



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 03:07 AM BST

PDB ID : 4OU3
Title : Crystal structure of porcine aminopeptidase N complexed with CNGRCG tumor-homing peptide
Authors : Liu, C.; Yang, Y.; Chen, L.; Lin, Y.-L.; Li, F.
Deposited on : 2014-02-14
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

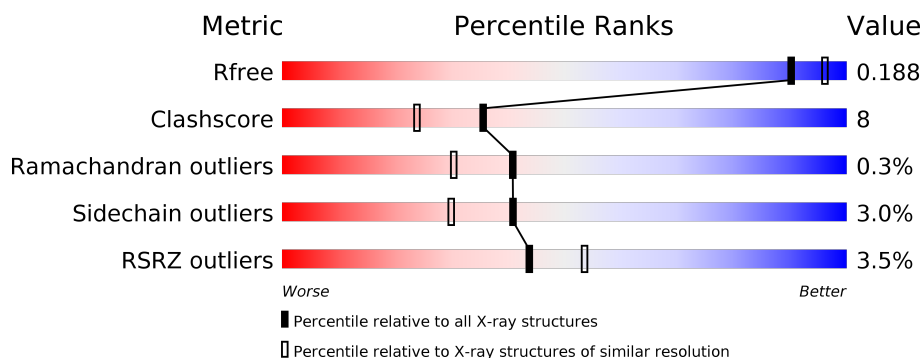
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



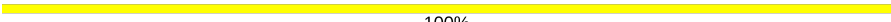


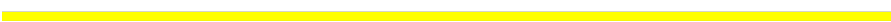
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	908	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
2	B	6	<div> <div>17%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>
3	D	2	<div> <div></div> <div>100%</div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 50% 50%
3	J	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
6	SO4	A	1022	-	-	X	-
6	SO4	A	1027	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8498 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	902	7249	4626	1212	1381	30	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	PHE	LEU	conflict	UNP P15145
A	964	SER	-	expression tag	UNP P15145
A	965	HIS	-	expression tag	UNP P15145
A	966	HIS	-	expression tag	UNP P15145
A	967	HIS	-	expression tag	UNP P15145
A	968	HIS	-	expression tag	UNP P15145
A	969	HIS	-	expression tag	UNP P15145
A	970	HIS	-	expression tag	UNP P15145

- Molecule 2 is a protein called tumor-homing peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	6	40	20	10	8	2	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
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

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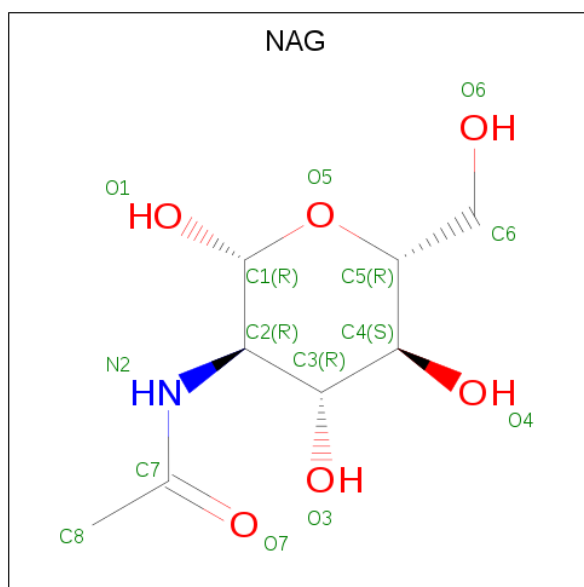
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

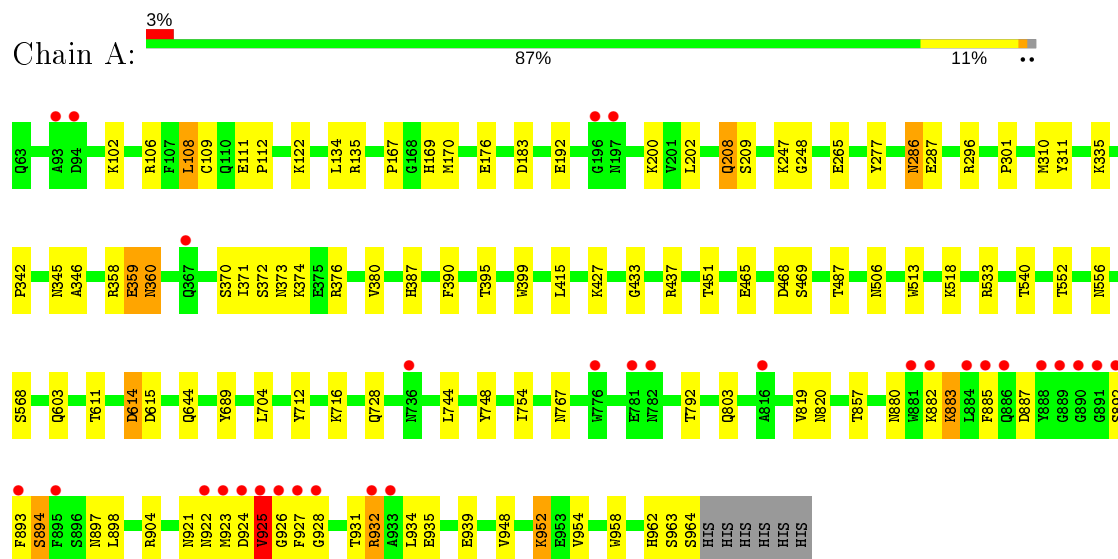
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	904	Total 904	O 904	0	0
7	B	2	Total 2	O 2	0	0

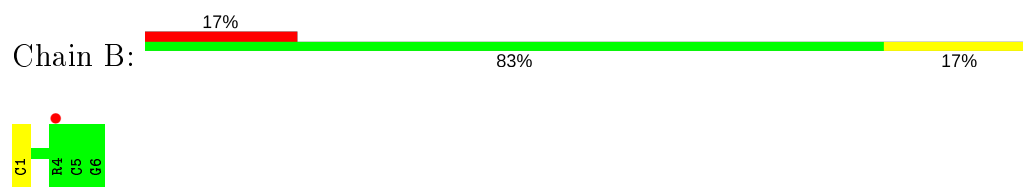
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

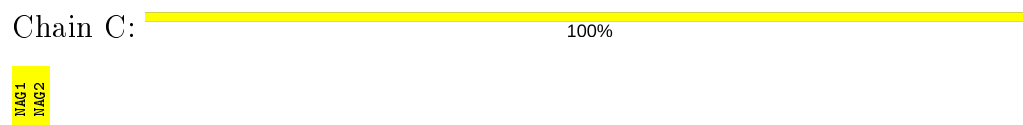
- Molecule 1: Aminopeptidase N



- Molecule 2: tumor-homing peptide



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



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



MAG1
MAG2

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

Chain E:  100%MAG1
MAG2

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

Chain F:  100%MAG1
MAG2

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

Chain G:  100%MAG1
MAG2

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

Chain H:  50% 50%MAG1
MAG2

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

Chain I:  50% 50%MAG1
MAG2

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

Chain J:  100%MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	260.32Å 62.88Å 82.02Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 47.68 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-1.95) 97.8 (47.68-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.140 , 0.190 0.145 , 0.188	Depositor DCC
R_{free} test set	4710 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/7437	0.73	3/10135 (0.0%)
2	B	1.11	0/39	1.34	0/48
All	All	0.64	0/7476	0.74	3/10183 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	GLU	CB-CA-C	-5.95	98.50	110.40
1	A	135	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	176	GLU	CG-CD-OE2	-5.20	107.90	118.30

