



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:11 AM UTC

PDB ID : 6WIX / pdb_00006wix
Title : Crystal Structure of HIV-1 MI369 RnS-DS.SOSIP Prefusion Env Trimer in Complex with Human Antibodies 3H109L and 35O22 at 3.5 Angstrom
Authors : Lai, Y.-T.; Olia, A.; Kwong, P.D.
Deposited on : 2020-04-10
Resolution : 2.67 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

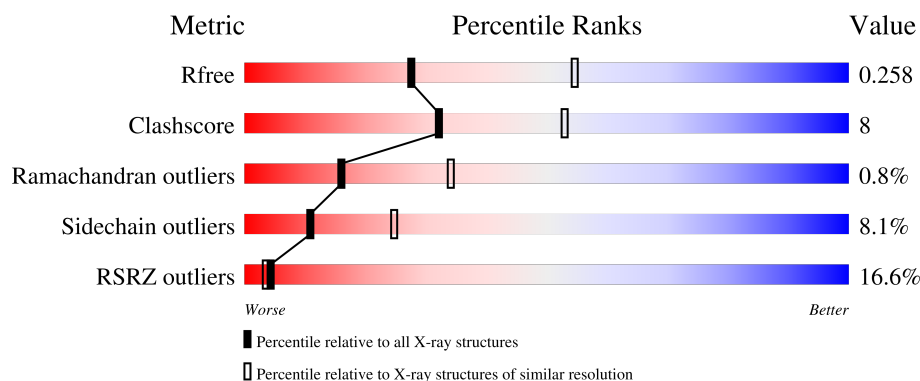
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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.



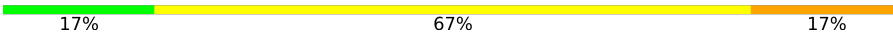
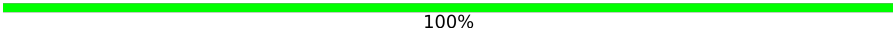
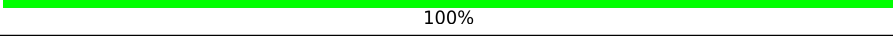
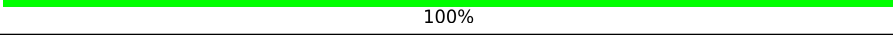
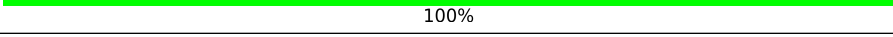
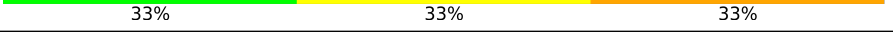
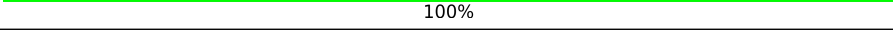
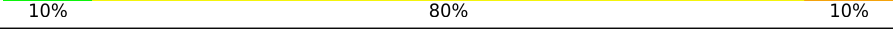
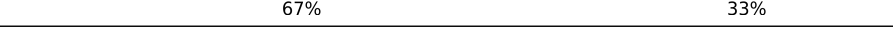
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	B	153	9% 58% 18% • 22%
2	D	134	41% 69% 23% • •
3	E	114	32% 68% 22% • 8%
4	G	498	6% 64% 19% • 15%
5	H	244	20% 69% 20% • 7%

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Mol	Chain	Length	Quality of chain
6	L	217	
7	A	6	
8	C	2	
8	F	2	
8	J	2	
8	M	2	
8	P	2	
9	I	3	
9	O	3	
10	K	10	
11	N	3	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9952 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	120	Total	C	N	O	S	0	0	0
			967	623	162	177	5			

- Molecule 2 is a protein called 35O22 scFv heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	128	Total	C	N	O	S	0	0	0
			994	628	169	192	5			

- Molecule 3 is a protein called 35O22 scFv light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	105	Total	C	N	O	S	0	0	0
			805	506	133	160	6			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	425	Total	C	N	O	S	0	0	0
			3363	2118	601	616	28			

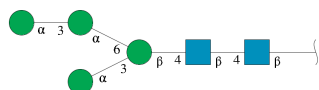
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1715	1093	278	338	6			

- Molecule 6 is a protein called 3H109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1604	1009	276	312	7			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(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.



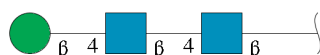
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



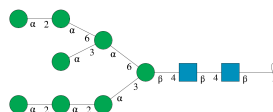
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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.



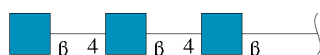
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



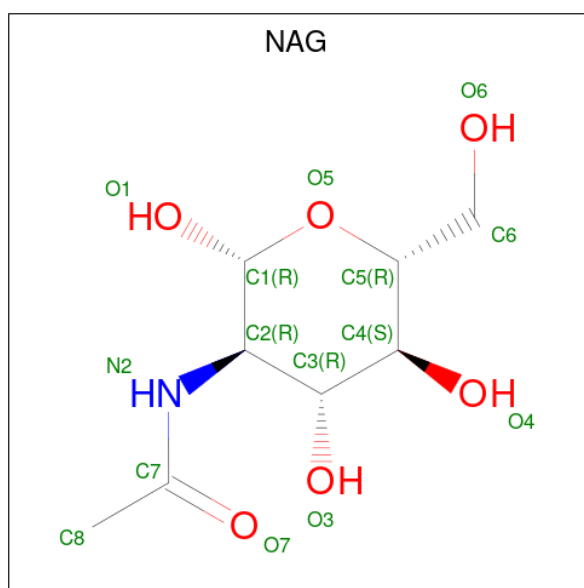
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 11 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
11	N	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

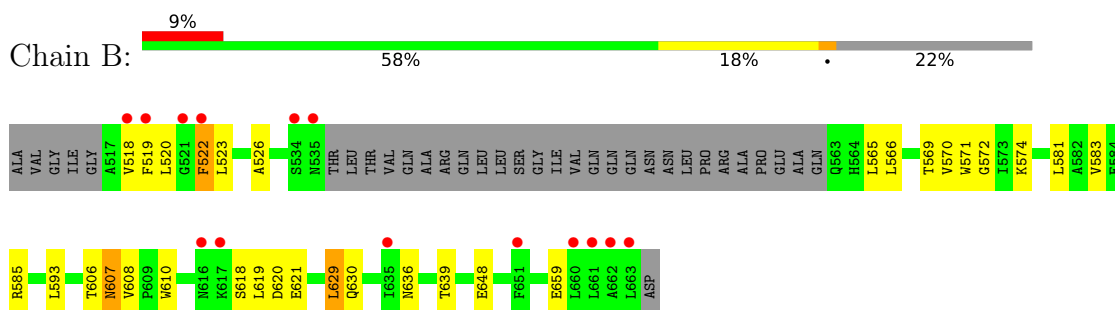


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	G	1	Total	C	N	O	0	0
			14	8	1	5		

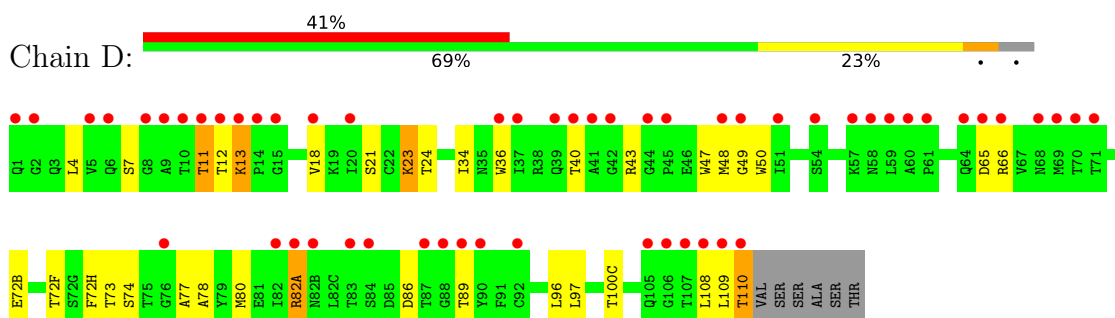
3 Residue-property plots [i](#)

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

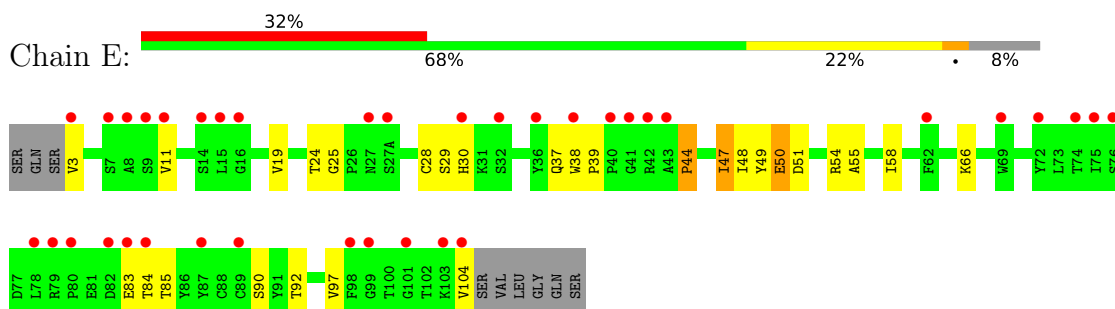
- Molecule 1: Envelope glycoprotein gp41



- Molecule 2: 35O22 scFv heavy chain

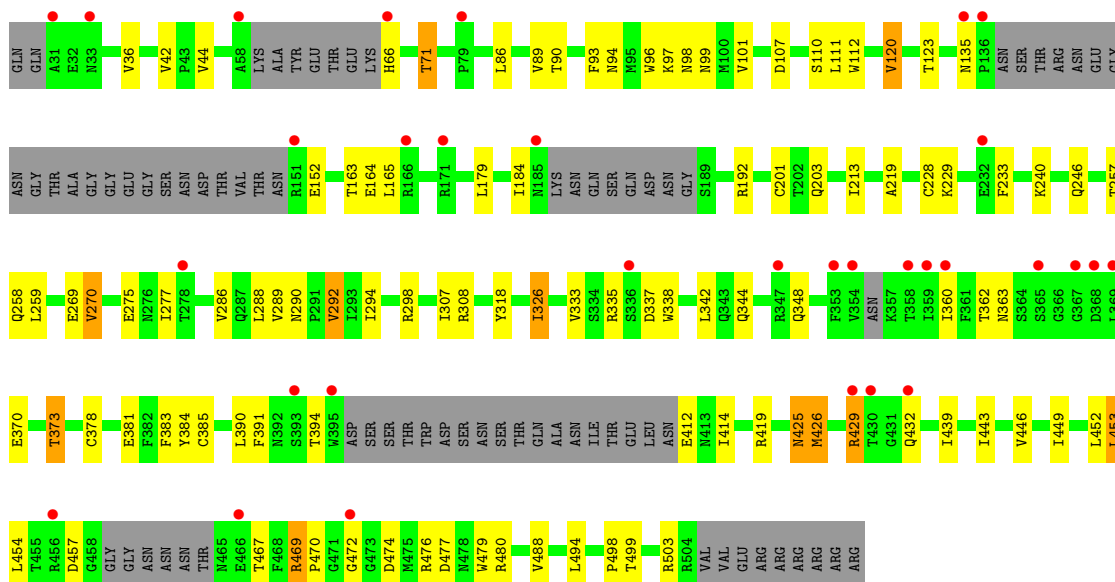


- Molecule 3: 35O22 scFv light chain

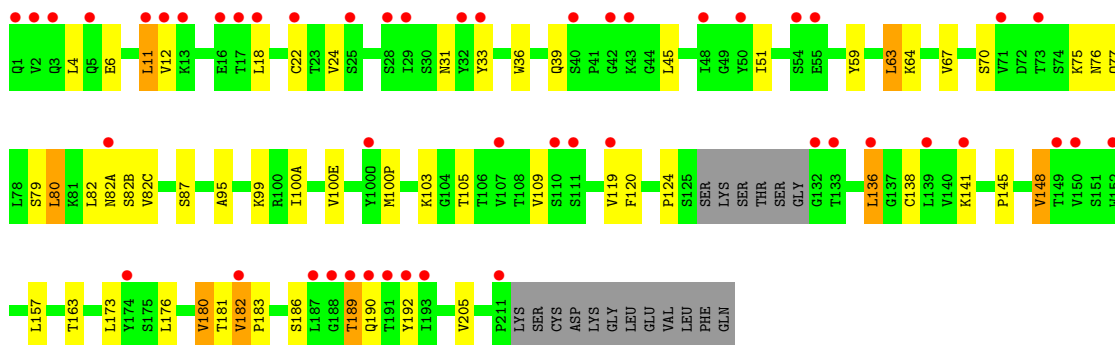


- Molecule 4: Envelope glycoprotein gp120

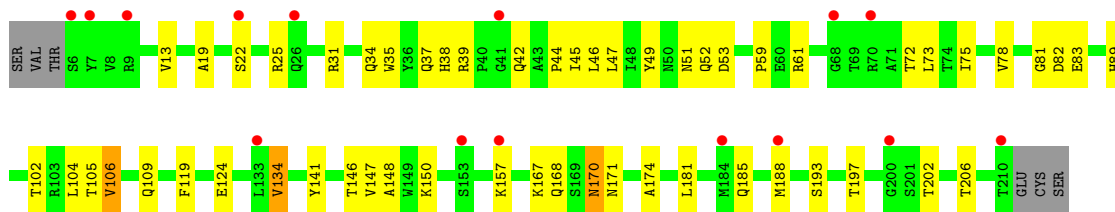




• Molecule 5: 3H109L Fab heavy chain

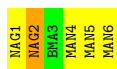


• Molecule 6: 3H109L Fab light chain



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(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





- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

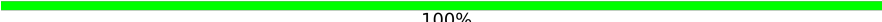


- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%

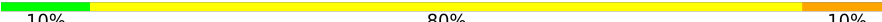


- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
EMA3

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  10% 80% 10%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

- Molecule 11: 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 N:  67% 33%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.86Å 131.86Å 316.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.39 – 2.67 42.39 – 2.67	Depositor EDS
% Data completeness (in resolution range)	39.4 (42.39-2.67) 39.4 (42.39-2.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.270 (Not available) , 0.258	Depositor DCC
R_{free} test set	1724 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.072 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9952	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: BMA, NAG, MAN

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	B	0.44	0/987	0.49	1/1340 (0.1%)
2	D	0.08	0/1021	0.27	0/1390
3	E	0.10	0/829	0.32	0/1133
4	G	0.10	0/3434	0.30	0/4658
5	H	0.11	0/1758	0.30	0/2397
6	L	0.09	0/1647	0.28	0/2247
All	All	0.17	0/9676	0.32	1/13165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	522	PHE	N-CA-C	-8.09	102.46	111.28

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	B	967	0	954	13	0
2	D	994	0	953	21	0
3	E	805	0	752	13	0
4	G	3363	0	3308	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1715	0	1687	26	0
6	L	1604	0	1553	30	0
7	A	72	0	61	3	0
8	C	28	0	25	0	0
8	F	28	0	25	0	0
8	J	28	0	25	0	0
8	M	28	0	25	0	0
8	P	28	0	25	0	0
9	I	39	0	34	2	0
9	O	39	0	34	0	0
10	K	116	0	97	2	0
11	N	42	0	37	1	0
12	G	56	0	52	0	0
All	All	9952	0	9647	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (156) 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)
6:L:37:GLN:HE21	6:L:45:ILE:HD11	1.53	0.74
6:L:61:ARG:NH1	6:L:82:ASP:OD2	2.23	0.71
4:G:270:VAL:HG23	4:G:348:GLN:HG3	1.72	0.69
4:G:270:VAL:HG12	4:G:288:LEU:HA	1.76	0.68
4:G:360:ILE:HG23	4:G:394:THR:HG22	1.76	0.68
5:H:24:VAL:HB	5:H:76:ASN:HB3	1.77	0.66
4:G:429:ARG:HH21	4:G:432:GLN:HG2	1.60	0.66
1:B:569:THR:HG23	1:B:572:GLY:H	1.60	0.65
4:G:90:THR:HG22	4:G:240:LYS:HA	1.79	0.64
4:G:474:ASP:OD2	4:G:476:ARG:NH1	2.30	0.64
4:G:219:ALA:O	4:G:246:GLN:NE2	2.32	0.62
4:G:286:VAL:HB	4:G:452:LEU:HB2	1.82	0.62
6:L:39:ARG:NH2	6:L:81:GLY:O	2.30	0.62
4:G:360:ILE:HB	4:G:467:THR:HG22	1.81	0.62
4:G:101:VAL:HG21	4:G:480:ARG:HG2	1.80	0.61
6:L:52:GLN:NE2	6:L:53:ASP:OD1	2.33	0.61
6:L:34:GLN:HB2	6:L:89:HIS:HB3	1.82	0.61
3:E:28:CYS:HB3	3:E:66:LYS:HE2	1.83	0.60
2:D:40:THR:HB	2:D:43:ARG:HB2	1.83	0.59
6:L:34:GLN:NE2	6:L:49:TYR:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2:NAG:H3	7:A:2:NAG:H83	1.84	0.59
1:B:574:LYS:NZ	4:G:107:ASP:OD2	2.33	0.58
5:H:59:TYR:HB2	5:H:64:LYS:HD2	1.84	0.58
3:E:83:GLU:HA	3:E:104:VAL:HG23	1.86	0.57
1:B:522:PHE:N	1:B:522:PHE:CD1	2.73	0.56
10:K:1:NAG:H83	10:K:1:NAG:H3	1.87	0.56
2:D:96:LEU:HG	2:D:97:LEU:HG	1.87	0.55
4:G:270:VAL:HG13	4:G:289:VAL:HG12	1.87	0.55
2:D:36:TRP:HB3	2:D:48:MET:HE3	1.89	0.55
4:G:257:THR:O	4:G:259:LEU:N	2.39	0.55
6:L:119:PHE:HB2	6:L:134:VAL:HG13	1.90	0.54
6:L:13:VAL:HG22	6:L:104:LEU:HD11	1.89	0.54
6:L:150:LYS:HB2	6:L:193:SER:HB2	1.89	0.54
4:G:370:GLU:HG3	4:G:384:TYR:HE2	1.72	0.53
4:G:298:ARG:NH1	4:G:381:GLU:OE2	2.42	0.53
6:L:185:GLN:HA	6:L:188:MET:HG2	1.90	0.53
1:B:523:LEU:O	4:G:86:LEU:HD22	2.08	0.53
2:D:72(B):GLU:HB2	2:D:74:SER:HB3	1.90	0.53
2:D:7:SER:HB3	2:D:21:SER:H	1.73	0.53
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.90	0.53
2:D:11:THR:HB	2:D:110:THR:HA	1.89	0.52
9:I:1:NAG:H61	9:I:2:NAG:N2	2.24	0.52
2:D:89:THR:HG22	2:D:108:LEU:HG	1.90	0.52
5:H:70:SER:HB2	5:H:79:SER:HB3	1.91	0.52
4:G:259:LEU:HD23	4:G:452:LEU:HD21	1.92	0.52
6:L:83:GLU:HG3	6:L:105:THR:HA	1.90	0.52
2:D:18:VAL:HG11	2:D:109:LEU:HD11	1.92	0.52
1:B:629:LEU:HD23	4:G:44:VAL:HG23	1.92	0.52
4:G:335:ARG:HD2	4:G:412:GLU:HG3	1.93	0.51
2:D:72(F):THR:HG22	2:D:73:THR:HB	1.91	0.50
5:H:189:THR:OG1	5:H:190:GLN:N	2.42	0.50
4:G:335:ARG:C	4:G:337:ASP:H	2.19	0.50
4:G:163:THR:HG23	4:G:165:LEU:H	1.77	0.50
3:E:54:ARG:HH11	3:E:58:ILE:HG22	1.77	0.50
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.94	0.50
5:H:63:LEU:HD13	5:H:67:VAL:HG21	1.94	0.49
4:G:96:TRP:CG	4:G:275:GLU:HG2	2.48	0.49
1:B:618:SER:HB3	1:B:621:GLU:HG3	1.94	0.49
5:H:163:THR:HG23	5:H:176:LEU:HD21	1.95	0.49
4:G:373:THR:OG1	4:G:385:CYS:O	2.30	0.48
9:I:1:NAG:H61	9:I:2:NAG:HN2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:71:THR:OG1	4:G:213:ILE:HD11	2.13	0.48
5:H:124:PRO:HB3	5:H:136:LEU:HB3	1.94	0.48
2:D:23:LYS:HA	2:D:77:ALA:HA	1.96	0.48
4:G:453:LEU:HB2	4:G:472:GLY:HA2	1.95	0.48
5:H:39:GLN:HB2	5:H:45:LEU:HD23	1.95	0.48
1:B:607:ASN:ND2	4:G:503:ARG:O	2.46	0.48
2:D:66:ARG:NH2	2:D:86:ASP:OD2	2.46	0.48
6:L:38:HIS:CD2	6:L:44:PRO:HG3	2.49	0.48
10:K:1:NAG:O6	11:N:1:NAG:O7	2.28	0.48
4:G:425:ASN:N	4:G:425:ASN:OD1	2.46	0.47
6:L:146:THR:HB	6:L:197:THR:HB	1.96	0.47
4:G:457:ASP:OD2	4:G:469:ARG:NH1	2.48	0.47
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.33	0.47
5:H:11:LEU:HG	5:H:145:PRO:HG3	1.97	0.47
2:D:72(F):THR:HG23	2:D:72(H):PHE:H	1.79	0.47
4:G:98:ASN:OD1	4:G:99:ASN:N	2.47	0.47
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.47	0.46
3:E:90:SER:HB3	3:E:97:VAL:HB	1.97	0.46
4:G:381:GLU:HG3	4:G:439:ILE:HD13	1.97	0.46
5:H:6:GLU:HG3	5:H:22:CYS:SG	2.56	0.46
4:G:292:VAL:HG22	4:G:449:ILE:HB	1.98	0.46
5:H:182:VAL:HG22	5:H:183:PRO:HD2	1.97	0.46
3:E:28:CYS:C	3:E:30:HIS:H	2.24	0.46
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.51	0.45
5:H:22:CYS:O	5:H:77:GLN:HA	2.17	0.45
5:H:157:LEU:HD21	5:H:180:VAL:HG21	1.98	0.45
6:L:148:ALA:HA	6:L:157:LYS:NZ	2.31	0.45
4:G:307:ILE:HG22	4:G:308:ARG:H	1.81	0.45
6:L:124:GLU:OE1	6:L:124:GLU:N	2.35	0.45
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.77	0.45
4:G:120:VAL:HG13	4:G:203:GLN:HG2	1.98	0.45
4:G:135:ASN:OD1	4:G:326:ILE:HD12	2.16	0.45
4:G:94:ASN:ND2	4:G:97:LYS:HB2	2.32	0.45
4:G:362:THR:OG1	4:G:363:ASN:N	2.49	0.45
6:L:168:GLN:NE2	6:L:170:ASN:OD1	2.50	0.44
5:H:36:TRP:CG	5:H:80:LEU:HD13	2.53	0.44
5:H:87:SER:HB3	5:H:109:VAL:HG23	1.99	0.44
6:L:168:GLN:OE1	6:L:174:ALA:HB2	2.17	0.44
5:H:148:VAL:HG12	5:H:176:LEU:HD13	1.99	0.44
6:L:19:ALA:HB3	6:L:75:ILE:HB	2.00	0.44
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:99:LYS:HE2	5:H:100(A):ILE:HD11	2.00	0.44
1:B:526:ALA:HB3	4:G:89:VAL:HG21	2.00	0.43
4:G:42:VAL:HG23	4:G:44:VAL:HG12	2.00	0.43
2:D:66:ARG:O	2:D:82(A):ARG:N	2.50	0.43
3:E:54:ARG:NH1	3:E:58:ILE:O	2.51	0.43
5:H:6:GLU:N	5:H:6:GLU:OE1	2.49	0.43
5:H:12:VAL:HG21	5:H:18:LEU:HD12	2.00	0.43
6:L:109:GLN:HB2	6:L:141:TYR:CE1	2.54	0.43
6:L:46:LEU:HD21	6:L:49:TYR:HB3	2.00	0.43
1:B:630:GLN:HB3	2:D:72(H):PHE:CZ	2.54	0.43
2:D:4:LEU:HG	2:D:24:THR:HG22	2.01	0.43
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.53	0.43
4:G:93:PHE:HB2	4:G:233:PHE:HZ	1.84	0.43
1:B:570:VAL:HG11	4:G:110:SER:HB3	2.00	0.42
4:G:294:ILE:HD12	4:G:449:ILE:HD11	2.01	0.42
5:H:120:PHE:HE2	5:H:141:LYS:HD3	1.84	0.42
5:H:100(A):ILE:HD13	5:H:100(E):VAL:HG22	1.99	0.42
6:L:31:ARG:NH1	6:L:51:ASN:OD1	2.52	0.42
4:G:112:TRP:CZ3	4:G:426:MET:HE2	2.54	0.42
4:G:179:LEU:HD12	4:G:179:LEU:H	1.84	0.42
4:G:391:PHE:CD1	4:G:470:PRO:HG3	2.55	0.42
3:E:38:TRP:CE2	3:E:44:PRO:HG3	2.54	0.42
4:G:439:ILE:HB	4:G:443:ILE:HD11	2.00	0.42
6:L:59:PRO:HB2	6:L:61:ARG:HG2	2.01	0.42
1:B:606:THR:OG1	4:G:36:VAL:O	2.25	0.42
3:E:47:ILE:HG23	3:E:48:ILE:HG12	2.02	0.42
4:G:203:GLN:HE22	4:G:318:TYR:HD2	1.68	0.42
2:D:36:TRP:CH2	2:D:78:ALA:HB1	2.55	0.42
3:E:51:ASP:CG	3:E:66:LYS:HD3	2.45	0.42
4:G:333:VAL:HG11	4:G:390:LEU:HD21	2.02	0.42
5:H:95:ALA:HA	5:H:100(P):MET:HG3	2.02	0.42
5:H:33:TYR:HB2	5:H:95:ALA:O	2.19	0.42
6:L:39:ARG:HB2	6:L:42:GLN:HB3	2.02	0.42
2:D:13:LYS:HD2	2:D:13:LYS:HA	1.70	0.41
4:G:93:PHE:CE1	4:G:228:CYS:HB2	2.55	0.41
2:D:100(C):THR:HG21	7:A:2:NAG:H3	2.02	0.41
6:L:78:VAL:HG13	6:L:82:ASP:HB2	2.01	0.41
3:E:49:TYR:CD2	3:E:50:GLU:HG2	2.55	0.41
6:L:167:LYS:HE2	6:L:171:ASN:HA	2.01	0.41
3:E:24:THR:OG1	3:E:25:GLY:N	2.54	0.41
2:D:80:MET:HE3	2:D:80:MET:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1:NAG:H61	7:A:2:NAG:H82	2.02	0.41
4:G:338:TRP:O	4:G:342:LEU:HB2	2.20	0.41
6:L:22:SER:HA	6:L:72:THR:HG22	2.03	0.41
1:B:571:TRP:CZ2	4:G:111:LEU:HD11	2.56	0.41
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.56	0.41
4:G:184:ILE:HD11	4:G:192:ARG:HB2	2.02	0.41
6:L:35:TRP:CD2	6:L:73:LEU:HB2	2.56	0.41
3:E:39:PRO:HG3	3:E:84:THR:HG21	2.02	0.41
5:H:103:LYS:HD2	5:H:103:LYS:N	2.36	0.40
5:H:186:SER:O	5:H:186:SER:OG	2.39	0.40
3:E:55:ALA:HB3	3:E:58:ILE:HD13	2.03	0.40
6:L:106:VAL:HG13	6:L:109:GLN:NE2	2.36	0.40
5:H:182:VAL:HG11	5:H:192:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	116/153 (76%)	108 (93%)	6 (5%)	2 (2%)	7	17
2	D	126/134 (94%)	113 (90%)	12 (10%)	1 (1%)	16	34
3	E	103/114 (90%)	81 (79%)	19 (18%)	3 (3%)	3	8
4	G	411/498 (82%)	377 (92%)	31 (8%)	3 (1%)	18	37
5	H	222/244 (91%)	198 (89%)	24 (11%)	0	100	100
6	L	209/217 (96%)	195 (93%)	14 (7%)	0	100	100
All	All	1187/1360 (87%)	1072 (90%)	106 (9%)	9 (1%)	16	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	VAL
1	B	565	LEU
3	E	29	SER
3	E	50	GLU
4	G	269	GLU
4	G	426	MET
4	G	258	GLN
2	D	82(A)	ARG
3	E	44	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	B	104/130 (80%)	88 (85%)	16 (15%)	2	6
2	D	107/112 (96%)	100 (94%)	7 (6%)	15	34
3	E	92/100 (92%)	85 (92%)	7 (8%)	12	27
4	G	382/445 (86%)	357 (94%)	25 (6%)	15	34
5	H	196/212 (92%)	174 (89%)	22 (11%)	6	13
6	L	175/181 (97%)	166 (95%)	9 (5%)	21	44
All	All	1056/1180 (90%)	970 (92%)	86 (8%)	11	25

