Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 08:36 AM EDT

PDB ID	:	8DFY
Title	:	Crystal structure of Human BTN2A1 Ectodomain
Authors	:	Fulford, T.S.; Soliman, C.; Castle, R.G.; Rigau, M.; Ruan, Z.; Dolezal, O.; Seneviratna, R.; Brown, H.G.; Hanssen, E.; Hammet, A.; Li, S.; Redmond, S.J.; Chung, A.; Gorman, M.A.; Parker, M.W.; Patel, O.; Peat, T.S.; Newman, J.; Behren, A.; Gherardin, N.A.; Godfrey, D.I.; Uldrich, A.P.
Deposited on	:	2022-06-22
Resolution	:	3.55 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

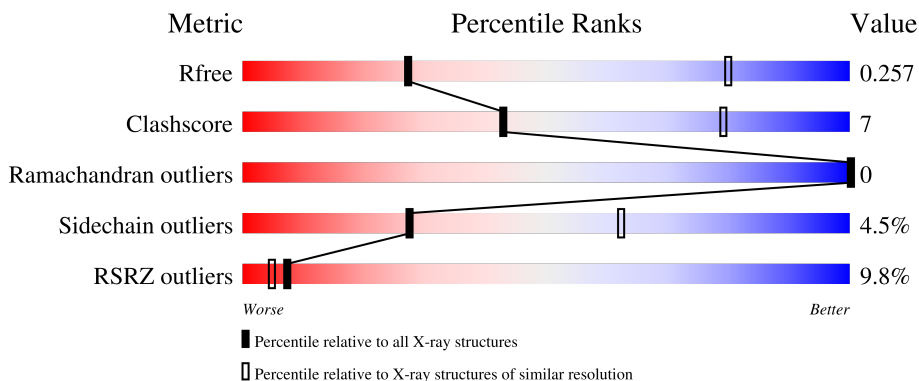|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.55 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		4.5%
RSRZ outliers		9.8%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
⫿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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 <=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	226	5% / 77% / 18% · ·
1	B	226	4% / 78% / 16% · ·
1	C	226	15% / 80% / 15% · ·
1	D	226	12% / 76% / 20% ·

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Mol	Chain	Length	Quality of chain
1	E	226	11% / 79% / 16%
2	F	3	33% / 67%
2	G	3	67% / 33%
2	H	3	67% / 33%
2	I	3	33% / 33% / 33%
2	J	3	33% / 33% / 33%
2	L	3	33% / 67%
2	M	3	67% / 33%
3	K	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
2	BMA	F	3	-	-	-	X
2	NAG	M	1	-	-	-	X
2	NAG	M	2	-	-	-	X
2	BMA	M	3	-	-	-	X
3	NAG	K	1	-	-	-	X
4	NAG	B	303	-	-	-	X
4	NAG	E	301	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8993 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total 1709	C 1078	N 299	O 321	S 11	0	0	0
1	B	218	Total 1709	C 1078	N 299	O 321	S 11	0	0	0
1	C	217	Total 1702	C 1074	N 298	O 319	S 11	0	0	0
1	D	217	Total 1702	C 1074	N 298	O 319	S 11	0	0	0
1	E	217	Total 1702	C 1074	N 298	O 319	S 11	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP Q7KYR7
A	-1	THR	-	expression tag	UNP Q7KYR7
A	0	GLY	-	expression tag	UNP Q7KYR7
A	218	HIS	-	expression tag	UNP Q7KYR7
A	219	HIS	-	expression tag	UNP Q7KYR7
A	220	HIS	-	expression tag	UNP Q7KYR7
A	221	HIS	-	expression tag	UNP Q7KYR7
A	222	HIS	-	expression tag	UNP Q7KYR7
A	223	HIS	-	expression tag	UNP Q7KYR7
B	-2	GLU	-	expression tag	UNP Q7KYR7
B	-1	THR	-	expression tag	UNP Q7KYR7
B	0	GLY	-	expression tag	UNP Q7KYR7
B	218	HIS	-	expression tag	UNP Q7KYR7
B	219	HIS	-	expression tag	UNP Q7KYR7
B	220	HIS	-	expression tag	UNP Q7KYR7
B	221	HIS	-	expression tag	UNP Q7KYR7
B	222	HIS	-	expression tag	UNP Q7KYR7
B	223	HIS	-	expression tag	UNP Q7KYR7
C	-2	GLU	-	expression tag	UNP Q7KYR7

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	THR	-	expression tag	UNP Q7KYR7
C	0	GLY	-	expression tag	UNP Q7KYR7
C	218	HIS	-	expression tag	UNP Q7KYR7
C	219	HIS	-	expression tag	UNP Q7KYR7
C	220	HIS	-	expression tag	UNP Q7KYR7
C	221	HIS	-	expression tag	UNP Q7KYR7
C	222	HIS	-	expression tag	UNP Q7KYR7
C	223	HIS	-	expression tag	UNP Q7KYR7
D	-2	GLU	-	expression tag	UNP Q7KYR7
D	-1	THR	-	expression tag	UNP Q7KYR7
D	0	GLY	-	expression tag	UNP Q7KYR7
D	218	HIS	-	expression tag	UNP Q7KYR7
D	219	HIS	-	expression tag	UNP Q7KYR7
D	220	HIS	-	expression tag	UNP Q7KYR7
D	221	HIS	-	expression tag	UNP Q7KYR7
D	222	HIS	-	expression tag	UNP Q7KYR7
D	223	HIS	-	expression tag	UNP Q7KYR7
E	-2	GLU	-	expression tag	UNP Q7KYR7
E	-1	THR	-	expression tag	UNP Q7KYR7
E	0	GLY	-	expression tag	UNP Q7KYR7
E	218	HIS	-	expression tag	UNP Q7KYR7
E	219	HIS	-	expression tag	UNP Q7KYR7
E	220	HIS	-	expression tag	UNP Q7KYR7
E	221	HIS	-	expression tag	UNP Q7KYR7
E	222	HIS	-	expression tag	UNP Q7KYR7
E	223	HIS	-	expression tag	UNP Q7KYR7

- Molecule 2 is an oligosaccharide called beta-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
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	3	Total 39	C 22	N 2	O 15	0	0	0
2	J	3	Total 39	C 22	N 2	O 15	0	0	0
2	L	3	Total 39	C 22	N 2	O 15	0	0	0
2	M	3	Total 39	C 22	N 2	O 15	0	0	0

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

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.
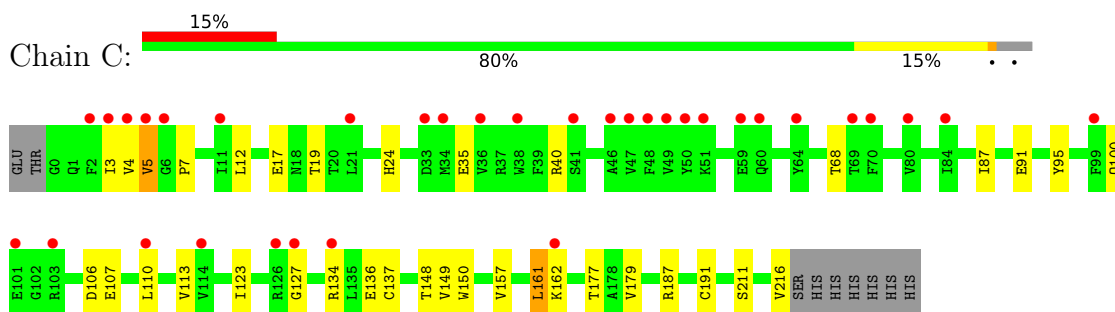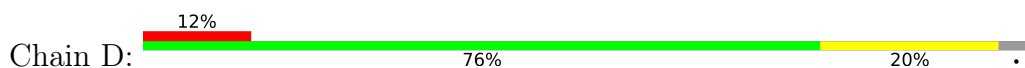
• Molecule 1: Butyrophilin subfamily 2 member A1

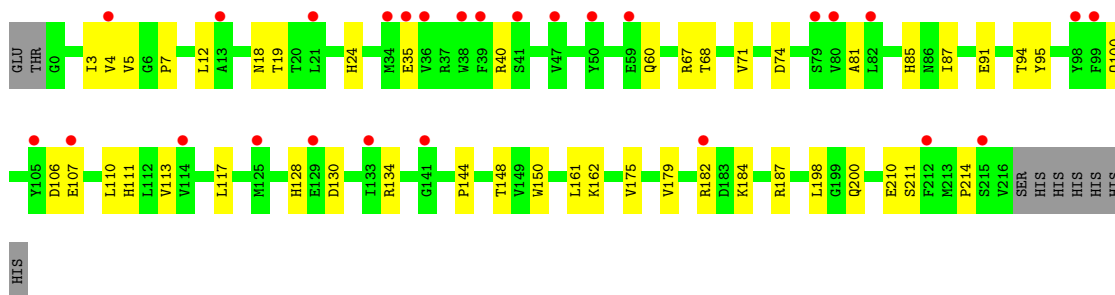• Molecule 1: Butyrophilin subfamily 2 member A1