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	7249	0	7000	117	0
2	B	40	0	35	1	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	2	0
3	J	28	0	25	0	0
4	A	1	0	0	0	0
5	A	28	0	26	1	0
6	A	50	0	0	7	0
7	A	904	0	0	43	0
7	B	2	0	0	0	0
All	All	8498	0	7261	120	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 8.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:THR:HG22	1:A:893:PHE:CZ	1.65	1.31
1:A:106:ARG:HD3	7:A:1905:HOH:O	1.43	1.16
1:A:310:MET:HE3	7:A:1730:HOH:O	1.48	1.11
1:A:857:THR:HG22	1:A:893:PHE:CE1	1.89	1.06
1:A:857:THR:CG2	1:A:893:PHE:CE1	2.38	1.06
1:A:857:THR:CG2	1:A:893:PHE:CZ	2.38	1.05
1:A:451:THR:HG22	7:A:1848:HOH:O	1.56	1.03
1:A:924:ASP:O	1:A:925:VAL:HG13	1.59	1.02
1:A:265:GLU:HG3	7:A:1247:HOH:O	1.60	1.02
1:A:465:GLU:HG2	7:A:1824:HOH:O	1.59	1.00
1:A:346:ALA:HB3	7:A:1906:HOH:O	1.66	0.96
1:A:358:ARG:HG2	6:A:1022:SO4:O3	1.70	0.92
1:A:108:LEU:HD12	1:A:109:CYS:N	1.85	0.91
1:A:894:SER:HB3	7:A:1797:HOH:O	1.71	0.91
7:A:1564:HOH:O	3:I:2:NAG:H83	1.68	0.91
1:A:183:ASP:HB2	7:A:1862:HOH:O	1.77	0.84
1:A:468:ASP:HB2	6:A:1027:SO4:O4	1.78	0.83
1:A:373:ASN:HD21	1:A:820:ASN:HD22	1.28	0.80
1:A:893:PHE:HZ	1:A:898:LEU:HD22	1.47	0.80
1:A:247:LYS:HB2	7:A:1991:HOH:O	1.83	0.78
1:A:894:SER:CB	7:A:1797:HOH:O	2.32	0.73
1:A:373:ASN:HD21	1:A:820:ASN:ND2	1.86	0.73
1:A:893:PHE:CZ	1:A:898:LEU:HD22	2.24	0.73
1:A:170:MET:SD	7:A:1905:HOH:O	2.47	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:ASP:O	1:A:925:VAL:CG1	2.35	0.71
1:A:924:ASP:C	1:A:925:VAL:HG13	2.11	0.71
1:A:927:PHE:HB2	1:A:931:THR:HA	1.74	0.69
1:A:415:LEU:HD22	1:A:427:LYS:HE2	1.73	0.69
1:A:857:THR:HG23	1:A:893:PHE:CE1	2.28	0.67
1:A:346:ALA:CB	7:A:1906:HOH:O	2.32	0.67
1:A:102:LYS:HE3	7:A:1879:HOH:O	1.96	0.66
1:A:208:GLN:HE21	1:A:209:SER:HA	1.62	0.64
1:A:102:LYS:HG3	7:A:1879:HOH:O	1.97	0.64
1:A:469:SER:N	6:A:1027:SO4:O4	2.24	0.63
1:A:552:THR:HB	1:A:611:THR:HG22	1.80	0.63
1:A:611:THR:HG21	7:A:1340:HOH:O	1.99	0.62
1:A:932:ARG:C	1:A:934:LEU:N	2.52	0.62
1:A:924:ASP:O	1:A:925:VAL:HG22	2.00	0.61
1:A:108:LEU:HD12	1:A:109:CYS:H	1.64	0.61
1:A:892:SER:O	1:A:893:PHE:HB3	2.00	0.60
1:A:170:MET:HB3	7:A:1905:HOH:O	2.01	0.60
1:A:372:SER:HB3	7:A:1392:HOH:O	2.02	0.59
1:A:518:LYS:HE3	7:A:1638:HOH:O	2.01	0.59
1:A:556:ASN:HD22	5:A:1016:NAG:H83	1.67	0.59
1:A:954:VAL:HG23	7:A:1841:HOH:O	2.01	0.59
1:A:248:GLY:N	7:A:1991:HOH:O	2.36	0.59
1:A:359:GLU:CD	7:A:1927:HOH:O	2.40	0.59
1:A:345:ASN:HB2	7:A:1923:HOH:O	2.04	0.56
1:A:376:ARG:NH2	6:A:1029:SO4:O4	2.39	0.55
1:A:342:PRO:HB3	7:A:1927:HOH:O	2.07	0.55
1:A:857:THR:CG2	1:A:893:PHE:CD1	2.90	0.55
1:A:932:ARG:C	1:A:934:LEU:H	2.09	0.54
1:A:819:VAL:HG23	7:A:1670:HOH:O	2.07	0.54
1:A:926:GLY:C	1:A:927:PHE:CD1	2.81	0.54
1:A:712:TYR:CE2	1:A:716:LYS:HD2	2.42	0.54
1:A:310:MET:HB3	7:A:1730:HOH:O	2.07	0.53
1:A:803:GLN:NE2	7:A:1922:HOH:O	2.41	0.53
1:A:704:LEU:HD21	1:A:904:ARG:HG2	1.90	0.53
1:A:921:ASN:OD1	1:A:921:ASN:O	2.27	0.53
1:A:286:ASN:HB3	1:A:296:ARG:HG2	1.90	0.53
1:A:380:VAL:HG13	7:A:1461:HOH:O	2.09	0.53
1:A:924:ASP:O	1:A:925:VAL:CB	2.56	0.52
7:A:1949:HOH:O	3:H:1:NAG:H81	2.10	0.52
1:A:932:ARG:O	1:A:935:GLU:N	2.42	0.52
7:A:1564:HOH:O	3:I:2:NAG:C8	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:THR:CG2	1:A:893:PHE:CE2	2.93	0.51
1:A:857:THR:HG21	1:A:893:PHE:CZ	2.42	0.51
1:A:370:SER:O	1:A:373:ASN:HB3	2.11	0.51
1:A:122:LYS:CE	7:A:1984:HOH:O	2.58	0.50
1:A:552:THR:HB	1:A:611:THR:CG2	2.42	0.50
1:A:122:LYS:HE3	7:A:1984:HOH:O	2.11	0.50
1:A:433:GLY:O	1:A:437:ARG:HD2	2.11	0.50
1:A:857:THR:HG21	1:A:893:PHE:CE2	2.47	0.50
1:A:373:ASN:ND2	1:A:820:ASN:ND2	2.59	0.50
1:A:358:ARG:HD2	1:A:360:ASN:OD1	2.11	0.50
1:A:451:THR:CG2	7:A:1848:HOH:O	2.34	0.49
1:A:451:THR:HG23	1:A:540:THR:HB	1.95	0.49
1:A:614:ASP:N	1:A:614:ASP:OD1	2.32	0.49
1:A:108:LEU:HD12	1:A:108:LEU:C	2.34	0.48
1:A:932:ARG:HH21	1:A:932:ARG:CG	2.26	0.48
1:A:108:LEU:HD13	1:A:169:HIS:O	2.13	0.48
1:A:880:ASN:O	1:A:883:LYS:HD2	2.14	0.48
1:A:399:TRP:CZ3	6:A:1028:SO4:O1	2.67	0.48
1:A:415:LEU:CD2	1:A:427:LYS:HE2	2.42	0.48
1:A:893:PHE:O	1:A:894:SER:CB	2.61	0.48
1:A:894:SER:OG	1:A:897:ASN:ND2	2.47	0.48
1:A:371:ILE:CG1	1:A:744:LEU:HD12	2.45	0.47
1:A:111:GLU:HG2	7:A:1541:HOH:O	2.15	0.46
1:A:963:SER:O	1:A:964:SER:HB3	2.16	0.46
1:A:924:ASP:C	1:A:925:VAL:CG1	2.80	0.46
1:A:712:TYR:CD2	1:A:716:LYS:HD2	2.51	0.46
1:A:958:TRP:O	1:A:962:HIS:HD2	1.99	0.45
1:A:754:ILE:HG22	1:A:792:THR:HG21	1.98	0.45
1:A:948:VAL:O	1:A:952:LYS:HB2	2.16	0.45
1:A:883:LYS:O	1:A:887:ASP:HB2	2.18	0.44
1:A:924:ASP:O	1:A:925:VAL:CG2	2.64	0.44
1:A:202:LEU:C	1:A:202:LEU:HD12	2.38	0.44
1:A:371:ILE:HG13	1:A:744:LEU:HD12	1.99	0.44
1:A:311:TYR:CE1	1:A:374:LYS:HE3	2.53	0.43
1:A:927:PHE:CD1	1:A:927:PHE:N	2.86	0.43
1:A:962:HIS:HE1	7:A:1914:HOH:O	2.01	0.43
1:A:122:LYS:HD3	7:A:1885:HOH:O	2.17	0.43
1:A:932:ARG:HD3	7:A:1597:HOH:O	2.18	0.43
1:A:106:ARG:CD	7:A:1905:HOH:O	2.26	0.42
1:A:387:HIS:HA	1:A:390:PHE:O	2.18	0.42
1:A:112:PRO:HD3	1:A:167:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HG2	2:B:1:CYS:HB2	2.00	0.42
1:A:611:THR:OG1	1:A:615:ASP:CB	2.67	0.42
1:A:468:ASP:CB	6:A:1027:SO4:O4	2.59	0.42
1:A:395:THR:O	1:A:506:ASN:HA	2.20	0.42
1:A:893:PHE:O	1:A:894:SER:HB3	2.20	0.42
1:A:928:GLY:O	1:A:931:THR:OG1	2.31	0.41
1:A:904:ARG:NH2	7:A:1764:HOH:O	2.52	0.41
1:A:301:PRO:HD2	7:A:1145:HOH:O	2.20	0.41
1:A:122:LYS:HE2	7:A:1984:HOH:O	2.21	0.41
1:A:728:GLN:HG3	7:A:1644:HOH:O	2.20	0.41
1:A:192:GLU:HA	1:A:200:LYS:O	2.21	0.41
1:A:310:MET:CE	7:A:1730:HOH:O	2.32	0.41
1:A:360:ASN:HB3	6:A:1022:SO4:O2	2.21	0.40
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	901/908 (99%)	872 (97%)	26 (3%)	3 (0%)	41	30
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	905/914 (99%)	876 (97%)	26 (3%)	3 (0%)	41	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	894	SER
1	A	925	VAL
1	A	487	THR

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	798/803 (99%)	774 (97%)	24 (3%)	41	30
2	B	4/4 (100%)	4 (100%)	0	100	100
All	All	802/807 (99%)	778 (97%)	24 (3%)	41	30

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	134	LEU
1	A	208	GLN
1	A	277	TYR
1	A	286	ASN
1	A	287	GLU
1	A	335	LYS
1	A	360	ASN
1	A	513	TRP
1	A	533	ARG
1	A	568	SER
1	A	603	GLN
1	A	614	ASP
1	A	644	GLN
1	A	767	ASN
1	A	882	LYS
1	A	883	LYS
1	A	885	PHE
1	A	922	ASN
1	A	923	MET
1	A	925	VAL
1	A	932	ARG
1	A	939	GLU
1	A	952	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	360	ASN
1	A	767	ASN
1	A	820	ASN
1	A	897	ASN
1	A	962	HIS

