



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:52 PM UTC

PDB ID : 3BT6 / pdb_00003bt6
Title : Crystal Structure of Influenza B Virus Hemagglutinin
Authors : Wang, Q.; Cheng, F.; Lu, M.; Tian, X.; Ma, J.
Deposited on : 2007-12-27
Resolution : 2.80 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

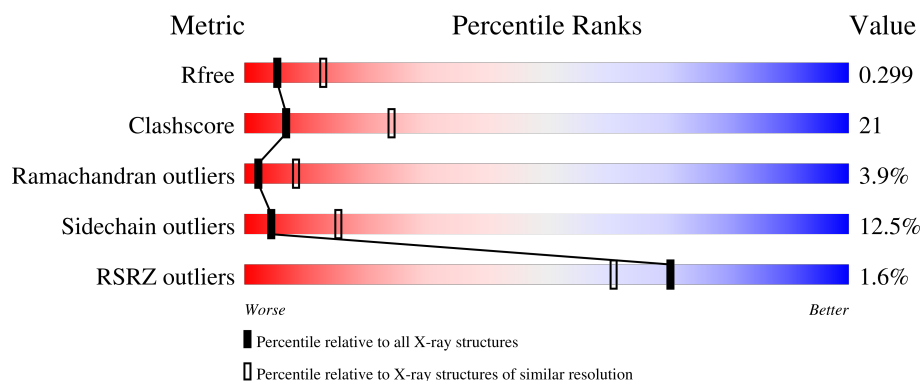
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	342	2% 52% 37% 10%
2	B	169	% 63% 31% 5%
3	C	2	50% 50%
3	E	2	100%
4	D	2	100%

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Mol	Chain	Length	Quality of chain
4	F	2	 100%

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
5	NAG	A	345	X	-	-	-
6	SO4	B	171	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4024 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 Influenza B hemagglutinin (HA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2583	1626	457	484	16			

- Molecule 2 is a protein called Influenza B hemagglutinin (HA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			

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



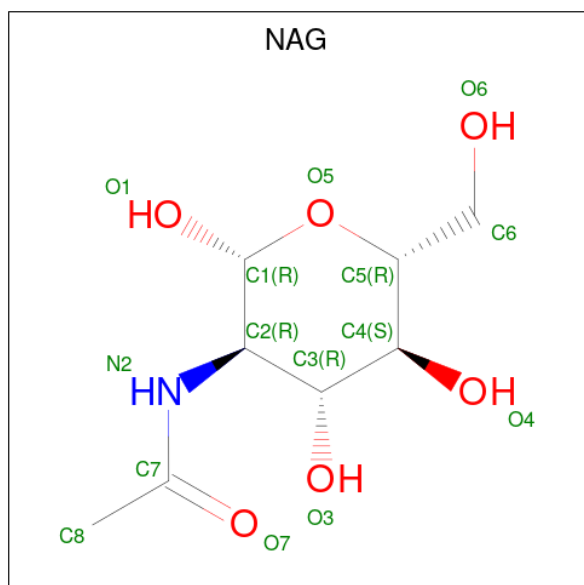
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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



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

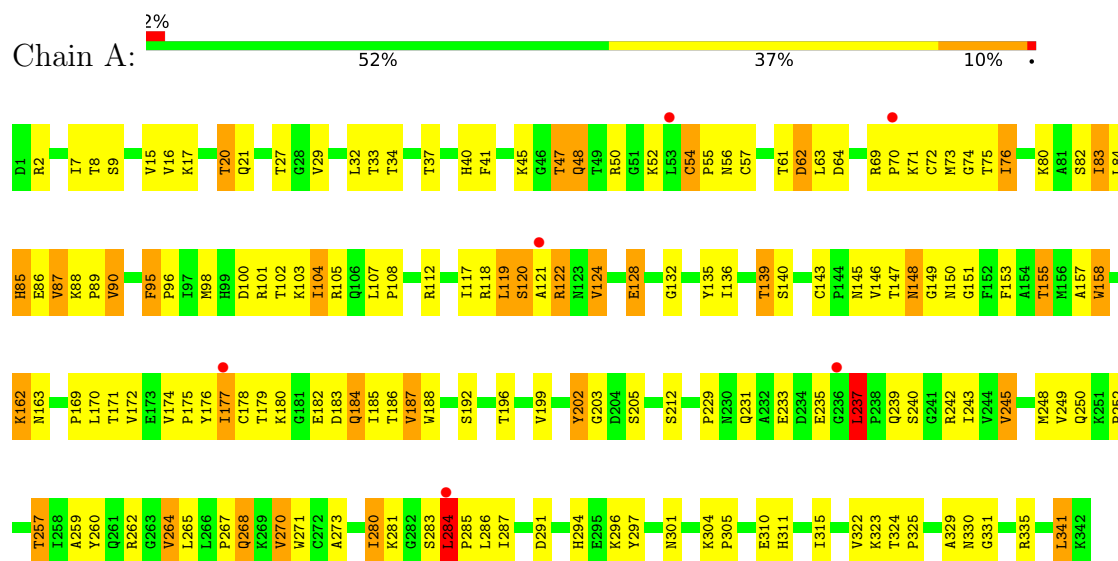
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		

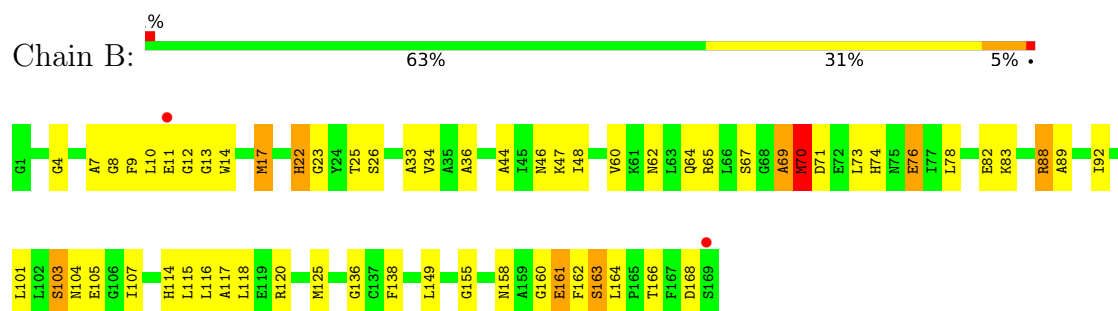
3 Residue-property plots [i](#)

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: Influenza B hemagglutinin (HA)



- Molecule 2: Influenza B hemagglutinin (HA)



