



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:46 PM UTC

PDB ID : 3KW7 / pdb_00003kw7
Title : Crystal structure of LacB from Trametes sp. AH28-2
Authors : Ge, H.H.; Teng, M.K.; Niu, L.W.
Deposited on : 2009-12-01
Resolution : 3.44 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

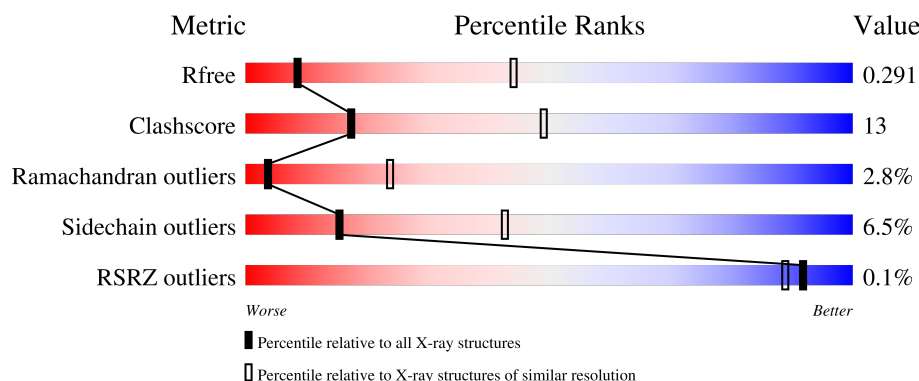
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	502	69% 26% 5%
1	B	502	71% 25% .
2	C	2	50% 50%
2	D	2	50% 50%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7825 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 Laccase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	5	0	0
			3809	2416	631	753	9			
1	B	502	Total	C	N	O	S	18	0	0
			3808	2416	631	752	9			

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

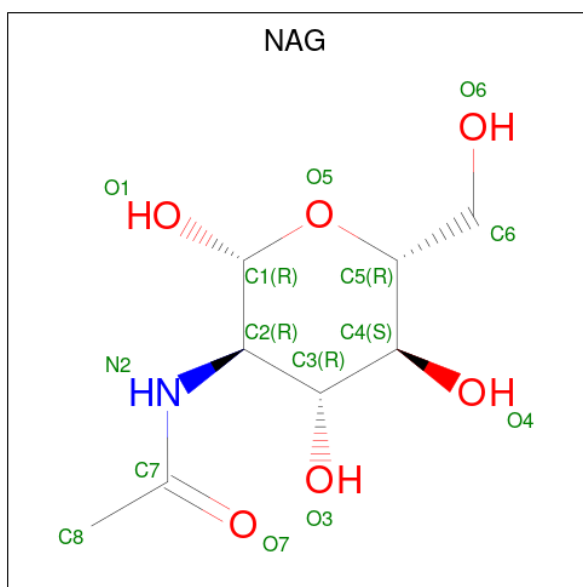


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		
3	B	4	Total	Cu	0	0
			4	4		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

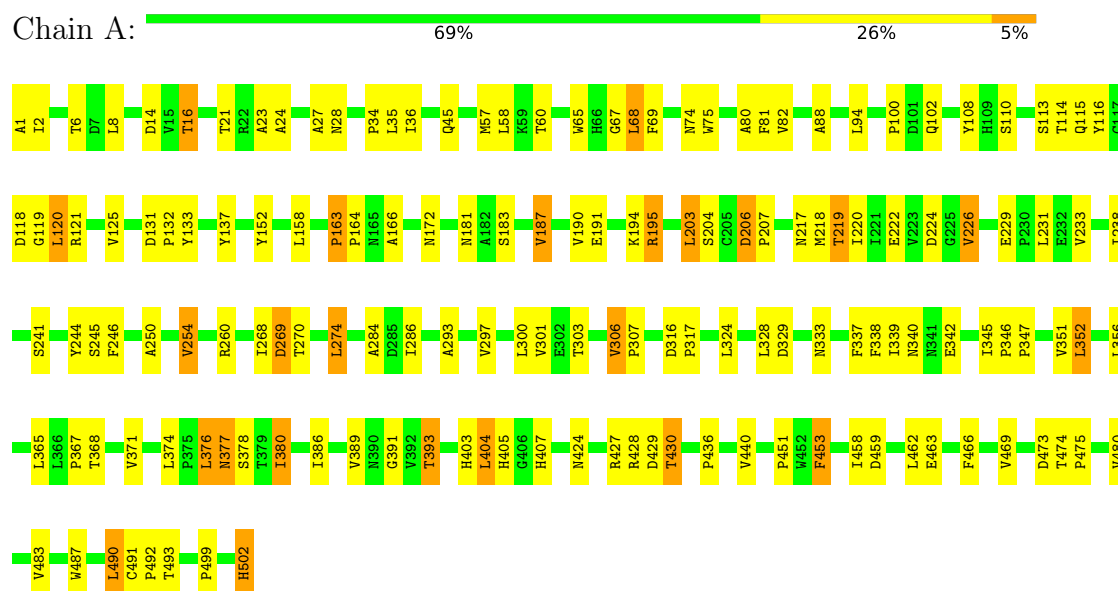
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	13	Total	O	0	0
			13	13		