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 ⓘ

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.74	0	17,19,21	1.70	4 (23%)
3	NAG	C	2	3	14,14,15	0.63	0	17,19,21	2.00	6 (35%)
3	NAG	D	1	1,3	14,14,15	0.59	0	17,19,21	1.14	3 (17%)
3	NAG	D	2	3	14,14,15	0.66	0	17,19,21	1.71	3 (17%)
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	1.68	4 (23%)
3	NAG	E	2	3	14,14,15	0.75	1 (7%)	17,19,21	1.04	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.13	1 (5%)
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	1.60	1 (5%)
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	1.46	3 (17%)
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	1.91	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	H	2	3	14,14,15	0.73	0	17,19,21	0.97	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.50	0	17,19,21	2.38	7 (41%)
3	NAG	I	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.80	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.96	1 (7%)	17,19,21	1.70	4 (23%)
3	NAG	J	2	3	14,14,15	0.51	0	17,19,21	2.27	4 (23%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	2	NAG	C1-C2	2.34	1.55	1.52
3	G	1	NAG	O4-C4	-2.26	1.37	1.43
3	F	1	NAG	C1-C2	2.21	1.55	1.52
3	E	2	NAG	O5-C1	-2.08	1.40	1.43
3	J	1	NAG	O5-C1	-2.01	1.40	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	O5-C5-C6	5.62	116.01	107.20
3	I	1	NAG	C1-O5-C5	5.53	119.69	112.19
3	C	2	NAG	C4-C3-C2	4.97	118.30	111.02
3	J	2	NAG	O5-C1-C2	-4.71	103.85	111.29
3	D	2	NAG	C4-C3-C2	4.60	117.76	111.02
3	J	2	NAG	C2-N2-C7	-4.57	116.39	122.90
3	I	1	NAG	O5-C1-C2	-4.26	104.56	111.29
3	H	1	NAG	O5-C5-C6	4.21	113.80	107.20
3	G	1	NAG	O5-C1-C2	-4.11	104.80	111.29
3	J	1	NAG	O5-C5-C6	4.00	113.48	107.20
3	I	1	NAG	C1-C2-N2	-3.95	103.74	110.49
3	E	1	NAG	O5-C5-C6	3.92	113.34	107.20
3	D	2	NAG	C1-C2-N2	-3.69	104.19	110.49
3	C	1	NAG	C1-O5-C5	3.62	117.10	112.19
3	G	2	NAG	C4-C3-C2	3.48	116.12	111.02
3	J	2	NAG	C1-O5-C5	3.39	116.79	112.19
3	C	2	NAG	C8-C7-N2	3.15	121.44	116.10
3	E	1	NAG	C2-N2-C7	-2.92	118.75	122.90
3	I	1	NAG	C4-C3-C2	2.89	115.26	111.02
3	J	2	NAG	C4-C3-C2	-2.81	106.90	111.02
3	I	1	NAG	C3-C4-C5	-2.81	105.23	110.24
3	I	1	NAG	C2-N2-C7	-2.80	118.91	122.90
3	C	1	NAG	O5-C1-C2	-2.80	106.87	111.29
3	H	1	NAG	O5-C1-C2	-2.75	106.94	111.29
3	H	2	NAG	C4-C3-C2	-2.72	107.03	111.02
3	H	1	NAG	O3-C3-C4	-2.71	104.09	110.35
3	H	1	NAG	C4-C3-C2	2.70	114.98	111.02
3	G	2	NAG	O5-C1-C2	-2.68	107.05	111.29
3	C	1	NAG	O3-C3-C2	-2.60	104.09	109.47
3	F	2	NAG	C1-O5-C5	2.58	115.68	112.19
3	C	2	NAG	O5-C1-C2	-2.53	107.30	111.29
3	D	1	NAG	O7-C7-C8	-2.49	117.44	122.06
3	E	1	NAG	O7-C7-C8	-2.45	117.50	122.06
3	J	1	NAG	C3-C4-C5	-2.34	106.06	110.24
3	E	2	NAG	C3-C4-C5	-2.34	106.07	110.24
3	J	1	NAG	O5-C1-C2	-2.33	107.60	111.29
3	E	1	NAG	C1-O5-C5	-2.32	109.05	112.19
3	D	2	NAG	O4-C4-C3	-2.25	105.15	110.35
3	I	2	NAG	C3-C4-C5	-2.24	106.24	110.24
3	J	1	NAG	C6-C5-C4	-2.24	107.76	113.00
3	I	1	NAG	O4-C4-C5	2.22	114.81	109.30
3	C	2	NAG	O5-C5-C6	2.21	110.67	107.20
3	H	1	NAG	C2-N2-C7	2.20	126.03	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O7-C7-C8	-2.08	118.19	122.06
3	F	1	NAG	O4-C4-C3	-2.08	105.54	110.35
3	D	1	NAG	C2-N2-C7	2.05	125.82	122.90
3	D	1	NAG	O7-C7-N2	2.03	125.68	121.95
3	C	2	NAG	C1-O5-C5	-2.03	109.44	112.19
3	C	2	NAG	O7-C7-C8	-2.02	118.30	122.06
3	G	2	NAG	O5-C5-C6	2.01	110.36	107.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

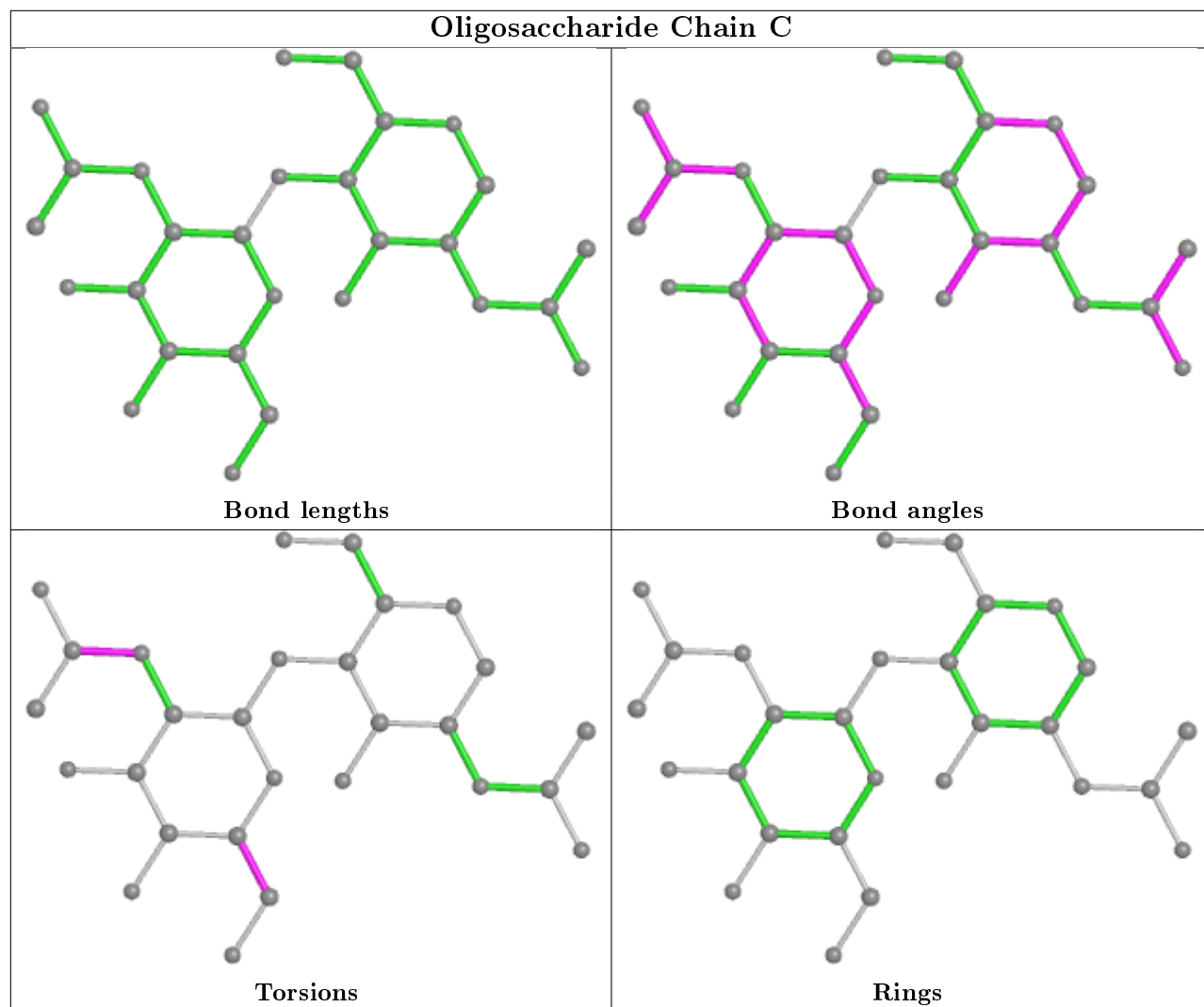
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

