A:782:ILE:HG12	1.75	0.67
1:A:295:GLU:HB3	1:A:329:VAL:HG22	1.77	0.66
1:A:171:LYS:HE3	1:A:315:ASP:OD2	1.95	0.66
1:A:889:LYS:HG2	3:A:1688:HOH:O	1.95	0.66
1:A:874:ASN:C	1:A:874:ASN:HD22	2.04	0.66
1:A:708:LYS:HD3	1:A:715:GLU:HG3	1.78	0.66
1:A:546:ALA:HB1	3:A:1058:HOH:O	1.98	0.64
1:A:335:PHE:CE2	1:A:353:MET:HE2	2.34	0.63
1:A:288:VAL:HG13	1:A:294:TYR:OH	1.99	0.63
1:A:821:ASN:ND2	1:A:823:THR:H	1.95	0.63
1:A:178:LEU:HD11	1:A:363:LEU:HD23	1.81	0.62
1:A:821:ASN:C	1:A:821:ASN:HD22	2.06	0.62
1:A:607:GLY:C	1:A:610:PRO:HD2	2.25	0.62
1:A:336:ARG:HH12	2:B:1:NAG:H2	1.64	0.61
1:A:705:ASN:HB3	3:A:1240:HOH:O	2.00	0.61
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.65	0.61
1:A:603:HIS:ND1	3:A:1444:HOH:O	2.31	0.60
1:A:711:VAL:CG2	1:A:754:MET:HE1	2.32	0.59
1:A:189:GLN:HG2	3:A:1546:HOH:O	2.03	0.59
1:A:286:SER:O	1:A:288:VAL:HG12	2.03	0.59
1:A:663:THR:HB	1:A:688:SER:HB3	1.85	0.58
1:A:821:ASN:HD22	1:A:823:THR:H	1.50	0.58
1:A:492:GLU:HG3	1:A:493:THR:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:LYS:HB2	1:A:886:VAL:HG12	1.84	0.58
1:A:652:THR:HB	3:A:1281:HOH:O	2.03	0.57
1:A:764:LYS:HD2	1:A:772:ASP:HB3	1.86	0.57
1:A:205:LEU:O	1:A:209:VAL:HG13	2.05	0.57
1:A:713:ASP:C	1:A:714:LYS:HD2	2.30	0.57
1:A:411:VAL:HG13	3:A:1623:HOH:O	2.03	0.57
1:A:254:ASN:ND2	1:A:256:SER:H	2.03	0.57
1:A:717:SER:O	1:A:723:LYS:HE3	2.06	0.56
1:A:585:ARG:HG3	1:A:766:ILE:HG22	1.88	0.56
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.88	0.55
1:A:888:LYS:O	1:A:889:LYS:HB2	2.06	0.55
1:A:711:VAL:HG22	1:A:754:MET:HE1	1.89	0.54
1:A:254:ASN:C	1:A:254:ASN:HD22	2.15	0.54
1:A:355:ARG:HH11	1:A:418:GLN:NE2	2.06	0.54
1:A:376:SER:O	1:A:379:GLN:HG2	2.08	0.53
1:A:174:TYR:CD2	1:A:365:LYS:HG2	2.43	0.53
1:A:235:SER:HB2	1:A:293:ASP:HB2	1.90	0.53
1:A:889:LYS:HD3	3:A:1688:HOH:O	2.07	0.53
1:A:288:VAL:HG22	1:A:288:VAL:O	2.09	0.53
1:A:386:GLN:NE2	3:A:1635:HOH:O	2.41	0.52
1:A:420:LEU:HD22	1:A:435:MET:HE3	1.91	0.52
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.37	0.52
1:A:495:GLN:CA	1:A:495:GLN:HE21	2.23	0.52
