Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 03:00 PM JST

PDB ID	:	5XGR
Title	:	Structure of the S1 subunit C-terminal domain from bat-derived coronavirus HKU5 spike protein
Authors	:	Xue, H.; Qi, J.; Song, H.; Qihui, W.; Shi, Y.; Gao, G.F.
Deposited on	:	2017-04-16
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) 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 2.10 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.
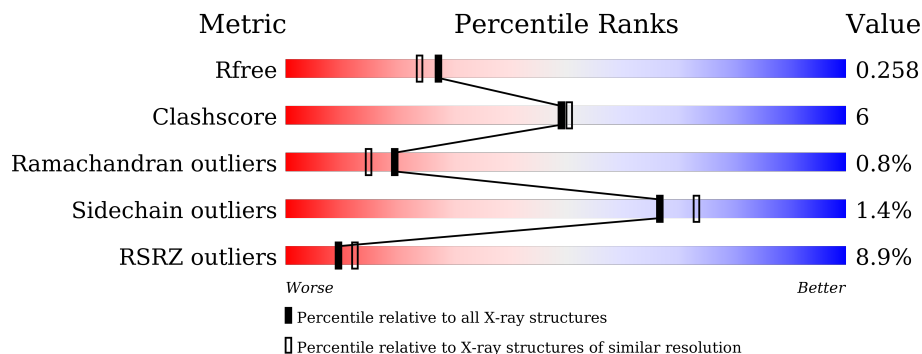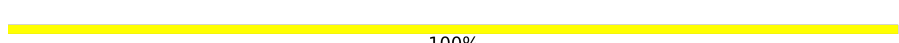

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	204	6% / 89% / 8% ·
1	B	204	9% / 85% / 10% ··
1	C	204	6% / 87% / 9% ·
1	D	204	2% / 85% / 11% ·
1	E	204	12% / 81% / 15% ··
1	F	204	11% / 80% / 17% ·

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Mol	Chain	Length	Quality of chain
1	G	204	13% / 82% / 14%
1	H	204	10% / 84% / 11%
2	I	2	50% / 50%
2	J	2	100%
2	K	2	50% / 50%
2	L	2	100%
2	M	2	100%
2	N	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	NAG	K	2	-	-	-	X
3	NAG	G	603	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13125 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	B	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	C	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	D	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	E	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	F	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	G	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0
1	H	198	Total 1538	C 981	N 241	O 304	S 12	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	HIS	-	expression tag	UNP A3EXD0
A	200	HIS	-	expression tag	UNP A3EXD0
A	201	HIS	-	expression tag	UNP A3EXD0
A	202	HIS	-	expression tag	UNP A3EXD0
A	203	HIS	-	expression tag	UNP A3EXD0
A	204	HIS	-	expression tag	UNP A3EXD0
B	199	HIS	-	expression tag	UNP A3EXD0
B	200	HIS	-	expression tag	UNP A3EXD0
B	201	HIS	-	expression tag	UNP A3EXD0
B	202	HIS	-	expression tag	UNP A3EXD0
B	203	HIS	-	expression tag	UNP A3EXD0
B	204	HIS	-	expression tag	UNP A3EXD0
C	199	HIS	-	expression tag	UNP A3EXD0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	200	HIS	-	expression tag	UNP A3EXD0
C	201	HIS	-	expression tag	UNP A3EXD0
C	202	HIS	-	expression tag	UNP A3EXD0
C	203	HIS	-	expression tag	UNP A3EXD0
C	204	HIS	-	expression tag	UNP A3EXD0
D	199	HIS	-	expression tag	UNP A3EXD0
D	200	HIS	-	expression tag	UNP A3EXD0
D	201	HIS	-	expression tag	UNP A3EXD0
D	202	HIS	-	expression tag	UNP A3EXD0
D	203	HIS	-	expression tag	UNP A3EXD0
D	204	HIS	-	expression tag	UNP A3EXD0
E	199	HIS	-	expression tag	UNP A3EXD0
E	200	HIS	-	expression tag	UNP A3EXD0
E	201	HIS	-	expression tag	UNP A3EXD0
E	202	HIS	-	expression tag	UNP A3EXD0
E	203	HIS	-	expression tag	UNP A3EXD0
E	204	HIS	-	expression tag	UNP A3EXD0
F	199	HIS	-	expression tag	UNP A3EXD0
F	200	HIS	-	expression tag	UNP A3EXD0
F	201	HIS	-	expression tag	UNP A3EXD0
F	202	HIS	-	expression tag	UNP A3EXD0
F	203	HIS	-	expression tag	UNP A3EXD0
F	204	HIS	-	expression tag	UNP A3EXD0
G	199	HIS	-	expression tag	UNP A3EXD0
G	200	HIS	-	expression tag	UNP A3EXD0
G	201	HIS	-	expression tag	UNP A3EXD0
G	202	HIS	-	expression tag	UNP A3EXD0
G	203	HIS	-	expression tag	UNP A3EXD0
G	204	HIS	-	expression tag	UNP A3EXD0
H	199	HIS	-	expression tag	UNP A3EXD0
H	200	HIS	-	expression tag	UNP A3EXD0
H	201	HIS	-	expression tag	UNP A3EXD0
H	202	HIS	-	expression tag	UNP A3EXD0
H	203	HIS	-	expression tag	UNP A3EXD0
H	204	HIS	-	expression tag	UNP A3EXD0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
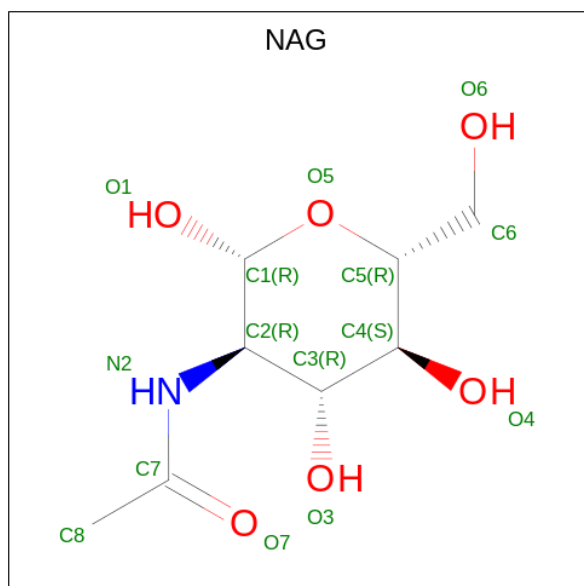
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	E	1	Total 14	C 8	N 1	O 5	0	0
3	F	1	Total 14	C 8	N 1	O 5	0	0
3	G	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total 59	O 59	0	0
4	B	60	Total 60	O 60	0	0
4	C	102	Total 102	O 102	0	0
4	D	101	Total 101	O 101	0	0
4	E	54	Total 54	O 54	0	0
4	F	36	Total 36	O 36	0	0
4	G	57	Total 57	O 57	0	0
4	H	58	Total 58	O 58	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.
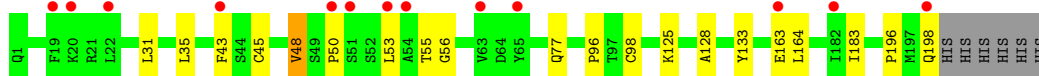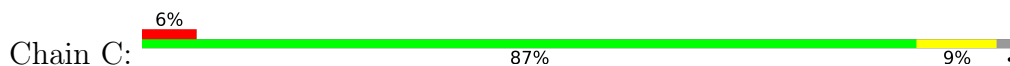
• Molecule 1: Spike protein S1
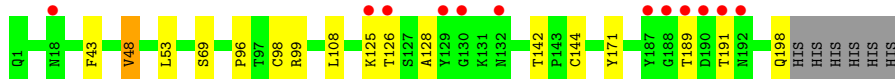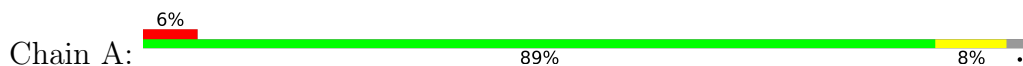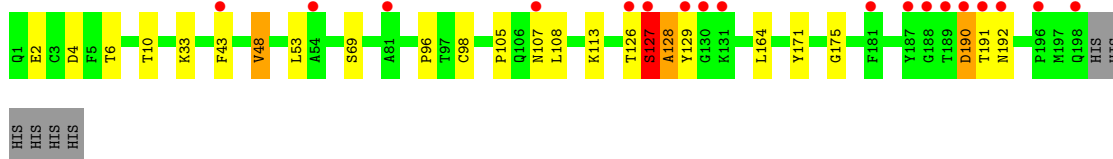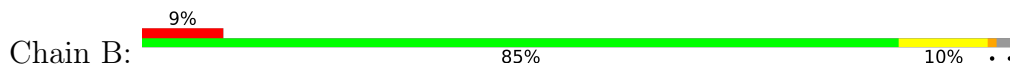
• Molecule 1: Spike protein S1

• Molecule 1: Spike protein S1

• Molecule 1: Spike protein S1
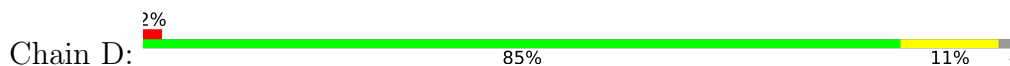

• Molecule 1: Spike protein S1

• Molecule 1: Spike protein S1
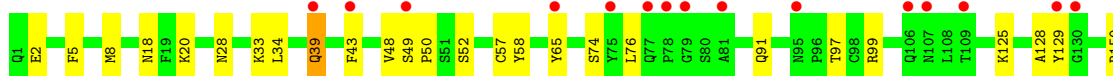
Chain F:

