



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:04 PM UTC

PDB ID : 1AZX / pdb_00001azx
Title : ANTITHROMBIN/PENTASACCHARIDE COMPLEX
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Deposited on : 1997-11-23
Resolution : 2.90 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

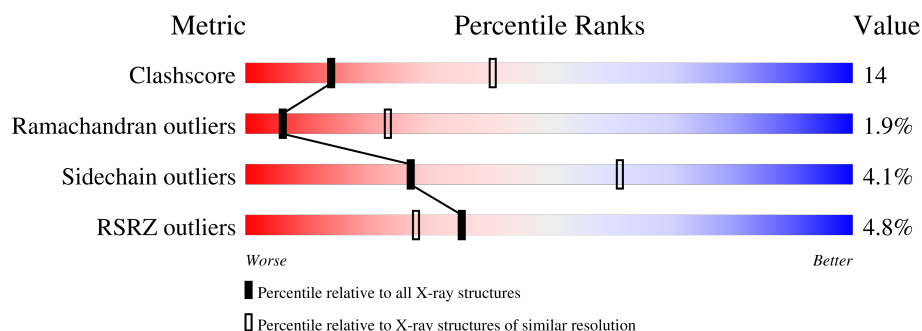
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	I	432	6% 64% 29% • •
1	L	432	4% 62% 31% • •
2	A	5	60% 40%
2	B	5	40% 60%

2 Entry composition [i](#)

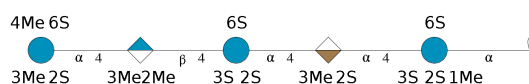
There are 3 unique types of molecules in this entry. The entry contains 6881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANTITHROMBIN.

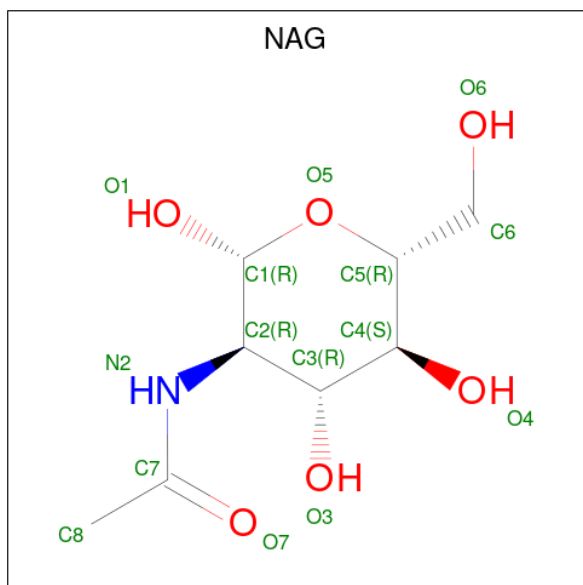
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	417	Total	C	N	O	S	0	0	0
			3328	2121	562	627	18			
1	L	414	Total	C	N	O	S	0	0	0
			3311	2111	559	623	18			

- Molecule 2 is an oligosaccharide called 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	5	Total	C	O	S	0	0	0
			100	36	55	9			
2	B	5	Total	C	O	S	0	0	0
			100	36	55	9			