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



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

Chain E:  100%

HA01
HA02

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

Chain D:  100%

HA01
HA02

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

Chain F:  100%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.30Å 98.30Å 135.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.6 (50.00-2.80) 83.6 (50.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.280 , 0.309 0.268 , 0.299	Depositor DCC
R_{free} test set	1758 reflections (7.35%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4024	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: SO4, NDG, 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	0.57	1/2642 (0.0%)	1.02	14/3592 (0.4%)
2	B	0.54	0/1300	0.95	3/1752 (0.2%)
All	All	0.56	1/3942 (0.0%)	1.00	17/5344 (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	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CA-C	5.13	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	LEU	CA-C-N	-7.67	111.56	121.91
1	A	237	LEU	C-N-CA	-7.67	111.56	121.91
2	B	161	GLU	N-CA-C	-7.32	103.61	112.54
1	A	69	ARG	CA-C-N	7.17	128.81	119.84
1	A	69	ARG	C-N-CA	7.17	128.81	119.84
1	A	237	LEU	N-CA-C	6.99	125.25	109.81
1	A	162	LYS	N-CA-C	-6.24	102.13	110.55
1	A	284	LEU	CA-C-N	5.93	127.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	LEU	C-N-CA	5.93	127.25	119.84
1	A	124	VAL	N-CA-C	5.79	115.98	110.42
1	A	76	ILE	N-CA-C	5.70	113.52	107.76
2	B	62	ASN	N-CA-C	5.66	117.90	111.11
1	A	104	ILE	N-CA-C	5.50	116.13	110.36
1	A	284	LEU	N-CA-C	5.48	120.91	108.74
2	B	136	GLY	N-CA-C	-5.11	107.76	115.32
1	A	95	PHE	CA-C-N	5.08	126.19	119.84
1	A	95	PHE	C-N-CA	5.08	126.19	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	LEU	Peptide
2	B	70	MET	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	2583	0	2602	135	0
2	B	1281	0	1251	43	0
3	C	28	0	25	1	0
3	E	28	0	25	0	0
4	D	28	0	24	0	0
4	F	28	0	24	0	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
6	B	5	0	0	0	10
7	A	1	0	0	0	0
All	All	4024	0	3990	170	10