• Molecule 1: Spike protein S1

Chain G:

• Molecule 1: Spike protein S1

Chain H:

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

Chain I:

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

Chain J:
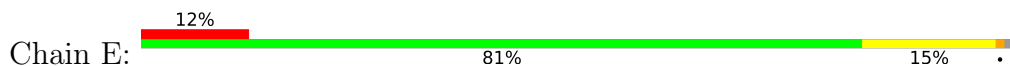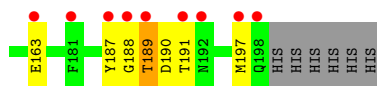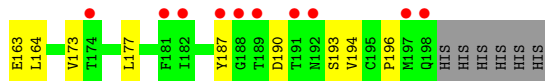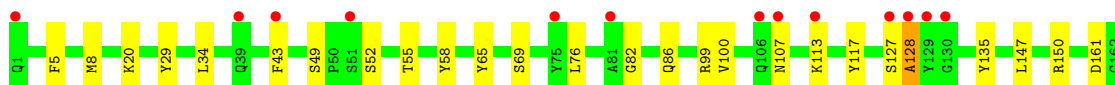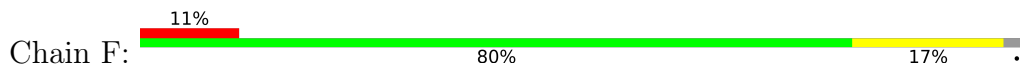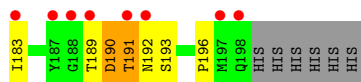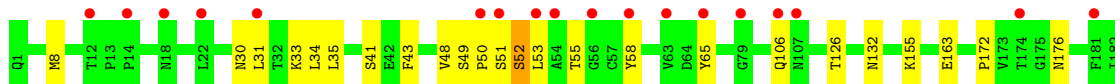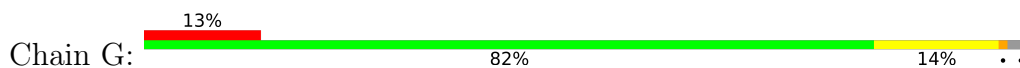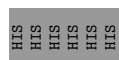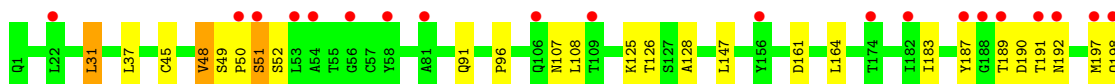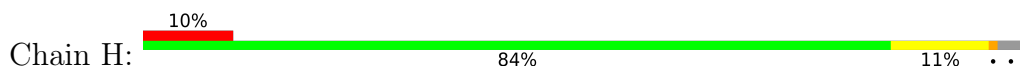
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain K:

50%   50%

MAG1 NAG2

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

Chain L:

100%

NAG1 NAG2

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

Chain M:

100%

MAG1 NAG2

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

Chain N:

100%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.61Å 212.66Å 87.94Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	37.80 – 2.10 38.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.80-2.10) 99.6 (38.26-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.216 , 0.259 0.218 , 0.258	Depositor DCC
R_{free} test set	5244 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13125	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3008e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/1580	0.51	0/2159
1	B	0.33	0/1580	0.56	2/2159 (0.1%)
1	C	0.33	0/1580	0.52	0/2159
1	D	0.32	0/1580	0.52	0/2159
1	E	0.35	0/1580	0.55	0/2159
1	F	0.29	0/1580	0.47	0/2159
1	G	0.36	0/1580	0.55	0/2159
1	H	0.31	0/1580	0.49	0/2159
All	All	0.32	0/12640	0.52	2/17272 (0.0%)

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	B	0	2
1	H	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	SER	N-CA-C	6.60	128.81	111.00
1	B	190	ASP	CB-CG-OD1	6.46	124.12	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	B	126	THR	Peptide
1	B	127	SER	Peptide
1	H	50	PRO	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	1538	0	1465	13	0
1	B	1538	0	1465	20	0
1	C	1538	0	1465	15	0
1	D	1538	0	1465	18	0
1	E	1538	0	1465	24	0
1	F	1538	0	1465	26	0
1	G	1538	0	1465	18	0
1	H	1538	0	1466	17	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	2	0
2	N	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
3	C	14	0	13	0	0
3	D	14	0	13	1	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
3	G	14	0	13	2	0
4	A	59	0	0	3	0
4	B	60	0	0	0	0
4	C	102	0	0	2	1
4	D	101	0	0	4	1
4	E	54	0	0	3	0
4	F	36	0	0	2	0
4	G	57	0	0	4	0
4	H	58	0	0	4	0
All	All	13125	0	11988	146	1

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 6.

