



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:22 AM EDT

PDB ID : 3GXT / pdb_00003gxt
Title : Crystal structure of alpha-galactosidase A at pH 4.5 complexed with 1-deoxy galactonijirimycin
Authors : Lieberman, R.L.
Deposited on : 2009-04-02
Resolution : 2.70 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

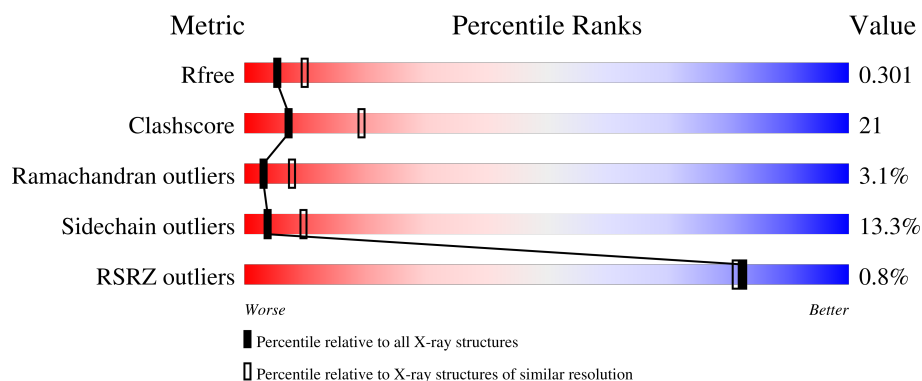
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	398	53% 36% 8% ..
1	B	398	56% 34% 7% ..
2	C	2	100%
2	D	2	100%
2	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	E	2	 50%50%
4	G	4	 100%
5	H	3	 33%67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	E	2	X	-	-	-
4	NAG	G	1	X	-	-	-
4	MAN	G	3	X	-	-	-
5	MAN	H	3	X	-	-	-
6	SO4	A	2	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6573 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 Alpha-galactosidase A.

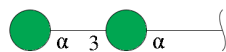
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	391	Total	C	N	O	S	0	0	0
			3131	1993	536	576	26			

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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			22	12	10			

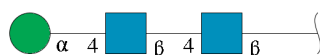
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.

ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



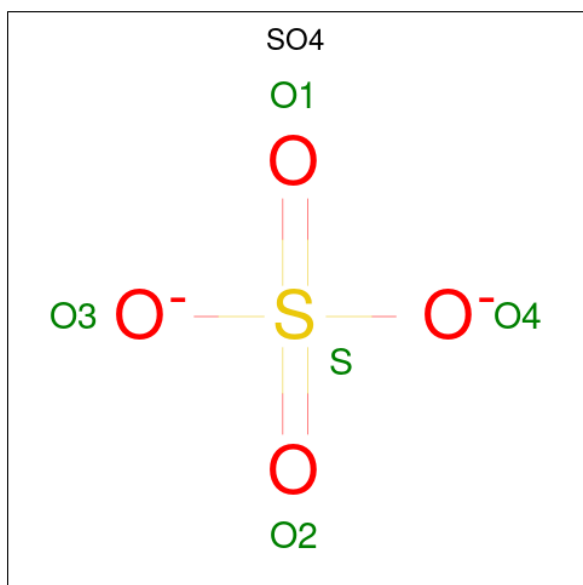
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



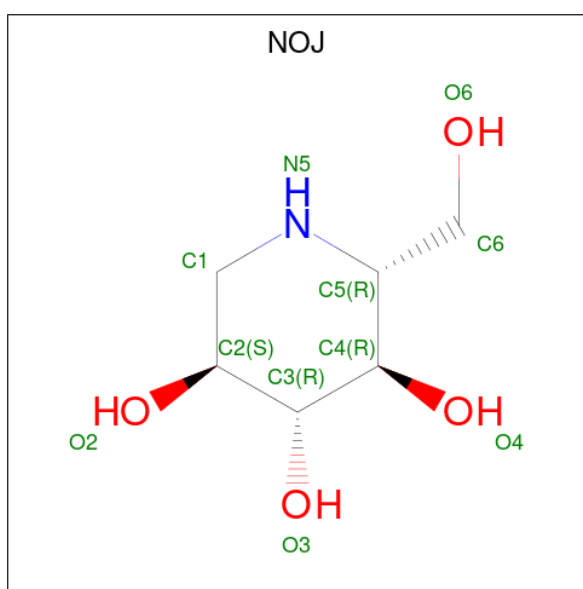
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

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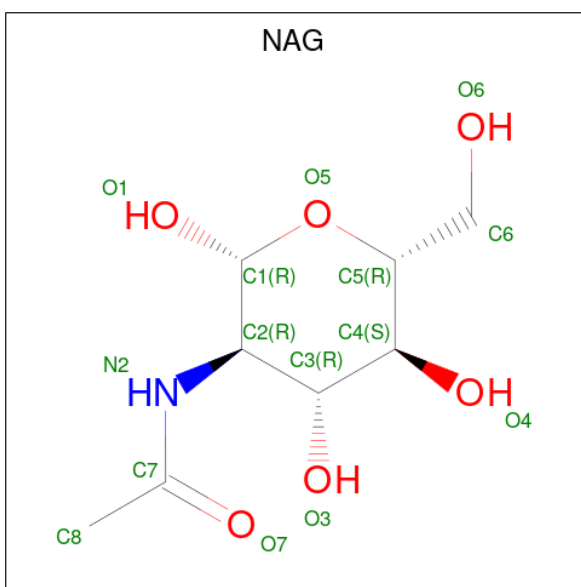
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	6	1	4		
7	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

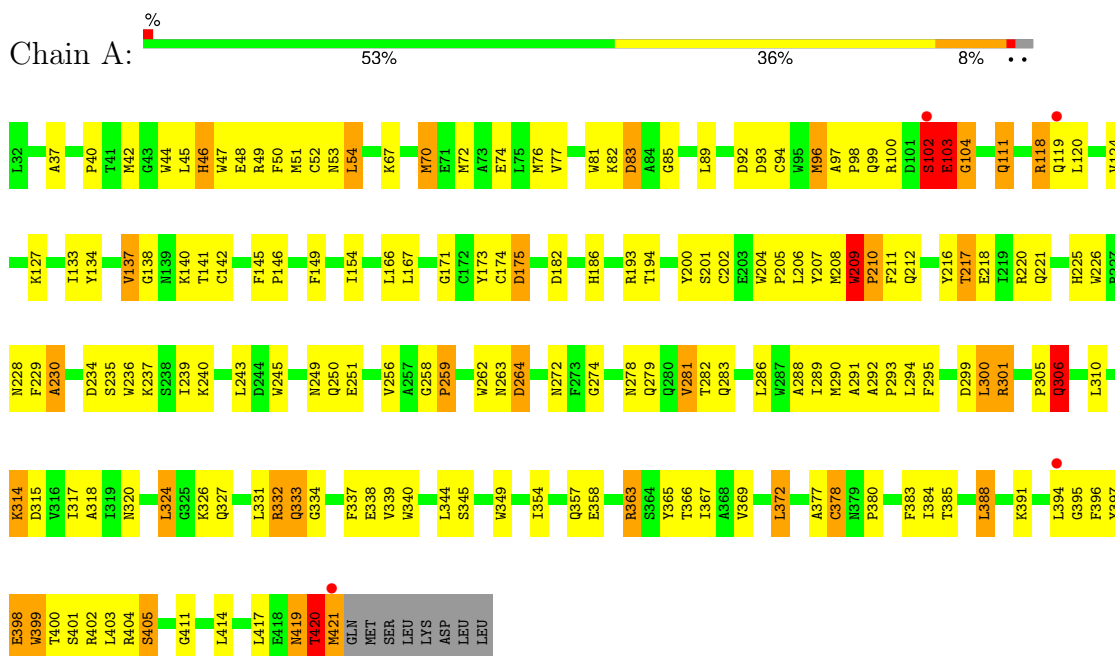
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	36	Total	O	0	0
			36	36		
9	B	28	Total	O	0	0
			28	28		

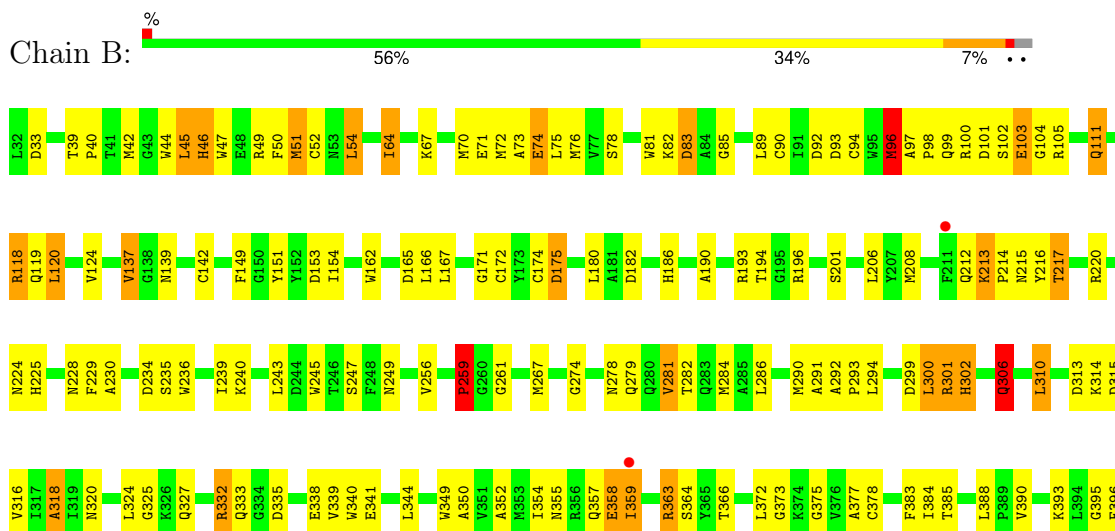
3 Residue-property plots

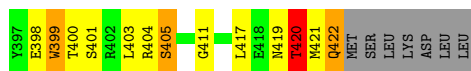
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-galactosidase A