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 (170) 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:139:THR:HB	1:A:150:ASN:HB3	1.16	1.12
1:A:9:SER:HB2	2:B:13:GLY:HA3	1.40	1.02
1:A:268:GLN:HE21	1:A:268:GLN:HA	1.19	1.00
1:A:61:THR:HG21	1:A:90:VAL:O	1.65	0.94
1:A:139:THR:HB	1:A:150:ASN:CB	2.01	0.90
1:A:260:TYR:HD1	1:A:264:VAL:HG21	1.38	0.88
1:A:291:ASP:HB2	1:A:301:ASN:HA	1.57	0.87
1:A:155:THR:HG23	1:A:187:VAL:CG2	2.05	0.86
2:B:26:SER:HB2	2:B:149:LEU:HD13	1.57	0.85
2:B:160:GLY:HA2	2:B:164:LEU:H	1.39	0.84
2:B:26:SER:HB3	2:B:33:ALA:HB3	1.58	0.84
1:A:119:LEU:O	1:A:120:SER:HB2	1.78	0.83
1:A:83:ILE:HG21	1:A:284:LEU:HG	1.63	0.81
1:A:41:PHE:HB2	1:A:284:LEU:CD2	2.13	0.79
1:A:268:GLN:HA	1:A:268:GLN:NE2	1.95	0.77
1:A:260:TYR:CD1	1:A:264:VAL:HG21	2.20	0.77
1:A:280:ILE:HD12	1:A:315:ILE:HG12	1.66	0.76
2:B:69:ALA:O	2:B:74:HIS:ND1	2.19	0.75
1:A:124:VAL:HG12	1:A:177:ILE:HD13	1.69	0.74
2:B:125:MET:HE1	2:B:155:GLY:HA2	1.70	0.73
1:A:243:ILE:CG2	1:A:245:VAL:HG23	2.19	0.72
1:A:284:LEU:HD13	1:A:286:LEU:HG	1.74	0.69
1:A:158:TRP:HH2	1:A:202:TYR:OH	1.76	0.69
1:A:155:THR:HG23	1:A:187:VAL:HG21	1.73	0.69
1:A:7:ILE:HD11	1:A:335:ARG:HG3	1.73	0.69
1:A:98:MET:HE3	1:A:229:PRO:HD2	1.76	0.68
1:A:139:THR:CB	1:A:150:ASN:HB3	2.09	0.67
1:A:330:ASN:HA	2:B:48:ILE:HD13	1.77	0.66
1:A:52:LYS:C	1:A:54:CYS:H	2.04	0.65
1:A:291:ASP:OD2	1:A:301:ASN:HB2	1.95	0.65
1:A:260:TYR:HD1	1:A:264:VAL:CG2	2.08	0.64
1:A:61:THR:HB	1:A:64:ASP:H	1.62	0.63
1:A:9:SER:HB2	2:B:13:GLY:CA	2.23	0.63
1:A:41:PHE:CB	1:A:284:LEU:HD21	2.28	0.63
1:A:85:HIS:CD2	1:A:85:HIS:H	2.15	0.63
1:A:41:PHE:HB2	1:A:284:LEU:HD21	1.80	0.63
1:A:170:LEU:O	1:A:259:ALA:HA	1.99	0.62
1:A:20:THR:HG22	1:A:21:GLN:HG3	1.81	0.61
1:A:76:ILE:HG21	1:A:117:ILE:CG1	2.30	0.61
1:A:89:PRO:HG2	1:A:105:ARG:O	2.00	0.61
1:A:98:MET:CE	1:A:229:PRO:HD2	2.31	0.61
1:A:155:THR:HG23	1:A:187:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:O	1:A:177:ILE:HG22	1.98	0.61
2:B:17:MET:HE3	2:B:36:ALA:HA	1.84	0.60
2:B:7:ALA:O	2:B:9:PHE:N	2.35	0.59
1:A:132:GLY:HA3	1:A:135:TYR:OH	2.02	0.59
1:A:155:THR:CG2	1:A:187:VAL:HB	2.32	0.59
1:A:155:THR:HG23	1:A:187:VAL:CB	2.32	0.58
1:A:231:GLN:HE22	1:A:237:LEU:H	1.51	0.58
1:A:177:ILE:O	1:A:177:ILE:CG2	2.51	0.58
1:A:268:GLN:HE21	1:A:268:GLN:CA	2.03	0.58
1:A:329:ALA:H	2:B:104:ASN:ND2	2.01	0.58
1:A:107:LEU:HD11	1:A:185:ILE:HG21	1.85	0.58
1:A:83:ILE:HD12	1:A:284:LEU:HD11	1.86	0.57
1:A:57:CYS:SG	1:A:74:GLY:HA3	2.44	0.57
2:B:160:GLY:HA2	2:B:164:LEU:N	2.15	0.57
1:A:82:SER:HB3	1:A:112:ARG:HG2	1.87	0.57
1:A:324:THR:OG1	1:A:325:PRO:HD2	2.03	0.57
2:B:76:GLU:H	2:B:76:GLU:CD	2.11	0.57
2:B:17:MET:CE	2:B:36:ALA:HA	2.34	0.57
2:B:11:GLU:O	2:B:11:GLU:HG3	2.04	0.57
1:A:176:TYR:O	1:A:184:GLN:NE2	2.30	0.56
2:B:4:GLY:HA2	2:B:9:PHE:HD1	1.70	0.56
1:A:237:LEU:C	1:A:239:GLN:H	2.14	0.56
2:B:44:ALA:HB2	2:B:114:HIS:CE1	2.41	0.55
2:B:103:SER:O	2:B:107:ILE:HG13	2.07	0.55
1:A:243:ILE:HG22	1:A:245:VAL:HG23	1.87	0.55
1:A:199:VAL:HG22	1:A:205:SER:HB2	1.90	0.54
2:B:46:ASN:O	2:B:47:LYS:C	2.49	0.54
1:A:311:HIS:CE1	2:B:89:ALA:HB2	2.42	0.54
1:A:102:THR:C	1:A:104:ILE:H	2.16	0.54
1:A:140:SER:C	1:A:150:ASN:HA	2.33	0.53
1:A:76:ILE:HG21	1:A:117:ILE:HG13	1.88	0.53
1:A:140:SER:O	1:A:150:ASN:HA	2.08	0.53
1:A:176:TYR:OH	1:A:182:GLU:O	2.18	0.53
1:A:176:TYR:CZ	1:A:252:PRO:HA	2.43	0.53
1:A:147:THR:O	1:A:148:ASN:HB2	2.08	0.53
1:A:87:VAL:HG23	1:A:88:LYS:HG3	1.91	0.53
2:B:88:ARG:C	2:B:88:ARG:HD2	2.34	0.53
1:A:304:LYS:HB3	1:A:305:PRO:HD2	1.90	0.52
1:A:83:ILE:HG21	1:A:284:LEU:CG	2.38	0.52
1:A:329:ALA:H	2:B:104:ASN:HD21	1.56	0.52
1:A:40:HIS:ND1	1:A:287:ILE:HB	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TRP:CH2	1:A:202:TYR:OH	2.54	0.51
1:A:186:THR:HB	1:A:248:MET:HB3	1.93	0.51
2:B:160:GLY:HA2	2:B:163:SER:HA	1.93	0.51
1:A:145:ASN:OD1	1:A:146:VAL:N	2.43	0.51
1:A:184:GLN:HB3	1:A:250:GLN:HB2	1.91	0.51
1:A:8:THR:HG22	1:A:9:SER:N	2.26	0.51
2:B:17:MET:HE1	2:B:22:HIS:C	2.36	0.51
1:A:107:LEU:N	1:A:108:PRO:HD2	2.26	0.51
1:A:48:GLN:HE21	1:A:48:GLN:N	2.09	0.50
1:A:55:PRO:O	1:A:56:ASN:HB3	2.10	0.50
1:A:95:PHE:N	1:A:143:CYS:SG	2.85	0.50
1:A:178:CYS:SG	1:A:184:GLN:HG3	2.51	0.50
1:A:71:LYS:HD3	1:A:146:VAL:HG22	1.93	0.50
1:A:239:GLN:O	1:A:240:SER:C	2.54	0.50
1:A:172:VAL:HG23	1:A:260:TYR:CE2	2.47	0.49
1:A:157:ALA:O	1:A:265:LEU:HA	2.12	0.49
2:B:160:GLY:CA	2:B:164:LEU:H	2.17	0.49
1:A:27:THR:HB	1:A:331:GLY:HA3	1.95	0.48
2:B:60:VAL:HG12	2:B:88:ARG:HH21	1.78	0.48
1:A:71:LYS:C	1:A:73:MET:H	2.21	0.48
2:B:70:MET:HB2	2:B:74:HIS:HD1	1.78	0.48
1:A:61:THR:HG22	1:A:63:LEU:H	1.78	0.48
1:A:202:TYR:HB3	1:A:262:ARG:HG2	1.95	0.48
2:B:73:LEU:HD23	2:B:74:HIS:CE1	2.49	0.48
1:A:98:MET:HE1	1:A:101:ARG:NH2	2.27	0.47
1:A:260:TYR:CD1	1:A:264:VAL:CG2	2.92	0.47
2:B:158:ASN:O	2:B:161:GLU:HB2	2.14	0.47
1:A:84:LEU:HD11	1:A:86:GLU:O	2.14	0.47
1:A:176:TYR:CE1	1:A:252:PRO:HA	2.50	0.47
1:A:50:ARG:HB2	1:A:82:SER:HA	1.96	0.47
2:B:60:VAL:HG12	2:B:88:ARG:NH2	2.30	0.47
1:A:128:GLU:H	1:A:128:GLU:HG2	1.56	0.46
1:A:162:LYS:O	1:A:163:ASN:HB3	2.15	0.46
1:A:118:ARG:HH22	1:A:179:THR:CB	2.27	0.46
1:A:124:VAL:HG21	1:A:267:PRO:HB2	1.96	0.46
1:A:237:LEU:C	1:A:239:GLN:N	2.73	0.46
1:A:7:ILE:HD11	1:A:335:ARG:CG	2.44	0.46
1:A:185:ILE:HG12	1:A:249:VAL:HG22	1.98	0.46
3:C:1:NAG:H62	3:C:2:NAG:HN2	1.81	0.46
1:A:61:THR:HG22	1:A:62:ASP:N	2.31	0.46
1:A:86:GLU:OE1	1:A:89:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLN:HB3	1:A:242:ARG:NH1	2.30	0.46
1:A:212:SER:HA	1:A:257:THR:O	2.16	0.46
1:A:283:SER:O	1:A:284:LEU:HD23	2.17	0.45
2:B:65:ARG:NH2	2:B:71:ASP:OD2	2.50	0.45
1:A:183:ASP:N	1:A:273:ALA:O	2.46	0.45
1:A:105:ARG:NH2	1:A:233:GLU:OE2	2.49	0.45
1:A:20:THR:HB	2:B:105:GLU:OE2	2.17	0.45
1:A:61:THR:CG2	1:A:90:VAL:O	2.53	0.45
1:A:143:CYS:CB	1:A:151:GLY:O	2.65	0.45
1:A:294:HIS:CD2	1:A:296:LYS:H	2.35	0.45
1:A:280:ILE:CG2	1:A:281:LYS:N	2.80	0.45
1:A:2:ARG:HA	2:B:138:PHE:O	2.17	0.44
1:A:148:ASN:CG	1:A:149:GLY:H	2.25	0.44
1:A:95:PHE:HA	1:A:96:PRO:HD2	1.74	0.44
2:B:117:ALA:O	2:B:120:ARG:N	2.51	0.44
2:B:168:ASP:N	2:B:168:ASP:OD1	2.50	0.44
1:A:184:GLN:OE1	1:A:186:THR:OG1	2.31	0.44
1:A:55:PRO:C	1:A:57:CYS:H	2.26	0.43
1:A:296:LYS:CD	1:A:310:GLU:OE1	2.67	0.43
2:B:17:MET:HE1	2:B:23:GLY:N	2.34	0.43
1:A:76:ILE:HD11	1:A:271:TRP:HZ3	1.83	0.43
1:A:341:LEU:HD11	2:B:14:TRP:CH2	2.54	0.43
1:A:231:GLN:OE1	1:A:239:GLN:HG2	2.19	0.43
1:A:54:CYS:HB3	1:A:57:CYS:HB2	1.85	0.43
1:A:280:ILE:HG23	1:A:281:LYS:N	2.33	0.43
1:A:143:CYS:HB3	1:A:151:GLY:O	2.18	0.42
1:A:121:ALA:O	1:A:122:ARG:CB	2.67	0.42
1:A:148:ASN:CG	1:A:149:GLY:N	2.77	0.42
1:A:179:THR:HG22	1:A:180:LYS:CG	2.49	0.42
1:A:47:THR:CG2	1:A:80:LYS:HB2	2.50	0.42
1:A:76:ILE:HG21	1:A:117:ILE:HD11	2.00	0.42
1:A:187:VAL:O	1:A:188:TRP:HB3	2.20	0.42
1:A:185:ILE:HB	1:A:271:TRP:HB2	2.02	0.41
1:A:61:THR:O	1:A:64:ASP:HB2	2.20	0.41
1:A:76:ILE:HD11	1:A:271:TRP:CZ3	2.55	0.41
1:A:294:HIS:HD2	1:A:297:TYR:H	1.69	0.41
1:A:29:VAL:HG12	1:A:329:ALA:HA	2.02	0.41
1:A:98:MET:HE2	1:A:98:MET:HB3	1.91	0.41
2:B:10:LEU:C	2:B:12:GLY:H	2.28	0.41
2:B:4:GLY:HA2	2:B:9:PHE:CD1	2.53	0.41
2:B:160:GLY:HA2	2:B:163:SER:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HA	1:A:175:PRO:HD3	1.88	0.40
2:B:82:GLU:O	2:B:83:LYS:C	2.63	0.40
2:B:162:PHE:O	2:B:164:LEU:HG	2.20	0.40
2:B:114:HIS:O	2:B:115:LEU:C	2.65	0.40
1:A:186:THR:HA	1:A:270:VAL:HG22	2.03	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:171:SO4:O1	6:B:171:SO4:O2[2_655]	0.81	1.39
6:B:171:SO4:O2	6:B:171:SO4:O3[2_655]	0.99	1.21
6:B:171:SO4:S	6:B:171:SO4:O3[2_655]	1.27	0.93
6:B:171:SO4:O1	6:B:171:SO4:O3[3_665]	1.31	0.89
6:B:171:SO4:S	6:B:171:SO4:O1[3_665]	1.37	0.83
6:B:171:SO4:O4	6:B:171:SO4:O4[2_655]	1.44	0.76
6:B:171:SO4:S	6:B:171:SO4:O4[3_665]	1.61	0.59
6:B:171:SO4:O3	6:B:171:SO4:O4[3_665]	1.71	0.49
6:B:171:SO4:S	6:B:171:SO4:O2[2_655]	1.81	0.39
6:B:171:SO4:O1	6:B:171:SO4:O1[2_655]	1.86	0.34