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

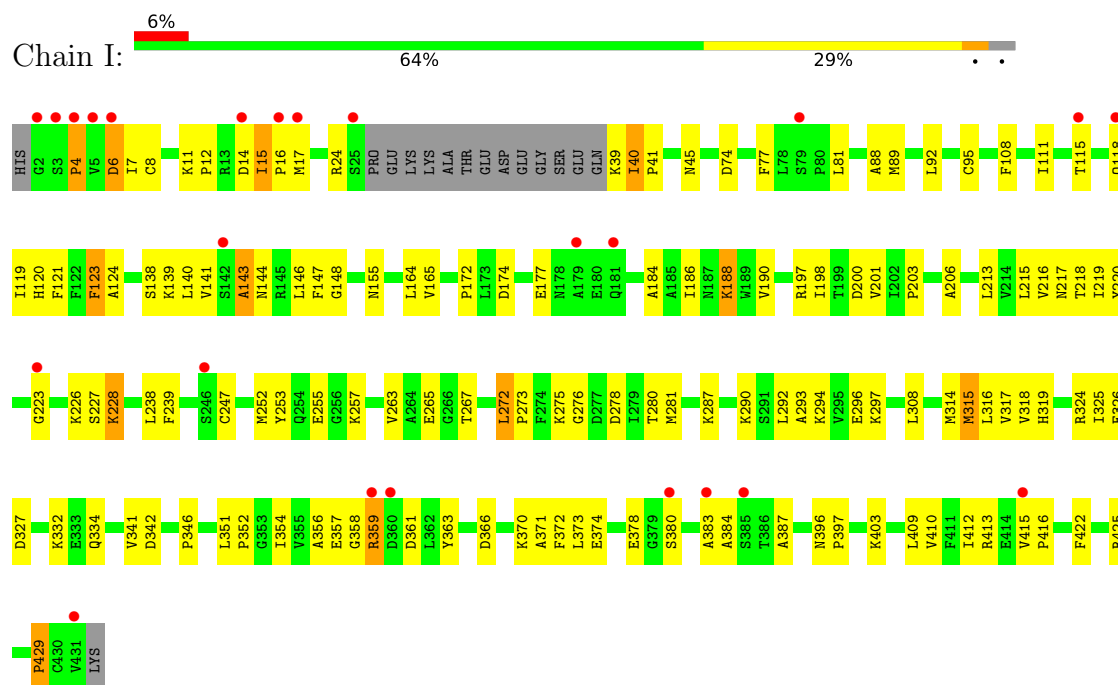


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

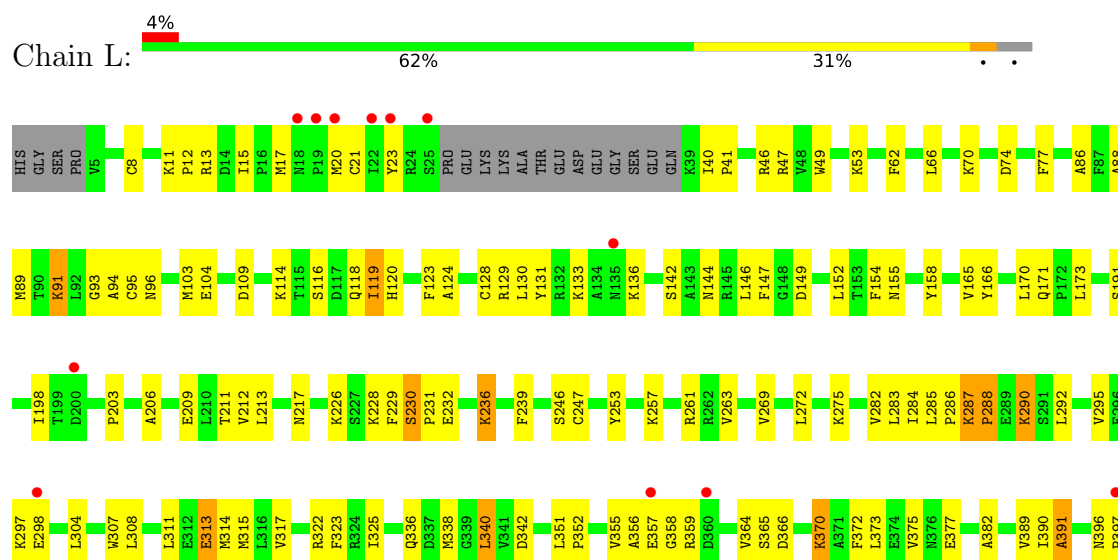
3 Residue-property plots [i](#)

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: ANTITHROMBIN



• Molecule 1: ANTITHROMBIN





- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain A: 60% 40%



- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain B: 40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.44Å 86.97Å 97.22Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.90) 94.4 (30.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.90Å)	Xtriage
Refinement program	TNT 5D	Depositor
R, R_{free}	0.195 , 0.280 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: GU6, Z9L, Z9H, GU1, Z9K, NAG

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	I	0.40	0/3394	0.88	3/4582 (0.1%)
1	L	0.42	0/3376	0.90	12/4557 (0.3%)
All	All	0.41	0/6770	0.89	15/9139 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	322	ARG	N-CA-C	-6.92	97.94	108.67
1	L	287	LYS	CA-C-N	6.80	128.34	119.84
1	L	287	LYS	C-N-CA	6.80	128.34	119.84
1	L	226	LYS	N-CA-C	-6.11	104.70	111.36
1	I	88	ALA	N-CA-C	-5.97	104.90	111.82
1	I	387	ALA	N-CA-C	-5.78	100.16	108.60
1	L	123	PHE	N-CA-C	-5.73	104.64	111.69
1	L	230	SER	CA-C-N	5.59	125.26	119.56
1	L	230	SER	C-N-CA	5.59	125.26	119.56
1	L	342	ASP	N-CA-C	5.32	117.50	111.11
1	L	323	PHE	N-CA-C	5.32	116.35	108.86
1	L	88	ALA	N-CA-C	-5.31	105.66	111.82
1	L	119	ILE	N-CA-C	5.23	115.67	110.23
1	I	123	PHE	N-CA-C	-5.12	105.78	111.36
1	L	400	VAL	N-CA-C	5.03	114.99	108.35