All (146) 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:D:142:THR:HG22	1:D:144:CYS:H	1.31	0.94
1:B:127:SER:OG	1:B:128:ALA:N	2.05	0.88
1:F:113:LYS:HG2	1:F:177:LEU:HB2	1.60	0.82
1:D:156:TYR:O	4:D:701:HOH:O	1.97	0.81
1:H:126:THR:O	4:H:701:HOH:O	1.99	0.80
1:A:142:THR:HG22	1:A:144:CYS:H	1.48	0.78
1:H:125:LYS:HG3	1:H:164:LEU:HD23	1.65	0.77
1:A:125:LYS:HD2	1:A:126:THR:N	1.98	0.77
1:B:127:SER:HG	1:B:128:ALA:H	1.31	0.76
1:E:129:TYR:OH	1:F:113:LYS:HE2	1.88	0.74
1:H:48:VAL:HG13	1:H:96:PRO:HB3	1.72	0.71
4:G:701:HOH:O	2:M:2:NAG:O3	2.09	0.71
1:A:108:LEU:O	4:A:701:HOH:O	2.09	0.70
1:B:190:ASP:O	1:B:192:ASN:N	2.25	0.70
1:H:96:PRO:HG2	1:H:187:TYR:HE2	1.57	0.68
1:B:2:GLU:OE2	1:B:33:LYS:NZ	2.22	0.67
1:B:127:SER:HB2	1:B:129:TYR:H	1.60	0.67
1:E:18:ASN:OD1	4:E:701:HOH:O	2.14	0.65
1:C:77:GLN:NE2	4:C:705:HOH:O	2.29	0.65
1:H:197:MET:O	1:H:198:GLN:HG3	1.96	0.65
1:E:189:THR:OG1	1:E:190:ASP:N	2.30	0.64
1:E:125:LYS:HE3	1:E:163:GLU:HB2	1.80	0.63
1:G:55:THR:HA	1:G:196:PRO:HG3	1.81	0.63
1:A:142:THR:HG23	4:A:711:HOH:O	1.99	0.62
1:A:43:PHE:CZ	1:C:50:PRO:HB3	2.35	0.62
1:H:37:LEU:O	4:H:702:HOH:O	2.16	0.61
3:G:603:NAG:O3	3:G:603:NAG:H82	1.99	0.61
1:A:48:VAL:HG22	1:A:96:PRO:HB3	1.83	0.61
4:G:706:HOH:O	2:M:1:NAG:H2	1.99	0.61
1:F:86:GLN:HB3	1:F:135:TYR:HD1	1.65	0.60
1:E:43:PHE:CZ	1:E:50:PRO:HB3	2.36	0.60
1:A:198:GLN:O	4:A:702:HOH:O	2.16	0.60
1:C:133:TYR:OH	4:C:701:HOH:O	2.16	0.60
1:D:77:GLN:NE2	4:D:706:HOH:O	2.33	0.60
1:E:74:SER:OG	4:E:702:HOH:O	2.15	0.60
1:E:43:PHE:HZ	1:E:50:PRO:HB3	1.66	0.60
1:G:155:LYS:NZ	1:H:189:THR:HG21	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:HG23	4:D:717:HOH:O	2.03	0.58
1:F:82:GLY:O	1:F:86:GLN:HG3	2.03	0.58
1:G:41:SER:OG	4:G:702:HOH:O	2.17	0.58
1:B:43:PHE:CZ	1:D:50:PRO:HB3	2.39	0.58
1:E:39:GLN:NE2	1:E:39:GLN:HA	2.19	0.57
1:H:45:CYS:HB3	1:H:48:VAL:HG23	1.86	0.57
1:B:48:VAL:HG22	1:B:96:PRO:HB3	1.87	0.57
1:B:69:SER:OG	1:B:171:TYR:OH	2.21	0.57
1:G:49:SER:O	1:G:52:SER:HB3	2.05	0.56
1:C:31:LEU:HD21	1:C:183:ILE:HD13	1.87	0.56
1:F:49:SER:OG	1:F:52:SER:OG	2.22	0.56
1:B:107:ASN:OD1	1:B:108:LEU:N	2.39	0.56
1:E:28:ASN:HB3	1:E:197:MET:HG3	1.86	0.56
1:F:86:GLN:HB3	1:F:135:TYR:CD1	2.41	0.56
1:H:31:LEU:HD21	1:H:183:ILE:HD13	1.88	0.56
1:D:8:MET:HE2	1:D:34:LEU:HD11	1.88	0.56
1:B:105:PRO:HB3	3:B:602:NAG:H83	1.88	0.55
1:C:50:PRO:O	1:C:53:LEU:HB3	2.07	0.55
1:G:126:THR:O	4:G:703:HOH:O	2.18	0.54
1:D:125:LYS:HG3	1:D:164:LEU:HD23	1.90	0.54
1:H:49:SER:O	1:H:52:SER:N	2.28	0.54
1:E:8:MET:HE2	1:E:34:LEU:HD11	1.89	0.54
1:F:55:THR:HA	1:F:196:PRO:HG3	1.91	0.53
1:A:125:LYS:HD2	1:A:126:THR:H	1.70	0.53
1:B:127:SER:HB2	1:B:129:TYR:N	2.22	0.53
1:G:8:MET:HG2	1:G:65:TYR:CE2	2.43	0.53
1:F:8:MET:HG2	1:F:65:TYR:CE2	2.45	0.52
1:D:105:PRO:HB2	1:D:107:ASN:OD1	2.10	0.52
1:E:20:LYS:HD3	1:E:65:TYR:OH	2.10	0.51
1:C:53:LEU:HD22	1:C:98:CYS:SG	2.50	0.51
1:D:50:PRO:O	1:D:53:LEU:HB3	2.11	0.51
1:D:48:VAL:HG22	1:D:96:PRO:HB3	1.92	0.50
1:G:172:PRO:HD2	1:H:189:THR:HB	1.93	0.50
1:C:198:GLN:HA	2:I:1:NAG:H81	1.94	0.50
1:B:4:ASP:OD1	1:B:6:THR:OG1	2.24	0.50
1:A:69:SER:OG	1:A:171:TYR:OH	2.28	0.50
1:F:147:LEU:HD21	1:F:161:ASP:HB3	1.94	0.49
1:E:129:TYR:OH	1:F:113:LYS:HB2	2.12	0.49
1:H:49:SER:O	1:H:52:SER:OG	2.26	0.49
1:D:125:LYS:HG2	1:D:163:GLU:HG2	1.95	0.49
1:F:163:GLU:HG3	1:F:164:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:MET:HE2	1:F:34:LEU:HD11	1.94	0.48
1:C:48:VAL:HG22	1:C:96:PRO:HB3	1.96	0.48
1:F:150:ARG:NH2	4:F:701:HOH:O	2.38	0.48
1:C:125:LYS:HG3	1:C:164:LEU:HD23	1.96	0.48
1:E:49:SER:HB3	1:E:52:SER:OG	2.14	0.47
1:D:8:MET:HG2	1:D:65:TYR:CE2	2.49	0.47
1:F:127:SER:OG	1:F:128:ALA:N	2.46	0.47
1:A:43:PHE:CE1	1:C:45:CYS:HB2	2.49	0.47
1:B:113:LYS:NZ	1:B:175:GLY:O	2.46	0.47
1:F:76:LEU:HB3	1:F:99:ARG:HD2	1.96	0.47
1:A:43:PHE:HZ	1:C:43:PHE:CE2	2.33	0.47
1:C:125:LYS:HG2	1:C:163:GLU:HG3	1.95	0.47
1:E:150:ARG:NH1	4:E:703:HOH:O	2.29	0.47
1:D:155:LYS:HE3	1:D:169:TYR:CE1	2.50	0.47
1:H:96:PRO:HG2	1:H:187:TYR:CE2	2.43	0.47
1:G:190:ASP:O	1:G:193:SER:N	2.48	0.46
1:E:58:TYR:HD1	1:E:187:TYR:CE1	2.33	0.46
1:B:127:SER:HA	1:B:129:TYR:CE2	2.50	0.46
1:H:147:LEU:HD21	1:H:161:ASP:HB3	1.97	0.46
1:D:53:LEU:HD22	1:D:98:CYS:SG	2.55	0.46
1:B:53:LEU:HD22	1:B:98:CYS:SG	2.55	0.46
1:B:190:ASP:O	1:B:190:ASP:OD1	2.34	0.46
1:F:190:ASP:HB3	1:F:193:SER:HB2	1.98	0.46
1:E:57:CYS:HB3	1:E:191:THR:O	2.15	0.46
1:G:190:ASP:O	1:G:192:ASN:N	2.49	0.45
1:F:58:TYR:HD1	1:F:187:TYR:CE1	2.35	0.45
1:D:8:MET:HG2	1:D:65:TYR:CD2	2.51	0.45
1:F:107:ASN:ND2	3:F:603:NAG:H61	2.31	0.45
1:F:20:LYS:HD3	1:F:65:TYR:OH	2.17	0.45
1:F:117:TYR:CE2	1:F:173:VAL:HG13	2.51	0.45
1:H:108:LEU:O	4:H:703:HOH:O	2.21	0.45
1:G:191:THR:OG1	1:G:192:ASN:N	2.49	0.45
1:E:91:GLN:HE21	1:E:97:THR:CG2	2.30	0.44
1:D:49:SER:HB3	1:D:52:SER:OG	2.18	0.44
1:E:188:GLY:O	1:E:191:THR:HG23	2.18	0.44
1:G:53:LEU:HA	1:G:58:TYR:OH	2.17	0.44
3:D:603:NAG:O3	4:D:702:HOH:O	2.20	0.44
1:H:91:GLN:OE1	4:H:704:HOH:O	2.21	0.44
1:F:43:PHE:HB2	1:F:100:VAL:HG22	2.00	0.44
1:G:31:LEU:HD21	1:G:183:ILE:HD13	2.00	0.44
1:B:43:PHE:HE2	1:D:48:VAL:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:MET:HE2	1:G:34:LEU:HD11	1.98	0.43
1:G:50:PRO:C	1:G:53:LEU:H	2.22	0.43
3:G:603:NAG:O6	3:G:603:NAG:O4	2.20	0.43
1:F:86:GLN:HA	4:F:711:HOH:O	2.18	0.43
1:A:53:LEU:HD22	1:A:98:CYS:SG	2.58	0.43
1:E:49:SER:HA	1:E:50:PRO:HD2	1.89	0.43
1:C:55:THR:HA	1:C:196:PRO:HG3	2.01	0.42
1:E:39:GLN:HA	1:E:39:GLN:HE21	1.83	0.42
1:G:106:GLN:HG3	1:G:176:ASN:OD1	2.19	0.42
1:E:2:GLU:HG3	1:E:197:MET:SD	2.60	0.42
1:G:30:ASN:O	1:G:33:LYS:HB2	2.20	0.42
1:F:29:TYR:HD2	1:F:194:VAL:HG12	1.85	0.42
1:G:35:LEU:HD21	1:G:43:PHE:HE2	1.84	0.42
1:A:43:PHE:HA	1:A:99:ARG:O	2.20	0.42
1:C:56:GLY:O	1:C:196:PRO:HD3	2.20	0.42
1:B:43:PHE:CE2	1:D:45:CYS:HB2	2.54	0.41
1:B:6:THR:O	1:B:10:THR:HG23	2.20	0.41
1:E:48:VAL:HG22	1:E:49:SER:O	2.21	0.41
1:G:51:SER:O	1:G:55:THR:OG1	2.28	0.41
1:H:191:THR:OG1	1:H:192:ASN:OD1	2.38	0.41
1:E:76:LEU:HB3	1:E:99:ARG:HD2	2.03	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.88	0.41
1:E:5:PHE:CG	1:E:34:LEU:HD22	2.56	0.41
1:F:5:PHE:CG	1:F:34:LEU:HD22	2.56	0.41
1:F:43:PHE:HA	1:F:99:ARG:O	2.21	0.41
1:F:29:TYR:CD2	1:F:194:VAL:HG12	2.56	0.40
1:C:163:GLU:HG2	1:C:164:LEU:HG	2.04	0.40

All (1) 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)
4:C:798:HOH:O	4:D:798:HOH:O[1_554]	2.11	0.09

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	196/204 (96%)	187 (95%)	6 (3%)	3 (2%)	10	5
1	B	196/204 (96%)	187 (95%)	7 (4%)	2 (1%)	15	11
1	C	196/204 (96%)	189 (96%)	6 (3%)	1 (0%)	29	26
1	D	196/204 (96%)	191 (97%)	4 (2%)	1 (0%)	29	26
1	E	196/204 (96%)	184 (94%)	10 (5%)	2 (1%)	15	11
1	F	196/204 (96%)	189 (96%)	6 (3%)	1 (0%)	29	26
1	G	196/204 (96%)	187 (95%)	8 (4%)	1 (0%)	29	26
1	H	196/204 (96%)	187 (95%)	7 (4%)	2 (1%)	15	11
All	All	1568/1632 (96%)	1501 (96%)	54 (3%)	13 (1%)	19	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	A	189	THR
1	A	191	THR
1	B	191	THR
1	E	189	THR
1	G	191	THR
1	H	51	SER
1	B	128	ALA
1	C	128	ALA
1	D	128	ALA
1	F	128	ALA
1	H	128	ALA
1	E	128	ALA