1:A:560:LYS:NZ	3:A:1232:HOH:O	2.43	0.51
1:A:420:LEU:HD13	1:A:435:MET:CE	2.41	0.51
1:A:254:ASN:ND2	1:A:254:ASN:C	2.69	0.51
1:A:462:ARG:HD3	1:A:577:GLU:OE2	2.10	0.50
1:A:355:ARG:NH2	3:A:1623:HOH:O	2.44	0.50
1:A:173:THR:O	1:A:176:ASP:HB2	2.11	0.50
1:A:566:LEU:HD23	3:A:1062:HOH:O	2.10	0.50
1:A:623:THR:HB	1:A:690:ASP:HB2	1.93	0.50
1:A:213:LEU:HD11	1:A:265:VAL:HG22	1.93	0.50
1:A:230:SER:O	1:A:232:TYR:N	2.45	0.50
1:A:661:ASN:C	1:A:661:ASN:HD22	2.20	0.50
1:A:806:PHE:O	1:A:810:ILE:HG23	2.11	0.49
1:A:239:THR:HG22	1:A:243:ARG:HD2	1.94	0.49
1:A:322:THR:OG1	1:A:364:ARG:NH1	2.44	0.49
1:A:216:ILE:HD12	1:A:226:TRP:CZ2	2.47	0.49
1:A:723:LYS:HD3	3:A:1203:HOH:O	2.12	0.49
1:A:224:TYR:CD2	1:A:230:SER:HB3	2.47	0.49
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:TYR:HA	3:A:1444:HOH:O	2.13	0.48
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.78	0.48
1:A:228:LYS:HD2	1:A:229:PHE:CE1	2.48	0.48
1:A:420:LEU:HD13	1:A:435:MET:HE3	1.96	0.48
1:A:598:ASN:HB2	1:A:739:LYS:O	2.14	0.48
1:A:303:ASN:HB3	1:A:359:ILE:HG21	1.96	0.47
1:A:303:ASN:HB3	1:A:359:ILE:CG2	2.44	0.47
1:A:701:LEU:HD12	1:A:778:GLU:HG2	1.96	0.47
1:A:374:ILE:O	1:A:378:GLU:HG3	2.15	0.47
1:A:634:LYS:HD2	3:A:1459:HOH:O	2.15	0.47
1:A:585:ARG:NH1	1:A:629:ASP:OD2	2.48	0.47
1:A:229:PHE:HE2	1:A:244:LYS:HE2	1.80	0.47
1:A:504:ILE:HG23	3:A:1016:HOH:O	2.15	0.47
1:A:354:GLY:O	1:A:358:VAL:HB	2.15	0.47
1:A:722:GLU:HG2	1:A:753:SER:OG	2.15	0.47
1:A:850:GLN:O	1:A:889:LYS:HD2	2.14	0.46
1:A:708:LYS:HD3	1:A:715:GLU:CG	2.45	0.46
1:A:585:ARG:HH11	1:A:629:ASP:CG	2.23	0.46
1:A:888:LYS:O	1:A:889:LYS:CB	2.64	0.46
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.98	0.46
1:A:295:GLU:HB3	1:A:329:VAL:CG2	2.46	0.46
1:A:667:HIS:HD2	3:A:1142:HOH:O	1.99	0.45
1:A:764:LYS:HA	1:A:767:ASN:O	2.16	0.45
1:A:329:VAL:HG12	1:A:357:LYS:HD2	1.98	0.45
1:A:381:PHE:O	1:A:437:THR:HG21	2.17	0.45
1:A:277:HIS:CD2	3:A:1528:HOH:O	2.69	0.45
1:A:581:LYS:O	1:A:584:LYS:HD2	2.15	0.45
1:A:643:THR:HB	3:A:1058:HOH:O	2.16	0.45
1:A:708:LYS:CD	1:A:715:GLU:HG3	2.46	0.45