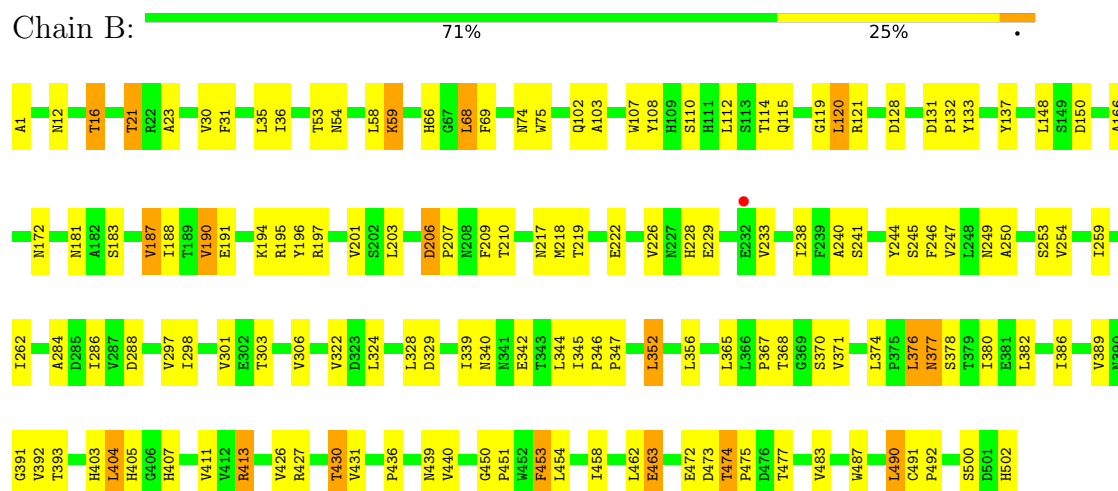
3 Residue-property plots

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: Laccase B



• Molecule 1: Laccase B



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

Chain C:  50% 50%

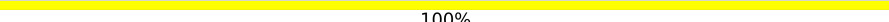
MAG1
MAG2

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	98.78Å 98.78Å 149.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.44 30.00 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-3.44) 99.1 (30.00-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.292 0.223 , 0.291	Depositor DCC
R_{free} test set	978 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7825	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 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	A	0.96	4/3919 (0.1%)	1.06	8/5396 (0.1%)
1	B	1.00	6/3918 (0.2%)	1.08	13/5396 (0.2%)
All	All	0.98	10/7837 (0.1%)	1.07	21/10792 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	500	SER	CB-OG	-17.27	1.07	1.42
1	B	30	VAL	CB-CG1	-11.35	1.15	1.52
1	A	274	LEU	CG-CD2	-8.38	1.24	1.52
1	B	21	THR	CB-CG2	-7.48	1.27	1.52
1	A	306	VAL	CA-CB	7.29	1.60	1.54
1	B	112	LEU	CG-CD1	-5.88	1.33	1.52
1	A	345	ILE	CA-C	5.72	1.58	1.52
1	B	21	THR	CB-OG1	5.26	1.52	1.43
1	B	59	LYS	CE-NZ	5.21	1.65	1.49
1	A	393	THR	CA-CB	5.18	1.62	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	VAL	CA-CB-CG2	-13.65	87.19	110.40
1	B	30	VAL	CG1-CB-CG2	11.64	136.40	110.80
1	B	112	LEU	CD1-CG-CD2	10.11	133.03	110.80
1	B	346	PRO	CA-C-N	8.22	128.17	120.03
1	B	346	PRO	C-N-CA	8.22	128.17	120.03
1	B	253	SER	N-CA-CB	6.94	120.73	109.69
1	A	82	VAL	N-CA-C	-6.87	106.20	111.62
1	A	483	VAL	N-CA-C	6.67	115.24	107.77
1	A	346	PRO	CA-C-N	6.60	126.56	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	PRO	C-N-CA	6.60	126.56	120.03
1	A	113	SER	CB-CA-C	-6.23	109.37	116.54
1	B	500	SER	CA-CB-OG	5.83	122.76	111.10
1	B	288	ASP	CA-C-N	5.65	125.66	119.90
1	B	288	ASP	C-N-CA	5.65	125.66	119.90
1	B	483	VAL	N-CA-C	5.61	114.67	108.05
1	A	187	VAL	N-CA-C	5.53	115.50	106.72
1	A	163	PRO	CA-C-N	5.50	124.85	118.85
1	A	163	PRO	C-N-CA	5.50	124.85	118.85
1	B	392	VAL	N-CA-C	5.33	116.41	111.45
1	B	21	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	187	VAL	N-CA-C	5.03	115.10	107.75