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	340/342 (99%)	277 (82%)	48 (14%)	15 (4%)		
2	B	167/169 (99%)	146 (87%)	16 (10%)	5 (3%)		
All	All	507/511 (99%)	423 (83%)	64 (13%)	20 (4%)		

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	120	SER
1	A	148	ASN
2	B	8	GLY
1	A	72	CYS
1	A	122	ARG
1	A	264	VAL
2	B	163	SER
1	A	100	ASP
1	A	103	LYS
1	A	153	PHE
1	A	177	ILE
1	A	285	PRO
2	B	17	MET
2	B	69	ALA
1	A	237	LEU
2	B	70	MET
1	A	70	PRO
1	A	169	PRO
1	A	203	GLY

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	287/287 (100%)	248 (86%)	39 (14%)	3	13
2	B	136/136 (100%)	122 (90%)	14 (10%)	7	23
All	All	423/423 (100%)	370 (88%)	53 (12%)	4	15

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	16	VAL
1	A	17	LYS
1	A	20	THR

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Mol	Chain	Res	Type
1	A	32	LEU
1	A	33	THR
1	A	34	THR
1	A	37	THR
1	A	47	THR
1	A	48	GLN
1	A	54	CYS
1	A	62	ASP
1	A	75	THR
1	A	83	ILE
1	A	85	HIS
1	A	87	VAL
1	A	90	VAL
1	A	119	LEU
1	A	128	GLU
1	A	136	ILE
1	A	139	THR
1	A	155	THR
1	A	158	TRP
1	A	171	THR
1	A	184	GLN
1	A	187	VAL
1	A	192	SER
1	A	196	THR
1	A	202	TYR
1	A	237	LEU
1	A	245	VAL
1	A	257	THR
1	A	268	GLN
1	A	270	VAL
1	A	280	ILE
1	A	284	LEU
1	A	322	VAL
1	A	323	LYS
1	A	341	LEU
2	B	22	HIS
2	B	25	THR
2	B	34	VAL
2	B	64	GLN
2	B	67	SER
2	B	76	GLU
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	88	ARG
2	B	92	ILE
2	B	101	LEU
2	B	103	SER
2	B	116	LEU
2	B	118	LEU
2	B	166	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	14	HIS
1	A	48	GLN
1	A	85	HIS
1	A	126	ASN
1	A	239	GLN
1	A	250	GLN
1	A	294	HIS
1	A	311	HIS
2	B	42	GLN
2	B	64	GLN
2	B	104	ASN
2	B	142	HIS
2	B	146	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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	1.90	3 (17%)
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	0.63	0
4	NAG	D	1	1,4	14,14,15	0.89	0	17,19,21	1.89	4 (23%)
4	NDG	D	2	4	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.48	0	17,19,21	1.75	3 (17%)
3	NAG	E	2	3	14,14,15	0.73	0	17,19,21	1.20	3 (17%)
4	NAG	F	1	1,4	14,14,15	0.56	0	17,19,21	2.50	6 (35%)
4	NDG	F	2	4	14,14,15	0.86	1 (7%)	17,19,21	1.48	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NDG	D	2	4	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	6/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NDG	F	2	4	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NDG	C1-C2	2.09	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C4-C3-C2	-7.12	100.58	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	5.23	119.19	112.19
3	E	1	NAG	C1-O5-C5	4.73	118.53	112.19
3	C	1	NAG	C1-O5-C5	4.70	118.48	112.19
4	F	2	NDG	C4-C3-C2	4.25	117.25	111.02
3	C	1	NAG	O5-C1-C2	-3.92	105.23	111.29
4	F	1	NAG	C1-O5-C5	3.78	117.25	112.19
4	F	1	NAG	O4-C4-C5	3.74	118.54	109.32
4	D	1	NAG	O4-C4-C5	3.35	117.56	109.32
3	E	1	NAG	C2-N2-C7	3.14	127.11	122.90
4	D	1	NAG	C4-C3-C2	3.03	115.45	111.02
4	F	1	NAG	O4-C4-C3	2.86	117.12	110.38
3	E	1	NAG	C4-C3-C2	-2.84	106.85	111.02
4	F	1	NAG	C1-C2-N2	2.73	114.74	110.43
4	D	2	NDG	C1-O5-C5	2.65	115.73	112.19
3	C	1	NAG	C2-N2-C7	2.58	126.36	122.90
4	F	2	NDG	C2-N2-C7	2.44	126.18	122.90
3	E	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	E	2	NAG	C1-O5-C5	2.31	115.28	112.19
4	D	1	NAG	O4-C4-C3	-2.17	105.27	110.38
4	F	1	NAG	O5-C1-C2	-2.15	107.97	111.29
3	E	2	NAG	C2-N2-C7	2.13	125.75	122.90

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NDG	C3-C2-N2-C7
4	F	2	NDG	C8-C7-N2-C2
4	F	2	NDG	O7-C7-N2-C2