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	176/182 (97%)	175 (99%)	1 (1%)	86	90
1	B	176/182 (97%)	175 (99%)	1 (1%)	86	90
1	C	176/182 (97%)	174 (99%)	2 (1%)	73	79
1	D	176/182 (97%)	174 (99%)	2 (1%)	73	79
1	E	176/182 (97%)	174 (99%)	2 (1%)	73	79
1	F	176/182 (97%)	175 (99%)	1 (1%)	86	90
1	G	176/182 (97%)	170 (97%)	6 (3%)	37	39
1	H	176/182 (97%)	171 (97%)	5 (3%)	43	47
All	All	1408/1456 (97%)	1388 (99%)	20 (1%)	67	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	B	48	VAL
1	C	35	LEU
1	C	48	VAL
1	D	48	VAL
1	D	109	THR
1	E	33	LYS
1	E	39	GLN
1	F	69	SER
1	G	48	VAL
1	G	52	SER
1	G	132	ASN
1	G	163	GLU
1	G	189	THR
1	G	190	ASP
1	H	31	LEU
1	H	48	VAL
1	H	51	SER
1	H	107	ASN
1	H	190	ASP

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

Mol	Chain	Res	Type
1	A	77	GLN
1	A	192	ASN

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Mol	Chain	Res	Type
1	E	39	GLN
1	G	132	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

12 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	I	1	2,1	14,14,15	0.40	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.33	0
2	NAG	J	1	2,1	14,14,15	0.44	0	17,19,21	0.56	0
2	NAG	J	2	2	14,14,15	0.19	0	17,19,21	0.36	0
2	NAG	K	1	2,1	14,14,15	0.59	1 (7%)	17,19,21	0.68	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.35	0
2	NAG	L	1	2,1	14,14,15	0.55	0	17,19,21	0.61	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	M	1	2,1	14,14,15	0.40	0	17,19,21	0.51	0
2	NAG	M	2	2	14,14,15	0.48	0	17,19,21	0.42	0
2	NAG	N	1	2,1	14,14,15	0.27	0	17,19,21	0.65	0
2	NAG	N	2	2	14,14,15	0.45	0	17,19,21	0.41	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
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	O5-C1	-2.09	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	NAG	1	0
2	I	1	NAG	1	0
2	M	1	NAG	1	0

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

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths
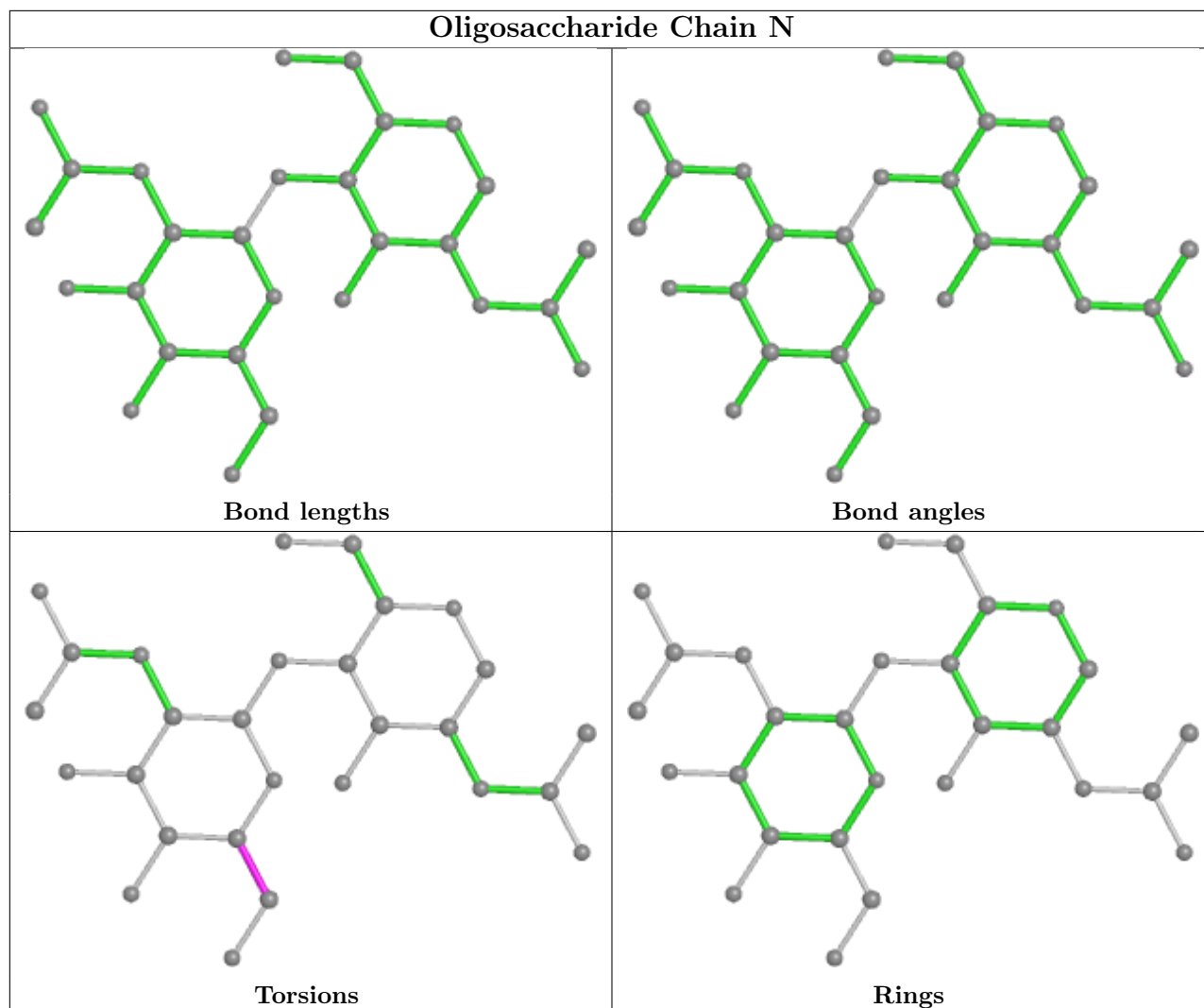