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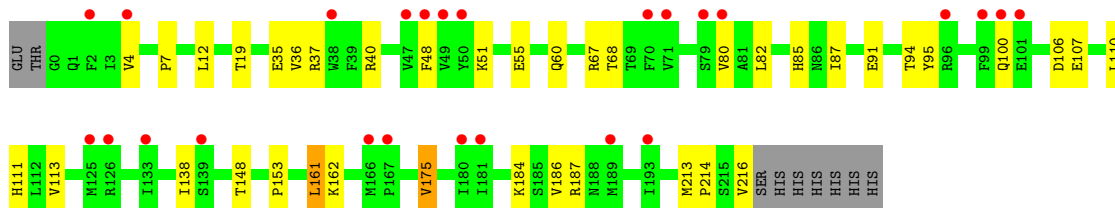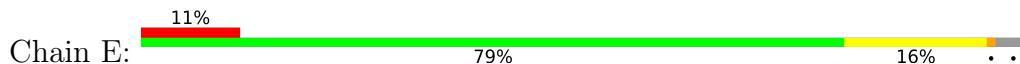
- Molecule 1: Butyrophilin subfamily 2 member A1

Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

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

Chain L:

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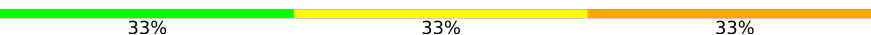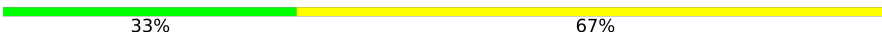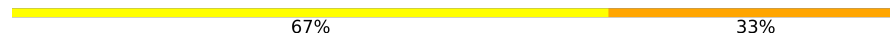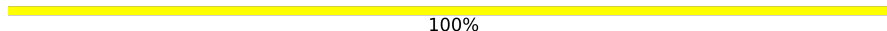
Chain M:

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

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	237.01Å 94.19Å 134.72Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	49.75 – 3.55 49.76 – 3.55	Depositor EDS
% Data completeness (in resolution range)	64.4 (49.75-3.55) 64.3 (49.76-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.4 (11-DEC-2020)	Depositor
R, R_{free}	0.255 , 0.268 0.251 , 0.257	Depositor DCC
R_{free} test set	1102 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	111.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 238.1	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8993	wwPDB-VP
Average B, all atoms (Å^2)	268.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, 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	0.49	0/1746	0.62	0/2363
1	B	0.46	0/1746	0.64	0/2363
1	C	0.42	0/1739	0.59	0/2353
1	D	0.39	0/1739	0.56	0/2353
1	E	0.35	0/1739	0.55	0/2353
All	All	0.43	0/8709	0.59	0/11785

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1709	0	1690	23	0
1	B	1709	0	1690	19	0
1	C	1702	0	1683	28	0
1	D	1702	0	1683	28	0
1	E	1702	0	1683	22	0
2	F	39	0	34	0	0
2	G	39	0	34	2	0
2	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	34	1	0
2	J	39	0	34	1	0
2	L	39	0	34	0	0
2	M	39	0	34	1	0
3	K	28	0	25	0	0
4	A	42	0	39	0	0
4	B	42	0	39	0	0
4	C	28	0	26	1	0
4	D	28	0	26	0	0
4	E	28	0	26	0	0
All	All	8993	0	8848	122	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 7.