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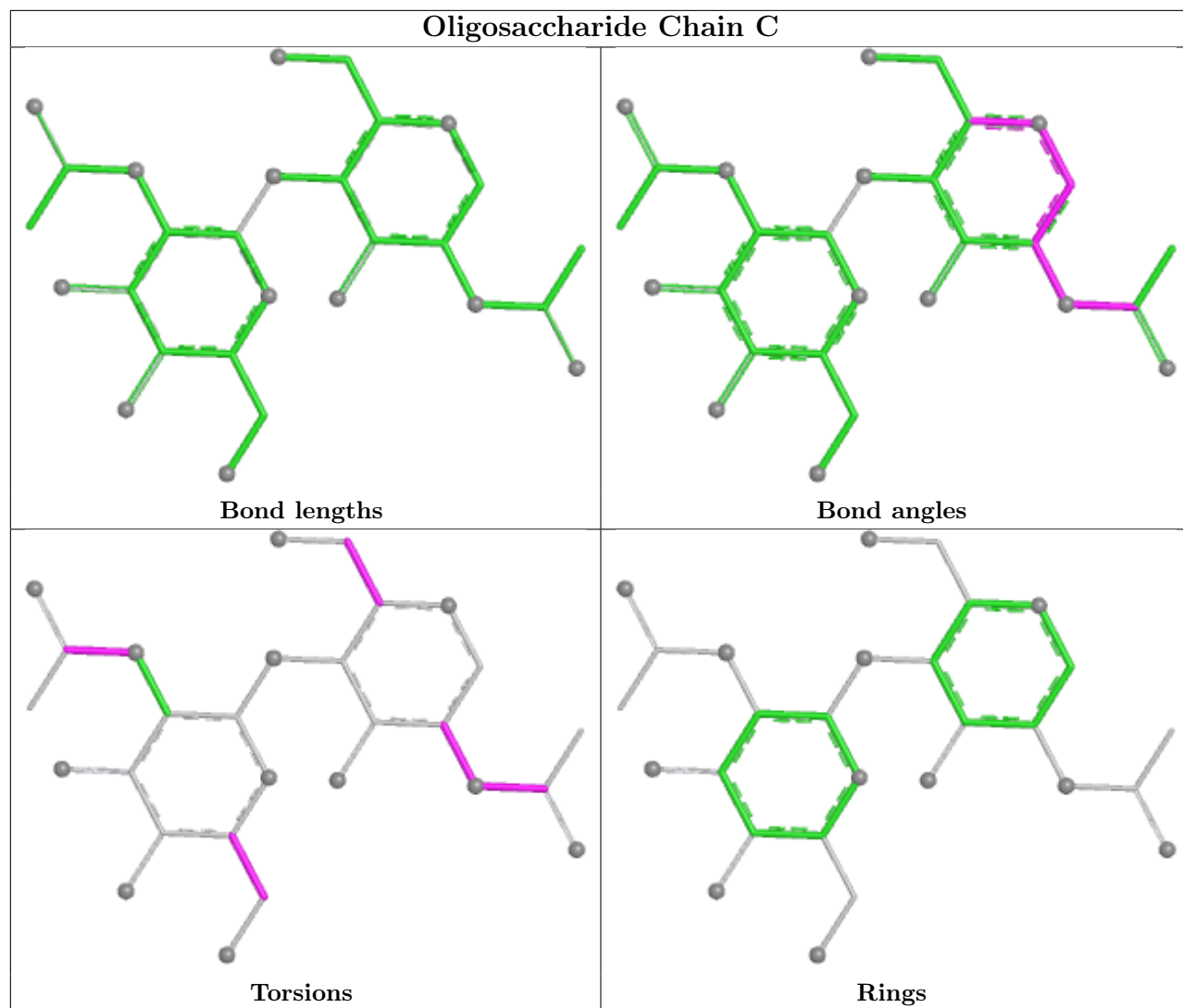
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
4	D	2	NDG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
4	D	2	NDG	C4-C5-C6-O6
4	F	2	NDG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C3-C2-N2-C7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

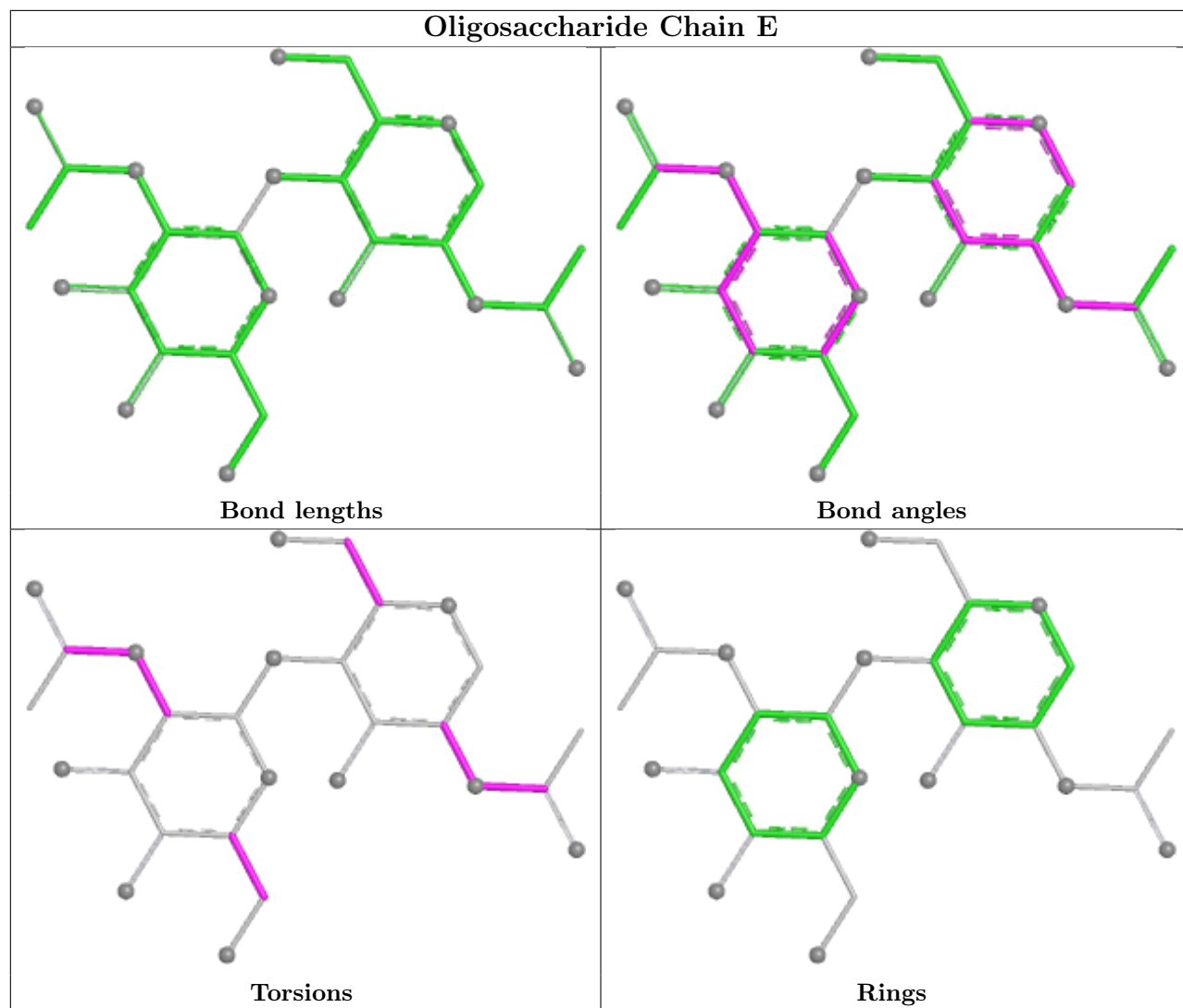
There are no ring outliers.