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	PHE
1	B	520	LEU
1	B	566	LEU
1	B	581	LEU
1	B	583	VAL
1	B	585	ARG
1	B	593	LEU
1	B	607	ASN
1	B	608	VAL
1	B	619	LEU

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Mol	Chain	Res	Type
1	B	620	ASP
1	B	629	LEU
1	B	636	ASN
1	B	639	THR
1	B	648	GLU
1	B	659	GLU
2	D	11	THR
2	D	12	THR
2	D	13	LYS
2	D	23	LYS
2	D	34	ILE
2	D	65	ASP
2	D	110	THR
3	E	3	VAL
3	E	11	VAL
3	E	19	VAL
3	E	37	GLN
3	E	47	ILE
3	E	85	THR
3	E	92	THR
4	G	66	HIS
4	G	71	THR
4	G	120	VAL
4	G	123	THR
4	G	152	GLU
4	G	164	GLU
4	G	201	CYS
4	G	229	LYS
4	G	270	VAL
4	G	277	ILE
4	G	290	ASN
4	G	292	VAL
4	G	326	ILE
4	G	344	GLN
4	G	373	THR
4	G	414	ILE
4	G	419	ARG
4	G	425	ASN
4	G	429	ARG
4	G	446	VAL
4	G	453	LEU
4	G	454	LEU

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Mol	Chain	Res	Type
4	G	469	ARG
4	G	488	VAL
4	G	499	THR
5	H	4	LEU
5	H	11	LEU
5	H	31	ASN
5	H	51	ILE
5	H	63	LEU
5	H	75	LYS
5	H	80	LEU
5	H	82	LEU
5	H	82(A)	ASN
5	H	82(B)	SER
5	H	82(C)	VAL
5	H	105	THR
5	H	119	VAL
5	H	136	LEU
5	H	138	CYS
5	H	148	VAL
5	H	173	LEU
5	H	180	VAL
5	H	181	THR
5	H	182	VAL
5	H	189	THR
5	H	205	VAL
6	L	25	ARG
6	L	102	THR
6	L	106	VAL
6	L	134	VAL
6	L	147	VAL
6	L	170	ASN
6	L	181	LEU
6	L	202	THR
6	L	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	611	ASN
4	G	66	HIS
4	G	80	ASN
4	G	99	ASN

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Mol	Chain	Res	Type
4	G	287	GLN
4	G	348	GLN
4	G	465	ASN
5	H	97	GLN
5	H	169	GLN
5	H	197	ASN
6	L	34	GLN
6	L	37	GLN
6	L	109	GLN
6	L	168	GLN
6	L	170	ASN
6	L	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

35 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	$\# Z > 2$
7	NAG	A	1	7,4	14,14,15	0.34	0	17,19,21	0.46	0
7	NAG	A	2	7	14,14,15	0.42	0	17,19,21	1.31	1 (5%)
7	BMA	A	3	7	11,11,12	0.81	0	15,15,17	0.73	0
7	MAN	A	4	7	11,11,12	1.05	1 (9%)	15,15,17	1.52	3 (20%)
7	MAN	A	5	7	11,11,12	1.58	2 (18%)	15,15,17	2.09	3 (20%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	1	4,8	14,14,15	0.30	0	17,19,21	0.44	0
8	NAG	C	2	8	14,14,15	0.27	0	17,19,21	0.45	0
8	NAG	F	1	4,8	14,14,15	0.50	0	17,19,21	0.85	1 (5%)
8	NAG	F	2	8	14,14,15	0.33	0	17,19,21	0.43	0
9	NAG	I	1	4,9	14,14,15	0.28	0	17,19,21	0.58	0
9	NAG	I	2	9	14,14,15	0.32	0	17,19,21	0.79	1 (5%)
9	BMA	I	3	9	11,11,12	0.91	0	15,15,17	0.77	0
8	NAG	J	1	4,8	14,14,15	0.29	0	17,19,21	0.45	0
8	NAG	J	2	8	14,14,15	0.23	0	17,19,21	0.51	0
10	NAG	K	1	4,10	14,14,15	0.49	0	17,19,21	1.40	2 (11%)
10	MAN	K	10	10	11,11,12	1.02	1 (9%)	15,15,17	1.19	2 (13%)
10	NAG	K	2	10	14,14,15	0.31	0	17,19,21	0.45	0
10	BMA	K	3	10	11,11,12	0.63	0	15,15,17	1.25	1 (6%)
10	MAN	K	4	10	11,11,12	0.86	1 (9%)	15,15,17	1.50	2 (13%)
10	MAN	K	5	10	11,11,12	0.50	0	15,15,17	0.97	2 (13%)
10	MAN	K	6	10	11,11,12	0.65	0	15,15,17	0.95	2 (13%)
10	MAN	K	7	10	11,11,12	0.76	0	15,15,17	1.10	2 (13%)
10	MAN	K	8	10	11,11,12	0.66	0	15,15,17	1.11	1 (6%)
10	MAN	K	9	10	11,11,12	0.80	0	15,15,17	1.44	2 (13%)
8	NAG	M	1	4,8	14,14,15	0.40	0	17,19,21	0.53	0
8	NAG	M	2	8	14,14,15	0.36	0	17,19,21	0.54	0
11	NAG	N	1	4,11	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
11	NAG	N	2	11	14,14,15	0.36	0	17,19,21	0.57	0
11	NAG	N	3	11	14,14,15	0.35	0	17,19,21	0.55	0
9	NAG	O	1	4,9	14,14,15	0.25	0	17,19,21	0.48	0
9	NAG	O	2	9	14,14,15	0.29	0	17,19,21	0.49	0
9	BMA	O	3	9	11,11,12	0.60	0	15,15,17	0.68	0
8	NAG	P	1	4,8	14,14,15	0.24	0	17,19,21	0.56	0
8	NAG	P	2	8	14,14,15	0.26	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	6/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	4	7	-	2/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	NAG	F	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
9	NAG	I	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
8	NAG	J	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
10	NAG	K	1	4,10	-	5/6/23/26	0/1/1/1
10	MAN	K	10	10	-	0/2/19/22	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	2/2/19/22	0/1/1/1
10	MAN	K	6	10	-	0/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1
10	MAN	K	8	10	-	2/2/19/22	0/1/1/1
10	MAN	K	9	10	-	0/2/19/22	0/1/1/1
8	NAG	M	1	4,8	-	1/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
11	NAG	N	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	0/6/23/26	0/1/1/1
11	NAG	N	3	11	-	2/6/23/26	0/1/1/1
9	NAG	O	1	4,9	-	4/6/23/26	0/1/1/1
9	NAG	O	2	9	-	1/6/23/26	0/1/1/1
9	BMA	O	3	9	-	0/2/19/22	0/1/1/1
8	NAG	P	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5	MAN	C1-C2	4.08	1.62	1.52
7	A	5	MAN	O5-C1	2.92	1.48	1.43
10	K	10	MAN	C1-C2	2.79	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4	MAN	C1-C2	2.74	1.58	1.52
10	K	4	MAN	C1-C2	2.27	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5	MAN	C1-O5-C5	6.75	121.24	112.19
10	K	1	NAG	C2-N2-C7	4.68	129.18	122.90
10	K	9	MAN	C1-O5-C5	4.67	118.45	112.19
7	A	2	NAG	C2-N2-C7	4.58	129.03	122.90
10	K	4	MAN	C1-O5-C5	4.27	117.90	112.19
7	A	6	MAN	C1-O5-C5	3.83	117.32	112.19
7	A	4	MAN	C1-C2-C3	3.50	114.74	109.64
7	A	4	MAN	C1-O5-C5	3.44	116.80	112.19
10	K	8	MAN	C1-O5-C5	3.10	116.35	112.19
10	K	3	BMA	C1-O5-C5	3.00	116.20	112.19
10	K	7	MAN	C1-O5-C5	2.89	116.06	112.19
7	A	5	MAN	C1-C2-C3	2.63	113.48	109.64
10	K	6	MAN	C1-O5-C5	2.47	115.50	112.19
10	K	5	MAN	C1-O5-C5	2.35	115.33	112.19
10	K	10	MAN	C1-C2-C3	2.31	113.00	109.64
8	F	1	NAG	C1-O5-C5	2.29	115.26	112.19
10	K	6	MAN	O2-C2-C3	-2.20	105.59	110.15
10	K	5	MAN	O2-C2-C3	-2.20	105.59	110.15
7	A	6	MAN	O2-C2-C3	-2.19	105.61	110.15
10	K	9	MAN	O2-C2-C3	-2.17	105.65	110.15
10	K	1	NAG	C1-C2-N2	2.14	113.81	110.43
7	A	4	MAN	O2-C2-C3	-2.12	105.77	110.15
7	A	5	MAN	O2-C2-C3	-2.10	105.81	110.15
9	I	2	NAG	O4-C4-C3	-2.09	105.45	110.38
10	K	7	MAN	O2-C2-C3	-2.05	105.90	110.15
10	K	10	MAN	O2-C2-C3	-2.03	105.94	110.15
10	K	4	MAN	O2-C2-C3	-2.03	105.94	110.15
11	N	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3	BMA	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	K	5	MAN	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
11	N	1	NAG	C4-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
11	N	1	NAG	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
10	K	5	MAN	C4-C5-C6-O6
11	N	3	NAG	C4-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
10	K	4	MAN	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
9	I	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
8	M	2	NAG	C8-C7-N2-C2
8	M	2	NAG	O7-C7-N2-C2
9	O	1	NAG	C8-C7-N2-C2
9	O	1	NAG	O7-C7-N2-C2
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
10	K	4	MAN	C4-C5-C6-O6
8	F	2	NAG	C4-C5-C6-O6
11	N	3	NAG	O5-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
10	K	8	MAN	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
7	A	5	MAN	O5-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
8	M	1	NAG	O5-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
10	K	1	NAG	C1-C2-N2-C7
10	K	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
10	K	1	NAG	C3-C2-N2-C7
7	A	4	MAN	C4-C5-C6-O6
10	K	8	MAN	C4-C5-C6-O6