All (122) 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:C:137:CYS:HB3	1:C:177:THR:HG23	1.42	0.98
1:B:148:THR:HG21	1:B:175:VAL:HG21	1.48	0.93
1:C:137:CYS:HB3	1:C:177:THR:CG2	2.02	0.89
1:E:148:THR:HG21	1:E:175:VAL:HG21	1.54	0.89
2:G:2:NAG:H61	2:G:3:BMA:H2	1.61	0.82
1:D:134:ARG:HH12	1:D:162:LYS:NZ	1.80	0.79
1:D:134:ARG:NH1	1:D:162:LYS:NZ	2.30	0.79
1:A:148:THR:HG21	1:A:175:VAL:HG21	1.68	0.75
1:D:148:THR:HG21	1:D:175:VAL:HG21	1.70	0.73
1:C:134:ARG:HH12	1:C:162:LYS:HZ1	1.38	0.71
1:D:134:ARG:NH1	1:D:162:LYS:HZ2	1.91	0.69
1:E:60:GLN:HE22	1:E:68:THR:HG21	1.57	0.68
2:I:2:NAG:H61	2:I:3:BMA:C1	2.25	0.67
1:E:37:ARG:HH21	1:E:51:LYS:NZ	1.93	0.66
1:C:134:ARG:HH12	1:C:162:LYS:NZ	1.94	0.66
1:A:18:ASN:OD1	1:A:85:HIS:HA	1.96	0.65
1:D:5:VAL:HG23	1:D:24:HIS:CE1	2.31	0.65
1:B:9:ASP:HB3	1:B:10:PRO:HD2	1.79	0.65
1:C:150:TRP:NE1	1:C:179:VAL:HG13	2.11	0.65
1:D:60:GLN:HE22	1:D:68:THR:HG21	1.62	0.64
1:E:48:PHE:CE1	1:E:55:GLU:HG3	2.33	0.63
1:B:163:GLU:HG3	1:B:177:THR:HB	1.80	0.63
1:E:184:LYS:HG2	1:E:213:MET:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG23	1:A:24:HIS:CE1	2.36	0.61
1:E:37:ARG:NH2	1:E:51:LYS:NZ	2.49	0.60
1:E:7:PRO:HD2	1:E:110:LEU:HG	1.83	0.59
1:B:147:LEU:HD21	1:B:196:THR:HG23	1.85	0.58
1:B:216:VAL:HB	1:C:216:VAL:HA	1.85	0.58
1:D:134:ARG:NH1	1:D:162:LYS:HZ1	2.01	0.58
1:C:5:VAL:HG21	1:C:24:HIS:NE2	2.18	0.57
1:C:149:VAL:HG13	1:C:157:VAL:HG13	1.87	0.57
1:A:19:THR:HG22	1:A:87:ILE:HD11	1.86	0.57
1:A:5:VAL:HG21	1:A:24:HIS:NE2	2.20	0.57
1:B:149:VAL:HG13	1:B:157:VAL:HG13	1.86	0.56
1:C:123:ILE:HD11	1:C:191:CYS:HB3	1.87	0.56
1:A:145:LYS:HD3	1:A:165:SER:HB3	1.87	0.55
1:A:9:ASP:HB3	1:A:10:PRO:HD2	1.88	0.54
1:A:5:VAL:CG2	1:A:24:HIS:NE2	2.72	0.53
1:D:144:PRO:HB3	2:J:1:NAG:H82	1.90	0.53
1:D:187:ARG:NE	1:D:187:ARG:HA	2.24	0.53
1:B:94:THR:HG23	1:B:109:ILE:HG23	1.91	0.52
1:E:19:THR:HG22	1:E:87:ILE:HD11	1.92	0.52
1:A:4:VAL:HG23	1:A:106:ASP:HB3	1.91	0.51
1:C:17:GLU:HA	4:C:302:NAG:H83	1.92	0.51
1:D:4:VAL:HG23	1:D:106:ASP:HB3	1.91	0.51
1:B:19:THR:HG22	1:B:87:ILE:HD11	1.92	0.51
1:C:5:VAL:CG2	1:C:24:HIS:NE2	2.74	0.50
1:A:163:GLU:HG3	1:A:177:THR:HB	1.94	0.50
1:A:12:LEU:HA	1:A:113:VAL:HG13	1.92	0.50
1:A:115:ALA:HB2	1:A:197:LEU:HD12	1.93	0.50
1:D:35:GLU:HB3	1:D:100:GLN:HB3	1.92	0.50
1:E:94:THR:HG22	1:E:111:HIS:CE1	2.47	0.49
1:D:117:LEU:HD21	1:D:200:GLN:HB2	1.93	0.49
1:A:7:PRO:HD2	1:A:110:LEU:HG	1.94	0.49
1:B:138:ILE:HD11	1:B:140:ARG:NH2	2.27	0.49
1:C:7:PRO:HD2	1:C:110:LEU:HG	1.93	0.49
1:E:67:ARG:HG2	1:E:85:HIS:O	2.13	0.48
1:E:187:ARG:NE	1:E:187:ARG:HA	2.29	0.48
1:D:19:THR:HG22	1:D:87:ILE:HD11	1.95	0.47
1:B:4:VAL:HG23	1:B:106:ASP:HB3	1.97	0.47
1:D:5:VAL:CG2	1:D:24:HIS:NE2	2.77	0.47
1:A:94:THR:HG22	1:A:111:HIS:CE1	2.50	0.47
1:D:130:ASP:HB3	1:D:182:ARG:HH21	1.78	0.47
1:E:37:ARG:NH2	1:E:51:LYS:HZ3	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ARG:HD3	1:E:95:TYR:CD2	2.50	0.47
1:A:5:VAL:CG2	1:A:24:HIS:CE1	2.98	0.46
1:C:4:VAL:HG23	1:C:106:ASP:HB3	1.96	0.46
1:C:187:ARG:NE	1:C:187:ARG:HA	2.30	0.46
1:A:187:ARG:NE	1:A:187:ARG:HA	2.30	0.46
1:D:7:PRO:HD2	1:D:110:LEU:HG	1.96	0.46
1:B:187:ARG:HA	1:B:187:ARG:NE	2.30	0.46
1:B:21:LEU:HB3	1:B:110:LEU:HD22	1.98	0.46
1:E:12:LEU:HA	1:E:113:VAL:HG13	1.97	0.46
1:A:35:GLU:HB3	1:A:100:GLN:HB3	1.97	0.46
1:C:137:CYS:HB2	1:C:150:TRP:CH2	2.51	0.46
1:B:126:ARG:HB2	1:B:134:ARG:HG2	1.99	0.45
1:C:150:TRP:CD1	1:C:179:VAL:CG1	3.00	0.45
1:D:94:THR:HG22	1:D:111:HIS:CE1	2.51	0.45
1:C:12:LEU:HA	1:C:113:VAL:HG13	1.99	0.45
1:C:150:TRP:CD1	1:C:179:VAL:HG13	2.52	0.45
1:D:5:VAL:CG2	1:D:24:HIS:CE1	2.99	0.45
1:D:198:LEU:HB3	1:D:200:GLN:HE21	1.81	0.45
1:E:35:GLU:HB3	1:E:100:GLN:HB3	1.99	0.44
1:D:150:TRP:NE1	1:D:179:VAL:HG13	2.31	0.44
1:C:5:VAL:CG2	1:C:24:HIS:CD2	2.99	0.44
1:C:19:THR:HG22	1:C:87:ILE:HD11	1.99	0.44
1:E:4:VAL:HG23	1:E:106:ASP:HB3	1.98	0.44
1:C:5:VAL:HG23	1:C:24:HIS:CE1	2.52	0.44
1:B:40:ARG:HD3	1:B:95:TYR:CD2	2.52	0.44
1:C:161:LEU:HD12	1:C:162:LYS:HG3	2.00	0.44
1:D:18:ASN:OD1	1:D:85:HIS:HA	2.18	0.44
1:A:4:VAL:HG12	1:A:108:ALA:HB2	1.99	0.44
1:B:35:GLU:HB3	1:B:100:GLN:HB3	2.00	0.43
1:D:40:ARG:HD3	1:D:95:TYR:CD2	2.54	0.43
1:E:153:PRO:HD3	1:E:186:VAL:HG13	2.01	0.43
2:M:1:NAG:H62	2:M:2:NAG:C7	2.47	0.43
1:B:123:ILE:HD11	1:B:191:CYS:HB3	2.01	0.43
1:C:40:ARG:HD3	1:C:95:TYR:CD2	2.53	0.43
1:E:37:ARG:HH21	1:E:51:LYS:HZ1	1.64	0.43
1:E:161:LEU:HD12	1:E:162:LYS:HE3	2.02	0.42
1:D:5:VAL:HG21	1:D:24:HIS:NE2	2.34	0.42
1:C:150:TRP:CE2	1:C:179:VAL:HG13	2.54	0.42
1:B:118:GLY:HA3	1:B:142:TRP:CE2	2.55	0.42
1:D:71:VAL:HB	1:D:81:ALA:HB3	2.02	0.42
1:D:128:HIS:CD2	1:D:214:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:THR:OG1	1:E:82:LEU:HD11	2.20	0.42
1:D:184:LYS:HG2	1:D:210:GLU:HG3	2.01	0.42
1:B:60:GLN:HE22	1:B:68:THR:HG21	1.85	0.41
1:A:13:ALA:HB2	1:A:112:LEU:HD11	2.01	0.41
1:E:214:PRO:HB2	1:E:216:VAL:HG13	2.01	0.41
1:A:115:ALA:HA	1:A:143:TYR:O	2.21	0.41
1:C:5:VAL:HG23	1:C:24:HIS:CD2	2.56	0.41
1:D:67:ARG:HG2	1:D:85:HIS:O	2.20	0.41
2:G:2:NAG:H61	2:G:3:BMA:C2	2.43	0.41
1:C:148:THR:HG21	1:C:177:THR:HG21	2.02	0.41
1:E:36:VAL:HG11	1:E:80:VAL:HG21	2.03	0.41
1:A:40:ARG:HD3	1:A:95:TYR:CD2	2.56	0.40
1:A:212:PHE:CE2	1:C:127:GLY:HA2	2.56	0.40
1:B:121:PRO:HB2	1:B:137:CYS:SG	2.61	0.40
1:C:35:GLU:HB3	1:C:100:GLN:HB3	2.02	0.40
1:D:12:LEU:HA	1:D:113:VAL:HG13	2.03	0.40
1:A:40:ARG:NH2	1:A:90:GLN:O	2.55	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	216/226 (96%)	210 (97%)	6 (3%)	0	100	100
1	B	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
1	C	215/226 (95%)	208 (97%)	7 (3%)	0	100	100
1	D	215/226 (95%)	207 (96%)	8 (4%)	0	100	100
1	E	215/226 (95%)	208 (97%)	7 (3%)	0	100	100
All	All	1077/1130 (95%)	1042 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	188/196 (96%)	175 (93%)	13 (7%)	15	48
1	B	188/196 (96%)	178 (95%)	10 (5%)	22	58
1	C	187/196 (95%)	179 (96%)	8 (4%)	29	63
1	D	187/196 (95%)	181 (97%)	6 (3%)	39	70
1	E	187/196 (95%)	182 (97%)	5 (3%)	44	74
All	All	937/980 (96%)	895 (96%)	42 (4%)	27	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	51	LYS
1	A	68	THR
1	A	91	GLU
1	A	107	GLU
1	A	138	ILE
1	A	145	LYS
1	A	147	LEU
1	A	148	THR
1	A	161	LEU
1	A	175	VAL
1	A	197	LEU
1	A	211	SER
1	B	33	ASP
1	B	68	THR
1	B	107	GLU
1	B	113	VAL
1	B	147	LEU
1	B	148	THR
1	B	161	LEU
1	B	175	VAL

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Mol	Chain	Res	Type
1	B	196	THR
1	B	211	SER
1	C	3	ILE
1	C	5	VAL
1	C	68	THR
1	C	91	GLU
1	C	107	GLU
1	C	136	GLU
1	C	161	LEU
1	C	211	SER
1	D	3	ILE
1	D	74	ASP
1	D	91	GLU
1	D	107	GLU
1	D	161	LEU
1	D	211	SER
1	E	91	GLU
1	E	107	GLU
1	E	138	ILE
1	E	161	LEU
1	E	175	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	GLN
1	D	60	GLN
1	D	200	GLN
1	E	60	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 (i)

23 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	F	1	1,2	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
2	NAG	F	2	2	14,14,15	0.35	0	17,19,21	1.54	4 (23%)
2	BMA	F	3	2	11,11,12	0.39	0	15,15,17	0.55	0
2	NAG	G	1	1,2	14,14,15	0.33	0	17,19,21	1.06	1 (5%)
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	1.58	3 (17%)
2	BMA	G	3	2	11,11,12	0.37	0	15,15,17	0.50	0
2	NAG	H	1	1,2	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
2	BMA	H	3	2	11,11,12	0.36	0	15,15,17	0.40	0
2	NAG	I	1	1,2	14,14,15	0.30	0	17,19,21	0.60	0
2	NAG	I	2	2	14,14,15	0.41	0	17,19,21	1.63	4 (23%)
2	BMA	I	3	2	11,11,12	0.39	0	15,15,17	0.42	0
2	NAG	J	1	1,2	14,14,15	0.34	0	17,19,21	1.23	1 (5%)
2	NAG	J	2	2	14,14,15	0.33	0	17,19,21	1.60	3 (17%)
2	BMA	J	3	2	11,11,12	0.29	0	15,15,17	0.61	0
3	NAG	K	1	3,1	14,14,15	0.42	0	17,19,21	1.08	2 (11%)
3	NAG	K	2	3	14,14,15	0.53	0	17,19,21	1.50	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.27	0	17,19,21	1.08	1 (5%)
2	NAG	L	2	2	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
2	BMA	L	3	2	11,11,12	0.37	0	15,15,17	0.55	0
2	NAG	M	1	1,2	14,14,15	0.35	0	17,19,21	0.74	0
2	NAG	M	2	2	14,14,15	0.54	0	17,19,21	1.69	4 (23%)
2	BMA	M	3	2	11,11,12	0.42	0	15,15,17	0.68	1 (6%)

