



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 AM UTC

PDB ID : 6MSU / pdb_00006msu
Title : Integrin alphaVBeta3 in complex with EETI-II 2.5F
Authors : van Agthoven, J.F.; Arnaout, M.A.
Deposited on : 2018-10-18
Resolution : 3.11 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

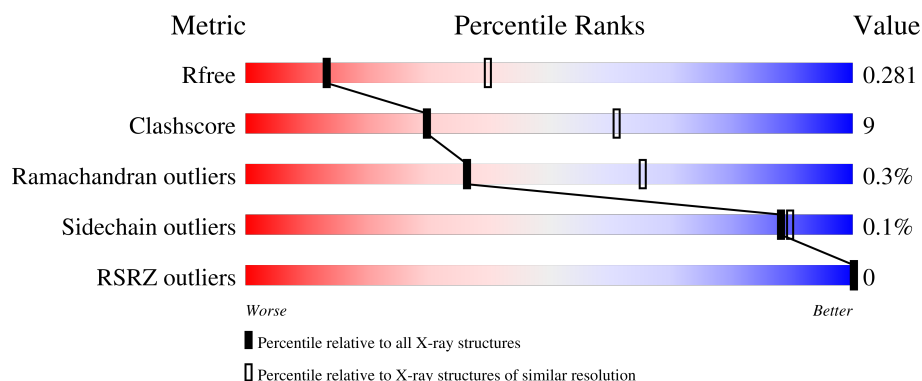
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



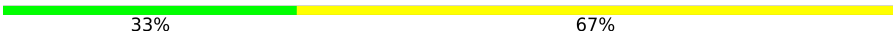
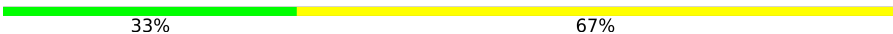
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	967	 77% 18% . .
2	B	695	 79% 20% .
3	C	32	 62% 38%
4	D	4	 50% 50%
4	G	4	 75% 25%

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Mol	Chain	Length	Quality of chain
5	E	2	 50% 50%
5	H	2	 100%
5	I	2	 50% 50%
5	K	2	 50% 50%
6	F	6	 33% 17% 50%
7	J	3	 33% 67%
7	L	3	 33% 67%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13158 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Engineered EETI-II 2.5F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	32	Total	C	N	O	S	0	0	0
			224	132	42	44	6			

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



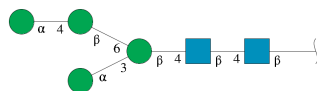
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



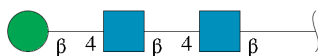
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranos e-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total	Mn	0	0
			5	5		
9	B	3	Total	Mn	0	0
			3	3		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Cl	0	0
			1	1		

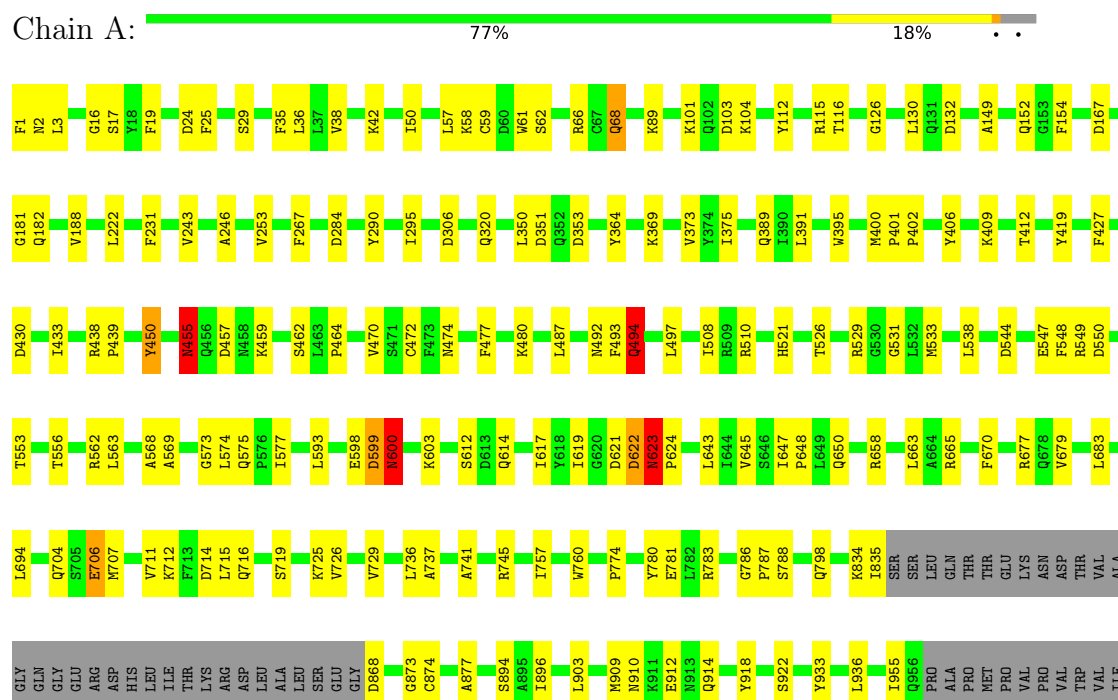
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	O 1	0	0
11	B	2	Total 2	O 2	0	0

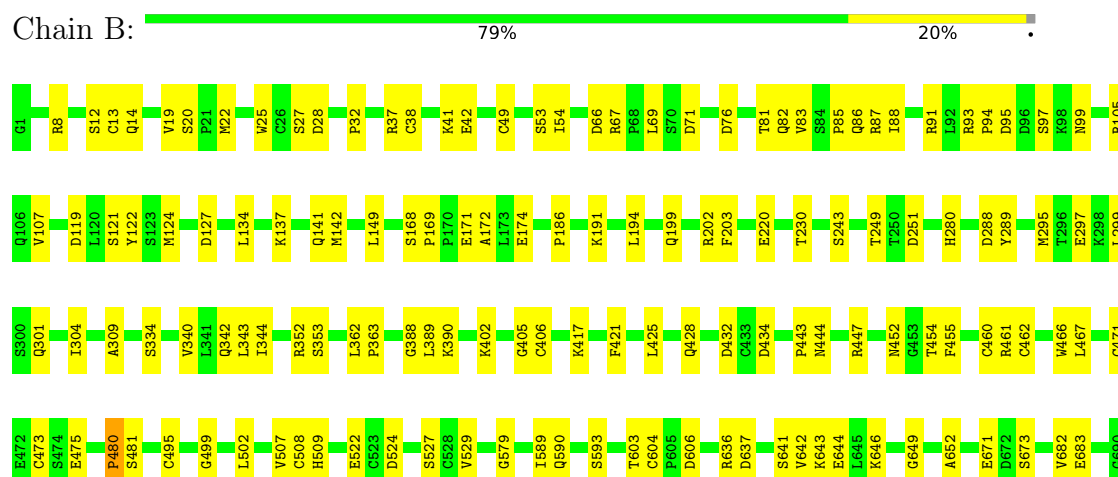
3 Residue-property plots

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

• Molecule 1: Integrin alpha-V



• Molecule 2: Integrin beta-3



PRO
ASP
ILE
LEU
VAL

- Molecule 3: Engineered EETI-II 2.5F

Chain C:  62% 38%

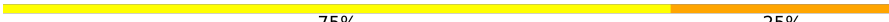
C2 P3 R4 P5 D8 I9 P10 P11 L12 T13 C14 D17 C20 C24 V25 C26 G33

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

Chain D:  50% 50%

MAG1
MAG2
BMA3
MAN4

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

Chain G:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 6: α -D-mannopyranose-(1-4)- β -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  33% 17% 50%



- Molecule 7: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  33% 67%



- Molecule 7: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain L:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.89Å 129.89Å 305.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	3.21 – 3.11 3.21 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (3.21-3.11) 5.2 (3.21-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	(Not available) , (Not available) 0.235 , 0.281	Depositor DCC
R_{free} test set	2624 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 0.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	13158	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MN, MAN, BMA, CL

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	0.31	1/7352 (0.0%)	0.76	17/9967 (0.2%)
2	B	0.24	0/5390	0.48	0/7289
3	C	0.26	0/229	0.58	0/309
All	All	0.28	1/12971 (0.0%)	0.65	17/17565 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	ASN	CA-C	5.33	1.60	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	GLN	CG-CD-NE2	-25.98	77.43	116.40
1	A	623	ASN	CB-CG-ND2	-22.56	82.55	116.40
1	A	494	GLN	CG-CD-OE1	18.41	157.63	120.80
1	A	494	GLN	OE1-CD-NE2	-17.61	104.99	122.60
1	A	622	ASP	CA-C-N	15.13	142.39	121.20
1	A	622	ASP	C-N-CA	15.13	142.39	121.20
1	A	623	ASN	CB-CG-OD1	12.95	146.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASN	OD1-CG-ND2	-9.92	112.68	122.60
1	A	599	ASP	CA-C-N	8.93	135.35	122.40
1	A	599	ASP	C-N-CA	8.93	135.35	122.40
1	A	623	ASN	O-C-N	7.90	128.02	121.31
1	A	600	ASN	CB-CA-C	-7.62	99.47	111.51
1	A	455	ASN	CB-CA-C	-6.44	99.24	109.80
1	A	494	GLN	CB-CG-CD	5.50	121.95	112.60
1	A	600	ASN	CB-CG-ND2	-5.49	108.16	116.40
1	A	455	ASN	CA-C-N	-5.20	112.05	121.14
1	A	455	ASN	C-N-CA	-5.20	112.05	121.14

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LYS	Peptide
1	A	450	TYR	Peptide
1	A	455	ASN	Sidechain
1	A	494	GLN	Sidechain
1	A	600	ASN	Sidechain
1	A	623	ASN	Sidechain
1	A	68	GLN	Sidechain
2	B	495	CYS	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	7196	0	7013	119	0
2	B	5294	0	5024	93	0
3	C	224	0	201	9	0
4	D	50	0	43	0	0
4	G	50	0	43	2	0
5	E	28	0	25	2	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	72	0	61	2	0
7	J	39	0	34	1	0
7	L	39	0	34	0	0
8	A	42	0	39	0	0
8	B	28	0	26	1	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	B	2	0	0	0	0
All	All	13158	0	12618	220	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 9.

