



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:16 AM UTC

PDB ID : 1NWT / pdb_00001nwt
Title : Crystal structure of human cartilage gp39 (HC-gp39) in complex with chitopentaose
Authors : Fusetti, F.; Pijning, T.; Kalk, K.H.; Bos, E.; Dijkstra, B.W.
Deposited on : 2003-02-06
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

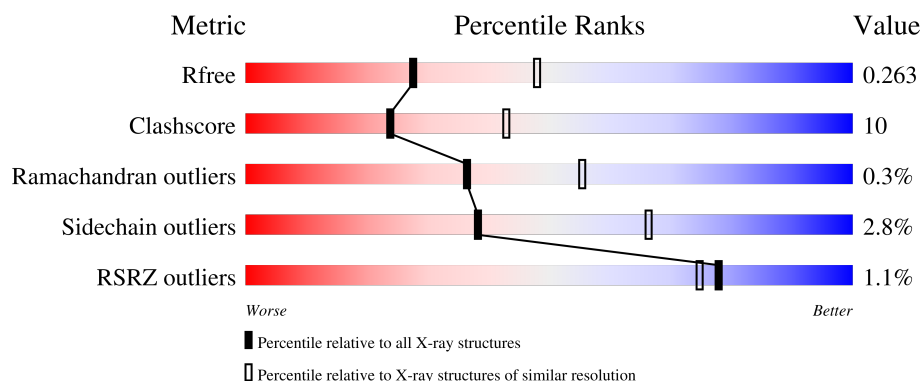
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



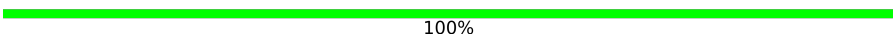
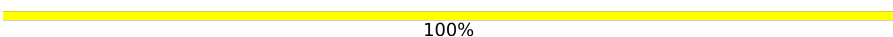
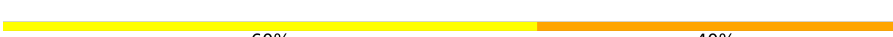
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	362	2% 81% 17%
1	B	362	% 76% 22%
1	C	362	% 80% 18%
1	D	362	% 77% 20%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	 50% 50%
2	I	2	 100%
2	K	2	 100%
3	F	6	 17% 50% 33%
3	J	6	 33% 17% 50%
3	L	6	 17% 33% 50%
4	H	5	 60% 40%

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
3	NAG	J	3	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12269 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 Chitinase-3 like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2838	1816	483	528	11			
1	B	362	Total	C	N	O	S	0	0	0
			2839	1816	483	529	11			
1	C	362	Total	C	N	O	S	0	0	0
			2839	1816	483	529	11			
1	D	362	Total	C	N	O	S	0	0	0
			2845	1819	486	529	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	conflict	UNP P36222
B	311	ILE	THR	conflict	UNP P36222
C	311	ILE	THR	conflict	UNP P36222
D	311	ILE	THR	conflict	UNP P36222

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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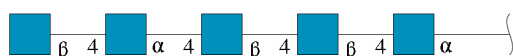
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-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	F	6	Total	C	N	O	0	0	0
			85	48	6	31			
3	J	6	Total	C	N	O	0	0	0
			85	48	6	31			
3	L	6	Total	C	N	O	0	0	0
			85	48	6	31			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			71	40	5	26			

- Molecule 5 is water.

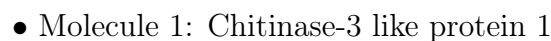
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	83	Total	O	0	0
			83	83		
5	C	104	Total	O	0	0
			104	104		

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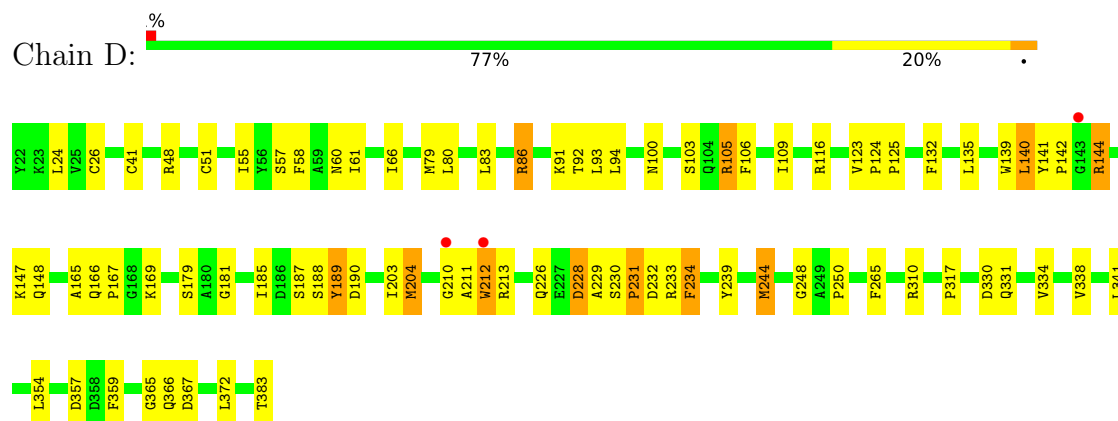
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	155	Total	O	0	0
			155	155		

- Molecule 1: Chitinase-3 like protein 1



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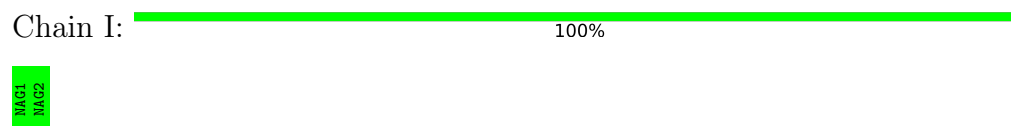
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



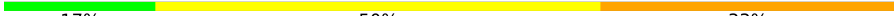
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 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-alpha-D-glucopyranose-(1-4)-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 F:  17% 50% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-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 J:  33% 17% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-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 L:  17% 33% 50%



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

Chain H:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	128.32Å 128.32Å 108.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.50 29.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.92-2.50) 98.4 (29.92-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.253 0.231 , 0.263	Depositor DCC
R_{free} test set	8851 reflections (13.13%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 47.30 % 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 1.0122e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, NDG

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	1/2914 (0.0%)	0.87	6/3951 (0.2%)
1	B	0.32	1/2915 (0.0%)	0.87	7/3952 (0.2%)
1	C	0.34	1/2915 (0.0%)	0.86	6/3952 (0.2%)
1	D	0.34	1/2921 (0.0%)	0.88	8/3959 (0.2%)
All	All	0.34	4/11665 (0.0%)	0.87	27/15814 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	204	MET	SD-CE	-6.82	1.62	1.79
1	A	204	MET	SD-CE	-6.17	1.64	1.79
1	C	204	MET	SD-CE	-5.64	1.65	1.79
1	B	204	MET	SD-CE	-5.56	1.65	1.79

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ARG	N-CA-C	-9.13	99.92	113.61
1	C	144	ARG	N-CA-C	-7.56	103.32	112.54
1	B	144	ARG	N-CA-C	-7.54	103.34	112.54
1	A	144	ARG	N-CA-C	-7.54	103.34	112.54
1	D	144	ARG	N-CA-C	-7.51	103.38	112.54
1	D	189	TYR	N-CA-C	6.83	120.81	109.95
1	B	189	TYR	N-CA-C	6.76	120.70	109.95
1	A	229	ALA	N-CA-C	6.60	120.03	112.57
1	A	189	TYR	N-CA-C	6.56	120.38	109.95
1	A	357	ASP	N-CA-C	-6.54	102.10	110.53
1	D	357	ASP	N-CA-C	-6.53	102.11	110.53
1	C	357	ASP	N-CA-C	-6.48	102.18	110.53
1	C	190	ASP	N-CA-C	-6.47	99.92	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	N-CA-C	-6.45	102.21	110.53
1	B	190	ASP	N-CA-C	-6.45	99.95	109.11
1	D	190	ASP	N-CA-C	-6.45	99.95	109.11
1	C	189	TYR	N-CA-C	6.43	120.18	109.95
1	A	190	ASP	N-CA-C	-6.41	100.00	109.11
1	D	66	ILE	N-CA-C	-5.74	102.18	109.58
1	A	66	ILE	N-CA-C	-5.71	102.22	109.58
1	B	230	SER	CA-C-N	5.70	126.96	119.84
1	B	230	SER	C-N-CA	5.70	126.96	119.84
1	B	66	ILE	N-CA-C	-5.66	102.28	109.58
1	D	229	ALA	N-CA-C	5.61	118.92	112.97
1	C	66	ILE	N-CA-C	-5.57	102.39	109.58
1	D	228	ASP	N-CA-C	5.25	116.81	111.14
1	C	229	ALA	N-CA-C	5.08	119.11	113.01

There are no chirality outliers.

There are no planarity outliers.

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	2838	0	2742	52	0
1	B	2839	0	2742	60	0
1	C	2839	0	2742	47	0
1	D	2845	0	2753	63	0
2	E	28	0	25	0	0
2	G	28	0	25	1	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
3	F	85	0	74	10	0
3	J	85	0	74	8	0
3	L	85	0	74	8	0
4	H	71	0	59	10	0
5	A	128	0	0	5	0
5	B	83	0	0	1	0
5	C	104	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	155	0	0	6	0
All	All	12269	0	11360	233	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 10.

All (233) 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:86:ARG:HH11	1:A:86:ARG:HB3	1.35	0.92
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.35	0.92
1:D:204:MET:HE2	3:L:3:NAG:H62	1.52	0.91
1:A:204:MET:HE2	3:F:3:NAG:H62	1.49	0.91
1:D:86:ARG:HH11	1:D:86:ARG:HB3	1.35	0.91
1:C:86:ARG:HB3	1:C:86:ARG:HH11	1.35	0.89
1:D:231:PRO:HG2	1:D:232:ASP:H	1.38	0.86
1:B:203:ILE:HD12	1:B:244:MET:HG3	1.59	0.85
1:B:234:PHE:HB3	1:B:239:TYR:CD2	2.12	0.85
1:B:204:MET:HE2	4:H:2:NAG:H62	1.59	0.84
1:D:212:TRP:CZ3	3:L:1:NAG:H4	2.13	0.83
3:F:3:NAG:O3	3:F:4:NAG:H4	1.87	0.73
1:D:61:ILE:HG21	1:D:109:ILE:HD13	1.71	0.73
3:L:3:NAG:O3	3:L:4:NAG:H4	1.90	0.72
1:C:61:ILE:HG21	1:C:109:ILE:HD13	1.71	0.72
1:B:61:ILE:HG21	1:B:109:ILE:HD13	1.71	0.71
1:A:61:ILE:HG21	1:A:109:ILE:HD13	1.70	0.71
4:H:2:NAG:O3	4:H:3:NAG:H4	1.93	0.68
1:A:204:MET:CE	3:F:3:NAG:H62	2.24	0.67
1:B:86:ARG:HB3	1:B:86:ARG:NH1	2.09	0.67
3:J:2:NAG:H62	3:J:3:NAG:H82	1.76	0.66
1:A:86:ARG:HB3	1:A:86:ARG:NH1	2.10	0.65
1:B:100:ASN:CG	4:H:4:NDG:H6C2	2.23	0.64
1:D:103:SER:HB2	5:D:537:HOH:O	1.98	0.64
1:D:86:ARG:HB3	1:D:86:ARG:NH1	2.10	0.64
1:C:86:ARG:HB3	1:C:86:ARG:NH1	2.10	0.63
1:D:231:PRO:CG	1:D:232:ASP:H	2.11	0.63
1:C:253:LYS:HA	5:C:467:HOH:O	1.98	0.63
1:A:234:PHE:HB3	1:A:239:TYR:CD2	2.35	0.62
1:B:92:THR:HG22	1:B:132:PHE:CD1	2.35	0.62
1:B:92:THR:HG22	1:B:132:PHE:HD1	1.64	0.62
1:B:204:MET:CE	4:H:2:NAG:H62	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HH11	1:C:86:ARG:CB	2.11	0.62
1:D:92:THR:HG22	1:D:132:PHE:CD1	2.36	0.61
1:A:92:THR:HG22	1:A:132:PHE:HD1	1.65	0.61
1:A:92:THR:HG22	1:A:132:PHE:CD1	2.35	0.61
1:D:92:THR:HG22	1:D:132:PHE:HD1	1.66	0.61
1:A:100:ASN:CG	3:F:5:NDG:H6C2	2.26	0.60
1:B:86:ARG:HH11	1:B:86:ARG:CB	2.10	0.60
1:C:92:THR:HG22	1:C:132:PHE:CD1	2.36	0.60
1:B:204:MET:CE	4:H:3:NAG:C1	2.80	0.60
1:C:92:THR:HG22	1:C:132:PHE:HD1	1.66	0.59
1:C:204:MET:HE2	3:J:3:NAG:H62	1.85	0.59
1:D:226:GLN:HE21	1:D:228:ASP:CB	2.16	0.59
1:A:86:ARG:HH11	1:A:86:ARG:CB	2.11	0.59
1:A:124:PRO:HB2	1:A:125:PRO:HD3	1.85	0.58
1:D:124:PRO:HB2	1:D:125:PRO:HD3	1.85	0.58
1:D:226:GLN:HE21	1:D:228:ASP:HB3	1.67	0.58
1:B:234:PHE:HB3	1:B:239:TYR:CE2	2.38	0.58
1:B:166:GLN:N	1:B:167:PRO:HD2	2.19	0.58
1:C:166:GLN:N	1:C:167:PRO:HD2	2.19	0.58
1:D:166:GLN:N	1:D:167:PRO:HD2	2.19	0.58
1:C:80:LEU:HD12	1:C:83:LEU:HD12	1.86	0.58
1:B:80:LEU:HD12	1:B:83:LEU:HD12	1.84	0.58
1:D:80:LEU:HD12	1:D:83:LEU:HD12	1.86	0.58
1:D:204:MET:CE	3:L:3:NAG:H62	2.30	0.58
1:D:86:ARG:HH11	1:D:86:ARG:CB	2.10	0.57
1:C:124:PRO:HB2	1:C:125:PRO:HD3	1.87	0.57
1:A:166:GLN:N	1:A:167:PRO:HD2	2.19	0.57
1:A:80:LEU:HD12	1:A:83:LEU:HD12	1.86	0.56
1:A:352:TRP:CZ3	3:F:4:NAG:H83	2.40	0.56
1:B:124:PRO:HB2	1:B:125:PRO:HD3	1.87	0.56
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.88	0.56
1:D:123:VAL:HB	1:D:124:PRO:HD3	1.88	0.55
1:A:310:ARG:NH2	1:A:330:ASP:OD2	2.39	0.55
1:A:147:LYS:HE3	1:A:189:TYR:O	2.07	0.55
1:B:147:LYS:HE3	1:B:189:TYR:O	2.06	0.55
1:B:210:GLY:O	1:B:213:ARG:HG3	2.05	0.55
1:C:141:TYR:CE1	1:C:179:SER:HB2	2.42	0.55
1:B:141:TYR:CE1	1:B:179:SER:HB2	2.42	0.55
1:B:94:LEU:O	1:B:135:LEU:HD12	2.06	0.55
1:A:94:LEU:O	1:A:135:LEU:HD12	2.07	0.55
1:C:94:LEU:O	1:C:135:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:TYR:CE1	1:D:179:SER:HB2	2.42	0.55
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.90	0.54
1:D:212:TRP:CH2	3:L:1:NAG:H4	2.41	0.54
1:D:231:PRO:HG2	1:D:232:ASP:N	2.15	0.54
1:A:99:TRP:CH2	3:F:2:NAG:H61	2.43	0.54
1:A:204:MET:CE	3:F:4:NAG:C1	2.86	0.54
1:D:211:ALA:N	1:D:265:PHE:HE1	2.06	0.54
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.89	0.54
1:C:310:ARG:NH2	1:C:330:ASP:OD2	2.41	0.54
1:D:204:MET:CE	3:L:4:NAG:C1	2.85	0.54
1:D:94:LEU:O	1:D:135:LEU:HD12	2.08	0.53
4:H:4:NDG:H6C1	4:H:5:NAG:HN2	1.73	0.53
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.43	0.53
1:C:147:LYS:HE3	1:C:189:TYR:O	2.07	0.53
1:C:204:MET:CE	3:J:3:NAG:H62	2.38	0.53
1:D:147:LYS:HE3	1:D:189:TYR:O	2.09	0.53
1:A:105:ARG:HH11	1:A:105:ARG:HB3	1.73	0.53
1:D:310:ARG:NH2	1:D:330:ASP:OD2	2.42	0.52
1:B:26:CYS:HB3	1:B:354:LEU:HG	1.91	0.52
1:C:105:ARG:HB3	1:C:105:ARG:HH11	1.74	0.52
1:B:105:ARG:HH11	1:B:105:ARG:HB3	1.75	0.52
1:D:48:ARG:HG2	5:D:544:HOH:O	2.10	0.51
1:B:310:ARG:NH2	1:B:330:ASP:OD2	2.43	0.51
1:D:100:ASN:CG	3:L:5:NDG:H6C2	2.36	0.51
1:B:181:GLY:O	1:B:185:ILE:HG13	2.11	0.50
1:B:41:CYS:HB2	1:B:359:PHE:CZ	2.46	0.50
1:A:105:ARG:HB3	1:A:105:ARG:NH1	2.27	0.50
1:B:55:ILE:HG12	1:B:93:LEU:HB2	1.94	0.50
1:C:105:ARG:HB3	1:C:105:ARG:NH1	2.27	0.50
1:D:234:PHE:HB3	1:D:239:TYR:CD2	2.47	0.49
1:D:26:CYS:HB3	1:D:354:LEU:HG	1.95	0.49
1:B:144:ARG:HA	1:B:187:SER:O	2.12	0.49
1:D:105:ARG:HH11	1:D:105:ARG:HB3	1.76	0.49
1:D:212:TRP:CD1	1:D:212:TRP:H	2.30	0.49
1:D:55:ILE:HG12	1:D:93:LEU:HB2	1.94	0.49
1:B:383:THR:HG22	1:B:383:THR:O	2.13	0.49
1:B:22:TYR:CZ	1:B:342:LYS:HG2	2.47	0.49
1:B:81:ASN:HB3	5:B:459:HOH:O	2.13	0.49
1:D:334:VAL:O	1:D:338:VAL:HG23	2.13	0.49
1:C:55:ILE:HG12	1:C:93:LEU:HB2	1.95	0.48
1:C:181:GLY:O	1:C:185:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLN:NE2	5:D:557:HOH:O	2.41	0.48
1:A:234:PHE:HB3	1:A:239:TYR:CE2	2.48	0.48
1:A:55:ILE:HG12	1:A:93:LEU:HB2	1.96	0.48
1:B:214:GLY:C	1:B:278:ILE:HG12	2.39	0.48
1:B:334:VAL:O	1:B:338:VAL:HG23	2.14	0.48
1:A:26:CYS:HB3	1:A:354:LEU:HG	1.96	0.48
1:B:105:ARG:HB3	1:B:105:ARG:NH1	2.28	0.48
1:A:223:PHE:HB2	1:A:313:GLY:O	2.14	0.47
1:C:144:ARG:HA	1:C:187:SER:O	2.13	0.47
1:D:144:ARG:HA	1:D:187:SER:O	2.14	0.47
1:C:204:MET:CE	3:J:4:NAG:C1	2.92	0.47
1:C:383:THR:O	1:C:383:THR:HG22	2.14	0.47
1:A:212:TRP:CE2	1:A:213:ARG:HG2	2.49	0.47
1:D:105:ARG:HB3	1:D:105:ARG:NH1	2.29	0.47
1:A:57:SER:HA	1:A:58:PHE:HA	1.65	0.47
1:D:383:THR:HG22	1:D:383:THR:O	2.14	0.47
1:A:144:ARG:HA	1:A:187:SER:O	2.14	0.47
1:D:181:GLY:O	1:D:185:ILE:HG13	2.15	0.47
1:B:230:SER:HA	1:B:231:PRO:HD3	1.69	0.47
1:C:57:SER:HA	1:C:58:PHE:HA	1.65	0.47
1:C:334:VAL:O	1:C:338:VAL:HG23	2.15	0.47
1:C:223:PHE:HB2	1:C:313:GLY:O	2.14	0.47
1:C:121:LYS:HE3	5:C:534:HOH:O	2.13	0.47
5:C:464:HOH:O	1:D:169:LYS:HE2	2.14	0.47
1:A:332:GLU:HB2	5:A:512:HOH:O	2.14	0.46
1:A:181:GLY:O	1:A:185:ILE:HG13	2.16	0.46
1:A:341:LEU:HD12	1:A:341:LEU:C	2.41	0.46
1:D:203:ILE:HD12	1:D:244:MET:HG3	1.98	0.46
1:A:334:VAL:O	1:A:338:VAL:HG23	2.14	0.46
1:B:248:GLY:O	1:B:250:PRO:HD3	2.15	0.46
1:B:223:PHE:HB2	1:B:313:GLY:O	2.16	0.45
1:C:341:LEU:HD12	1:C:341:LEU:C	2.41	0.45
1:C:99:TRP:CD2	3:J:3:NAG:H3	2.52	0.45
1:D:341:LEU:C	1:D:341:LEU:HD12	2.41	0.45
3:J:2:NAG:C6	3:J:3:NAG:H82	2.43	0.45
1:B:338:VAL:O	1:B:341:LEU:HG	2.17	0.45
1:A:331:GLN:NE2	5:A:470:HOH:O	2.49	0.45
1:C:142:PRO:HD2	1:C:188:SER:HB3	1.98	0.45
1:D:211:ALA:C	1:D:213:ARG:H	2.25	0.45
1:B:341:LEU:C	1:B:341:LEU:HD12	2.42	0.44
4:H:4:NDG:H6C1	4:H:5:NAG:N2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLY:C	1:A:278:ILE:HG12	2.43	0.44
1:C:26:CYS:HB3	1:C:354:LEU:HG	1.99	0.44
1:B:142:PRO:HD2	1:B:188:SER:HB3	1.99	0.44
4:H:2:NAG:O4	4:H:3:NAG:H4	2.16	0.44
1:A:139:TRP:CD1	1:A:139:TRP:C	2.96	0.44
1:A:360:GLN:NE2	5:A:531:HOH:O	2.51	0.44
1:B:57:SER:HA	1:B:58:PHE:HA	1.65	0.43
1:B:330:ASP:HA	1:B:372:LEU:HD21	2.00	0.43
1:A:330:ASP:HB2	5:A:470:HOH:O	2.18	0.43
1:A:330:ASP:HA	1:A:372:LEU:HD21	2.01	0.43
1:B:243:TYR:CE2	1:B:247:LEU:HD11	2.53	0.43
1:D:79:MET:HE3	1:D:79:MET:HB2	1.94	0.43
1:B:139:TRP:CD1	1:B:139:TRP:C	2.96	0.43
1:B:366:GLN:N	1:B:366:GLN:CD	2.77	0.43
1:C:366:GLN:CD	1:C:366:GLN:N	2.76	0.43
2:G:1:NAG:O6	2:G:2:NAG:H82	2.19	0.43
1:C:338:VAL:O	1:C:341:LEU:HG	2.19	0.43
1:D:57:SER:HA	1:D:58:PHE:HA	1.65	0.43
1:A:142:PRO:HD2	1:A:188:SER:HB3	2.00	0.43
1:B:178:LEU:HD12	1:B:201:ILE:HG21	2.01	0.43
1:C:330:ASP:HA	1:C:372:LEU:HD21	2.00	0.43
1:D:139:TRP:CD1	1:D:139:TRP:C	2.96	0.43
1:B:227:GLU:O	1:B:227:GLU:HG2	2.18	0.42
1:A:338:VAL:O	1:A:341:LEU:HG	2.19	0.42
1:D:330:ASP:HB2	5:D:481:HOH:O	2.18	0.42
1:B:34:TYR:OH	1:B:70:GLU:HG3	2.20	0.42
1:D:142:PRO:HD2	1:D:188:SER:HB3	2.00	0.42
1:C:34:TYR:OH	1:C:70:GLU:HG3	2.20	0.42
1:C:204:MET:HE2	3:J:3:NAG:C6	2.49	0.42
1:D:330:ASP:HA	1:D:372:LEU:HD21	2.01	0.42
1:B:352:TRP:HA	1:B:353:ALA:HA	1.76	0.42
1:D:338:VAL:O	1:D:341:LEU:HG	2.20	0.42
1:D:366:GLN:N	1:D:366:GLN:CD	2.76	0.42
1:A:140:LEU:HA	1:A:141:TYR:CD1	2.55	0.42
1:A:352:TRP:HA	1:A:353:ALA:HA	1.76	0.42
1:B:99:TRP:CH2	4:H:1:NDG:H6C1	2.55	0.41
1:D:230:SER:HB3	5:D:500:HOH:O	2.20	0.41
1:C:99:TRP:CG	3:J:3:NAG:H3	2.55	0.41
1:C:140:LEU:HA	1:C:141:TYR:CD1	2.55	0.41
1:C:234:PHE:HB3	1:C:239:TYR:CD2	2.55	0.41
1:D:41:CYS:HB2	1:D:359:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASN:CG	1:D:61:ILE:H	2.28	0.41
1:B:47:ASP:C	1:B:47:ASP:OD1	2.63	0.41
1:B:204:MET:HE3	4:H:3:NAG:C7	2.51	0.41
1:C:139:TRP:CD1	1:C:139:TRP:C	2.97	0.41
1:A:165:ALA:C	1:A:167:PRO:HD2	2.45	0.41
1:B:24:LEU:O	1:B:51:CYS:HB3	2.20	0.41
1:A:224:ARG:NE	1:A:230:SER:OG	2.39	0.41
1:C:165:ALA:C	1:C:167:PRO:HD2	2.45	0.41
1:A:100:ASN:HB2	3:F:5:NDG:H6C2	2.03	0.41
1:B:205:THR:HG21	1:B:237:THR:HG23	2.03	0.41
1:C:47:ASP:OD1	1:C:47:ASP:C	2.63	0.41
1:D:210:GLY:C	1:D:265:PHE:HE1	2.27	0.41
1:A:79:MET:HE3	1:A:79:MET:HB2	1.94	0.41
1:B:165:ALA:C	1:B:167:PRO:HD2	2.45	0.41
1:D:24:LEU:O	1:D:51:CYS:HB3	2.21	0.41
1:A:34:TYR:OH	1:A:70:GLU:HG3	2.21	0.41
1:D:116:ARG:NH2	5:D:564:HOH:O	2.54	0.41
1:D:139:TRP:O	1:D:141:TYR:HA	2.21	0.41
1:B:35:ARG:O	1:B:40:SER:HB2	2.21	0.41
1:C:365:GLY:C	1:C:367:ASP:H	2.29	0.41
1:D:248:GLY:O	1:D:250:PRO:HD3	2.21	0.41
3:L:3:NAG:O4	3:L:4:NAG:H4	2.21	0.41
1:B:330:ASP:O	1:B:334:VAL:HG22	2.21	0.40
1:C:24:LEU:O	1:C:51:CYS:HB3	2.21	0.40
1:D:140:LEU:HA	1:D:141:TYR:CD1	2.56	0.40
1:D:365:GLY:C	1:D:367:ASP:H	2.29	0.40
5:A:422:HOH:O	3:F:2:NAG:H83	2.20	0.40
1:B:147:LYS:HE3	1:B:189:TYR:C	2.47	0.40
1:C:210:GLY:O	1:C:212:TRP:N	2.54	0.40
1:A:100:ASN:CB	3:F:5:NDG:H6C2	2.51	0.40
1:B:60:ASN:CG	1:B:61:ILE:H	2.29	0.40
1:C:214:GLY:C	1:C:278:ILE:HG12	2.46	0.40
1:D:165:ALA:C	1:D:167:PRO:HD2	2.46	0.40
1:D:226:GLN:HE21	1:D:228:ASP:HB2	1.85	0.40
1:B:140:LEU:HA	1:B:141:TYR:CD1	2.56	0.40
1:A:139:TRP:O	1:A:141:TYR:HA	2.21	0.40
1:A:366:GLN:CD	1:A:366:GLN:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/362 (99%)	344 (96%)	16 (4%)	0	100	100
1	B	360/362 (99%)	343 (95%)	16 (4%)	1 (0%)	36	55
1	C	360/362 (99%)	343 (95%)	16 (4%)	1 (0%)	36	55
1	D	360/362 (99%)	342 (95%)	16 (4%)	2 (1%)	21	38
All	All	1440/1448 (99%)	1372 (95%)	64 (4%)	4 (0%)	36	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	211	ALA
1	D	212	TRP
1	D	231	PRO
1	B	231	PRO

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	298/302 (99%)	291 (98%)	7 (2%)	44	72
1	B	298/302 (99%)	289 (97%)	9 (3%)	36	64
1	C	298/302 (99%)	290 (97%)	8 (3%)	39	67
1	D	299/302 (99%)	290 (97%)	9 (3%)	36	64
All	All	1193/1208 (99%)	1160 (97%)	33 (3%)	38	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	91	LYS
1	A	105	ARG
1	A	106	PHE
1	A	140	LEU
1	A	234	PHE
1	A	331	GLN
1	B	86	ARG
1	B	91	LYS
1	B	105	ARG
1	B	106	PHE
1	B	140	LEU
1	B	227	GLU
1	B	234	PHE
1	B	317	PRO
1	B	331	GLN
1	C	86	ARG
1	C	91	LYS
1	C	105	ARG
1	C	106	PHE
1	C	140	LEU
1	C	227	GLU
1	C	317	PRO
1	C	331	GLN
1	D	86	ARG
1	D	91	LYS
1	D	105	ARG
1	D	106	PHE
1	D	140	LEU
1	D	234	PHE
1	D	244	MET
1	D	317	PRO
1	D	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	196	GLN
1	A	314	GLN
1	A	331	GLN

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	360	GLN
1	B	171	GLN
1	B	196	GLN
1	B	226	GLN
1	B	314	GLN
1	B	345	GLN
1	C	196	GLN
1	C	226	GLN
1	C	345	GLN
1	D	196	GLN
1	D	226	GLN
1	D	345	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

31 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	E	1	1,2	14,14,15	0.56	0	17,19,21	0.69	1 (5%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.94	1 (5%)
3	NAG	F	1	3	15,15,15	0.45	0	21,21,21	0.64	0
3	NAG	F	2	3	14,14,15	0.65	0	17,19,21	0.70	0
3	NAG	F	3	3	14,14,15	0.65	0	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	4	3	14,14,15	0.93	1 (7%)	17,19,21	1.25	2 (11%)
3	NDG	F	5	3	14,14,15	1.00	1 (7%)	17,19,21	1.23	3 (17%)
3	NAG	F	6	3	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.54	0	17,19,21	0.81	1 (5%)
2	NAG	G	2	2	14,14,15	0.60	0	17,19,21	0.67	0
4	NDG	H	1	4	15,15,15	0.60	0	21,21,21	0.69	0
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	0.89	0
4	NAG	H	3	4	14,14,15	0.96	1 (7%)	17,19,21	1.25	1 (5%)
4	NDG	H	4	4	14,14,15	0.96	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	H	5	4	14,14,15	0.58	0	17,19,21	0.65	0
2	NAG	I	1	1,2	14,14,15	0.50	0	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.53	0	17,19,21	0.65	0
3	NAG	J	1	3	15,15,15	0.46	0	21,21,21	0.59	0
3	NAG	J	2	3	14,14,15	0.79	1 (7%)	17,19,21	0.72	0
3	NAG	J	3	3	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
3	NAG	J	4	3	14,14,15	0.82	1 (7%)	17,19,21	0.98	2 (11%)
3	NDG	J	5	3	14,14,15	0.83	0	17,19,21	0.86	1 (5%)
3	NAG	J	6	3	14,14,15	0.50	0	17,19,21	0.68	0
2	NAG	K	1	1,2	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
2	NAG	K	2	2	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
3	NAG	L	1	3	15,15,15	0.44	0	21,21,21	0.68	0
3	NAG	L	2	3	14,14,15	0.59	0	17,19,21	0.67	0
3	NAG	L	3	3	14,14,15	0.66	0	17,19,21	0.90	1 (5%)
3	NAG	L	4	3	14,14,15	0.94	1 (7%)	17,19,21	1.23	1 (5%)
3	NDG	L	5	3	14,14,15	1.07	1 (7%)	17,19,21	1.26	3 (17%)
3	NAG	L	6	3	14,14,15	0.52	0	17,19,21	0.73	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3	-	4/6/26/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	4	3	-	0/6/23/26	0/1/1/1
3	NDG	F	5	3	-	2/6/23/26	0/1/1/1
3	NAG	F	6	3	-	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
4	NDG	H	1	4	-	0/6/26/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	3	4	-	0/6/23/26	0/1/1/1
4	NDG	H	4	4	-	4/6/23/26	0/1/1/1
4	NAG	H	5	4	-	4/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1	3	-	0/6/26/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	3	3	-	2/6/23/26	0/1/1/1
3	NAG	J	4	3	-	2/6/23/26	0/1/1/1
3	NDG	J	5	3	-	1/6/23/26	0/1/1/1
3	NAG	J	6	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	2/6/26/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	3	3	-	0/6/23/26	0/1/1/1
3	NAG	L	4	3	-	0/6/23/26	0/1/1/1
3	NDG	L	5	3	-	2/6/23/26	0/1/1/1
3	NAG	L	6	3	-	4/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	5	NDG	C1-C2	3.22	1.56	1.52
4	H	4	NDG	C1-C2	2.90	1.56	1.52
3	F	5	NDG	C1-C2	2.89	1.56	1.52
4	H	3	NAG	C1-C2	2.44	1.55	1.52
3	L	4	NAG	C1-C2	2.16	1.55	1.52
3	F	4	NAG	C1-C2	2.09	1.55	1.52
3	J	4	NAG	C1-C2	2.08	1.55	1.52
3	J	2	NAG	C1-C2	2.04	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4	NAG	C2-N2-C7	-2.86	119.07	122.90
3	F	4	NAG	C2-N2-C7	-2.69	119.29	122.90
4	H	3	NAG	C2-N2-C7	-2.59	119.44	122.90
3	L	5	NDG	C3-C4-C5	-2.57	105.56	110.23
2	K	2	NAG	C2-N2-C7	-2.52	119.52	122.90
2	G	1	NAG	C2-N2-C7	-2.50	119.55	122.90
2	E	2	NAG	C2-N2-C7	-2.49	119.57	122.90
3	F	5	NDG	C3-C4-C5	-2.40	105.89	110.23
3	J	4	NAG	C1-O5-C5	2.32	115.29	112.19
2	K	1	NAG	C2-N2-C7	-2.30	119.82	122.90
3	J	4	NAG	C2-N2-C7	-2.29	119.83	122.90
3	F	5	NDG	C1-O5-C5	2.29	115.26	112.19
3	L	5	NDG	C2-N2-C7	-2.26	119.88	122.90
3	J	3	NAG	C2-N2-C7	-2.22	119.92	122.90
3	F	4	NAG	C1-O5-C5	2.20	115.14	112.19
3	F	5	NDG	C2-N2-C7	-2.13	120.04	122.90
3	L	3	NAG	C4-C3-C2	2.13	114.14	111.02
3	F	6	NAG	C2-N2-C7	-2.12	120.06	122.90
3	J	5	NDG	C2-N2-C7	-2.12	120.06	122.90
3	L	6	NAG	C2-N2-C7	-2.11	120.08	122.90
4	H	4	NDG	C2-N2-C7	-2.08	120.11	122.90
2	E	1	NAG	C2-N2-C7	-2.07	120.12	122.90
3	L	5	NDG	O5-C1-C2	2.03	114.44	111.29

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
4	H	5	NAG	C8-C7-N2-C2
4	H	5	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
3	L	6	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	L	5	NDG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6

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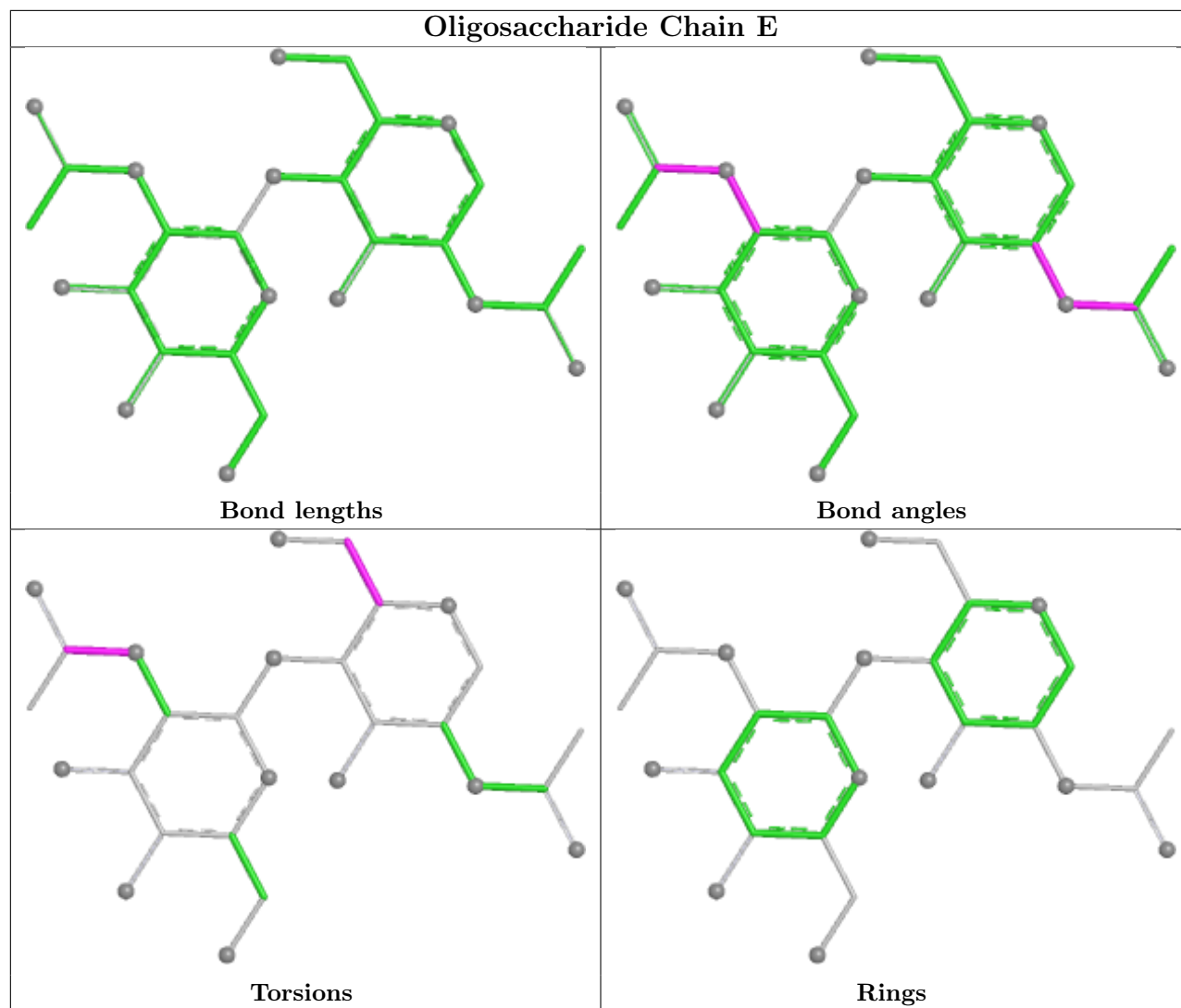
Mol	Chain	Res	Type	Atoms
3	F	6	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	L	5	NDG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	3	NAG	C8-C7-N2-C2
3	J	4	NAG	C8-C7-N2-C2
3	J	6	NAG	O5-C5-C6-O6
3	L	6	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	F	6	NAG	C4-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
3	F	5	NDG	O5-C5-C6-O6
4	H	5	NAG	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
3	J	3	NAG	O7-C7-N2-C2
3	J	4	NAG	O7-C7-N2-C2
3	L	6	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	L	6	NAG	O7-C7-N2-C2
3	J	6	NAG	C4-C5-C6-O6
2	I	2	NAG	C8-C7-N2-C2
4	H	4	NDG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
4	H	4	NDG	C8-C7-N2-C2
3	F	5	NDG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
4	H	5	NAG	C4-C5-C6-O6
2	I	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	F	6	NAG	C8-C7-N2-C2
4	H	4	NDG	O7-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
3	J	5	NDG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
4	H	4	NDG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	6	NAG	O7-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2

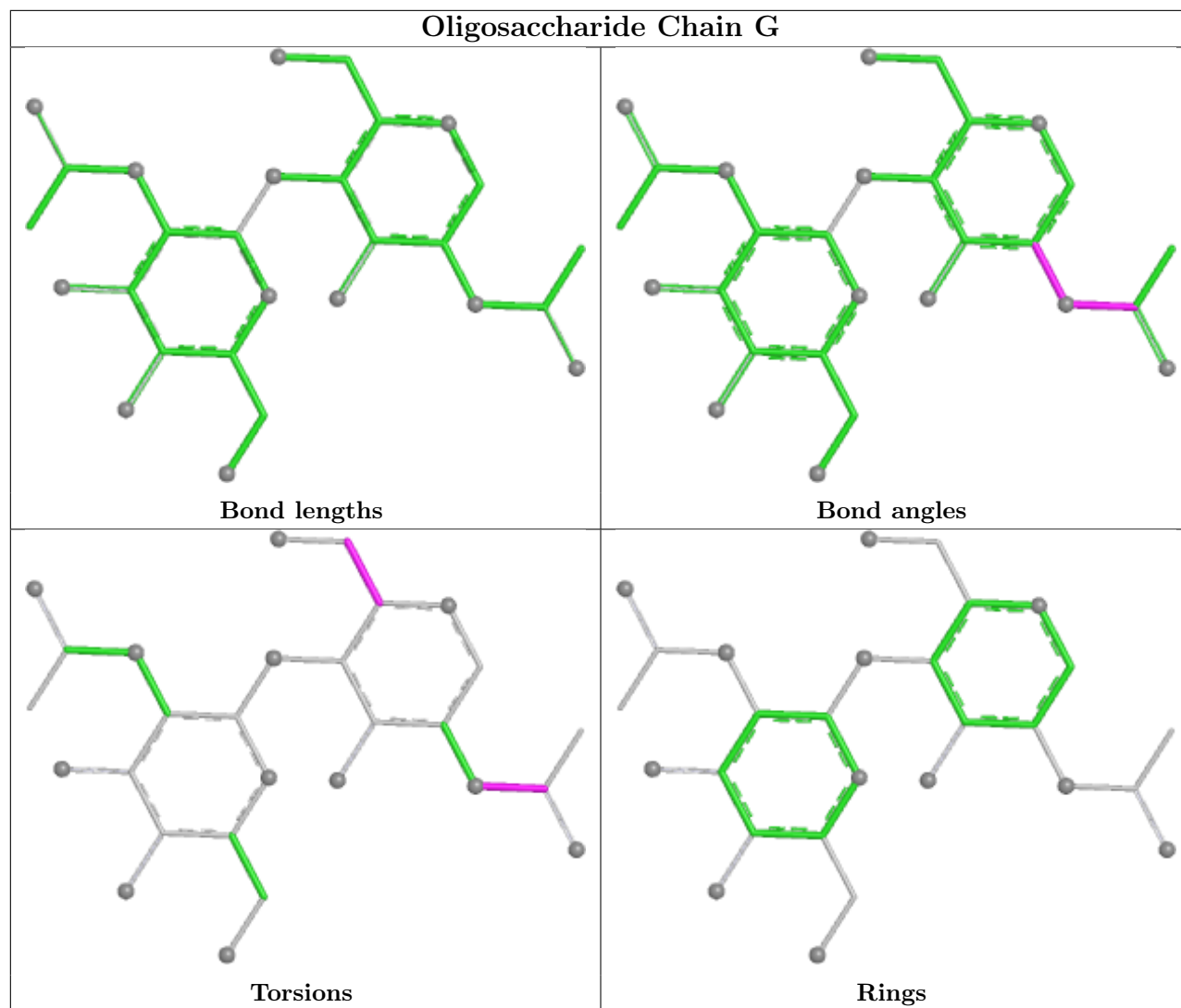
There are no ring outliers.

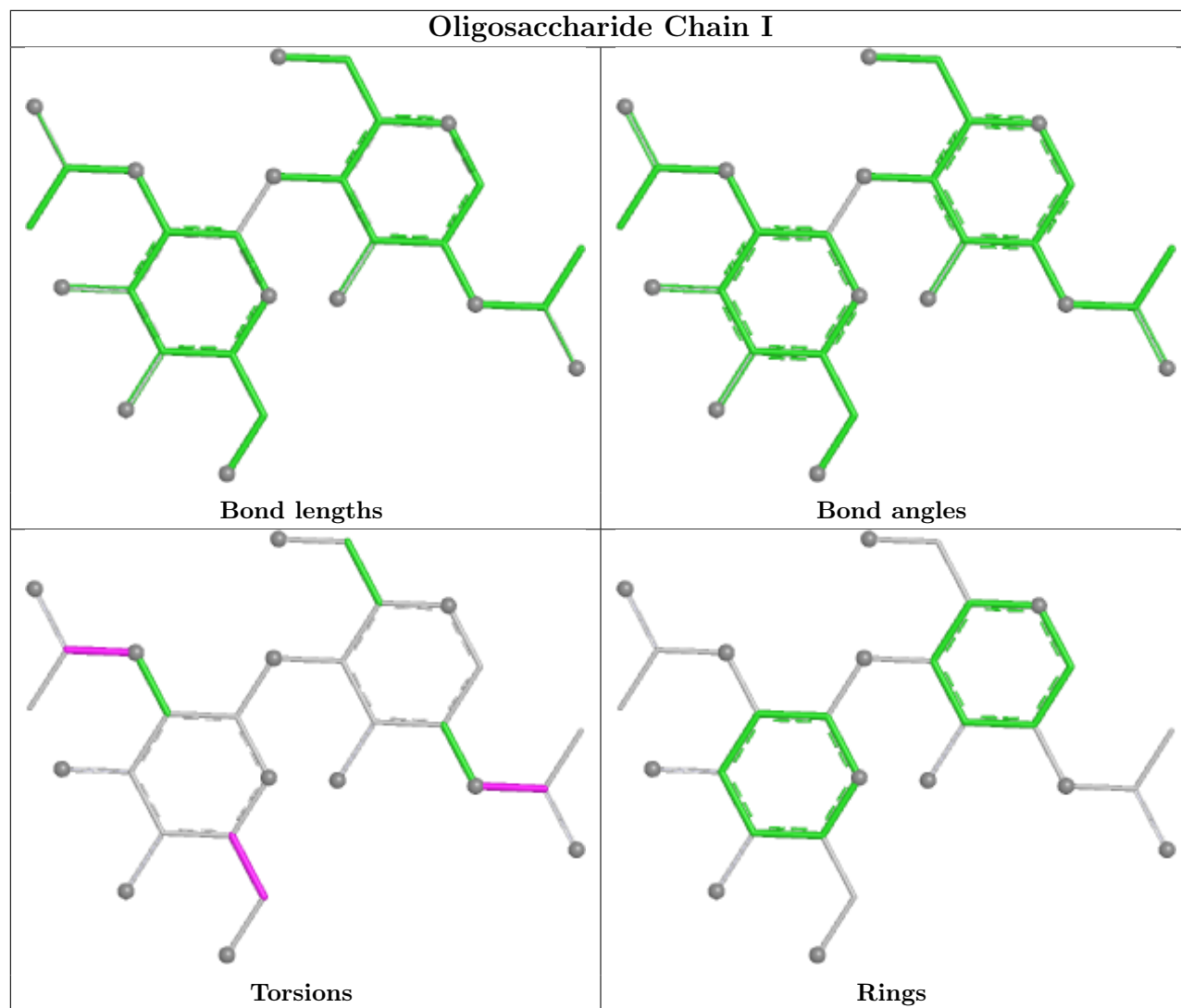
18 monomers are involved in 37 short contacts:

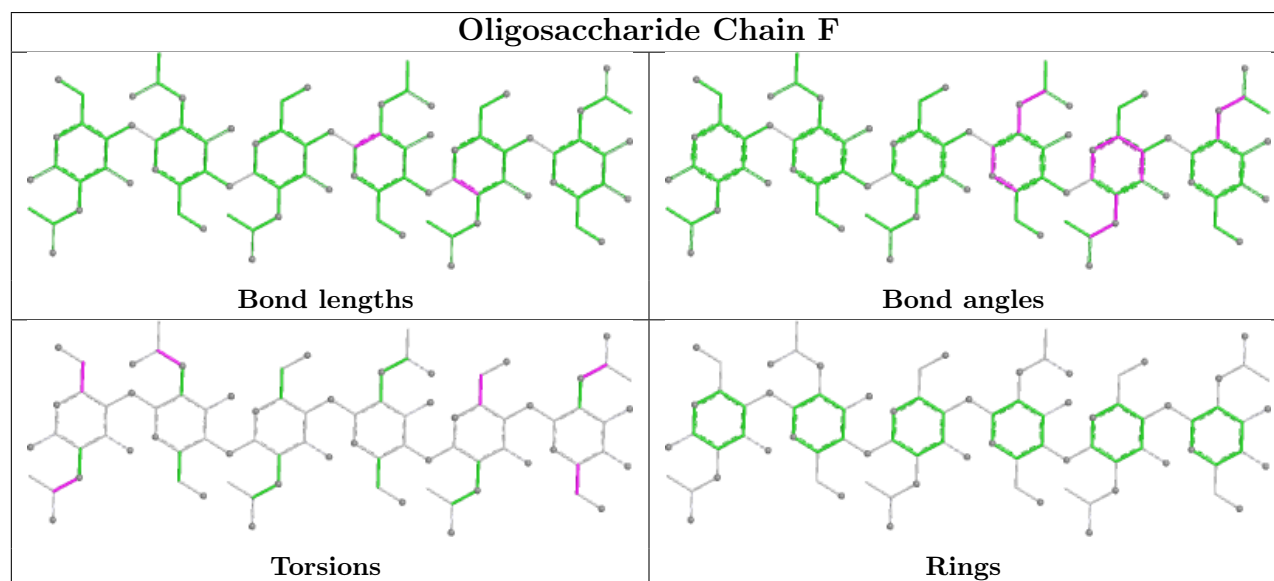
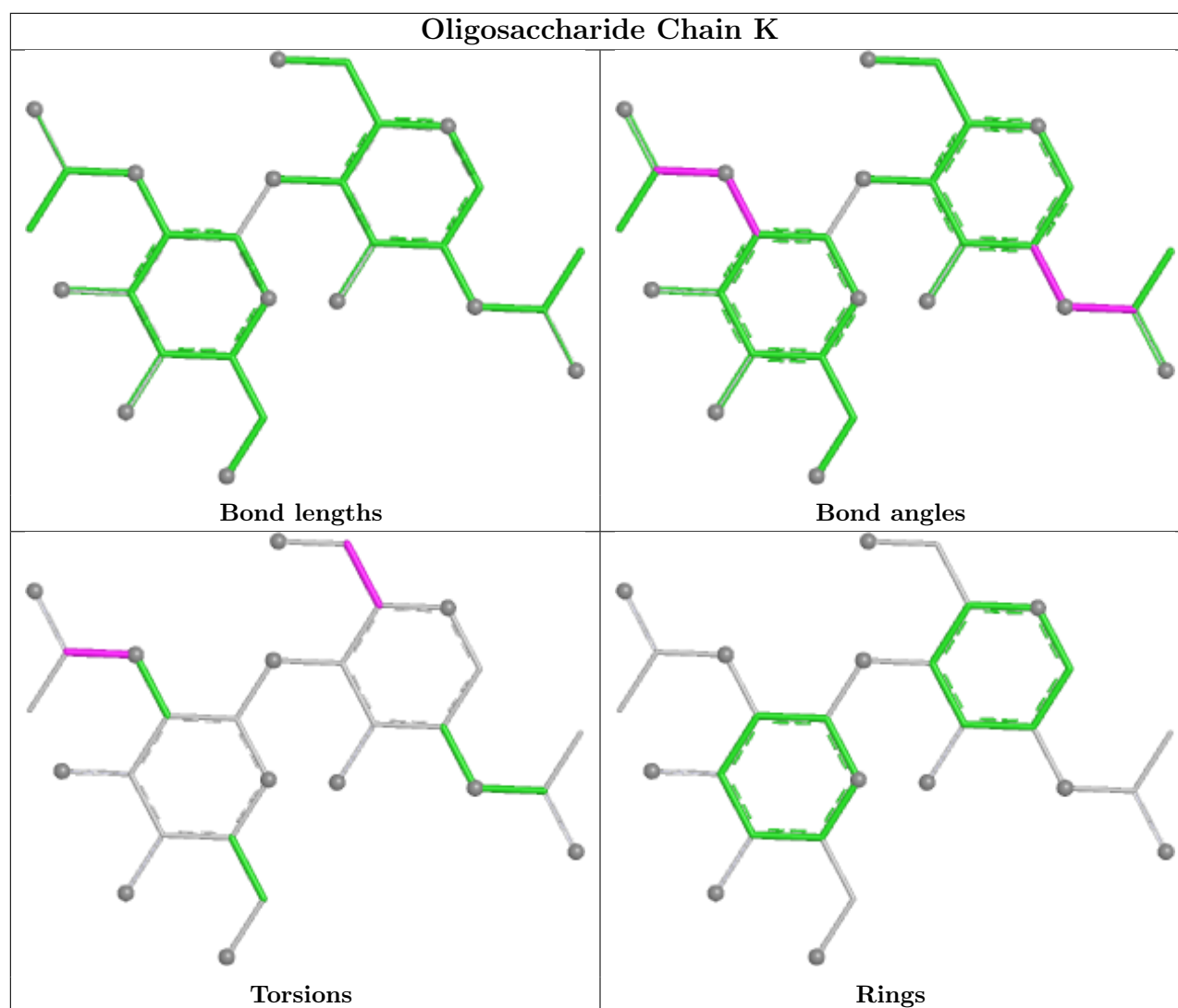
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	2	0
3	J	3	NAG	7	0
2	G	2	NAG	1	0
3	F	2	NAG	2	0
4	H	1	NDG	1	0
3	L	1	NAG	2	0
3	L	5	NDG	1	0
4	H	4	NDG	3	0
2	G	1	NAG	1	0
3	F	3	NAG	3	0
3	F	5	NDG	3	0
4	H	3	NAG	4	0
3	L	4	NAG	3	0
3	L	3	NAG	4	0
4	H	2	NAG	4	0
3	F	4	NAG	3	0
4	H	5	NAG	2	0
3	J	4	NAG	1	0

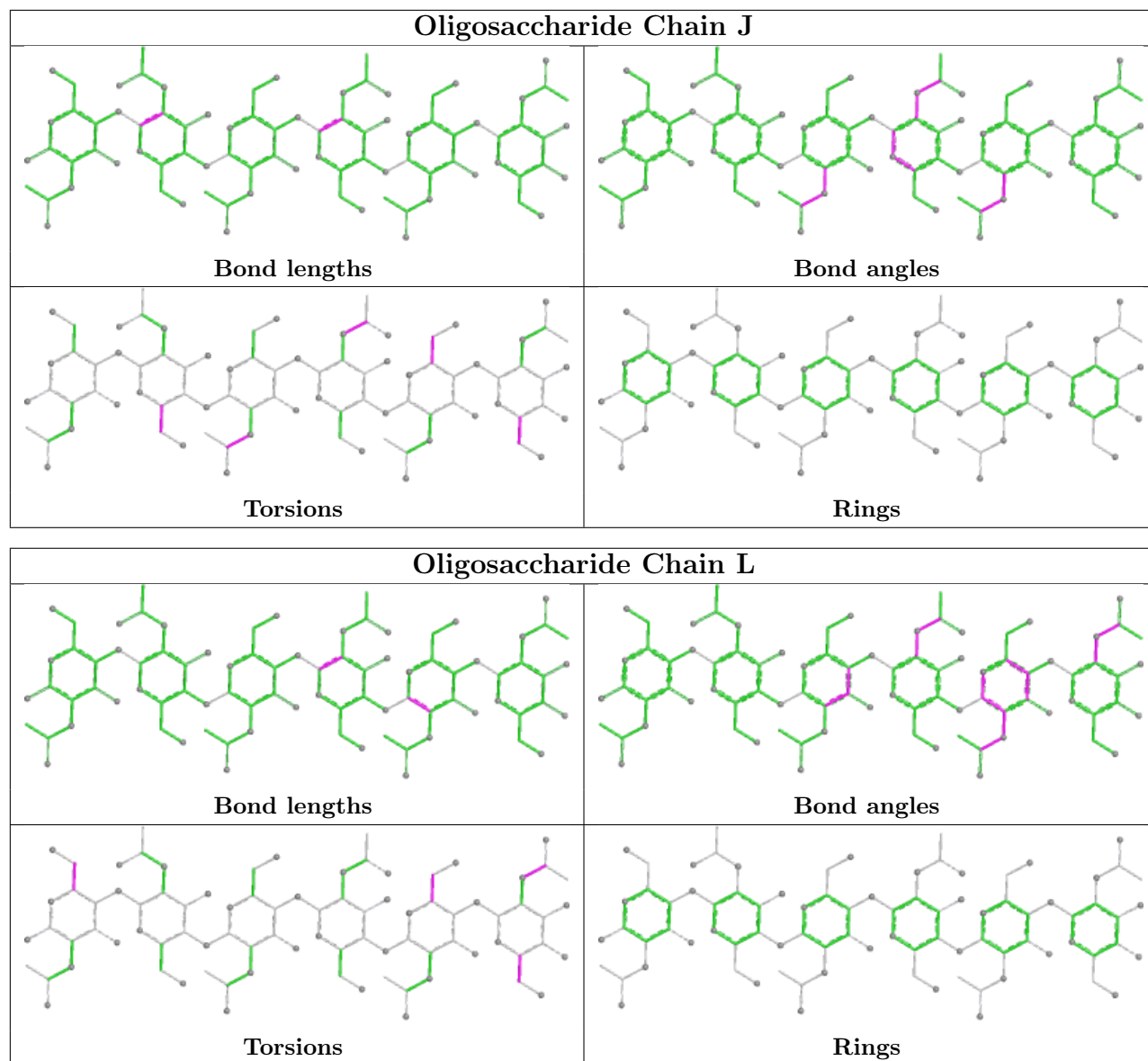
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

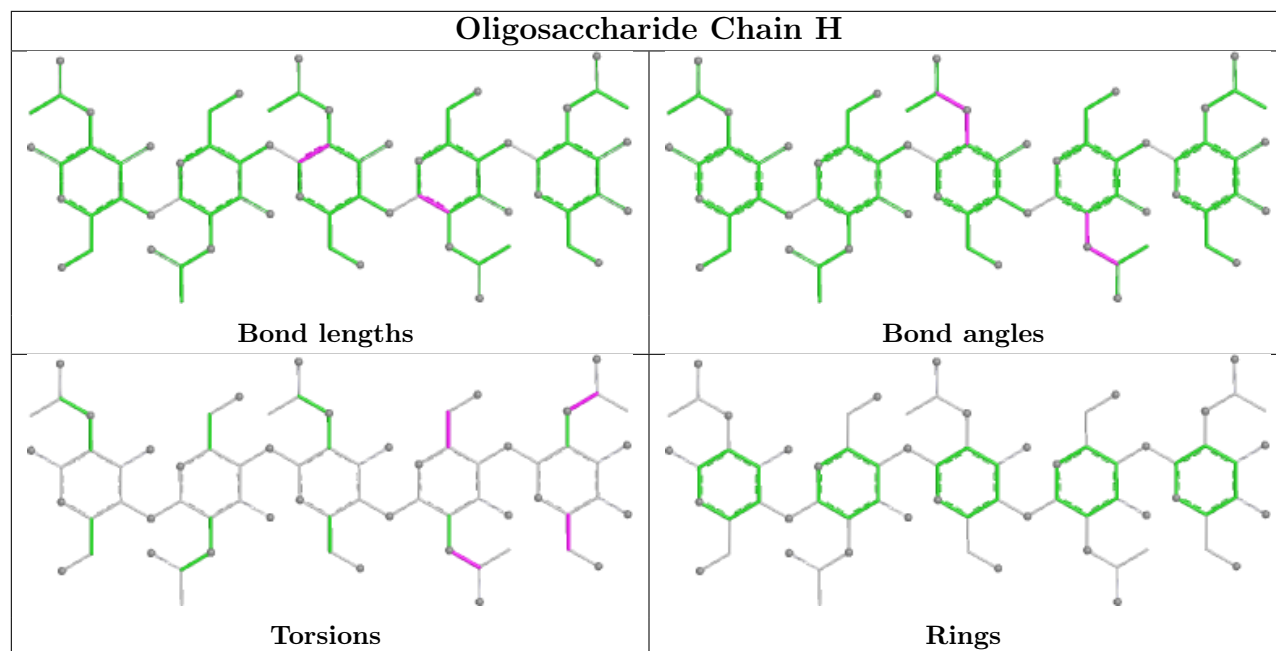












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/362 (100%)	-0.09	6 (1%) 69 65	17, 31, 55, 78	0
1	B	362/362 (100%)	0.19	4 (1%) 78 75	20, 38, 60, 80	0
1	C	362/362 (100%)	-0.04	3 (0%) 82 80	16, 33, 59, 81	0
1	D	362/362 (100%)	-0.12	3 (0%) 82 80	16, 30, 60, 81	0
All	All	1448/1448 (100%)	-0.02	16 (1%) 78 75	16, 33, 59, 81	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	GLY	3.1
1	A	383	THR	2.8
1	C	111	SER	2.6
1	A	104	GLN	2.5
1	B	113	THR	2.4
1	C	167	PRO	2.4
1	D	143	GLY	2.2
1	D	210	GLY	2.2
1	A	365	GLY	2.2
1	A	228	ASP	2.2
1	D	212	TRP	2.2
1	C	365	GLY	2.1
1	A	108	LYS	2.1
1	B	109	ILE	2.1
1	A	212	TRP	2.1
1	B	368	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

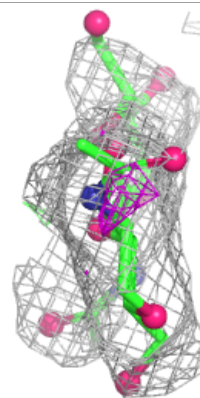
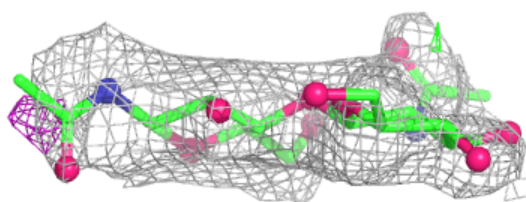
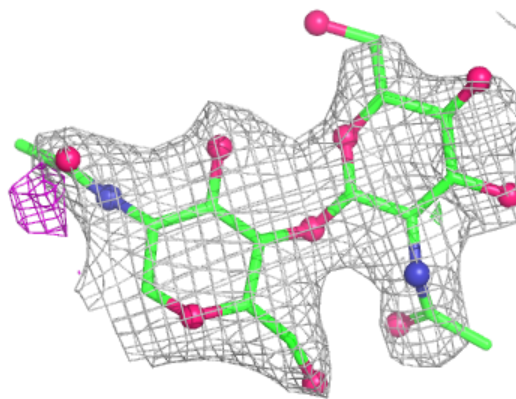
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	J	1	15/15	0.49	0.28	52,54,60,60	15
3	NAG	F	1	15/15	0.58	0.25	32,36,41,46	15
2	NAG	I	2	14/15	0.60	0.15	84,89,91,95	0
3	NAG	L	1	15/15	0.60	0.27	41,50,54,55	15
2	NAG	E	2	14/15	0.70	0.15	74,82,86,90	0
2	NAG	G	2	14/15	0.71	0.14	80,83,86,87	0
2	NAG	K	2	14/15	0.76	0.14	62,71,74,75	0
3	NAG	F	6	14/15	0.76	0.18	13,21,23,25	14
4	NDG	H	1	15/15	0.79	0.14	52,58,63,72	0
2	NAG	I	1	14/15	0.80	0.13	57,66,72,80	0
2	NAG	G	1	14/15	0.80	0.13	58,68,74,76	0
3	NAG	L	3	14/15	0.81	0.18	44,57,61,63	0
4	NAG	H	5	14/15	0.81	0.15	65,69,74,77	0
3	NAG	J	6	14/15	0.82	0.21	20,26,30,36	14
3	NAG	J	2	14/15	0.84	0.15	50,58,65,66	0
3	NAG	F	3	14/15	0.84	0.17	52,59,64,67	0
4	NAG	H	2	14/15	0.85	0.12	42,56,61,61	0
4	NAG	H	3	14/15	0.86	0.12	25,38,43,43	0
3	NAG	L	2	14/15	0.86	0.14	47,60,62,64	0
2	NAG	E	1	14/15	0.87	0.10	43,49,58,62	0
3	NAG	L	4	14/15	0.88	0.11	22,32,39,42	0
3	NAG	L	6	14/15	0.88	0.15	10,12,17,18	14
3	NAG	F	4	14/15	0.89	0.10	24,33,39,43	0
3	NAG	J	3	14/15	0.89	0.15	49,53,55,56	0
3	NDG	L	5	14/15	0.90	0.10	18,27,31,35	0
3	NAG	F	2	14/15	0.90	0.10	35,49,57,59	0
4	NDG	H	4	14/15	0.90	0.10	34,39,47,54	0
2	NAG	K	1	14/15	0.90	0.10	40,47,52,54	0
3	NAG	J	4	14/15	0.93	0.08	27,33,37,42	0
3	NDG	J	5	14/15	0.93	0.08	20,34,41,42	0
3	NDG	F	5	14/15	0.94	0.08	12,28,35,37	0

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

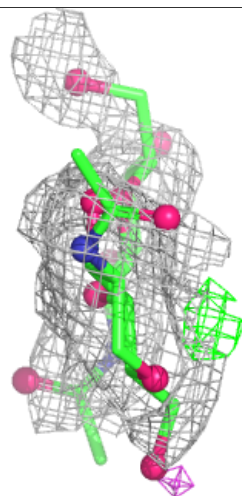
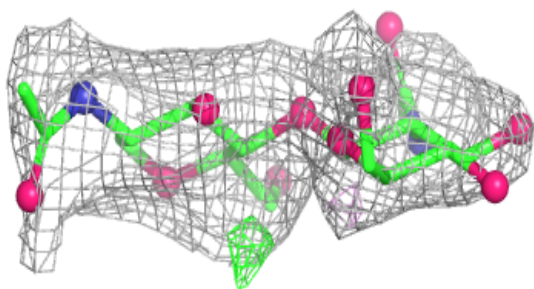
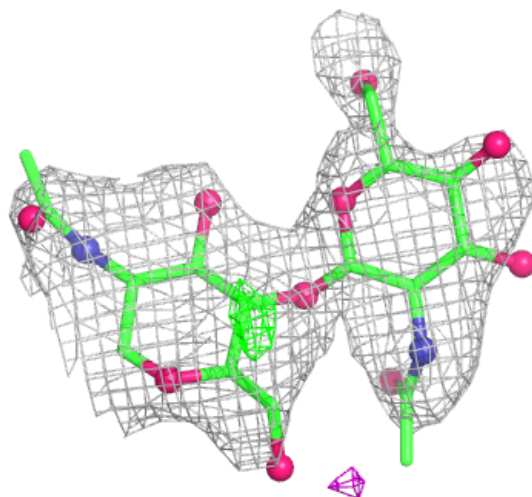
Electron density around Chain E:

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



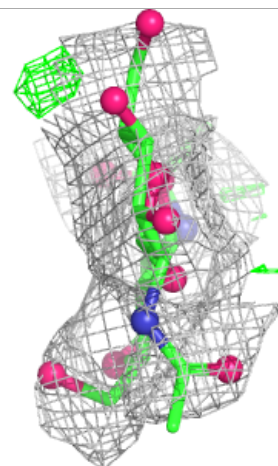
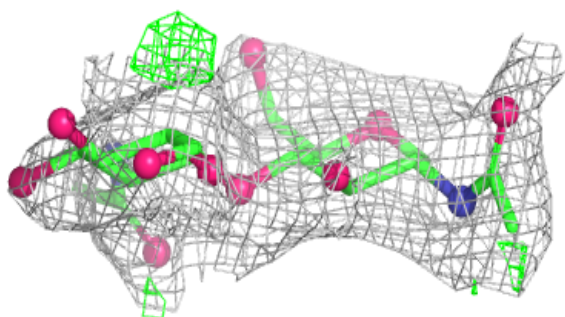
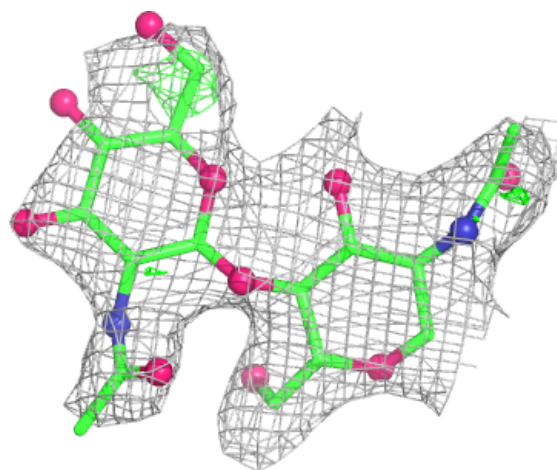
Electron density around Chain G:

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



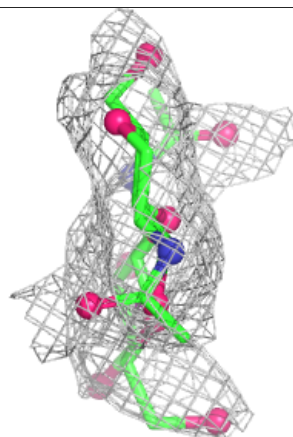
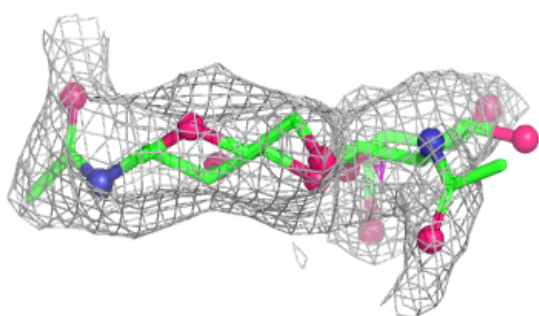
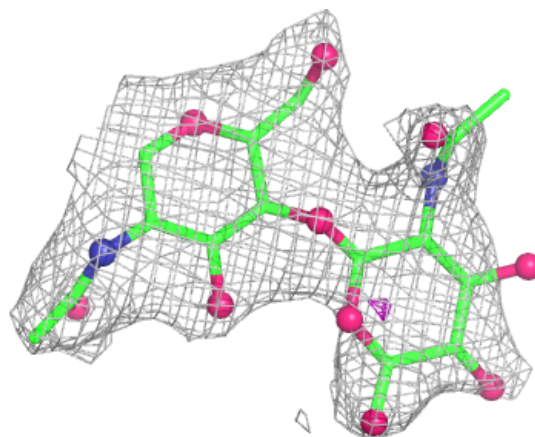
Electron density around Chain I:

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

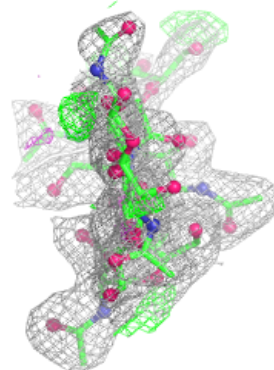
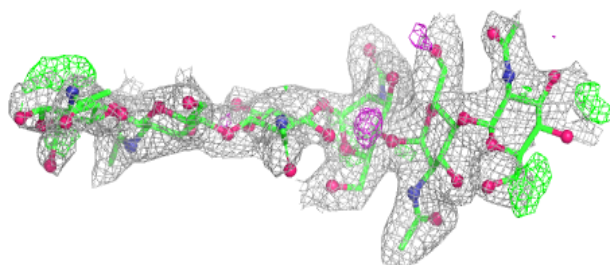
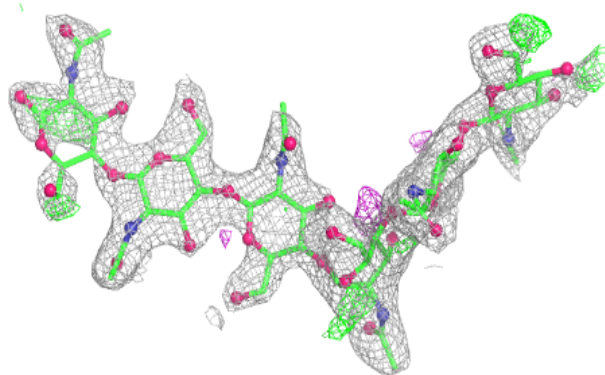


Electron density around Chain K:

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

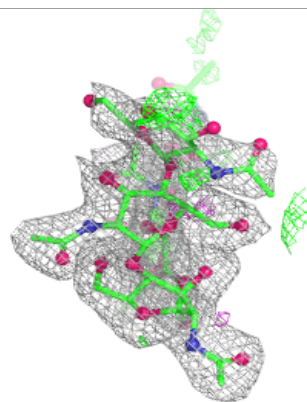
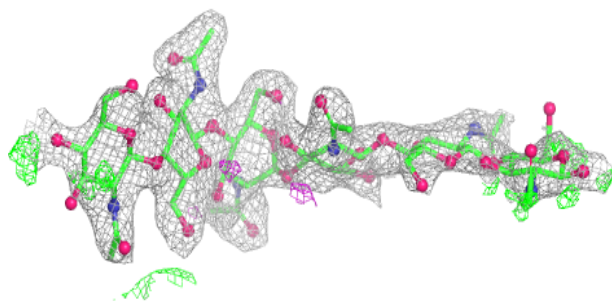
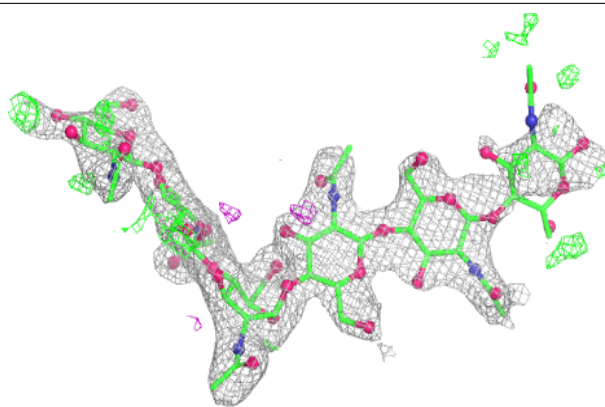
**Electron density around Chain F:**

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

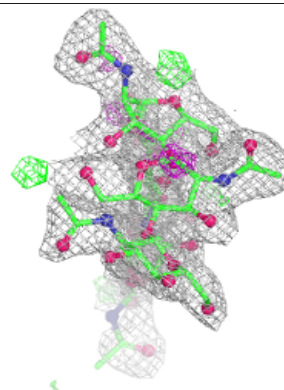
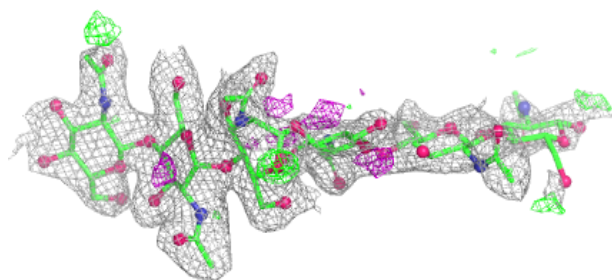
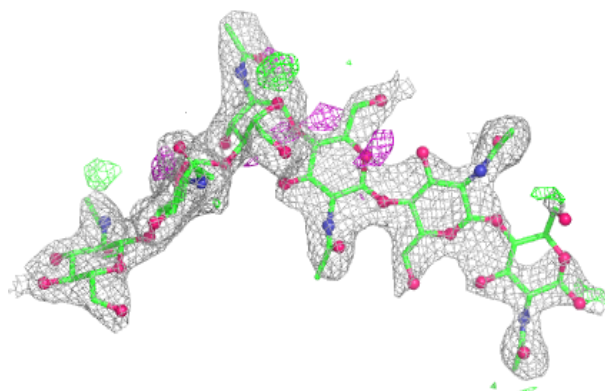


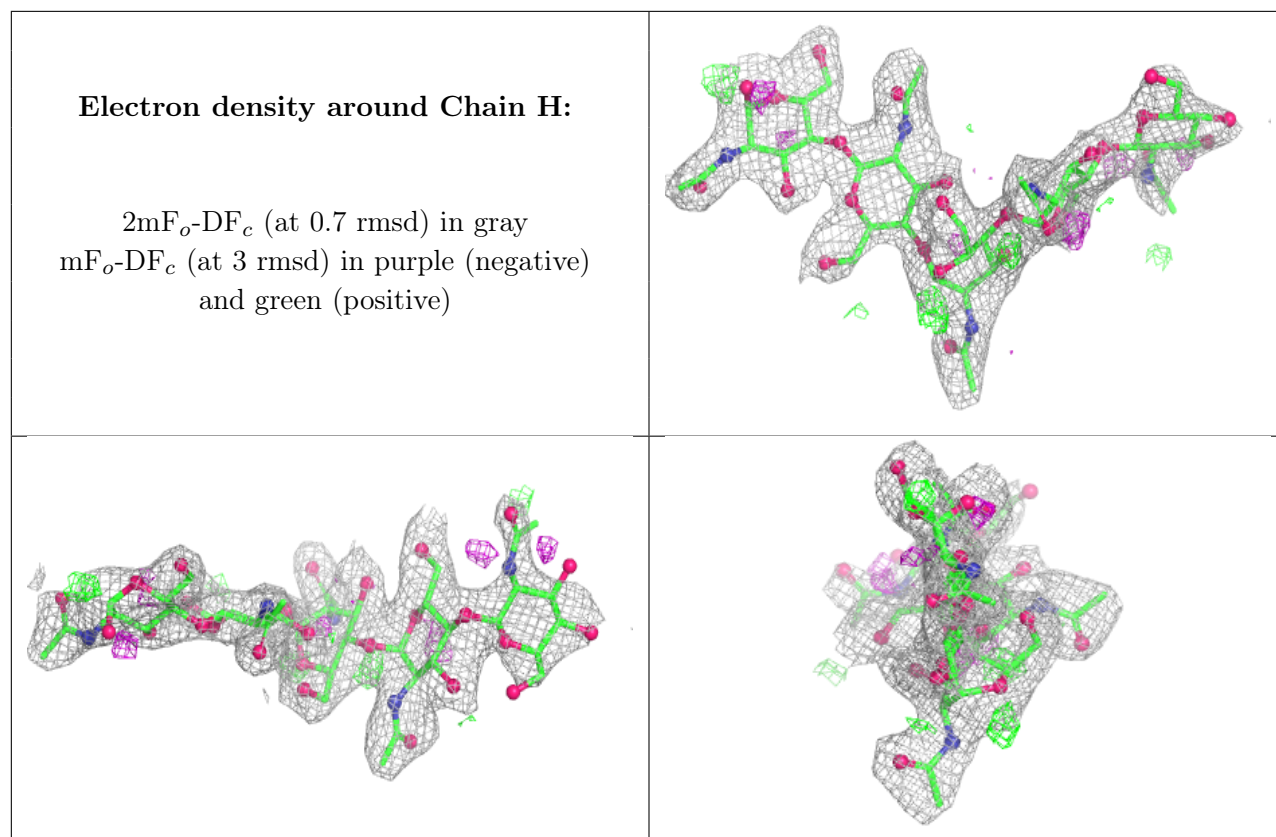
Electron density around Chain J:

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

**Electron density around Chain L:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.