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	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C1-O5-C5	4.89	118.82	112.19
2	J	1	NAG	C1-C2-N2	-4.39	102.98	110.49
2	M	2	NAG	C1-C2-N2	4.19	117.64	110.49
2	G	2	NAG	C1-O5-C5	4.16	117.83	112.19
2	J	2	NAG	O5-C1-C2	-4.10	104.82	111.29
2	F	2	NAG	C1-O5-C5	3.87	117.44	112.19
2	I	2	NAG	C1-O5-C5	3.77	117.30	112.19
2	M	2	NAG	C1-O5-C5	3.76	117.29	112.19
2	J	2	NAG	C1-O5-C5	3.68	117.18	112.19
2	L	1	NAG	C1-C2-N2	-3.47	104.57	110.49
2	I	2	NAG	O4-C4-C5	3.36	117.63	109.30
3	K	2	NAG	O5-C1-C2	3.27	116.45	111.29
3	K	1	NAG	C1-C2-N2	3.25	116.05	110.49
2	M	2	NAG	C2-N2-C7	3.20	127.46	122.90
2	G	1	NAG	C1-C2-N2	-3.19	105.04	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	O5-C1-C2	-3.14	106.33	111.29
2	L	2	NAG	C1-O5-C5	3.03	116.30	112.19
2	I	2	NAG	O5-C1-C2	2.97	115.97	111.29
2	F	2	NAG	C1-C2-N2	2.96	115.55	110.49
2	H	2	NAG	C1-O5-C5	2.75	115.92	112.19
2	G	2	NAG	C1-C2-N2	2.71	115.11	110.49
2	J	2	NAG	C1-C2-N2	2.59	114.91	110.49
2	F	1	NAG	C1-C2-N2	-2.31	106.54	110.49
2	M	2	NAG	O4-C4-C5	2.28	114.97	109.30
2	L	2	NAG	C1-C2-N2	2.20	114.24	110.49
2	M	3	BMA	C1-O5-C5	2.17	115.14	112.19
2	F	2	NAG	O5-C1-C2	-2.14	107.90	111.29
2	F	2	NAG	O4-C4-C5	2.12	114.56	109.30
2	I	2	NAG	C1-C2-N2	-2.07	106.96	110.49
3	K	1	NAG	C2-N2-C7	2.03	125.79	122.90

There are no chirality outliers.
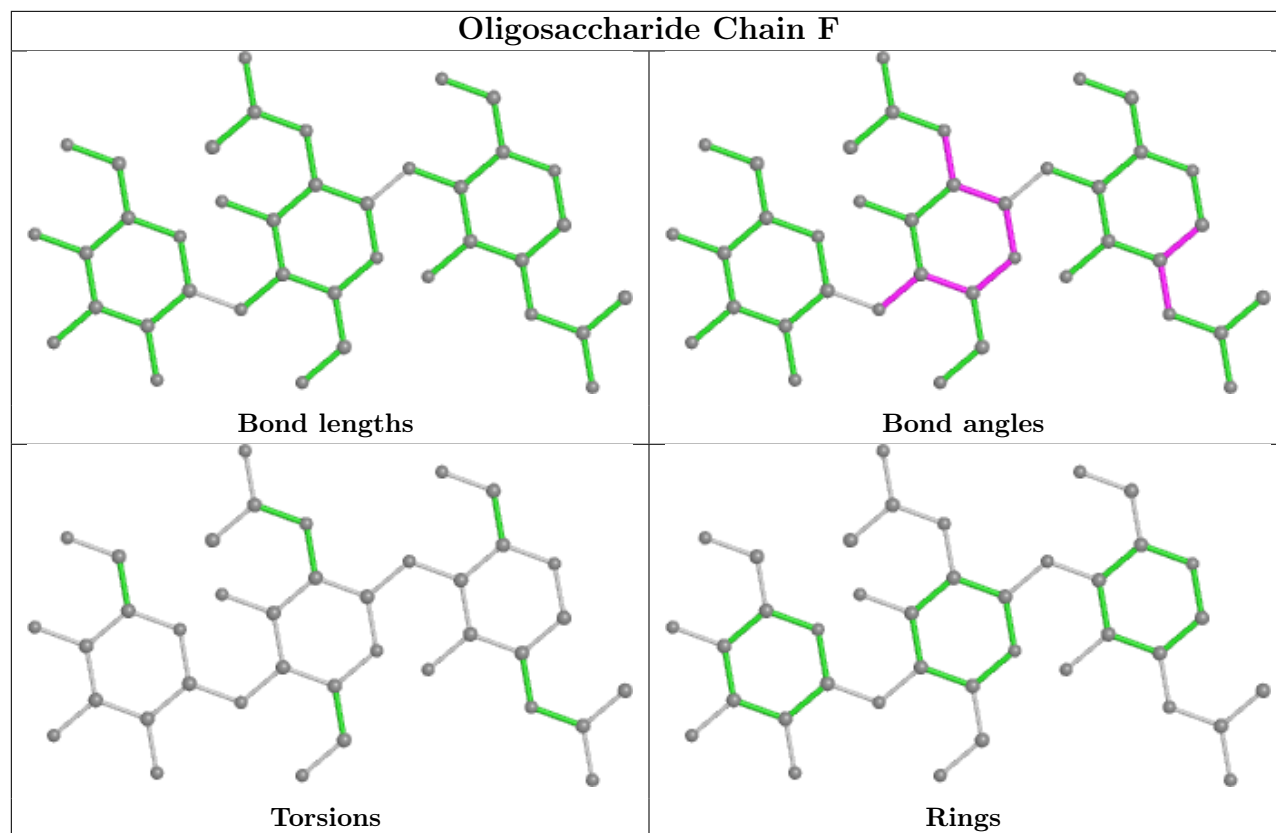
All (4) torsion outliers are listed below:

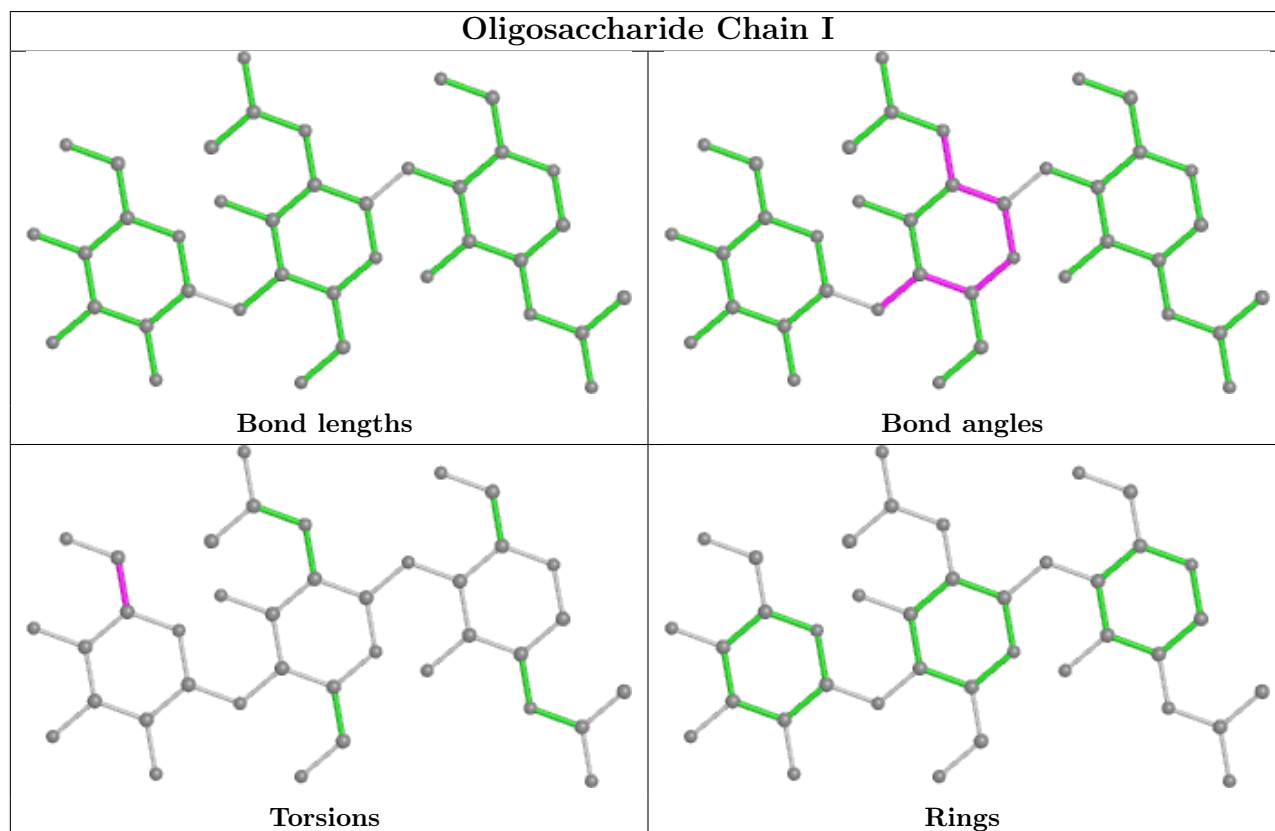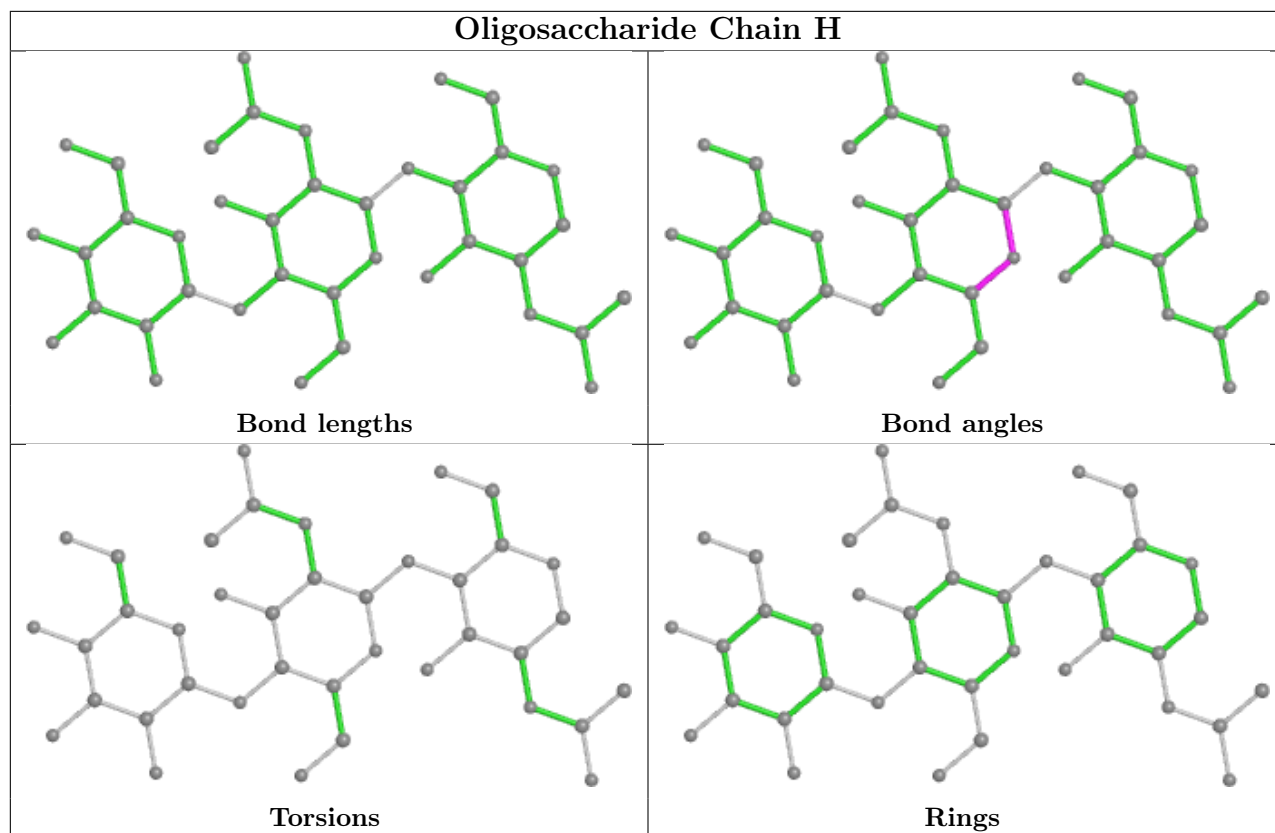| Mol	Chain	Res	Type	Atoms
2	I	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C3-C2-N2-C7
2	M	2	NAG	C3-C2-N2-C7