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	I	3328	0	3333	93	0
1	L	3311	0	3323	94	0
2	A	100	0	16	4	0
2	B	100	0	16	5	0
3	I	14	0	13	5	0
3	L	28	0	26	3	0
All	All	6881	0	6727	191	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 (191) 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:I:356:ALA:O	3:I:501:NAG:H81	1.60	1.01
1:L:129:ARG:HD3	1:L:417:LEU:HD21	1.56	0.87
1:L:20:MET:HA	3:L:501:NAG:H61	1.55	0.87
1:I:17:MET:HB2	1:I:120:HIS:HE1	1.39	0.86
1:I:144:ASN:HB3	1:I:217:ASN:HA	1.67	0.77
1:I:324:ARG:HG2	1:I:374:GLU:HG3	1.67	0.75
2:B:2:Z9K:O10	2:B:3:GU6:H5	1.91	0.71
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.73	0.69
1:I:155:ASN:HD22	3:I:501:NAG:H83	1.55	0.69
2:B:4:GU1:H83	2:B:4:GU1:H72	1.75	0.69
1:I:356:ALA:O	3:I:501:NAG:C8	2.41	0.68
1:I:108:PHE:O	1:I:111:ILE:HG12	1.94	0.67
1:I:228:LYS:HB3	1:I:228:LYS:HZ2	1.60	0.67
1:I:358:GLY:O	1:I:359:ARG:HD3	1.94	0.66
1:L:20:MET:CA	3:L:501:NAG:H61	2.26	0.66
1:L:355:VAL:HG21	1:L:359:ARG:HB2	1.78	0.65
1:I:17:MET:HB2	1:I:120:HIS:CE1	2.28	0.65
1:L:17:MET:HE2	1:L:165:VAL:HG22	1.79	0.65
1:I:139:LYS:HZ3	1:I:197:ARG:HH22	1.45	0.65
1:I:257:LYS:HA	1:I:314:MET:O	1.96	0.65
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:ARG:NH1	1:L:114:LYS:HB3	2.11	0.64
1:I:308:LEU:HD13	1:I:413:ARG:NH1	2.14	0.63
1:I:255:GLU:HG2	1:I:317:VAL:HG22	1.80	0.62
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.81	0.62
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.80	0.62
1:L:229:PHE:O	1:L:377:GLU:HB3	2.00	0.62
1:I:15:ILE:HG12	1:I:17:MET:HE3	1.82	0.61
1:I:17:MET:SD	1:I:121:PHE:HB2	2.40	0.61
1:L:313:GLU:H	1:L:313:GLU:CD	2.08	0.61
1:L:257:LYS:HG2	1:L:315:MET:HG2	1.82	0.61
1:L:286:PRO:HD3	1:L:292:LEU:HD13	1.81	0.61
1:L:247:CYS:HG	1:L:430:CYS:CB	2.13	0.60
1:I:239:PHE:HB3	1:I:247:CYS:HB3	1.83	0.60
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.66	0.60
1:I:412:ILE:HB	1:I:422:PHE:HB2	1.84	0.59
1:L:152:LEU:HD13	1:L:212:VAL:HG13	1.83	0.59
1:L:211:THR:HA	1:L:391:ALA:O	2.01	0.59
1:L:370:LYS:HB2	1:L:370:LYS:HZ2	1.68	0.59
1:L:407:PRO:HB3	1:L:427:ALA:HA	1.85	0.59
1:I:265:GLU:O	1:I:287:LYS:HD2	2.03	0.58
1:I:140:LEU:HD11	1:I:219:ILE:HD11	1.85	0.58
1:I:198:ILE:HG23	1:I:370:LYS:HD3	1.87	0.57
1:L:272:LEU:HD11	1:L:283:LEU:HD11	1.87	0.57
1:L:364:VAL:HG22	1:L:390:ILE:HD13	1.88	0.56
1:L:21:CYS:SG	1:L:95:CYS:CB	2.94	0.56
1:I:4:PRO:HB2	1:I:8:CYS:SG	2.46	0.55
1:L:308:LEU:HA	1:L:311:LEU:HG	1.88	0.55
1:I:138:SER:HB3	1:I:223:GLY:HA2	1.88	0.55
1:L:355:VAL:CG2	1:L:359:ARG:HB2	2.36	0.55
1:L:17:MET:HE2	1:L:165:VAL:CG2	2.36	0.55
1:L:116:SER:O	1:L:119:ILE:HG12	2.07	0.55
1:I:143:ALA:HB3	1:I:218:THR:OG1	2.07	0.55
1:L:95:CYS:SG	1:L:96:ASN:ND2	2.80	0.55
1:L:62:PHE:CD1	1:L:338:MET:HE1	2.42	0.54
1:L:21:CYS:SG	1:L:95:CYS:HB2	2.47	0.54
1:L:236:LYS:NZ	1:L:236:LYS:HB2	2.22	0.54
1:I:356:ALA:O	3:I:501:NAG:O7	2.26	0.53
1:L:12:PRO:HB3	1:L:118:GLN:NE2	2.24	0.53
1:I:238:LEU:HA	1:I:247:CYS:O	2.10	0.52
1:L:253:TYR:CE1	1:L:317:VAL:HG13	2.45	0.52
1:L:40:ILE:HB	1:L:41:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:LEU:HG	1:I:215:LEU:HG	1.91	0.52
1:L:130:LEU:HD23	1:L:414:GLU:OE1	2.11	0.51
1:L:365:SER:HB3	1:L:389:VAL:HG23	1.91	0.51
2:A:4:GU1:H72	2:A:4:GU1:H83	1.92	0.51
1:I:147:PHE:CE2	1:I:186:ILE:HG23	2.45	0.51
1:L:20:MET:HA	3:L:501:NAG:C6	2.36	0.51
1:L:257:LYS:HA	1:L:314:MET:O	2.10	0.51
1:L:287:LYS:HB3	1:L:290:LYS:HG3	1.91	0.51
1:L:370:LYS:HB2	1:L:370:LYS:NZ	2.25	0.51
1:I:15:ILE:N	1:I:15:ILE:HD13	2.26	0.51
1:I:174:ASP:OD2	1:I:177:GLU:HB2	2.11	0.51
1:I:40:ILE:HG13	1:I:41:PRO:HD2	1.94	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.12	0.50
1:L:23:TYR:CD1	1:L:103:MET:HG3	2.47	0.50
1:I:184:ALA:O	1:I:188:LYS:HD2	2.12	0.50
1:I:253:TYR:HA	1:I:318:VAL:O	2.12	0.50
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.46	0.50
1:L:402:PHE:HD1	1:L:402:PHE:O	1.95	0.50
1:I:220:TYR:HD1	1:I:372:PHE:HB3	1.77	0.49
1:L:86:ALA:O	1:L:89:MET:HB2	2.12	0.49
1:I:380:SER:HB2	1:I:384:ALA:HB2	1.94	0.49
1:I:314:MET:HG2	1:I:315:MET:N	2.26	0.49
1:I:290:LYS:HD2	1:I:294:LYS:HD3	1.93	0.49
1:L:120:HIS:HD2	1:L:166:TYR:OH	1.96	0.49
1:I:17:MET:HG3	1:I:118:GLN:HE22	1.77	0.49
1:L:93:GLY:O	1:L:351:LEU:HA	2.13	0.49
1:L:91:LYS:NZ	1:L:120:HIS:NE2	2.61	0.49
1:I:326:GLU:HA	1:I:371:ALA:O	2.13	0.49
1:I:358:GLY:C	1:I:359:ARG:HD3	2.37	0.49
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.13	0.48
1:L:149:ASP:HA	1:L:173:LEU:O	2.13	0.48
1:L:21:CYS:HG	1:L:95:CYS:HG	0.48	0.48
1:L:203:PRO:HG2	1:L:206:ALA:HB2	1.94	0.48
1:I:12:PRO:HD2	2:A:3:GU6:O14	2.14	0.48