• Molecule 1: Alpha-galactosidase A





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

Chain C: 100%



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

Chain D: 100%



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

Chain F: 50% 50%



- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose

Chain E: 50% 50%



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.61Å 89.61Å 216.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.90-2.70) 97.0 (19.90-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.306 0.238 , 0.301	Depositor DCC
R_{free} test set	1400 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6573	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, NOJ, MAN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	0/3209	1.21	16/4358 (0.4%)
1	B	0.96	2/3218 (0.1%)	1.18	12/4370 (0.3%)
All	All	0.99	2/6427 (0.0%)	1.20	28/8728 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	VAL	CA-CB	6.62	1.62	1.54
1	B	302	HIS	CA-C	-5.12	1.48	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	210	PRO	N-CA-C	-12.07	99.26	114.35
1	B	267	MET	N-CA-C	8.33	121.07	110.24
1	B	47	TRP	N-CA-C	7.46	119.10	110.97
1	A	102	SER	CA-C-N	7.06	134.40	121.70
1	A	102	SER	C-N-CA	7.06	134.40	121.70
1	A	264	ASP	CA-C-N	7.01	129.13	121.00
1	A	264	ASP	C-N-CA	7.01	129.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	THR	CA-C-N	6.62	133.62	121.70
1	A	420	THR	C-N-CA	6.62	133.62	121.70
1	A	405	SER	N-CA-C	6.34	118.03	108.46
1	B	103	GLU	N-CA-C	-6.19	97.62	110.80
1	A	281	VAL	N-CA-CB	6.18	117.78	110.55
1	A	394	LEU	N-CA-C	-5.92	100.35	109.52
1	A	420	THR	N-CA-C	5.91	123.39	110.80
1	B	96	MET	N-CA-C	5.86	118.46	110.55
1	B	97	ALA	CA-C-N	5.74	127.02	119.84
1	B	97	ALA	C-N-CA	5.74	127.02	119.84
1	B	339	VAL	N-CA-C	5.62	115.94	107.80
1	B	420	THR	CA-C-N	5.54	131.67	121.70
1	B	420	THR	C-N-CA	5.54	131.67	121.70
1	A	97	ALA	CA-C-N	5.45	126.66	119.84
1	A	97	ALA	C-N-CA	5.45	126.66	119.84
1	A	96	MET	N-CA-C	5.41	117.86	110.55
1	B	120	LEU	N-CA-C	-5.27	105.54	111.28
1	B	281	VAL	N-CA-CB	5.27	117.32	110.57
1	A	53	ASN	N-CA-C	5.24	117.01	108.63
1	B	90	CYS	N-CA-C	5.23	117.05	108.52
1	A	295	PHE	N-CA-C	5.02	117.52	107.62

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	SER	Peptide
1	A	103	GLU	Peptide
1	A	104	GLY	Peptide
1	A	209	TRP	Peptide
1	B	102	SER	Peptide
1	B	420	THR	Peptide

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	3122	0	2981	133	0
1	B	3131	0	2991	117	0
2	C	28	0	25	4	0
2	D	28	0	25	5	0
2	F	28	0	25	1	0
3	E	22	0	19	1	0
4	G	50	0	43	3	0
5	H	39	0	34	6	0
6	A	15	0	0	3	0
6	B	10	0	0	2	0
7	A	11	0	13	2	0
7	B	11	0	13	3	0
8	B	14	0	13	2	0
9	A	36	0	0	3	0
9	B	28	0	0	9	0
All	All	6573	0	6182	262	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 21.