There are no ring outliers.

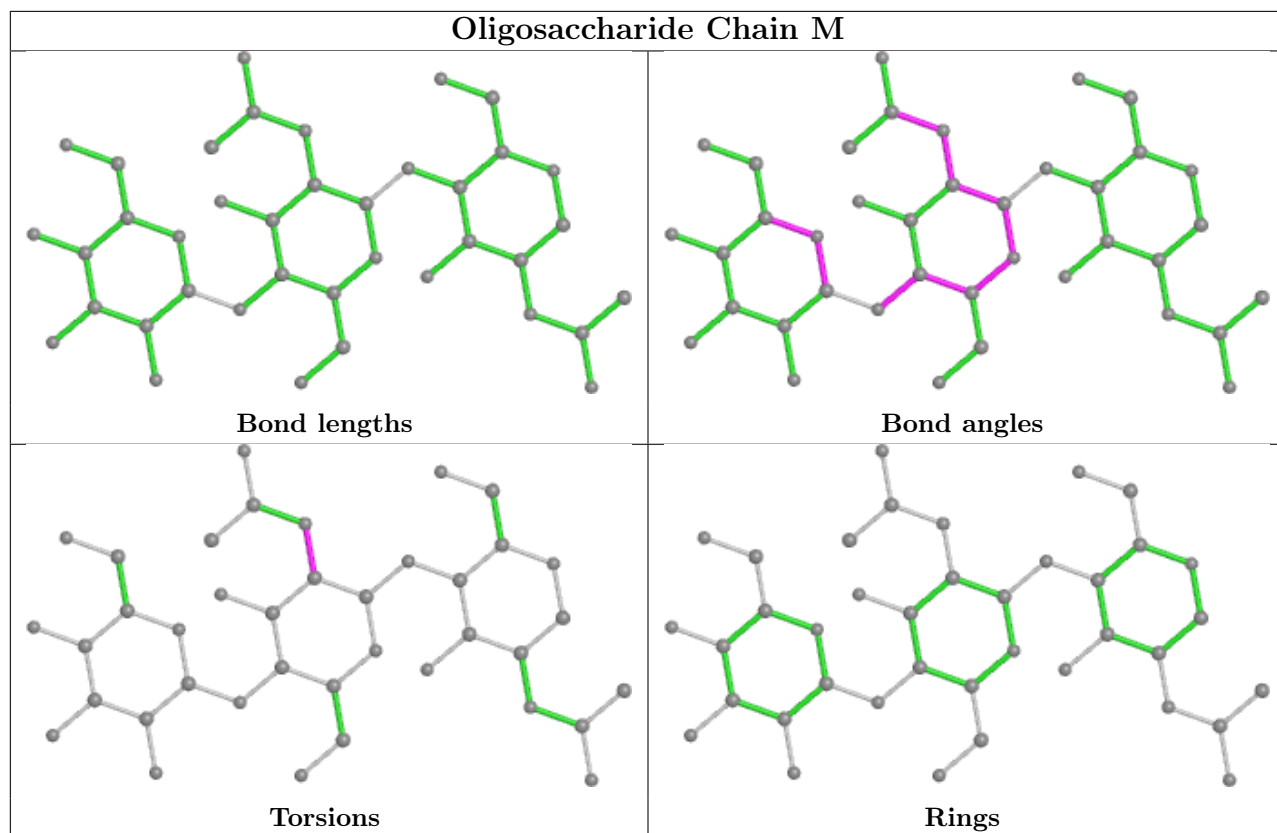7 monomers are involved in 5 short contacts:

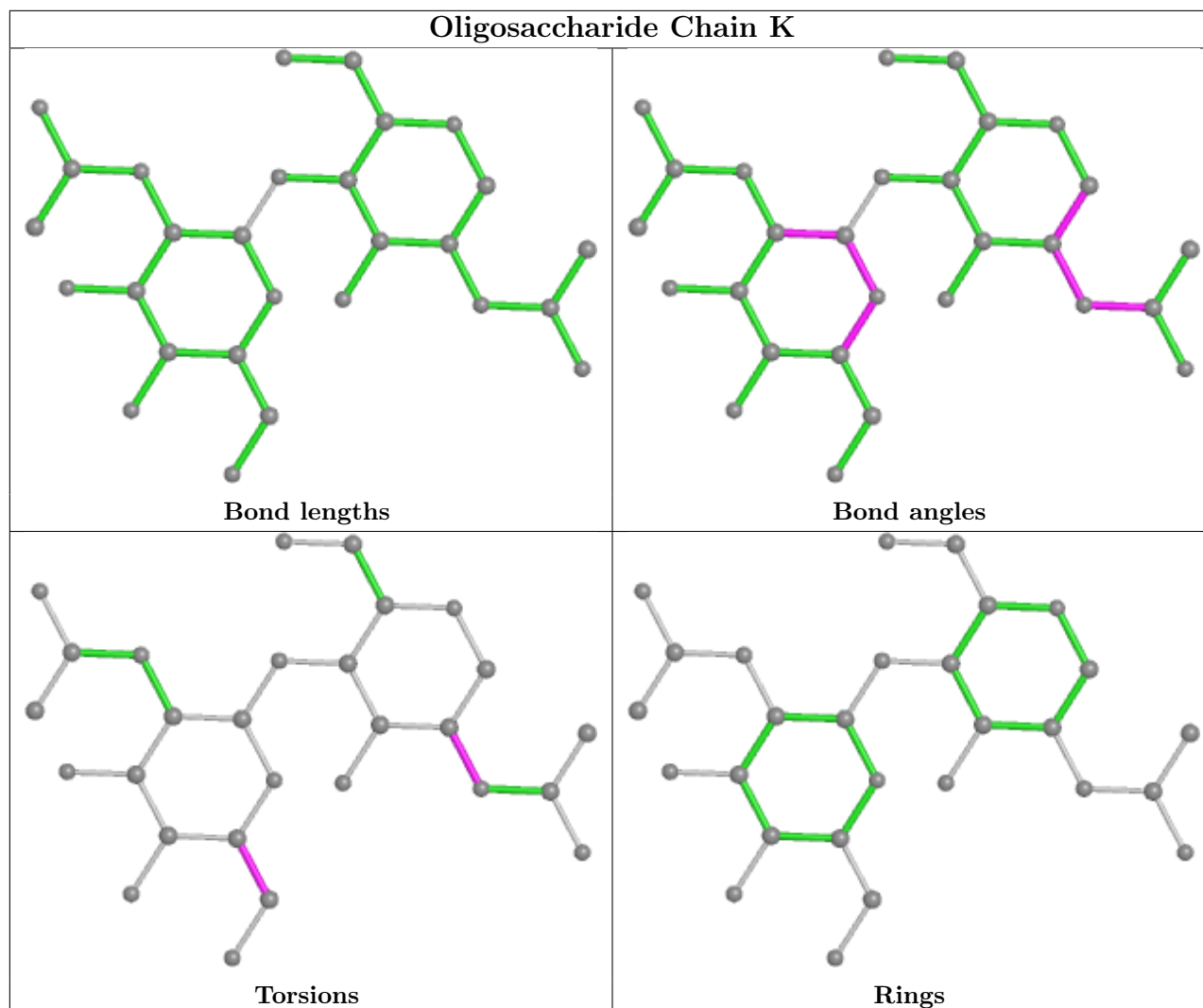| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	NAG	1	0
2	I	2	NAG	1	0
2	I	3	BMA	1	0
2	G	2	NAG	2	0
2	J	1	NAG	1	0
2	M	2	NAG	1	0
2	G	3	BMA	2	0