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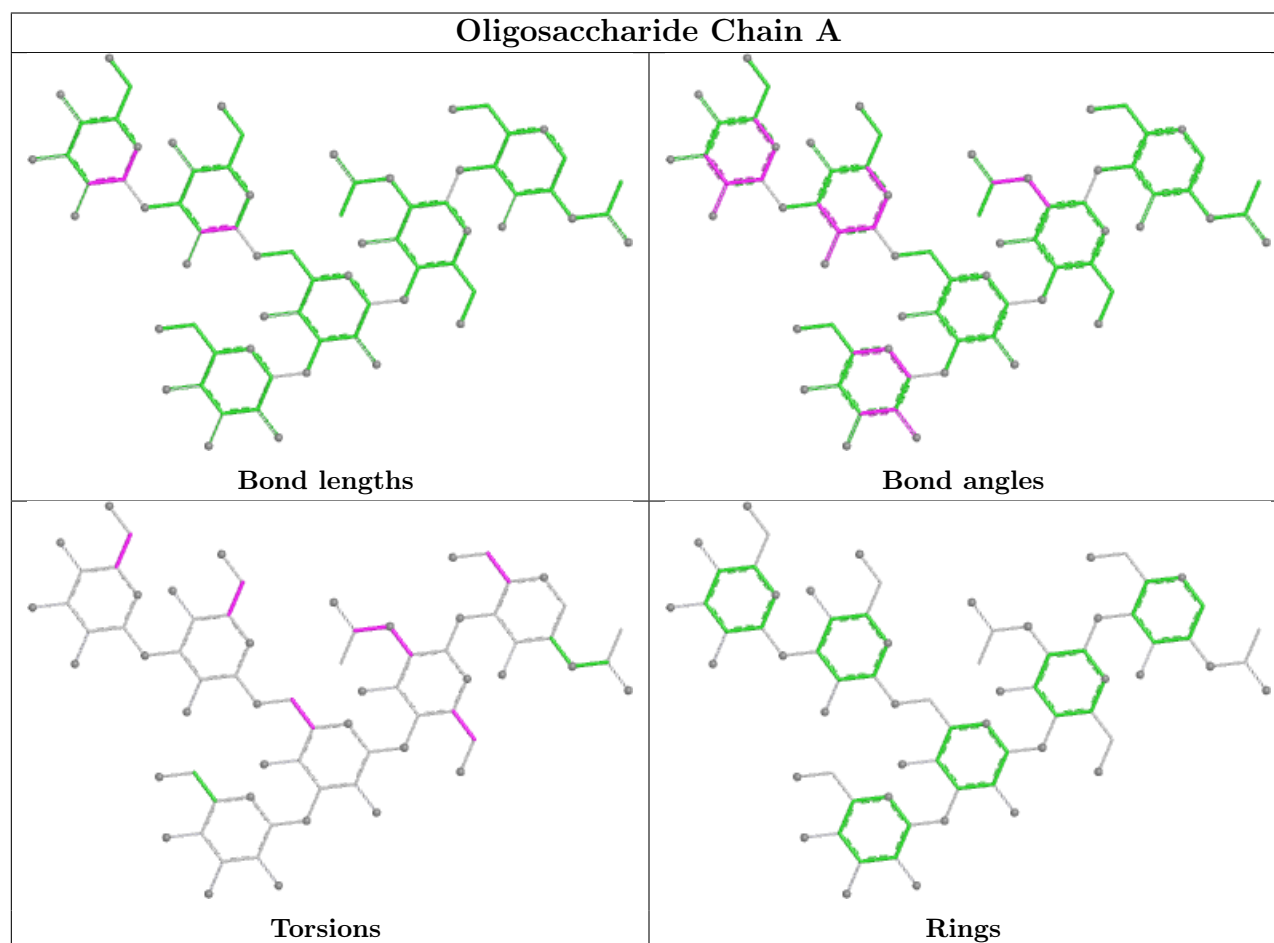
Mol	Chain	Res	Type	Atoms
8	J	2	NAG	C4-C5-C6-O6

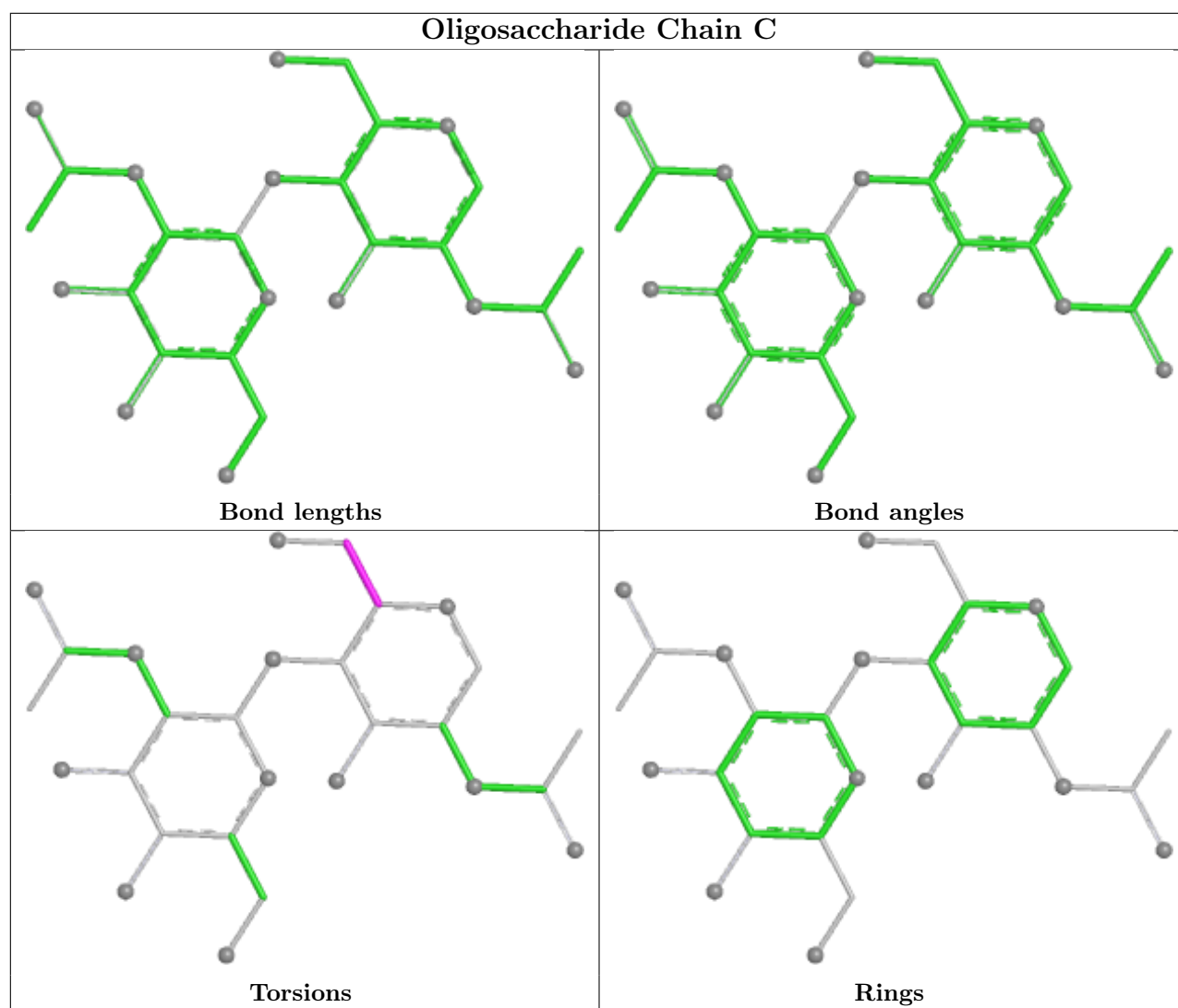
There are no ring outliers.

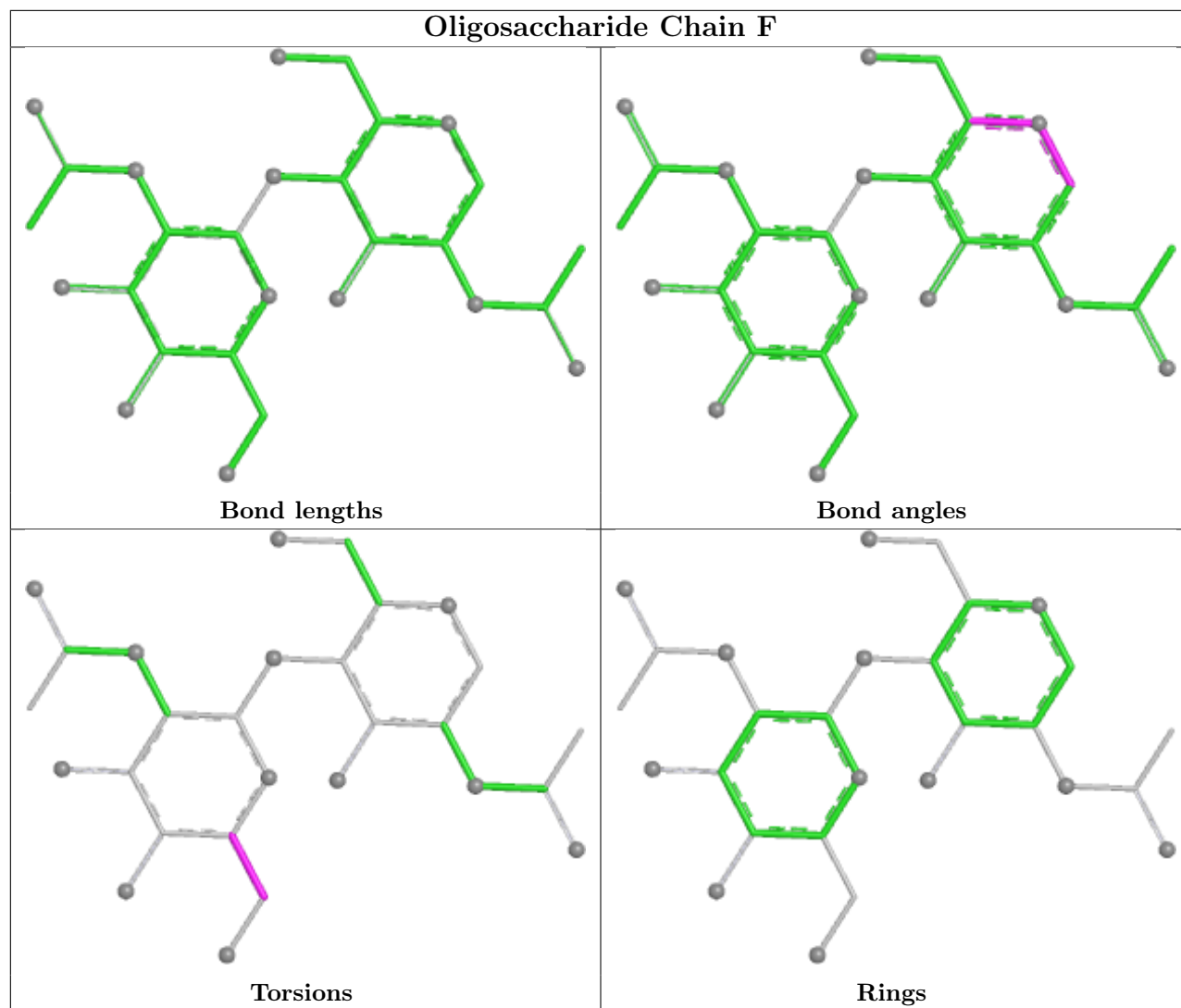
6 monomers are involved in 7 short contacts:

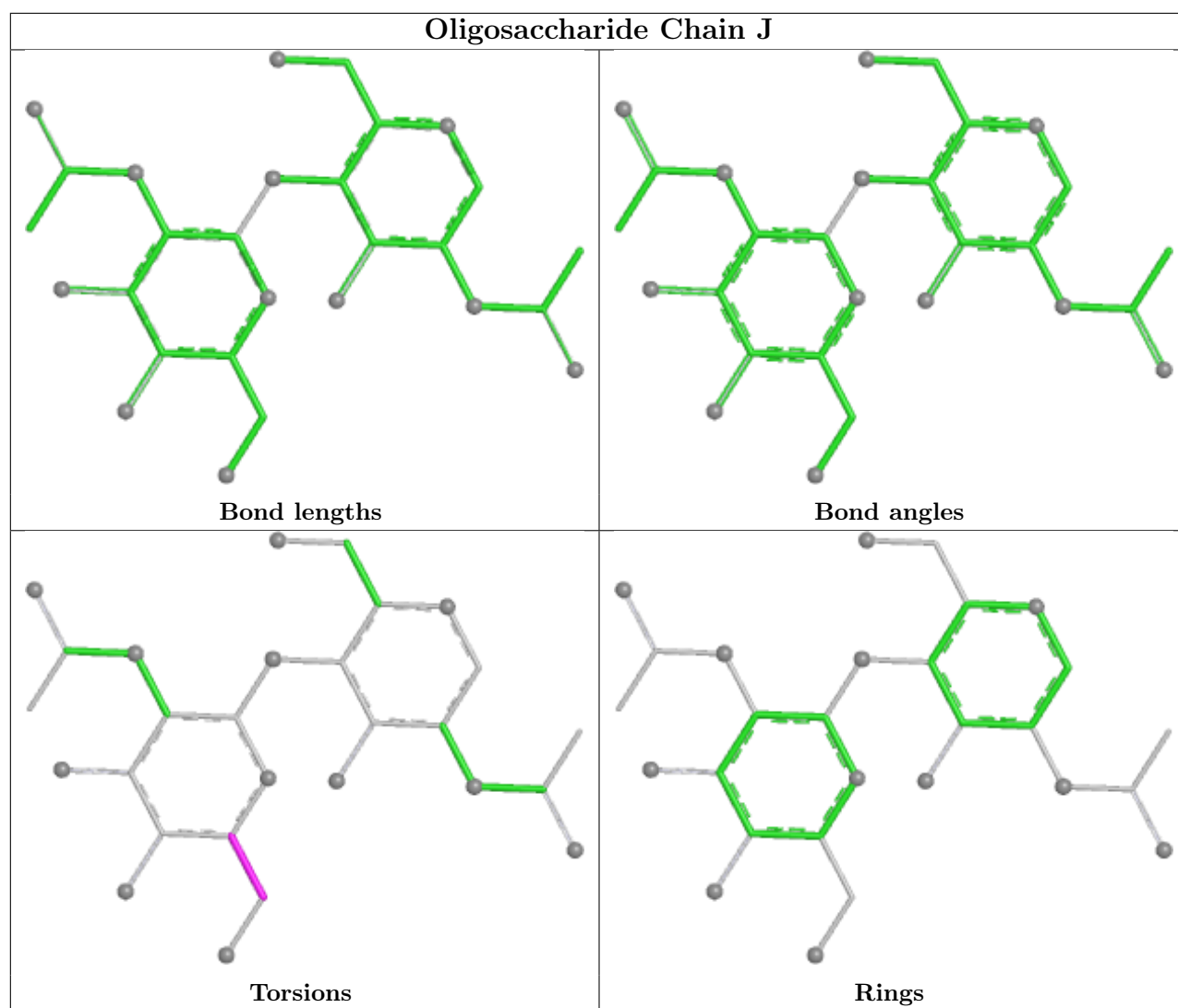
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	NAG	1	0
9	I	1	NAG	2	0
11	N	1	NAG	1	0
7	A	2	NAG	3	0
9	I	2	NAG	2	0
10	K	1	NAG	2	0

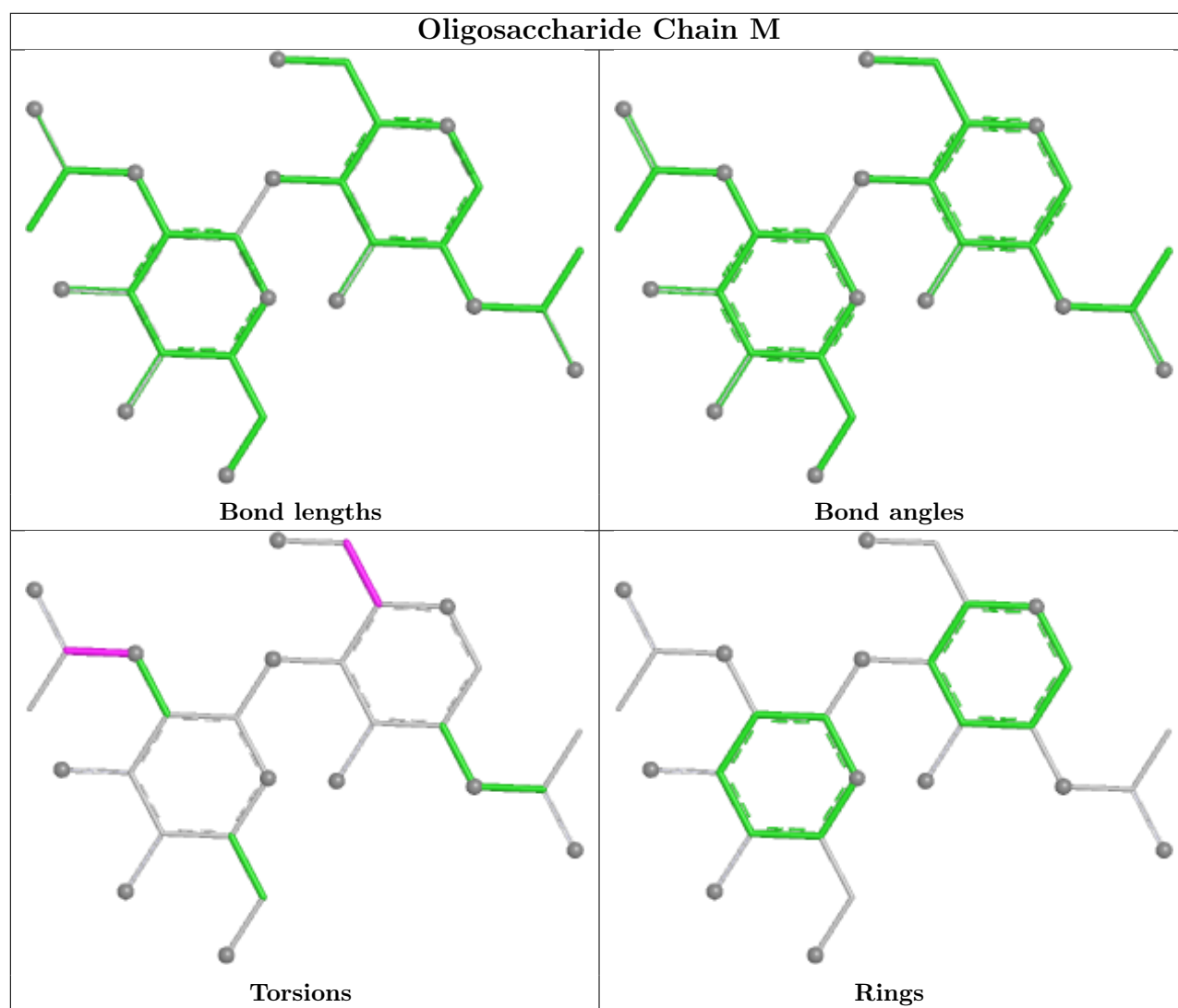
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