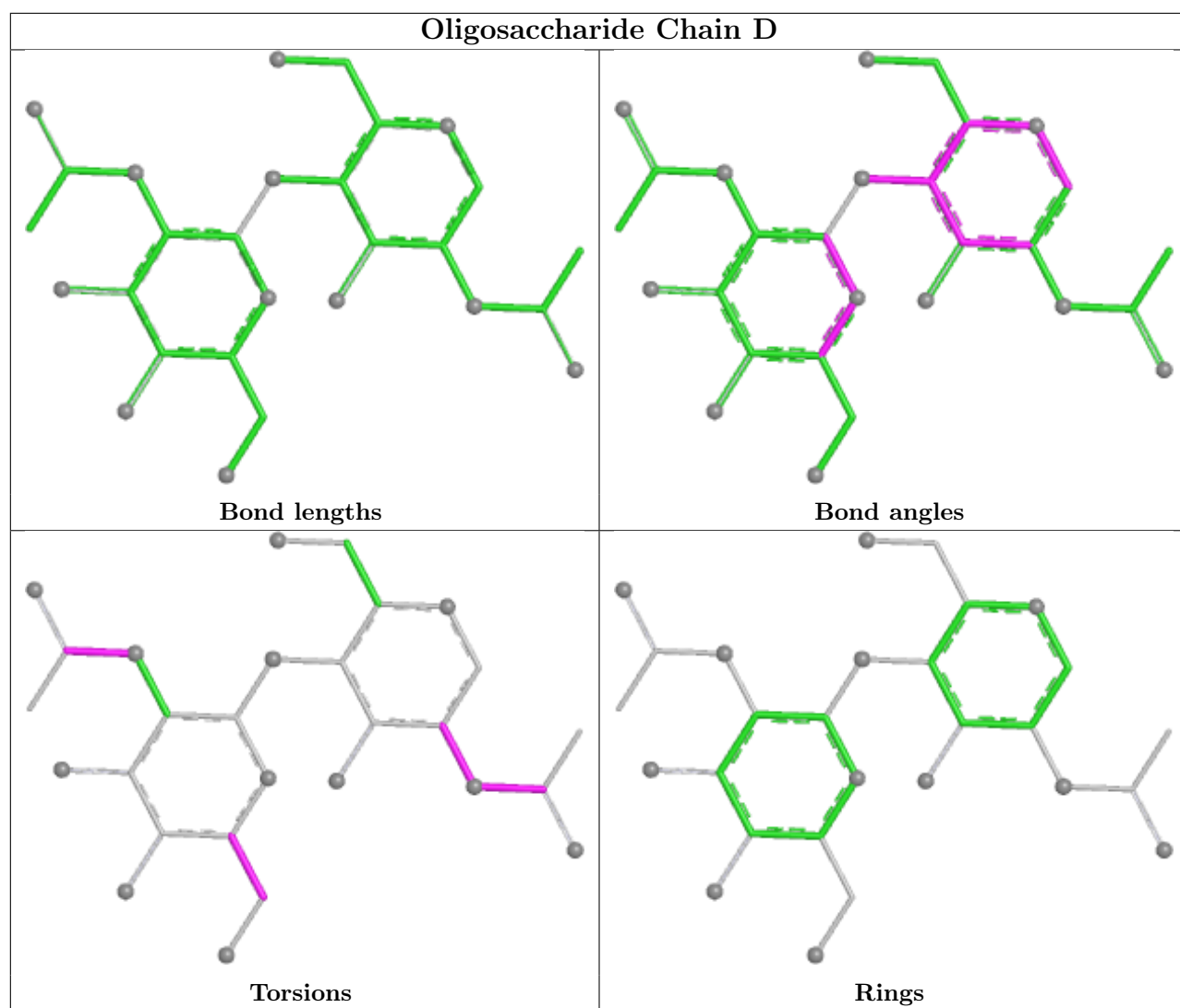
2 monomers are involved in 1 short contact:

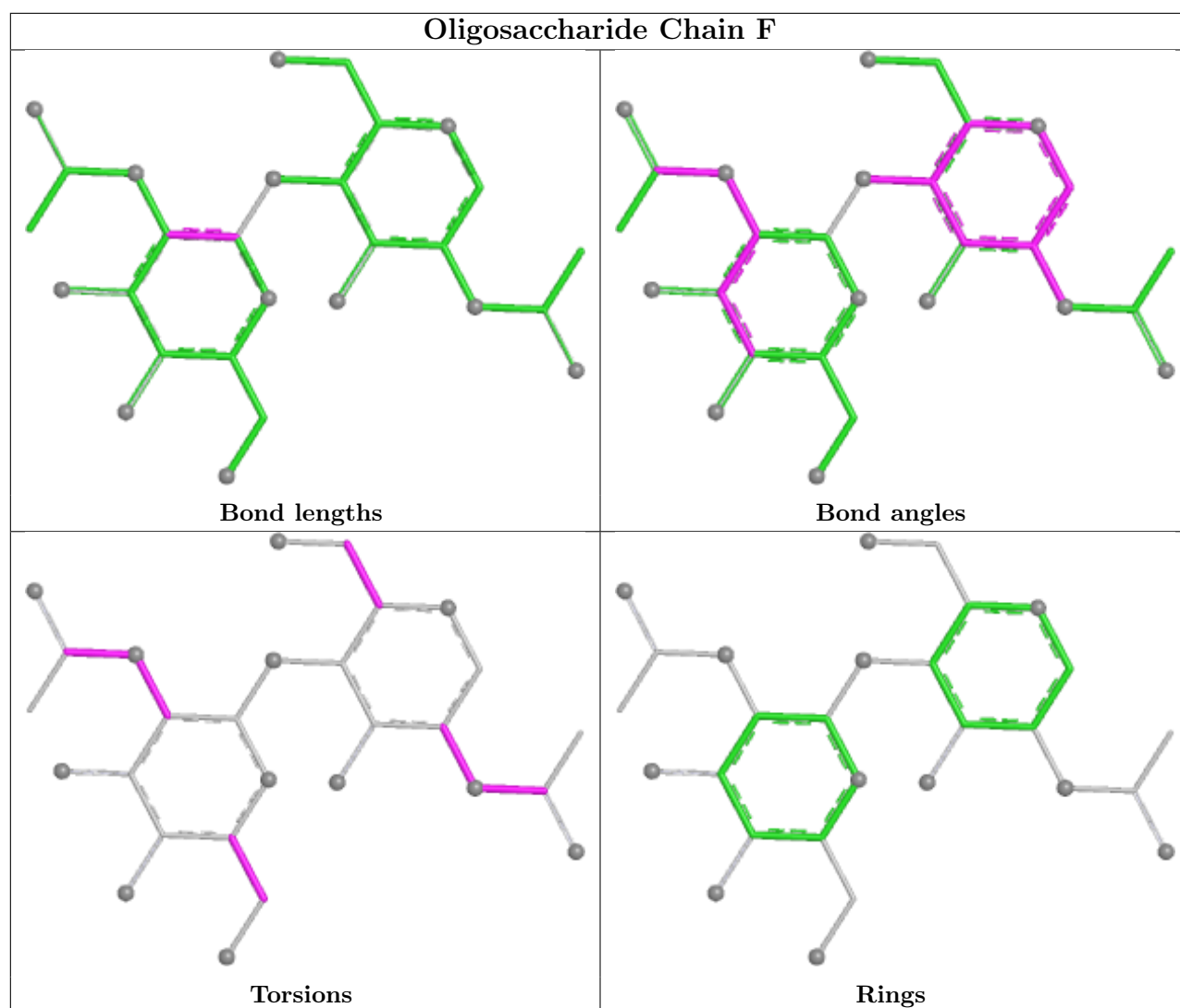
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0