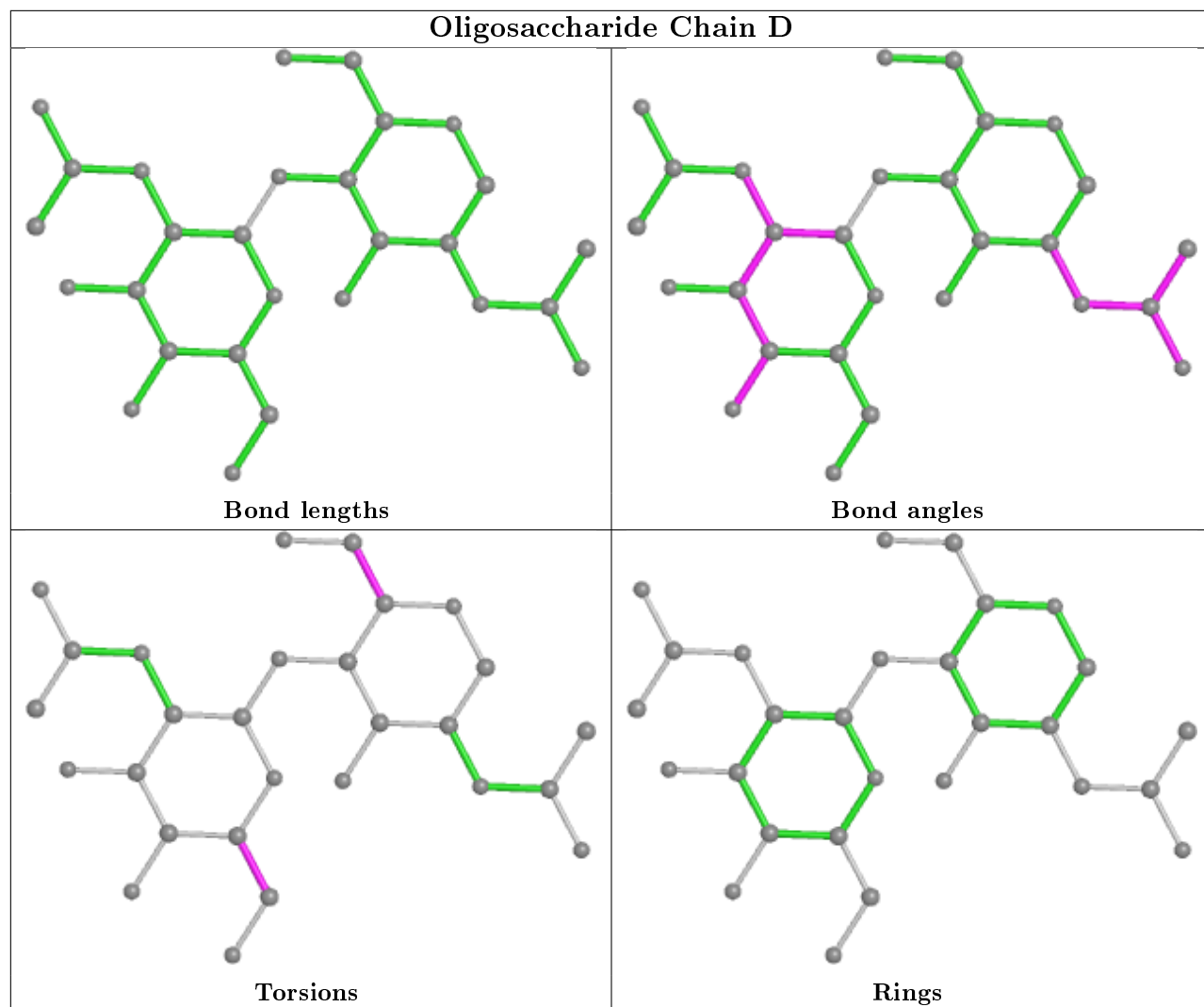
There are no ring outliers.

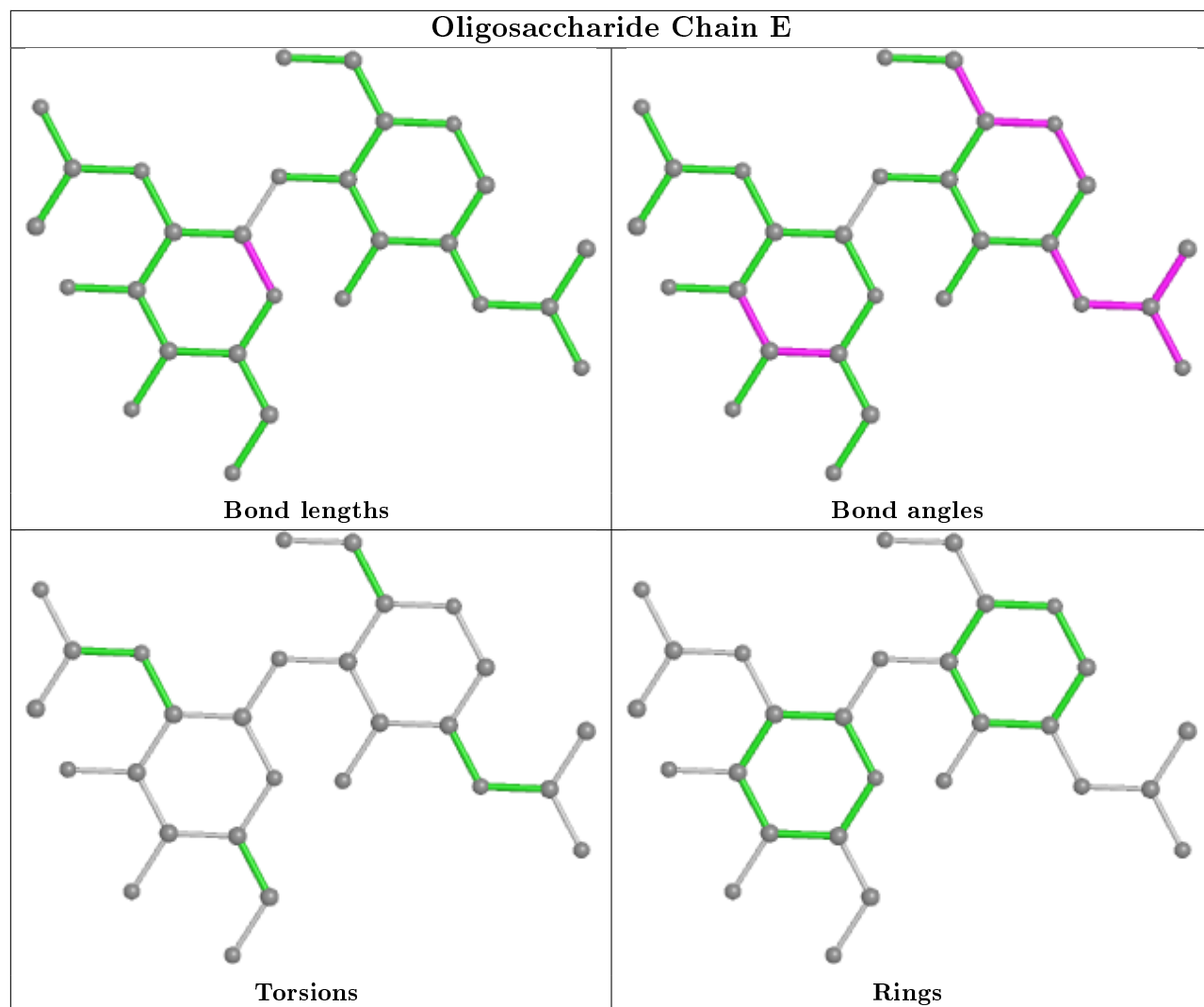
2 monomers are involved in 3 short contacts:

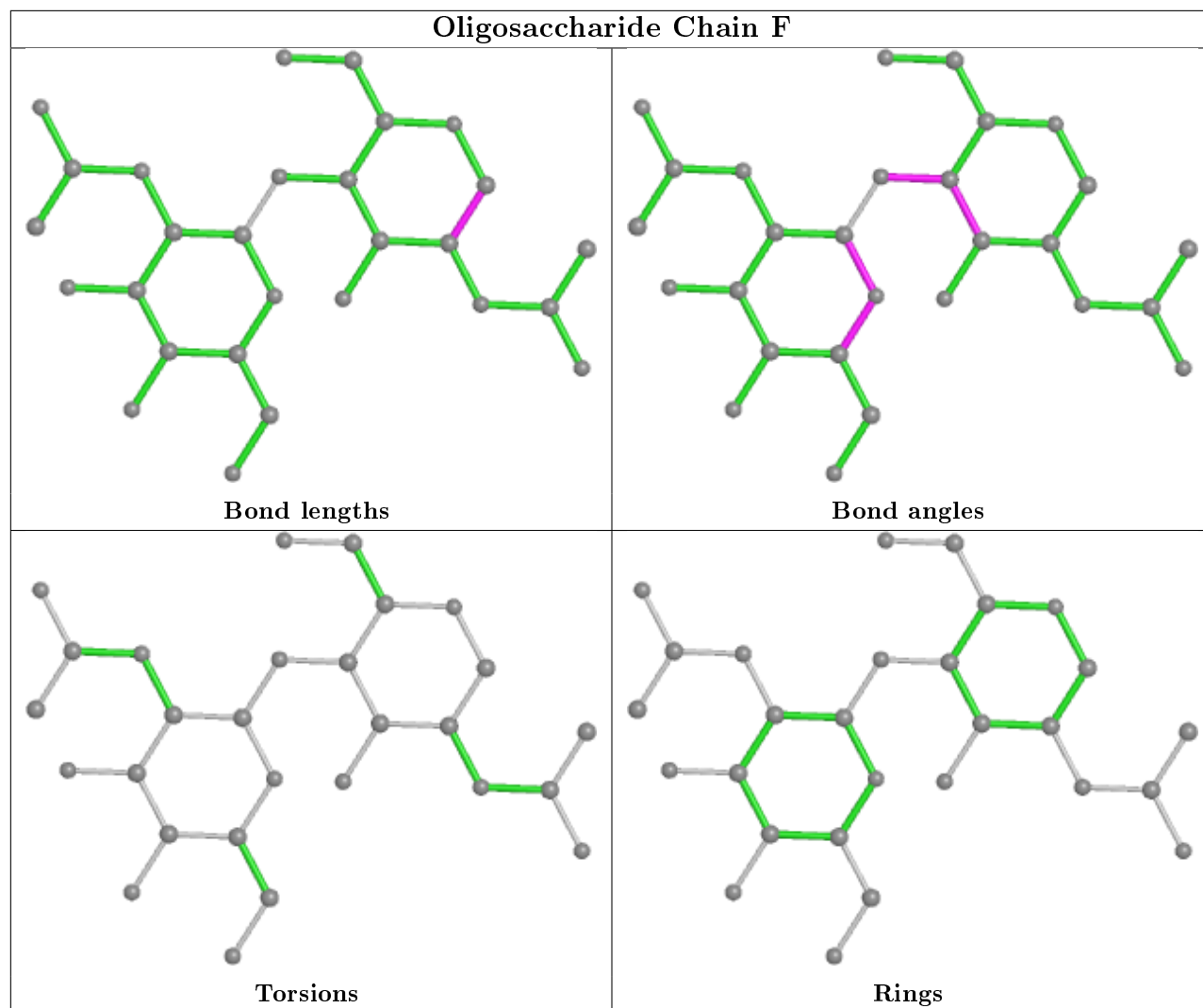
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	I	2	NAG	2	0

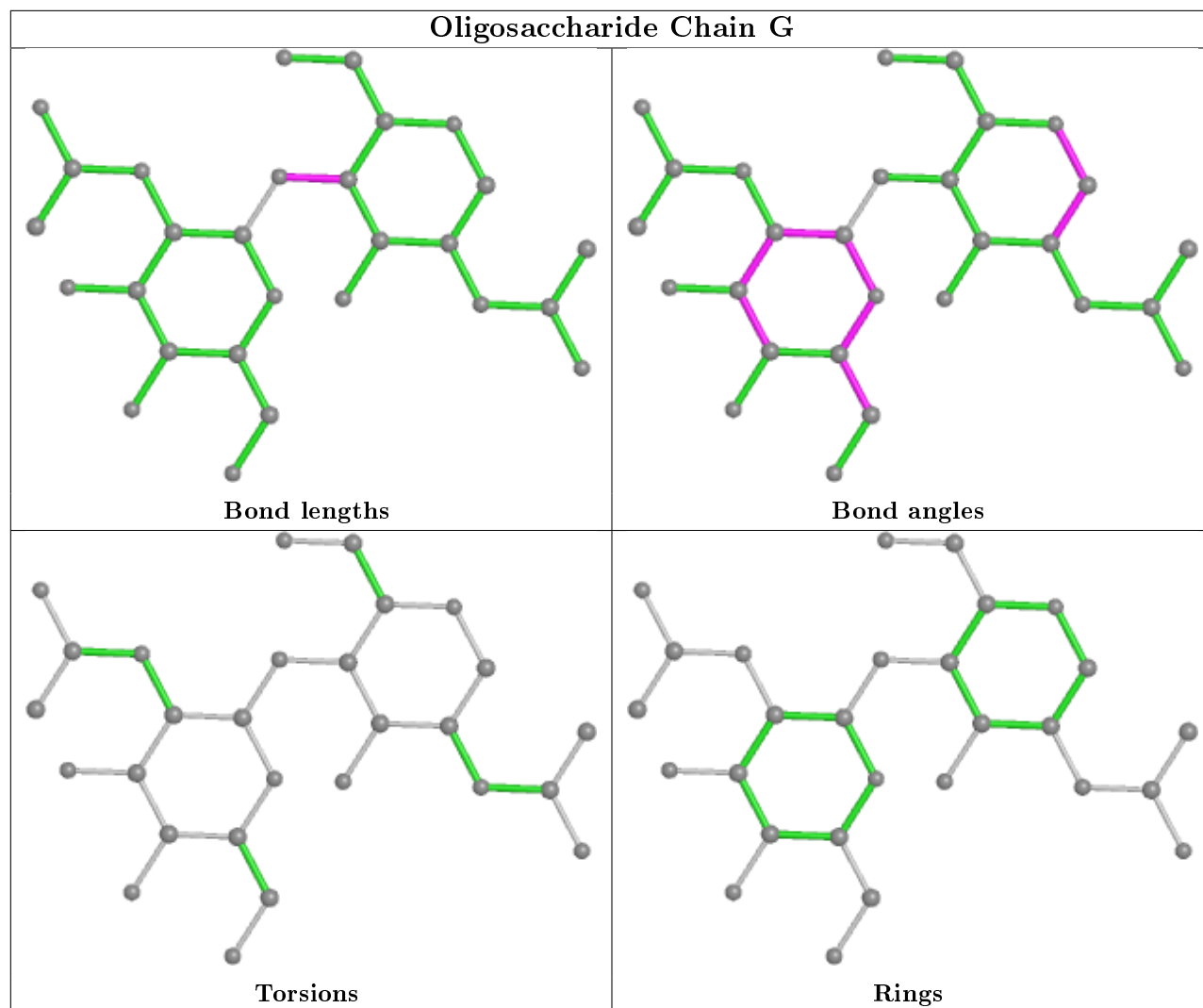
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

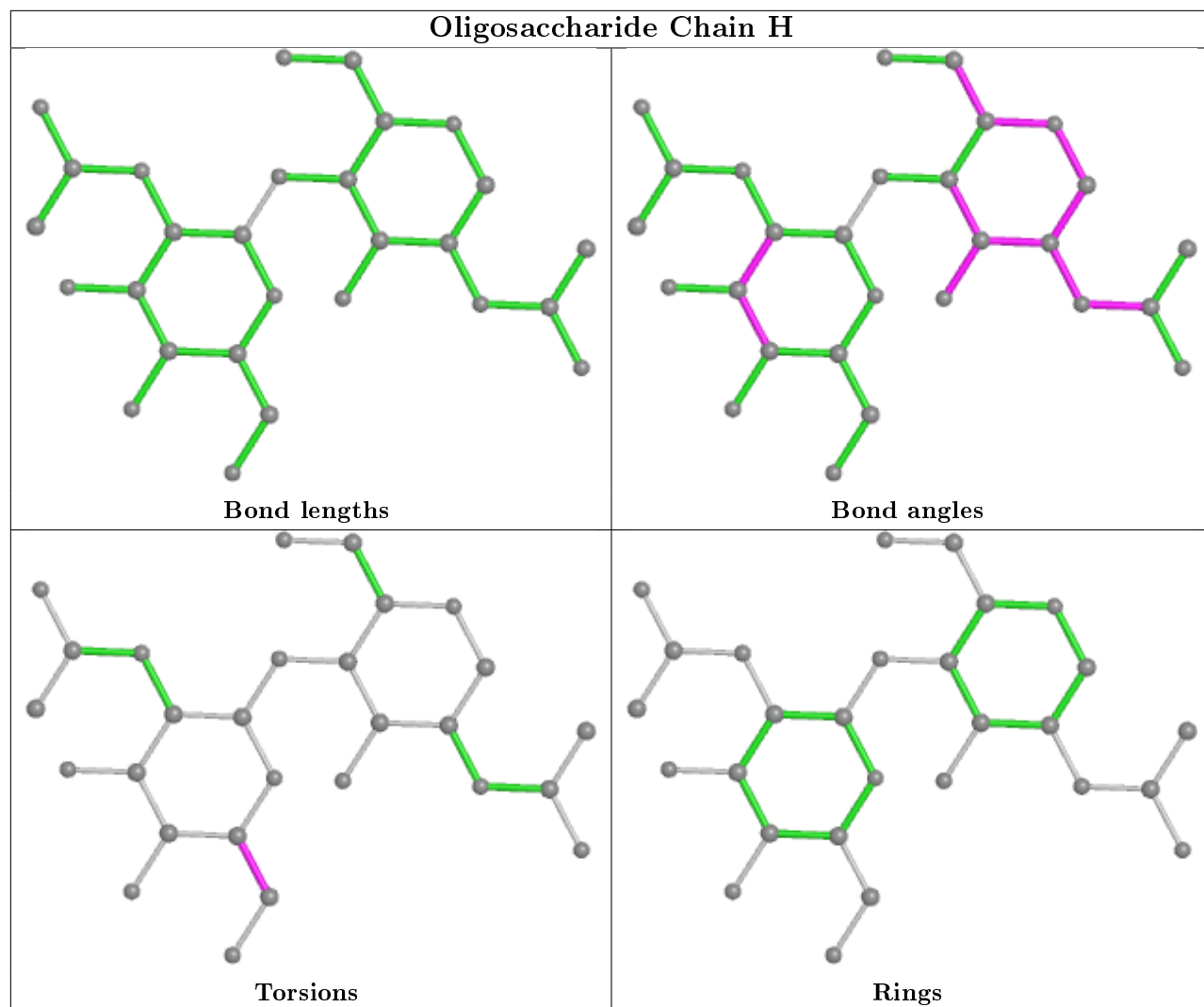


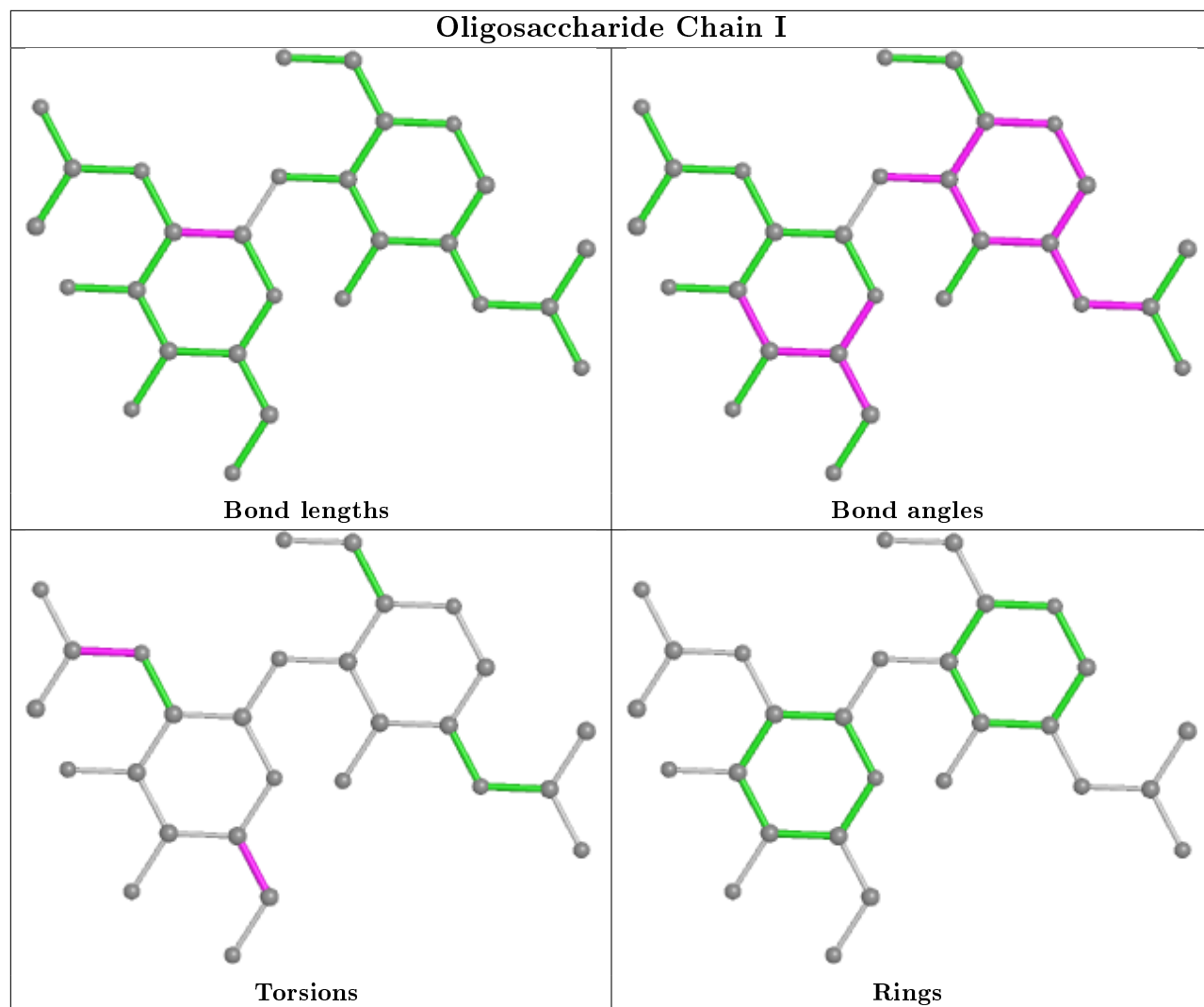


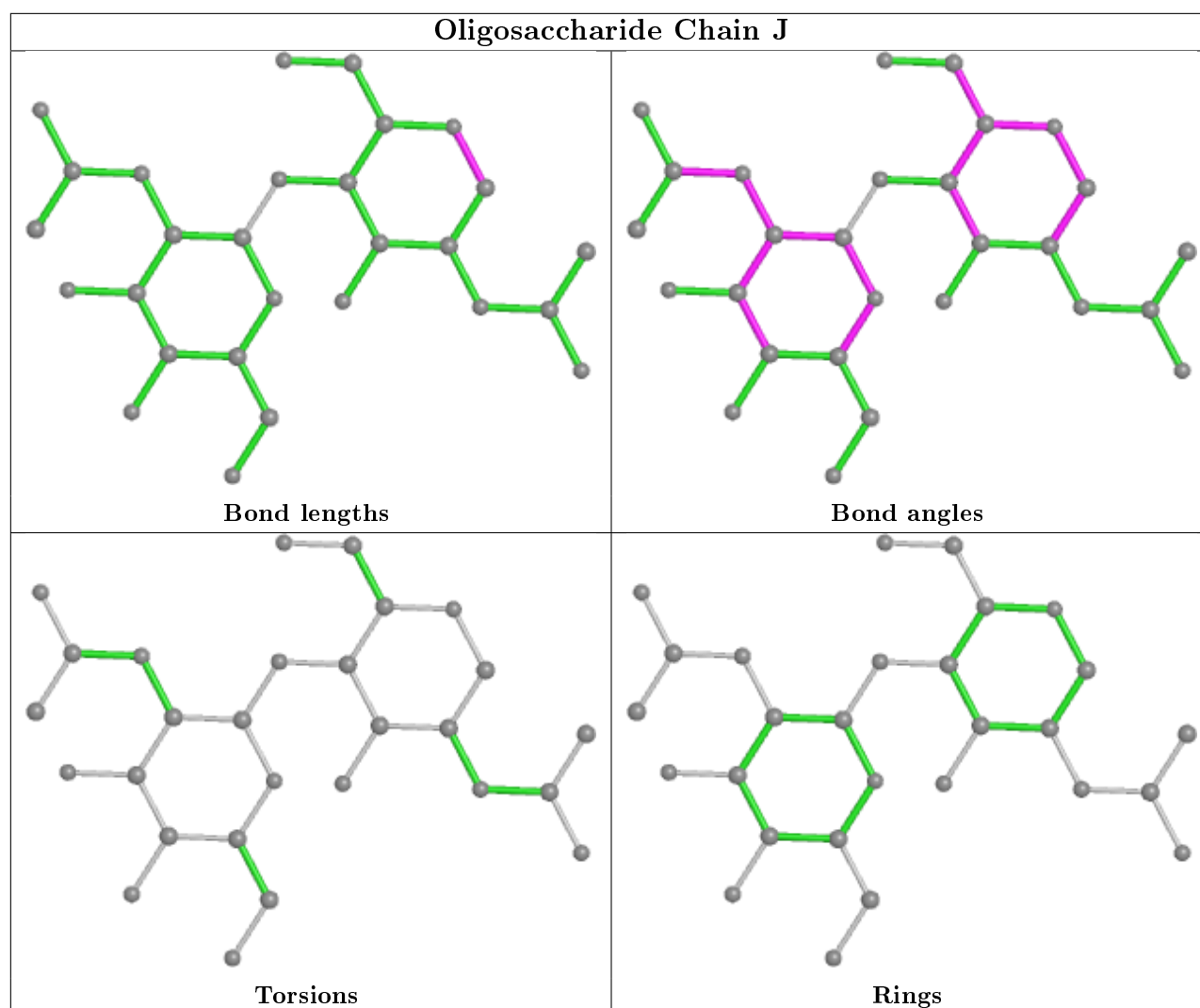












5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	1027	-	4,4,4	0.85	0	6,6,6	0.64	0
6	SO4	A	1023	-	4,4,4	0.76	0	6,6,6	0.69	0
6	SO4	A	1024	-	4,4,4	0.81	0	6,6,6	0.41	0
6	SO4	A	1026	-	4,4,4	1.02	0	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1029	-	4,4,4	0.36	0	6,6,6	0.28	0
6	SO4	A	1022	-	4,4,4	0.79	0	6,6,6	0.27	0
6	SO4	A	1028	-	4,4,4	0.50	0	6,6,6	1.71	1 (16%)
6	SO4	A	1025	-	4,4,4	0.70	0	6,6,6	0.50	0
5	NAG	A	1019	1	14,14,15	0.61	0	17,19,21	1.40	3 (17%)
6	SO4	A	1021	-	4,4,4	0.63	0	6,6,6	0.46	0
5	NAG	A	1016	1	14,14,15	0.61	0	17,19,21	2.57	5 (29%)
6	SO4	A	1020	-	4,4,4	0.83	0	6,6,6	0.45	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
5	NAG	A	1016	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1019	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1016	NAG	O5-C1-C2	-5.25	103.00	111.29
5	A	1016	NAG	O5-C5-C6	4.89	114.87	107.20
5	A	1016	NAG	C8-C7-N2	4.55	123.80	116.10
5	A	1016	NAG	C2-N2-C7	4.44	129.23	122.90
5	A	1019	NAG	C1-O5-C5	3.32	116.69	112.19
5	A	1016	NAG	O7-C7-C8	-2.81	116.84	122.06
6	A	1028	SO4	O4-S-O2	2.73	123.55	109.31
5	A	1019	NAG	O5-C5-C6	2.39	110.94	107.20
5	A	1019	NAG	C4-C3-C2	2.26	114.33	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1016	NAG	O5-C5-C6-O6
5	A	1016	NAG	C4-C5-C6-O6
5	A	1016	NAG	C8-C7-N2-C2
5	A	1016	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1027	SO4	3	0
6	A	1029	SO4	1	0
6	A	1022	SO4	2	0
6	A	1028	SO4	1	0
5	A	1016	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	902/908 (99%)	-0.12	31 (3%) 45 55	21, 42, 82, 198	0
2	B	6/6 (100%)	0.88	1 (16%) 1 2	34, 39, 46, 56	0
All	All	908/914 (99%)	-0.11	32 (3%) 44 53	21, 42, 82, 198	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	893	PHE	19.1
1	A	885	PHE	14.0
1	A	891	GLY	11.4
1	A	888	TYR	10.9
1	A	889	GLY	9.7
1	A	925	VAL	8.0
1	A	886	GLN	6.6
1	A	923	MET	5.6
1	A	927	PHE	5.3
1	A	932	ARG	4.4
1	A	882	LYS	4.2
1	A	928	GLY	3.8
1	A	924	ASP	3.6
1	A	197	ASN	3.6
1	A	926	GLY	3.4
1	A	933	ALA	3.3
1	A	892	SER	3.2
1	A	890	GLY	2.9
1	A	922	ASN	2.9
1	A	196	GLY	2.9
1	A	93	ALA	2.9
1	A	367	GLN	2.7
1	A	884	LEU	2.7
1	A	895	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	781	GLU	2.5
1	A	881	TRP	2.3
2	B	4	ARG	2.3
1	A	782	ASN	2.2
1	A	776	TRP	2.2
1	A	736	ASN	2.1
1	A	816	ALA	2.1
1	A	94	ASP	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](#)

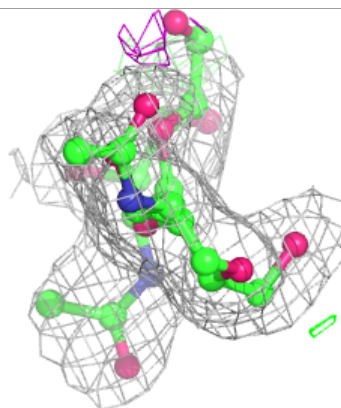
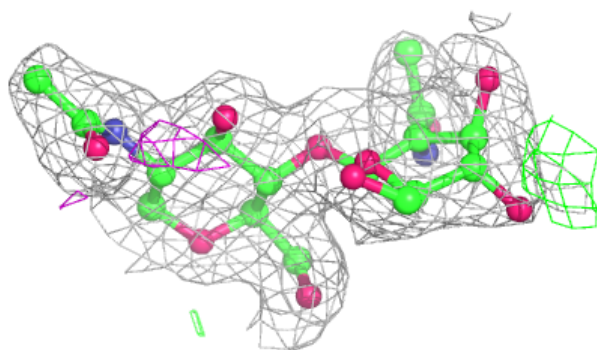
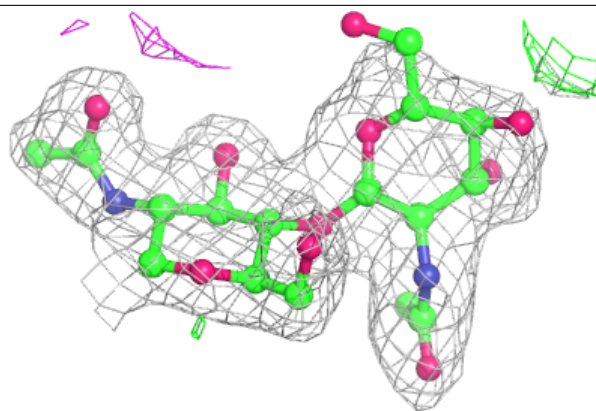
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	J	2	14/15	0.80	0.22	85,107,125,137	0
3	NAG	D	2	14/15	0.81	0.41	85,113,151,153	0
3	NAG	H	1	14/15	0.83	0.14	56,112,171,179	0
3	NAG	F	2	14/15	0.86	0.22	65,103,163,188	0
3	NAG	H	2	14/15	0.89	0.26	56,89,111,138	0
3	NAG	I	2	14/15	0.91	0.19	54,77,130,151	0
3	NAG	G	2	14/15	0.92	0.18	60,102,131,145	0
3	NAG	J	1	14/15	0.92	0.11	56,99,169,169	0
3	NAG	F	1	14/15	0.94	0.09	49,76,108,114	0
3	NAG	D	1	14/15	0.95	0.13	40,56,82,88	0
3	NAG	G	1	14/15	0.96	0.16	56,72,112,119	0
3	NAG	I	1	14/15	0.97	0.07	34,42,50,51	0
3	NAG	E	1	14/15	0.97	0.07	29,41,55,58	0
3	NAG	E	2	14/15	0.97	0.17	49,64,79,91	0
3	NAG	C	1	14/15	0.98	0.08	32,40,48,50	0
3	NAG	C	2	14/15	0.98	0.17	58,85,187,216	0

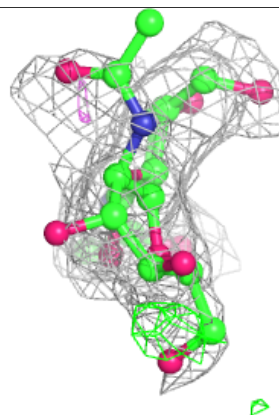
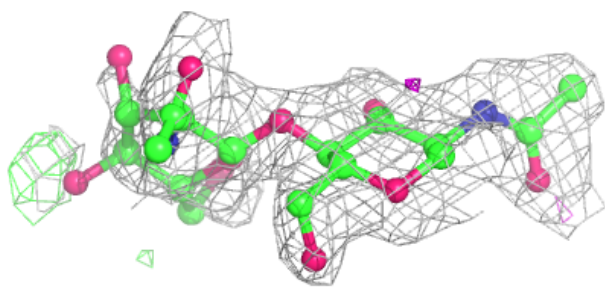
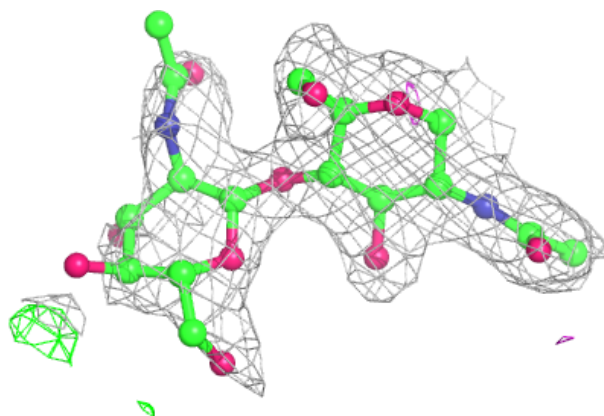
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

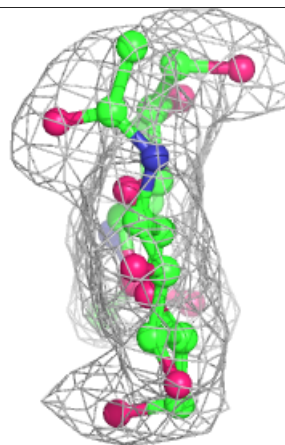
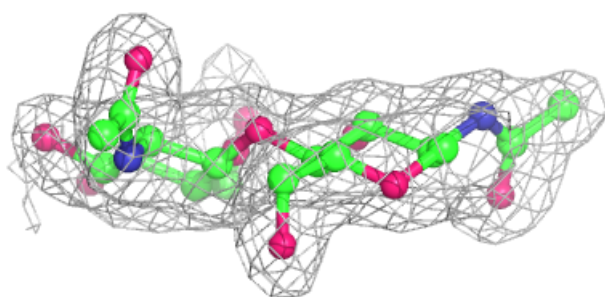
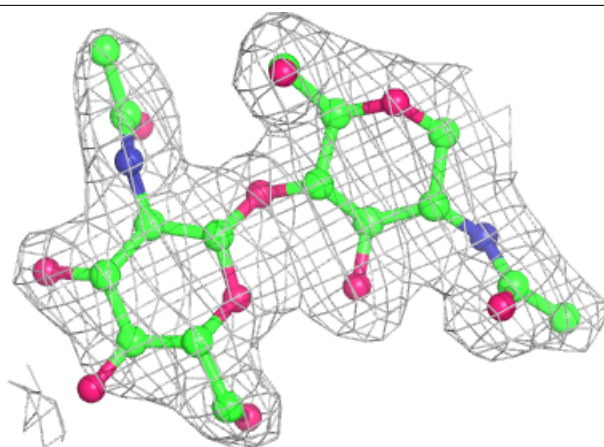
**Electron density around Chain D:**

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



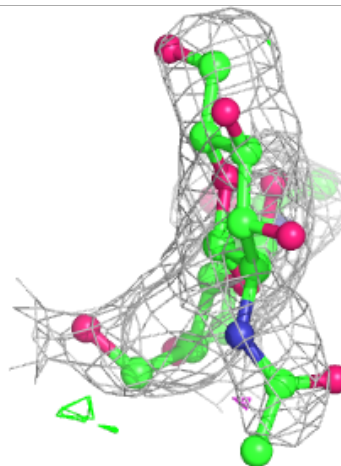
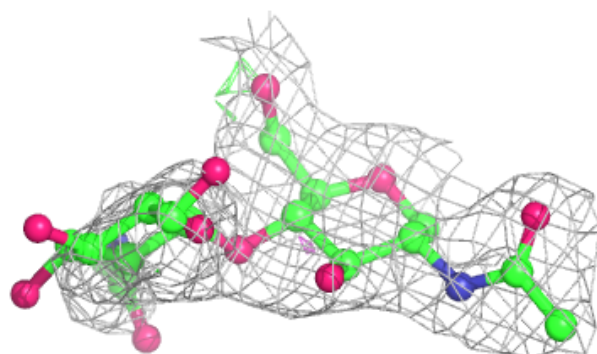
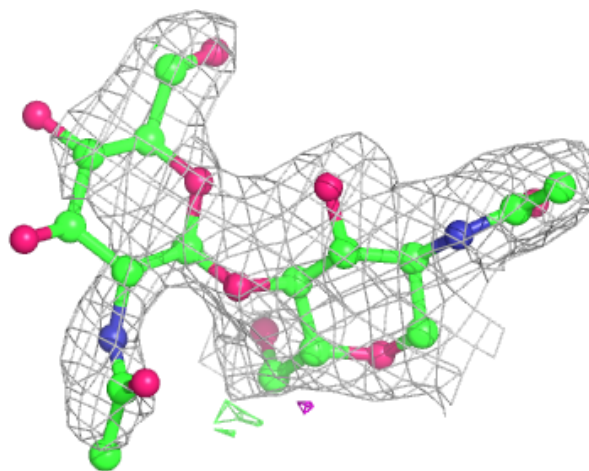
Electron density around Chain E:

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



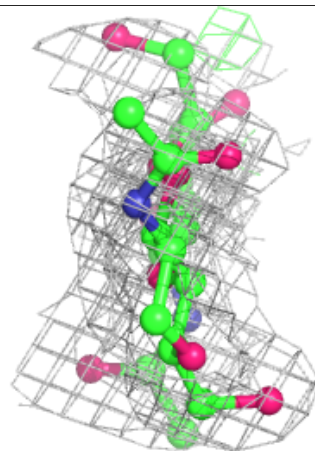
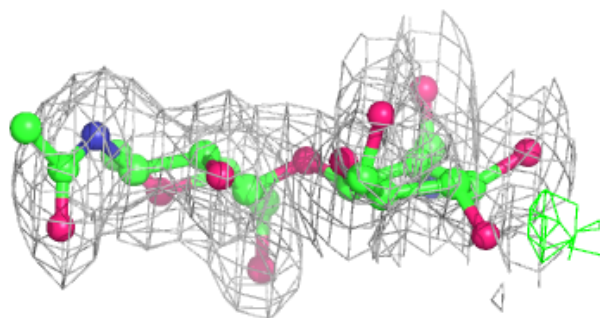
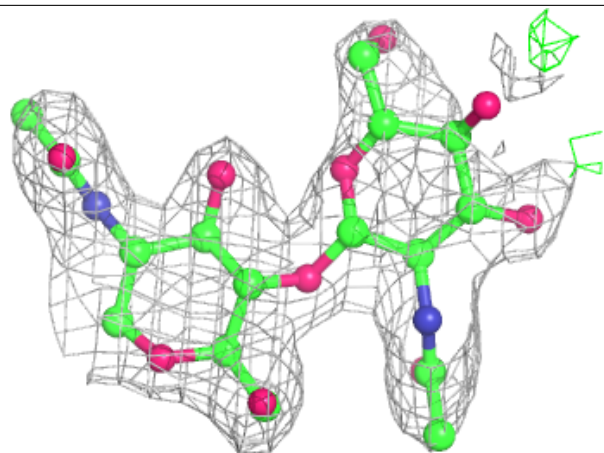
Electron density around Chain F:

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



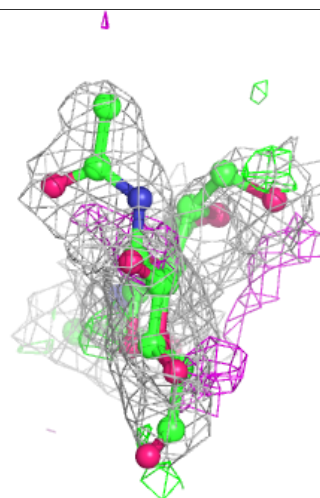
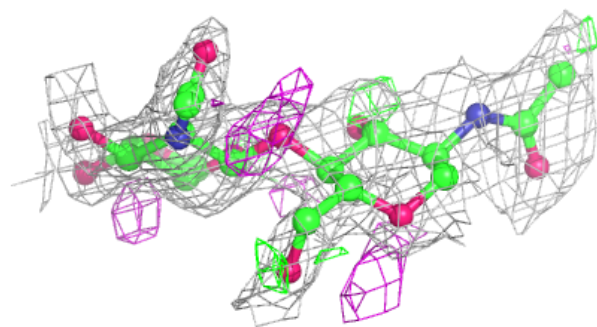
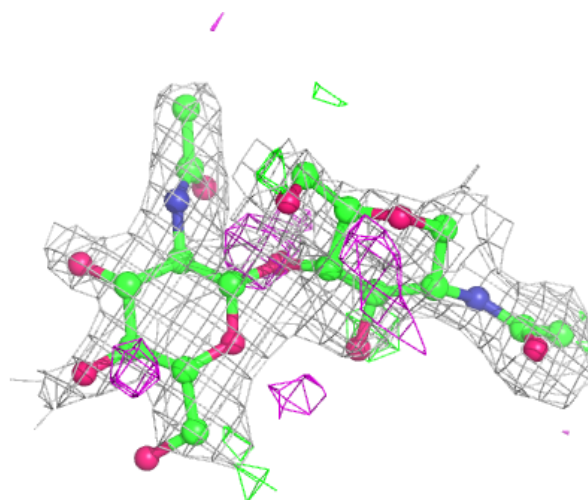
Electron density around Chain G:

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



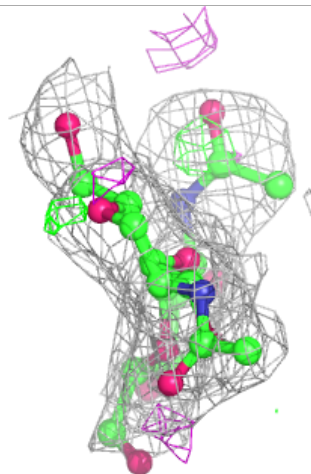
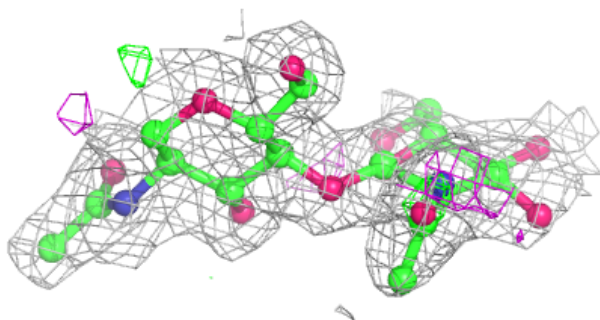
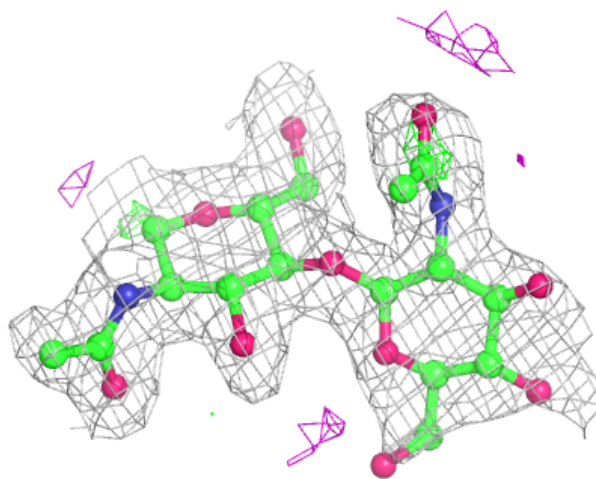
Electron density around Chain H:

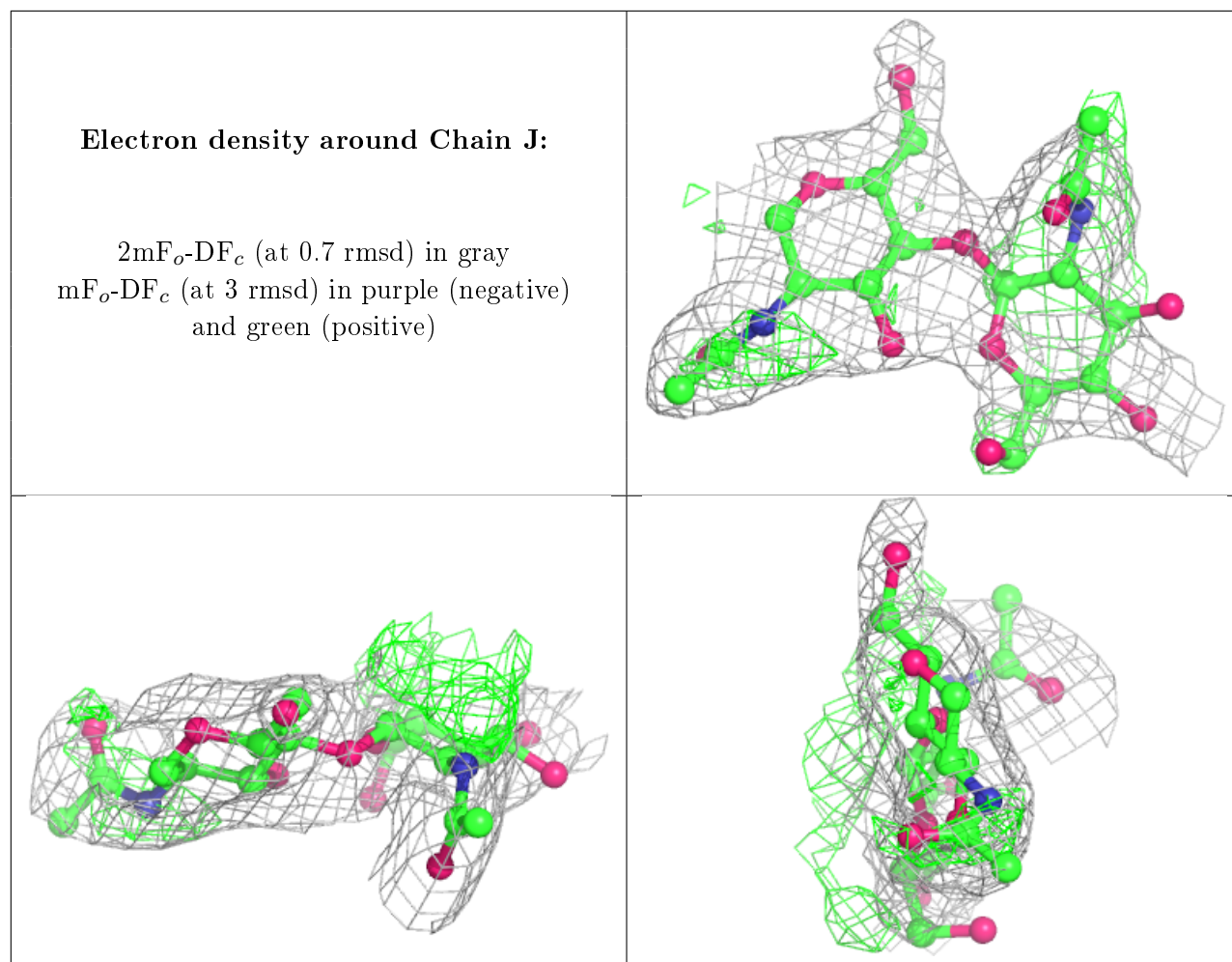
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	NAG	A	1016	14/15	0.84	0.17	87,115,160,185	0
5	NAG	A	1019	14/15	0.85	0.36	87,105,127,141	0
6	SO4	A	1026	5/5	0.90	0.24	64,64,81,81	0
6	SO4	A	1028	5/5	0.92	0.21	40,41,60,65	0
6	SO4	A	1027	5/5	0.93	0.23	60,66,75,76	0
6	SO4	A	1023	5/5	0.93	0.22	56,57,73,76	0
6	SO4	A	1022	5/5	0.94	0.23	62,65,81,86	0
6	SO4	A	1025	5/5	0.94	0.21	64,71,74,87	0
6	SO4	A	1021	5/5	0.95	0.26	64,70,73,85	0
6	SO4	A	1029	5/5	0.95	0.24	64,69,76,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	A	1024	5/5	0.96	0.29	60,63,75,91	0
6	SO4	A	1020	5/5	0.96	0.18	51,56,68,77	0
4	ZN	A	1001	1/1	1.00	0.11	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.