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	3809	0	3600	96	0
1	B	3808	0	3600	86	0
2	C	28	0	25	1	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	28	0	26	3	0
4	B	28	0	26	3	0
5	A	19	0	0	3	0
5	B	13	0	0	3	0
All	All	7825	0	7352	185	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 (185) 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:217:ASN:HD21	4:A:701:NAG:C1	1.67	1.08
1:B:1:ALA:HB3	1:B:35:LEU:O	1.52	1.07
1:A:1:ALA:HB3	1:A:35:LEU:O	1.57	1.03
1:B:23:ALA:HB1	5:B:515:HOH:O	1.61	0.98
1:B:376:LEU:O	1:B:378:SER:N	1.98	0.96
1:A:376:LEU:O	1:A:378:SER:N	2.01	0.92
1:B:376:LEU:HD12	1:B:473:ASP:CG	1.95	0.92
1:B:217:ASN:HD21	4:B:705:NAG:C1	1.82	0.91
1:A:376:LEU:HD12	1:A:473:ASP:CB	2.01	0.91
1:B:376:LEU:CD1	1:B:473:ASP:OD2	2.20	0.90
1:A:376:LEU:HD12	1:A:473:ASP:CG	1.97	0.88
5:B:510:HOH:O	2:F:2:NAG:H82	1.75	0.85
1:B:376:LEU:HD12	1:B:473:ASP:CB	2.07	0.84
1:B:1:ALA:CB	1:B:35:LEU:O	2.26	0.83
1:A:376:LEU:CD1	1:A:473:ASP:OD2	2.28	0.82
1:B:328:LEU:HD23	1:B:339:ILE:HG21	1.61	0.81
1:B:376:LEU:HD12	1:B:473:ASP:OD2	1.79	0.80
1:A:217:ASN:ND2	4:A:701:NAG:C1	2.46	0.79
1:B:427:ARG:HH11	1:B:427:ARG:HG2	1.46	0.79
1:A:376:LEU:HD12	1:A:473:ASP:HB2	1.65	0.78
1:A:328:LEU:HD23	1:A:339:ILE:HG21	1.65	0.77
1:B:181:ASN:HD22	1:B:183:SER:HB3	1.50	0.75
1:B:254:VAL:HG12	1:B:284:ALA:HB2	1.67	0.75
1:A:222:GLU:HB3	1:A:245:SER:HB2	1.70	0.72
1:B:222:GLU:HB3	1:B:245:SER:HB2	1.72	0.71
1:A:206:ASP:HB3	1:A:207:PRO:HD3	1.73	0.71
1:B:23:ALA:CB	5:B:515:HOH:O	2.30	0.70
1:A:181:ASN:HD22	1:A:183:SER:HB3	1.56	0.69
1:B:427:ARG:HG2	1:B:427:ARG:NH1	2.07	0.68
1:A:254:VAL:HG12	1:A:284:ALA:HB2	1.74	0.68
1:A:376:LEU:HD12	1:A:473:ASP:OD2	1.91	0.66
1:B:228:HIS:NE2	1:B:426:VAL:HG23	2.11	0.66
1:B:229:GLU:HB2	1:B:306:VAL:HG23	1.78	0.66
1:B:206:ASP:HB3	1:B:207:PRO:HD3	1.77	0.66
1:A:352:LEU:HD22	1:A:356:LEU:CD1	2.25	0.65
1:B:376:LEU:HD12	1:B:473:ASP:HB2	1.78	0.64
1:A:347:PRO:HD3	1:A:367:PRO:HD3	1.78	0.64
1:B:217:ASN:ND2	4:B:705:NAG:C1	2.58	0.64
1:B:376:LEU:C	1:B:378:SER:H	2.06	0.64
1:A:376:LEU:O	1:A:377:ASN:C	2.41	0.63
1:B:328:LEU:HD23	1:B:339:ILE:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASN:HD22	1:B:53:THR:H	1.47	0.62
1:B:103:ALA:HB1	1:B:128:ASP:HB2	1.81	0.62
1:B:386:ILE:O	1:B:436:PRO:HA	2.00	0.62
1:B:191:GLU:HB2	1:B:194:LYS:HD2	1.82	0.61
1:A:386:ILE:O	1:A:436:PRO:HA	1.99	0.61
1:A:203:LEU:HD12	1:A:203:LEU:H	1.65	0.61
1:A:328:LEU:HD23	1:A:339:ILE:CG2	2.30	0.61
1:A:203:LEU:HD12	1:A:203:LEU:N	2.15	0.60
1:B:12:ASN:ND2	1:B:54:ASN:H	2.00	0.60
1:B:352:LEU:HD22	1:B:356:LEU:CD1	2.30	0.60
1:B:218:MET:HG2	1:B:246:PHE:CD1	2.37	0.60
1:B:352:LEU:HD22	1:B:356:LEU:HD12	1.84	0.59
1:A:365:LEU:HD13	1:A:371:VAL:HG11	1.85	0.59
1:A:376:LEU:C	1:A:378:SER:H	2.10	0.59
1:B:487:TRP:HA	1:B:490:LEU:HD22	1.84	0.59
1:A:8:LEU:HD22	1:A:27:ALA:HB1	1.83	0.59
1:B:75:TRP:HB2	1:B:487:TRP:CD1	2.38	0.58
1:A:191:GLU:HB2	1:A:194:LYS:HD2	1.86	0.58
1:A:220:ILE:CD1	1:A:300:LEU:HD13	2.33	0.58
1:B:413:ARG:NH1	1:B:439:ASN:HB3	2.19	0.58
1:A:137:TYR:HA	1:A:195:ARG:HB2	1.85	0.57
1:B:203:LEU:HD12	1:B:203:LEU:N	2.19	0.57
1:A:376:LEU:C	1:A:378:SER:N	2.62	0.57
1:B:195:ARG:HG2	1:B:249:ASN:OD1	2.05	0.56
1:A:218:MET:HG2	1:A:246:PHE:CD1	2.40	0.56
1:B:68:LEU:HA	1:B:102:GLN:HE22	1.71	0.56
1:A:352:LEU:HD22	1:A:356:LEU:HD12	1.87	0.55
5:A:519:HOH:O	2:D:2:NAG:C8	2.55	0.55
1:A:352:LEU:HD22	1:A:356:LEU:HD11	1.87	0.54
1:B:324:LEU:HB3	1:B:380:ILE:HG13	1.90	0.54
1:B:491:CYS:N	1:B:492:PRO:HD2	2.23	0.54
1:B:181:ASN:ND2	1:B:183:SER:HB3	2.21	0.54
1:B:403:HIS:HB2	1:B:430:THR:HB	1.88	0.54
1:B:188:ILE:HD12	1:B:259:ILE:HD13	1.90	0.54
1:B:196:TYR:O	1:B:247:VAL:HA	2.08	0.54
5:A:519:HOH:O	2:D:2:NAG:H82	2.07	0.53
1:A:329:ASP:H	1:A:340:ASN:ND2	2.07	0.53
1:B:217:ASN:HD21	4:B:705:NAG:C2	2.21	0.53
1:B:329:ASP:H	1:B:340:ASN:ND2	2.07	0.53
1:A:376:LEU:CD1	1:A:473:ASP:CG	2.74	0.53
1:A:224:ASP:OD2	1:A:428:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG23	1:A:238:ILE:O	2.08	0.52
1:A:45:GLN:HB3	1:A:94:LEU:HD11	1.92	0.52
1:A:1:ALA:CB	1:A:35:LEU:O	2.46	0.51
1:A:14:ASP:HA	1:A:23:ALA:HA	1.91	0.51
1:B:376:LEU:HD13	1:B:473:ASP:OD2	2.05	0.51
1:A:119:GLY:O	1:A:121:ARG:N	2.42	0.50
1:A:487:TRP:HA	1:A:490:LEU:HD22	1.92	0.50
1:A:429:ASP:OD1	1:A:430:THR:HG22	2.11	0.50
1:A:241:SER:OG	1:A:430:THR:HG21	2.11	0.50
1:A:268:ILE:O	1:A:269:ASP:HB2	2.12	0.49
1:A:68:LEU:HA	1:A:102:GLN:HE22	1.77	0.49
1:A:491:CYS:N	1:A:492:PRO:HD2	2.28	0.49
1:A:376:LEU:HD13	1:A:473:ASP:OD2	2.11	0.49
1:B:203:LEU:HD12	1:B:203:LEU:H	1.77	0.49
1:A:57:MET:HE3	2:C:1:NAG:O6	2.12	0.49
1:B:69:PHE:HD2	1:B:102:GLN:CD	2.21	0.49
1:B:474:THR:HG23	1:B:475:PRO:HD3	1.93	0.49
1:A:75:TRP:HB2	1:A:487:TRP:CD1	2.48	0.48
1:A:229:GLU:HB2	1:A:306:VAL:HG23	1.94	0.48
1:B:238:ILE:HG23	1:B:238:ILE:O	2.13	0.48
1:B:365:LEU:HD13	1:B:371:VAL:HG11	1.95	0.48
1:A:301:VAL:HG12	1:A:303:THR:HG22	1.96	0.48
1:A:28:ASN:HD22	1:A:34:PRO:HG3	1.79	0.48
1:A:69:PHE:HD2	1:A:102:GLN:CD	2.22	0.48
1:B:238:ILE:HD12	1:B:244:TYR:HD2	1.78	0.48
1:B:240:ALA:O	1:B:241:SER:OG	2.29	0.48
1:A:405:HIS:CD2	1:A:453:PHE:HB3	2.48	0.48
1:B:376:LEU:O	1:B:377:ASN:C	2.52	0.47
1:A:24:ALA:HB1	1:A:118:ASP:O	2.14	0.47
1:A:324:LEU:HB3	1:A:380:ILE:HG13	1.96	0.47
1:B:407:HIS:NE2	1:B:472:GLU:OE1	2.41	0.47
1:B:188:ILE:HD12	1:B:259:ILE:CD1	2.44	0.47
1:A:333:ASN:HB3	1:A:338:PHE:HE2	1.80	0.47
1:B:131:ASP:C	1:B:133:TYR:H	2.22	0.47
1:B:137:TYR:CG	1:B:197:ARG:HB2	2.50	0.47
1:A:226:VAL:HG11	1:A:427:ARG:HD2	1.95	0.47
1:B:376:LEU:HD23	1:B:377:ASN:H	1.80	0.47
1:A:16:THR:HB	1:A:21:THR:HA	1.97	0.47
1:A:260:ARG:CZ	1:A:293:ALA:HB2	2.45	0.47
1:A:403:HIS:HB2	1:A:430:THR:HB	1.97	0.47
1:A:206:ASP:HA	1:A:458:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASP:C	1:A:133:TYR:H	2.23	0.46
1:B:16:THR:HB	1:B:21:THR:HA	1.98	0.46
1:A:35:LEU:HD11	1:A:125:VAL:HG23	1.98	0.46
1:A:376:LEU:HD23	1:A:377:ASN:H	1.81	0.46
1:A:490:LEU:HA	1:A:493:THR:HG22	1.98	0.45
1:B:206:ASP:HA	1:B:458:ILE:HG23	1.98	0.45
1:B:74:ASN:CG	1:B:451:PRO:HD2	2.41	0.45
1:B:53:THR:O	1:B:59:LYS:HE3	2.17	0.45
1:A:23:ALA:HB1	5:A:507:HOH:O	2.17	0.45
1:A:131:ASP:O	1:A:133:TYR:N	2.49	0.45
1:B:119:GLY:O	1:B:121:ARG:N	2.48	0.45
1:B:66:HIS:CE1	1:B:241:SER:HB2	2.52	0.44
1:A:337:PHE:HB3	1:A:466:PHE:CD1	2.53	0.44
1:B:31:PHE:CD2	1:B:31:PHE:C	2.95	0.44
1:B:131:ASP:O	1:B:133:TYR:N	2.50	0.44
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.85	0.44
1:A:217:ASN:HD21	4:A:701:NAG:C2	2.26	0.44
1:A:65:TRP:HB3	1:A:68:LEU:HD23	2.00	0.44
1:B:450:GLY:HA2	1:B:477:THR:HG23	1.98	0.44
1:A:474:THR:HG23	1:A:475:PRO:HD3	1.99	0.44
1:A:67:GLY:O	1:A:102:GLN:NE2	2.51	0.44
1:A:351:VAL:HG11	1:A:469:VAL:HG11	1.99	0.43
1:A:238:ILE:HD12	1:A:244:TYR:HD2	1.83	0.43
1:A:110:SER:HB2	1:A:120:LEU:HD23	2.00	0.43
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.83	0.43
1:B:150:ASP:HB2	1:B:166:ALA:HB2	2.01	0.43
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.46	0.43
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.93	0.43
1:A:60:THR:HG22	1:A:88:ALA:HA	2.00	0.43
1:A:306:VAL:HA	1:A:307:PRO:HD3	1.82	0.43
1:B:218:MET:HG2	1:B:246:PHE:CE1	2.53	0.43
1:A:80:ALA:O	1:A:81:PHE:HB2	2.19	0.43
1:A:219:THR:HA	1:A:231:LEU:O	2.19	0.43
1:A:74:ASN:CG	1:A:451:PRO:HD2	2.44	0.42
1:A:204:SER:OG	1:A:207:PRO:HD2	2.19	0.42
1:B:426:VAL:HG22	1:B:427:ARG:N	2.35	0.42
1:A:480:VAL:HG12	1:A:480:VAL:O	2.19	0.42
1:B:110:SER:OG	1:B:115:GLN:HB3	2.20	0.42
1:B:301:VAL:HG12	1:B:303:THR:HG22	2.01	0.42
1:B:36:ILE:HD12	1:B:108:TYR:CD1	2.55	0.42
1:B:411:VAL:HG11	1:B:431:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HB3	1:B:209:PHE:CE2	2.54	0.42
1:A:404:LEU:HD13	1:A:407:HIS:HB2	2.01	0.41
1:A:499:PRO:O	1:A:502:HIS:HB2	2.20	0.41
1:B:190:VAL:HG12	1:B:196:TYR:CE1	2.54	0.41
1:B:367:PRO:HG2	1:B:370:SER:HB2	2.02	0.41
1:B:107:TRP:HB3	1:B:201:VAL:HG11	2.03	0.41
1:B:114:THR:HG23	1:B:463:GLU:HG3	2.03	0.41
1:A:36:ILE:HD12	1:A:108:TYR:CD1	2.55	0.41
1:B:352:LEU:HD22	1:B:356:LEU:HD11	1.99	0.41
1:A:2:ILE:HB	1:A:6:THR:HG21	2.02	0.41
1:A:114:THR:HG23	1:A:463:GLU:HG3	2.03	0.41
1:A:28:ASN:HB2	1:A:34:PRO:HG3	2.02	0.41
1:A:110:SER:OG	1:A:115:GLN:HB3	2.21	0.41
1:A:152:TYR:CE2	1:A:166:ALA:HA	2.56	0.41
1:B:328:LEU:HD11	1:B:382:LEU:HD22	2.03	0.41
1:B:347:PRO:HD3	1:B:367:PRO:HD3	2.02	0.41
1:B:404:LEU:HG	1:B:454:LEU:HD13	2.04	0.40
1:A:23:ALA:O	1:A:57:MET:HE1	2.21	0.40
1:A:114:THR:HA	1:A:459:ASP:OD1	2.21	0.40
1:A:424:ASN:O	1:A:424:ASN:OD1	2.40	0.40
1:B:405:HIS:CD2	1:B:453:PHE:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	500/502 (100%)	455 (91%)	29 (6%)	16 (3%)	3	22
1	B	500/502 (100%)	455 (91%)	33 (7%)	12 (2%)	4	26
All	All	1000/1004 (100%)	910 (91%)	62 (6%)	28 (3%)	4	24