All (262) 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:103:GLU:HB3	1:A:104:GLY:HA3	1.15	1.15
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.08	1.12
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.28	0.95
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.34	0.93
1:A:103:GLU:HB3	1:A:104:GLY:CA	2.04	0.88
9:B:441:HOH:O	5:H:2:NAG:H83	1.75	0.86
1:A:175:ASP:OD2	2:C:1:NAG:O7	1.94	0.83
1:A:332:ARG:HH11	1:A:332:ARG:CG	1.90	0.83
1:A:332:ARG:HG3	1:A:332:ARG:NH1	1.86	0.82
1:B:224:ASN:O	1:B:261:GLY:HA2	1.80	0.82
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.15	0.81
1:A:290:MET:O	1:A:327:GLN:HG3	1.83	0.79
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.18	0.78
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.47	0.78
1:A:175:ASP:OD2	1:A:175:ASP:N	2.09	0.76
1:B:42:MET:HE3	1:B:294:LEU:HD12	1.68	0.75
9:B:21:HOH:O	5:H:1:NAG:H5	1.85	0.75
1:B:215:ASN:HD21	5:H:1:NAG:C1	2.00	0.74
2:D:1:NAG:H61	2:D:2:NAG:H82	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASN:ND2	5:H:1:NAG:O5	2.19	0.72
1:A:142:CYS:HB2	7:A:430:NOJ:O6	1.89	0.72
1:A:377:ALA:O	1:A:378:CYS:HB2	1.89	0.71
1:B:335:ASP:OD1	9:B:440:HOH:O	2.07	0.71
1:A:332:ARG:NH1	9:A:25:HOH:O	2.20	0.71
1:A:42:MET:HE3	1:A:294:LEU:HD12	1.73	0.69
1:A:120:LEU:O	1:A:124:VAL:HG23	1.93	0.69
1:A:100:ARG:HD3	1:A:104:GLY:O	1.93	0.68
6:A:2:SO4:O4	9:A:12:HOH:O	2.11	0.68
1:B:83:ASP:OD2	1:B:83:ASP:N	2.26	0.67
1:A:103:GLU:CB	1:A:104:GLY:HA3	2.08	0.67
1:B:290:MET:O	1:B:327:GLN:HG3	1.95	0.67
1:B:332:ARG:HH11	1:B:332:ARG:CG	2.05	0.67
1:B:228:ASN:HB3	1:B:245:TRP:HH2	1.59	0.66
1:A:290:MET:O	1:A:327:GLN:CG	2.43	0.66
1:A:380:PRO:HD3	1:A:421:MET:HG3	1.79	0.65
1:B:208:MET:HE2	1:B:212:GLN:HE21	1.62	0.65
1:B:299:ASP:OD1	1:B:301:ARG:HB2	1.97	0.64
1:B:73:ALA:HB2	1:B:89:LEU:HD22	1.79	0.64
1:B:142:CYS:HB2	7:B:1:NOJ:H62	1.79	0.63
1:A:54:LEU:HD12	1:A:54:LEU:H	1.64	0.62
1:A:299:ASP:OD1	1:A:301:ARG:HB2	1.99	0.62
1:B:340:TRP:HB2	1:B:352:ALA:HB3	1.82	0.62
2:D:1:NAG:C6	2:D:2:NAG:H82	2.29	0.62
1:A:118:ARG:HA	1:A:118:ARG:HE	1.65	0.61
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.83	0.61
1:A:46:HIS:CD2	1:A:92:ASP:H	2.18	0.60
1:B:142:CYS:HB2	7:B:1:NOJ:C6	2.32	0.60
1:A:210:PRO:HD2	1:A:211:PHE:HD2	1.67	0.59
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.37	0.59
1:B:422:GLN:HE21	1:B:422:GLN:C	2.10	0.59
1:A:377:ALA:O	1:A:378:CYS:CB	2.49	0.59
1:B:422:GLN:C	1:B:422:GLN:NE2	2.60	0.59
1:A:77:VAL:HG21	1:A:127:LYS:HD2	1.85	0.58
1:B:338:GLU:HB2	1:B:354:ILE:HB	1.86	0.58
1:A:243:LEU:HD22	1:A:286:LEU:HD22	1.86	0.58
1:B:72:MET:O	1:B:76:MET:HG3	2.04	0.57
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.39	0.57
1:B:118:ARG:NH2	1:B:162:TRP:O	2.37	0.57
1:B:175:ASP:OD2	1:B:175:ASP:N	2.36	0.57
1:B:39:THR:HB	1:B:40:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:OD1	1:B:274:GLY:N	2.38	0.56
1:B:215:ASN:ND2	5:H:1:NAG:C1	2.67	0.56
1:A:237:LYS:HD3	9:A:439:HOH:O	2.04	0.56
1:B:315:ASP:O	1:B:318:ALA:HB3	2.06	0.56
1:A:250:GLN:O	1:A:251:GLU:C	2.48	0.56
4:G:1:NAG:H5	4:G:2:NAG:H82	1.86	0.56
1:B:120:LEU:O	1:B:124:VAL:HG23	2.06	0.56
1:A:380:PRO:CD	1:A:421:MET:HG3	2.36	0.55
1:B:67:LYS:HA	1:B:70:MET:HB2	1.87	0.55
1:B:332:ARG:HG3	1:B:332:ARG:NH1	2.06	0.55
1:A:83:ASP:OD2	1:A:83:ASP:N	2.39	0.55
1:A:286:LEU:HD21	1:A:354:ILE:HD11	1.89	0.55
1:B:118:ARG:HE	1:B:118:ARG:HA	1.72	0.55
1:B:72:MET:SD	1:B:300:LEU:HB2	2.47	0.55
1:B:196:ARG:NH1	6:B:4:SO4:O4	2.38	0.55
1:B:234:ASP:OD1	1:B:274:GLY:HA3	2.06	0.55
9:B:442:HOH:O	4:G:3:MAN:H62	2.06	0.55
1:A:72:MET:O	1:A:76:MET:HG3	2.06	0.54
1:B:111:GLN:HE21	1:B:111:GLN:H	1.54	0.54
1:B:76:MET:SD	1:B:89:LEU:HD13	2.48	0.54
1:A:363:ARG:HH11	1:A:363:ARG:CG	2.15	0.54
1:B:175:ASP:OD2	8:B:639:NAG:O7	2.25	0.54
1:A:166:LEU:HD23	1:A:167:LEU:N	2.23	0.54
1:A:76:MET:SD	1:A:89:LEU:HD13	2.48	0.54
1:A:111:GLN:H	1:A:111:GLN:HE21	1.56	0.53
1:B:341:GLU:HA	1:B:350:ALA:O	2.08	0.53
1:A:292:ALA:O	1:A:320:ASN:ND2	2.35	0.53
1:A:216:TYR:HB3	1:A:256:VAL:HG21	1.90	0.53
1:A:264:ASP:OD1	1:A:264:ASP:C	2.52	0.53
1:A:208:MET:O	1:A:209:TRP:C	2.51	0.53
1:A:154:ILE:HD12	1:A:154:ILE:N	2.24	0.53
1:A:286:LEU:CD2	1:A:354:ILE:HD11	2.39	0.52
1:B:358:GLU:O	1:B:359:ILE:HB	2.10	0.52
1:A:118:ARG:HE	1:A:118:ARG:CA	2.22	0.52
1:B:302:HIS:HA	9:B:7:HOH:O	2.09	0.52
1:A:337:PHE:CE2	1:A:365:TYR:HB2	2.45	0.52
1:A:67:LYS:HA	1:A:70:MET:HB2	1.92	0.52
1:A:72:MET:SD	1:A:300:LEU:HB2	2.49	0.52
1:A:243:LEU:HD22	1:A:286:LEU:CD2	2.40	0.51
1:B:236:TRP:CD1	1:B:240:LYS:HE2	2.45	0.51
1:B:278:ASN:HB3	1:B:411:GLY:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLN:N	9:B:444:HOH:O	2.08	0.51
1:A:193:ARG:O	1:A:194:THR:C	2.53	0.51
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.92	0.51
1:B:349:TRP:CD1	1:B:377:ALA:HB2	2.46	0.51
2:D:1:NAG:H61	2:D:2:NAG:C8	2.37	0.51
1:B:100:ARG:HD3	1:B:104:GLY:O	2.10	0.51
1:B:290:MET:O	1:B:327:GLN:CG	2.58	0.51
1:B:217:THR:HG21	5:H:1:NAG:H82	1.92	0.50
1:A:40:PRO:HB2	1:A:293:PRO:HA	1.93	0.50
1:A:154:ILE:HD12	1:A:154:ILE:H	1.77	0.50
1:B:383:PHE:HD1	1:B:396:PHE:CE1	2.29	0.50
1:A:175:ASP:OD2	2:C:1:NAG:C7	2.59	0.50
1:A:363:ARG:HG2	1:A:363:ARG:NH1	2.12	0.50
2:D:2:NAG:O4	3:E:1:MAN:H4	2.12	0.50
1:A:93:ASP:OD1	1:A:94:CYS:N	2.45	0.50
1:A:236:TRP:CD1	1:A:240:LYS:HE2	2.47	0.50
1:A:317:ILE:O	1:A:318:ALA:C	2.54	0.49
1:A:337:PHE:CZ	1:A:365:TYR:HB2	2.47	0.49
1:A:366:THR:HG22	1:A:404:ARG:HA	1.94	0.49
1:B:234:ASP:O	1:B:274:GLY:HA3	2.12	0.49
1:B:363:ARG:HH11	1:B:363:ARG:CG	2.22	0.49
1:B:281:VAL:O	1:B:282:THR:C	2.53	0.49
1:A:420:THR:CA	1:A:421:MET:HB2	2.43	0.49
1:A:200:TYR:CE2	1:A:202:CYS:SG	3.06	0.49
1:B:193:ARG:O	1:B:194:THR:C	2.55	0.49
1:A:209:TRP:C	1:A:211:PHE:H	2.18	0.49
1:B:139:ASN:HD21	8:B:639:NAG:C7	2.25	0.49
1:B:236:TRP:CE3	1:B:279:GLN:HG2	2.47	0.49
1:A:37:ALA:HB1	1:A:262:TRP:HE1	1.78	0.49
1:A:228:ASN:HB3	1:A:245:TRP:HH2	1.73	0.48
1:B:71:GLU:CD	1:B:301:ARG:HD2	2.37	0.48
1:B:82:LYS:O	1:B:85:GLY:N	2.47	0.48
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.94	0.48
1:B:373:GLY:C	1:B:375:GLY:H	2.20	0.48
1:B:93:ASP:OD1	1:B:94:CYS:N	2.47	0.48
1:A:141:THR:HG23	1:A:145:PHE:O	2.13	0.48
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.95	0.48
1:B:234:ASP:OD1	1:B:274:GLY:CA	2.62	0.48
1:A:333:GLN:HE21	1:A:333:GLN:C	2.22	0.48
1:A:338:GLU:HB2	1:A:354:ILE:HB	1.96	0.48
1:B:313:ASP:CG	1:B:316:VAL:HG23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:HB2	1:A:173:TYR:CD2	2.50	0.47
1:A:226:TRP:NE1	1:A:263:ASN:OD1	2.42	0.47
1:B:355:ASN:HD21	1:B:363:ARG:HD3	1.79	0.47
1:A:76:MET:HA	1:A:81:TRP:CD1	2.50	0.47
1:A:258:GLY:O	1:A:259:PRO:C	2.58	0.47
1:A:340:TRP:CD1	1:A:340:TRP:N	2.81	0.47
1:A:377:ALA:HA	1:A:419:ASN:HB2	1.96	0.47
1:B:46:HIS:CD2	1:B:92:ASP:H	2.33	0.47
1:B:75:LEU:O	1:B:78:SER:N	2.48	0.47
1:A:367:ILE:HD11	1:A:372:LEU:HD11	1.97	0.47
1:B:40:PRO:HB2	1:B:293:PRO:HA	1.97	0.47
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.50	0.47
1:B:340:TRP:CD1	1:B:340:TRP:N	2.81	0.47
2:C:1:NAG:H62	2:C:2:NAG:C1	2.45	0.47
1:A:281:VAL:O	1:A:282:THR:C	2.57	0.46
1:B:201:SER:HB2	1:B:225:HIS:CE1	2.51	0.46
1:A:388:LEU:HB2	1:A:414:LEU:HB3	1.97	0.46
1:B:52:CYS:O	1:B:54:LEU:HD12	2.16	0.46
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.97	0.46
1:A:52:CYS:SG	1:A:52:CYS:O	2.73	0.46
1:A:138:GLY:O	1:A:149:PHE:HB3	2.15	0.46
1:A:208:MET:HE2	1:A:212:GLN:HE21	1.81	0.46
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.51	0.46
1:A:288:ALA:HA	1:A:320:ASN:HB2	1.97	0.46
1:B:332:ARG:NH2	6:B:3:SO4:O1	2.49	0.46
1:B:378:CYS:O	1:B:399:TRP:HD1	1.99	0.46
1:A:291:ALA:HB3	1:A:327:GLN:HG3	1.98	0.46
1:B:206:LEU:HD12	1:B:206:LEU:O	2.16	0.46
1:B:284:MET:HG2	1:B:310:LEU:HD22	1.98	0.46
1:A:324:LEU:CD1	1:A:326:LYS:HG3	2.46	0.46
1:A:378:CYS:H	1:A:419:ASN:HB2	1.81	0.45
1:A:182:ASP:O	1:A:186:HIS:HB2	2.16	0.45
1:A:209:TRP:C	1:A:211:PHE:N	2.74	0.45
1:A:331:LEU:N	1:A:339:VAL:O	2.50	0.45
1:B:166:LEU:HD23	1:B:167:LEU:C	2.42	0.45
1:B:239:ILE:O	1:B:240:LYS:C	2.56	0.45
1:A:333:GLN:HG2	1:A:334:GLY:N	2.32	0.45
1:B:153:ASP:HB2	1:B:154:ILE:HD12	1.99	0.45
1:B:383:PHE:HD1	1:B:396:PHE:CD1	2.35	0.45
1:B:390:VAL:HG22	9:B:443:HOH:O	2.17	0.45
1:A:225:HIS:HB3	1:A:262:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:O	1:A:240:LYS:C	2.59	0.45
1:B:71:GLU:OE1	1:B:301:ARG:HD2	2.17	0.45
1:B:355:ASN:ND2	1:B:363:ARG:HD3	2.32	0.45
1:A:378:CYS:SG	1:A:417:LEU:HD23	2.57	0.44
1:B:49:ARG:CG	1:B:50:PHE:CE2	3.00	0.44
1:A:278:ASN:HB3	1:A:411:GLY:CA	2.46	0.44
1:A:363:ARG:CG	1:A:363:ARG:NH1	2.78	0.44
1:B:291:ALA:HB3	1:B:327:GLN:HG3	1.98	0.44
1:A:205:PRO:O	1:A:206:LEU:C	2.61	0.44
1:B:259:PRO:HD3	1:B:325:GLY:HA3	2.00	0.44
1:A:82:LYS:O	1:A:85:GLY:N	2.47	0.44
1:A:419:ASN:OD1	1:A:419:ASN:C	2.60	0.44
1:B:51:MET:O	1:B:64:ILE:HD11	2.17	0.44
1:B:76:MET:HA	1:B:81:TRP:CD1	2.53	0.44
1:A:402:ARG:NH2	6:A:2:SO4:O1	2.48	0.44
1:B:166:LEU:HD23	1:B:167:LEU:N	2.32	0.44
1:B:393:LYS:NZ	9:B:435:HOH:O	2.50	0.44
1:B:216:TYR:HB3	1:B:256:VAL:HG21	2.00	0.44
9:B:438:HOH:O	4:G:4:MAN:O3	2.16	0.44
1:A:49:ARG:HG3	1:A:50:PHE:CD2	2.53	0.44
1:B:213:LYS:HA	1:B:214:PRO:HD3	1.79	0.44
1:A:48:GLU:CD	1:A:48:GLU:C	2.85	0.43
1:B:49:ARG:HG3	1:B:50:PHE:CD2	2.53	0.43
1:B:137:VAL:HG11	1:B:180:LEU:HD12	2.00	0.43
1:B:49:ARG:NH1	1:B:299:ASP:HB2	2.33	0.43
2:D:1:NAG:H61	2:D:2:NAG:C7	2.49	0.43
1:A:102:SER:HA	1:A:103:GLU:C	2.43	0.43
1:B:292:ALA:O	1:B:320:ASN:ND2	2.43	0.43
1:A:324:LEU:HB2	1:A:345:SER:HB3	2.01	0.43
1:B:220:ARG:NH1	1:B:256:VAL:O	2.50	0.43
1:B:417:LEU:N	1:B:417:LEU:HD12	2.33	0.43
1:A:383:PHE:HD1	1:A:396:PHE:CE1	2.37	0.42
1:A:207:TYR:O	1:A:210:PRO:CD	2.67	0.42
1:A:218:GLU:O	1:A:221:GLN:HB2	2.19	0.42
1:B:182:ASP:O	1:B:186:HIS:HB2	2.18	0.42
1:A:42:MET:HB2	1:A:85:GLY:O	2.18	0.42
1:A:234:ASP:O	1:A:274:GLY:HA3	2.18	0.42
1:A:324:LEU:HD11	1:A:326:LYS:HG3	2.01	0.42
1:A:378:CYS:O	1:A:399:TRP:HD1	2.01	0.42
1:B:142:CYS:CB	7:B:1:NOJ:H62	2.47	0.42
1:B:366:THR:HG22	1:B:404:ARG:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:NH1	1:A:256:VAL:O	2.53	0.42
1:B:50:PHE:CD2	1:B:50:PHE:N	2.87	0.42
1:B:363:ARG:HG2	1:B:363:ARG:NH1	2.26	0.42
1:A:305:PRO:O	1:A:306:GLN:C	2.62	0.42
1:B:42:MET:HB2	1:B:85:GLY:O	2.20	0.42
1:B:96:MET:HE3	1:B:96:MET:HB2	1.96	0.42
1:A:54:LEU:HD12	1:A:54:LEU:N	2.32	0.42
1:A:229:PHE:CD1	1:A:230:ALA:N	2.86	0.42
1:A:76:MET:HA	1:A:81:TRP:HB2	2.01	0.42
1:A:315:ASP:O	1:A:318:ALA:HB3	2.19	0.42
1:A:383:PHE:HD1	1:A:396:PHE:CD1	2.38	0.42
1:B:103:GLU:HB3	1:B:104:GLY:H	1.20	0.42
1:B:190:ALA:O	1:B:194:THR:HG23	2.20	0.42
1:A:239:ILE:HD12	1:A:283:GLN:HG3	2.02	0.41
1:A:333:GLN:HG2	1:A:334:GLY:H	1.85	0.41
1:A:50:PHE:CD2	1:A:50:PHE:N	2.88	0.41
1:A:314:LYS:O	1:A:315:ASP:C	2.63	0.41
1:B:364:SER:HA	1:B:405:SER:O	2.21	0.41
1:A:47:TRP:O	1:A:48:GLU:C	2.63	0.41
1:A:174:CYS:HA	2:C:1:NAG:O7	2.19	0.41
1:B:154:ILE:HD12	1:B:154:ILE:N	2.35	0.41
1:A:142:CYS:CB	7:A:430:NOJ:O6	2.66	0.41
1:A:217:THR:CG2	2:F:1:NAG:H5	2.51	0.41
1:A:237:LYS:N	6:A:1:SO4:O3	2.52	0.41
1:B:236:TRP:CD2	1:B:279:GLN:HG2	2.55	0.41
1:B:373:GLY:C	1:B:375:GLY:N	2.78	0.41
1:A:133:ILE:CG1	1:A:134:TYR:H	2.34	0.41
1:A:216:TYR:CB	1:A:256:VAL:HG21	2.51	0.41
1:B:286:LEU:HD21	1:B:354:ILE:HD11	2.03	0.41
1:B:243:LEU:HD22	1:B:286:LEU:HD22	2.02	0.41
1:B:45:LEU:HD22	1:B:92:ASP:HB2	2.03	0.40
1:B:149:PHE:C	1:B:151:TYR:H	2.29	0.40
1:B:76:MET:HA	1:B:81:TRP:HD1	1.86	0.40
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.80	0.40
1:B:101:ASP:OD2	1:B:105:ARG:HB2	2.22	0.40
1:A:236:TRP:CD2	1:A:279:GLN:HG2	2.57	0.40
1:B:49:ARG:HG3	1:B:50:PHE:CE2	2.57	0.40
1:B:229:PHE:CG	1:B:230:ALA:N	2.88	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	388/398 (98%)	332 (86%)	43 (11%)	13 (3%)	3	7
1	B	389/398 (98%)	333 (86%)	45 (12%)	11 (3%)	4	9
All	All	777/796 (98%)	665 (86%)	88 (11%)	24 (3%)	3	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	230	ALA
1	B	51	MET
1	B	359	ILE
1	B	420	THR
1	A	395	GLY
1	B	306	GLN
1	B	395	GLY
1	A	98	PRO
1	A	259	PRO
1	A	398	GLU
1	B	98	PRO
1	B	259	PRO
1	A	146	PRO
1	A	272	ASN
1	A	306	GLN
1	B	318	ALA
1	A	51	MET
1	A	378	CYS
1	A	420	THR
1	B	33	ASP
1	B	74	GLU
1	A	209	TRP
1	B	64	ILE