1:L:155:ASN:HB3	1:L:158:TYR:HB3	1.96	0.48
1:L:77:PHE:CE1	1:L:373:LEU:HD22	2.48	0.48
1:L:290:LYS:HB3	1:L:290:LYS:NZ	2.28	0.48
1:I:272:LEU:HD12	1:I:272:LEU:N	2.29	0.47
1:I:141:VAL:HG23	1:I:220:TYR:HB3	1.94	0.47
1:L:131:TYR:CE1	1:L:142:SER:HB2	2.49	0.47
1:L:144:ASN:OD1	1:L:217:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:239:PHE:O	1:L:246:SER:HA	2.13	0.47
1:L:407:PRO:HB2	1:L:425:ARG:HG2	1.97	0.47
1:L:154:PHE:HA	1:L:355:VAL:HA	1.96	0.47
1:L:247:CYS:SG	1:L:430:CYS:CB	3.03	0.47
1:L:47:ARG:HH12	1:L:114:LYS:HB3	1.78	0.47
1:I:188:LYS:N	1:I:188:LYS:HE3	2.30	0.46
1:L:8:CYS:HG	1:L:128:CYS:CB	2.26	0.46
1:I:119:ILE:O	1:I:123:PHE:HD2	1.98	0.46
1:I:293:ALA:O	1:I:297:LYS:HG3	2.16	0.46
1:L:13:ARG:NH1	2:B:3:GU6:O13	2.48	0.46
1:L:229:PHE:HB2	1:L:377:GLU:HA	1.96	0.46
1:I:273:PRO:HA	1:I:280:THR:HG22	1.97	0.46
1:I:276:GLY:C	1:I:278:ASP:H	2.24	0.46
1:L:47:ARG:CZ	1:L:114:LYS:HD3	2.46	0.46
1:L:282:VAL:HB	1:L:411:PHE:HB2	1.97	0.46
1:I:292:LEU:O	1:I:296:GLU:HG3	2.16	0.45
1:L:191:SER:HA	1:L:198:ILE:O	2.16	0.45
1:L:230:SER:HB3	1:L:232:GLU:CD	2.41	0.45
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.97	0.45
1:I:141:VAL:CG2	1:I:220:TYR:HB3	2.47	0.45
1:I:228:LYS:HZ2	1:I:378:GLU:HB2	1.82	0.45
1:I:147:PHE:O	1:I:213:LEU:HD12	2.18	0.44
1:I:324:ARG:HA	1:I:373:LEU:O	2.17	0.44
1:L:275:LYS:HA	1:L:275:LYS:HD2	1.79	0.44
1:L:133:LYS:O	1:L:136:LYS:HE2	2.17	0.44
1:I:95:CYS:SG	1:I:352:PRO:CG	3.05	0.44
1:L:261:ARG:HB2	1:L:311:LEU:HA	1.99	0.44
1:L:124:ALA:HB2	1:L:165:VAL:HG13	2.00	0.44
1:L:295:VAL:HG13	1:L:307:TRP:HH2	1.83	0.44
1:I:124:ALA:HB2	1:I:165:VAL:HG13	2.00	0.44
1:I:294:LYS:HZ2	1:I:294:LYS:HB3	1.82	0.44
1:L:66:LEU:O	1:L:70:LYS:HG3	2.17	0.44
1:L:338:MET:HE3	1:L:338:MET:HB2	1.88	0.44
1:I:325:ILE:O	1:I:372:PHE:HA	2.17	0.44
1:I:201:VAL:HG11	1:I:216:VAL:HG13	1.99	0.44
1:I:252:MET:O	1:I:319:HIS:HA	2.18	0.43
1:I:357:GLU:HB2	1:I:359:ARG:NH1	2.34	0.43
1:I:74:ASP:O	1:I:425:ARG:NH1	2.50	0.43
1:L:239:PHE:HB3	1:L:430:CYS:SG	2.58	0.43
1:I:341:VAL:HG23	1:I:342:ASP:H	1.83	0.43
1:L:287:LYS:HB3	1:L:290:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:336:GLN:HA	1:L:340:LEU:O	2.18	0.43
1:I:155:ASN:ND2	3:I:501:NAG:H83	2.28	0.43
1:I:281:MET:HE2	1:I:410:VAL:CG1	2.49	0.43
1:L:325:ILE:HD13	1:L:426:VAL:HG22	2.01	0.43
1:L:407:PRO:HB3	1:L:427:ALA:CA	2.48	0.43
1:I:198:ILE:HG21	1:I:218:THR:HB	2.01	0.42
1:I:11:LYS:HB3	2:A:3:GU6:O14	2.19	0.42
1:I:319:HIS:CB	1:I:403:LYS:HG3	2.49	0.42
1:L:147:PHE:HA	1:L:171:GLN:O	2.20	0.42
1:I:17:MET:HG3	1:I:118:GLN:OE1	2.20	0.42
1:I:203:PRO:HG2	1:I:206:ALA:HB2	2.00	0.42
1:I:139:LYS:HA	1:I:139:LYS:HD2	1.92	0.42
1:L:124:ALA:O	1:L:128:CYS:SG	2.78	0.42
1:I:14:ASP:HB2	1:I:15:ILE:HD13	2.02	0.42
1:L:285:LEU:HD12	1:L:285:LEU:N	2.35	0.42
1:I:6:ASP:CG	1:I:164:LEU:HD11	2.45	0.42
1:I:190:VAL:HG21	1:I:201:VAL:HG21	2.02	0.42
1:L:230:SER:HA	1:L:231:PRO:HD3	1.90	0.42
1:L:292:LEU:HD21	1:L:409:LEU:HG	2.01	0.41
1:I:39:LYS:O	1:I:40:ILE:HB	2.20	0.41
1:L:239:PHE:HZ	1:L:405:ASN:O	2.02	0.41
1:I:45:ASN:HA	2:A:4:GU1:H82	2.02	0.41
1:I:308:LEU:HD13	1:I:413:ARG:HH11	1.85	0.41
1:I:327:ASP:O	1:I:370:LYS:HA	2.20	0.41
1:I:351:LEU:HD13	1:I:354:ILE:HD12	2.01	0.41
1:L:20:MET:HG2	1:L:352:PRO:HG2	2.01	0.41
1:L:366:ASP:O	1:L:389:VAL:HG22	2.21	0.41
1:I:228:LYS:NZ	1:I:378:GLU:HB2	2.34	0.41
1:L:372:PHE:O	1:L:382:ALA:HA	2.20	0.41
1:L:11:LYS:HD3	2:B:3:GU6:H2	2.02	0.41
1:L:74:ASP:O	1:L:425:ARG:HD2	2.21	0.41
1:I:263:VAL:CG2	1:I:267:THR:HB	2.51	0.41
1:I:314:MET:HG2	1:I:315:MET:H	1.85	0.41
1:L:147:PHE:O	1:L:213:LEU:HD12	2.21	0.41
2:B:3:GU6:O15	2:B:3:GU6:C1	2.67	0.41
1:L:356:ALA:C	1:L:358:GLY:H	2.29	0.41
1:I:15:ILE:HA	1:I:16:PRO:HD2	1.87	0.40
1:I:346:PRO:HG3	1:I:363:TYR:CE2	2.56	0.40
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.03	0.40
1:L:146:LEU:HB2	1:L:170:LEU:HA	2.04	0.40
1:I:17:MET:HG3	1:I:118:GLN:NE2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:MET:O	1:I:92:LEU:HB3	2.21	0.40
1:I:226:LYS:HA	1:I:275:LYS:HD2	2.02	0.40
1:L:49:TRP:CZ2	1:L:53:LYS:HD3	2.56	0.40
1:L:269:VAL:HG13	1:L:284:ILE:HD13	2.04	0.40
1:I:115:THR:O	1:I:119:ILE:N	2.54	0.40
1:L:104:GLU:HA	1:L:109:ASP:OD1	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	I	413/432 (96%)	367 (89%)	36 (9%)	10 (2%)	4	18
1	L	410/432 (95%)	377 (92%)	27 (7%)	6 (2%)	8	28
All	All	823/864 (95%)	744 (90%)	63 (8%)	16 (2%)	6	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	4	PRO
1	I	200	ASP
1	I	359	ARG
1	L	404	ALA
1	L	288	PRO
1	I	6	ASP
1	I	383	ALA
1	I	429	PRO
1	L	357	GLU
1	I	143	ALA
1	I	361	ASP
1	L	391	ALA