1:A:748:LYS:O	1:A:749:LYS:C	2.59	0.45
1:A:607:GLY:O	1:A:610:PRO:HD2	2.16	0.45
1:A:502:LYS:HD3	1:A:537:SER:HB2	1.98	0.45
1:A:203:GLN:HG3	3:A:1374:HOH:O	2.17	0.45
1:A:768:GLU:HG3	3:A:1536:HOH:O	2.17	0.45
1:A:224:TYR:CG	1:A:230:SER:HB3	2.52	0.44
1:A:738:SER:O	1:A:800:ASN:HA	2.17	0.44
1:A:864:GLU:OE2	1:A:869:LYS:HD3	2.18	0.44
1:A:568:LEU:HD23	1:A:592:GLY:HA2	2.00	0.44
1:A:644:SER:HB2	1:A:873:TYR:HB3	1.98	0.44
1:A:244:LYS:HE2	3:A:1366:HOH:O	2.16	0.44
1:A:231:ASN:O	1:A:237:ASN:ND2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ARG:HD3	1:A:629:ASP:OD1	2.17	0.44
1:A:771:SER:OG	1:A:773:LYS:HB2	2.17	0.44
1:A:436:GLN:O	1:A:436:GLN:HG2	2.17	0.44
1:A:661:ASN:HD22	1:A:661:ASN:H	1.66	0.44
1:A:858:VAL:HG12	3:A:1281:HOH:O	2.17	0.44
1:A:790:GLY:HA2	3:A:1132:HOH:O	2.17	0.43
1:A:863:LYS:HD2	1:A:868:TYR:OH	2.18	0.43
1:A:512:ASP:HB3	1:A:515:LYS:HG3	2.00	0.43
1:A:278:LYS:HG2	1:A:279:HIS:CD2	2.53	0.43
1:A:664:LEU:HA	1:A:685:GLN:O	2.18	0.43
1:A:623:THR:HA	1:A:691:THR:O	2.18	0.43
1:A:332:PRO:O	1:A:353:MET:HG2	2.18	0.43
1:A:521:LYS:HA	1:A:521:LYS:HD2	1.80	0.43
1:A:681:GLY:O	1:A:792:SER:HB2	2.18	0.43
1:A:282:ASN:HD22	1:A:284:GLU:N	2.17	0.43
1:A:474:ALA:O	1:A:477:GLU:HB2	2.19	0.42
1:A:672:MET:HE1	3:A:1062:HOH:O	2.19	0.42
1:A:486:ALA:O	1:A:494:LYS:HG3	2.20	0.42
1:A:495:GLN:NE2	3:A:1005:HOH:O	2.51	0.42
1:A:488:MET:HE2	3:A:1602:HOH:O	2.19	0.42
1:A:882:PRO:O	1:A:885:GLU:HB2	2.19	0.42
1:A:223:ILE:N	1:A:223:ILE:HD13	2.34	0.42
1:A:496:ARG:HH11	1:A:496:ARG:HG3	1.85	0.42
1:A:457:ASP:HA	1:A:460:ARG:HG3	2.01	0.42
1:A:661:ASN:C	1:A:661:ASN:ND2	2.76	0.42
1:A:295:GLU:C	1:A:299:PRO:HG2	2.44	0.42
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.90	0.41
1:A:302:ILE:O	1:A:306:LEU:HG	2.19	0.41
1:A:175:THR:HA	1:A:178:LEU:HB2	2.02	0.41
1:A:350:LEU:O	1:A:353:MET:HB3	2.20	0.41
1:A:335:PHE:CZ	1:A:353:MET:HE2	2.54	0.41
1:A:438:MET:HG2	1:A:441:TRP:CZ3	2.55	0.41
1:A:521:LYS:HE3	1:A:525:LEU:HG	2.02	0.41
1:A:767:ASN:HB3	1:A:770:GLN:CG	2.51	0.41
1:A:822:GLU:HG2	1:A:823:THR:HG23	2.03	0.41