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	331/339 (98%)	289 (87%)	42 (13%)	4	11
1	B	332/339 (98%)	286 (86%)	46 (14%)	3	9
All	All	663/678 (98%)	575 (87%)	88 (13%)	4	10

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TRP
1	A	45	LEU
1	A	46	HIS
1	A	54	LEU
1	A	70	MET
1	A	74	GLU
1	A	83	ASP
1	A	96	MET
1	A	99	GLN
1	A	111	GLN
1	A	118	ARG
1	A	119	GLN
1	A	137	VAL
1	A	175	ASP
1	A	217	THR
1	A	235	SER
1	A	249	ASN
1	A	300	LEU
1	A	301	ARG
1	A	306	GLN
1	A	310	LEU
1	A	314	LYS
1	A	324	LEU
1	A	332	ARG
1	A	333	GLN
1	A	344	LEU
1	A	357	GLN

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Mol	Chain	Res	Type
1	A	358	GLU
1	A	363	ARG
1	A	369	VAL
1	A	372	LEU
1	A	385	THR
1	A	388	LEU
1	A	391	LYS
1	A	398	GLU
1	A	399	TRP
1	A	400	THR
1	A	401	SER
1	A	403	LEU
1	A	405	SER
1	A	419	ASN
1	A	421	MET
1	B	44	TRP
1	B	45	LEU
1	B	46	HIS
1	B	54	LEU
1	B	74	GLU
1	B	83	ASP
1	B	96	MET
1	B	99	GLN
1	B	111	GLN
1	B	118	ARG
1	B	119	GLN
1	B	137	VAL
1	B	165	ASP
1	B	172	CYS
1	B	174	CYS
1	B	175	ASP
1	B	213	LYS
1	B	217	THR
1	B	235	SER
1	B	247	SER
1	B	249	ASN
1	B	259	PRO
1	B	300	LEU
1	B	301	ARG
1	B	306	GLN
1	B	310	LEU
1	B	314	LYS

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Mol	Chain	Res	Type
1	B	324	LEU
1	B	332	ARG
1	B	333	GLN
1	B	344	LEU
1	B	357	GLN
1	B	358	GLU
1	B	363	ARG
1	B	372	LEU
1	B	385	THR
1	B	388	LEU
1	B	398	GLU
1	B	399	TRP
1	B	400	THR
1	B	401	SER
1	B	403	LEU
1	B	405	SER
1	B	419	ASN
1	B	421	MET
1	B	422	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	107	GLN
1	A	111	GLN
1	A	115	HIS
1	A	122	ASN
1	A	125	HIS
1	A	179	ASN
1	A	212	GLN
1	A	221	GLN
1	A	333	GLN
1	A	336	ASN
1	A	357	GLN
1	A	416	GLN
1	B	99	GLN
1	B	107	GLN
1	B	111	GLN
1	B	115	HIS
1	B	122	ASN
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	186	HIS
1	B	212	GLN
1	B	333	GLN
1	B	336	ASN
1	B	416	GLN
1	B	419	ASN
1	B	422	GLN

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 ⓘ

15 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	1,2	14,14,15	0.66	0	17,19,21	2.62	4 (23%)
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	2.10	4 (23%)
2	NAG	D	1	1,2	14,14,15	0.75	0	17,19,21	2.49	6 (35%)
2	NAG	D	2	2	14,14,15	0.98	0	17,19,21	2.50	3 (17%)
3	MAN	E	1	3	11,11,12	0.77	0	15,15,17	2.15	5 (33%)
3	MAN	E	2	3	11,11,12	0.93	1 (9%)	15,15,17	1.69	4 (26%)
2	NAG	F	1	1,2	14,14,15	0.83	0	17,19,21	1.61	4 (23%)
2	NAG	F	2	2	14,14,15	0.66	0	17,19,21	1.20	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.67	0	17,19,21	1.85	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2	4	14,14,15	0.70	0	17,19,21	1.36	2 (11%)
4	MAN	G	3	4	11,11,12	0.77	0	15,15,17	1.57	3 (20%)
4	MAN	G	4	4	11,11,12	1.08	1 (9%)	15,15,17	2.02	5 (33%)
5	NAG	H	1	5	14,14,15	0.60	0	17,19,21	2.39	8 (47%)
5	NAG	H	2	5	14,14,15	0.73	0	17,19,21	1.73	4 (23%)
5	MAN	H	3	5	11,11,12	0.83	0	15,15,17	2.42	3 (20%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
3	MAN	E	1	3	-	0/2/19/22	0/1/1/1
3	MAN	E	2	3	1/1/4/5	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	MAN	G	3	4	1/1/4/5	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	6/6/23/26	0/1/1/1
5	MAN	H	3	5	1/1/4/5	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	4	MAN	C2-C3	2.64	1.56	1.52
3	E	2	MAN	C2-C3	2.11	1.55	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	8.46	123.52	112.19
5	H	3	MAN	C1-O5-C5	7.73	122.55	112.19
2	D	1	NAG	C1-O5-C5	7.63	122.41	112.19
2	C	1	NAG	C1-O5-C5	6.62	121.05	112.19
5	H	1	NAG	C1-O5-C5	5.52	119.58	112.19
2	C	2	NAG	C1-O5-C5	5.37	119.39	112.19
2	C	1	NAG	C1-C2-N2	4.83	118.05	110.43
2	C	1	NAG	O5-C1-C2	-4.65	104.10	111.29
4	G	3	MAN	C3-C4-C5	4.40	118.21	110.23
4	G	1	NAG	C1-O5-C5	4.33	117.99	112.19
4	G	4	MAN	O5-C5-C6	4.29	116.01	107.66
5	H	1	NAG	C4-C3-C2	4.12	117.05	111.02
5	H	2	NAG	C1-O5-C5	3.92	117.44	112.19
3	E	1	MAN	O3-C3-C4	3.90	119.57	110.38
2	C	2	NAG	C2-N2-C7	3.87	128.09	122.90
2	D	1	NAG	C3-C4-C5	-3.87	103.22	110.23
2	C	2	NAG	O5-C1-C2	3.83	117.22	111.29
2	F	2	NAG	C1-O5-C5	3.62	117.04	112.19
2	F	1	NAG	C3-C4-C5	-3.53	103.83	110.23
3	E	2	MAN	C1-O5-C5	3.42	116.77	112.19
4	G	2	NAG	C1-O5-C5	3.41	116.76	112.19
5	H	2	NAG	O4-C4-C5	3.39	117.67	109.32
3	E	1	MAN	C3-C4-C5	-3.33	104.19	110.23
5	H	2	NAG	O4-C4-C3	-3.25	102.71	110.38
5	H	1	NAG	C3-C4-C5	3.25	116.13	110.23
3	E	1	MAN	C1-C2-C3	3.23	114.35	109.64
4	G	4	MAN	C2-C3-C4	3.20	116.49	110.86
2	D	2	NAG	O7-C7-C8	-3.05	116.63	122.05
4	G	4	MAN	C1-C2-C3	3.04	114.08	109.64
2	F	1	NAG	C4-C3-C2	3.00	115.41	111.02
4	G	1	NAG	O5-C1-C2	2.96	115.87	111.29
2	C	1	NAG	O3-C3-C4	2.94	117.31	110.38
4	G	1	NAG	O4-C4-C5	-2.91	102.16	109.32
4	G	4	MAN	O2-C2-C3	2.87	116.10	110.15
3	E	1	MAN	C2-C3-C4	-2.87	105.82	110.86
2	F	1	NAG	C2-N2-C7	2.82	126.69	122.90
3	E	1	MAN	O4-C4-C3	2.76	116.88	110.38
5	H	1	NAG	O5-C5-C6	2.75	113.02	107.66
4	G	2	NAG	C3-C4-C5	2.70	115.13	110.23
2	D	1	NAG	O5-C5-C6	2.62	112.77	107.66
3	E	2	MAN	C1-C2-C3	2.61	113.44	109.64
5	H	1	NAG	O5-C5-C4	2.60	117.15	110.83
2	D	2	NAG	O3-C3-C4	-2.56	104.34	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	MAN	O5-C5-C4	2.51	116.93	110.83
2	D	1	NAG	C6-C5-C4	-2.44	107.03	113.02
5	H	1	NAG	C1-C2-N2	2.39	114.19	110.43
5	H	1	NAG	O7-C7-C8	-2.32	117.92	122.05
5	H	1	NAG	C8-C7-N2	2.30	119.93	116.12
4	G	4	MAN	C1-O5-C5	-2.29	109.12	112.19
5	H	2	NAG	C8-C7-N2	2.25	119.85	116.12
4	G	3	MAN	C1-C2-C3	-2.23	106.39	109.64
3	E	2	MAN	C3-C4-C5	-2.20	106.25	110.23
2	D	1	NAG	O4-C4-C5	-2.14	104.06	109.32
4	G	3	MAN	O5-C5-C4	2.12	115.98	110.83
2	D	1	NAG	C2-N2-C7	2.10	125.71	122.90
5	H	3	MAN	C1-C2-C3	-2.09	106.59	109.64
2	F	1	NAG	O5-C5-C4	-2.09	105.74	110.83
3	E	2	MAN	O2-C2-C3	2.08	114.45	110.15
2	C	2	NAG	C4-C3-C2	2.01	113.97	111.02