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	389	VAL
1	B	377	ASN
1	B	389	VAL
1	A	269	ASP
1	B	250	ALA
1	B	286	ILE
1	B	393	THR
1	A	206	ASP
1	A	250	ALA
1	A	286	ILE
1	B	172	ASN
1	B	206	ASP
1	A	120	LEU
1	A	172	ASN
1	A	317	PRO
1	B	58	LEU
1	A	58	LEU
1	A	393	THR
1	A	440	VAL
1	B	120	LEU
1	A	132	PRO
1	A	391	GLY
1	B	391	GLY
1	A	254	VAL
1	B	440	VAL
1	B	132	PRO
1	A	100	PRO

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	A	423/423 (100%)	397 (94%)	26 (6%)	17	44
1	B	423/423 (100%)	394 (93%)	29 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	846/846 (100%)	791 (94%)	55 (6%)	15	43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	68	LEU
1	A	116	TYR
1	A	187	VAL
1	A	190	VAL
1	A	195	ARG
1	A	203	LEU
1	A	219	THR
1	A	226	VAL
1	A	233	VAL
1	A	270	THR
1	A	274	LEU
1	A	297	VAL
1	A	316	ASP
1	A	342	GLU
1	A	352	LEU
1	A	368	THR
1	A	374	LEU
1	A	376	LEU
1	A	380	ILE
1	A	404	LEU
1	A	430	THR
1	A	453	PHE
1	A	462	LEU
1	A	490	LEU
1	A	502	HIS
1	B	16	THR
1	B	68	LEU
1	B	120	LEU
1	B	187	VAL
1	B	190	VAL
1	B	210	THR
1	B	219	THR
1	B	226	VAL
1	B	233	VAL
1	B	262	ILE
1	B	297	VAL

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Mol	Chain	Res	Type
1	B	298	ILE
1	B	322	VAL
1	B	342	GLU
1	B	344	LEU
1	B	345	ILE
1	B	352	LEU
1	B	368	THR
1	B	374	LEU
1	B	376	LEU
1	B	404	LEU
1	B	413	ARG
1	B	430	THR
1	B	453	PHE
1	B	462	LEU
1	B	463	GLU
1	B	474	THR
1	B	490	LEU
1	B	502	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	45	GLN
1	A	70	GLN
1	A	71	HIS
1	A	91	ASN
1	A	102	GLN
1	A	115	GLN
1	A	181	ASN
1	A	192	GLN
1	A	217	ASN
1	A	275	ASN
1	A	340	ASN
1	A	341	ASN
1	A	481	ASN
1	A	502	HIS
1	B	12	ASN
1	B	43	ASN
1	B	45	GLN
1	B	70	GLN
1	B	71	HIS

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Mol	Chain	Res	Type
1	B	91	ASN
1	B	102	GLN
1	B	181	ASN
1	B	217	ASN
1	B	275	ASN
1	B	340	ASN
1	B	360	GLN
1	B	481	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 ⓘ

8 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	C	1	2,1	14,14,15	0.73	0	17,19,21	1.93	2 (11%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	1.48	2 (11%)
2	NAG	D	1	2,1	14,14,15	0.57	0	17,19,21	1.46	2 (11%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	1.78	6 (35%)
2	NAG	E	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	1.57	2 (11%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	1.87	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.69	0	17,19,21	1.37	2 (11%)
2	NAG	F	2	2	14,14,15	0.58	0	17,19,21	2.46	7 (41%)

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	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	2.64	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-6.64	114.01	122.90
2	F	2	NAG	C4-C3-C2	-6.39	101.65	111.02
2	E	2	NAG	C1-O5-C5	6.09	120.35	112.19
2	E	1	NAG	C1-O5-C5	4.18	117.79	112.19
2	F	2	NAG	C1-C2-N2	3.78	116.38	110.43
2	D	2	NAG	O4-C4-C5	3.71	118.46	109.32
2	E	1	NAG	C1-C2-N2	3.43	115.84	110.43
2	F	2	NAG	C1-O5-C5	3.38	116.72	112.19
2	C	2	NAG	C1-O5-C5	3.17	116.43	112.19
2	D	1	NAG	C1-O5-C5	2.91	116.08	112.19
2	D	2	NAG	C8-C7-N2	2.78	120.73	116.12
2	E	2	NAG	C4-C3-C2	2.76	115.06	111.02
2	F	1	NAG	O3-C3-C2	2.69	114.99	109.40
2	F	2	NAG	O5-C5-C4	2.62	117.21	110.83
2	D	2	NAG	C2-N2-C7	2.60	126.38	122.90
2	F	2	NAG	O4-C4-C5	2.59	115.70	109.32
2	F	1	NAG	O4-C4-C3	-2.59	104.27	110.38
2	D	2	NAG	O7-C7-C8	-2.54	117.54	122.05
2	D	1	NAG	O3-C3-C2	2.46	114.51	109.40
2	F	2	NAG	O5-C1-C2	-2.45	107.51	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C3-C4-C5	-2.16	106.32	110.23
2	C	1	NAG	O7-C7-C8	-2.09	118.34	122.05
2	D	2	NAG	C1-C2-N2	2.05	113.66	110.43
2	C	2	NAG	C4-C3-C2	2.04	114.01	111.02
2	F	2	NAG	O5-C5-C6	-2.03	103.71	107.66