1:A:282:ASN:HD22	1:A:284:GLU:H	1.67	0.41
1:A:420:LEU:HD12	1:A:488:MET:HE1	2.02	0.41
1:A:231:ASN:C	1:A:237:ASN:HD22	2.27	0.41
1:A:593:MET:HE2	1:A:595:TYR:CZ	2.55	0.41
1:A:821:ASN:HD21	1:A:824:LEU:N	2.07	0.41
1:A:195:ASN:CG	1:A:198:MET:HG3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:LYS:NZ	3:A:1442:HOH:O	2.55	0.40
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.57	0.40
1:A:869:LYS:N	1:A:869:LYS:HD2	2.36	0.40
1:A:234:THR:HG22	3:A:1533:HOH:O	2.20	0.40
1:A:281:TYR:CD2	1:A:324:VAL:HG11	2.57	0.40
1:A:391:TYR:CD2	1:A:549:LYS:HG3	2.57	0.40
1:A:821:ASN:ND2	1:A:821:ASN:C	2.76	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	717/721 (99%)	676 (94%)	38 (5%)	3 (0%)	30 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	848	SER
1	A	674	LYS

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	638/640 (100%)	576 (90%)	62 (10%)	80

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	A	196	ASP
1	A	209	VAL
1	A	219	GLN
1	A	221	ASP
1	A	222	ARG
1	A	230	SER
1	A	243	ARG
1	A	252	VAL
1	A	263	GLU
1	A	268	THR
1	A	278	LYS
1	A	280	VAL
1	A	283	SER
1	A	285	LYS
1	A	288	VAL
1	A	319	LYS
1	A	327	LYS
1	A	341	ASN
1	A	344	LYS
1	A	377	ILE
1	A	385	ASP
1	A	404	TYR
1	A	413	ILE
1	A	419	LEU
1	A	425	LYS
1	A	427	LYS
1	A	433	ASP
1	A	436	GLN
1	A	444	LYS
1	A	490	GLU
1	A	492	GLU
1	A	495	GLN
1	A	496	ARG
1	A	584	LYS
1	A	585	ARG
1	A	661	ASN
1	A	674	LYS

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Mol	Chain	Res	Type
1	A	690	ASP
1	A	708	LYS
1	A	721	GLN
1	A	722	GLU
1	A	723	LYS
1	A	727	GLU
1	A	748	LYS
1	A	749	LYS
1	A	753	SER
1	A	756	LYS
1	A	774	GLU
1	A	817	LEU
1	A	821	ASN
1	A	827	VAL
1	A	853	VAL
1	A	854	LEU
1	A	855	LYS
1	A	864	GLU
1	A	867	GLU
1	A	869	LYS
1	A	874	ASN
1	A	876	GLU
1	A	888	LYS
1	A	889	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	254	ASN
1	A	277	HIS
1	A	282	ASN
1	A	341	ASN
1	A	349	ASN
1	A	368	GLN
1	A	418	GLN
1	A	436	GLN
1	A	495	GLN
1	A	580	ASN
1	A	661	ASN
1	A	667	HIS
1	A	698	GLN

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Mol	Chain	Res	Type