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	MAN	C1
4	G	1	NAG	C1
4	G	3	MAN	C1
5	H	3	MAN	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	2	MAN	O5-C5-C6-O6
5	H	3	MAN	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
3	E	2	MAN	C4-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	3	MAN	C4-C5-C6-O6
5	H	3	MAN	O5-C5-C6-O6
5	H	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
5	H	2	NAG	C3-C2-N2-C7

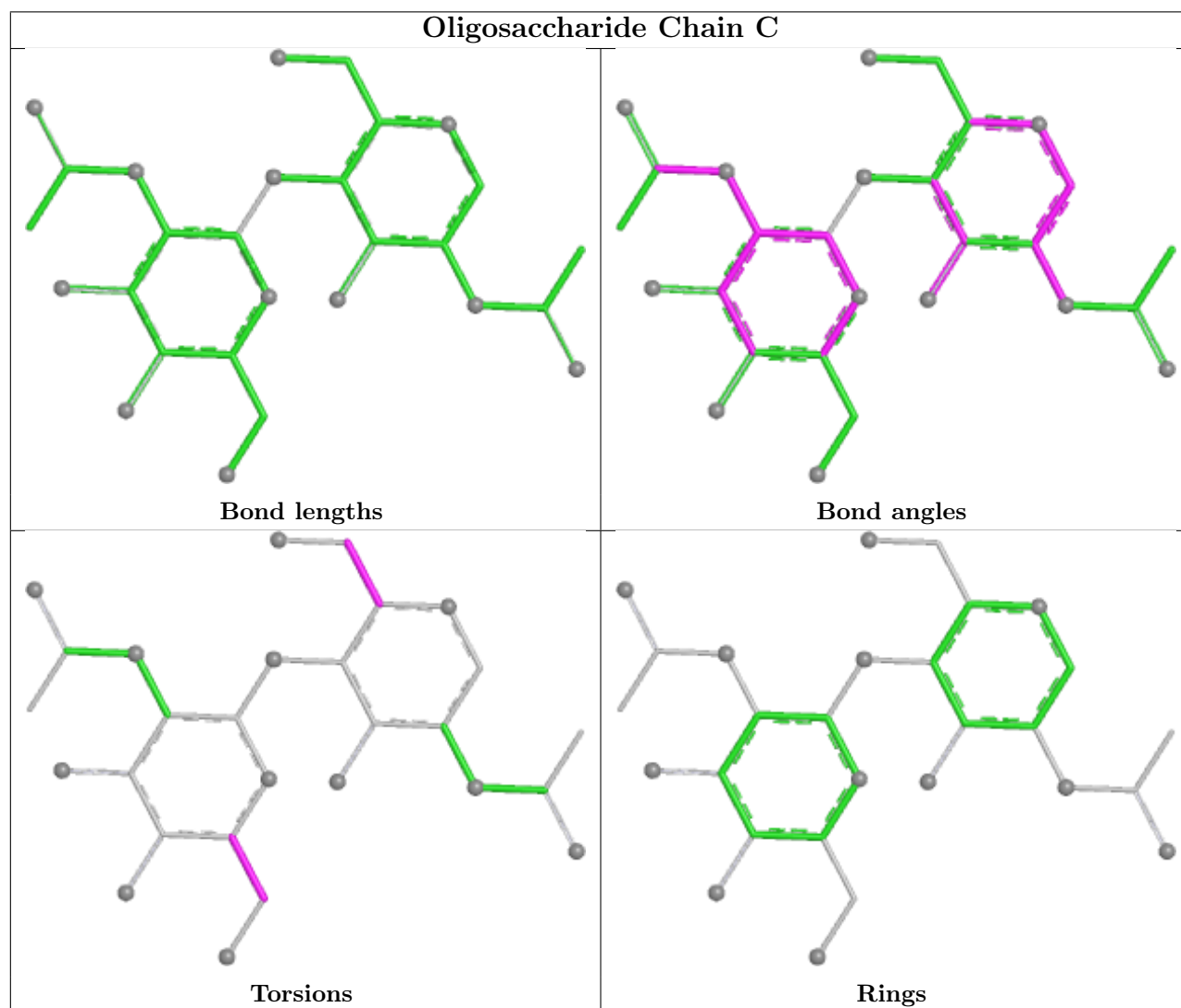
All (1) ring outliers are listed below:

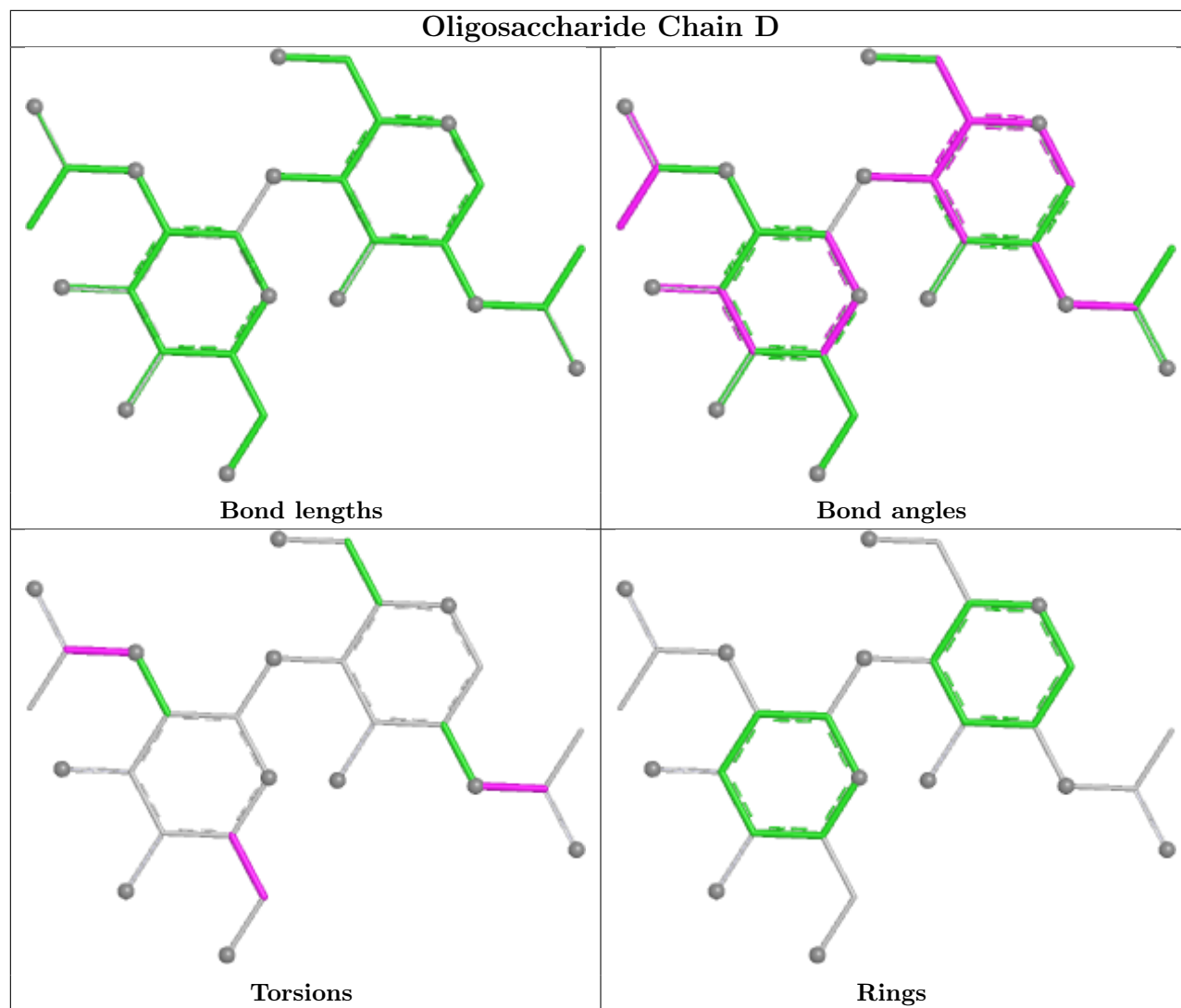
Mol	Chain	Res	Type	Atoms
3	E	2	MAN	C1-C2-C3-C4-C5-O5