Bond angles

Torsions

Rings

Oligosaccharide Chain N
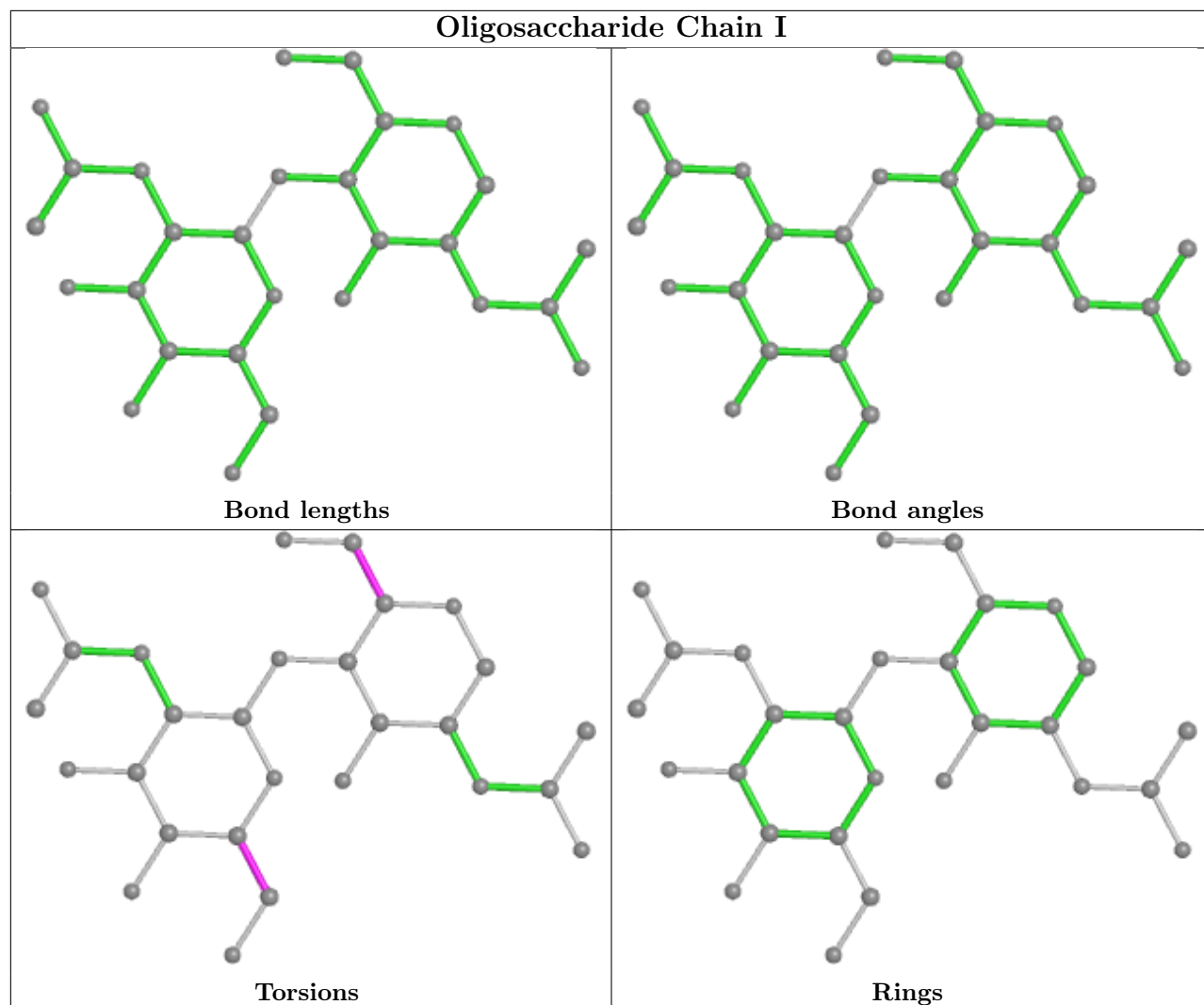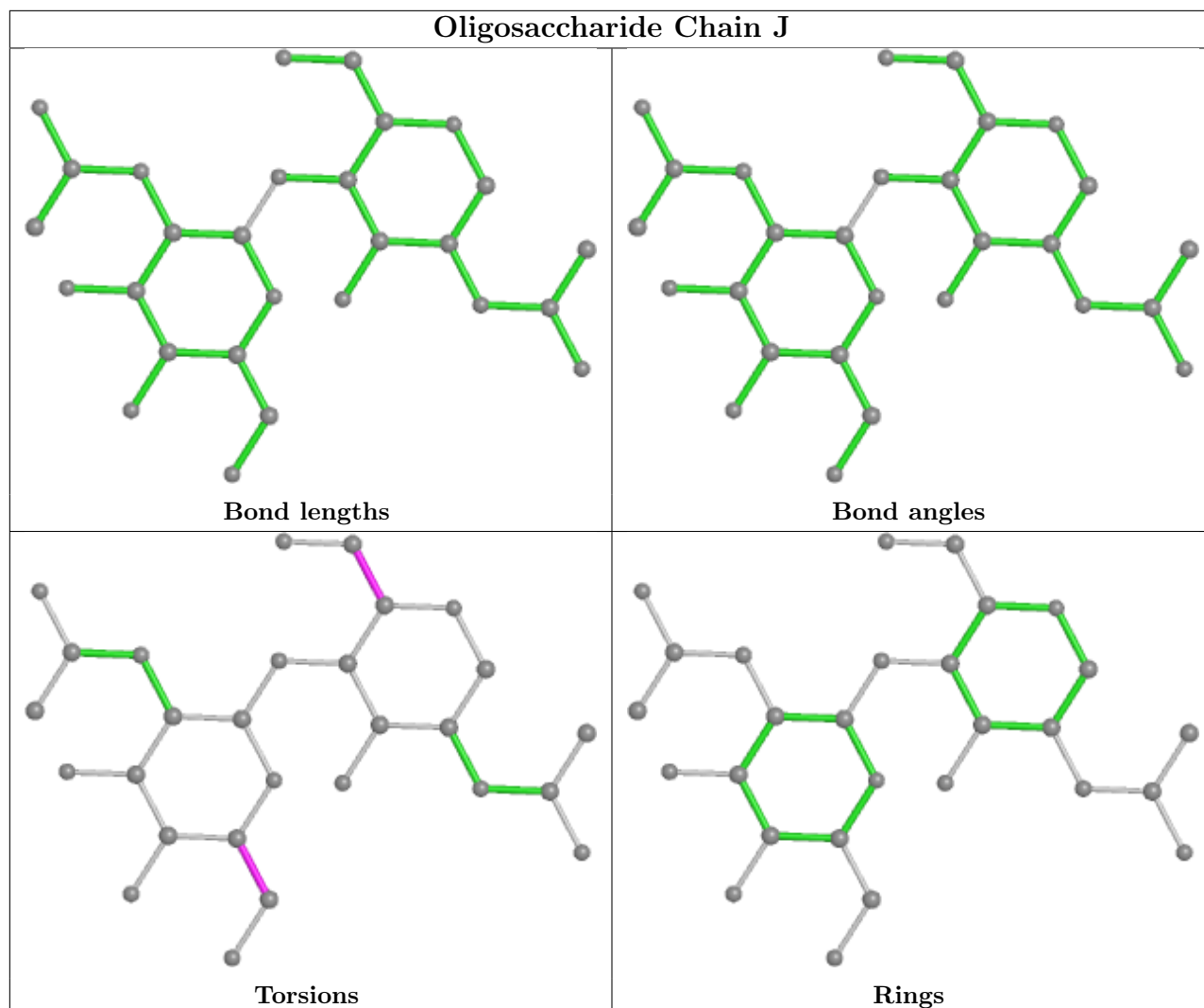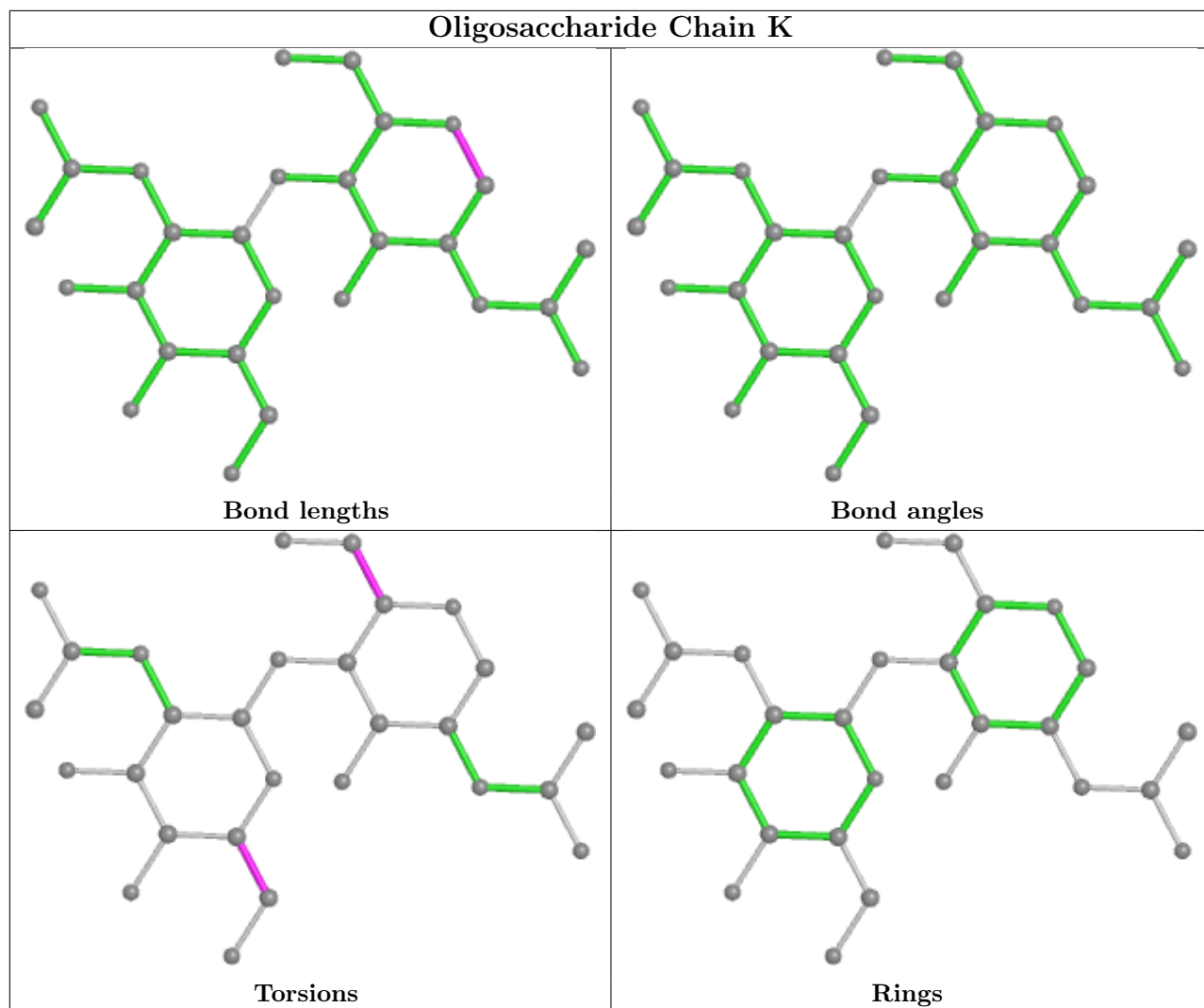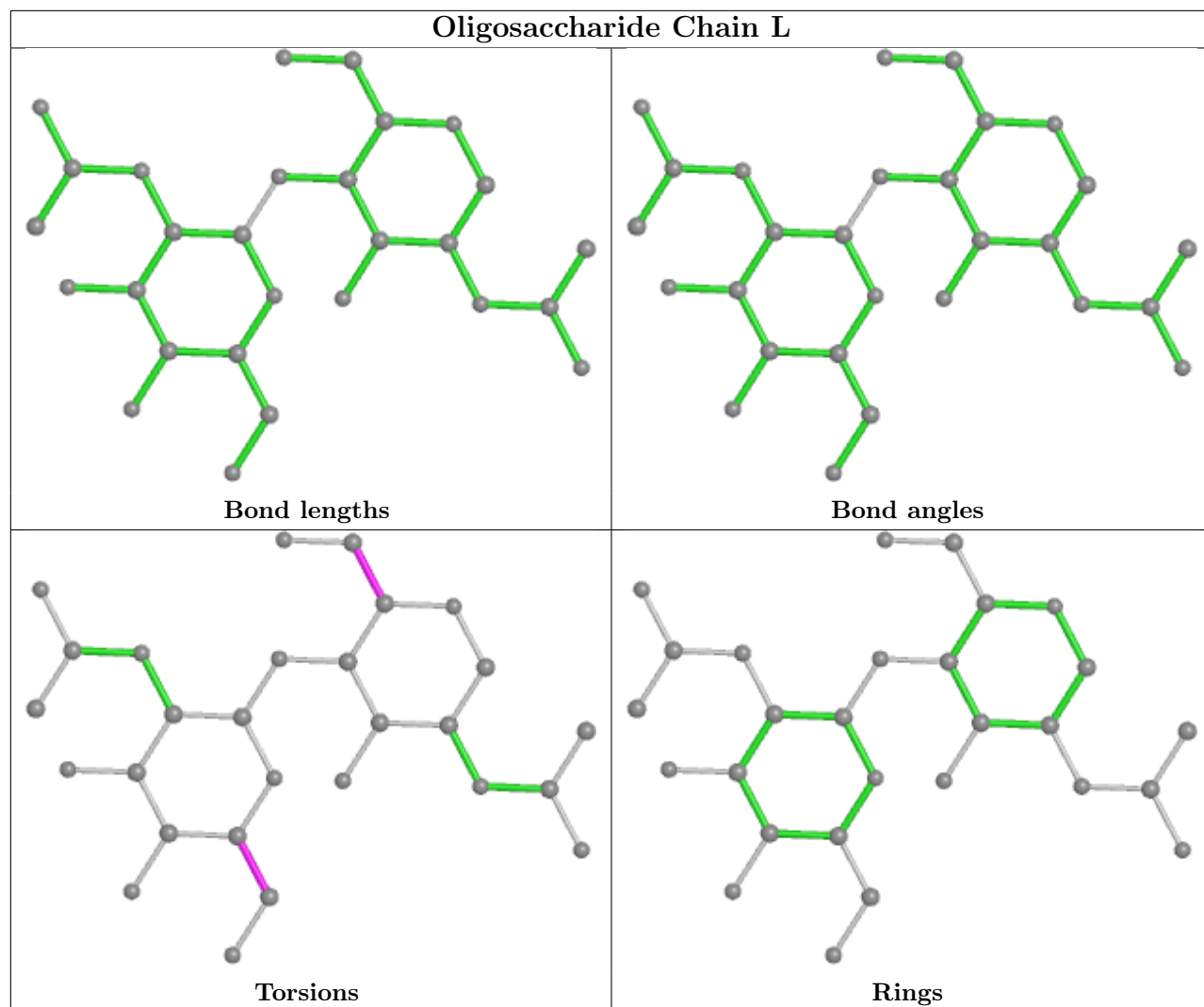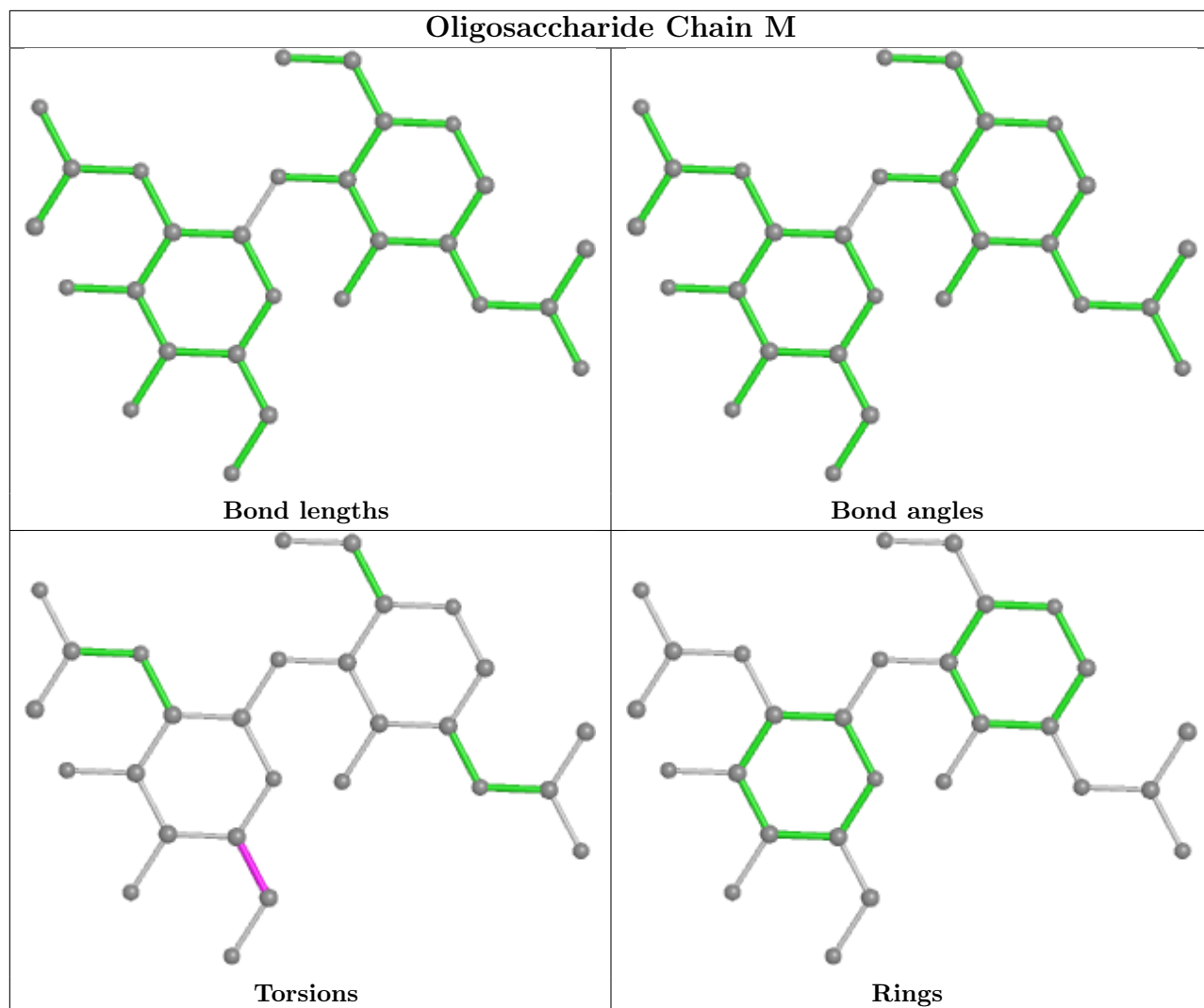
5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	B	602	1	14,14,15	0.63	0	17,19,21	0.85	1 (5%)
3	NAG	C	603	1	14,14,15	1.30	2 (14%)	17,19,21	1.08	1 (5%)
3	NAG	E	603	1	14,14,15	0.77	1 (7%)	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	G	603	1	14,14,15	1.53	2 (14%)	17,19,21	2.19	5 (29%)
3	NAG	B	601	1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	D	603	1	14,14,15	1.00	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	F	603	1	14,14,15	0.86	1 (7%)	17,19,21	0.89	1 (5%)
3	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	A	602	1	14,14,15	1.18	2 (14%)	17,19,21	0.98	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
3	NAG	B	602	1	-	4/6/23/26	0/1/1/1
3	NAG	C	603	1	-	4/6/23/26	0/1/1/1
3	NAG	E	603	1	-	4/6/23/26	0/1/1/1