1	A	705	ASN
1	A	729	GLN
1	A	759	GLN
1	A	784	GLN
1	A	820	ASN
1	A	821	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	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	15,15,15	2.24	7 (46%)	21,21,21	1.22	3 (14%)
2	BDP	B	2	2	12,12,13	5.66	3 (25%)	14,17,19	2.25	3 (21%)
2	NAG	B	3	2	14,14,15	2.59	6 (42%)	17,19,21	0.94	2 (11%)
2	BDP	B	4	2	12,12,13	3.19	4 (33%)	14,17,19	1.56	2 (14%)

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	-	2/6/26/26	0/1/1/1
2	BDP	B	2	2	-	1/4/21/24	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1
2	BDP	B	4	2	-	1/4/21/24	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BDP	C5-C6	-14.01	1.23	1.53
2	B	4	BDP	C4-C5	-9.77	1.37	1.53
2	B	2	BDP	C4-C5	9.42	1.68	1.53
2	B	2	BDP	O5-C5	9.13	1.61	1.43
2	B	3	NAG	O5-C1	6.16	1.54	1.43
2	B	1	NAG	O5-C1	4.29	1.53	1.42
2	B	1	NAG	C2-N2	4.02	1.52	1.45
2	B	3	NAG	C1-C2	3.69	1.57	1.52
2	B	3	NAG	O5-C5	3.60	1.50	1.43
2	B	3	NAG	C2-N2	3.54	1.52	1.46
2	B	1	NAG	C1-C2	3.00	1.56	1.52
2	B	4	BDP	O4-C4	2.81	1.49	1.43
2	B	1	NAG	C4-C5	2.75	1.58	1.53
2	B	4	BDP	C2-C3	2.69	1.56	1.52
2	B	1	NAG	C4-C3	2.39	1.58	1.52
2	B	3	NAG	C4-C5	2.34	1.58	1.53
2	B	1	NAG	C7-N2	2.30	1.41	1.34
2	B	3	NAG	C7-N2	2.29	1.41	1.34
2	B	4	BDP	O5-C5	2.29	1.47	1.43
2	B	1	NAG	O5-C5	2.26	1.49	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	BDP	C3-C4-C5	6.31	120.14	109.30
2	B	2	BDP	O4-C4-C5	-3.41	101.98	109.76
2	B	2	BDP	O5-C5-C6	3.04	117.44	106.59
2	B	4	BDP	O6B-C6-O6A	3.02	130.93	124.08
2	B	4	BDP	C1-C2-C3	-2.81	105.55	109.64
2	B	1	NAG	C8-C7-N2	-2.72	111.61	116.12
2	B	1	NAG	O5-C1-C2	2.45	111.97	109.52
2	B	1	NAG	O7-C7-N2	2.35	126.14	121.98
2	B	3	NAG	C8-C7-N2	-2.34	112.23	116.12
2	B	3	NAG	O7-C7-N2	2.20	125.87	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

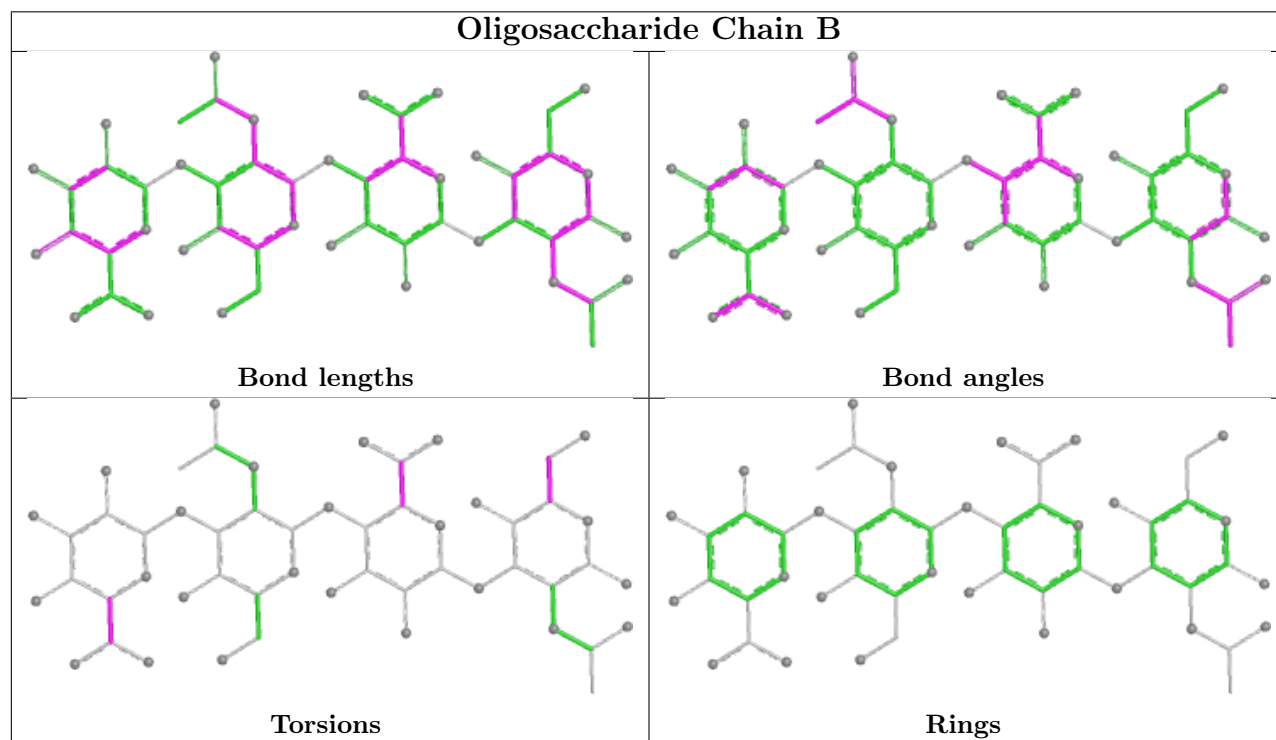
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	BDP	C4-C5-C6-O6A
2	B	4	BDP	O5-C5-C6-O6B

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 ⓘ

There are no ligands in this entry.