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

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths　　Bond angles

Torsions　　Rings

5.6 Ligand geometry ⓘ

12 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	$\#|Z| > 2$
4	NAG	D	301	1	14,14,15	0.37	0	17,19,21	0.92	2 (11%)
4	NAG	D	302	1	14,14,15	0.33	0	17,19,21	1.07	2 (11%)
4	NAG	A	302	1	14,14,15	0.36	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	C	301	1	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	A	301	1	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	C	302	1	14,14,15	0.31	0	17,19,21	0.82	1 (5%)
4	NAG	B	302	1	14,14,15	0.46	0	17,19,21	1.03	2 (11%)
4	NAG	B	301	1	14,14,15	0.35	0	17,19,21	0.98	2 (11%)
4	NAG	E	302	1	14,14,15	0.48	0	17,19,21	1.00	1 (5%)
4	NAG	E	301	1	14,14,15	0.38	0	17,19,21	0.83	0
4	NAG	B	303	1	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
4	NAG	A	303	1	14,14,15	0.43	0	17,19,21	1.26	3 (17%)

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	D	301	1	-	1/6/23/26	0/1/1/1
4	NAG	D	302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	301	1	-	1/6/23/26	0/1/1/1
4	NAG	E	302	1	-	2/6/23/26	0/1/1/1
4	NAG	E	301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	303	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	302	NAG	C1-O5-C5	2.86	116.06	112.19
4	B	301	NAG	C1-C2-N2	2.82	115.31	110.49
4	E	302	NAG	O5-C1-C2	2.78	115.68	111.29
4	A	303	NAG	C2-N2-C7	2.76	126.83	122.90
4	A	303	NAG	C1-O5-C5	2.73	115.89	112.19
4	B	302	NAG	C1-C2-N2	2.72	115.14	110.49
4	B	301	NAG	C1-O5-C5	2.67	115.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	302	NAG	O5-C1-C2	-2.63	107.14	111.29
4	D	301	NAG	C1-C2-N2	2.59	114.92	110.49
4	A	303	NAG	C1-C2-N2	2.40	114.59	110.49
4	C	301	NAG	O5-C1-C2	-2.38	107.53	111.29
4	D	301	NAG	C1-O5-C5	2.22	115.20	112.19
4	B	303	NAG	C1-O5-C5	2.16	115.12	112.19
4	C	302	NAG	C1-C2-N2	2.12	114.12	110.49
4	B	302	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	NAG	C1-C2-N2-C7
4	E	301	NAG	O5-C5-C6-O6
4	A	301	NAG	O5-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
4	D	301	NAG	O5-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6
4	E	302	NAG	O5-C5-C6-O6
4	A	302	NAG	O5-C5-C6-O6
4	C	302	NAG	C1-C2-N2-C7
4	B	303	NAG	C3-C2-N2-C7
4	E	302	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/226 (96%)	0.46	11 (5%)	28	18	171, 260, 288, 294	0
1	B	218/226 (96%)	0.52	10 (4%)	32	20	188, 246, 282, 287	0
1	C	217/226 (96%)	0.98	34 (15%)	2	1	165, 294, 300, 300	0
1	D	217/226 (96%)	0.78	27 (12%)	4	3	188, 285, 297, 300	0
1	E	217/226 (96%)	0.80	25 (11%)	4	4	271, 286, 299, 300	0
All	All	1087/1130 (96%)	0.71	107 (9%)	7	5	165, 282, 297, 300	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	VAL	7.2
1	C	59	GLU	6.8
1	E	101	GLU	6.5
1	C	99	PHE	5.9
1	E	125	MET	4.8
1	D	47	VAL	4.8
1	C	34	MET	4.8
1	C	2	PHE	4.8
1	E	79	SER	4.6
1	C	70	PHE	4.5
1	E	189	MET	4.4
1	A	131	GLY	4.3
1	C	47	VAL	4.2
1	D	215	SER	4.0
1	C	127	GLY	3.8
1	D	4	VAL	3.7
1	E	48	PHE	3.7
1	E	181	ILE	3.7
1	D	36	VAL	3.7
1	E	4	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	125	MET	3.6
1	D	79	SER	3.5
1	C	36	VAL	3.5
1	C	21	LEU	3.5
1	E	50	TYR	3.3
1	D	114	VAL	3.3
1	E	99	PHE	3.3
1	E	126	ARG	3.2
1	C	5	VAL	3.2
1	C	101	GLU	3.2
1	E	70	PHE	3.2
1	C	38	TRP	3.0
1	C	84	ILE	3.0
1	D	80	VAL	2.9
1	B	43	PHE	2.9
1	C	114	VAL	2.9
1	B	110	LEU	2.9
1	D	105	TYR	2.9
1	B	154	TYR	2.8
1	B	166	MET	2.8
1	B	153	PRO	2.8
1	A	69	THR	2.7
1	C	50	TYR	2.7
1	D	98	TYR	2.7
1	E	96	ARG	2.7
1	C	49	VAL	2.7
1	C	6	GLY	2.6
1	E	47	VAL	2.6
1	C	60	GLN	2.6
1	D	34	MET	2.5
1	D	13	ALA	2.5
1	C	110	LEU	2.5
1	D	182	ARG	2.5
1	C	103	ARG	2.5
1	E	167	PRO	2.5
1	C	41	SER	2.4
1	C	51	LYS	2.4
1	E	2	PHE	2.4
1	D	82	LEU	2.4
1	C	126	ARG	2.3
1	C	48	PHE	2.3
1	E	100	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	TYR	2.3
1	E	80	VAL	2.3
1	D	212	PHE	2.3
1	D	50	TYR	2.2
1	D	99	PHE	2.2
1	D	141	GLY	2.2
1	E	166	MET	2.2
1	C	134	ARG	2.2
1	A	-1	THR	2.2
1	D	59	GLU	2.2
1	B	12	LEU	2.2
1	C	3	ILE	2.2
1	C	69	THR	2.2
1	A	64	TYR	2.2
1	D	39	PHE	2.2
1	A	13	ALA	2.2
1	D	133	ILE	2.2
1	E	193	ILE	2.2
1	B	-1	THR	2.2
1	B	112	LEU	2.2
1	E	133	ILE	2.2
1	E	71	VAL	2.1
1	E	139	SER	2.1
1	D	107	GLU	2.1
1	C	162	LYS	2.1
1	A	99	PHE	2.1
1	B	47	VAL	2.1
1	D	41	SER	2.1
1	A	52	GLY	2.1
1	A	61	MET	2.1
1	C	46	ALA	2.1
1	D	129	GLU	2.1
1	D	21	LEU	2.1
1	E	49	VAL	2.1
1	E	180	ILE	2.1
1	A	65	ARG	2.1
1	C	33	ASP	2.0
1	C	80	VAL	2.0
1	C	11	ILE	2.0
1	E	38	TRP	2.0
1	B	4	VAL	2.0
1	A	49	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	38	TRP	2.0
1	D	35	GLU	2.0
1	A	7	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	BMA	F	3	11/12	0.47	0.42	280,281,284,284	0
2	BMA	I	3	11/12	0.48	0.33	278,280,282,282	0
2	BMA	M	3	11/12	0.49	0.86	300,300,300,300	0
2	NAG	M	2	14/15	0.57	0.56	300,300,300,300	0
3	NAG	K	1	14/15	0.57	0.54	280,281,281,282	0
2	NAG	M	1	14/15	0.65	0.49	296,299,300,300	0
2	BMA	J	3	11/12	0.70	0.22	290,292,295,295	0
2	NAG	I	1	14/15	0.73	0.30	285,286,287,287	0
2	BMA	G	3	11/12	0.76	0.22	275,275,276,276	0
2	BMA	H	3	11/12	0.77	0.30	299,300,300,300	0
2	NAG	G	2	14/15	0.82	0.41	262,278,279,279	0
2	NAG	I	2	14/15	0.82	0.21	283,285,288,289	0
2	NAG	L	2	14/15	0.83	0.27	269,279,287,289	0
2	NAG	L	1	14/15	0.84	0.30	244,274,279,280	0
2	BMA	L	3	11/12	0.84	0.19	267,278,289,292	0
2	NAG	F	2	14/15	0.85	0.32	233,252,281,281	0
2	NAG	H	1	14/15	0.87	0.26	295,296,297,297	0
2	NAG	J	2	14/15	0.87	0.30	281,290,293,294	0
2	NAG	J	1	14/15	0.88	0.27	191,264,275,278	0
2	NAG	H	2	14/15	0.88	0.21	297,298,299,299	0
3	NAG	K	2	14/15	0.89	0.17	280,281,283,283	0
2	NAG	G	1	14/15	0.93	0.32	222,232,252,252	0
2	NAG	F	1	14/15	0.94	0.29	190,203,216,225	0