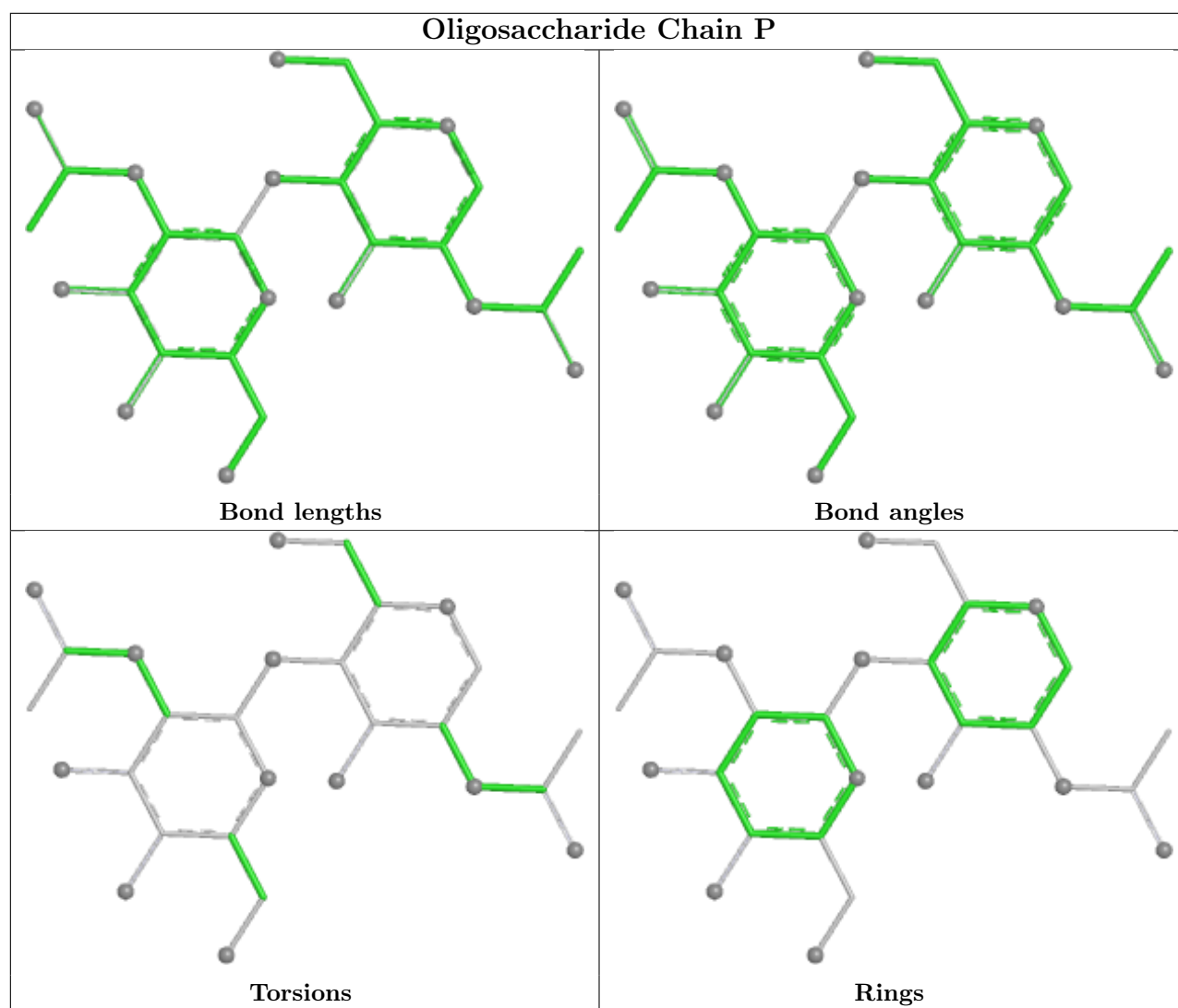


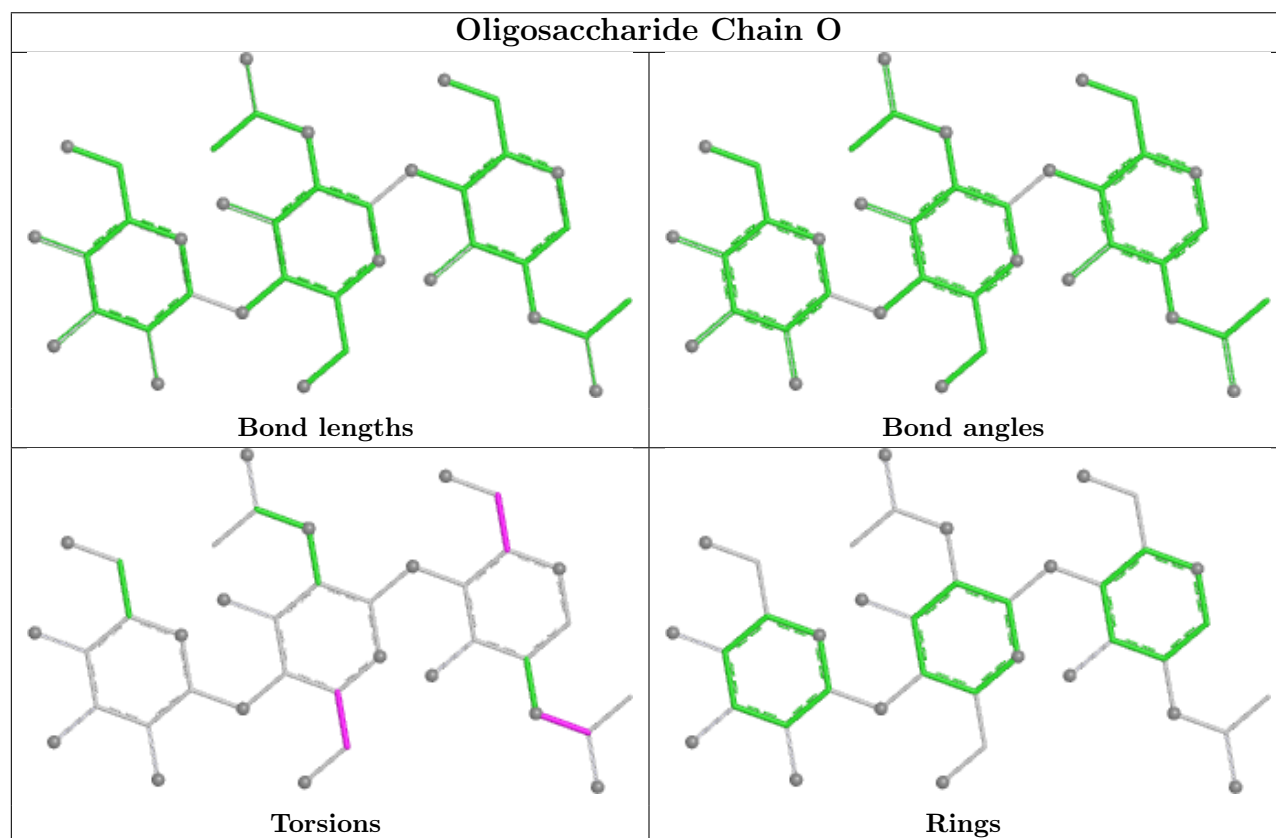
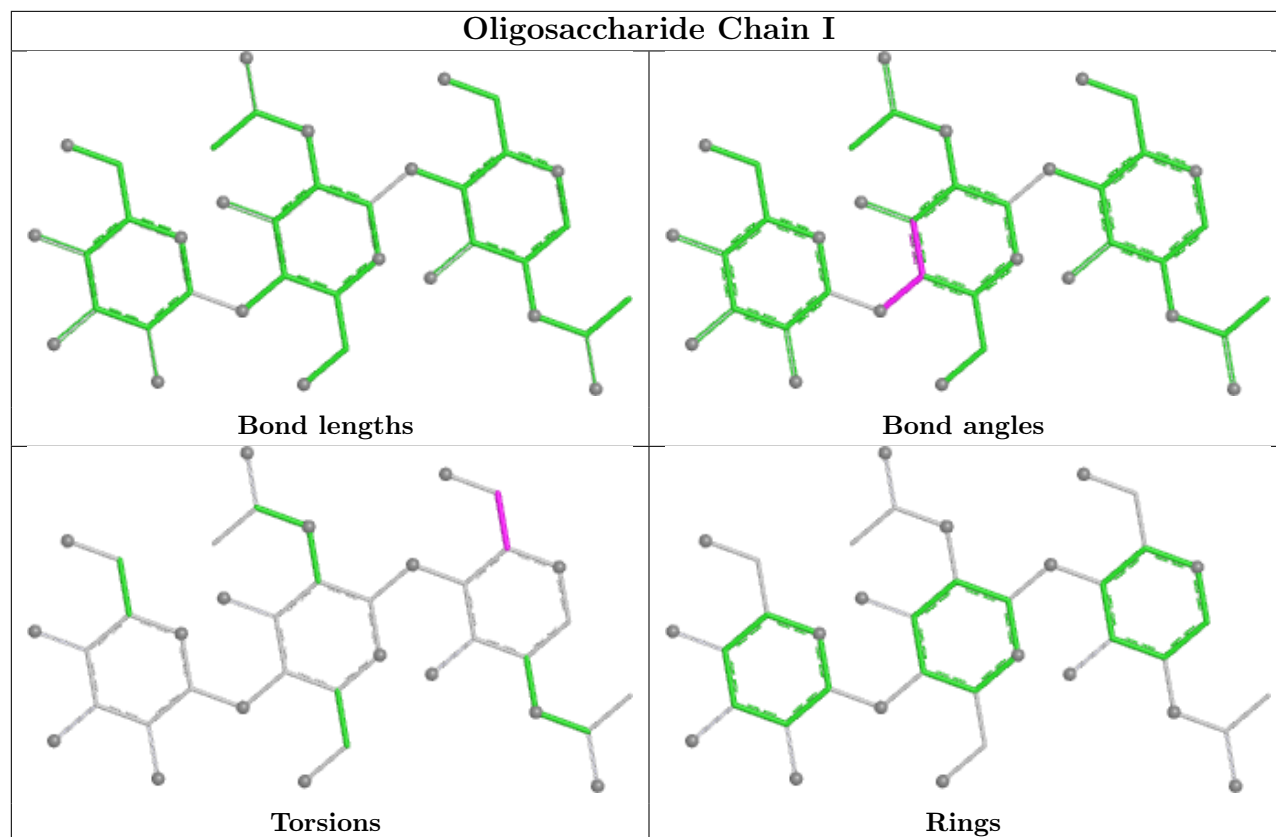


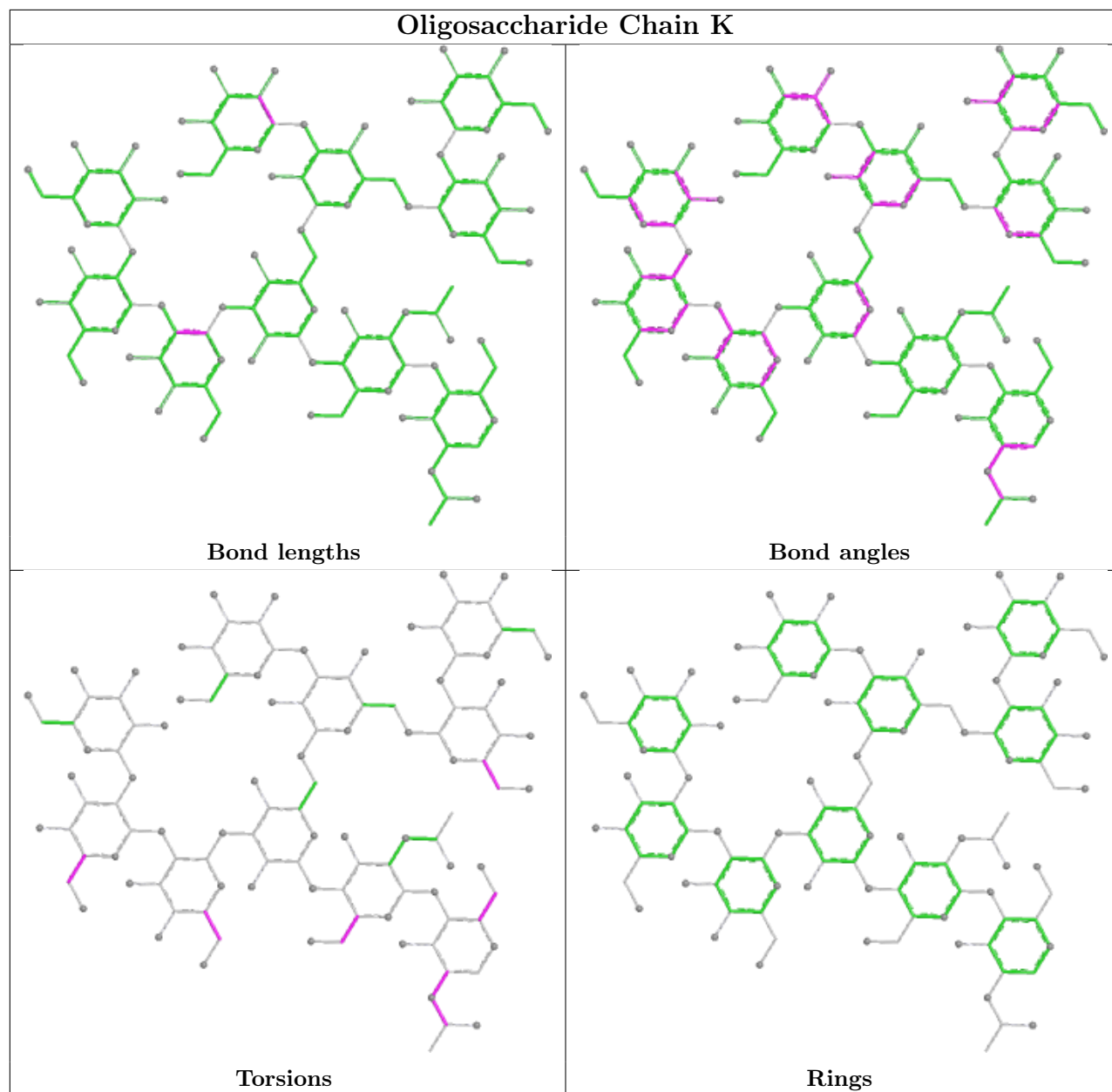


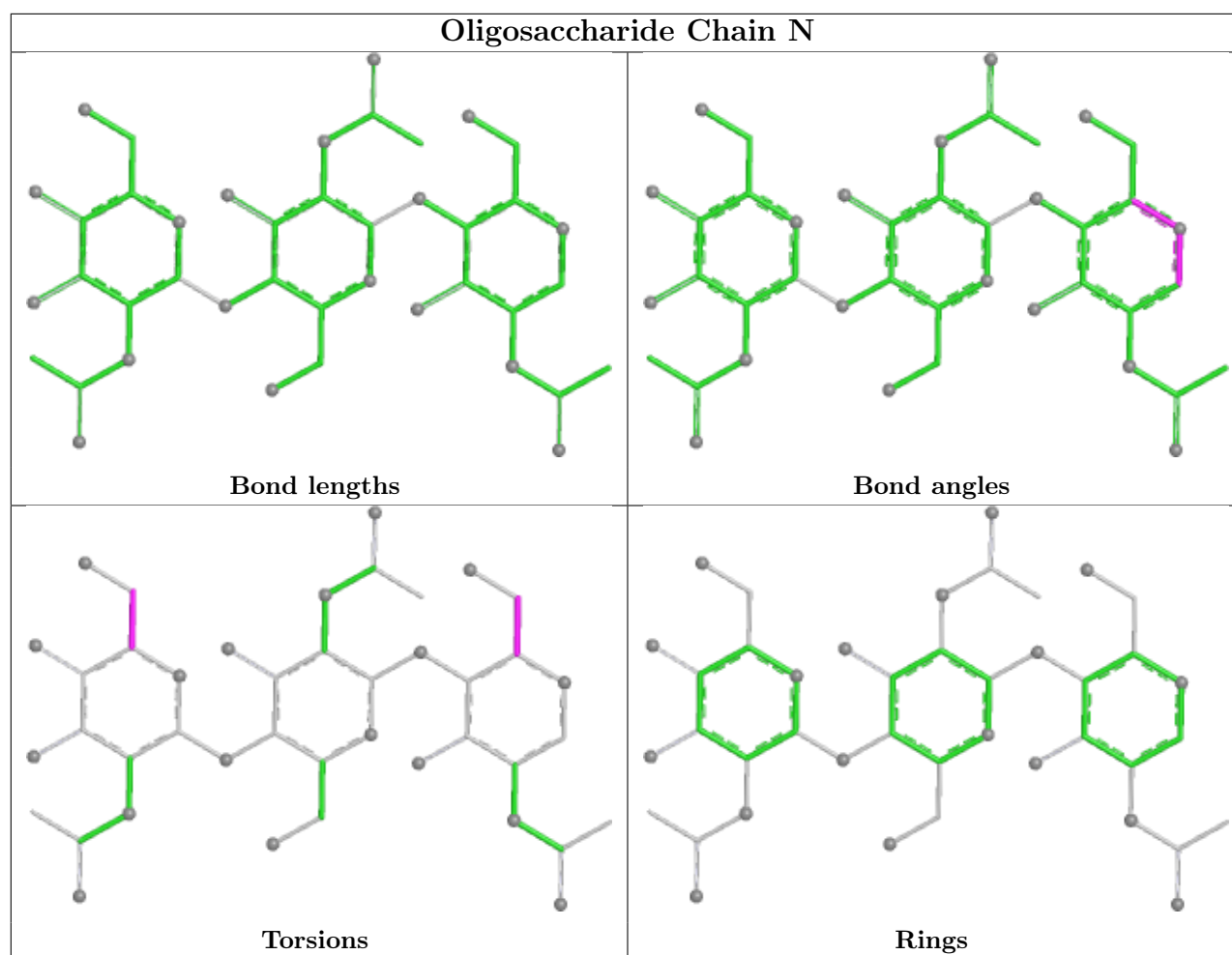












5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	NAG	G	601	4	14,14,15	0.33	0	17,19,21	0.45	0
12	NAG	G	604	4	14,14,15	0.29	0	17,19,21	0.51	0
12	NAG	G	602	4	14,14,15	0.36	0	17,19,21	0.56	0
12	NAG	G	603	4	14,14,15	0.24	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	G	601	4	-	2/6/23/26	0/1/1/1
12	NAG	G	604	4	-	0/6/23/26	0/1/1/1
12	NAG	G	602	4	-	2/6/23/26	0/1/1/1
12	NAG	G	603	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	NAG	O5-C5-C6-O6
12	G	603	NAG	O5-C5-C6-O6
12	G	601	NAG	C4-C5-C6-O6
12	G	602	NAG	C8-C7-N2-C2
12	G	602	NAG	O7-C7-N2-C2
12	G	603	NAG	C4-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