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 ⓘ

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	719/721 (99%)	1.72	235 (32%) ⓘ ⓘ	31, 41, 68, 98	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ALA	7.8
1	A	223	ILE	6.7
1	A	224	TYR	6.4
1	A	232	TYR	5.7
1	A	339	THR	5.5
1	A	342	PRO	5.3
1	A	229	PHE	5.1
1	A	209	VAL	5.0
1	A	716	ALA	5.0
1	A	225	LEU	5.0
1	A	226	TRP	4.8
1	A	430	ILE	4.7
1	A	280	VAL	4.6
1	A	221	ASP	4.4
1	A	288	VAL	4.4
1	A	286	SER	4.3
1	A	827	VAL	4.3
1	A	281	TYR	4.2
1	A	889	LYS	4.2
1	A	865	GLY	4.2
1	A	343	PHE	4.1
1	A	216	ILE	4.1
1	A	174	TYR	4.1
1	A	277	HIS	4.0
1	A	279	HIS	4.0
1	A	278	LYS	4.0
1	A	283	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	ASN	4.0
1	A	291	TRP	3.9
1	A	275	TRP	3.9
1	A	491	GLY	3.8
1	A	222	ARG	3.8
1	A	329	VAL	3.8
1	A	853	VAL	3.8
1	A	340	ASP	3.8
1	A	341	ASN	3.8
1	A	345	ALA	3.8
1	A	322	THR	3.8
1	A	238	LEU	3.7
1	A	689	THR	3.7
1	A	705	ASN	3.7
1	A	217	SER	3.6
1	A	296	ILE	3.6
1	A	335	PHE	3.6
1	A	196	ASP	3.6
1	A	292	TRP	3.6
1	A	338	THR	3.5
1	A	290	ASN	3.5
1	A	337	LYS	3.5
1	A	334	HIS	3.5
1	A	228	LYS	3.5
1	A	325	ILE	3.5
1	A	328	PHE	3.5
1	A	704	SER	3.5
1	A	289	GLY	3.5
1	A	219	GLN	3.5
1	A	437	THR	3.5
1	A	375	ARG	3.4
1	A	218	SER	3.4
1	A	171	LYS	3.4
1	A	268	THR	3.4
1	A	363	LEU	3.4
1	A	233	LYS	3.3
1	A	215	SER	3.3
1	A	864	GLU	3.3
1	A	294	TYR	3.3
1	A	213	LEU	3.3
1	A	210	ALA	3.3
1	A	725	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	330	PRO	3.2
1	A	231	ASN	3.2
1	A	230	SER	3.2
1	A	719	THR	3.2
1	A	855	LYS	3.2
1	A	433	ASP	3.2
1	A	323	ASP	3.1