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Mol	Chain	Res	Type
1	I	332	LYS
1	I	40	ILE
1	L	397	PRO
1	L	263	VAL

5.3.2 Protein sidechains ⓘ

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	I	370/383 (97%)	357 (96%)	13 (4%)	32	66
1	L	368/383 (96%)	351 (95%)	17 (5%)	24	57
All	All	738/766 (96%)	708 (96%)	30 (4%)	27	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	ILE
1	I	15	ILE
1	I	24	ARG
1	I	81	LEU
1	I	188	LYS
1	I	227	SER
1	I	228	LYS
1	I	272	LEU
1	I	315	MET
1	I	316	LEU
1	I	334	GLN
1	I	366	ASP
1	I	429	PRO
1	L	15	ILE
1	L	46	ARG
1	L	91	LYS
1	L	209	GLU
1	L	228	LYS
1	L	236	LYS

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Mol	Chain	Res	Type
1	L	288	PRO
1	L	290	LYS
1	L	297	LYS
1	L	298	GLU
1	L	304	LEU
1	L	313	GLU
1	L	340	LEU
1	L	370	LYS
1	L	375	VAL
1	L	396	ASN
1	L	402	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	55	ASN
1	I	127	ASN
1	I	233	ASN
1	I	428	ASN
1	L	96	ASN
1	L	118	GLN
1	L	120	HIS
1	L	127	ASN
1	L	268	GLN
1	L	305	GLN
1	L	336	GLN
1	L	396	ASN
1	L	418	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 ⓘ

10 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	Z9L	A	1	2	25,25,25	1.07	0	34,39,39	0.92	1 (2%)
2	Z9K	A	2	2	17,17,18	1.27	2 (11%)	17,25,27	1.17	1 (5%)
2	GU6	A	3	2	23,23,24	1.29	4 (17%)	28,36,38	1.10	1 (3%)
2	GU1	A	4	2	14,14,15	0.92	0	15,19,21	0.94	1 (6%)
2	Z9H	A	5	2	21,21,22	1.05	1 (4%)	26,31,33	1.15	1 (3%)
2	Z9L	B	1	2	25,25,25	1.02	0	34,39,39	0.96	1 (2%)
2	Z9K	B	2	2	17,17,18	1.32	2 (11%)	17,25,27	1.22	3 (17%)
2	GU6	B	3	2	23,23,24	1.19	3 (13%)	28,36,38	1.18	2 (7%)
2	GU1	B	4	2	14,14,15	0.78	0	15,19,21	0.94	1 (6%)
2	Z9H	B	5	2	21,21,22	1.12	1 (4%)	26,31,33	1.04	1 (3%)