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	B	120/153 (78%)	0.65	14 (11%) 9 7	11, 36, 74, 84	0
2	D	128/134 (95%)	1.85	55 (42%) 0 0	28, 72, 108, 124	0
3	E	105/114 (92%)	1.62	37 (35%) 1 0	31, 60, 105, 116	0
4	G	425/498 (85%)	0.52	32 (7%) 20 17	11, 30, 74, 115	0
5	H	226/244 (92%)	1.17	49 (21%) 2 2	23, 54, 90, 108	0
6	L	211/217 (97%)	0.42	15 (7%) 22 18	12, 36, 64, 115	0
All	All	1215/1360 (89%)	0.87	202 (16%) 4 3	11, 42, 93, 124	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	136	PRO	7.2
1	B	519	PHE	6.4
4	G	354	VAL	6.1
2	D	59	LEU	6.1
1	B	521	GLY	6.0
4	G	368	ASP	5.7
2	D	88	GLY	5.5
3	E	83	GLU	5.4
3	E	40	PRO	5.1
6	L	7	TYR	5.1
2	D	89	THR	5.1
2	D	110	THR	5.0
2	D	108	LEU	4.6
1	B	660	LEU	4.6
5	H	11	LEU	4.5
6	L	184	MET	4.5
3	E	14	SER	4.4
2	D	107	THR	4.4
2	D	45	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
5	H	110	SER	4.2
2	D	51	ILE	4.2
3	E	80	PRO	4.1
3	E	15	LEU	4.1
4	G	367	GLY	4.0
4	G	232	GLU	4.0
2	D	41	ALA	4.0
2	D	109	LEU	4.0
5	H	28	SER	3.9
2	D	18	VAL	3.9
5	H	73	THR	3.9
4	G	31	ALA	3.9
2	D	44	GLY	3.9
1	B	518	VAL	3.9
3	E	99	GLY	3.8
2	D	6	GLN	3.8
5	H	132	GLY	3.8
4	G	432	GLN	3.7
2	D	36	TRP	3.6
2	D	61	PRO	3.6
5	H	33	TYR	3.5
4	G	430	THR	3.5
1	B	535	ASN	3.5
6	L	9	ARG	3.5
5	H	111	SER	3.5
4	G	472	GLY	3.4
4	G	359	ILE	3.4
2	D	2	GLY	3.4
1	B	522	PHE	3.4
2	D	90	TYR	3.3
5	H	43	LYS	3.3
4	G	66	HIS	3.3
5	H	29	ILE	3.3
6	L	6	SER	3.3
2	D	1	GLN	3.3
4	G	135	ASN	3.3
2	D	60	ALA	3.2
3	E	8	ALA	3.2
2	D	14	PRO	3.2
5	H	13	LYS	3.2
5	H	189	THR	3.2
5	H	191	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	E	84	THR	3.2
3	E	16	GLY	3.1
5	H	22	CYS	3.1
2	D	5	VAL	3.1
4	G	171	ARG	3.1
3	E	87	TYR	3.1
2	D	84	SER	3.1
6	L	22	SER	3.1
3	E	89	CYS	3.0
5	H	100(O)	TYR	3.0
2	D	83	THR	3.0
5	H	42	GLY	3.0
3	E	3	VAL	3.0
2	D	64	GLN	3.0
3	E	9	SER	2.9
4	G	365	SER	2.9
2	D	68	ASN	2.9
2	D	70	THR	2.9
2	D	69	MET	2.9
5	H	71	VAL	2.9
3	E	30	HIS	2.9
4	G	429	ARG	2.9
5	H	152	TRP	2.9
2	D	82	ILE	2.9
4	G	395	TRP	2.8
4	G	360	ILE	2.8
1	B	662	ALA	2.8
6	L	70	ARG	2.8
3	E	69	TRP	2.8
3	E	104	VAL	2.8
4	G	58	ALA	2.8
2	D	15	GLY	2.8
3	E	11	VAL	2.8
3	E	36	TYR	2.8
3	E	7	SER	2.7
3	E	76	SER	2.7
3	E	72	TYR	2.7
3	E	103	LYS	2.7
3	E	27(A)	SER	2.7
1	B	651	PHE	2.7
6	L	26	GLN	2.7
5	H	50	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
6	L	133	LEU	2.7
3	E	42	ARG	2.7
3	E	32	SER	2.7
2	D	9	ALA	2.7
2	D	10	THR	2.7
2	D	39	GLN	2.6
2	D	12	THR	2.6
4	G	358	THR	2.6
2	D	20	ILE	2.6
2	D	58	ASN	2.6
3	E	62	PHE	2.6
4	G	79	PRO	2.6
5	H	192	TYR	2.6
4	G	347	ARG	2.6
2	D	87	THR	2.6
1	B	663	LEU	2.6
4	G	166	ARG	2.6
2	D	42	GLY	2.6
1	B	534	SER	2.5
5	H	139	LEU	2.5
5	H	149	THR	2.5
5	H	25	SER	2.5
4	G	456	ARG	2.5
2	D	57	LYS	2.5
2	D	82(B)	ASN	2.5
5	H	133	THR	2.5
6	L	153	SER	2.5
2	D	65	ASP	2.5
2	D	66	ARG	2.4
2	D	76	GLY	2.4
2	D	13	LYS	2.4
2	D	11	THR	2.4
2	D	82(A)	ARG	2.4
1	B	635	ILE	2.4
5	H	187	LEU	2.4
5	H	188	GLY	2.4
4	G	33	ASN	2.4
3	E	98	PHE	2.4
2	D	40	THR	2.4
5	H	193	ILE	2.4
5	H	141	LYS	2.4
6	L	157	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
5	H	119	VAL	2.4
2	D	71	THR	2.3
4	G	185	ASN	2.3
3	E	43	ALA	2.3
4	G	393	SER	2.3
3	E	41	GLY	2.3
5	H	17	THR	2.3
3	E	82	ASP	2.3
5	H	5	GLN	2.3
4	G	353	PHE	2.3
5	H	48	ILE	2.3
1	B	617	LYS	2.3
6	L	210	THR	2.3
5	H	54	SER	2.3
2	D	106	GLY	2.3
6	L	41	GLY	2.3
5	H	150	VAL	2.3
3	E	75	ILE	2.2
4	G	336	SER	2.2
5	H	190	GLN	2.2
2	D	48	MET	2.2
5	H	211	PRO	2.2
2	D	8	GLY	2.2
2	D	54	SER	2.2
3	E	78	LEU	2.2
5	H	16	GLU	2.2
4	G	278	THR	2.2
6	L	68	GLY	2.2
2	D	37	ILE	2.2
5	H	82(A)	ASN	2.1
2	D	92	CYS	2.1
1	B	661	LEU	2.1
5	H	107	VAL	2.1
4	G	151	ARG	2.1
3	E	74	THR	2.1
5	H	174	TYR	2.1
5	H	2	VAL	2.1
5	H	12	VAL	2.1
3	E	38	TRP	2.1
5	H	55	GLU	2.0
5	H	40	SER	2.0
6	L	188	MET	2.0

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Mol	Chain	Res	Type	RSRZ
5	H	1	GLN	2.0
5	H	3	GLN	2.0
5	H	136	LEU	2.0
3	E	101	GLY	2.0
5	H	32	TYR	2.0
5	H	182	VAL	2.0
3	E	79	ARG	2.0
4	G	466	GLU	2.0
2	D	105	GLN	2.0
4	G	369	LEU	2.0
5	H	18	LEU	2.0
1	B	616	ASN	2.0
2	D	49	GLY	2.0
3	E	27	ASN	2.0
6	L	200	GLY	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
7	NAG	A	1	14/15	-	-	21,30,41,45	0
7	NAG	A	2	14/15	-	-	29,35,47,48	0
7	BMA	A	3	11/12	-	-	33,45,57,59	0
7	MAN	A	4	11/12	-	-	55,78,98,104	0
7	MAN	A	5	11/12	-	-	79,94,110,110	0
7	MAN	A	6	11/12	-	-	31,40,47,50	0
8	NAG	C	1	14/15	-	-	31,49,83,88	0
8	NAG	C	2	14/15	-	-	68,107,123,129	0
8	NAG	F	1	14/15	-	-	49,93,105,114	0
8	NAG	F	2	14/15	-	-	49,100,112,114	0
8	NAG	M	2	14/15	0.57	0.26	93,103,115,115	0
8	NAG	P	2	14/15	0.64	0.23	78,104,121,132	0
10	NAG	K	2	14/15	0.68	0.20	29,54,68,69	0

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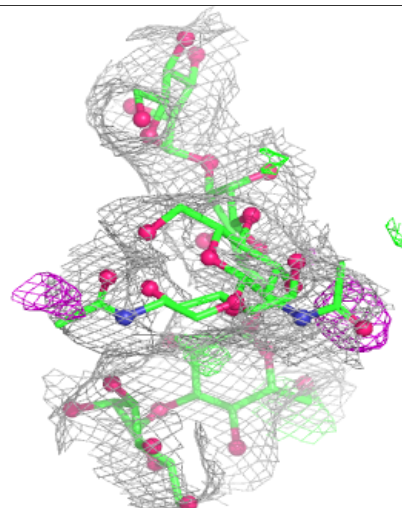
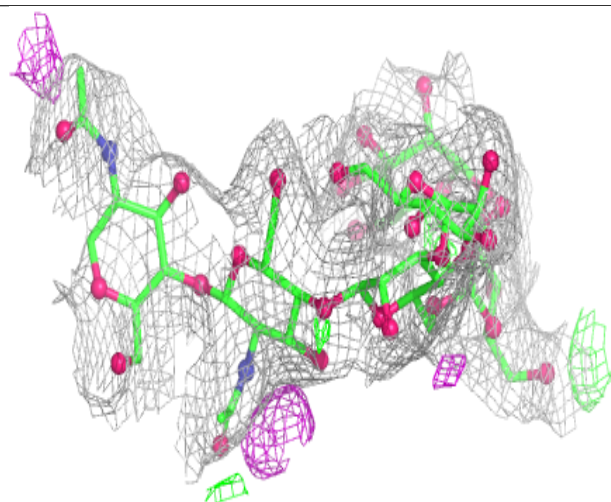
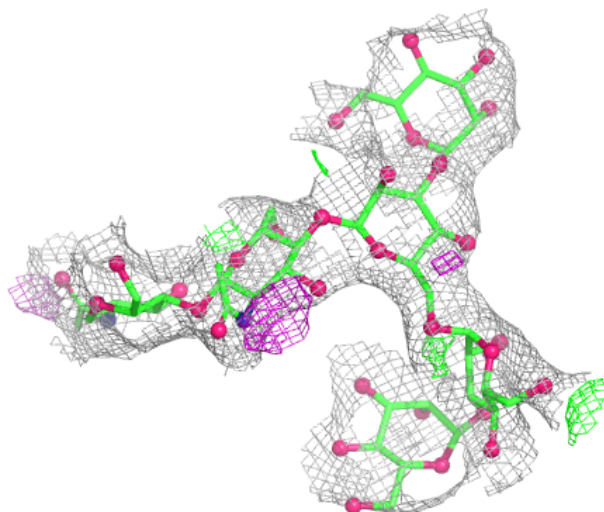
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	N	3	14/15	0.70	0.17	68,82,95,99	0
9	BMA	O	3	11/12	0.71	0.17	83,103,123,132	0
9	NAG	I	2	14/15	0.74	0.16	52,66,84,88	0
8	NAG	J	2	14/15	0.80	0.15	77,107,117,120	0
9	NAG	O	2	14/15	0.84	0.14	53,81,95,97	0
9	BMA	I	3	11/12	-	-	66,88,99,103	0
9	NAG	I	1	14/15	0.84	0.16	10,28,52,55	0
9	NAG	O	1	14/15	0.87	0.13	41,49,62,66	0
11	NAG	N	2	14/15	0.88	0.14	40,54,77,88	0
10	NAG	K	1	14/15	0.90	0.14	20,41,52,55	0
8	NAG	M	1	14/15	0.91	0.13	50,63,70,84	0
10	BMA	K	3	11/12	-	-	30,43,58,77	0
10	MAN	K	4	11/12	-	-	18,27,34,44	0
10	MAN	K	5	11/12	-	-	30,38,43,44	0
10	MAN	K	6	11/12	-	-	35,54,65,77	0
10	MAN	K	7	11/12	-	-	58,71,87,87	0
10	MAN	K	8	11/12	-	-	56,68,81,82	0
10	MAN	K	9	11/12	-	-	48,83,97,112	0
10	MAN	K	10	11/12	-	-	67,89,106,107	0
8	NAG	J	1	14/15	0.93	0.10	36,52,70,70	0
8	NAG	P	1	14/15	0.94	0.12	50,67,82,91	0
11	NAG	N	1	14/15	0.94	0.11	31,44,56,74	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.