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](#)

4 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	$\# Z > 2$
5	NAG	A	345	1	14,14,15	0.85	1 (7%)	17,19,21	1.36	1 (5%)
5	NAG	A	348	1	14,14,15	0.74	1 (7%)	17,19,21	1.16	0
6	SO4	B	171	-	4,4,4	1.87	1 (25%)	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	170	2	14,14,15	0.52	0	17,19,21	1.54	1 (5%)

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
5	NAG	A	345	1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	A	348	1	-	5/6/23/26	0/1/1/1
5	NAG	B	170	2	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	171	SO4	O1-S	2.61	1.60	1.44
5	A	345	NAG	C1-C2	2.26	1.55	1.52
5	A	348	NAG	C1-C2	2.09	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	170	NAG	C1-O5-C5	5.35	119.36	112.19
5	A	345	NAG	C3-C4-C5	-2.91	104.95	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	345	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	345	NAG	C3-C2-N2-C7
5	A	345	NAG	C8-C7-N2-C2
5	A	345	NAG	O7-C7-N2-C2
5	B	170	NAG	C8-C7-N2-C2
5	B	170	NAG	O7-C7-N2-C2
5	B	170	NAG	O5-C5-C6-O6
5	B	170	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	348	NAG	C8-C7-N2-C2
5	A	348	NAG	O7-C7-N2-C2
5	A	348	NAG	O5-C5-C6-O6
5	A	348	NAG	C4-C5-C6-O6
5	A	345	NAG	C4-C5-C6-O6
5	A	345	NAG	O5-C5-C6-O6
5	A	348	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	171	SO4	0	10

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	342/342 (100%)	0.11	6 (1%) 67 58	68, 96, 123, 139	0
2	B	169/169 (100%)	-0.15	2 (1%) 76 68	59, 83, 106, 120	0
All	All	511/511 (100%)	0.02	8 (1%) 70 61	59, 90, 120, 139	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	3.6
1	A	284	LEU	3.6
1	A	53	LEU	3.2
2	B	11	GLU	3.1
1	A	177	ILE	2.5
1	A	70	PRO	2.4
1	A	236	GLY	2.3
2	B	169	SER	2.1

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.

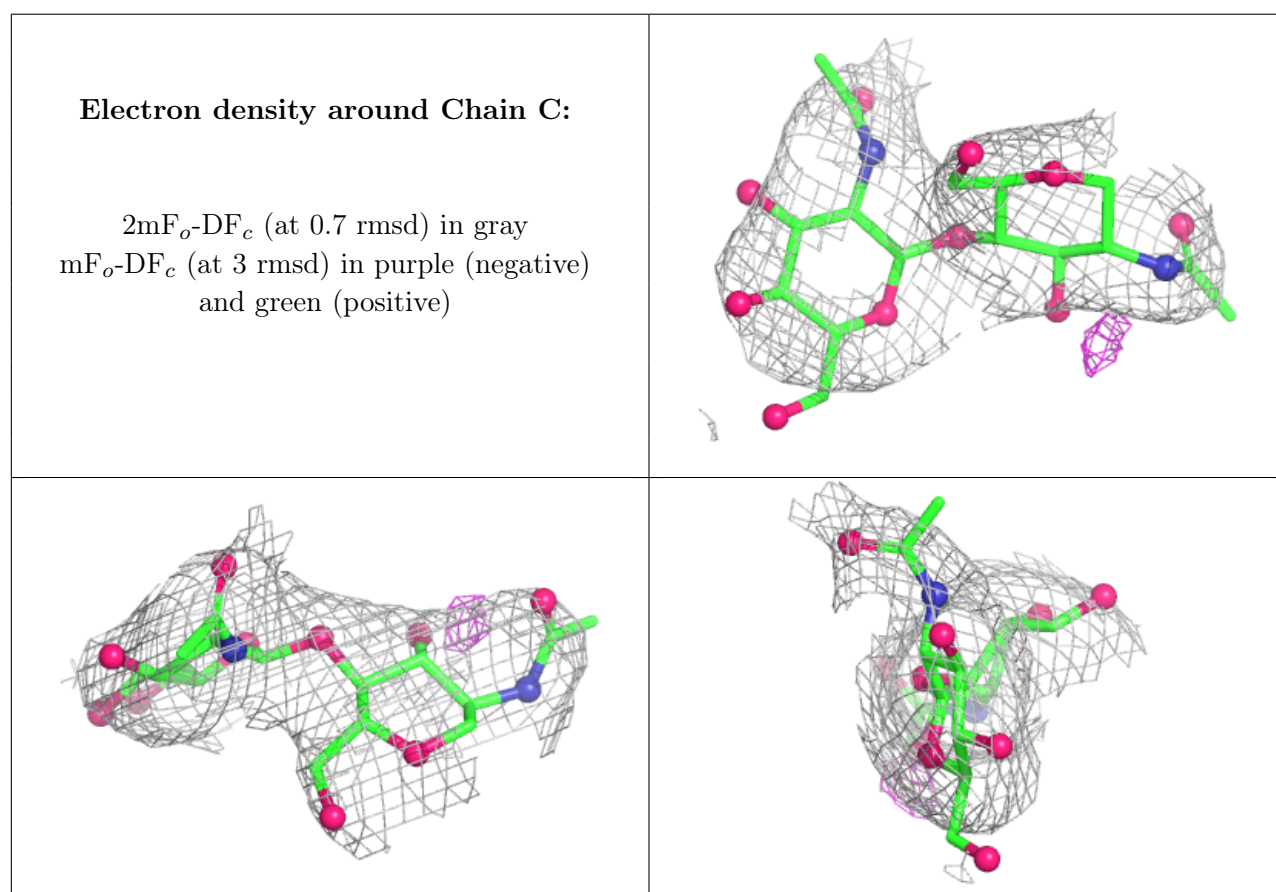
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NDG	F	2	14/15	0.47	0.09	119,124,126,126	0

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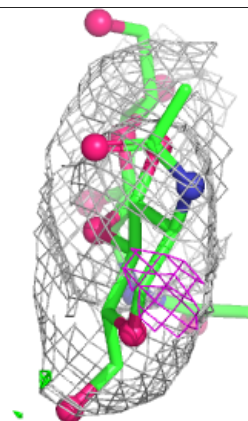
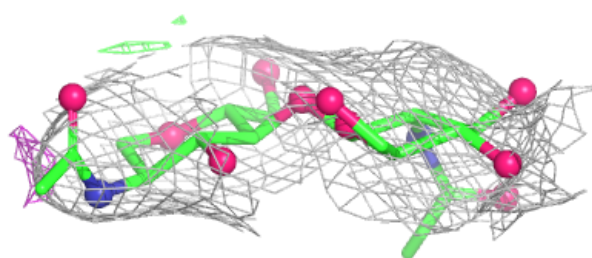
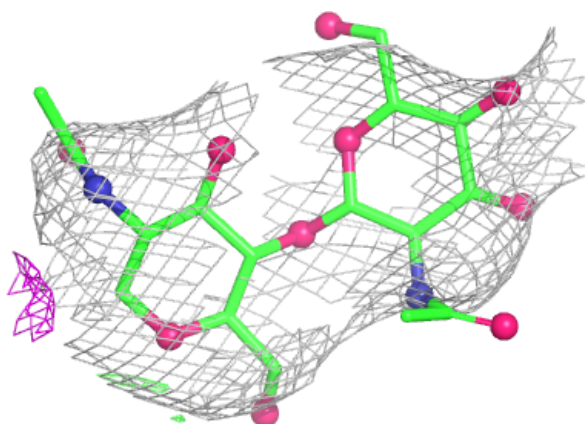
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NDG	D	2	14/15	0.51	0.11	168,170,170,171	0
3	NAG	E	2	14/15	0.65	0.10	137,142,145,146	0
3	NAG	C	2	14/15	0.77	0.08	129,133,134,136	0
4	NAG	D	1	14/15	0.78	0.09	156,161,163,167	0
3	NAG	E	1	14/15	0.86	0.11	115,118,124,129	0
3	NAG	C	1	14/15	0.91	0.09	103,111,115,123	0
4	NAG	F	1	14/15	0.94	0.07	94,103,112,112	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.