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

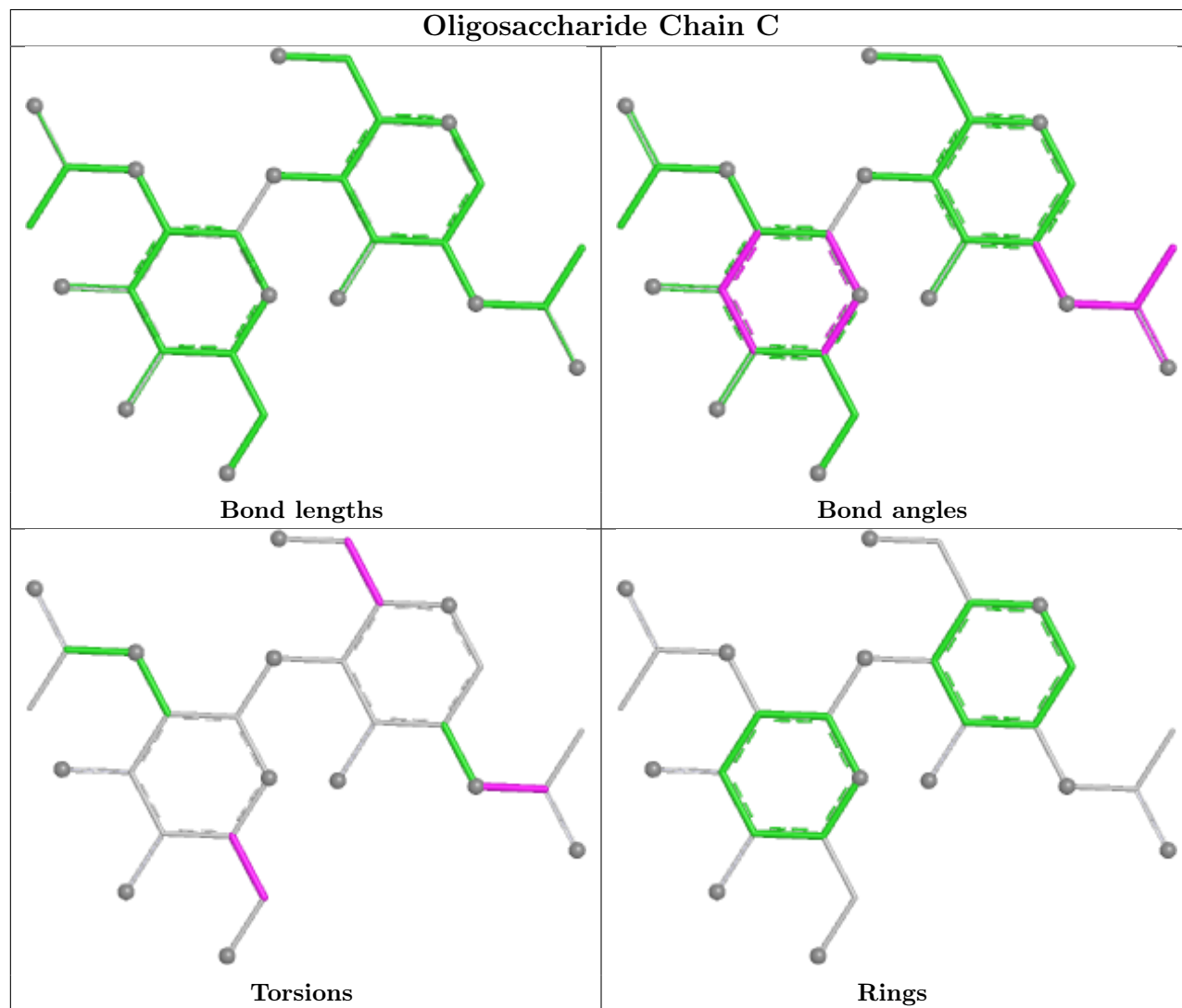
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
2	D	2	NAG	2	0