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	Z9L	A	1	2	-	8/18/38/38	0/1/1/1
2	Z9K	A	2	2	-	0/11/28/31	0/1/1/1
2	GU6	A	3	2	-	9/16/33/36	0/1/1/1
2	GU1	A	4	2	-	3/8/25/28	0/1/1/1
2	Z9H	A	5	2	-	5/15/32/35	0/1/1/1
2	Z9L	B	1	2	-	6/18/38/38	0/1/1/1
2	Z9K	B	2	2	-	0/11/28/31	0/1/1/1
2	GU6	B	3	2	-	8/16/33/36	0/1/1/1
2	GU1	B	4	2	-	2/8/25/28	0/1/1/1
2	Z9H	B	5	2	-	5/15/32/35	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	Z9H	O2-C2	-3.35	1.42	1.47
2	B	2	Z9K	O2-C2	-3.28	1.42	1.47
2	A	5	Z9H	O2-C2	-2.91	1.43	1.47
2	B	3	GU6	O2-C2	-2.86	1.43	1.47
2	A	2	Z9K	C1-C2	2.72	1.56	1.51
2	B	2	Z9K	C4-C5	2.58	1.57	1.53
2	A	3	GU6	C1-C2	2.54	1.55	1.51
2	A	3	GU6	O2-C2	-2.52	1.43	1.47
2	B	3	GU6	C1-C2	2.42	1.55	1.51
2	A	2	Z9K	O2-C2	-2.40	1.43	1.47
2	A	3	GU6	O3-C3	-2.23	1.41	1.46
2	A	3	GU6	O6-S6	2.23	1.62	1.56
2	B	3	GU6	O3-C3	-2.01	1.41	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	Z9H	O2-C2-C3	3.76	110.81	106.65
2	A	3	GU6	O2-C2-C3	3.49	110.52	106.65
2	B	3	GU6	O2-C2-C3	2.95	109.92	106.65
2	B	5	Z9H	O2-C2-C3	2.75	109.70	106.65
2	A	2	Z9K	O2-C2-C3	2.69	109.63	106.65
2	B	2	Z9K	O2-C2-C3	2.53	109.45	106.65
2	B	2	Z9K	O6-C6-O10	-2.37	118.71	124.08
2	A	4	GU1	O6B-C6-O6A	-2.21	119.06	124.08
2	A	1	Z9L	O2-C2-C1	2.20	110.54	107.58
2	B	3	GU6	O6-C6-C5	-2.19	103.67	107.57
2	B	4	GU1	O6B-C6-O6A	-2.12	119.27	124.08
2	B	1	Z9L	O2-C2-C1	2.11	110.41	107.58
2	B	2	Z9K	O5-C1-C2	2.05	113.65	109.51

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	Z9L	C6-O6-S1-O7
2	A	1	Z9L	C6-O6-S1-O11
2	A	3	GU6	C1-C2-O2-S2
2	A	3	GU6	C6-O6-S6-O19
2	A	3	GU6	C6-O6-S6-O20
2	A	3	GU6	C6-O6-S6-O21
2	A	5	Z9H	C4-C5-C6-O6