1	A	429	PRO	3.1
1	A	848	SER	3.1
1	A	360	ALA	3.1
1	A	811	LYS	3.1
1	A	867	GLU	3.1
1	A	336	ARG	3.1
1	A	379	GLN	3.1
1	A	399	HIS	3.0
1	A	775	VAL	3.0
1	A	321	TYR	3.0
1	A	610	PRO	3.0
1	A	721	GLN	3.0
1	A	813	LEU	3.0
1	A	854	LEU	3.0
1	A	265	VAL	3.0
1	A	175	THR	3.0
1	A	331	ASP	3.0
1	A	849	ASN	3.0
1	A	436	GLN	3.0
1	A	441	TRP	3.0
1	A	316	GLU	2.9
1	A	492	GLU	2.9
1	A	318	ILE	2.9
1	A	377	ILE	2.9
1	A	810	ILE	2.9
1	A	844	VAL	2.9
1	A	172	ASP	2.9
1	A	234	THR	2.9
1	A	381	PHE	2.9
1	A	368	GLN	2.9
1	A	817	LEU	2.9
1	A	714	LYS	2.9
1	A	374	ILE	2.9
1	A	173	THR	2.9
1	A	787	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	236	ALA	2.8
1	A	385	ASP	2.8
1	A	332	PRO	2.8
1	A	580	ASN	2.8
1	A	227	GLU	2.8
1	A	354	GLY	2.8
1	A	178	LEU	2.8
1	A	324	VAL	2.8
1	A	392	GLN	2.8
1	A	757	ALA	2.8
1	A	585	ARG	2.8
1	A	772	ASP	2.8
1	A	490	GLU	2.8
1	A	814	GLU	2.8
1	A	488	MET	2.8
1	A	425	LYS	2.8
1	A	366	ASP	2.7
1	A	264	THR	2.7
1	A	426	THR	2.7
1	A	295	GLU	2.7
1	A	370	ILE	2.7
1	A	427	LYS	2.7
1	A	432	LYS	2.7
1	A	726	PRO	2.7
1	A	815	SER	2.7
1	A	505	VAL	2.7
1	A	287	ILE	2.7
1	A	240	ALA	2.7
1	A	428	ASN	2.7
1	A	367	ASP	2.7
1	A	297	GLY	2.6
1	A	709	VAL	2.6
1	A	495	GLN	2.6
1	A	723	LYS	2.6
1	A	818	ILE	2.6
1	A	868	TYR	2.6
1	A	276	MET	2.6
1	A	862	ARG	2.6
1	A	344	LYS	2.6
1	A	263	GLU	2.6
1	A	314	SER	2.6
1	A	419	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	239	THR	2.5
1	A	632	THR	2.5
1	A	284	GLU	2.5
1	A	350	LEU	2.5
1	A	176	ASP	2.5
1	A	364	ARG	2.5
1	A	348	GLY	2.5
1	A	687	THR	2.5
1	A	788	GLN	2.5
1	A	271	ASP	2.5
1	A	691	THR	2.5
1	A	192	ASP	2.5
1	A	315	ASP	2.5