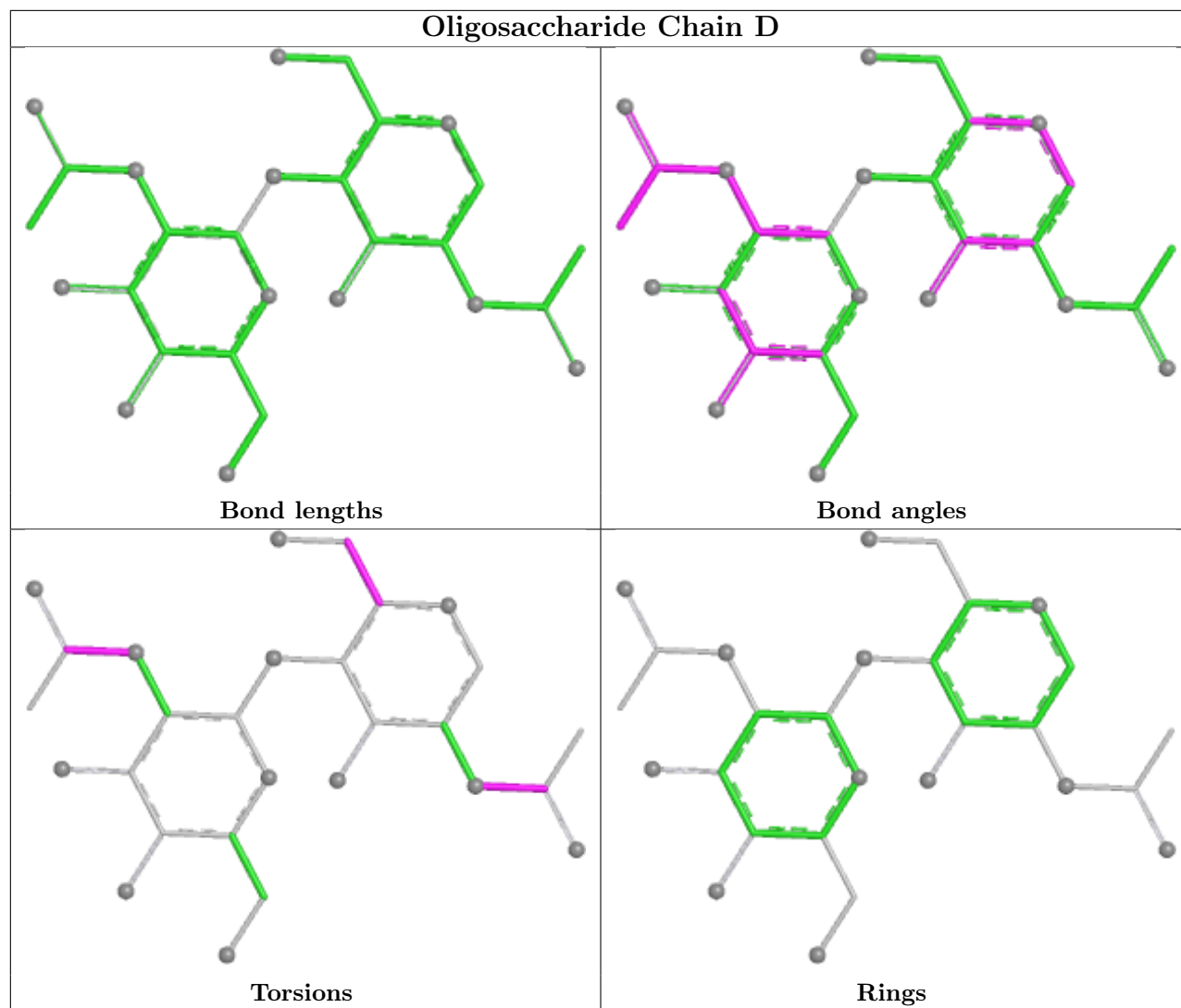
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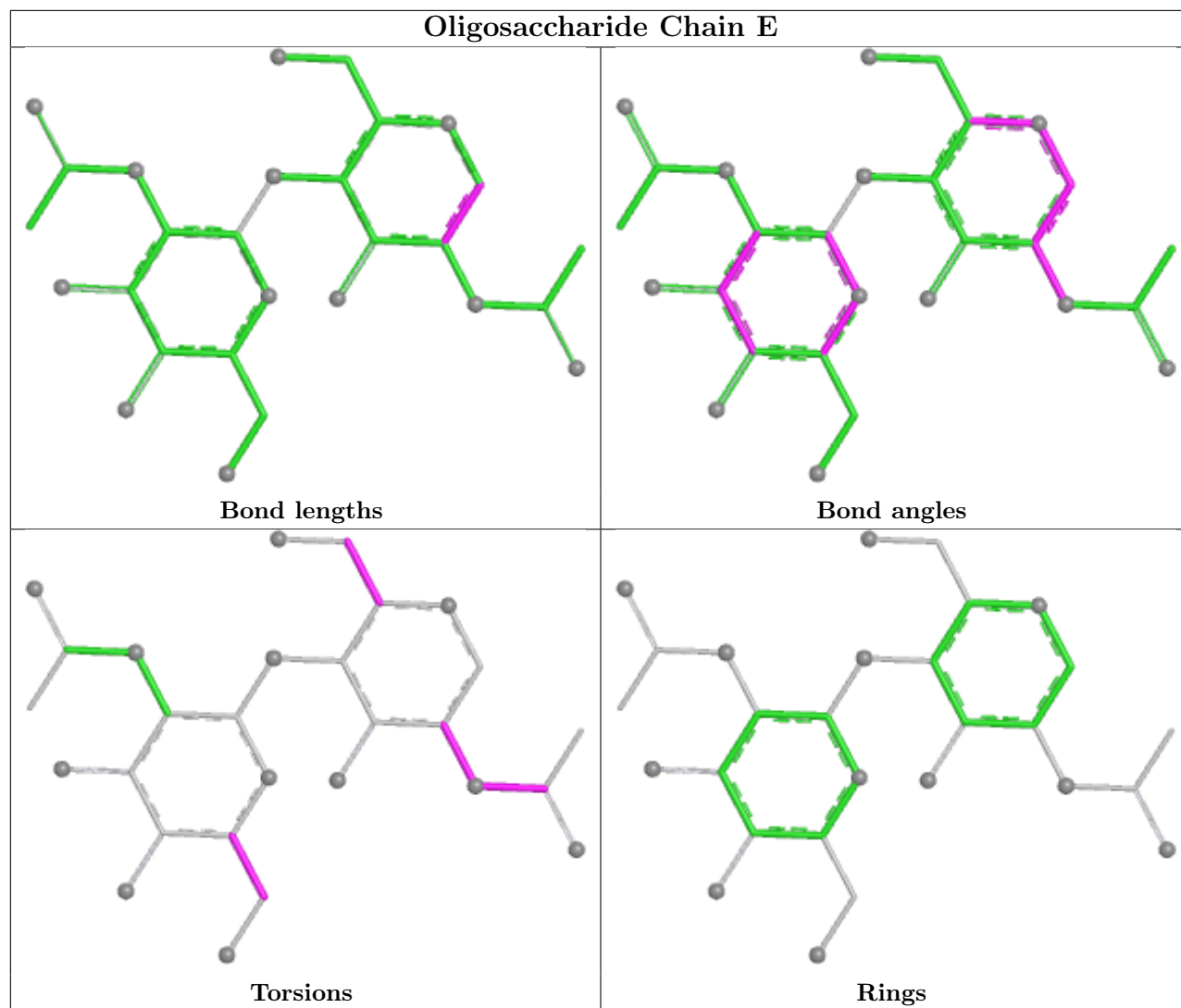
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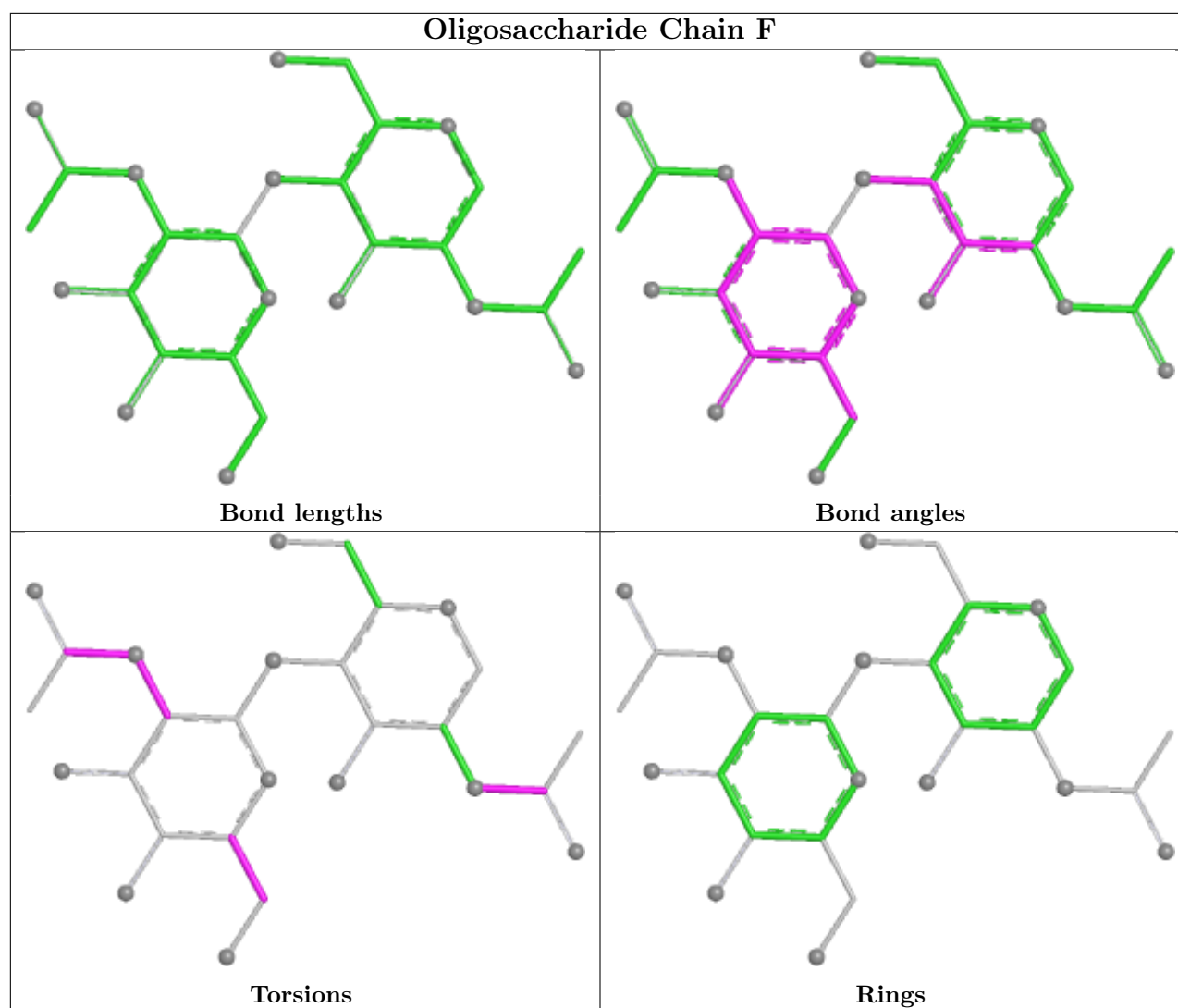
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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 12 ligands modelled in this entry, 8 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	$\# Z > 2$
4	NAG	A	701	-	14,14,15	0.61	0	17,19,21	1.46	3 (17%)
4	NAG	B	705	-	14,14,15	0.57	0	17,19,21	1.43	2 (11%)
4	NAG	B	706	1	14,14,15	1.02	1 (7%)	17,19,21	2.07	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	706	1	14,14,15	0.73	1 (7%)	17,19,21	1.83	6 (35%)