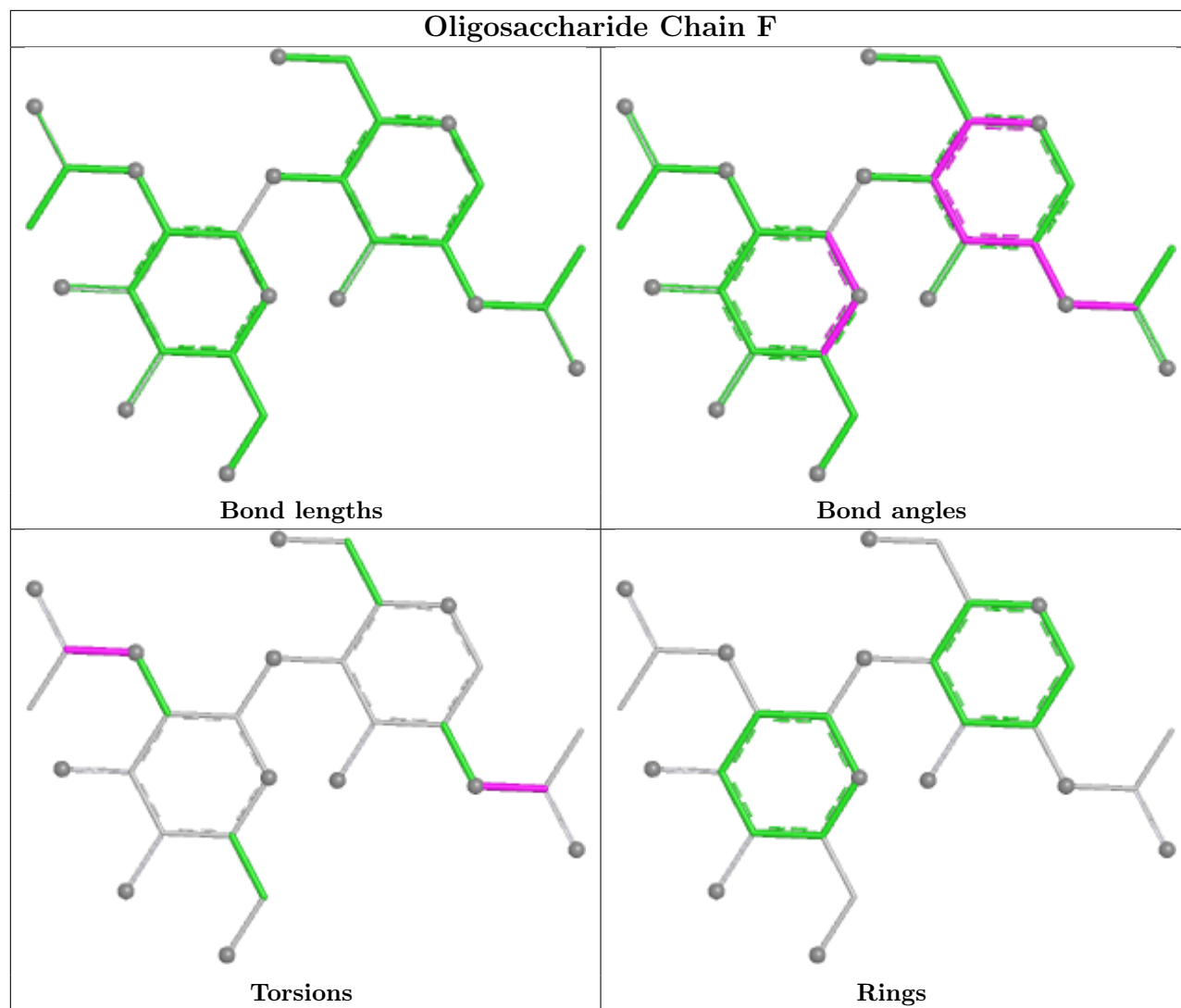
12 monomers are involved in 19 short contacts:

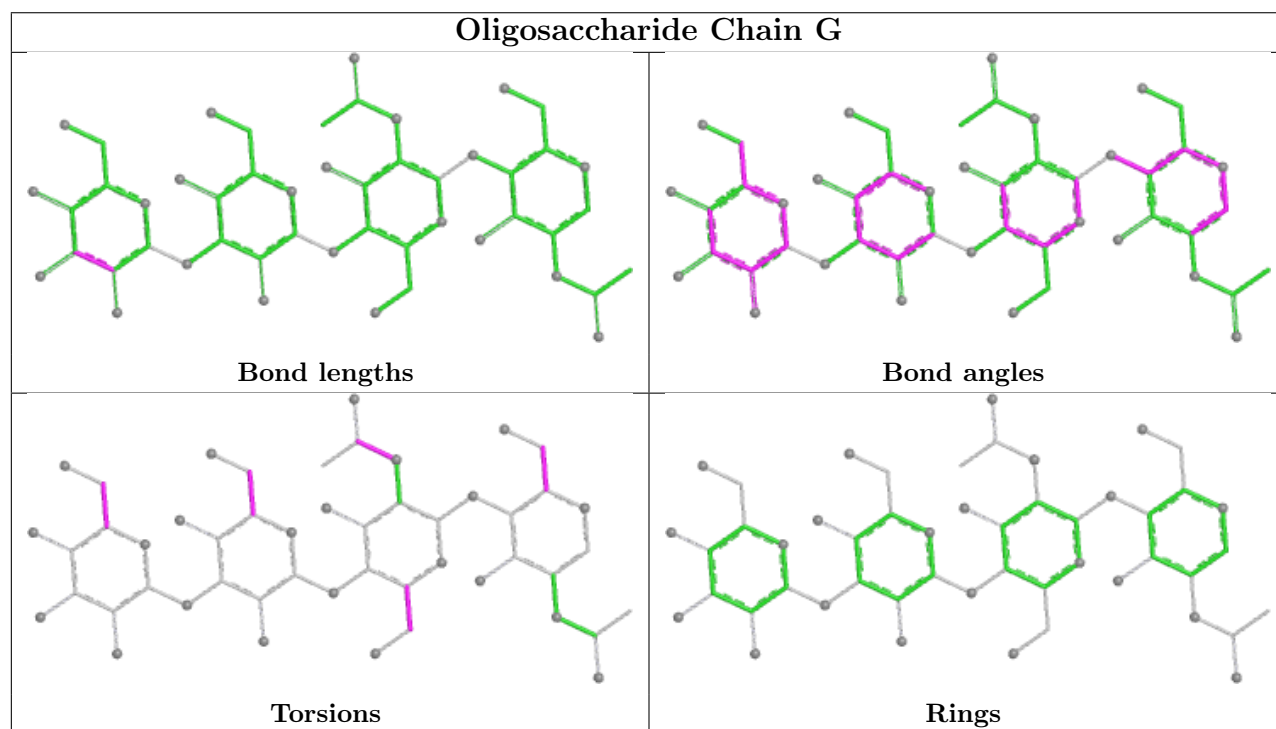
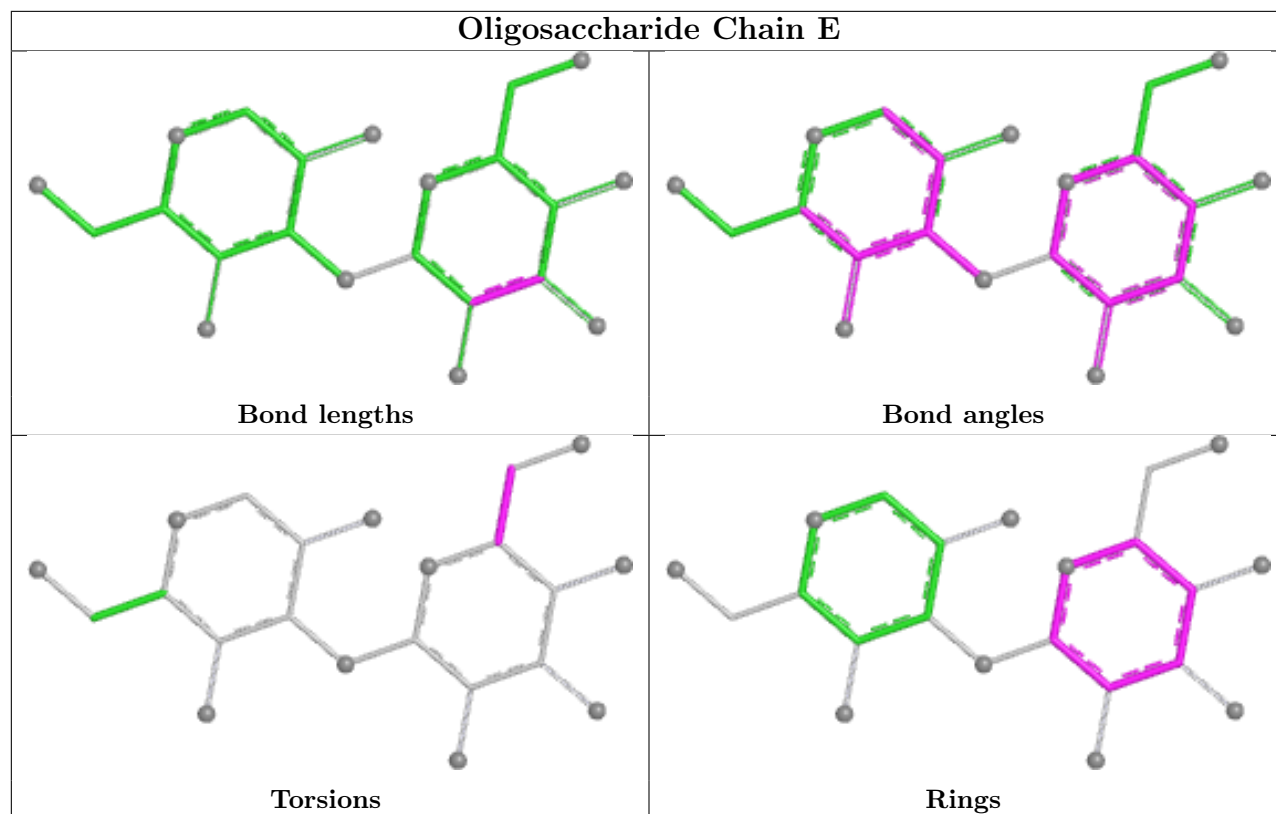
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	5	0
2	D	1	NAG	4	0
4	G	1	NAG	1	0
4	G	2	NAG	1	0
4	G	3	MAN	1	0
2	F	1	NAG	1	0
3	E	1	MAN	1	0
4	G	4	MAN	1	0
5	H	2	NAG	1	0
2	C	1	NAG	4	0
5	H	1	NAG	5	0
2	C	2	NAG	1	0