3	NAG	G	603	1	-	6/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	D	603	1	-	2/6/23/26	0/1/1/1
3	NAG	F	603	1	-	3/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	4/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	NAG	O5-C1	4.04	1.50	1.43
3	G	603	NAG	O5-C1	-3.92	1.37	1.43
3	A	602	NAG	O5-C1	3.62	1.49	1.43
3	D	603	NAG	C1-C2	3.38	1.57	1.52
3	G	603	NAG	C1-C2	-3.14	1.47	1.52
3	F	603	NAG	O5-C1	3.01	1.48	1.43
3	C	603	NAG	C1-C2	2.55	1.56	1.52
3	E	603	NAG	O5-C1	2.40	1.47	1.43
3	A	602	NAG	C1-C2	2.37	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	603	NAG	C1-O5-C5	-5.55	104.67	112.19
3	C	603	NAG	C1-O5-C5	4.17	117.85	112.19
3	A	602	NAG	C1-O5-C5	3.72	117.23	112.19
3	G	603	NAG	C1-C2-N2	-3.54	104.44	110.49
3	D	603	NAG	C1-O5-C5	3.52	116.96	112.19
3	F	603	NAG	C1-O5-C5	3.40	116.81	112.19
3	E	603	NAG	C1-O5-C5	3.13	116.44	112.19
3	G	603	NAG	O5-C5-C4	-3.12	103.23	110.83
3	B	602	NAG	C1-O5-C5	2.87	116.08	112.19
3	G	603	NAG	C2-N2-C7	2.72	126.78	122.90
3	G	603	NAG	C8-C7-N2	2.05	119.56	116.10