All (220) 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:617:ILE:HB	1:A:623:ASN:ND2	1.82	0.95
2:B:443:PRO:HG2	2:B:460:CYS:HB3	1.51	0.90
1:A:914:GLN:HE22	1:A:955:ILE:HD12	1.43	0.83
1:A:455:ASN:HD22	1:A:593:LEU:HD22	1.43	0.83
3:C:4:ARG:HH21	3:C:5:PRO:HD2	1.48	0.79
2:B:97:SER:HB2	2:B:402:LYS:HD3	1.63	0.78
2:B:25:TRP:HE1	2:B:27:SER:HB3	1.49	0.77
1:A:741:ALA:H	1:A:786:GLY:HA3	1.51	0.75
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.69	0.74
1:A:617:ILE:HB	1:A:623:ASN:HD22	1.53	0.74
2:B:388:GLY:O	2:B:636:ARG:NH1	2.22	0.71
1:A:650:GLN:HG3	1:A:704:GLN:HB2	1.74	0.69
1:A:645:VAL:HG12	1:A:715:LEU:HG	1.73	0.69
1:A:487:LEU:O	1:A:529:ARG:NH2	2.27	0.68
2:B:91:ARG:NH2	2:B:432:ASP:OD2	2.26	0.68
2:B:83:VAL:O	2:B:86:GLN:NE2	2.24	0.68
1:A:549:ARG:HH12	2:B:480:PRO:HD3	1.59	0.67
2:B:69:LEU:HB2	2:B:105:ARG:HH21	1.59	0.67
1:A:455:ASN:OD1	1:A:457:ASP:HB3	1.95	0.66
2:B:646:LYS:HE2	2:B:682:VAL:HG21	1.78	0.65
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.78	0.65
2:B:417:LYS:NZ	2:B:421:PHE:O	2.30	0.65
1:A:757:ILE:HD13	1:A:774:PRO:HD3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:PRO:HB3	2:B:447:ARG:HB2	1.80	0.64
1:A:510:ARG:NH1	1:A:550:ASP:O	2.30	0.64
1:A:621:ASP:OD1	1:A:622:ASP:N	2.32	0.63
1:A:455:ASN:HD22	1:A:593:LEU:CD2	2.10	0.63
2:B:462:CYS:HB2	2:B:467:LEU:HA	1.81	0.62
1:A:438:ARG:HH11	1:A:577:ILE:HB	1.66	0.61
2:B:467:LEU:O	2:B:473:CYS:HB2	2.00	0.61
1:A:24:ASP:OD1	1:A:25:PHE:N	2.34	0.60
1:A:783:ARG:HD2	1:A:894:SER:HB3	1.83	0.60
2:B:390:LYS:HE3	2:B:636:ARG:HD2	1.83	0.60
2:B:342:GLN:O	2:B:344:ILE:N	2.34	0.60
1:A:480:LYS:HD2	1:A:531:GLY:HA2	1.83	0.60
1:A:617:ILE:HB	1:A:623:ASN:HD21	1.63	0.60
1:A:510:ARG:NH2	1:A:553:THR:OG1	2.36	0.59
1:A:781:GLU:HG3	1:A:896:ILE:HG12	1.84	0.59
1:A:494:GLN:HB2	1:A:562:ARG:HB3	1.85	0.58
3:C:17:ASP:OD1	3:C:26:CYS:HB2	2.03	0.58
5:E:1:NAG:H3	5:E:1:NAG:H83	1.85	0.58
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.85	0.58
2:B:649:GLY:HA2	2:B:652:ALA:HB2	1.85	0.58
1:A:66:ARG:NH2	1:A:68:GLN:OE1	2.37	0.58
2:B:444:ASN:HA	2:B:454:THR:HG22	1.86	0.58
1:A:472:CYS:O	4:G:1:NAG:O6	2.20	0.58
1:A:780:TYR:HH	1:A:922:SER:HG	1.52	0.57
2:B:590:GLN:NE2	2:B:604:CYS:SG	2.77	0.57
2:B:481:SER:O	2:B:481:SER:OG	2.21	0.57
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.86	0.57
3:C:25:VAL:HG12	3:C:26:CYS:H	1.69	0.57
2:B:14:GLN:NE2	2:B:434:ASP:OD1	2.36	0.57
2:B:67:ARG:NH2	2:B:81:THR:OG1	2.38	0.57
2:B:644:GLU:HA	2:B:682:VAL:HG13	1.87	0.57
1:A:455:ASN:ND2	1:A:593:LEU:CD2	2.67	0.56
2:B:480:PRO:O	2:B:481:SER:HB3	2.04	0.56
2:B:502:LEU:HB2	2:B:507:VAL:HG21	1.88	0.56
2:B:199:GLN:OE1	2:B:202:ARG:NH2	2.39	0.56
2:B:466:TRP:HE1	2:B:475:GLU:HB3	1.70	0.56
1:A:645:VAL:HG23	1:A:679:VAL:HB	1.87	0.55
2:B:142:MET:HB2	2:B:149:LEU:HD22	1.89	0.55
1:A:658:ARG:HG2	1:A:665:ARG:HG2	1.90	0.54
1:A:438:ARG:NH1	1:A:577:ILE:HB	2.22	0.54
2:B:637:ASP:OD1	2:B:637:ASP:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:OG	1:A:103:ASP:OD2	2.25	0.54
1:A:798:GLN:HB3	1:A:874:CYS:SG	2.48	0.54
2:B:82:GLN:HG2	2:B:107:VAL:HG13	1.90	0.54
2:B:499:GLY:HA2	2:B:508:CYS:HA	1.90	0.54
2:B:41:LYS:HG3	2:B:42:GLU:HG2	1.90	0.53
1:A:774:PRO:HD2	1:A:903:LEU:HB3	1.90	0.53
3:C:13:THR:HG22	3:C:14:CYS:H	1.73	0.53
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.44	0.53
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.90	0.53
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.90	0.53
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.91	0.53
3:C:20:CYS:SG	3:C:24:CYS:HB2	2.49	0.53
1:A:112:TYR:HB3	1:A:126:GLY:HA2	1.91	0.53
1:A:149:ALA:HB2	1:A:154:PHE:CD1	2.44	0.52
1:A:648:PRO:O	1:A:677:ARG:NH1	2.42	0.52
2:B:28:ASP:HA	2:B:53:SER:HB3	1.92	0.52
1:A:544:ASP:HB3	1:A:547:GLU:HG3	1.91	0.52
2:B:452:ASN:HB2	2:B:471:CYS:HB3	1.91	0.52
1:A:663:LEU:HD22	1:A:694:LEU:HB3	1.91	0.52
2:B:121:SER:CB	2:B:220:GLU:OE1	2.58	0.52
1:A:745:ARG:HB3	2:B:603:THR:HG21	1.91	0.51
2:B:12:SER:OG	2:B:13:CYS:N	2.41	0.51
2:B:455:PHE:CD2	2:B:461:ARG:HD3	2.46	0.51
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.91	0.51
1:A:351:ASP:OD2	1:A:353:ASP:OD2	2.29	0.51
1:A:647:ILE:HD11	1:A:670:PHE:HE2	1.76	0.50
1:A:284:ASP:OD2	1:A:290:TYR:N	2.44	0.50
2:B:122:TYR:CD2	3:C:10:PRO:HD3	2.46	0.50
1:A:643:LEU:HB2	1:A:683:LEU:HD11	1.94	0.50
2:B:71:ASP:OD1	2:B:71:ASP:N	2.40	0.50
2:B:134:LEU:HD12	2:B:137:LYS:HD3	1.92	0.50
2:B:25:TRP:HE3	2:B:38:CYS:HB2	1.76	0.50
1:A:17:SER:HA	1:A:42:LYS:HB3	1.92	0.49
2:B:461:ARG:HH21	2:B:467:LEU:HD22	1.76	0.49
1:A:645:VAL:CG2	1:A:679:VAL:HB	2.42	0.49
1:A:25:PHE:CD2	1:A:412:THR:HB	2.47	0.49
1:A:115:ARG:NH1	1:A:116:THR:O	2.44	0.49
2:B:249:THR:HA	2:B:309:ALA:O	2.11	0.49
2:B:342:GLN:C	2:B:344:ILE:H	2.19	0.49
2:B:606:ASP:N	2:B:606:ASP:OD1	2.44	0.49
1:A:599:ASP:OD2	1:A:603:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.95	0.48
1:A:2:ASN:OD1	1:A:2:ASN:N	2.47	0.48
1:A:725:LYS:HG3	1:A:726:VAL:HG13	1.95	0.48
2:B:88:ILE:HG13	2:B:425:LEU:HD11	1.96	0.48
2:B:99:ASN:OD1	2:B:99:ASN:N	2.45	0.48
2:B:641:SER:OG	2:B:683:GLU:HB3	2.15	0.47
7:J:1:NAG:H4	7:J:2:NAG:H2	1.60	0.47
2:B:466:TRP:HE1	2:B:475:GLU:CB	2.27	0.47
1:A:912:GLU:OE1	1:A:912:GLU:N	2.47	0.47
1:A:19:PHE:HE2	1:A:57:LEU:HD22	1.80	0.47
2:B:49:CYS:O	2:B:54:ILE:HG13	2.14	0.47
2:B:297:GLU:O	2:B:301:GLN:HG2	2.15	0.47
1:A:35:PHE:CD2	1:A:58:LYS:HE2	2.49	0.47
2:B:32:PRO:HB3	2:B:37:ARG:HH22	1.78	0.47
2:B:295:MET:O	2:B:299:LEU:HB2	2.15	0.47
1:A:104:LYS:HE3	1:A:132:ASP:OD2	2.15	0.46
1:A:395:TRP:HE1	1:A:433:ILE:HD11	1.79	0.46
1:A:621:ASP:HB2	1:A:787:PRO:HB3	1.96	0.46
2:B:642:VAL:HG22	2:B:643:LYS:H	1.79	0.46
2:B:671:GLU:O	2:B:673:SER:N	2.47	0.46
2:B:76:ASP:OD1	2:B:76:ASP:N	2.45	0.46
1:A:508:ILE:HD13	1:A:548:PHE:HB3	1.96	0.46
1:A:706:GLU:O	1:A:707:MET:HG2	2.16	0.46
1:A:711:VAL:HG23	1:A:736:LEU:HD21	1.97	0.46
1:A:130:LEU:HD21	1:A:188:VAL:HG13	1.97	0.46
2:B:99:ASN:HD22	8:B:701:NAG:H62	1.80	0.46
1:A:406:TYR:CG	1:A:427:PHE:HE2	2.34	0.46
2:B:466:TRP:HA	2:B:473:CYS:HB3	1.98	0.46
2:B:169:PRO:O	2:B:171:GLU:N	2.49	0.45
1:A:868:ASP:OD1	1:A:868:ASP:N	2.50	0.45
1:A:492:ASN:OD1	1:A:526:THR:OG1	2.34	0.45
1:A:510:ARG:HH22	1:A:553:THR:C	2.24	0.45
1:A:61:TRP:CG	1:A:62:SER:H	2.34	0.45
1:A:462:SER:C	1:A:464:PRO:HD2	2.41	0.45
1:A:568:ALA:O	1:A:573:GLY:HA2	2.17	0.45
1:A:231:PHE:O	1:A:320:GLN:NE2	2.50	0.45
1:A:306:ASP:OD1	1:A:306:ASP:N	2.40	0.45
1:A:480:LYS:HB3	1:A:533:MET:HA	1.98	0.45
1:A:788:SER:HB3	1:A:933:TYR:CE2	2.52	0.45
2:B:95:ASP:OD1	2:B:405:GLY:N	2.40	0.45
1:A:284:ASP:OD2	1:A:290:TYR:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLY:O	1:A:575:GLN:HG3	2.17	0.45
1:A:612:SER:C	1:A:614:GLN:H	2.25	0.45
1:A:910:ASN:OD1	1:A:910:ASN:N	2.46	0.44
2:B:122:TYR:HB3	3:C:8:ASP:O	2.18	0.44
2:B:191:LYS:HG3	2:B:280:HIS:CE1	2.52	0.44
3:C:12:LEU:O	3:C:13:THR:OG1	2.27	0.44
4:G:3:BMA:H3	4:G:4:MAN:H2	1.81	0.44
1:A:152:GLN:HE21	1:A:182:GLN:HE22	1.66	0.44
2:B:121:SER:HB2	3:C:8:ASP:OD1	2.18	0.44
1:A:253:VAL:HG21	1:A:295:ILE:HD13	1.98	0.44
2:B:20:SER:OG	2:B:22:MET:HG2	2.17	0.44
2:B:94:PRO:HB3	2:B:406:CYS:HB2	1.98	0.44
2:B:334:SER:O	2:B:340:VAL:HG21	2.18	0.44
1:A:834:LYS:HE3	1:A:835:ILE:HG22	1.98	0.44
2:B:243:SER:HB3	2:B:352:ARG:HH22	1.83	0.44
2:B:362:LEU:HD12	2:B:363:PRO:HD2	2.00	0.44
1:A:1:PHE:H2	1:A:375:ILE:HD11	1.83	0.43
1:A:493:PHE:CE2	1:A:563:LEU:HB2	2.52	0.43
1:A:736:LEU:HD13	1:A:736:LEU:HA	1.87	0.43
2:B:168:SER:O	2:B:169:PRO:C	2.60	0.43
2:B:466:TRP:HB3	2:B:473:CYS:H	1.83	0.43
1:A:253:VAL:HB	1:A:267:PHE:HB2	2.01	0.43
1:A:521:HIS:ND1	1:A:538:LEU:HD11	2.34	0.43
2:B:174:GLU:HA	2:B:186:PRO:HG3	2.00	0.43
2:B:522:GLU:H	2:B:522:GLU:CD	2.25	0.43
1:A:477:PHE:CE1	1:A:497:LEU:HD11	2.54	0.43
2:B:93:ARG:HB2	2:B:94:PRO:HD2	2.01	0.43
1:A:3:LEU:HG	1:A:350:LEU:HD21	2.00	0.43
1:A:167:ASP:O	1:A:188:VAL:HG23	2.19	0.43
1:A:598:GLU:C	1:A:600:ASN:H	2.27	0.43
1:A:619:ILE:HG13	1:A:737:ALA:O	2.19	0.43
1:A:3:LEU:HD21	1:A:350:LEU:HD11	2.01	0.43
1:A:19:PHE:CE1	1:A:38:VAL:HG11	2.53	0.43
1:A:510:ARG:NH2	1:A:553:THR:O	2.49	0.43
2:B:8:ARG:HB2	2:B:19:VAL:HG11	2.01	0.43
1:A:16:GLY:N	1:A:430:ASP:OD2	2.50	0.42
2:B:127:ASP:OD2	2:B:251:ASP:OD1	2.37	0.42
2:B:524:ASP:CG	2:B:527:SER:HB2	2.44	0.42
6:F:3:BMA:H62	6:F:4:BMA:H2	1.76	0.42
6:F:4:BMA:H4	6:F:5:MAN:H2	1.38	0.42
1:A:459:LYS:HB3	1:A:470:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1:NAG:H61	5:E:2:NAG:O5	2.19	0.42
1:A:623:ASN:HA	1:A:624:PRO:HD2	1.83	0.42
2:B:194:LEU:HD23	2:B:203:PHE:HD2	1.83	0.42
1:A:1:PHE:N	1:A:375:ILE:HD11	2.34	0.42
1:A:373:VAL:HB	1:A:391:LEU:HB2	2.02	0.42
1:A:619:ILE:HD11	1:A:936:LEU:HD22	2.00	0.42
2:B:288:ASP:OD1	2:B:289:TYR:N	2.51	0.42
2:B:353:SER:HA	2:B:389:LEU:O	2.20	0.42
1:A:364:TYR:O	1:A:369:LYS:HG3	2.19	0.42
1:A:873:GLY:O	1:A:877:ALA:HB3	2.19	0.42
2:B:119:ASP:HB3	2:B:124:MET:HG3	2.01	0.42
1:A:716:GLN:HB3	1:A:729:VAL:HG12	2.02	0.41
1:A:548:PHE:HD1	1:A:549:ARG:O	2.03	0.41
2:B:462:CYS:CB	2:B:467:LEU:HA	2.48	0.41
1:A:658:ARG:HH12	2:B:529:VAL:HG13	1.85	0.41
2:B:334:SER:H	2:B:340:VAL:HG21	1.85	0.41
1:A:549:ARG:NH1	2:B:480:PRO:HD3	2.31	0.41
1:A:912:GLU:HG3	1:A:918:TYR:OH	2.21	0.41
2:B:137:LYS:O	2:B:141:GLN:HG3	2.20	0.41
1:A:719:SER:OG	1:A:725:LYS:O	2.38	0.41
1:A:760:TRP:CZ3	1:A:909:MET:HE2	2.55	0.41
1:A:480:LYS:HB3	1:A:533:MET:HG3	2.03	0.41
1:A:574:LEU:HD12	1:A:574:LEU:HA	1.84	0.41
2:B:87:ARG:NE	2:B:428:GLN:OE1	2.47	0.41
2:B:590:GLN:O	2:B:593:SER:OG	2.30	0.41
2:B:642:VAL:HG12	2:B:682:VAL:HA	2.03	0.41
2:B:169:PRO:O	2:B:172:ALA:N	2.46	0.41
2:B:119:ASP:O	2:B:124:MET:HG3	2.21	0.40
1:A:401:PRO:HA	1:A:402:PRO:HD2	1.95	0.40
1:A:521:HIS:CG	1:A:538:LEU:HD11	2.55	0.40
1:A:400:MET:HB2	1:A:401:PRO:HD2	2.03	0.40
1:A:712:LYS:HE2	1:A:714:ASP:OD1	2.21	0.40
2:B:579:GLY:HA2	2:B:589:ILE:HG12	2.04	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	920/967 (95%)	850 (92%)	68 (7%)	2 (0%)	43	71
2	B	688/695 (99%)	606 (88%)	79 (12%)	3 (0%)	30	60
3	C	30/32 (94%)	24 (80%)	6 (20%)	0	100	100
All	All	1638/1694 (97%)	1480 (90%)	153 (9%)	5 (0%)	36	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	706	GLU
2	B	343	LEU
2	B	509	HIS
1	A	569	ALA
2	B	480	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	784/821 (96%)	783 (100%)	1 (0%)	88	90
2	B	612/617 (99%)	612 (100%)	0	100	100
3	C	26/26 (100%)	26 (100%)	0	100	100
All	All	1422/1464 (97%)	1421 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	THR

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	91	HIS
1	A	205	ASN
1	A	356	ASN
1	A	494	GLN
1	A	623	ASN
1	A	650	GLN
1	A	785	ASN
1	A	914	GLN
1	A	935	ASN
2	B	43	ASN
2	B	106	GLN
2	B	132	GLN
2	B	303	ASN
2	B	509	HIS
2	B	590	GLN
2	B	632	ASN
2	B	654	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 ⓘ

28 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.37	0	17,19,21	0.63	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	1.04	0	15,15,17	1.09	2 (13%)
4	MAN	D	4	4	11,11,12	0.90	0	15,15,17	1.11	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.47	0	17,19,21	1.40	2 (11%)
5	NAG	E	2	5	14,14,15	0.41	0	17,19,21	0.57	0
6	NAG	F	1	1,6	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	F	2	6	14,14,15	0.20	0	17,19,21	0.51	0
6	BMA	F	3	6	11,11,12	0.79	0	15,15,17	0.97	1 (6%)
6	BMA	F	4	6	11,11,12	1.80	4 (36%)	15,15,17	1.13	1 (6%)
6	MAN	F	5	6	11,11,12	1.08	2 (18%)	15,15,17	1.32	3 (20%)
6	MAN	F	6	6	11,11,12	1.04	1 (9%)	15,15,17	1.21	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.59	1 (7%)	17,19,21	0.64	0
4	BMA	G	3	4	11,11,12	0.94	0	15,15,17	0.68	0
4	MAN	G	4	4	11,11,12	0.85	0	15,15,17	1.05	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.37	0	17,19,21	0.53	0
5	NAG	H	2	5	14,14,15	0.45	0	17,19,21	0.44	0
5	NAG	I	1	1,5	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	I	2	5	14,14,15	0.40	0	17,19,21	0.92	2 (11%)
7	NAG	J	1	7,1	14,14,15	0.52	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.43	0	17,19,21	0.45	0
7	BMA	J	3	7	11,11,12	0.82	0	15,15,17	0.73	0
5	NAG	K	1	2,5	14,14,15	0.34	0	17,19,21	0.50	0
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.86	1 (5%)
7	NAG	L	1	7,2	14,14,15	0.34	0	17,19,21	0.62	0
7	NAG	L	2	7	14,14,15	0.98	1 (7%)	17,19,21	1.46	1 (5%)
7	BMA	L	3	7	11,11,12	1.28	2 (18%)	15,15,17	1.23	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
6	BMA	F	4	6	-	2/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	3/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
7	NAG	L	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	1/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	2	NAG	O5-C1	3.46	1.49	1.43
6	F	4	BMA	C4-C5	3.19	1.59	1.53
6	F	4	BMA	O5-C5	2.66	1.48	1.43
6	F	4	BMA	C4-C3	2.58	1.59	1.52
7	L	3	BMA	O5-C5	2.49	1.48	1.43
6	F	5	MAN	C1-C2	2.46	1.58	1.52
6	F	4	BMA	C2-C3	2.45	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	6	MAN	C1-C2	2.34	1.57	1.52
6	F	5	MAN	C2-C3	2.15	1.55	1.52
4	G	2	NAG	O5-C1	-2.12	1.40	1.43
7	L	3	BMA	C1-C2	2.08	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	2	NAG	C1-O5-C5	5.48	119.53	112.19
5	E	1	NAG	C2-N2-C7	4.71	129.21	122.90
7	L	3	BMA	C1-O5-C5	3.65	117.08	112.19
4	D	4	MAN	C1-O5-C5	3.16	116.42	112.19
6	F	3	BMA	C1-O5-C5	2.60	115.67	112.19
4	G	4	MAN	C1-O5-C5	2.57	115.63	112.19
6	F	5	MAN	C1-C2-C3	2.52	113.31	109.64
5	K	2	NAG	C1-O5-C5	2.50	115.54	112.19
5	I	2	NAG	C1-O5-C5	2.43	115.44	112.19
5	E	1	NAG	C1-C2-N2	2.40	114.21	110.43
6	F	5	MAN	C1-O5-C5	2.34	115.32	112.19
4	D	3	BMA	O3-C3-C2	2.34	114.83	110.05
5	I	2	NAG	C3-C4-C5	2.23	114.28	110.23
6	F	6	MAN	O2-C2-C3	-2.13	105.74	110.15
4	D	3	BMA	C1-O5-C5	2.10	115.00	112.19
6	F	5	MAN	O2-C2-C3	-2.06	105.89	110.15
6	F	4	BMA	C1-O5-C5	2.05	114.94	112.19
4	G	4	MAN	O2-C2-C3	-2.05	105.91	110.15

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
6	F	4	BMA	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
6	F	4	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
7	L	3	BMA	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7
6	F	2	NAG	C1-C2-N2-C7
7	J	2	NAG	C3-C2-N2-C7
5	I	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

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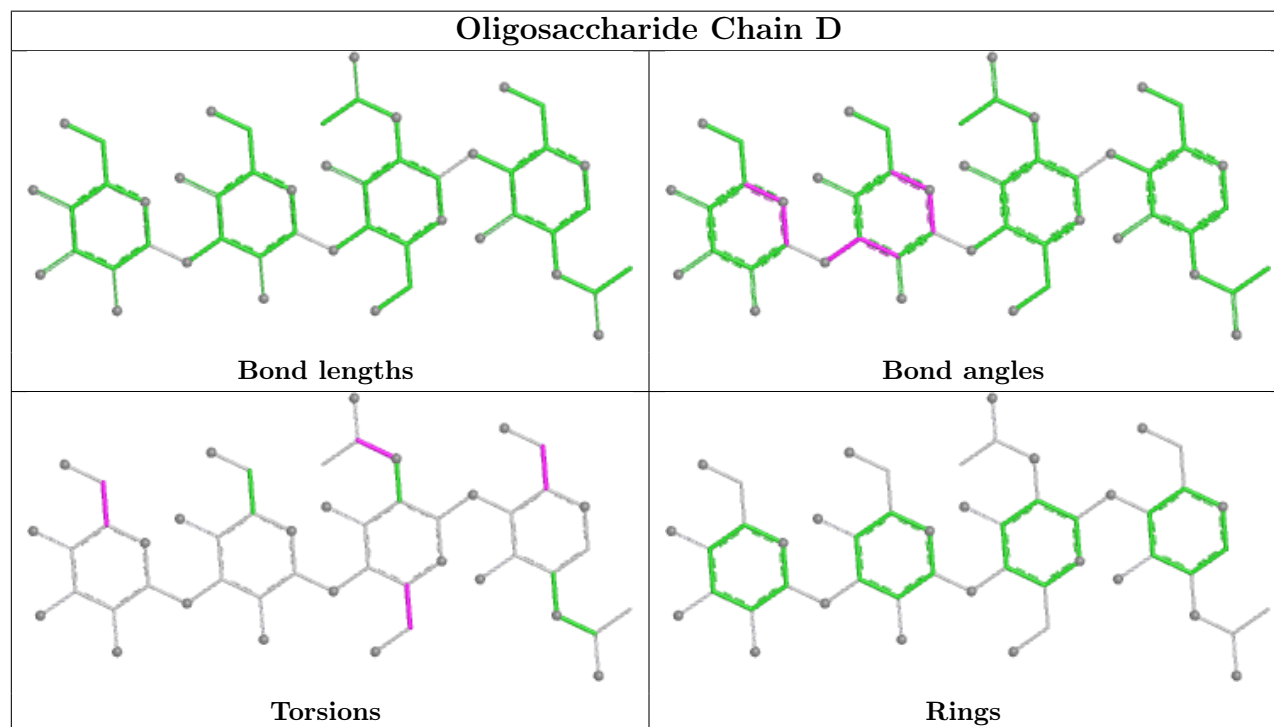
Mol	Chain	Res	Type	Atoms
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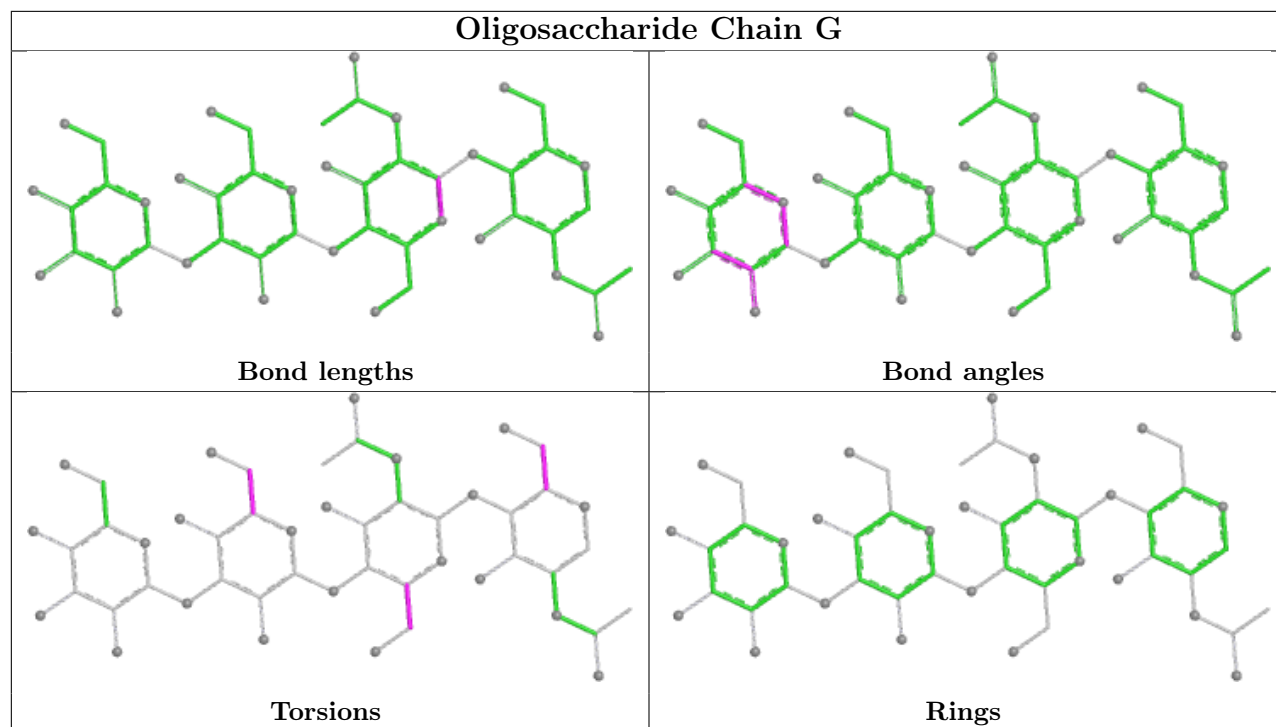
Mol	Chain	Res	Type	Atoms
7	L	3	BMA	C1-C2-C3-C4-C5-O5

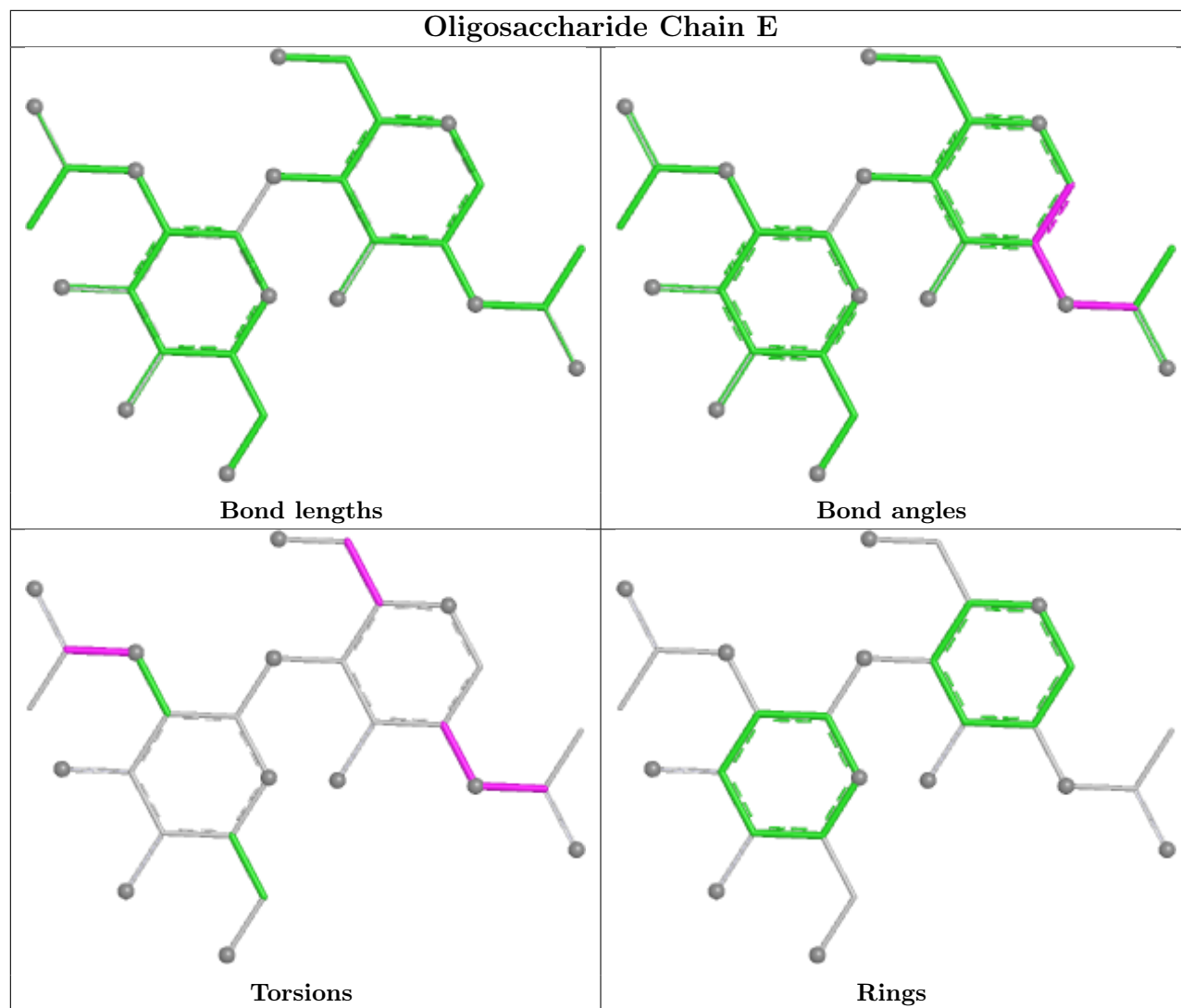
10 monomers are involved in 7 short contacts:

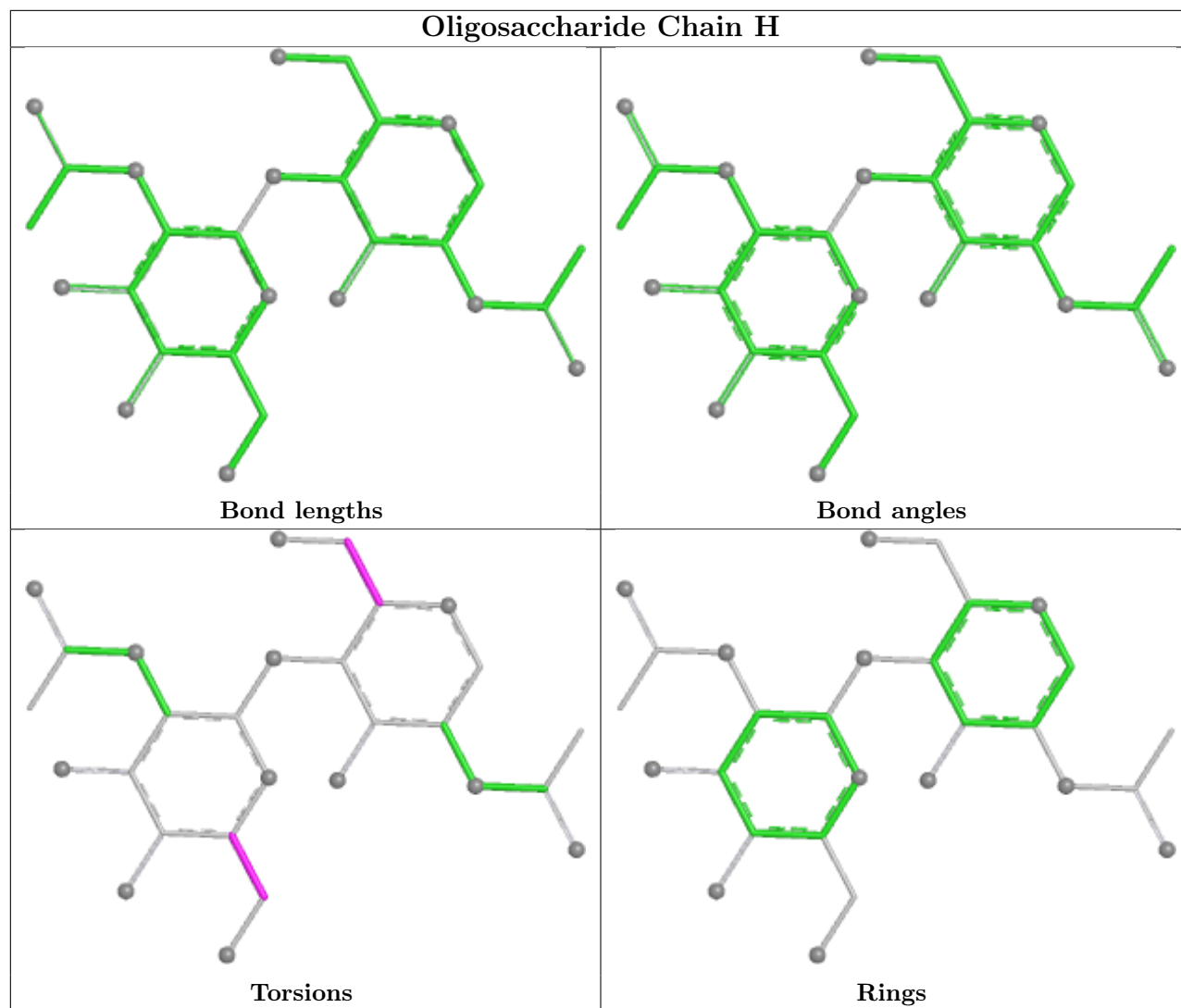
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	4	MAN	1	0
7	J	2	NAG	1	0
6	F	3	BMA	1	0
7	J	1	NAG	1	0
5	E	1	NAG	2	0
4	G	3	BMA	1	0
5	E	2	NAG	1	0
6	F	4	BMA	2	0
6	F	5	MAN	1	0
4	G	1	NAG	1	0

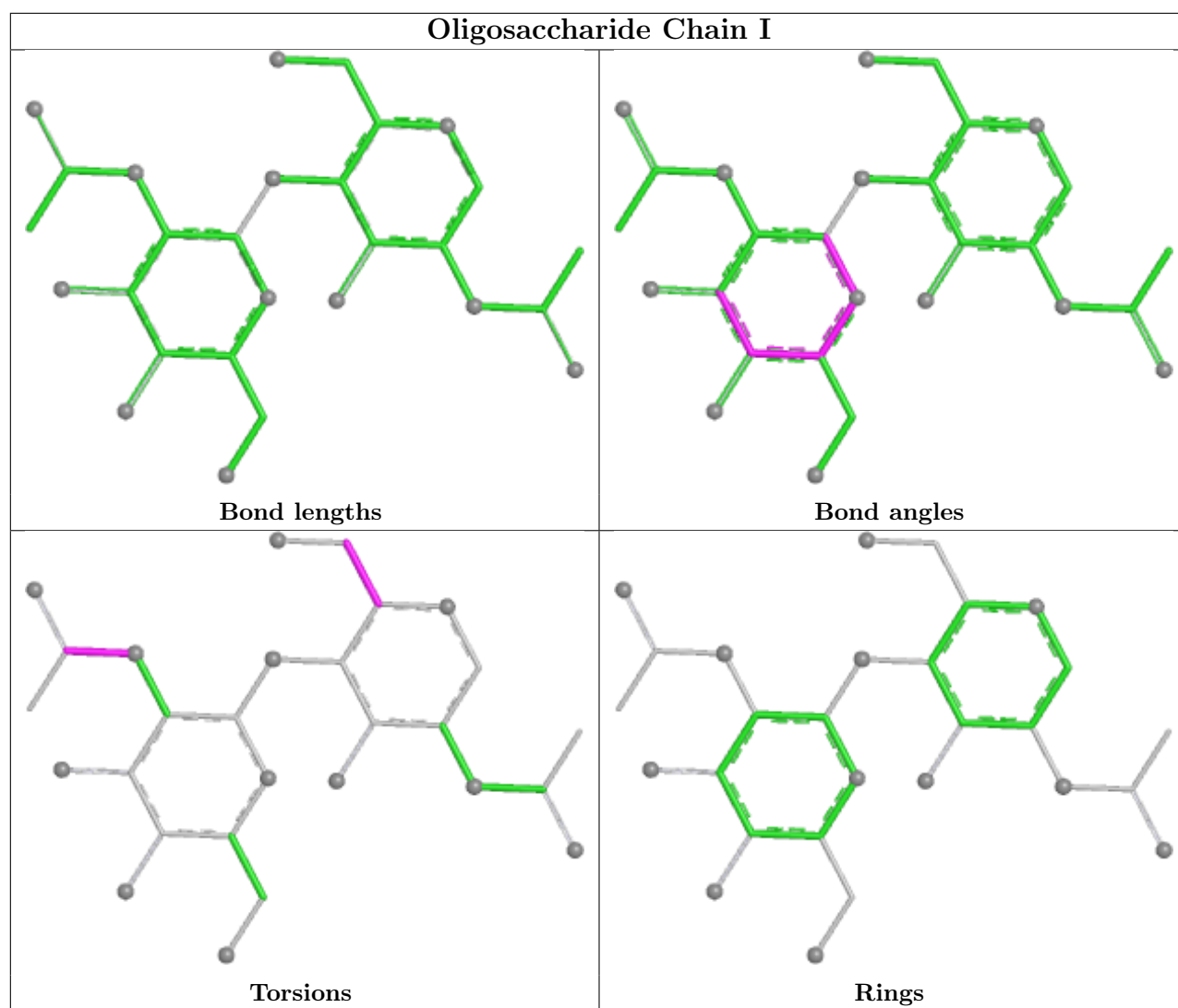
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

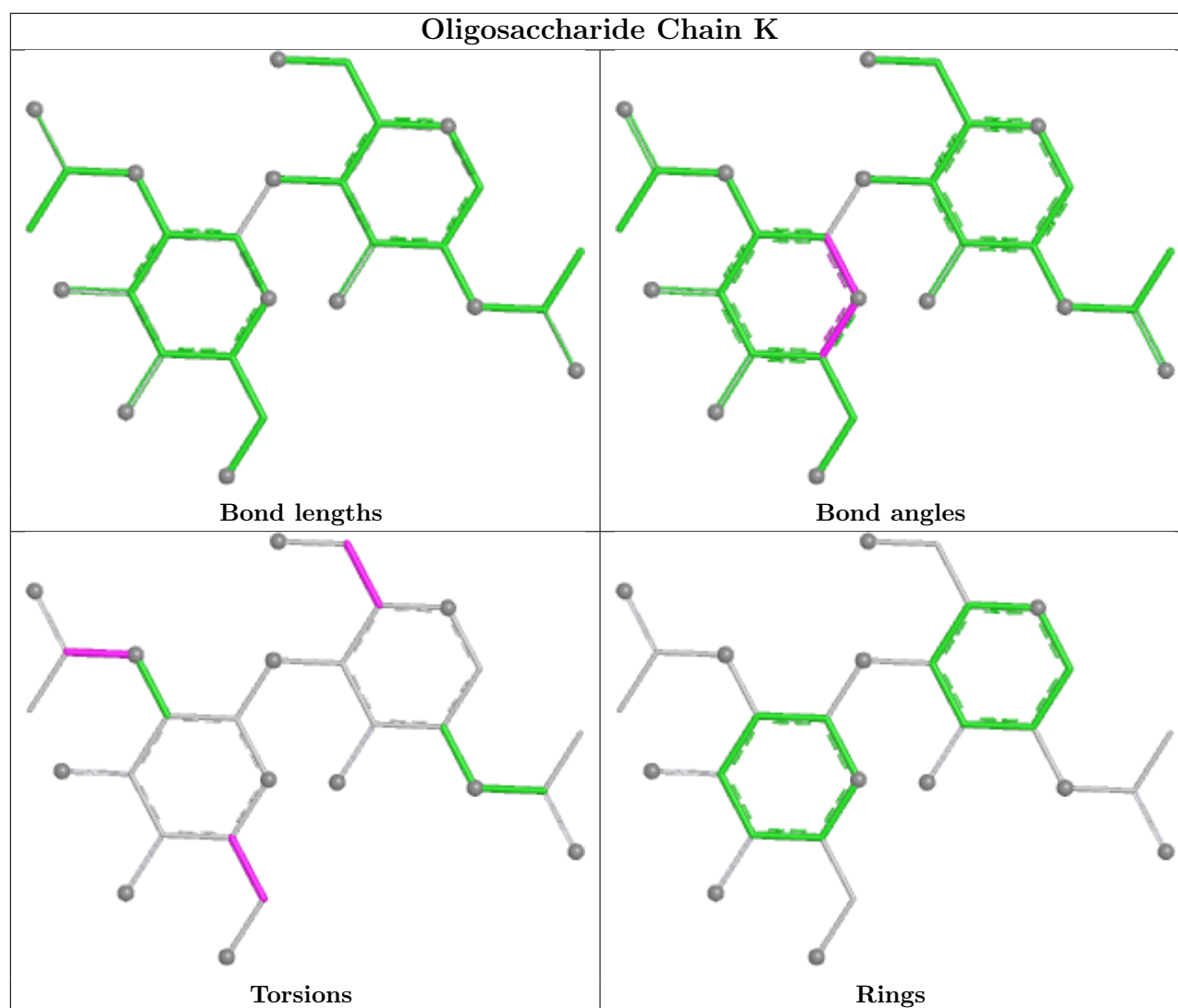




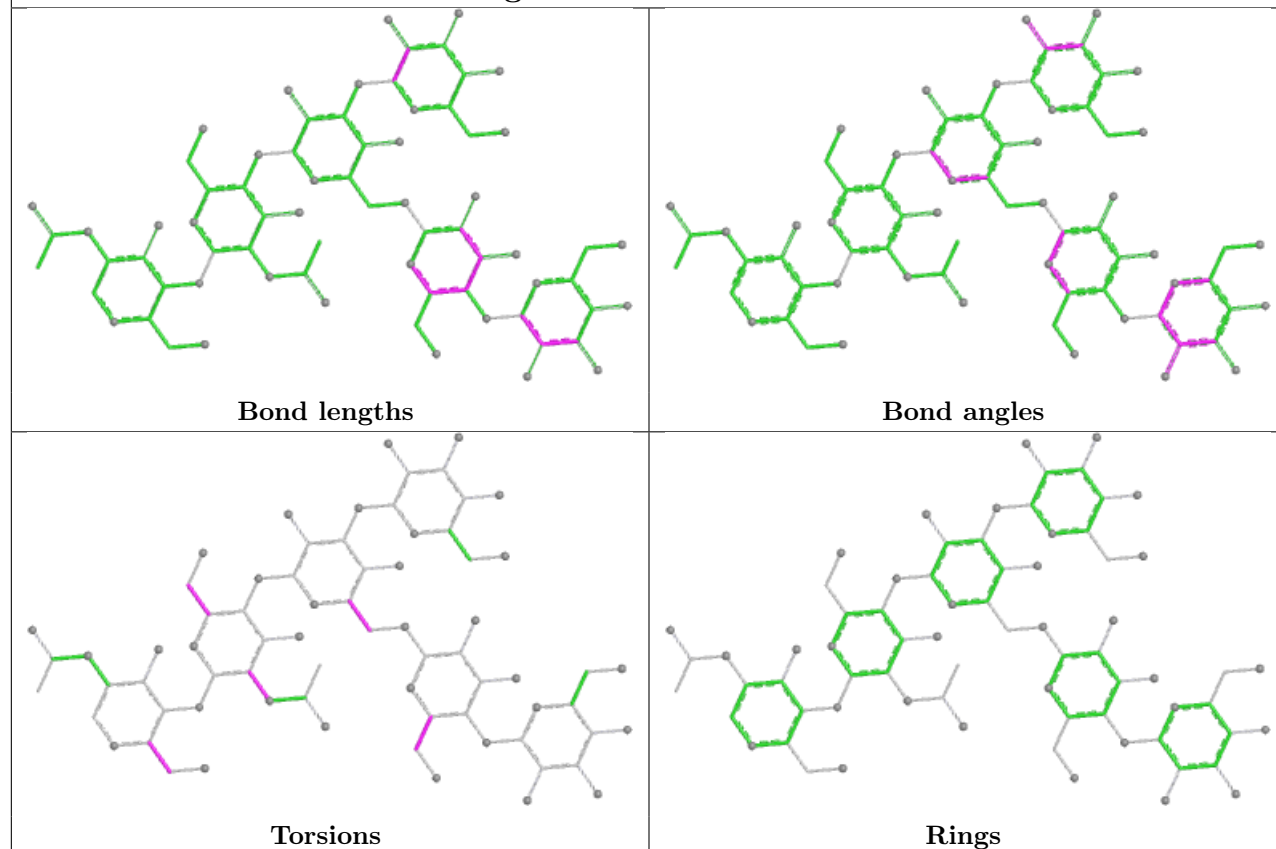




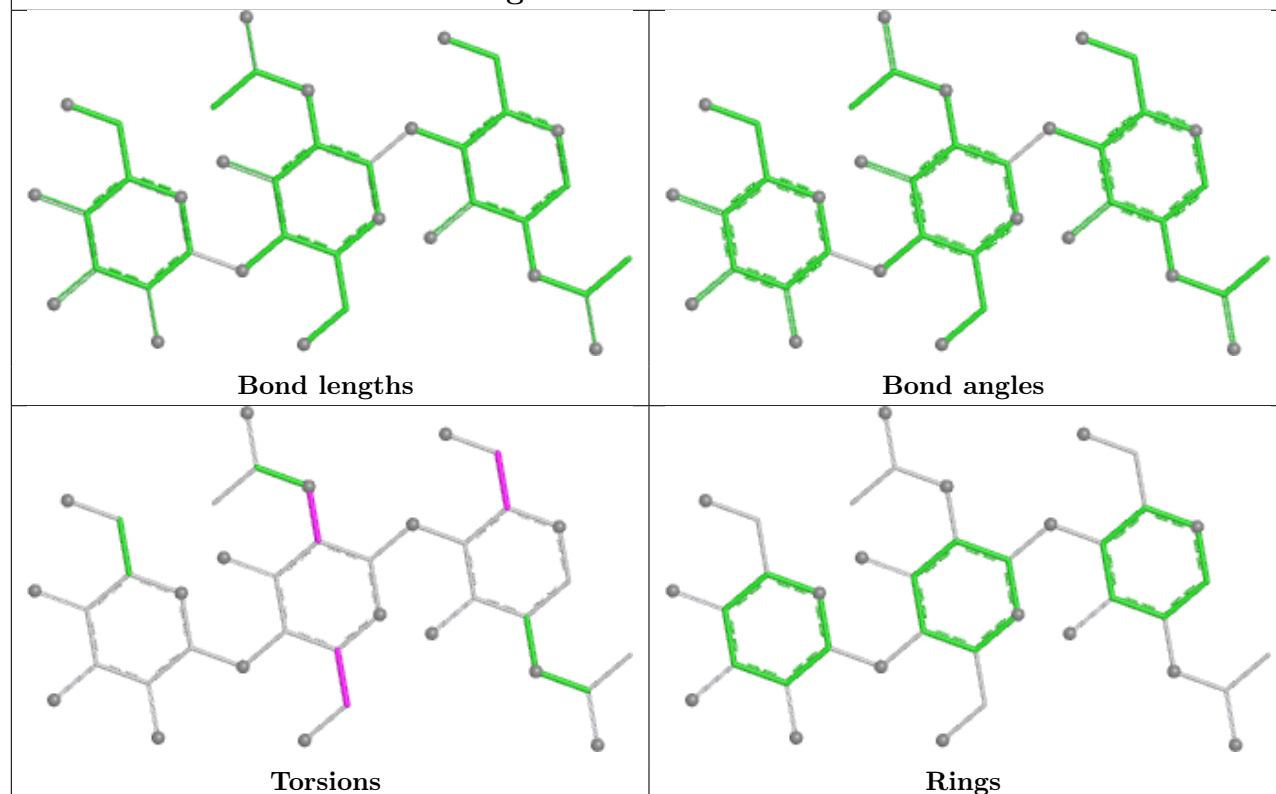


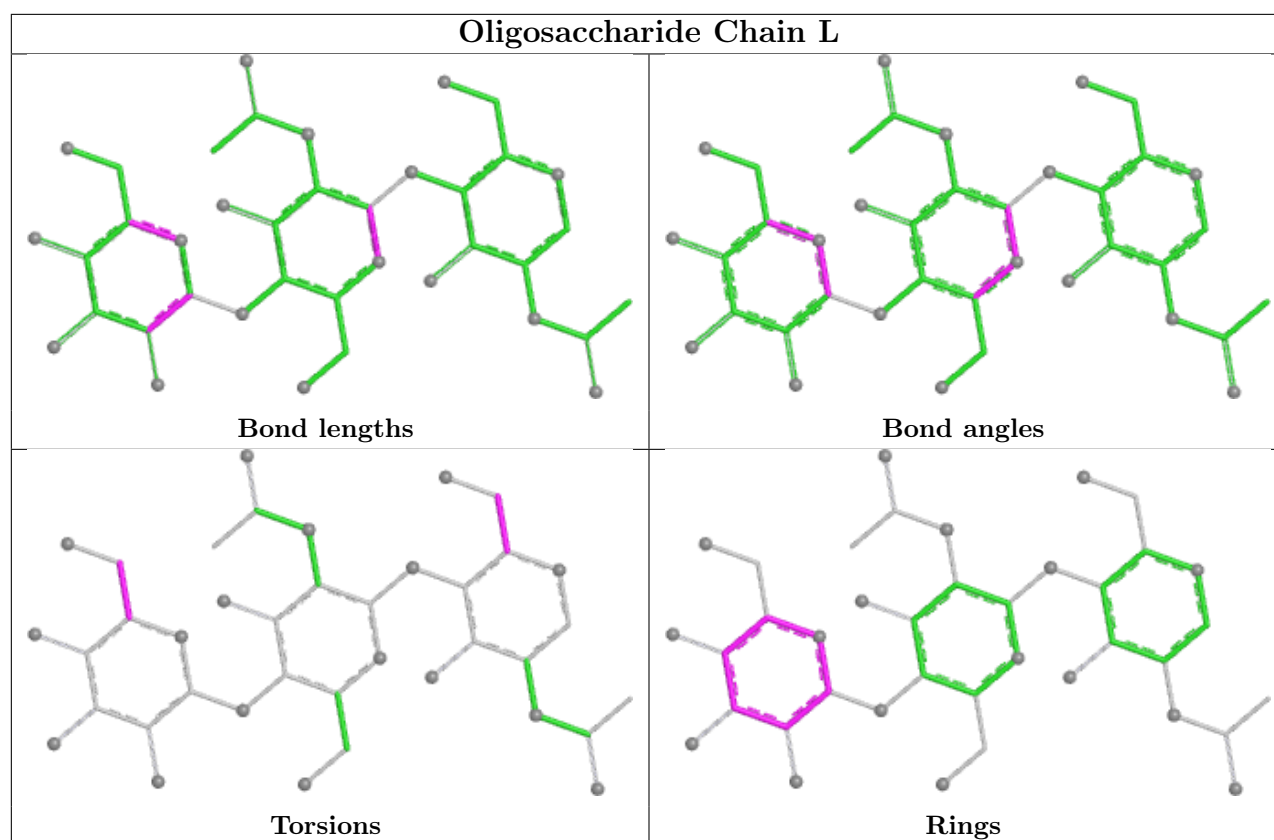


Oligosaccharide Chain F



Oligosaccharide Chain J





5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	$\# Z > 2$
8	NAG	A	1017	1	14,14,15	0.33	0	17,19,21	0.53	0
8	NAG	A	1020	1	14,14,15	0.69	1 (7%)	17,19,21	0.63	0
8	NAG	A	1021	1	14,14,15	0.47	0	17,19,21	0.59	1 (5%)
8	NAG	B	702	2	14,14,15	0.50	0	17,19,21	0.79	1 (5%)
8	NAG	B	701	2	14,14,15	0.85	1 (7%)	17,19,21	0.93	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
8	NAG	A	1017	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1020	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1021	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	2	-	1/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	NAG	O5-C1	2.41	1.47	1.43
8	A	1020	NAG	C1-C2	2.14	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	NAG	C1-O5-C5	3.56	116.96	112.19
8	B	702	NAG	C1-O5-C5	2.73	115.84	112.19
8	A	1021	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1017	NAG	C4-C5-C6-O6
8	A	1017	NAG	O5-C5-C6-O6
8	A	1020	NAG	O5-C5-C6-O6
8	A	1020	NAG	C4-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	A	1021	NAG	C4-C5-C6-O6
8	A	1021	NAG	O5-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	A	1020	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	701	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 [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	924/967 (95%)	-2.07	0 100 100	23, 51, 89, 118	0
2	B	690/695 (99%)	-2.07	0 100 100	23, 58, 113, 131	1 (0%)
3	C	32/32 (100%)	-2.03	0 100 100	35, 79, 97, 100	0
All	All	1646/1694 (97%)	-2.07	0 100 100	23, 54, 105, 131	1 (0%)

There are no RSRZ outliers to report.

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.

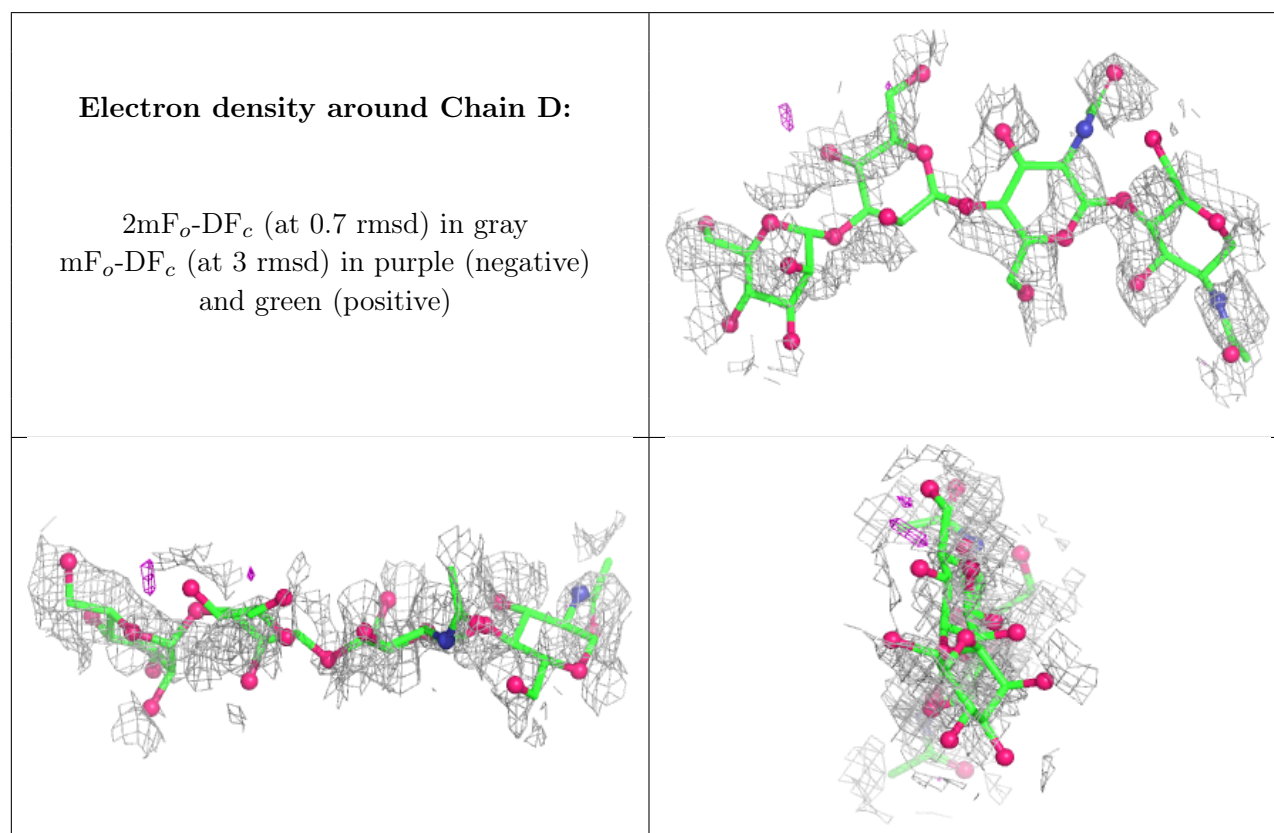
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	4	11/12	0.59	0.02	72,102,123,124	0
6	BMA	F	4	11/12	0.64	0.02	70,84,94,95	0
5	NAG	E	2	14/15	0.65	0.01	68,94,106,109	0
5	NAG	H	1	14/15	0.67	0.01	69,85,105,107	0
7	BMA	L	3	11/12	0.68	0.01	66,81,93,97	0
7	BMA	J	3	11/12	0.71	0.01	87,103,117,125	0
6	MAN	F	6	11/12	0.71	0.01	65,74,90,99	0
5	NAG	I	2	14/15	0.73	0.01	74,100,125,126	0
5	NAG	I	1	14/15	0.73	0.01	69,86,106,106	0
6	MAN	F	5	11/12	0.73	0.01	69,81,90,107	0

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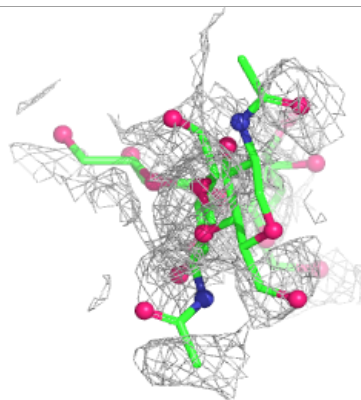
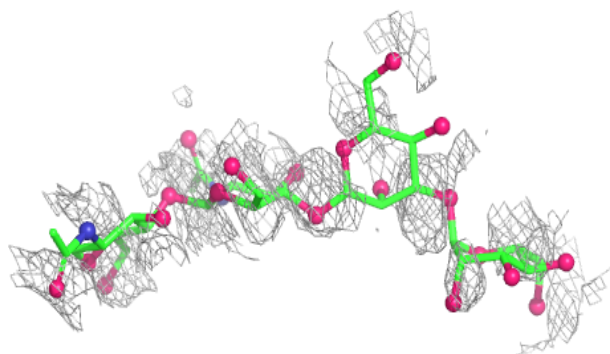
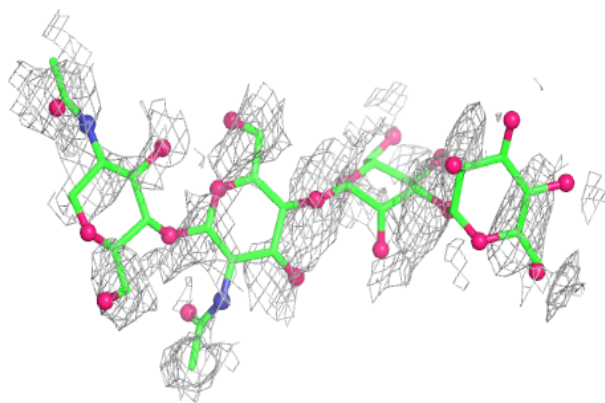
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	J	1	14/15	0.74	0.01	50,67,73,94	0
7	NAG	J	2	14/15	0.74	0.01	62,96,104,109	0
6	BMA	F	3	11/12	0.76	0.01	55,66,85,85	0
4	BMA	D	3	11/12	0.80	0.01	78,94,109,119	0
4	NAG	D	1	14/15	0.81	0.01	31,43,49,53	0
4	NAG	G	2	14/15	0.82	0.01	60,101,117,119	0
4	NAG	G	1	14/15	0.83	0.01	60,68,82,99	0
4	NAG	D	2	14/15	0.83	0.01	52,73,85,90	0
5	NAG	E	1	14/15	0.84	0.01	58,79,86,86	0
4	MAN	G	4	11/12	0.85	0.01	87,97,105,108	0
5	NAG	K	1	14/15	0.85	0.01	75,89,100,104	0
7	NAG	L	1	14/15	0.86	0.01	48,71,80,83	0
4	BMA	G	3	11/12	0.87	0.01	86,102,116,120	0
5	NAG	H	2	14/15	0.87	0.01	66,99,115,116	0
7	NAG	L	2	14/15	0.88	0.01	67,82,93,96	0
6	NAG	F	1	14/15	0.89	0.01	28,39,46,48	0
5	NAG	K	2	14/15	0.91	0.01	62,88,110,115	0
6	NAG	F	2	14/15	0.91	0.01	25,44,71,76	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.



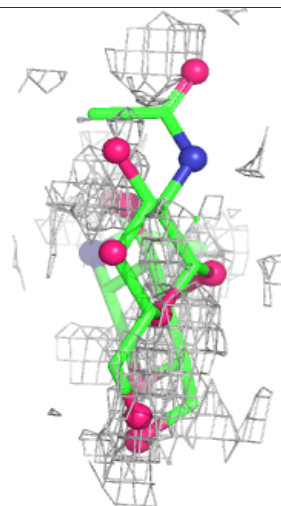
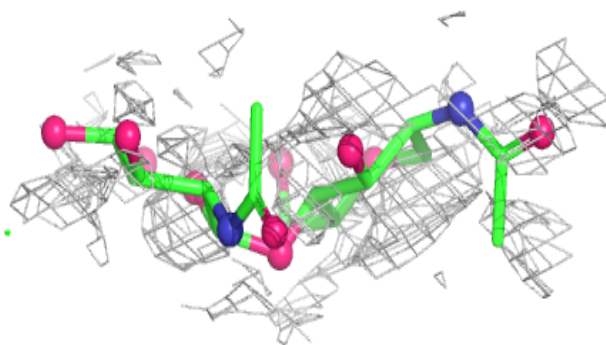
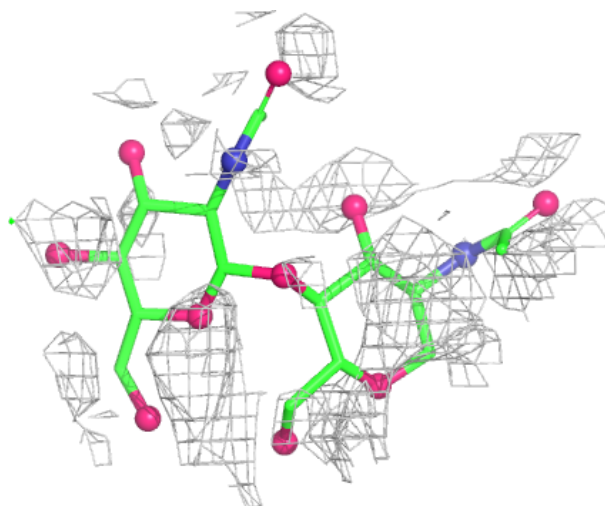
Electron density around Chain G:

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



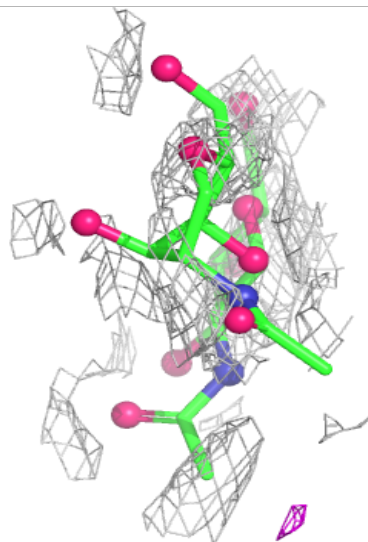
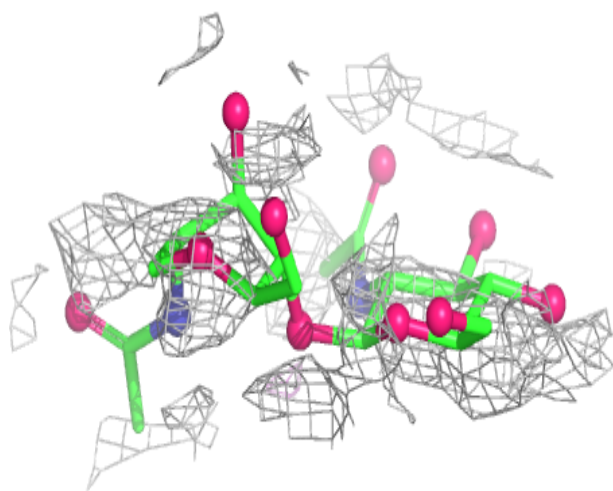
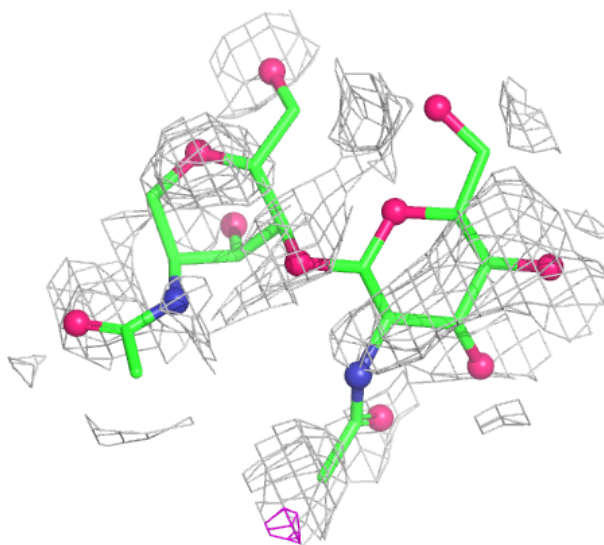
Electron density around Chain E:

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



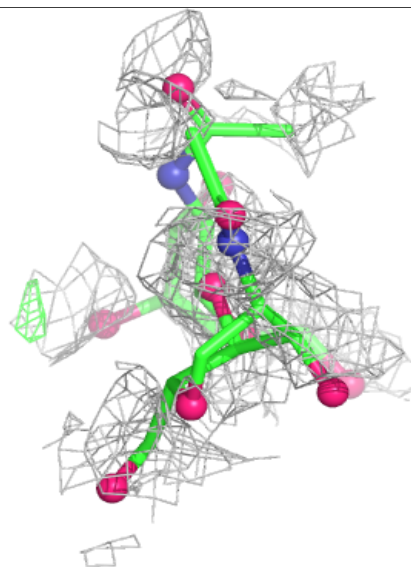
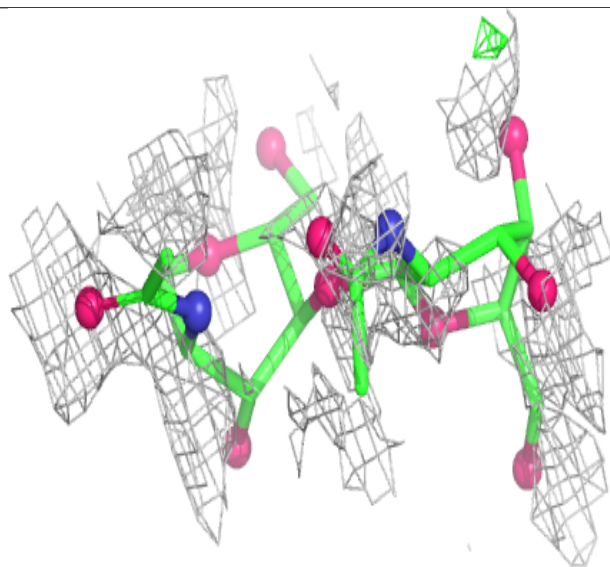
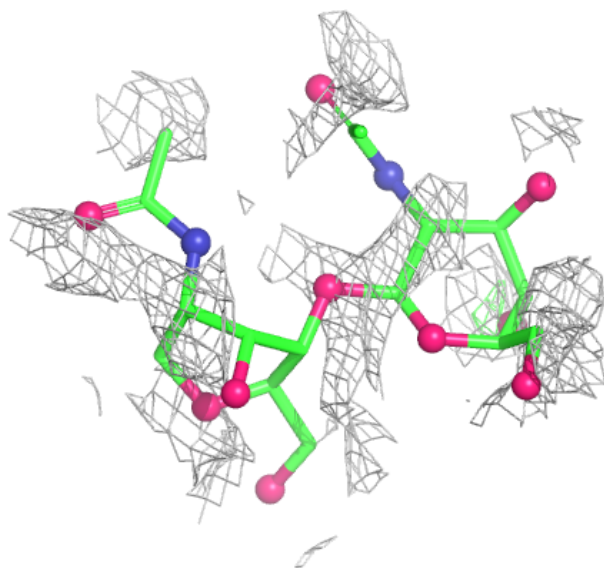
Electron density around Chain H:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



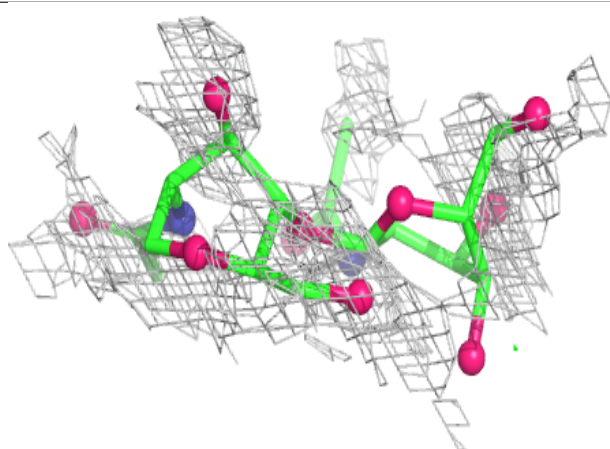
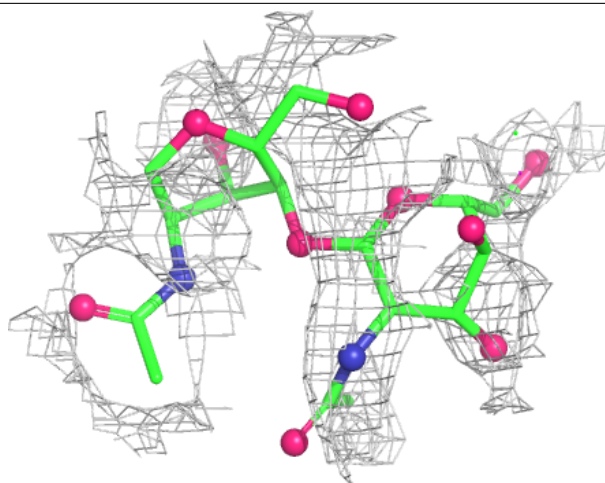
Electron density around Chain I:

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and green (positive)



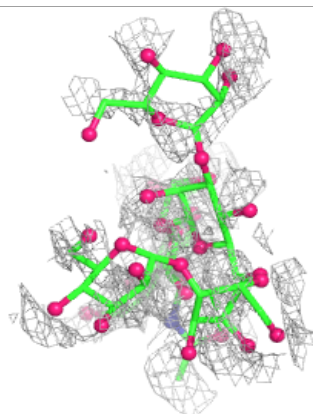
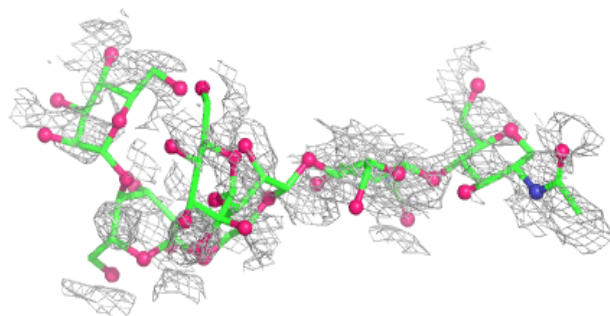
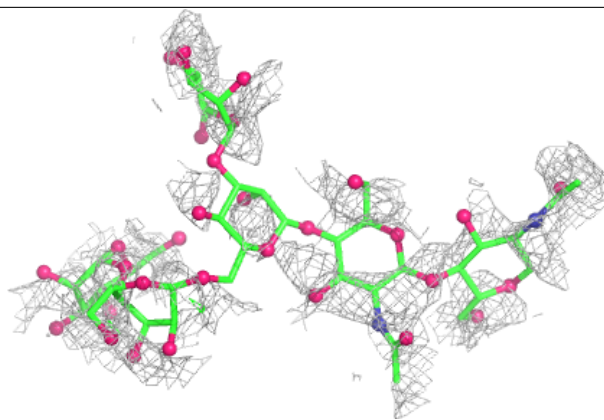
Electron density around Chain K:

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

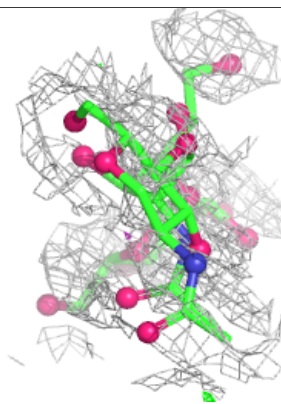
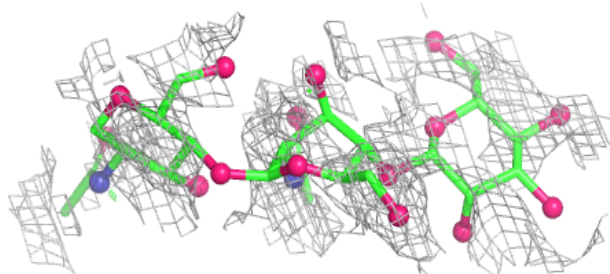
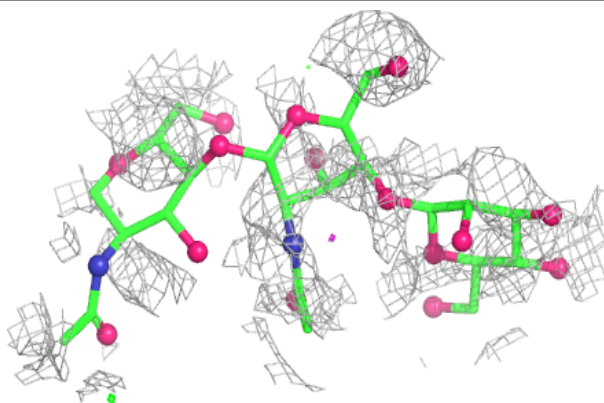


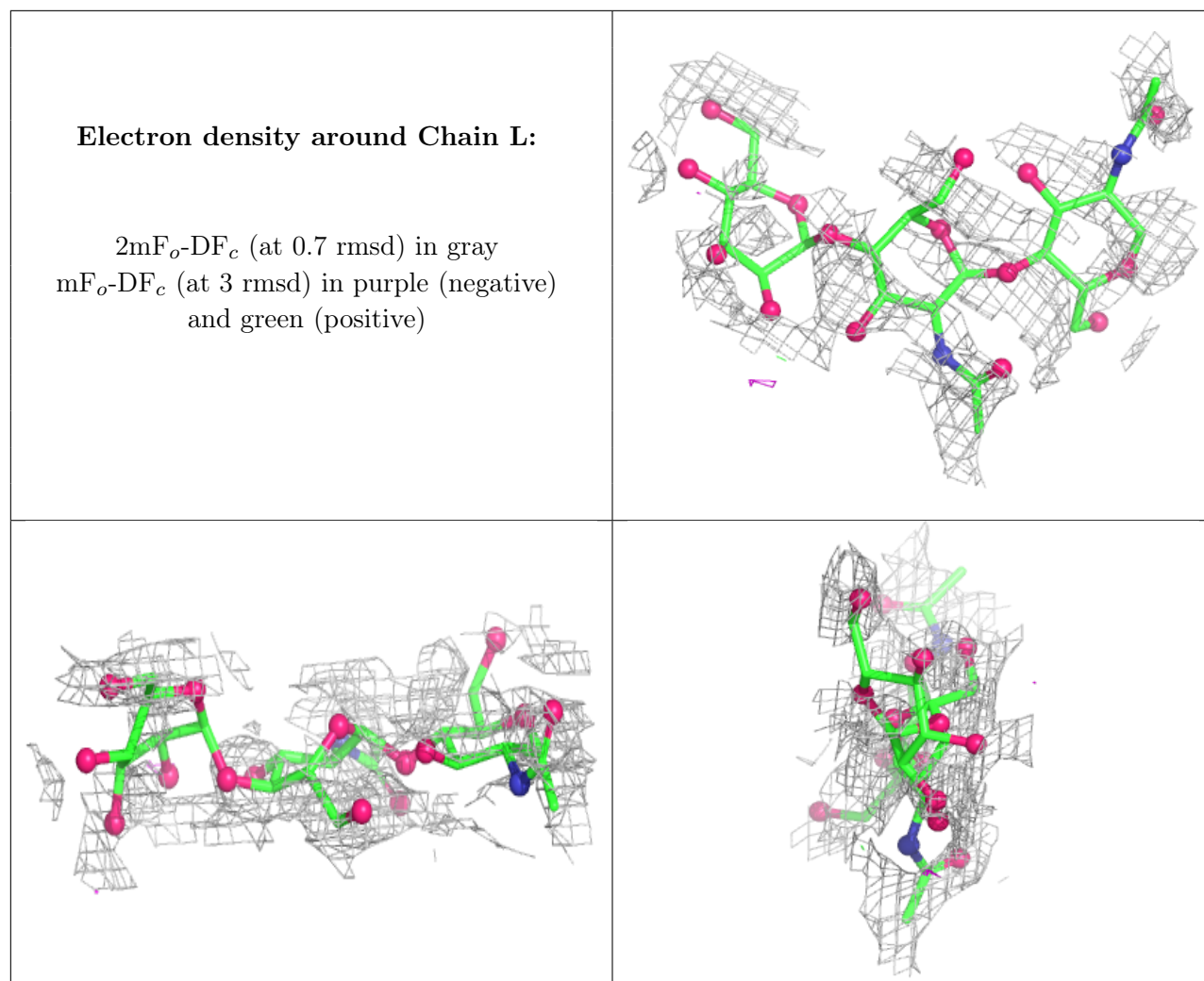
Electron density around Chain F:

$2mF_o-DF_c$ (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)





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($\text{\AA}^2$)	Q<0.9
9	MN	B	708	1/1	0.08	0.02	46,46,46,46	0
9	MN	A	1030	1/1	0.23	0.02	116,116,116,116	0
8	NAG	A	1020	14/15	0.49	0.01	67,106,128,131	0
8	NAG	A	1021	14/15	0.69	0.01	47,63,78,80	0
8	NAG	B	701	14/15	0.69	0.02	66,106,118,119	0
8	NAG	A	1017	14/15	0.78	0.01	75,95,108,108	0
9	MN	B	709	1/1	0.94	0.03	141,141,141,141	0
8	NAG	B	702	14/15	0.95	0.01	51,62,77,78	0
9	MN	A	1029	1/1	0.96	0.02	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MN	B	710	1/1	0.96	0.01	154,154,154,154	0
9	MN	A	1031	1/1	0.98	0.01	85,85,85,85	0
9	MN	A	1027	1/1	0.98	0.01	77,77,77,77	0
9	MN	A	1028	1/1	1.00	0.04	89,89,89,89	0
10	CL	C	101	1/1	-	0.02	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.