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
4	NAG	A	701	-	-	3/6/23/26	0/1/1/1
4	NAG	B	705	-	-	4/6/23/26	0/1/1/1
4	NAG	B	706	1	-	3/6/23/26	0/1/1/1
4	NAG	A	706	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	NAG	O6-C6	2.12	1.51	1.42
4	A	706	NAG	C3-C2	2.04	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	NAG	O5-C1-C2	-3.83	105.36	111.29
4	A	701	NAG	O5-C1-C2	-3.60	105.72	111.29
4	B	706	NAG	O4-C4-C5	3.53	118.02	109.32
4	B	705	NAG	O5-C1-C2	-3.42	106.00	111.29
4	A	706	NAG	O3-C3-C4	-3.28	102.65	110.38
4	B	706	NAG	C4-C3-C2	2.99	115.41	111.02
4	B	705	NAG	C3-C4-C5	2.91	115.51	110.23
4	A	701	NAG	C1-O5-C5	-2.89	108.31	112.19
4	B	706	NAG	C2-N2-C7	-2.85	119.08	122.90
4	A	706	NAG	C2-N2-C7	-2.85	119.08	122.90
4	A	706	NAG	O5-C1-C2	-2.75	107.03	111.29
4	B	706	NAG	O7-C7-C8	-2.55	117.51	122.05
4	B	706	NAG	C8-C7-N2	2.31	119.94	116.12
4	A	706	NAG	O3-C3-C2	2.27	114.11	109.40
4	B	706	NAG	O3-C3-C4	-2.27	105.03	110.38
4	A	706	NAG	C4-C3-C2	2.20	114.24	111.02
4	A	706	NAG	O7-C7-C8	-2.16	118.21	122.05
4	A	701	NAG	C3-C4-C5	2.14	114.11	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	A	706	NAG	C8-C7-N2-C2
4	A	706	NAG	O7-C7-N2-C2
4	B	705	NAG	C8-C7-N2-C2
4	B	705	NAG	O7-C7-N2-C2
4	B	706	NAG	C8-C7-N2-C2
4	B	706	NAG	O7-C7-N2-C2
4	B	705	NAG	O5-C5-C6-O6
4	B	705	NAG	C4-C5-C6-O6
4	A	706	NAG	O5-C5-C6-O6
4	A	706	NAG	C4-C5-C6-O6
4	B	706	NAG	O5-C5-C6-O6
4	A	701	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	NAG	3	0
4	B	705	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 [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	502/502 (100%)	-1.31	0 100 100	23, 48, 72, 82	26 (5%)
1	B	502/502 (100%)	-1.30	1 (0%) 91 84	22, 48, 71, 80	31 (6%)
All	All	1004/1004 (100%)	-1.30	1 (0%) 92 89	22, 48, 72, 82	57 (5%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	GLU	2.0

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

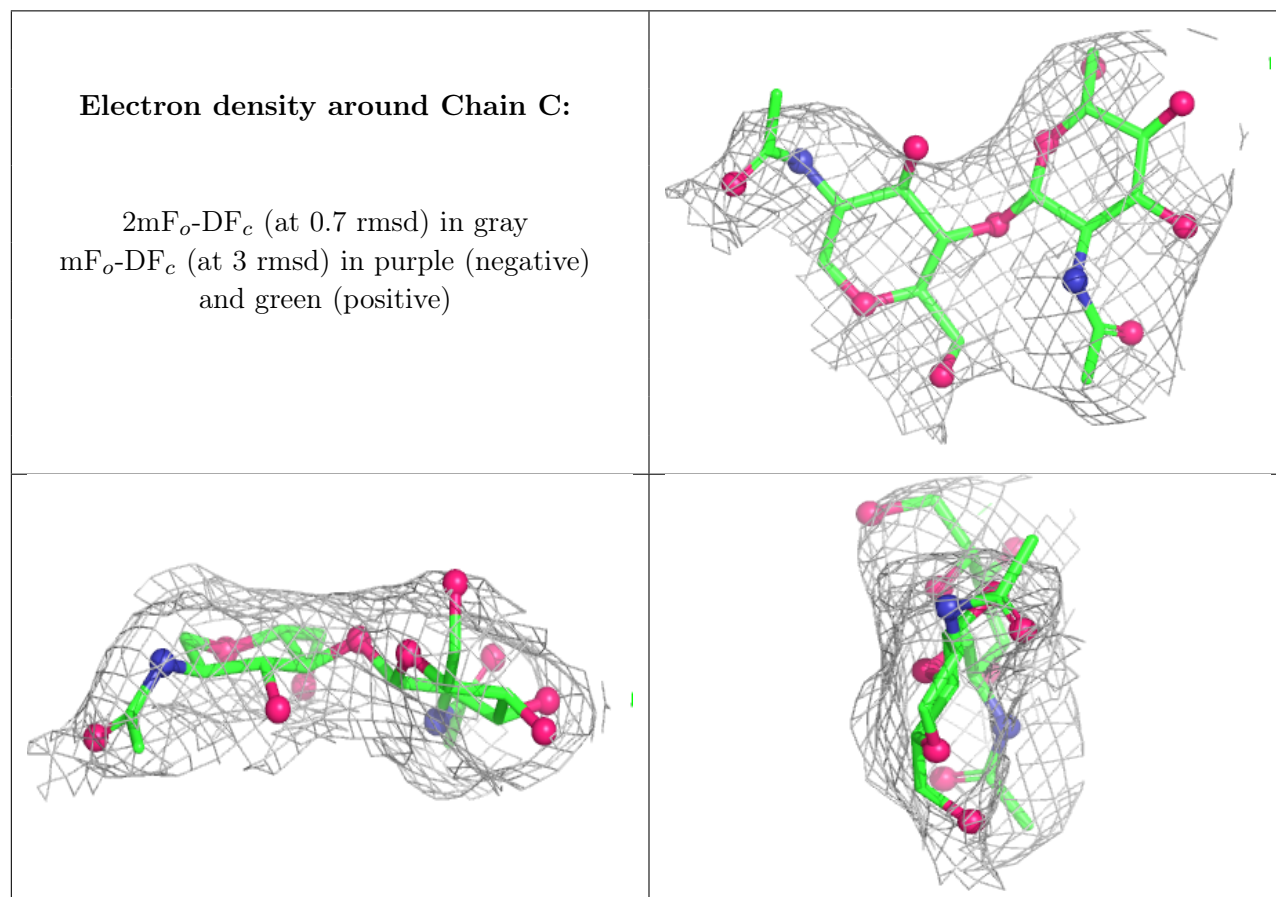
There are no non-standard protein/DNA/RNA residues in this entry.

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.