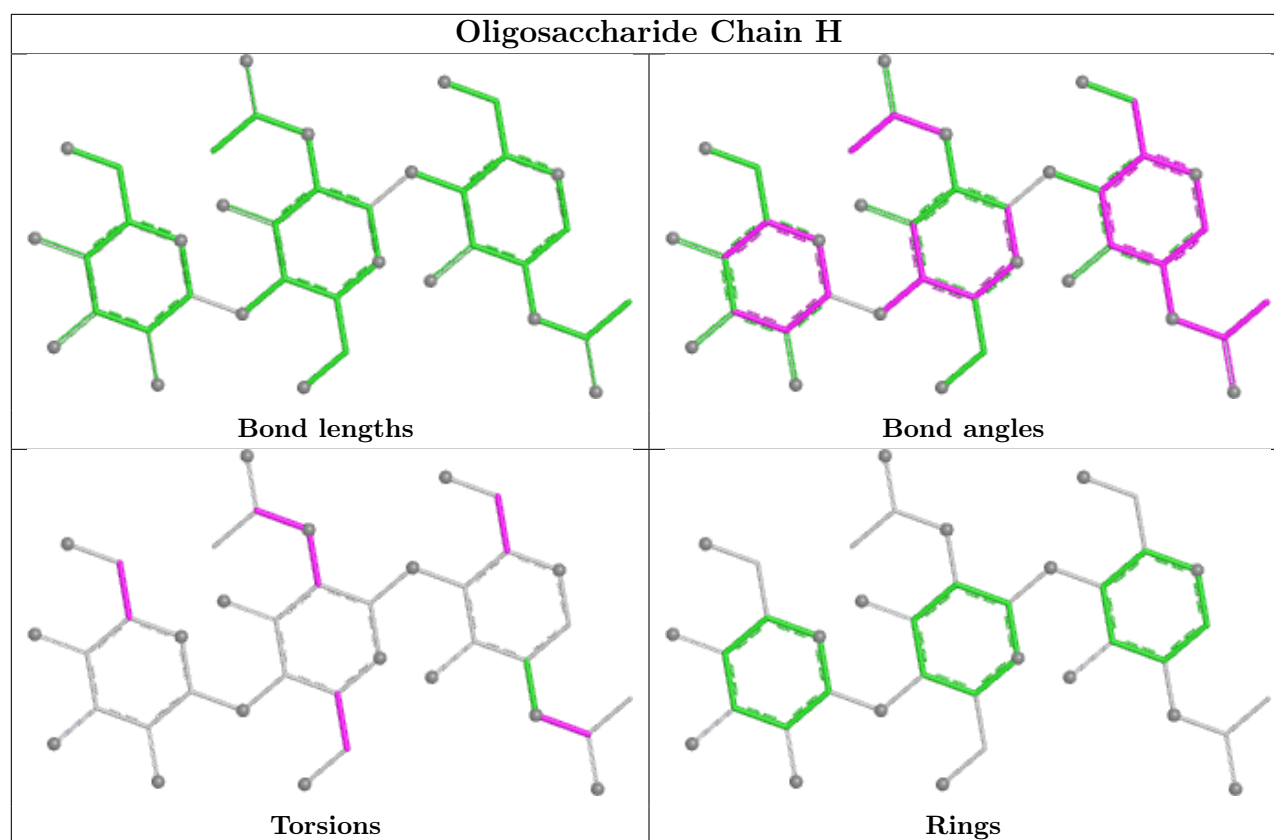
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
6	SO4	B	4	-	4,4,4	0.24	0	6,6,6	0.32	0
7	NOJ	B	1	-	11,11,11	1.76	1 (9%)	13,15,15	2.96	4 (30%)
6	SO4	A	1	-	4,4,4	0.47	0	6,6,6	1.29	0
6	SO4	B	3	-	4,4,4	0.23	0	6,6,6	0.36	0
8	NAG	B	639	-	14,14,15	0.70	0	17,19,21	2.39	7 (41%)
7	NOJ	A	430	-	11,11,11	1.00	1 (9%)	13,15,15	2.72	6 (46%)
6	SO4	A	5	-	4,4,4	0.48	0	6,6,6	0.19	0
6	SO4	A	2	-	4,4,4	0.35	0	6,6,6	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NOJ	B	1	-	-	0/2/19/19	0/1/1/1
8	NAG	B	639	-	-	1/6/23/26	0/1/1/1
7	NOJ	A	430	-	-	0/2/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1	NOJ	C1-C2	4.75	1.56	1.52
7	A	430	NOJ	C1-C2	2.47	1.54	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1	NOJ	C3-C4-C5	-8.94	97.92	111.02
7	A	430	NOJ	C2-C3-C4	-6.12	100.10	110.86
8	B	639	NAG	C1-O5-C5	5.52	119.59	112.19
7	A	430	NOJ	C3-C4-C5	-4.82	103.96	111.02
8	B	639	NAG	O5-C5-C4	3.54	119.44	110.83
7	B	1	NOJ	O3-C3-C2	3.44	117.08	110.05
8	B	639	NAG	C3-C4-C5	3.37	116.35	110.23
8	B	639	NAG	C2-N2-C7	3.12	127.08	122.90
7	A	430	NOJ	O3-C3-C2	3.00	116.17	110.05
8	B	639	NAG	O7-C7-C8	-2.85	116.97	122.05
7	A	430	NOJ	C1-C2-C3	-2.46	107.25	110.25
8	B	639	NAG	O3-C3-C4	-2.40	104.72	110.38
7	A	430	NOJ	O6-C6-C5	-2.35	105.41	111.10
7	B	1	NOJ	C4-C5-N5	-2.26	104.56	109.12
7	A	430	NOJ	O2-C2-C3	2.15	114.60	110.15
8	B	639	NAG	C4-C3-C2	2.05	114.03	111.02
7	B	1	NOJ	O4-C4-C5	2.03	113.63	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	639	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	4	SO4	1	0
7	B	1	NOJ	3	0
6	A	1	SO4	1	0
6	B	3	SO4	1	0
8	B	639	NAG	2	0
7	A	430	NOJ	2	0
6	A	2	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/398 (97%)	0.15	4 (1%) 79 78	54, 57, 59, 72	0
1	B	391/398 (98%)	0.29	2 (0%) 87 86	54, 57, 59, 71	0
All	All	781/796 (98%)	0.22	6 (0%) 82 81	54, 57, 59, 72	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	MET	2.7
1	B	211	PHE	2.5
1	B	359	ILE	2.3
1	A	102	SER	2.3
1	A	394	LEU	2.2
1	A	119	GLN	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.

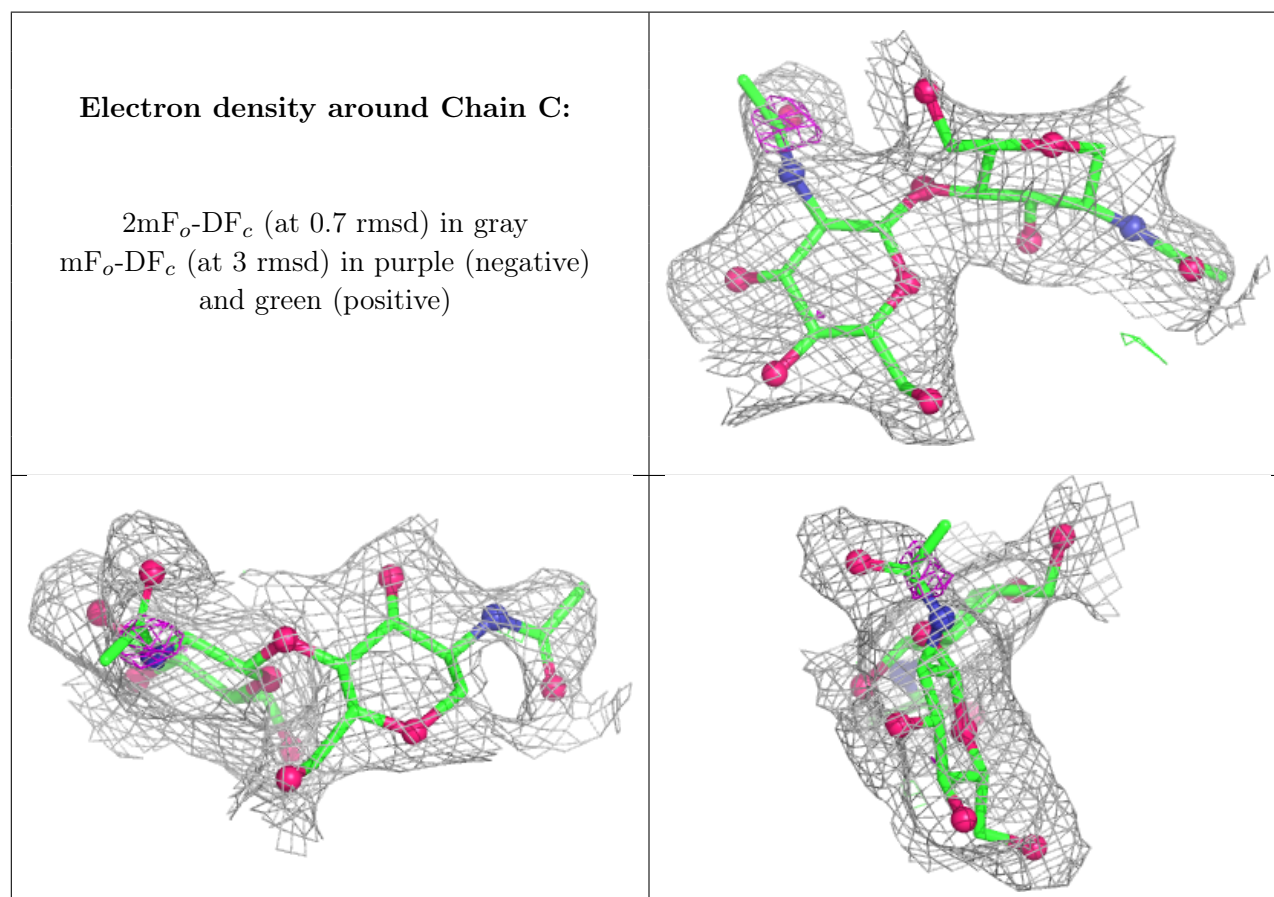
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	H	3	11/12	0.32	0.15	112,113,113,114	0
3	MAN	E	2	11/12	0.55	0.13	102,103,106,106	0
5	NAG	H	2	14/15	0.58	0.14	106,108,109,111	0