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

charide. Each fit is shown from different orientation to approximate a three-dimensional view.
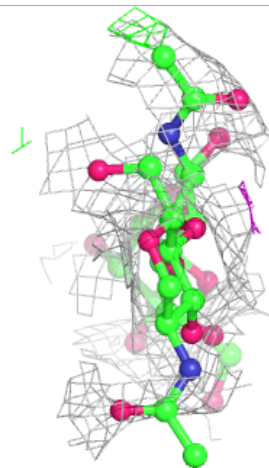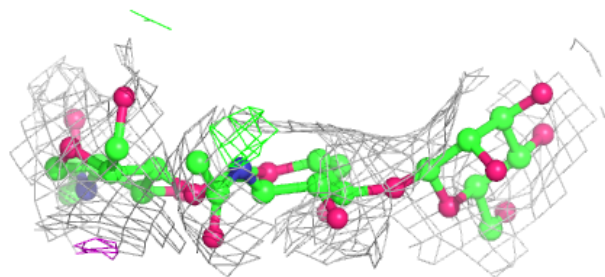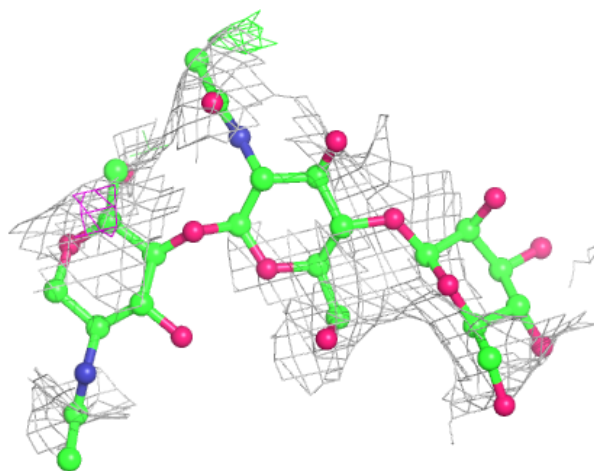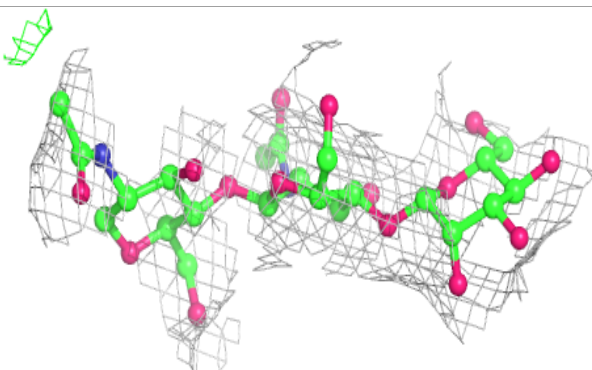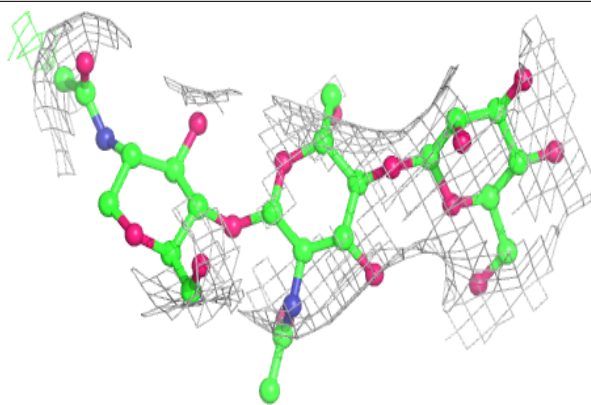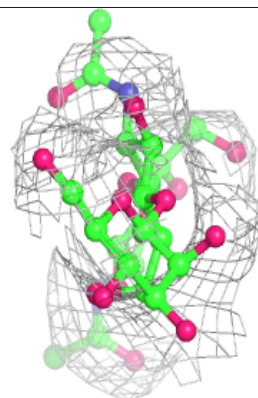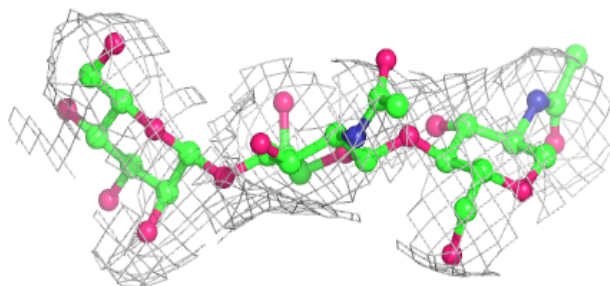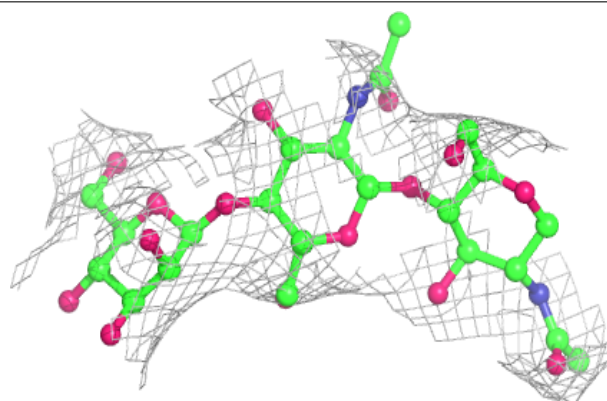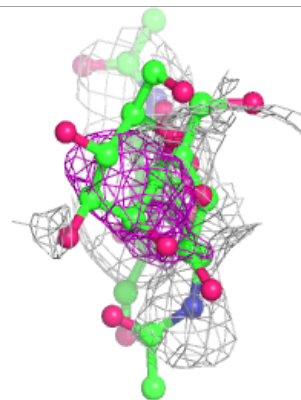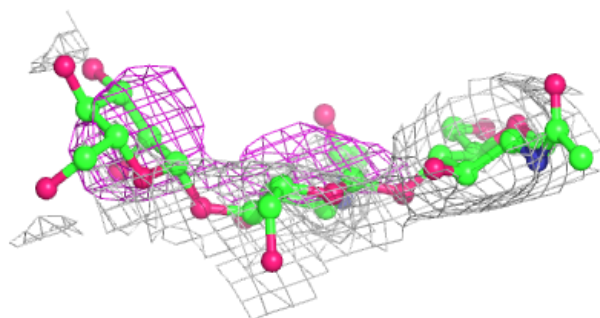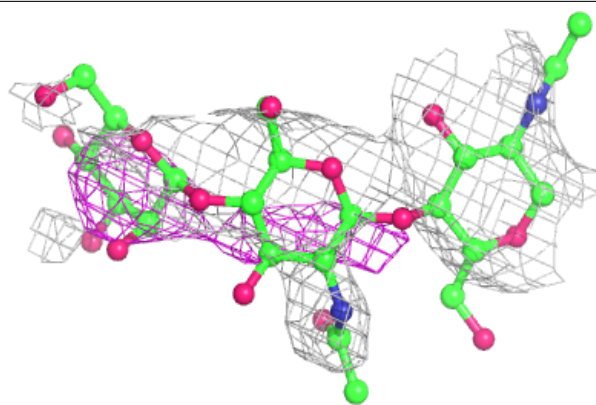
Electron density around Chain F:

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 G:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
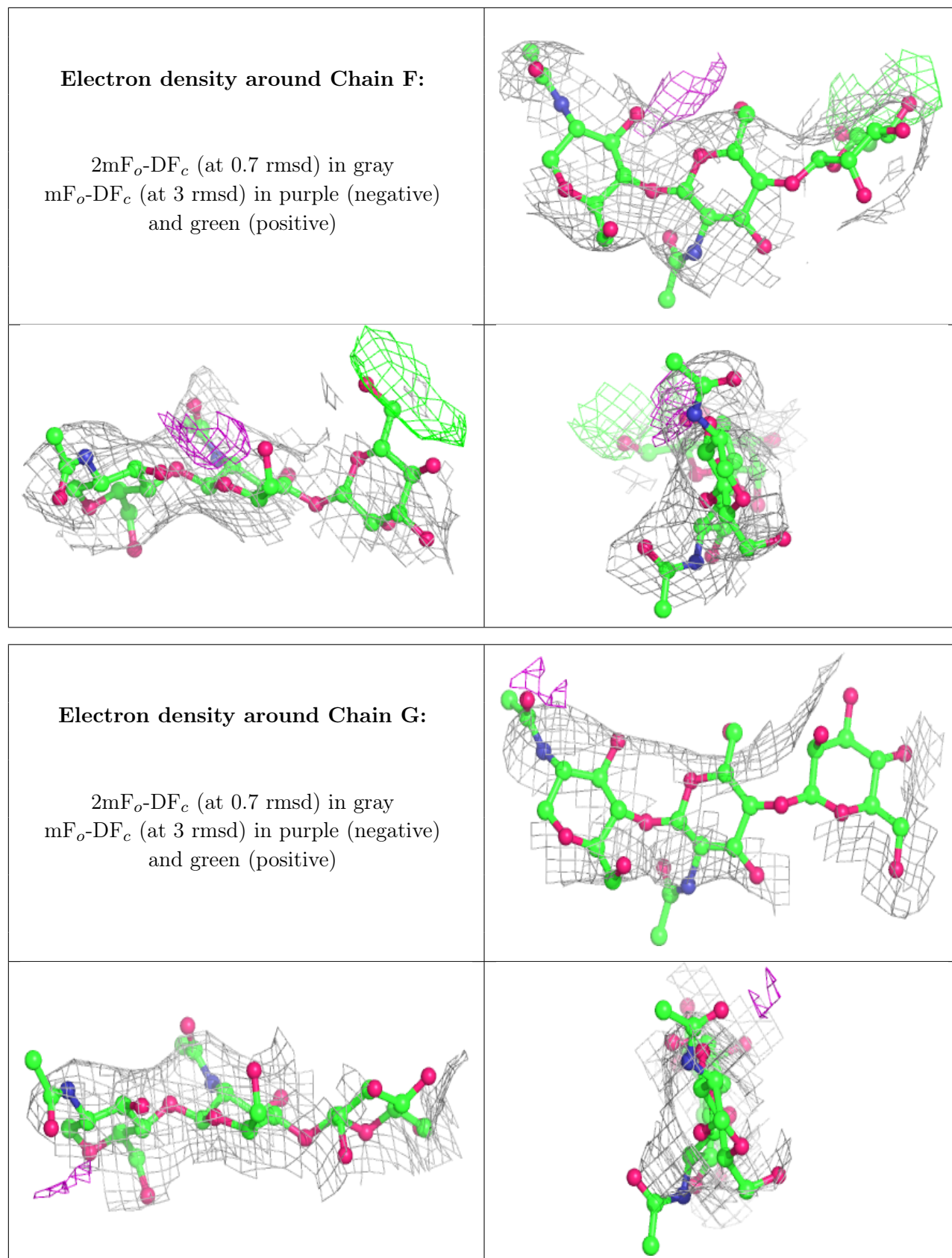
Electron density around Chain H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
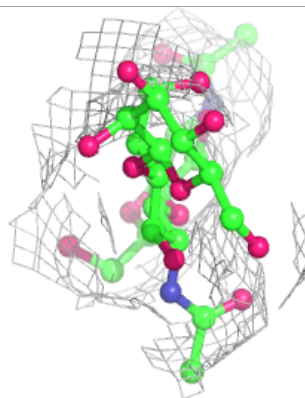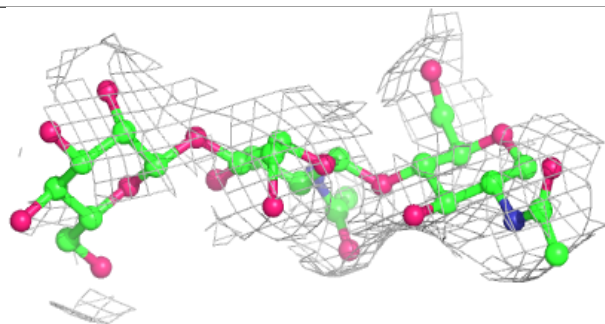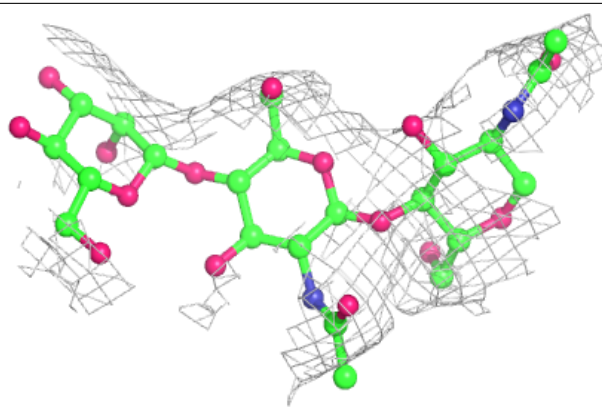
Electron density around Chain I:

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 J:

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 L:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
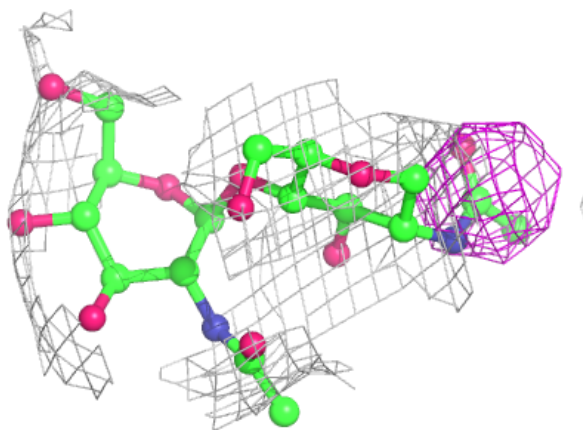and green (positive)

Electron density around Chain M:

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 K:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
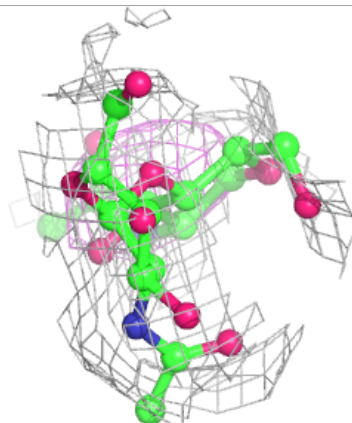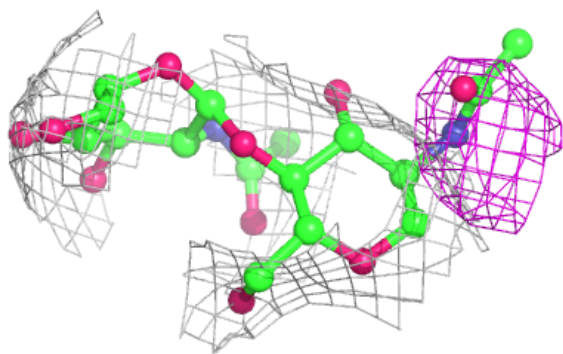
6.4 Ligands ⓘ

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(Å²)	Q<0.9
4	NAG	B	303	14/15	0.19	0.69	286,288,290,291	0
4	NAG	D	301	14/15	0.52	0.39	284,286,289,289	0
4	NAG	B	301	14/15	0.62	0.28	282,283,284,284	0
4	NAG	A	301	14/15	0.64	0.29	284,287,288,289	0
4	NAG	C	301	14/15	0.67	0.32	297,298,299,299	0
4	NAG	E	302	14/15	0.68	0.31	285,285,285,286	0
4	NAG	E	301	14/15	0.69	0.41	285,286,286,287	0
4	NAG	B	302	14/15	0.71	0.33	254,259,264,265	0
4	NAG	A	303	14/15	0.71	0.25	289,291,293,293	0
4	NAG	D	302	14/15	0.84	0.18	289,292,293,295	0
4	NAG	A	302	14/15	0.85	0.19	273,275,280,281	0
4	NAG	C	302	14/15	0.87	0.28	295,296,296,296	0

6.5 Other polymers ⓘ

There are no such residues in this entry.