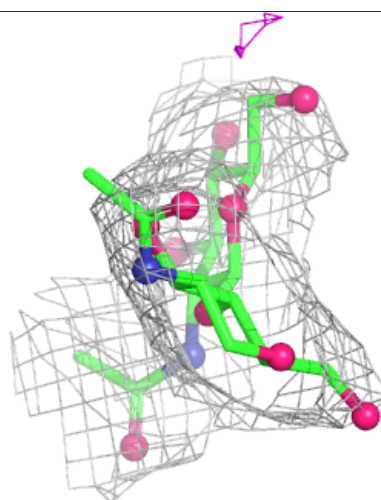
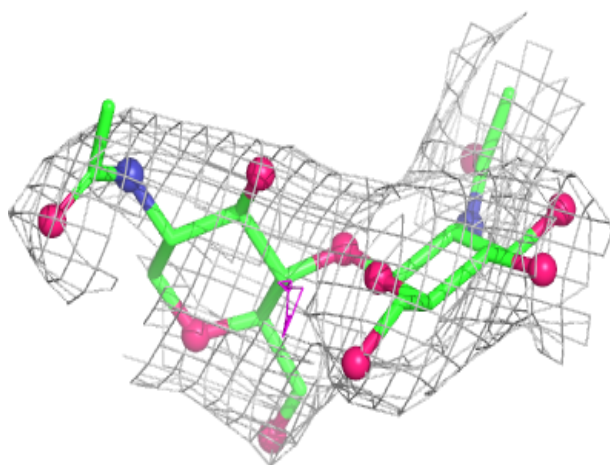
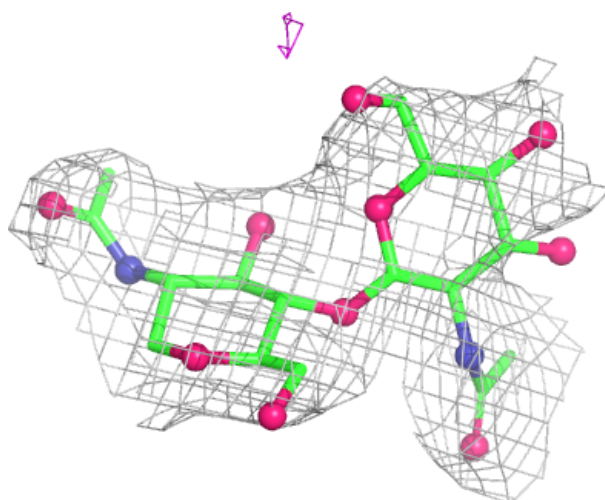
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.98	0.05	68,70,72,74	0
2	NAG	C	2	14/15	0.99	0.03	45,55,59,60	0
2	NAG	D	1	14/15	0.99	0.04	53,58,64,65	0
2	NAG	C	1	14/15	0.99	0.05	63,66,70,71	0
2	NAG	E	1	14/15	0.99	0.05	64,66,71,73	0
2	NAG	E	2	14/15	0.99	0.03	54,62,64,65	0
2	NAG	F	1	14/15	0.99	0.04	51,54,57,63	0
2	NAG	F	2	14/15	0.99	0.04	67,70,74,74	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.



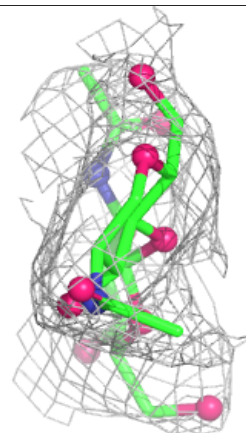
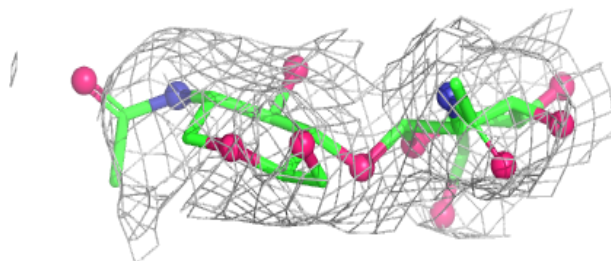
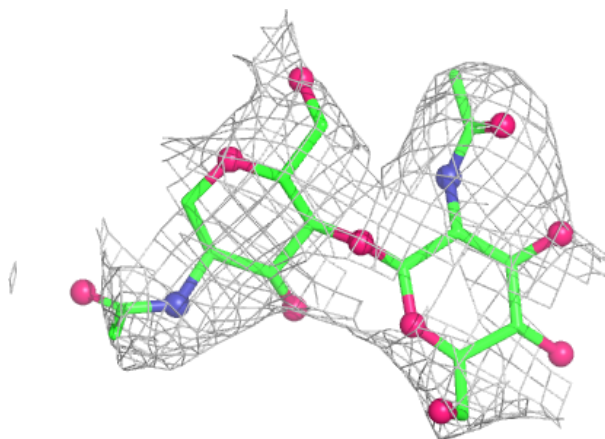
Electron density around Chain D:

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

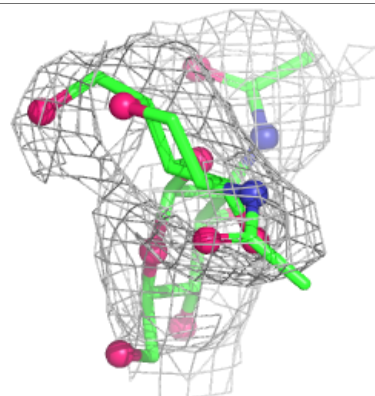
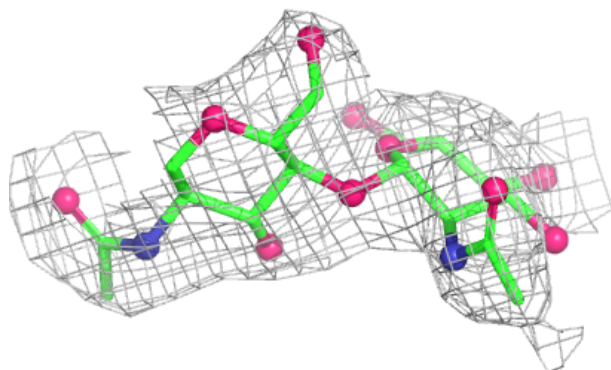
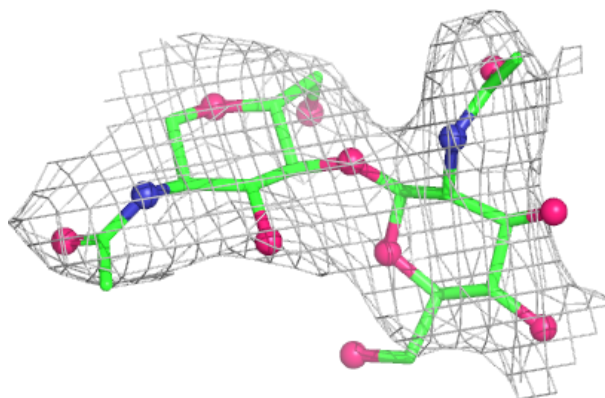


Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
4	NAG	A	701	14/15	0.98	0.05	87,88,89,90	0
4	NAG	A	706	14/15	0.99	0.05	41,47,49,51	0
4	NAG	B	705	14/15	0.99	0.05	93,94,95,96	0
4	NAG	B	706	14/15	0.99	0.05	50,54,58,59	0
3	CU	B	601	1/1	1.00	0.01	52,52,52,52	0
3	CU	B	602	1/1	1.00	0.02	60,60,60,60	0
3	CU	B	603	1/1	1.00	0.01	51,51,51,51	0
3	CU	B	604	1/1	1.00	0.01	67,67,67,67	0
3	CU	A	601	1/1	1.00	0.01	46,46,46,46	0
3	CU	A	602	1/1	1.00	0.02	58,58,58,58	0
3	CU	A	603	1/1	1.00	0.01	53,53,53,53	0
3	CU	A	604	1/1	1.00	0.02	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.