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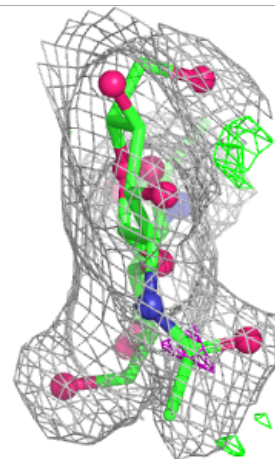
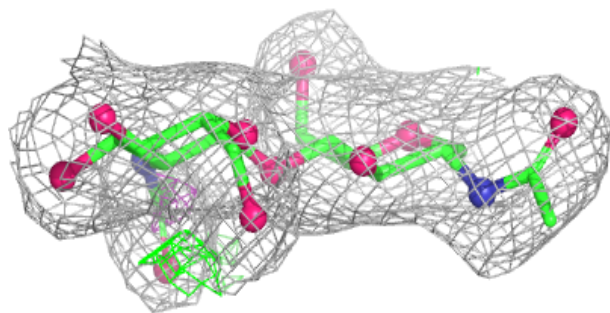
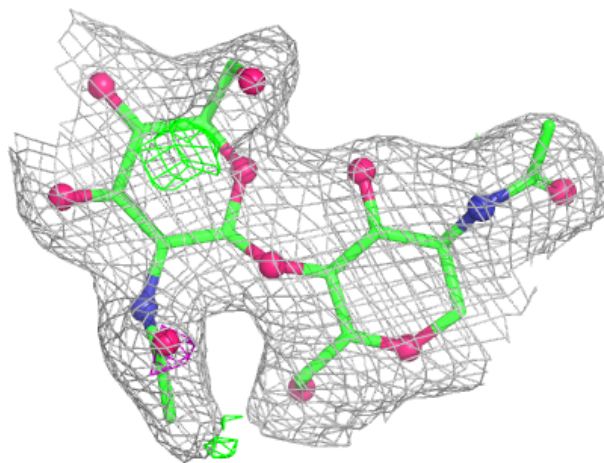
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	H	1	14/15	0.59	0.15	101,104,105,105	0
2	NAG	F	1	14/15	0.60	0.12	71,75,77,81	0
2	NAG	F	2	14/15	0.70	0.11	79,84,87,88	0
3	MAN	E	1	11/12	0.74	0.11	103,103,104,104	0
2	NAG	C	2	14/15	0.78	0.11	65,72,75,77	0
4	MAN	G	3	11/12	0.79	0.10	74,78,81,81	0
4	NAG	G	2	14/15	0.79	0.12	71,73,75,76	0
4	MAN	G	4	11/12	0.80	0.10	66,69,71,72	0
2	NAG	D	2	14/15	0.81	0.11	59,64,66,66	0
4	NAG	G	1	14/15	0.84	0.10	62,64,68,68	0
2	NAG	C	1	14/15	0.85	0.10	66,71,72,73	0
2	NAG	D	1	14/15	0.92	0.07	42,49,51,54	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.



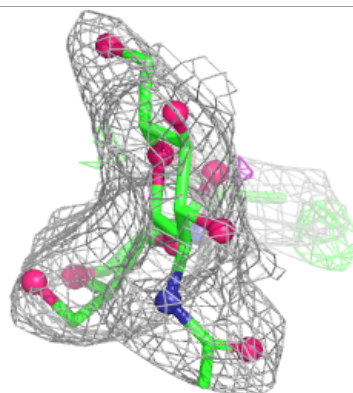
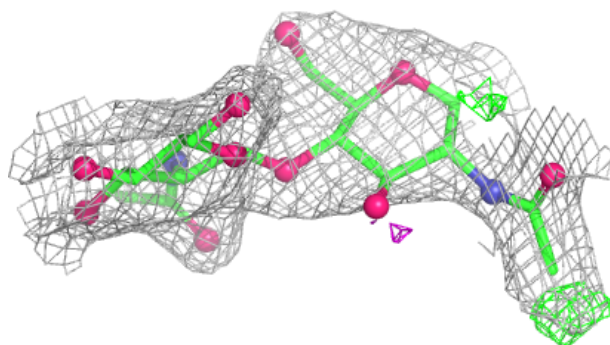
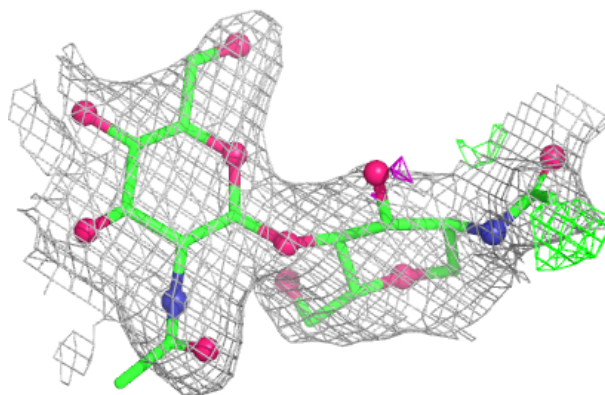
Electron density around Chain D:

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

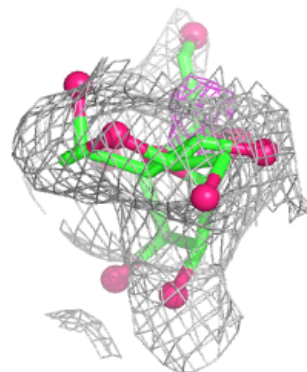
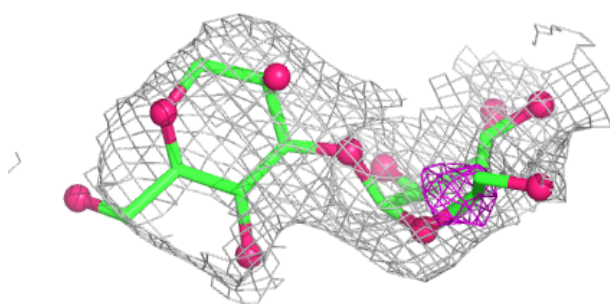
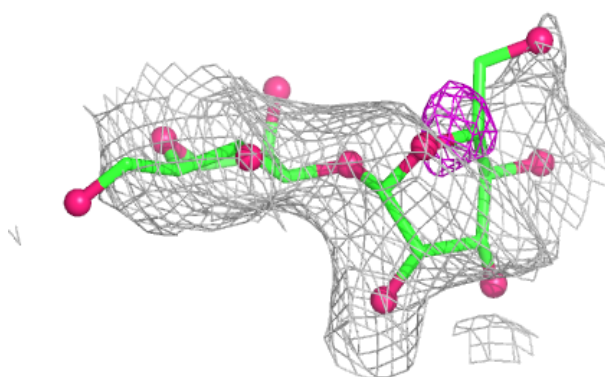


Electron density around Chain F:

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

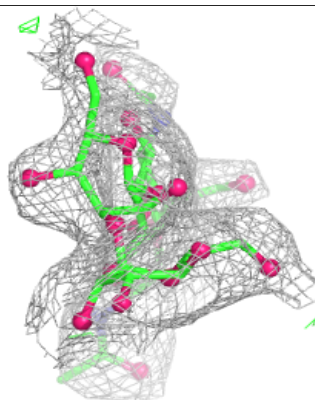
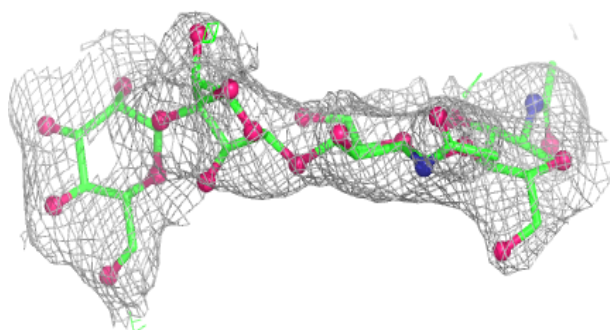
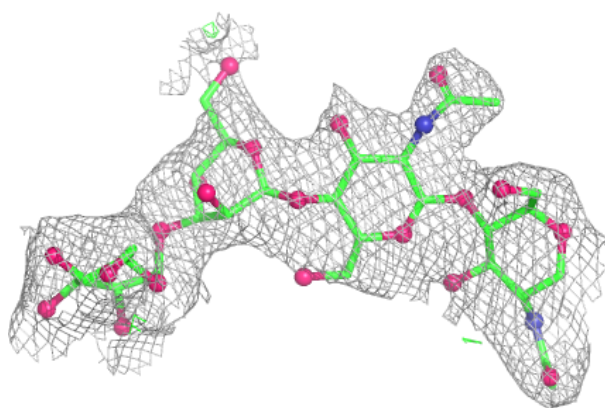
**Electron density around Chain E:**

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

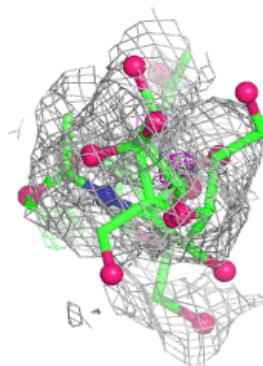
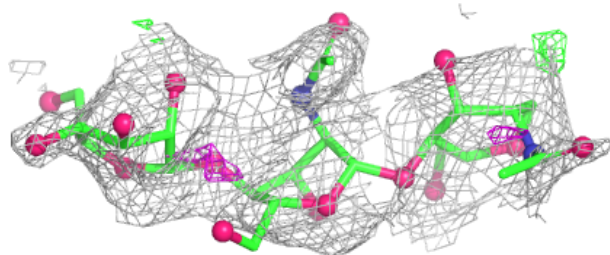
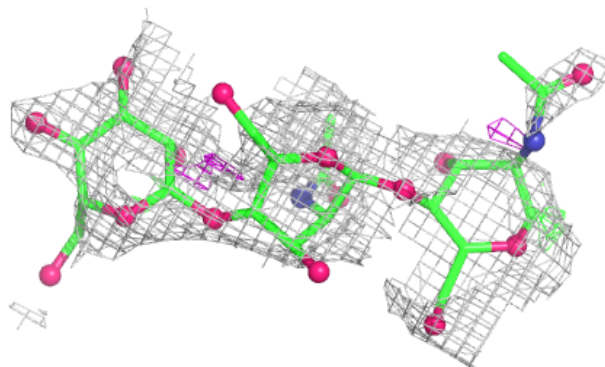


Electron density around Chain G:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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
6	SO4	A	5	5/5	0.64	0.18	115,116,116,116	0
8	NAG	B	639	14/15	0.64	0.15	107,109,110,110	0
7	NOJ	B	1	11/11	0.87	0.15	46,52,56,56	0
6	SO4	B	4	5/5	0.88	0.14	81,82,83,83	0
6	SO4	A	2	5/5	0.90	0.13	68,68,70,70	0
6	SO4	B	3	5/5	0.91	0.13	85,85,86,87	0
6	SO4	A	1	5/5	0.91	0.14	58,58,59,60	0
7	NOJ	A	430	11/11	0.93	0.08	55,57,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.