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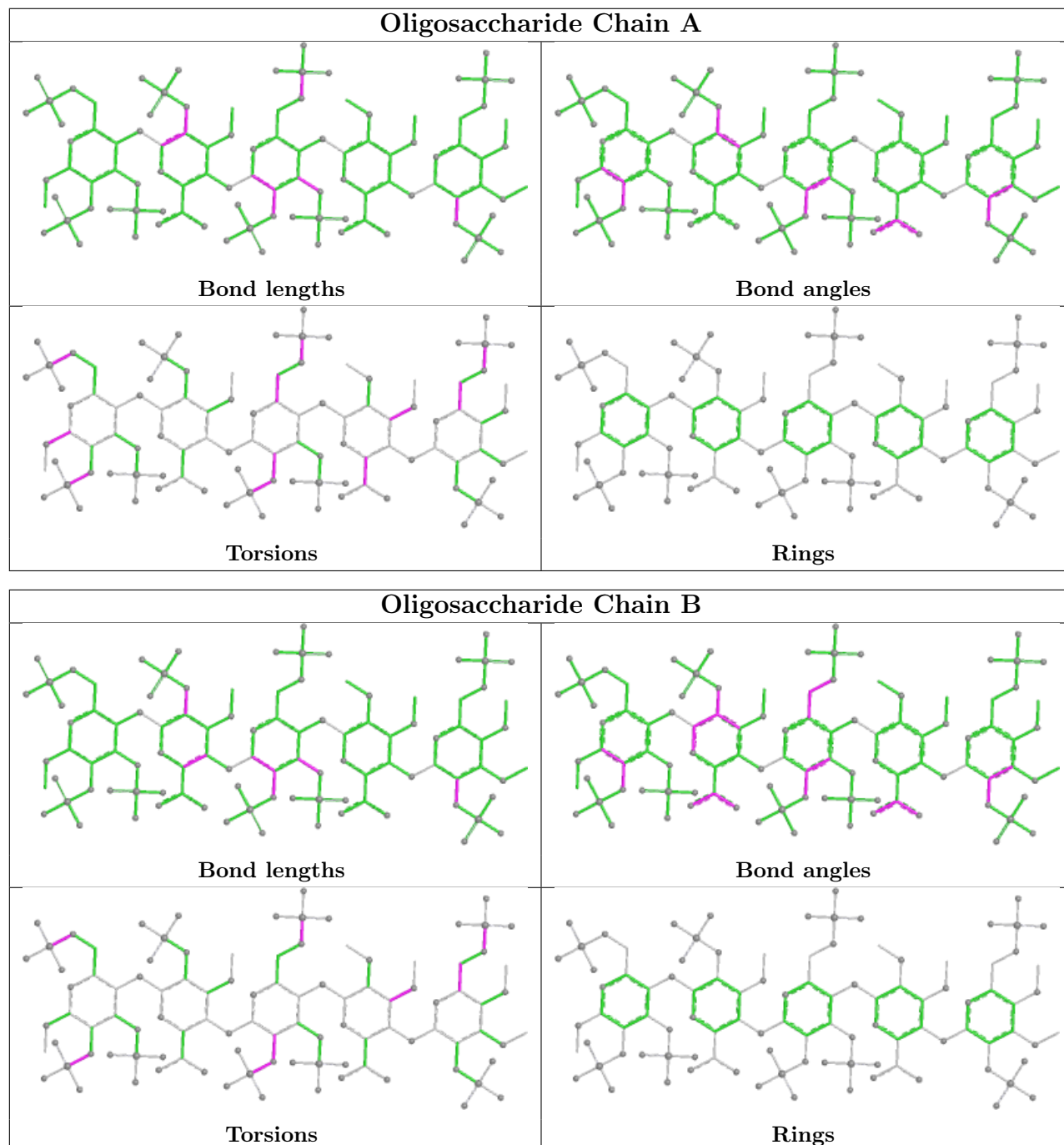
Mol	Chain	Res	Type	Atoms
2	A	5	Z9H	O5-C5-C6-O6
2	B	1	Z9L	C6-O6-S1-O7
2	B	1	Z9L	C6-O6-S1-O11
2	B	3	GU6	C1-C2-O2-S2
2	B	3	GU6	C3-C2-O2-S2
2	B	3	GU6	C6-O6-S6-O19
2	B	3	GU6	C6-O6-S6-O20
2	B	3	GU6	C6-O6-S6-O21
2	B	5	Z9H	C4-C5-C6-O6
2	B	5	Z9H	O5-C5-C6-O6
2	A	1	Z9L	O5-C1-O1-C7
2	A	1	Z9L	C2-C1-O1-C7
2	A	5	Z9H	C6-O6-S1-O8
2	A	5	Z9H	C6-O6-S1-O12
2	B	5	Z9H	C6-O6-S1-O8
2	B	5	Z9H	C6-O6-S1-O12
2	A	4	GU1	C2-C3-O3-C8
2	B	4	GU1	C2-C3-O3-C8
2	A	1	Z9L	C2-O2-S3-O13
2	A	1	Z9L	C2-O2-S3-O14
2	A	3	GU6	C2-O2-S2-O14
2	A	3	GU6	C2-O2-S2-O15
2	B	1	Z9L	C2-O2-S3-O13
2	B	1	Z9L	C2-O2-S3-O14
2	B	3	GU6	C2-O2-S2-O14
2	B	3	GU6	C2-O2-S2-O15
2	A	1	Z9L	C6-O6-S1-O15
2	A	5	Z9H	C6-O6-S1-O7
2	B	1	Z9L	C6-O6-S1-O15
2	B	5	Z9H	C6-O6-S1-O7
2	A	1	Z9L	C2-O2-S3-O12
2	A	3	GU6	C2-O2-S2-O13
2	B	1	Z9L	C2-O2-S3-O12
2	B	3	GU6	C2-O2-S2-O13
2	A	4	GU1	C4-C3-O3-C8
2	A	3	GU6	C3-C2-O2-S2
2	B	4	GU1	C4-C3-O3-C8
2	A	3	GU6	C4-C5-C6-O6
2	A	4	GU1	O5-C5-C6-O6A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4	GU1	2	0
2	B	3	GU6	4	0
2	B	4	GU1	1	0
2	A	3	GU6	2	0
2	B	2	Z9K	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

3 ligands 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$
3	NAG	L	502	1	14,14,15	0.86	0	17,19,21	1.67	4 (23%)
3	NAG	I	501	1	14,14,15	0.87	0	17,19,21	1.67	4 (23%)
3	NAG	L	501	1	14,14,15	0.86	0	17,19,21	1.68	4 (23%)

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	L	502	1	-	2/6/23/26	0/1/1/1
3	NAG	I	501	1	-	2/6/23/26	0/1/1/1
3	NAG	L	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	NAG	O5-C1-C2	-3.45	105.96	111.29
3	I	501	NAG	O5-C1-C2	-3.43	105.99	111.29
3	L	502	NAG	O5-C1-C2	-3.41	106.02	111.29
3	L	502	NAG	C1-O5-C5	3.06	116.28	112.19
3	I	501	NAG	C1-O5-C5	3.05	116.28	112.19
3	L	501	NAG	C1-O5-C5	3.05	116.27	112.19
3	L	501	NAG	O4-C4-C3	-2.97	103.37	110.38
3	L	502	NAG	O4-C4-C3	-2.97	103.37	110.38
3	I	501	NAG	O4-C4-C3	-2.97	103.38	110.38
3	L	501	NAG	O7-C7-C8	-2.31	117.95	122.05
3	L	502	NAG	O7-C7-C8	-2.31	117.95	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	501	NAG	O7-C7-C8	-2.27	118.01	122.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	501	NAG	C8-C7-N2-C2
3	I	501	NAG	O7-C7-N2-C2
3	L	501	NAG	C8-C7-N2-C2
3	L	501	NAG	O7-C7-N2-C2
3	L	502	NAG	C8-C7-N2-C2
3	L	502	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	501	NAG	5	0
3	L	501	NAG	3	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

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	I	417/432 (96%)	0.28	24 (5%) 29 22	2, 35, 78, 114	0
1	L	414/432 (95%)	0.11	16 (3%) 43 35	2, 27, 70, 97	0
All	All	831/864 (96%)	0.19	40 (4%) 35 28	2, 32, 74, 114	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	2	GLY	5.1
1	I	223	GLY	5.1
1	I	3	SER	4.8
1	I	25	SER	4.8
1	L	397	PRO	4.1
1	L	431	VAL	4.0
1	L	18	ASN	3.7
1	I	431	VAL	3.6
1	L	298	GLU	3.6
1	L	23	TYR	3.4
1	I	360	ASP	3.1
1	I	6	ASP	3.0
1	I	142	SER	3.0
1	I	17	MET	3.0
1	I	5	VAL	2.9
1	I	385	SER	2.8
1	I	79	SER	2.7
1	L	22	ILE	2.7
1	I	4	PRO	2.6
1	I	14	ASP	2.6
1	L	19	PRO	2.5
1	I	118	GLN	2.5
1	L	357	GLU	2.4
1	I	179	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	181	GLN	2.3
1	I	16	PRO	2.3
1	L	402	PHE	2.2
1	I	115	THR	2.2
1	I	246	SER	2.2
1	I	415	VAL	2.2
1	L	25	SER	2.2
1	L	135	ASN	2.1
1	L	200	ASP	2.1
1	I	359	ARG	2.1
1	L	406	ARG	2.1
1	I	380	SER	2.1
1	L	20	MET	2.1
1	L	399	ARG	2.0
1	I	383	ALA	2.0
1	L	360	ASP	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.