1	A	489	SER	2.4
1	A	717	SER	2.4
1	A	738	SER	2.4
1	A	836	GLY	2.4
1	A	242	TYR	2.4
1	A	420	LEU	2.4
1	A	302	ILE	2.4
1	A	752	ILE	2.4
1	A	847	ILE	2.4
1	A	308	LEU	2.4
1	A	241	THR	2.4
1	A	194	LYS	2.4
1	A	773	LYS	2.4
1	A	293	ASP	2.3
1	A	434	LYS	2.3
1	A	235	SER	2.3
1	A	306	LEU	2.3
1	A	789	ASN	2.3
1	A	313	PHE	2.3
1	A	708	LYS	2.3
1	A	888	LYS	2.3
1	A	285	LYS	2.3
1	A	435	MET	2.3
1	A	762	ALA	2.3
1	A	722	GLU	2.3
1	A	252	VAL	2.3
1	A	658	THR	2.3
1	A	190	TYR	2.3
1	A	579	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	346	LEU	2.2
1	A	758	LEU	2.2
1	A	312	TYR	2.2
1	A	828	TYR	2.2
1	A	533	ALA	2.2
1	A	812	GLU	2.2
1	A	365	LYS	2.2
1	A	351	VAL	2.2
1	A	383	LEU	2.2
1	A	333	GLU	2.2
1	A	693	ALA	2.2
1	A	493	THR	2.2
1	A	372	SER	2.2
1	A	269	VAL	2.2
1	A	319	LYS	2.2
1	A	866	ASP	2.1
1	A	703	SER	2.1
1	A	718	LEU	2.1
1	A	729	GLN	2.1
1	A	808	GLN	2.1
1	A	257	SER	2.1
1	A	272	SER	2.1
1	A	439	TYR	2.1
1	A	727	GLU	2.1
1	A	214	SER	2.1
1	A	371	SER	2.1
1	A	200	LYS	2.0
1	A	581	LYS	2.0
1	A	380	VAL	2.0
1	A	384	VAL	2.0
1	A	731	VAL	2.0
1	A	753	SER	2.0
1	A	258	ARG	2.0
1	A	299	PRO	2.0
1	A	720	GLU	2.0
1	A	356	VAL	2.0
1	A	358	VAL	2.0
1	A	422	VAL	2.0
1	A	529	LEU	2.0
1	A	688	SER	2.0

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

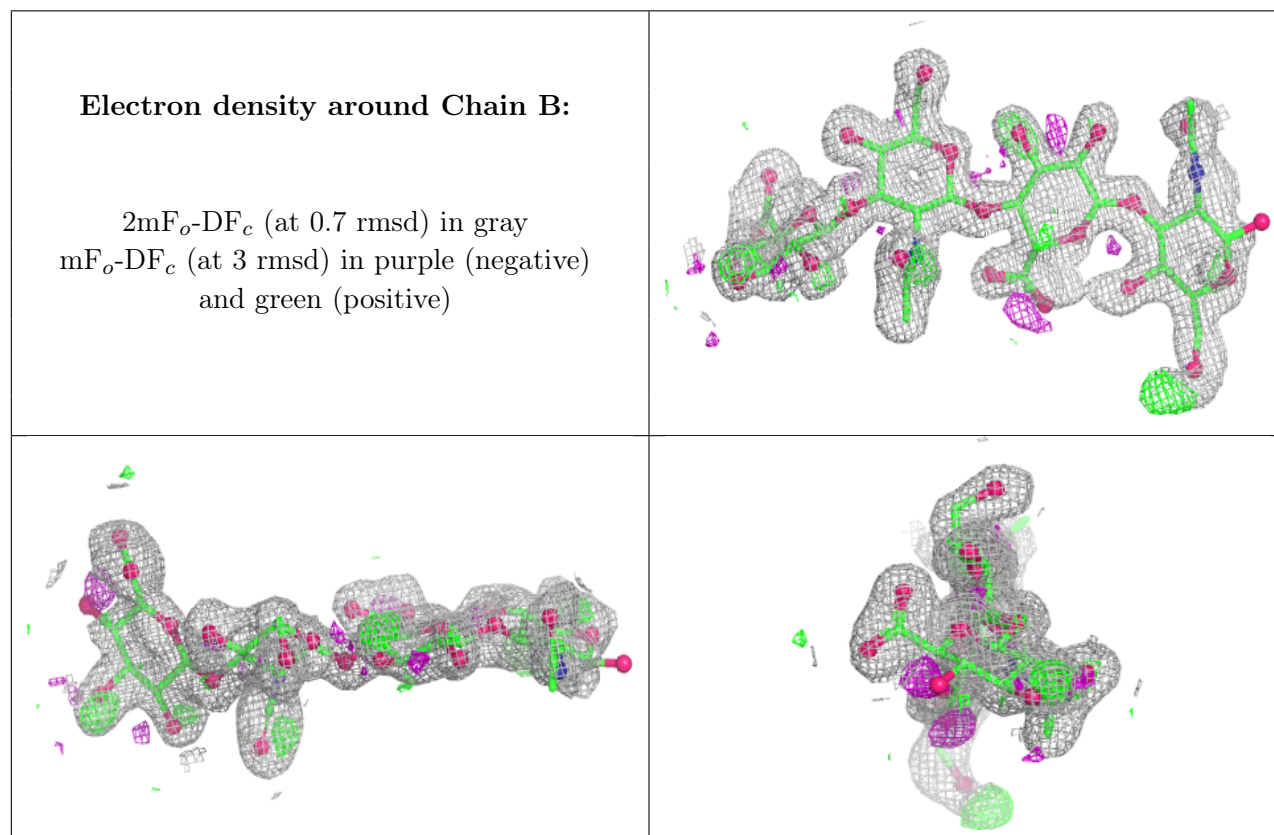
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	1	15/15	0.70	0.21	66,70,76,85	0
2	BDP	B	2	12/13	0.75	0.23	68,70,81,84	0
2	BDP	B	4	12/13	0.78	0.21	62,64,71,82	0
2	NAG	B	3	14/15	0.90	0.16	40,60,63,65	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.