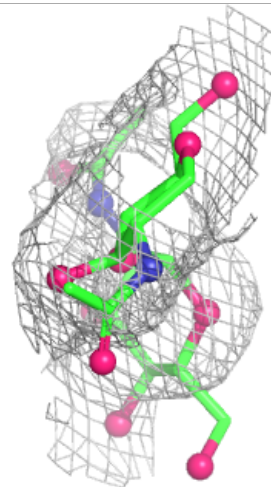
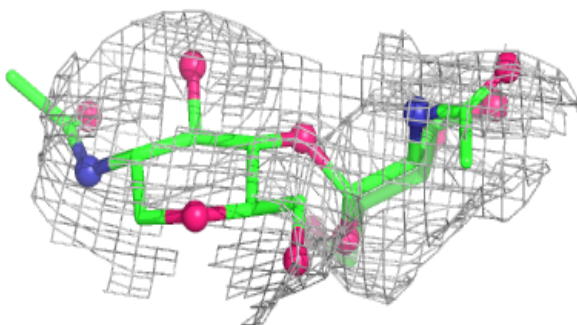
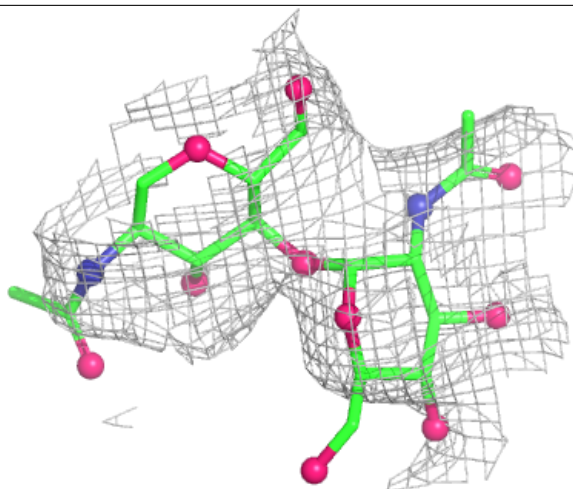
Electron density around Chain E:

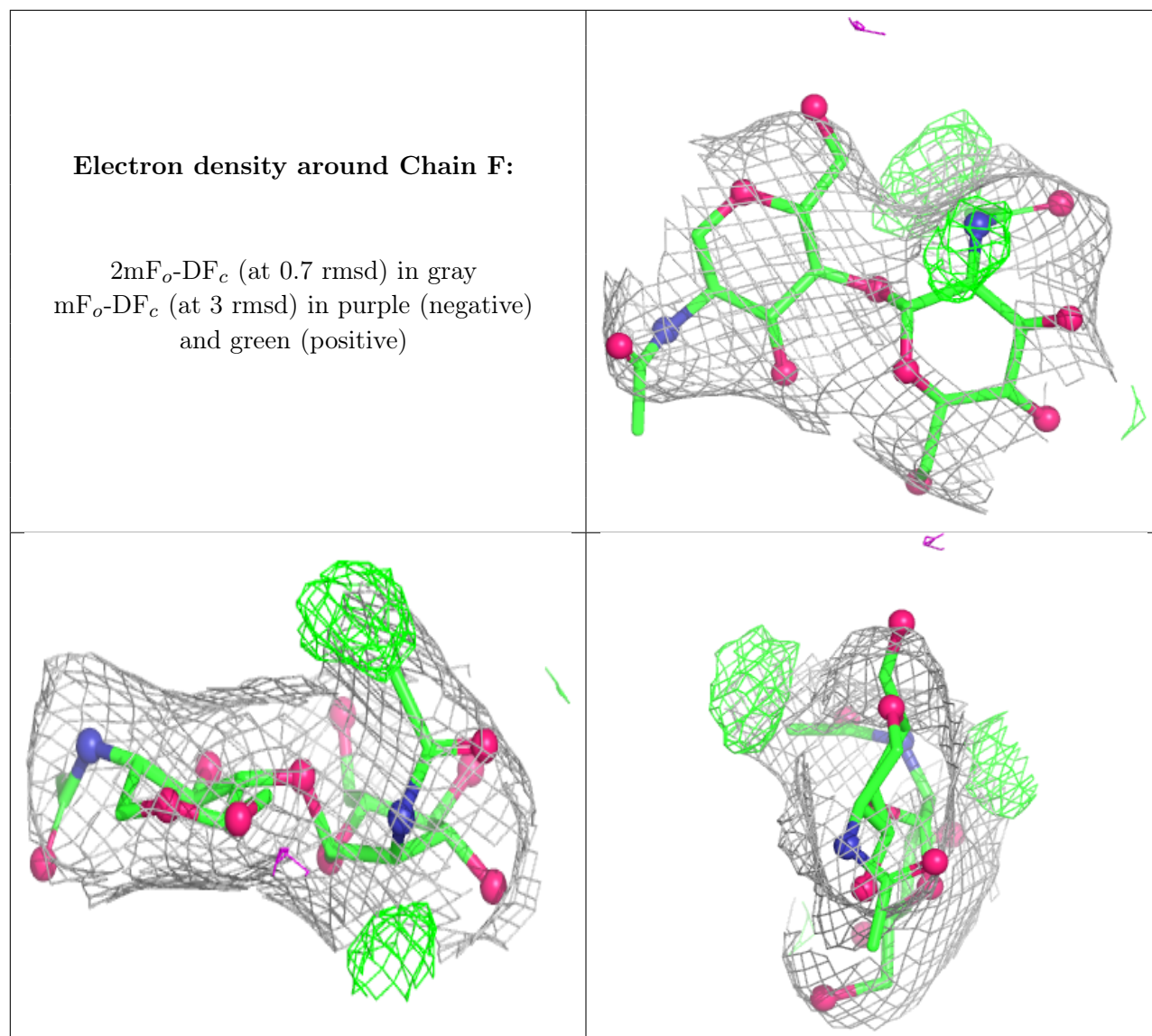
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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
5	NAG	A	348	14/15	0.24	0.13	144,149,152,153	0
5	NAG	B	170	14/15	0.68	0.09	124,129,131,133	0
5	NAG	A	345	14/15	0.81	0.09	102,104,110,110	0
6	SO4	B	171	5/5	0.93	0.34	52,61,63,65	1

6.5 Other polymers [i](#)

There are no such residues in this entry.