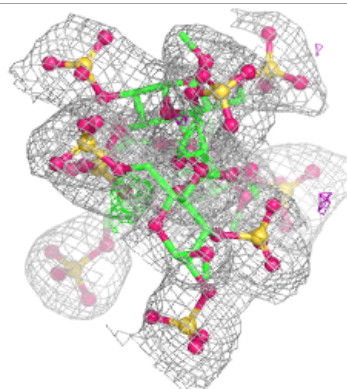
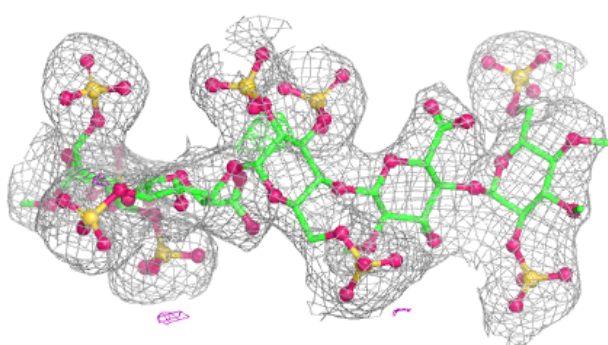
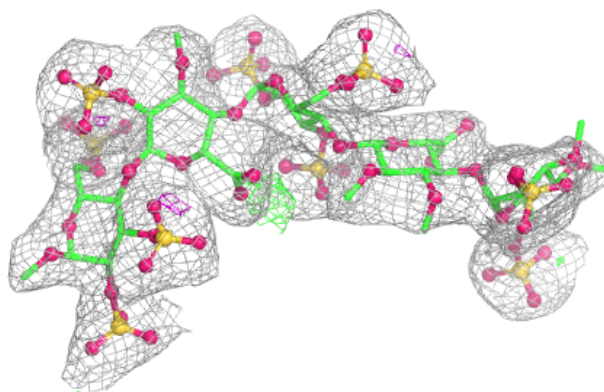
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Z9L	A	1	25/25	-	-	41,51,52,55	0
2	Z9K	A	2	17/18	-	-	35,55,71,71	0
2	GU6	A	3	23/24	-	-	30,50,65,65	0
2	GU1	A	4	14/15	-	-	37,40,53,53	0
2	Z9H	A	5	21/22	-	-	27,41,56,62	0
2	Z9L	B	1	25/25	-	-	21,30,44,44	0
2	Z9K	B	2	17/18	-	-	26,30,33,33	0
2	GU6	B	3	23/24	-	-	26,27,56,56	0
2	GU1	B	4	14/15	-	-	28,28,74,74	0
2	Z9H	B	5	21/22	-	-	36,38,45,67	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

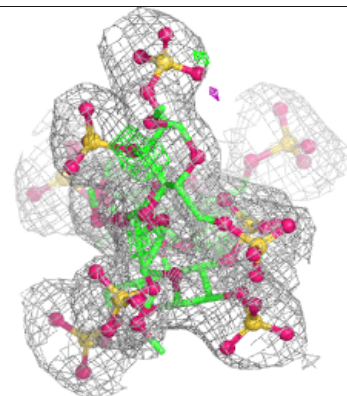
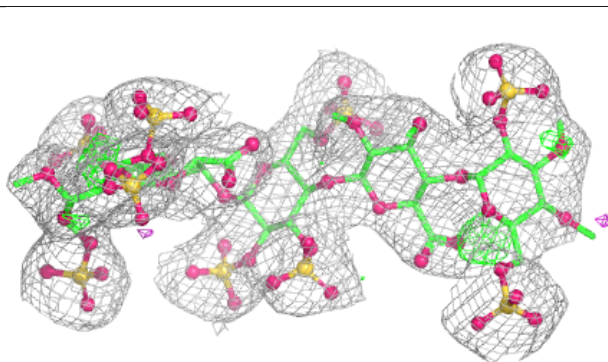
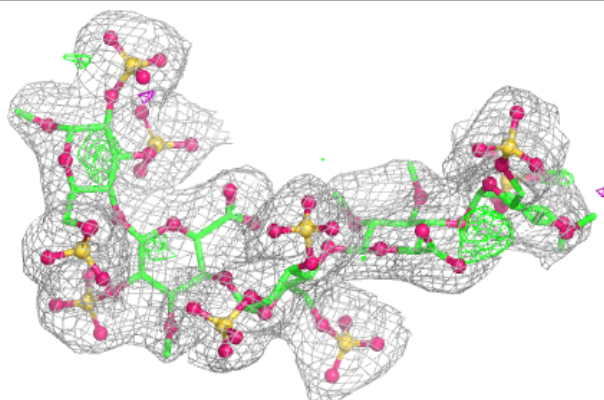
Electron density around Chain A:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
3	NAG	L	501	14/15	0.45	0.24	30,60,78,82	0
3	NAG	L	502	14/15	0.47	0.19	30,60,78,82	0
3	NAG	I	501	14/15	0.67	0.14	35,55,55,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.