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	603	NAG	C4-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	G	603	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
3	C	603	NAG	C8-C7-N2-C2
3	C	603	NAG	O7-C7-N2-C2
3	D	603	NAG	C8-C7-N2-C2
3	D	603	NAG	O7-C7-N2-C2
3	E	603	NAG	C8-C7-N2-C2
3	E	603	NAG	O7-C7-N2-C2
3	F	603	NAG	C8-C7-N2-C2
3	F	603	NAG	O7-C7-N2-C2
3	G	603	NAG	C8-C7-N2-C2
3	G	603	NAG	O7-C7-N2-C2
3	B	602	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	C	603	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	G	603	NAG	C1-C2-N2-C7
3	E	603	NAG	C4-C5-C6-O6
3	C	603	NAG	O5-C5-C6-O6
3	F	603	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	602	NAG	C4-C5-C6-O6
3	E	603	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	G	603	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAG	1	0
3	G	603	NAG	2	0
3	D	603	NAG	1	0
3	F	603	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	198/204 (97%)	0.56	12 (6%)	21	26	31, 48, 90, 124	0
1	B	198/204 (97%)	0.49	18 (9%)	9	12	26, 43, 107, 170	0
1	C	198/204 (97%)	0.36	13 (6%)	18	23	24, 38, 69, 142	0
1	D	198/204 (97%)	0.33	5 (2%)	57	62	23, 36, 64, 138	0
1	E	198/204 (97%)	0.74	24 (12%)	4	5	29, 51, 101, 154	0
1	F	198/204 (97%)	0.79	23 (11%)	4	6	31, 55, 106, 153	0
1	G	198/204 (97%)	0.77	26 (13%)	3	4	27, 54, 107, 168	0
1	H	198/204 (97%)	0.65	20 (10%)	7	9	25, 48, 101, 151	0
All	All	1584/1632 (97%)	0.59	141 (8%)	9	12	23, 47, 98, 170	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	188	GLY	10.4
1	G	50	PRO	9.3
1	F	188	GLY	8.9
1	H	50	PRO	8.3
1	F	129	TYR	7.7
1	B	191	THR	7.6
1	A	192	ASN	7.6
1	A	129	TYR	7.3
1	E	191	THR	7.2
1	E	129	TYR	6.9
1	F	189	THR	6.8
1	E	189	THR	6.4
1	G	187	TYR	6.3
1	E	192	ASN	6.2
1	H	54	ALA	5.8
1	A	189	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	H	198	GLN	5.6
1	H	187	TYR	5.5
1	A	191	THR	5.5
1	B	127	SER	5.4
1	B	188	GLY	5.3
1	C	51	SER	5.1
1	F	107	ASN	5.0
1	F	128	ALA	5.0
1	F	191	THR	5.0
1	D	51	SER	4.9
1	E	43	PHE	4.8
1	H	188	GLY	4.7
1	E	198	GLN	4.6
1	G	188	GLY	4.6
1	G	54	ALA	4.6
1	H	56	GLY	4.6
1	G	191	THR	4.6
1	D	50	PRO	4.5
1	H	53	LEU	4.5
1	G	189	THR	4.5
1	B	192	ASN	4.5
1	B	189	THR	4.5
1	B	130	GLY	4.3
1	G	198	GLN	4.3
1	C	50	PRO	4.2
1	H	189	THR	4.1
1	E	49	SER	4.0
1	H	192	ASN	4.0
1	G	51	SER	4.0
1	G	192	ASN	4.0
1	F	130	GLY	3.9
1	B	129	TYR	3.9
1	H	191	THR	3.7
1	G	107	ASN	3.6
1	A	187	TYR	3.6
1	F	192	ASN	3.6
1	F	39	GLN	3.5
1	G	53	LEU	3.5
1	G	56	GLY	3.5
1	D	198	GLN	3.5
1	F	106	GLN	3.4
1	B	190	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	51	SER	3.3
1	F	127	SER	3.3
1	H	197	MET	3.2
1	B	54	ALA	3.2
1	G	174	THR	3.2
1	A	130	GLY	3.1
1	G	197	MET	3.1
1	F	81	ALA	3.1
1	E	109	THR	3.1
1	E	78	PRO	3.0
1	H	22	LEU	3.0
1	C	198	GLN	3.0
1	E	187	TYR	2.9
1	B	126	THR	2.9
1	B	198	GLN	2.9
1	H	174	THR	2.9
1	B	187	TYR	2.8
1	F	197	MET	2.8
1	H	106	GLN	2.8
1	F	75	TYR	2.8
1	G	79	GLY	2.7
1	F	187	TYR	2.7
1	E	106	GLN	2.7
1	F	174	THR	2.6
1	B	43	PHE	2.6
1	B	181	PHE	2.6
1	A	190	ASP	2.6
1	E	130	GLY	2.6
1	C	65	TYR	2.6
1	B	81	ALA	2.5
1	C	43	PHE	2.5
1	G	58	TYR	2.5
1	A	188	GLY	2.5
1	E	107	ASN	2.5
1	G	181	PHE	2.5
1	E	197	MET	2.4
1	C	19	PHE	2.4
1	D	19	PHE	2.4
1	B	196	PRO	2.4
1	G	12	THR	2.4
1	B	107	ASN	2.4
1	G	14	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	81	ALA	2.4
1	E	39	GLN	2.3
1	A	126	THR	2.3
1	G	31	LEU	2.3
1	C	63	VAL	2.3
1	F	198	GLN	2.3
1	E	181	PHE	2.3
1	A	18	ASN	2.3
1	G	22	LEU	2.3
1	E	75	TYR	2.3
1	F	181	PHE	2.3
1	G	183	ILE	2.3
1	C	54	ALA	2.2
1	C	53	LEU	2.2
1	F	43	PHE	2.2
1	E	77	GLN	2.2
1	F	1	GLN	2.2
1	A	132	ASN	2.2
1	E	95	ASN	2.2
1	F	51	SER	2.2
1	H	156	TYR	2.2
1	H	182	ILE	2.2
1	G	18	ASN	2.2
1	E	79	GLY	2.2
1	F	113	LYS	2.2
1	C	22	LEU	2.1
1	E	65	TYR	2.1
1	B	131	LYS	2.1
1	C	163	GLU	2.1
1	C	182	ILE	2.1
1	H	81	ALA	2.1
1	E	163	GLU	2.1
1	G	106	GLN	2.1
1	D	63	VAL	2.1
1	H	109	THR	2.1
1	G	63	VAL	2.1
1	H	58	TYR	2.1
1	A	125	LYS	2.0
1	C	20	LYS	2.0
1	F	182	ILE	2.0
1	G	65	TYR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	M	2	14/15	0.60	0.35	100,113,120,126	0
2	NAG	K	2	14/15	0.61	0.42	118,134,143,147	0
2	NAG	N	2	14/15	0.61	0.37	102,112,120,122	0
2	NAG	L	2	14/15	0.74	0.36	111,124,132,135	0
2	NAG	J	2	14/15	0.75	0.33	95,99,108,112	0
2	NAG	I	2	14/15	0.76	0.30	106,111,120,123	0
2	NAG	K	1	14/15	0.83	0.19	79,87,96,102	0
2	NAG	N	1	14/15	0.85	0.18	76,82,89,93	0
2	NAG	M	1	14/15	0.85	0.14	75,80,86,90	0
2	NAG	J	1	14/15	0.87	0.23	68,72,77,83	0
2	NAG	I	1	14/15	0.89	0.22	76,81,88,95	0
2	NAG	L	1	14/15	0.90	0.18	77,82,92,92	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 I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
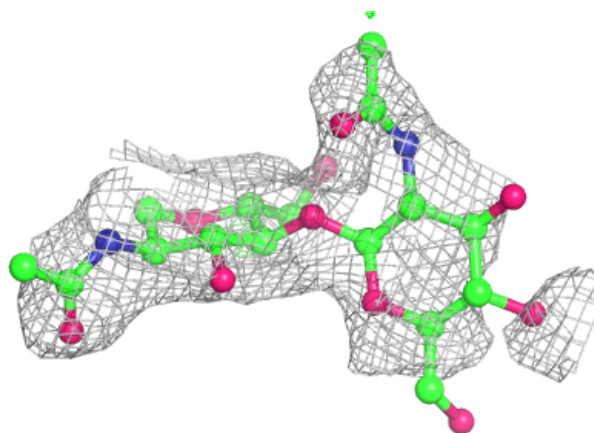and green (positive)
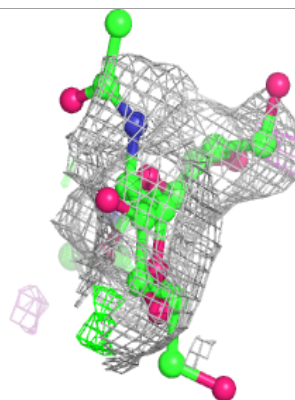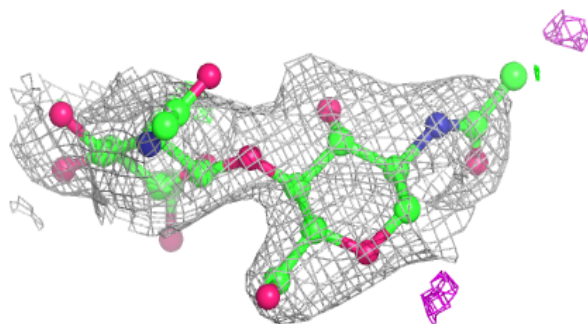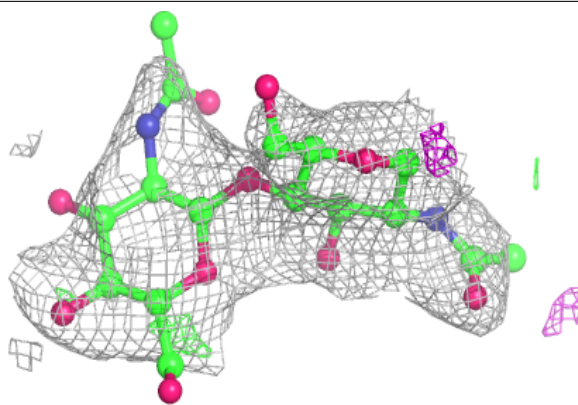
Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
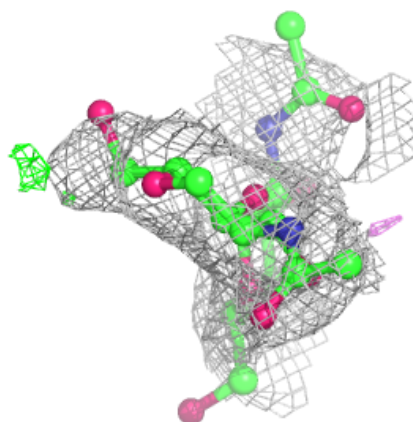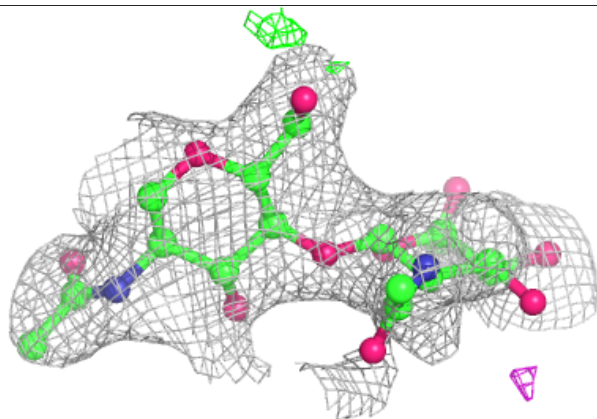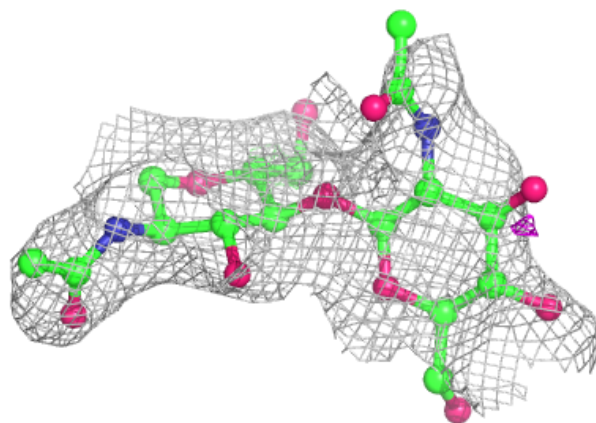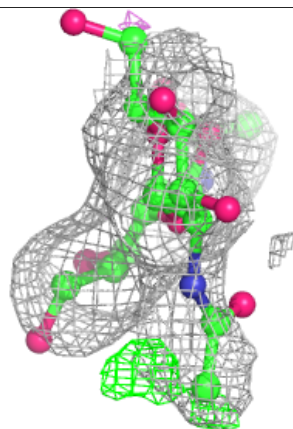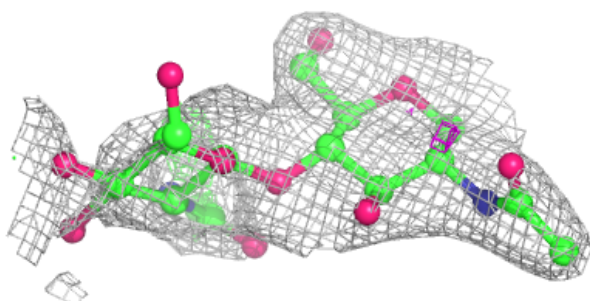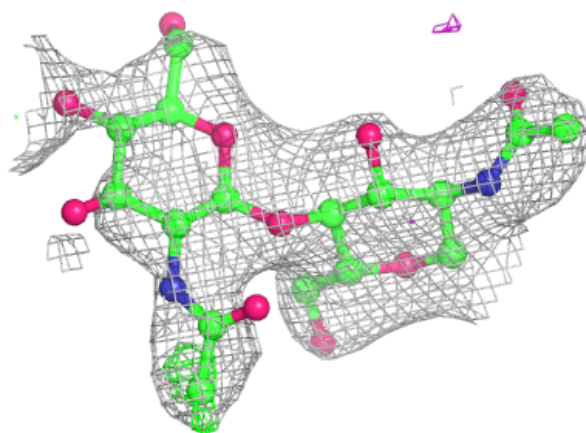mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
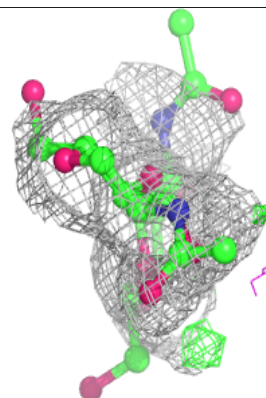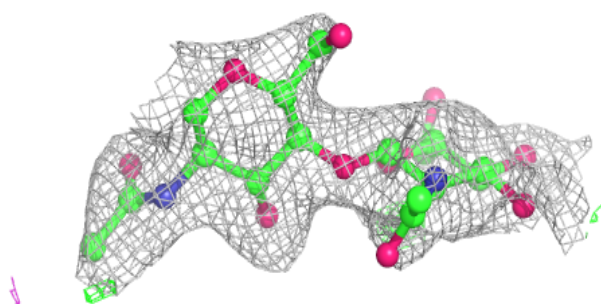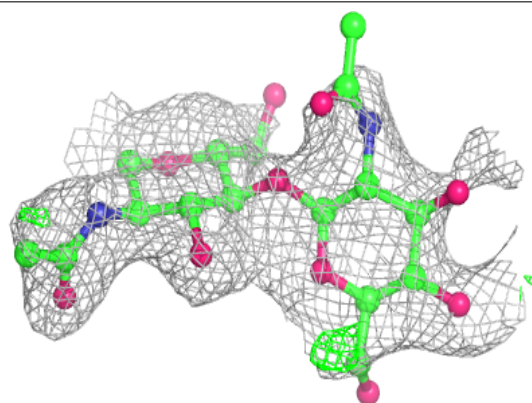
Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
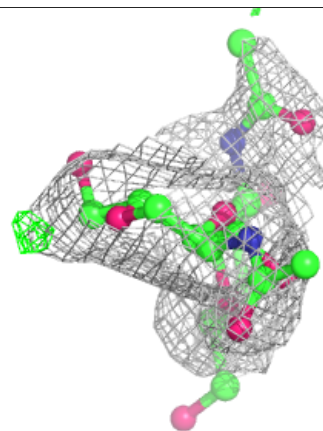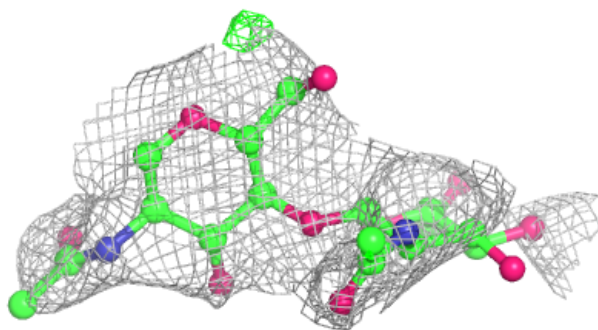
Electron density around Chain L:

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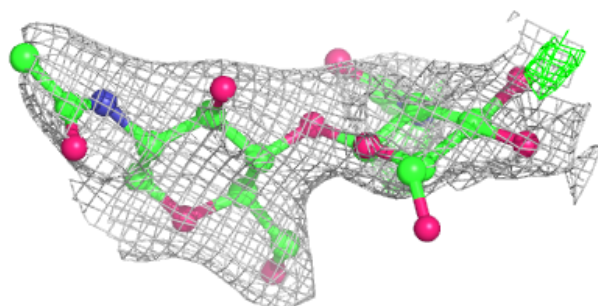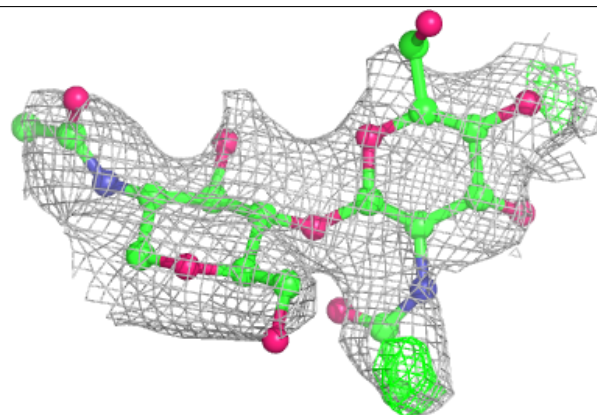and green (positive)

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 N:

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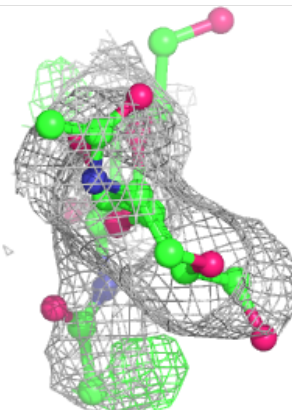
6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	NAG	G	603	14/15	0.06	0.61	144,151,152,155	0
3	NAG	A	602	14/15	0.46	0.35	100,110,119,120	0
3	NAG	B	602	14/15	0.59	0.38	105,111,119,119	0
3	NAG	E	603	14/15	0.61	0.28	97,103,107,107	0
3	NAG	F	603	14/15	0.67	0.28	115,117,122,124	0
3	NAG	D	603	14/15	0.69	0.26	94,99,104,106	0
3	NAG	C	603	14/15	0.69	0.26	90,95,98,99	0
3	NAG	B	601	14/15	0.81	0.25	98,108,114,114	0
3	NAG	A	601	14/15	0.82	0.24	98,102,112,114	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK