



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:50 PM EST

PDB ID : 4HOM
Title : Crystal structure of porcine aminopeptidase-N complexed with substance P
Authors : Chen, L.; Lin, Y.L.; Peng, G.; Li, F.
Deposited on : 2012-10-22
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

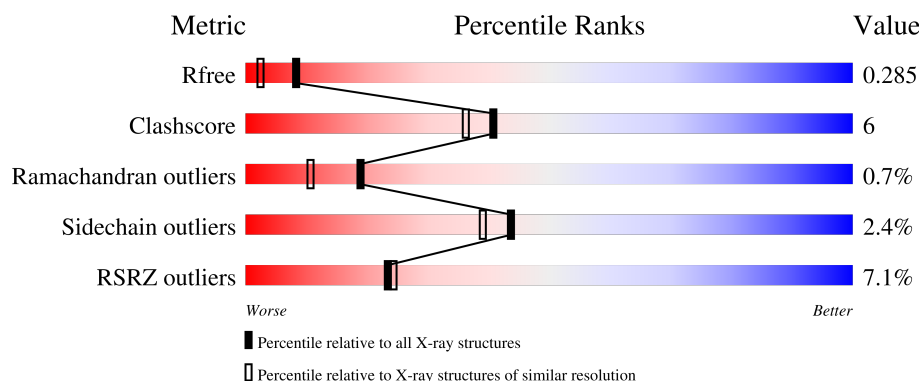
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	908	 6% 90% 8% ..
2	B	11	 18% 36% 36% 9%
3	C	3	 33% 67%
3	D	3	 33% 33% 33%
3	G	3	 100%
4	E	2	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	H	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	K	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9093 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
1	A	902	Total	C	N	O	S	0	0	0
			7241	4622	1210	1379	30			

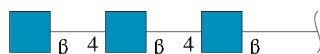
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ASN	PHE	conflict	UNP P15145
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 substance P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			95	63	17	14	1			

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



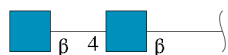
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			42	24	3	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			42	24	3	15			
3	G	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 4 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
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

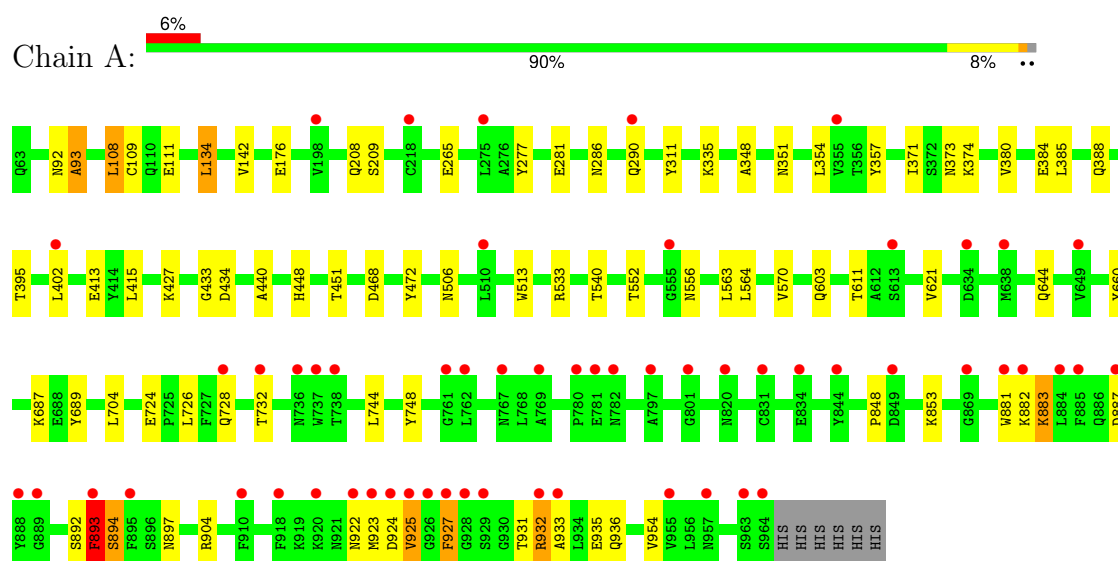
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1423	Total	O	0	0
			1423	1423		
7	B	11	Total	O	0	0
			11	11		

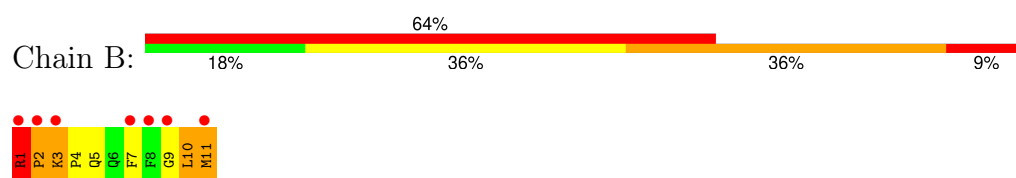
3 Residue-property plots

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. 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. 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



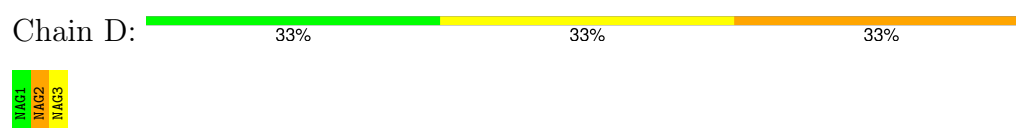
• Molecule 2: substance P



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

Chain G:  100%

NAG1
NAG2
NAG3

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

Chain E:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2

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

Chain H:  50% 50%

NAG1
NAG2

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

Chain I:  50% 50%

NAG1
NAG2

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

Chain J:  50% 50%

NAG1
NAG2

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

Chain K:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.57Å 62.60Å 81.55Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	37.18 – 1.90 37.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.18-1.90) 98.1 (37.18-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.147 , 0.201 0.255 , 0.285	Depositor DCC
R_{free} test set	5033 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.8	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	0.94	EDS
Total number of atoms	9093	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: NAG, ZN

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	0.34	0/7429	0.50	0/10124
2	B	0.65	0/98	1.50	4/128 (3.1%)
All	All	0.35	0/7527	0.53	4/10252 (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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1	ARG	C-N-CD	-7.80	103.43	120.60
2	B	2	PRO	N-CA-C	6.73	129.60	112.10
2	B	3	LYS	N-CA-C	6.52	128.60	111.00
2	B	2	PRO	CB-CA-C	-5.78	97.56	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	ARG	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	7241	0	6994	80	0
2	B	95	0	99	33	0
3	C	42	0	37	2	0
3	D	42	0	37	1	0
3	G	42	0	37	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
4	K	28	0	25	1	0
5	A	28	0	26	0	0
6	A	1	0	0	0	0
7	A	1423	0	0	18	2
7	B	11	0	0	0	0
All	All	9093	0	7380	96	2

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 (96) 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:348:ALA:HB3	2:B:2:PRO:HB3	1.28	1.08
2:B:2:PRO:O	2:B:4:PRO:HD3	1.60	0.99
1:A:384:GLU:OE1	2:B:2:PRO:HA	1.67	0.92
1:A:380:VAL:HG13	7:A:1847:HOH:O	1.70	0.91
1:A:265:GLU:HG3	7:A:1351:HOH:O	1.69	0.91
1:A:451:THR:HG22	7:A:2203:HOH:O	1.75	0.86
7:A:1269:HOH:O	2:B:1:ARG:HB3	1.73	0.86
2:B:3:LYS:HB3	2:B:5:GLN:OE1	1.77	0.83
1:A:556:ASN:HD22	4:J:1:NAG:H83	1.47	0.78
1:A:111:GLU:HG2	7:A:2218:HOH:O	1.85	0.76
1:A:348:ALA:CB	2:B:2:PRO:HB3	2.13	0.75
1:A:384:GLU:OE1	2:B:2:PRO:CA	2.35	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1269:HOH:O	2:B:1:ARG:CB	2.31	0.74
2:B:2:PRO:O	2:B:4:PRO:CD	2.36	0.72
1:A:371:ILE:HG13	1:A:744:LEU:HD12	1.75	0.69
1:A:373:ASN:HB3	7:A:2199:HOH:O	1.92	0.68
2:B:1:ARG:HB2	2:B:2:PRO:HD3	1.74	0.68
1:A:371:ILE:CG1	1:A:744:LEU:HD12	2.25	0.67
1:A:472:TYR:CD2	2:B:3:LYS:HB2	2.30	0.66
1:A:433:GLY:HA2	2:B:7:PHE:HA	1.77	0.66
1:A:927:PHE:HD2	1:A:931:THR:HG23	1.60	0.66
1:A:92:ASN:HB3	7:A:2014:HOH:O	1.95	0.65
1:A:564:LEU:HD13	2:B:11:MET:HG3	1.79	0.64
1:A:108:LEU:HD12	1:A:109:CYS:N	2.13	0.63
1:A:704:LEU:HD21	1:A:904:ARG:HG2	1.81	0.63
1:A:176:GLU:OE1	7:A:1512:HOH:O	2.16	0.63
1:A:892:SER:O	1:A:893:PHE:HB2	2.00	0.62
1:A:611:THR:HG21	7:A:1382:HOH:O	2.01	0.61
1:A:208:GLN:HE21	1:A:209:SER:HA	1.67	0.60
1:A:904:ARG:HD2	7:A:1894:HOH:O	2.02	0.60
1:A:932:ARG:N	1:A:932:ARG:HE	2.00	0.59
1:A:552:THR:HB	1:A:611:THR:HG22	1.86	0.58
1:A:448:HIS:HE1	1:A:468:ASP:OD2	1.87	0.57
1:A:92:ASN:O	1:A:93:ALA:HB3	2.05	0.56
1:A:564:LEU:CD1	2:B:11:MET:HG3	2.37	0.55
3:D:2:NAG:H61	3:D:3:NAG:O5	2.08	0.54
1:A:881:TRP:C	1:A:883:LYS:H	2.11	0.54
2:B:3:LYS:CB	2:B:5:GLN:OE1	2.52	0.54
1:A:434:ASP:OD1	2:B:5:GLN:HG3	2.10	0.52
1:A:954:VAL:HG23	7:A:1573:HOH:O	2.10	0.52
1:A:563:LEU:HD11	1:A:570:VAL:CG2	2.40	0.52
1:A:660:TYR:CD1	2:B:10:LEU:HG	2.45	0.51
1:A:660:TYR:HD1	2:B:10:LEU:HG	1.75	0.51
1:A:357:TYR:HE2	1:A:380:VAL:HG12	1.76	0.51
2:B:1:ARG:HB2	2:B:2:PRO:CD	2.42	0.50
2:B:4:PRO:C	2:B:5:GLN:HG2	2.31	0.50
1:A:395:THR:O	1:A:506:ASN:HA	2.12	0.50
1:A:451:THR:HG23	1:A:540:THR:HB	1.94	0.49
1:A:892:SER:O	1:A:893:PHE:CB	2.60	0.49
1:A:848:PRO:HG3	1:A:853:LYS:HE3	1.94	0.49
1:A:281:GLU:OE1	7:A:1541:HOH:O	2.20	0.49
7:A:1441:HOH:O	2:B:10:LEU:HD13	2.13	0.48
1:A:931:THR:HG22	1:A:932:ARG:NE	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ALA:HA	2:B:11:MET:HG2	1.96	0.48
1:A:357:TYR:CE2	1:A:380:VAL:HG12	2.49	0.47
1:A:927:PHE:CD2	1:A:931:THR:HG23	2.46	0.47
1:A:348:ALA:H	2:B:2:PRO:HG3	1.80	0.47
1:A:108:LEU:HD12	1:A:109:CYS:H	1.79	0.46
1:A:371:ILE:HG13	1:A:744:LEU:CD1	2.43	0.46
1:A:348:ALA:N	2:B:2:PRO:HG3	2.30	0.46
7:A:2191:HOH:O	3:C:3:NAG:H83	2.15	0.46
1:A:402:LEU:O	1:A:402:LEU:HG	2.12	0.46
2:B:4:PRO:O	2:B:5:GLN:HG2	2.17	0.45
1:A:448:HIS:CE1	1:A:468:ASP:OD2	2.69	0.45
1:A:208:GLN:HE21	1:A:209:SER:CA	2.29	0.45
1:A:415:LEU:HD22	1:A:427:LYS:HE3	1.97	0.45
1:A:556:ASN:HD22	4:J:1:NAG:C8	2.23	0.45
1:A:440:ALA:HB2	2:B:11:MET:H	1.81	0.45
7:A:2360:HOH:O	2:B:4:PRO:HB3	2.17	0.45
1:A:732:THR:HB	7:A:2161:HOH:O	2.17	0.44
1:A:351:ASN:HB2	1:A:354:LEU:O	2.18	0.44
1:A:563:LEU:HD11	1:A:570:VAL:HG23	2.00	0.44
1:A:924:ASP:O	1:A:925:VAL:HG22	2.18	0.44
7:A:1269:HOH:O	2:B:1:ARG:HB2	2.09	0.44
1:A:371:ILE:HG12	1:A:744:LEU:HD12	1.99	0.43
1:A:92:ASN:O	1:A:93:ALA:CB	2.66	0.43
1:A:208:GLN:HA	1:A:209:SER:HA	1.82	0.43
1:A:932:ARG:HA	1:A:935:GLU:HB2	2.00	0.43
1:A:385:LEU:HA	1:A:388:GLN:HG2	2.01	0.42
1:A:413:GLU:OE1	2:B:4:PRO:HB3	2.19	0.42
1:A:311:TYR:CE1	1:A:374:LYS:HE2	2.55	0.42
1:A:932:ARG:HE	1:A:932:ARG:H	1.67	0.42
1:A:440:ALA:CA	2:B:11:MET:HG2	2.49	0.41
3:C:2:NAG:H4	3:C:3:NAG:H2	1.81	0.41
1:A:472:TYR:CE2	2:B:3:LYS:HB2	2.55	0.41
1:A:621:VAL:HG11	4:K:1:NAG:H82	2.01	0.41
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.56	0.41
1:A:894:SER:OG	1:A:897:ASN:ND2	2.53	0.41
1:A:933:ALA:HA	1:A:936:GLN:OE1	2.21	0.41
1:A:134:LEU:HD13	1:A:142:VAL:CG2	2.51	0.41
1:A:380:VAL:HG22	2:B:4:PRO:HG2	2.03	0.41
1:A:413:GLU:OE2	2:B:4:PRO:HA	2.21	0.41
1:A:883:LYS:HG2	1:A:883:LYS:O	2.20	0.41
1:A:724:GLU:O	1:A:728:GLN:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:HG23	1:A:748:TYR:HE1	1.87	0.40
1:A:687:LYS:HA	1:A:726:LEU:HD13	2.03	0.40

All (2) 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)
7:A:2035:HOH:O	7:A:2035:HOH:O[2_556]	1.95	0.25
7:A:2351:HOH:O	7:A:2351:HOH:O[2_556]	1.98	0.22

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	900/908 (99%)	869 (97%)	26 (3%)	5 (1%)	22	13
2	B	9/11 (82%)	2 (22%)	6 (67%)	1 (11%)	0	0
All	All	909/919 (99%)	871 (96%)	32 (4%)	6 (1%)	19	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	LYS
1	A	893	PHE
1	A	925	VAL
2	B	9	GLY
1	A	93	ALA
1	A	894	SER

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	797/803 (99%)	780 (98%)	17 (2%)	48	45
2	B	10/10 (100%)	8 (80%)	2 (20%)	1	0
All	All	807/813 (99%)	788 (98%)	19 (2%)	44	39

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	134	LEU
1	A	277	TYR
1	A	286	ASN
1	A	290	GLN
1	A	335	LYS
1	A	513	TRP
1	A	533	ARG
1	A	603	GLN
1	A	644	GLN
1	A	883	LYS
1	A	887	ASP
1	A	893	PHE
1	A	922	ASN
1	A	923	MET
1	A	927	PHE
1	A	932	ARG
2	B	10	LEU
2	B	11	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	448	HIS
1	A	775	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	782	ASN
1	A	886	GLN
1	A	897	ASN
1	A	921	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 ⓘ

21 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	3,1	14,14,15	0.56	0	17,19,21	0.79	0
3	NAG	C	2	3	14,14,15	0.49	0	17,19,21	1.35	1 (5%)
3	NAG	C	3	3	14,14,15	0.75	0	17,19,21	1.35	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.57	0	17,19,21	0.84	0
3	NAG	D	2	3	14,14,15	0.72	0	17,19,21	1.56	1 (5%)
3	NAG	D	3	3	14,14,15	0.54	0	17,19,21	0.77	0
4	NAG	E	1	1,4	14,14,15	0.50	0	17,19,21	0.65	0
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	0.83	0
4	NAG	F	1	1,4	14,14,15	0.49	0	17,19,21	0.86	0
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.87	0
3	NAG	G	1	3,1	14,14,15	0.46	0	17,19,21	1.11	2 (11%)
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	1.18	1 (5%)
3	NAG	G	3	3	14,14,15	0.52	0	17,19,21	1.87	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	1,4	14,14,15	0.55	0	17,19,21	0.99	0
4	NAG	H	2	4	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.43	0	17,19,21	1.81	3 (17%)
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.89	0
4	NAG	J	1	1,4	14,14,15	0.51	0	17,19,21	1.43	5 (29%)
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	0.95	0
4	NAG	K	1	1,4	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
4	NAG	K	2	4	14,14,15	0.45	0	17,19,21	0.95	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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	C	3	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	3	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	3	3	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	NAG	C2-N2-C7	6.29	131.33	122.90
4	I	1	NAG	C1-O5-C5	5.88	120.06	112.19
3	D	2	NAG	C4-C3-C2	4.91	118.22	111.02
3	G	2	NAG	C4-C3-C2	3.82	116.61	111.02
3	C	3	NAG	C4-C3-C2	3.55	116.22	111.02
3	C	2	NAG	C4-C3-C2	3.13	115.60	111.02
3	G	1	NAG	C1-O5-C5	3.04	116.26	112.19
4	H	2	NAG	C1-O5-C5	2.86	116.02	112.19
4	K	1	NAG	C1-O5-C5	2.84	116.00	112.19
4	I	1	NAG	C2-N2-C7	-2.78	119.17	122.90
4	J	1	NAG	O5-C1-C2	-2.67	107.17	111.29
4	K	2	NAG	C1-O5-C5	2.64	115.73	112.19
4	I	1	NAG	C1-C2-N2	-2.55	106.42	110.43
3	G	3	NAG	C3-C4-C5	2.27	114.35	110.23
4	J	1	NAG	C8-C7-N2	2.26	119.87	116.12
4	J	1	NAG	C2-N2-C7	2.24	125.90	122.90
3	C	3	NAG	O5-C1-C2	2.21	114.71	111.29
4	J	1	NAG	C1-O5-C5	2.17	115.10	112.19
3	G	1	NAG	C1-C2-N2	2.14	113.81	110.43
3	G	3	NAG	O7-C7-N2	2.10	125.70	121.98
4	J	1	NAG	O7-C7-C8	-2.04	118.42	122.05

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	NAG	C3-C2-N2-C7
3	C	3	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	C	3	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

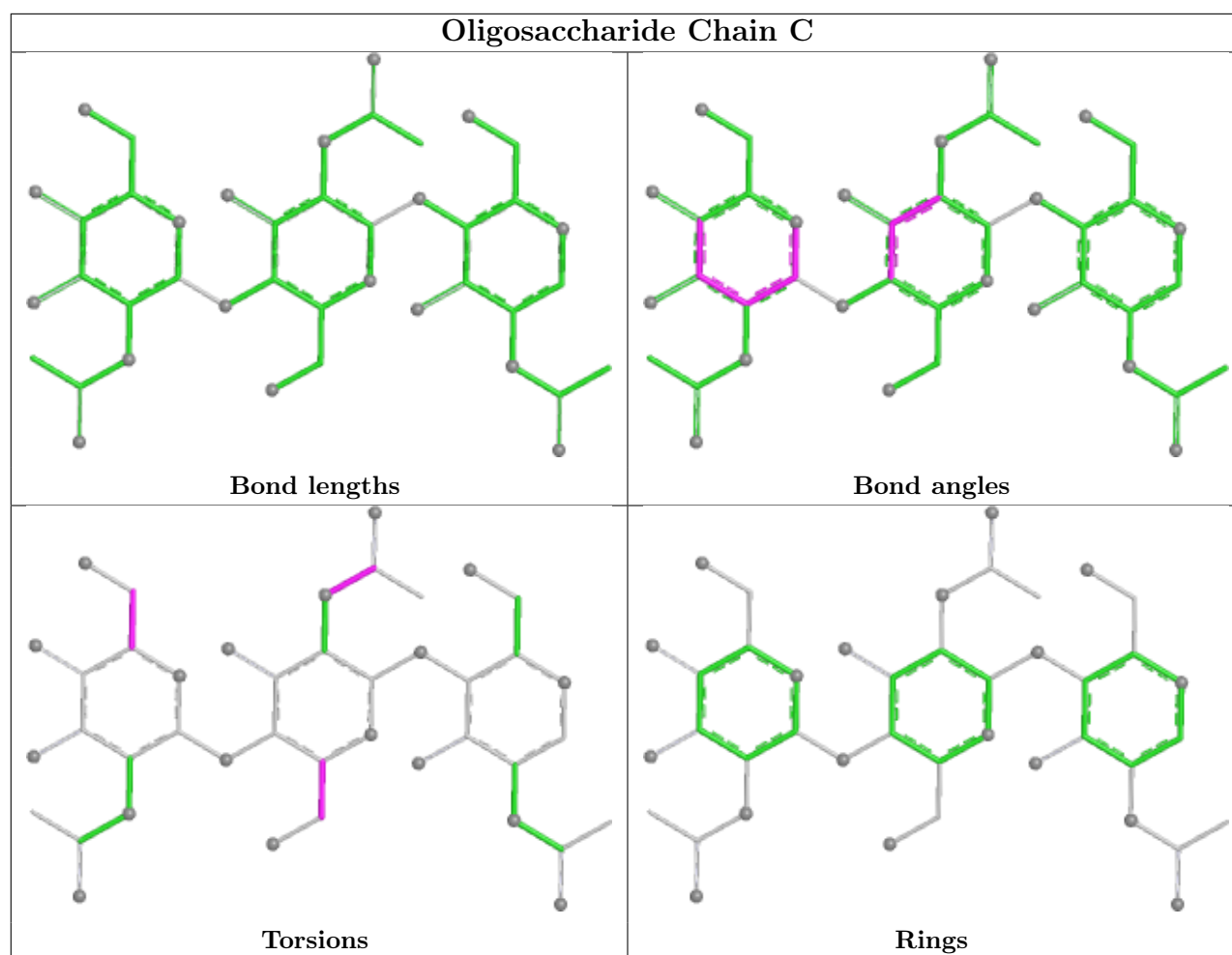
Mol	Chain	Res	Type	Atoms
3	G	3	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

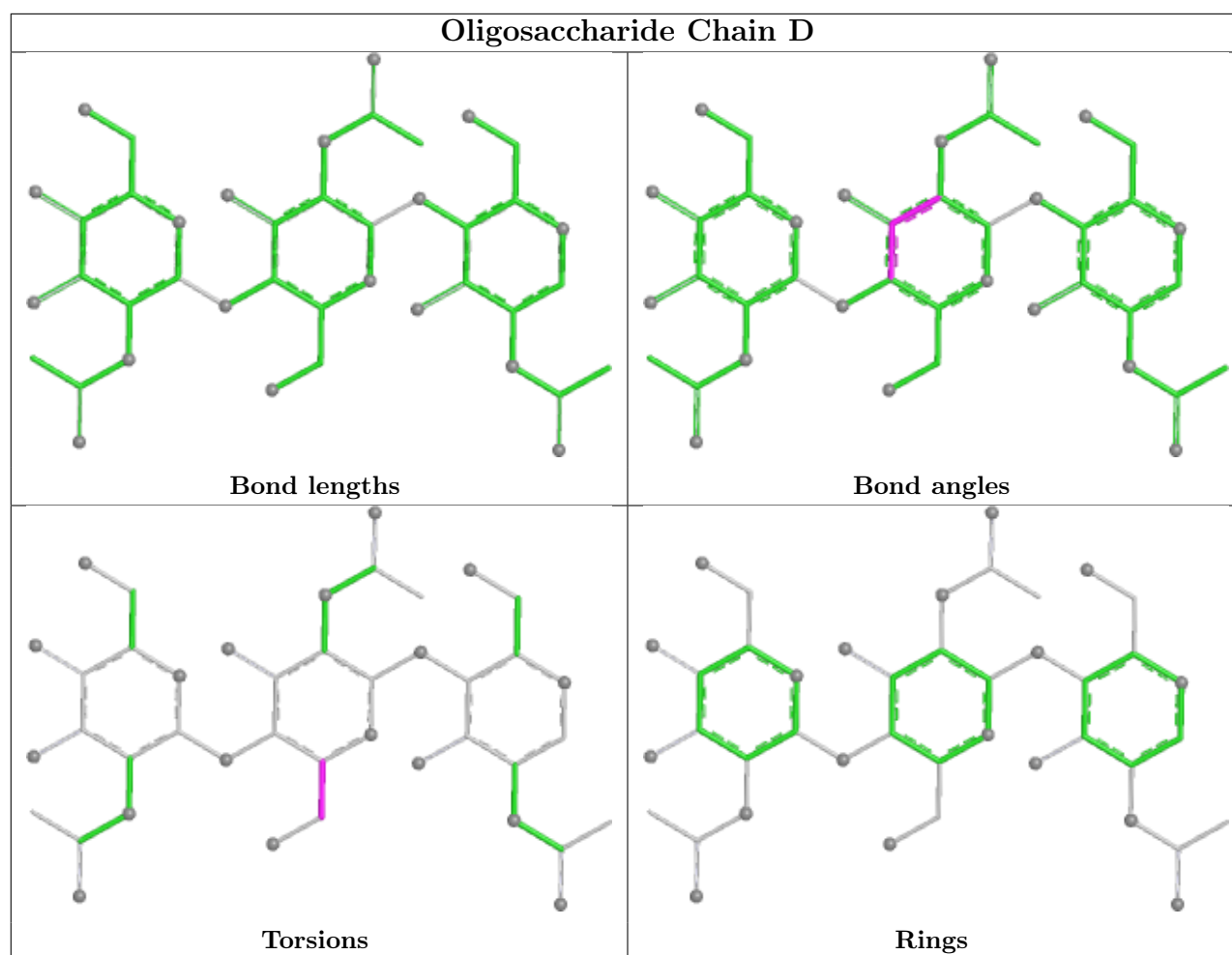
There are no ring outliers.

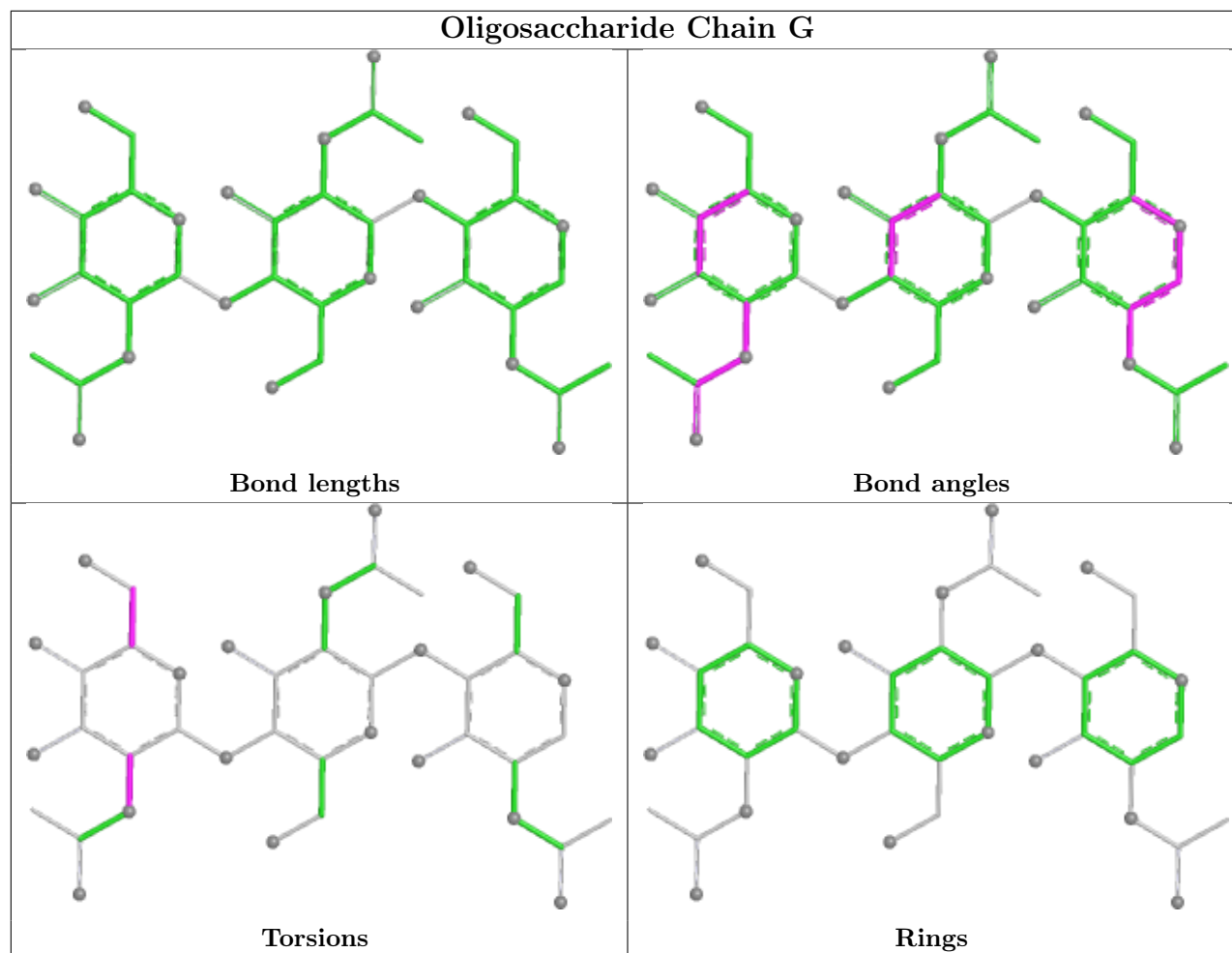
6 monomers are involved in 6 short contacts:

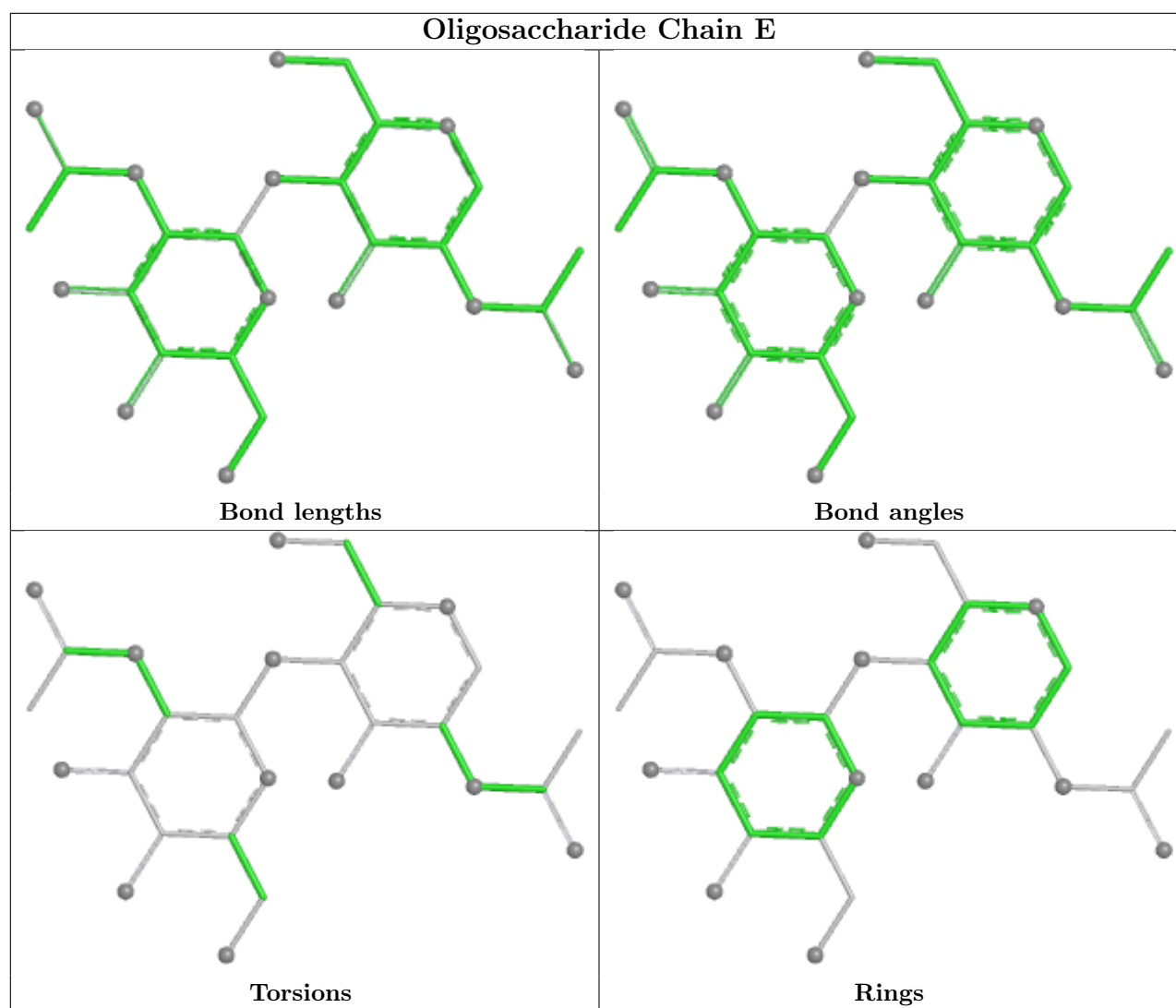
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	2	0
4	K	1	NAG	1	0
3	C	2	NAG	1	0
3	D	2	NAG	1	0
3	D	3	NAG	1	0
3	C	3	NAG	2	0

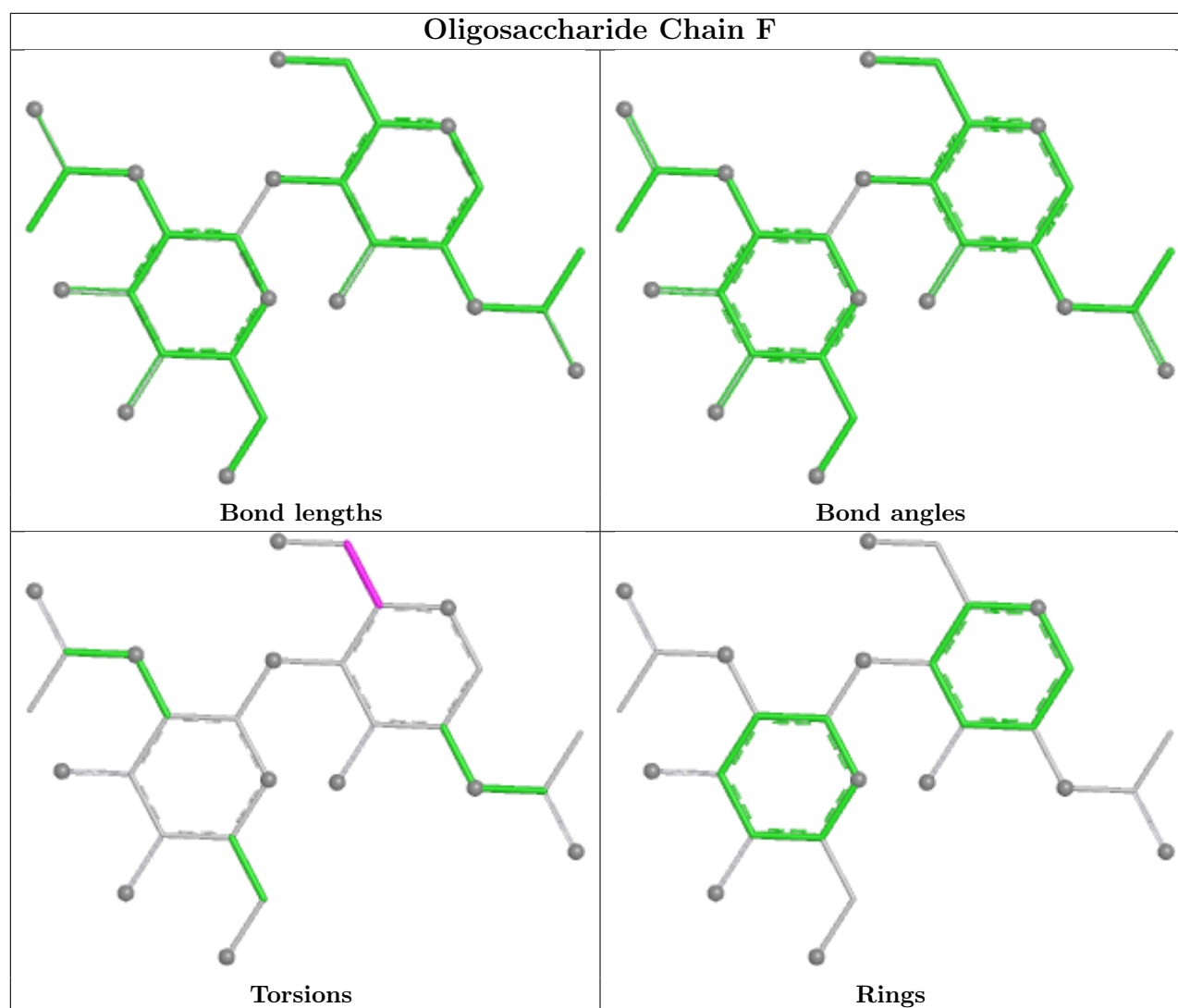
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

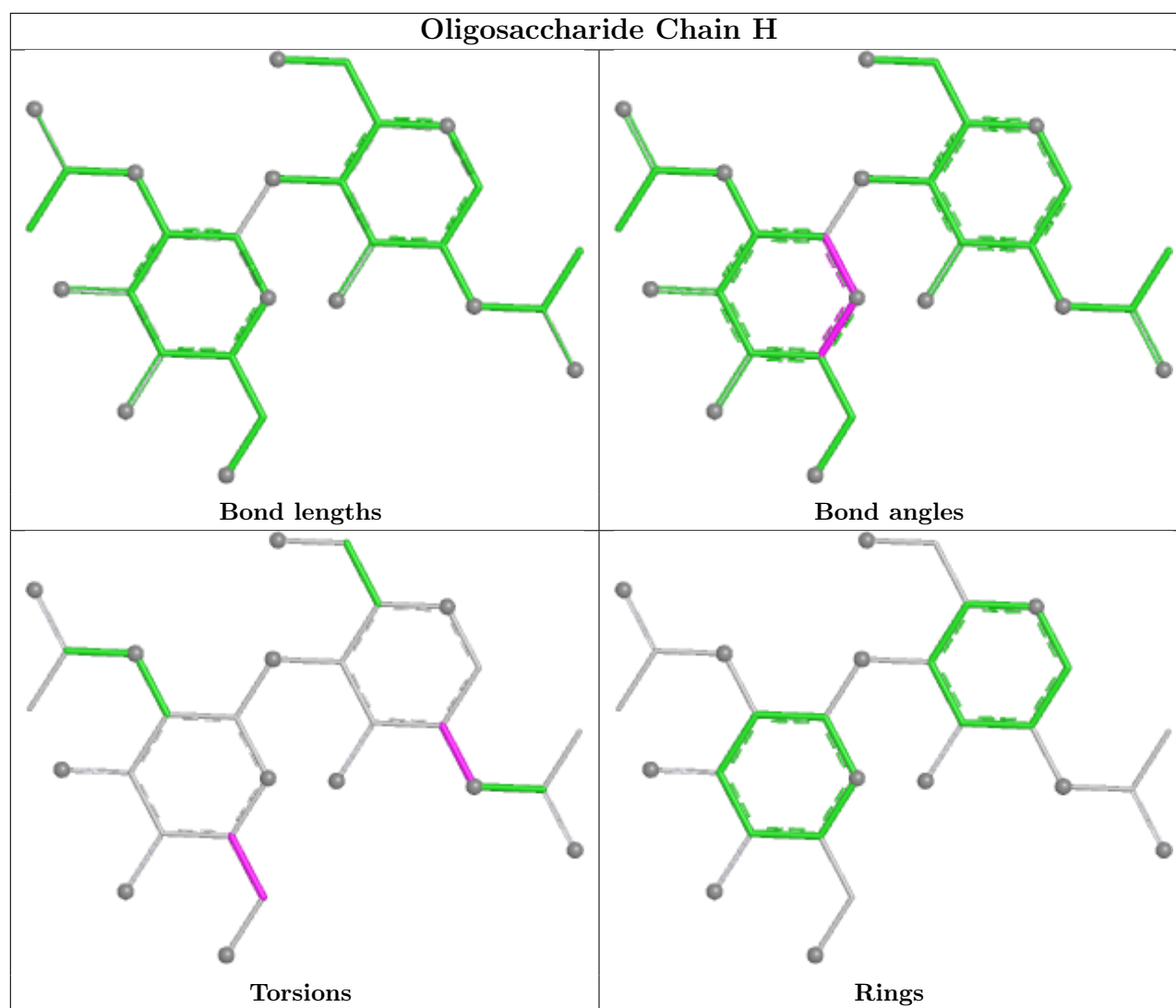


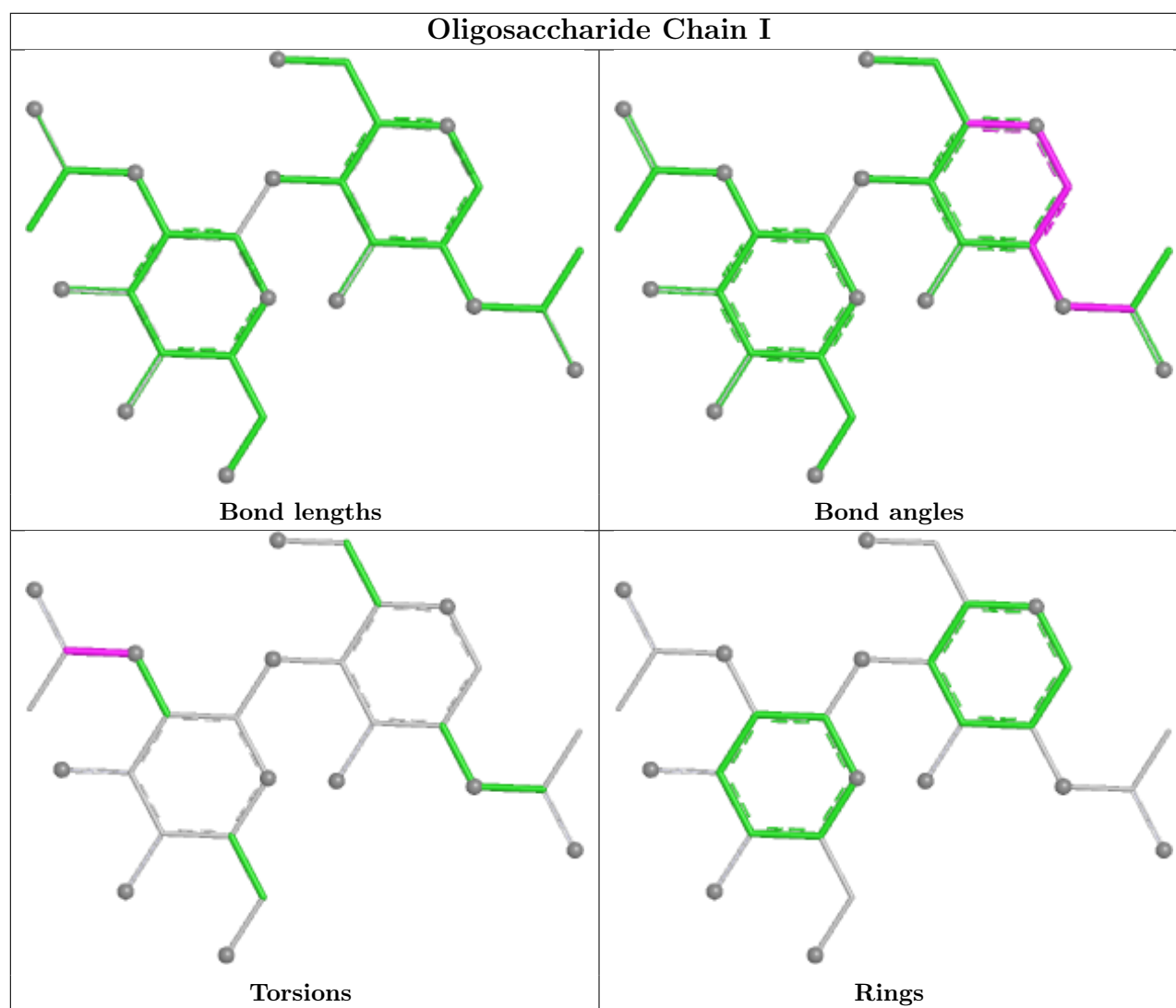


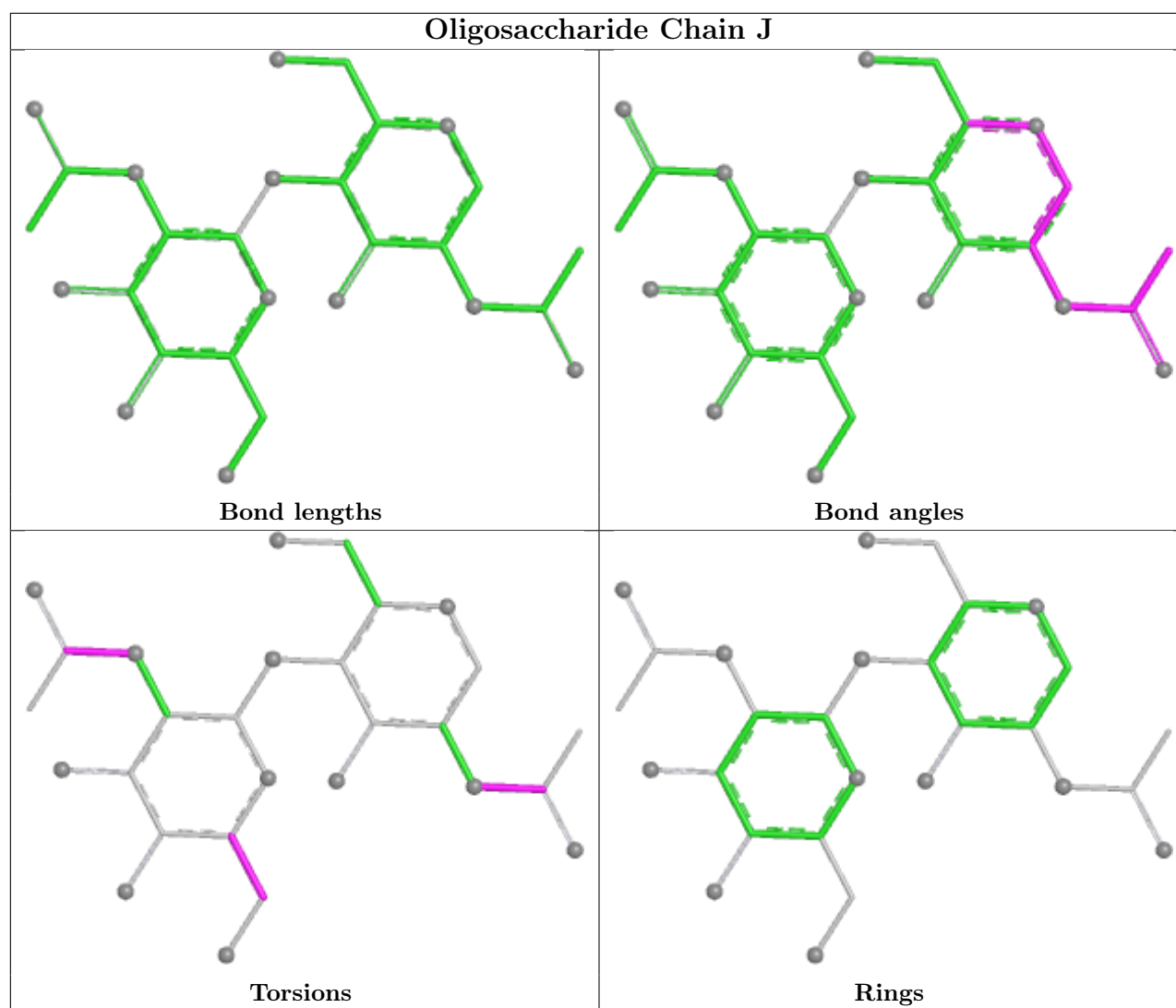


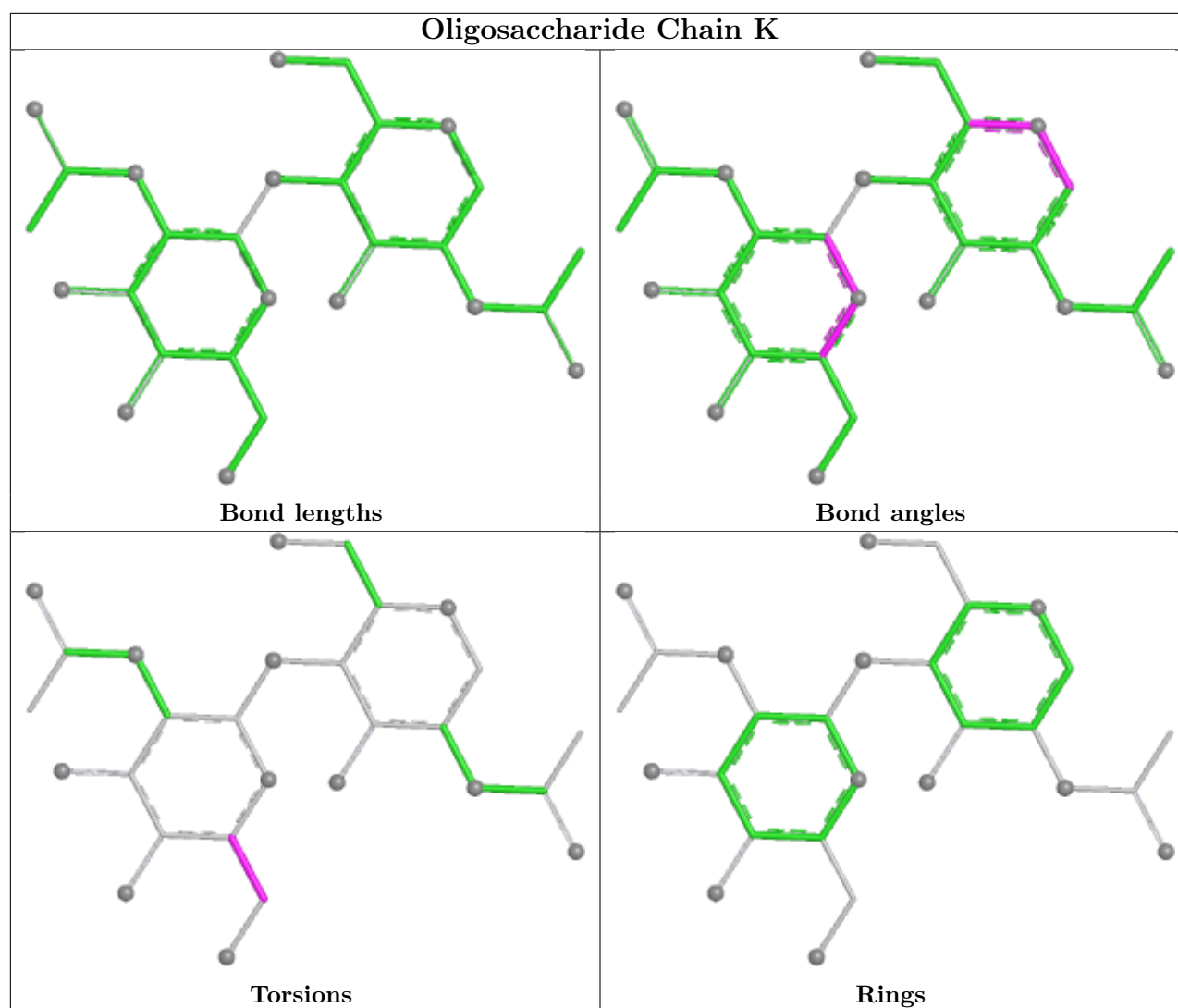












5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	NAG	A	1023	1	14,14,15	0.55	0	17,19,21	0.73	0
5	NAG	A	1020	1	14,14,15	0.50	0	17,19,21	1.42	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1023	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1020	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1020	NAG	C2-N2-C7	3.90	128.13	122.90
5	A	1020	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1020	NAG	C3-C2-N2-C7
5	A	1020	NAG	C4-C5-C6-O6
5	A	1020	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Warning: The R factor obtained from EDS is 0.255, which does not match the depositor's R factor of 0.1471. Please interpret the results in this section carefully.

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%)	0.64	58 (6%) 27 28	16, 23, 37, 54	0
2	B	11/11 (100%)	2.63	7 (63%) 0 0	63, 73, 84, 86	0
All	All	913/919 (99%)	0.67	65 (7%) 23 24	16, 23, 39, 86	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	885	PHE	5.0
1	A	888	TYR	5.0
2	B	2	PRO	4.3
1	A	925	VAL	3.9
1	A	728	GLN	3.7
1	A	932	ARG	3.7
1	A	964	SER	3.5
1	A	761	GLY	3.5
1	A	893	PHE	3.4
1	A	895	PHE	3.3
2	B	7	PHE	3.2
1	A	928	GLY	3.1
1	A	927	PHE	3.1
2	B	9	GLY	3.0
1	A	638	MET	3.0
2	B	1	ARG	3.0
1	A	882	LYS	3.0
2	B	11	MET	3.0
2	B	8	PHE	2.9
1	A	881	TRP	2.9
1	A	929	SER	2.9
1	A	781	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	3	LYS	2.9
1	A	634	ASP	2.8
1	A	738	THR	2.7
1	A	355	VAL	2.7
1	A	933	ALA	2.6
1	A	926	GLY	2.6
1	A	920	LYS	2.6
1	A	884	LEU	2.6
1	A	767	ASN	2.6
1	A	801	GLY	2.6
1	A	869	GLY	2.6
1	A	555	GLY	2.6
1	A	769	ALA	2.6
1	A	889	GLY	2.5
1	A	922	ASN	2.5
1	A	957	ASN	2.5
1	A	924	ASP	2.5
1	A	732	THR	2.5
1	A	198	VAL	2.5
1	A	955	VAL	2.5
1	A	736	ASN	2.4
1	A	887	ASP	2.4
1	A	275	LEU	2.4
1	A	402	LEU	2.4
1	A	918	PHE	2.4
1	A	218	CYS	2.3
1	A	820	ASN	2.3
1	A	923	MET	2.3
1	A	963	SER	2.3
1	A	910	PHE	2.3
1	A	737	TRP	2.3
1	A	831	CYS	2.3
1	A	780	PRO	2.2
1	A	849	ASP	2.2
1	A	844	TYR	2.1
1	A	782	ASN	2.1
1	A	510	LEU	2.0
1	A	290	GLN	2.0
1	A	834	GLU	2.0
1	A	649	VAL	2.0
1	A	797	ALA	2.0
1	A	613	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	762	LEU	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](#)

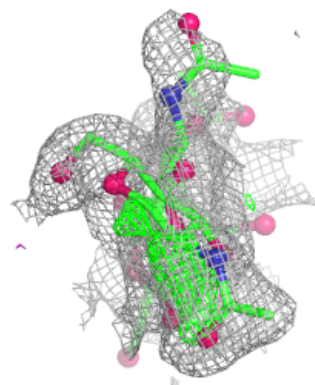
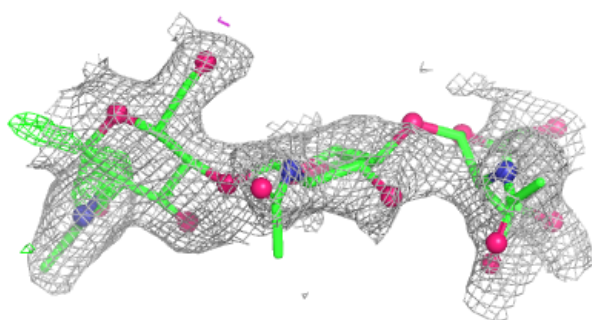
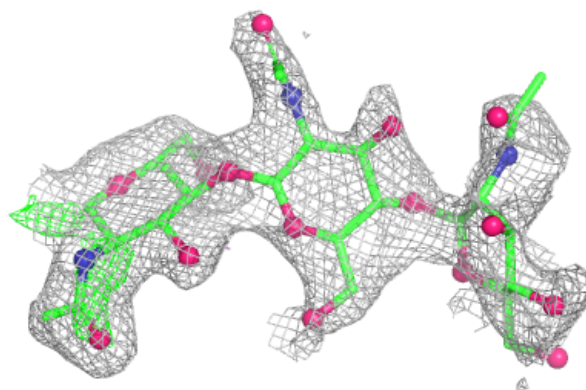
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	1	14/15	0.66	0.16	59,70,76,81	0
3	NAG	G	3	14/15	0.68	0.12	65,83,87,92	0
3	NAG	D	3	14/15	0.72	0.13	74,83,94,97	0
4	NAG	F	2	14/15	0.75	0.14	71,74,86,86	0
4	NAG	E	2	14/15	0.79	0.16	53,61,73,80	0
3	NAG	D	2	14/15	0.80	0.10	66,73,82,88	0
4	NAG	H	2	14/15	0.80	0.14	46,77,83,86	0
3	NAG	G	2	14/15	0.80	0.13	58,68,79,85	0
4	NAG	I	2	14/15	0.82	0.15	55,60,77,78	0
4	NAG	H	1	14/15	0.83	0.13	53,68,74,83	0
3	NAG	C	3	14/15	0.83	0.13	75,80,88,97	0
4	NAG	F	1	14/15	0.85	0.13	52,62,72,73	0
4	NAG	J	2	14/15	0.85	0.13	75,81,89,89	0
4	NAG	K	2	14/15	0.85	0.13	62,71,91,93	0
3	NAG	C	2	14/15	0.87	0.11	59,69,80,83	0
3	NAG	G	1	14/15	0.88	0.15	49,58,63,63	0
3	NAG	C	1	14/15	0.89	0.15	38,45,50,55	0
4	NAG	K	1	14/15	0.90	0.14	47,61,67,67	0
3	NAG	D	1	14/15	0.91	0.12	49,54,60,67	0
4	NAG	I	1	14/15	0.92	0.13	42,46,52,53	0
4	NAG	E	1	14/15	0.92	0.16	36,40,51,51	0

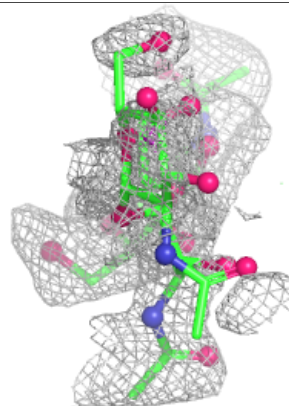
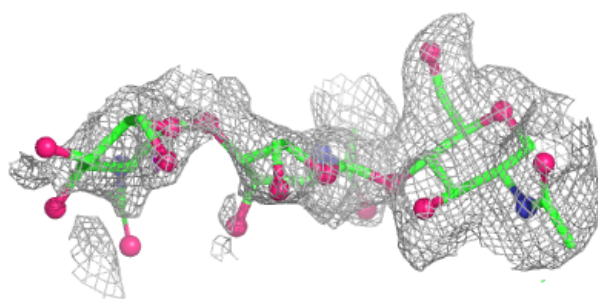
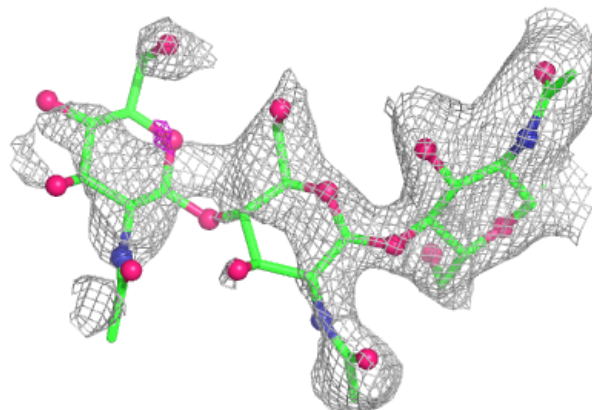
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

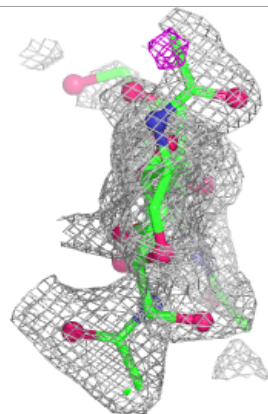
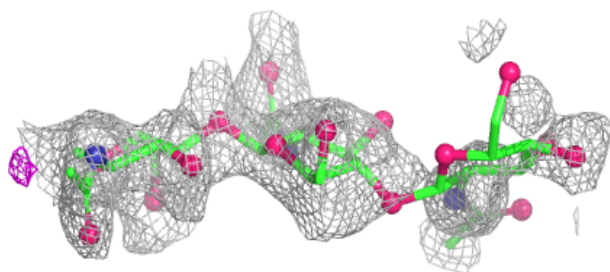
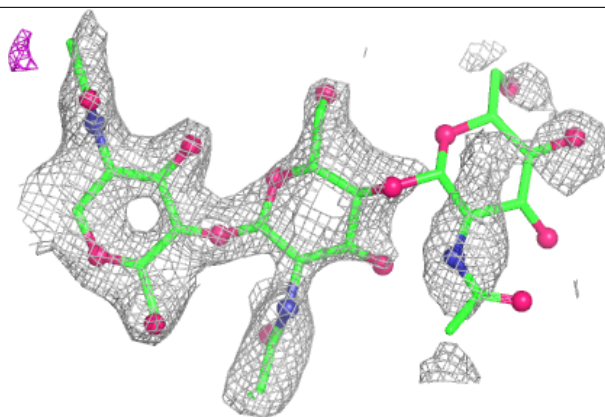
**Electron density around Chain D:**

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

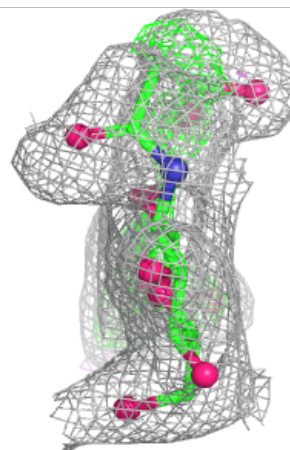
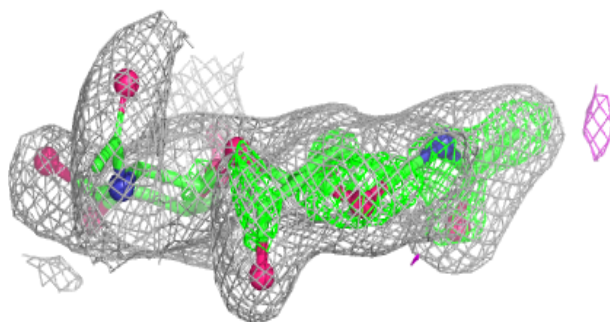
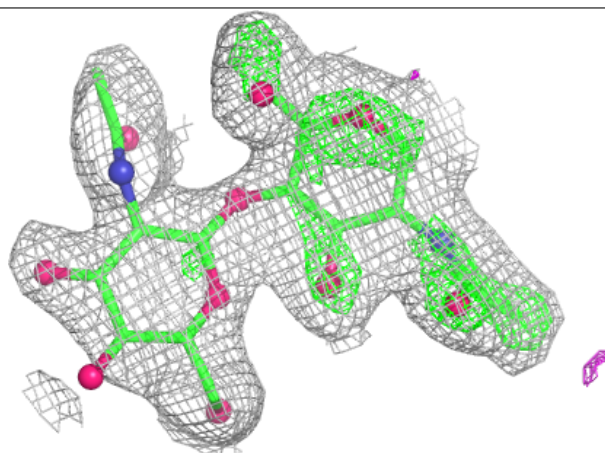


Electron density around Chain G:

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

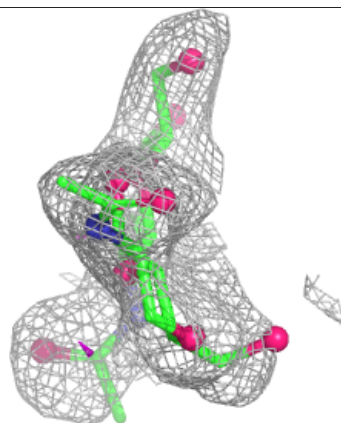
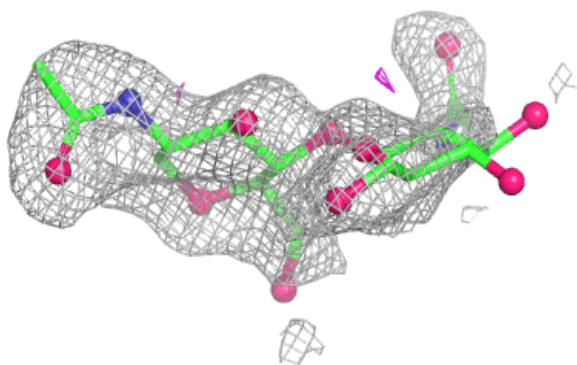
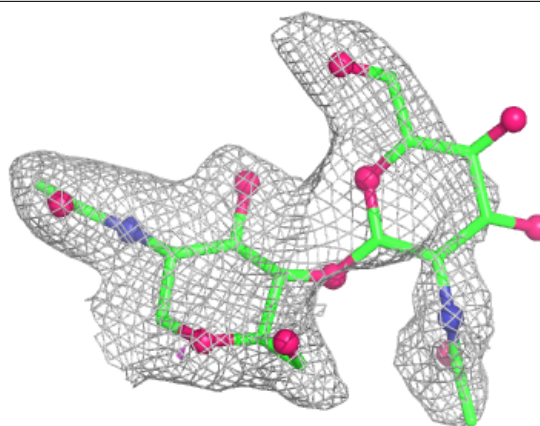
**Electron density around Chain E:**

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



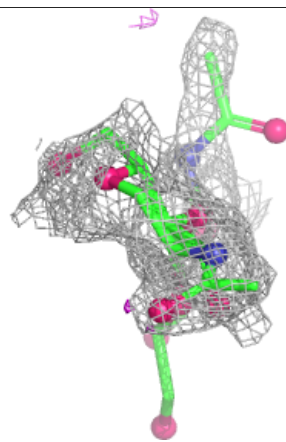
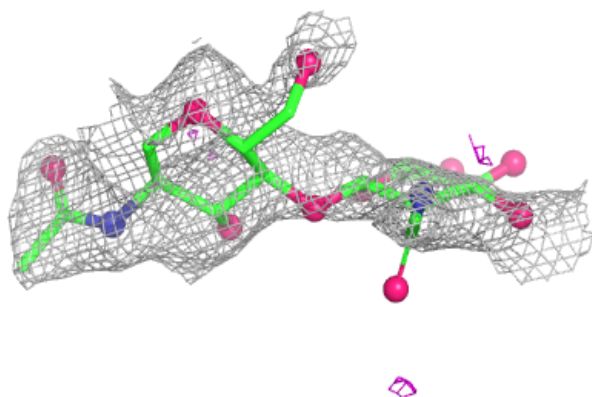
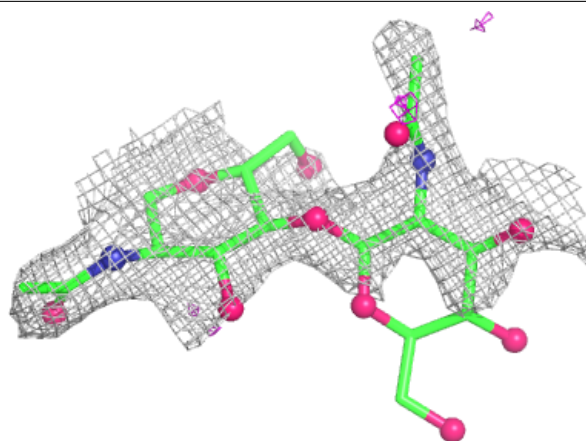
Electron density around Chain F:

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



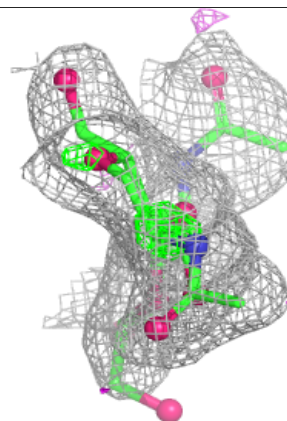
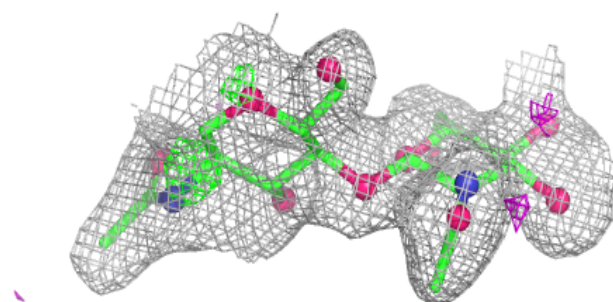
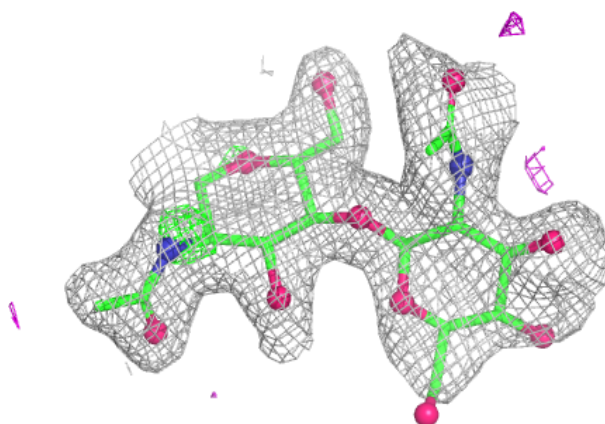
Electron density around Chain H:

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



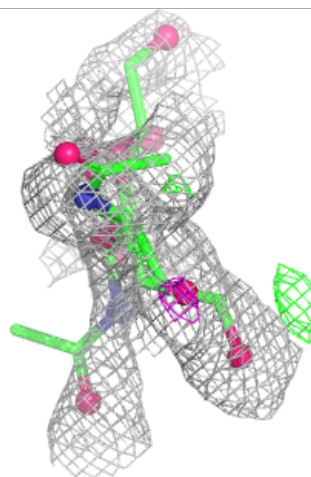
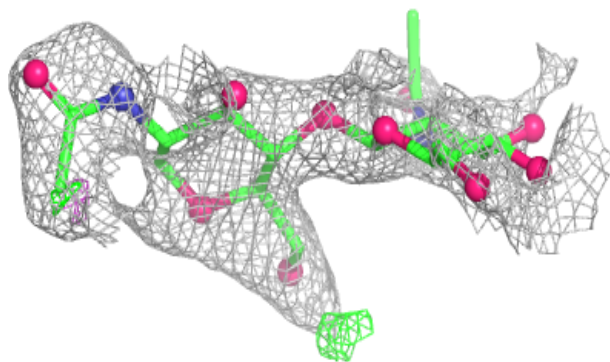
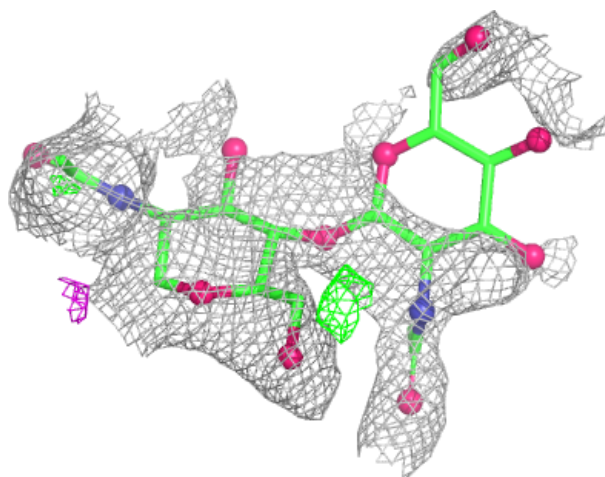
Electron density around Chain I:

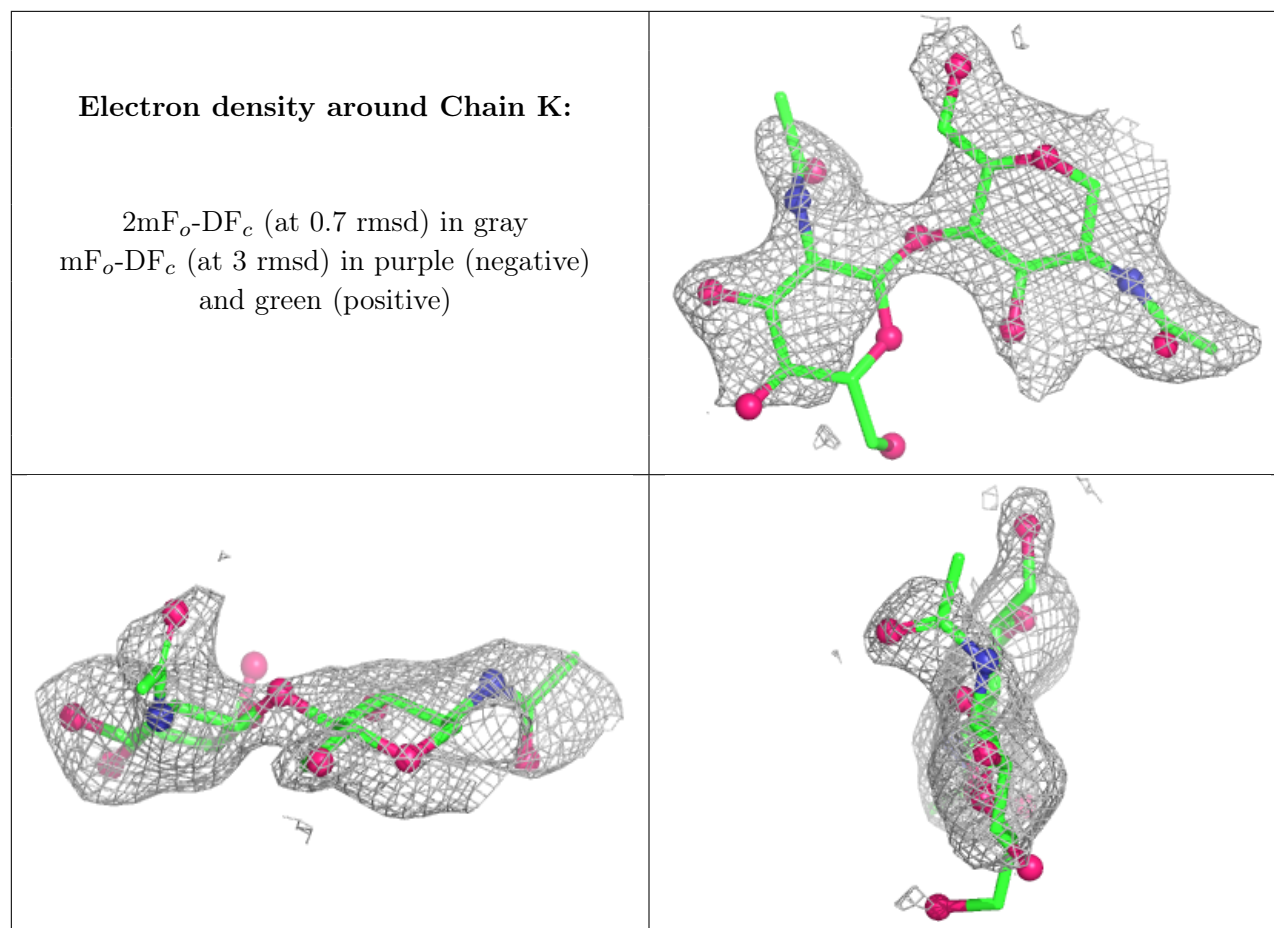
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	1020	14/15	0.59	0.13	68,81,97,99	0
5	NAG	A	1023	14/15	0.82	0.11	64,79,88,91	0
6	ZN	A	1024	1/1	0.99	0.17	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.