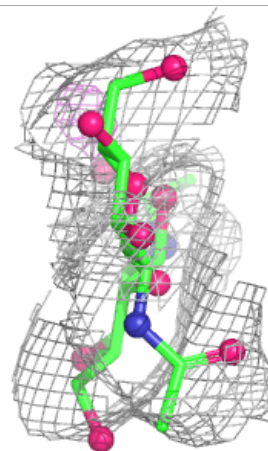
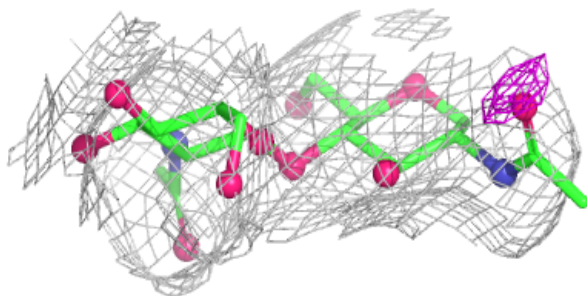
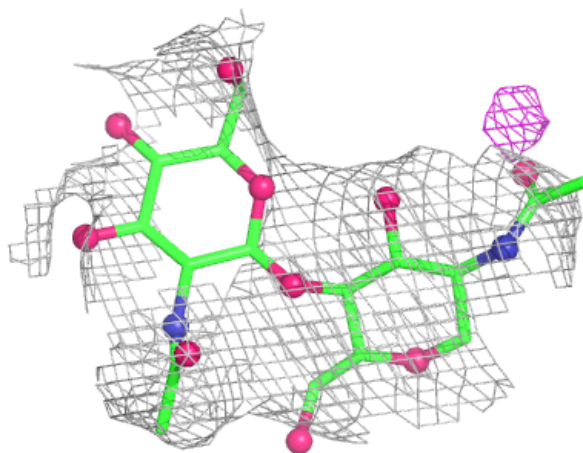
Electron density around Chain A:

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



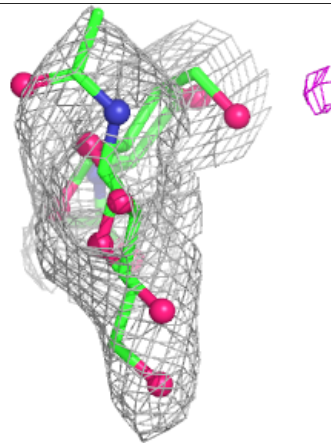
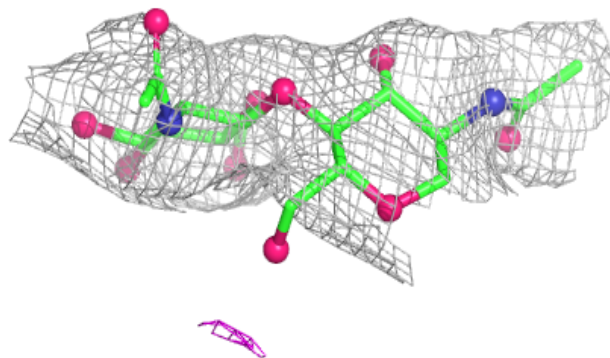
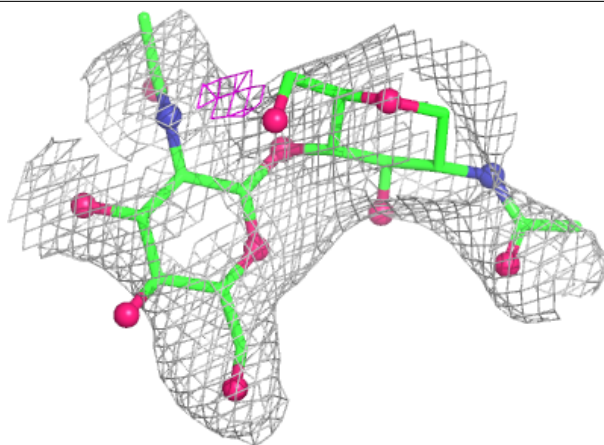
Electron density around Chain C:

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



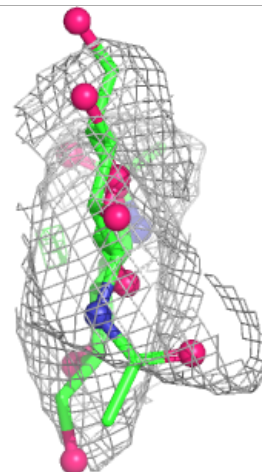
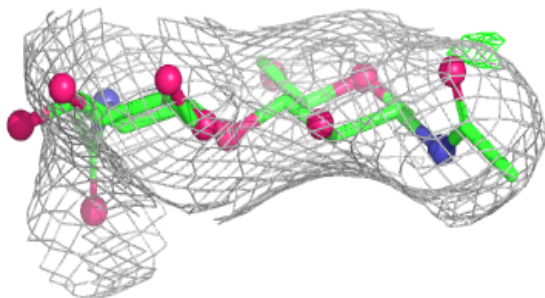
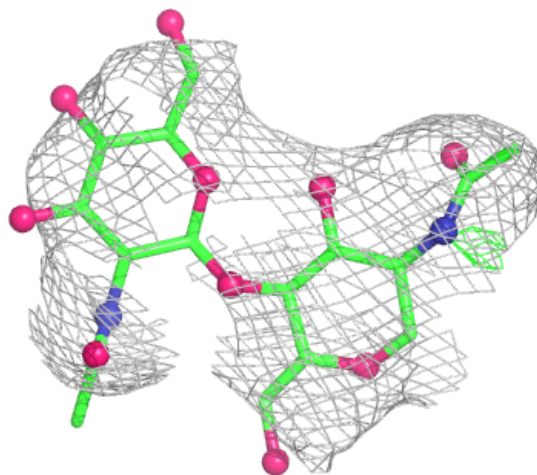
Electron density around Chain F:

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



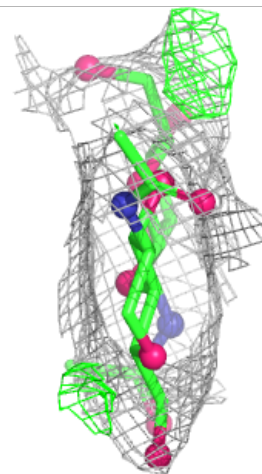
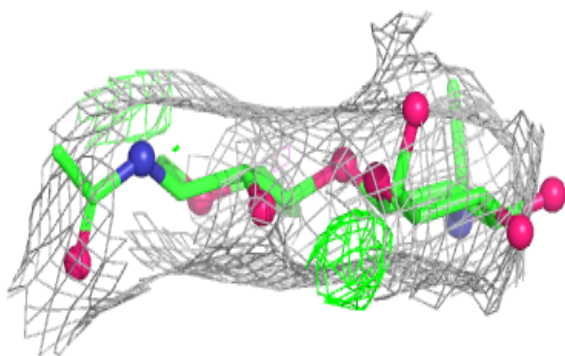
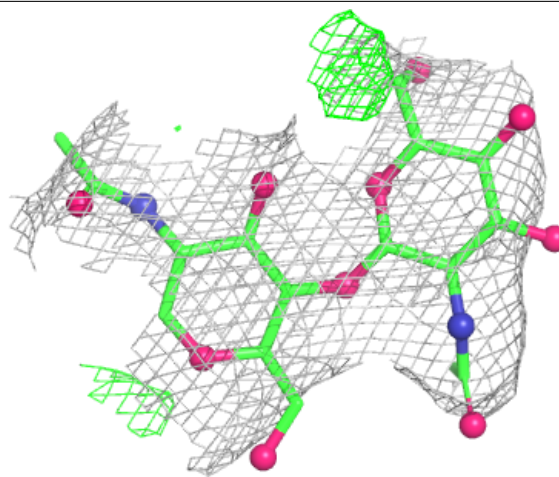
Electron density around Chain J:

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



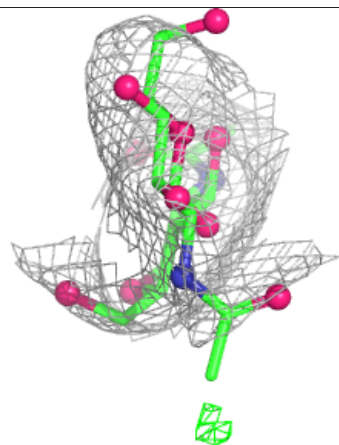
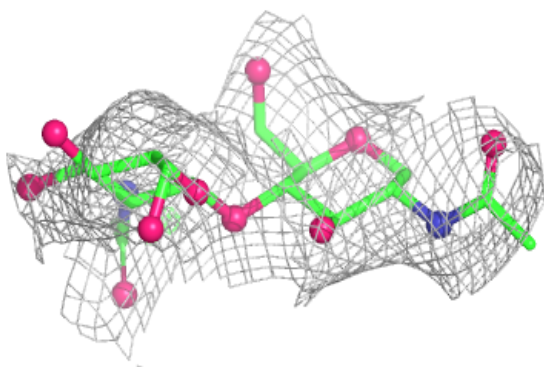
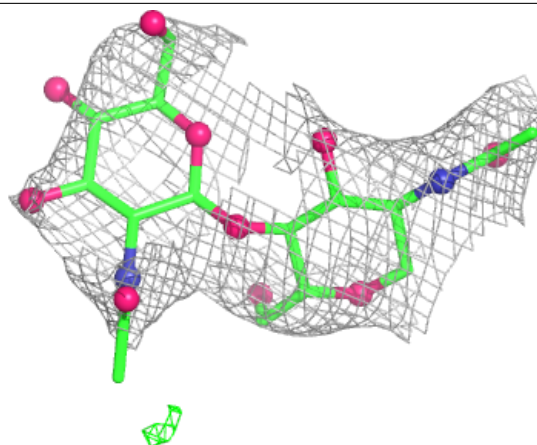
Electron density around Chain M:

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

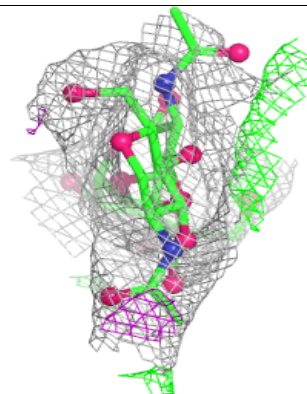
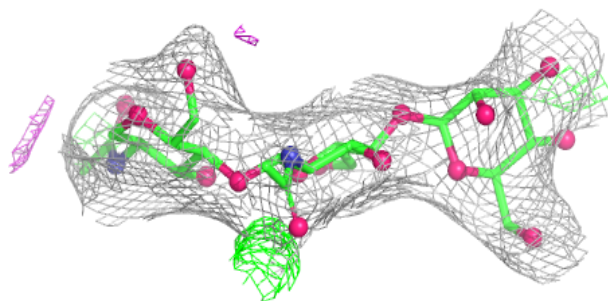
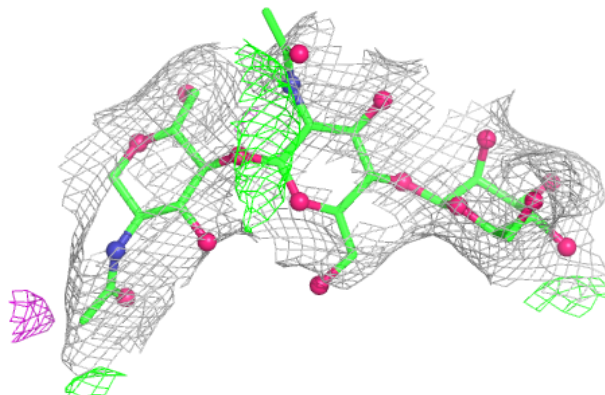


Electron density around Chain P:

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

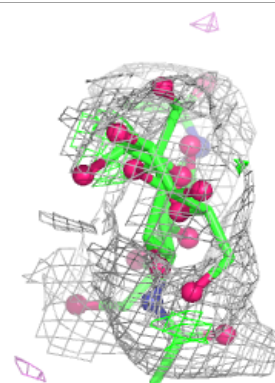
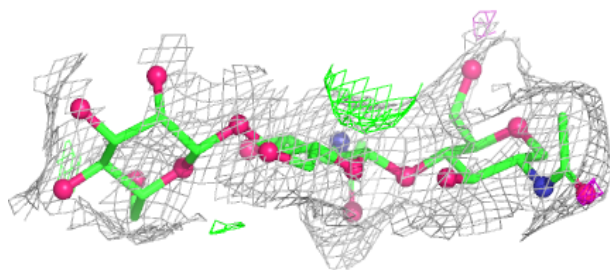
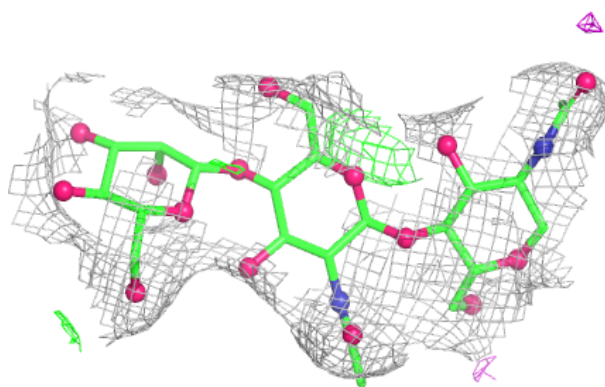
**Electron density around Chain I:**

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



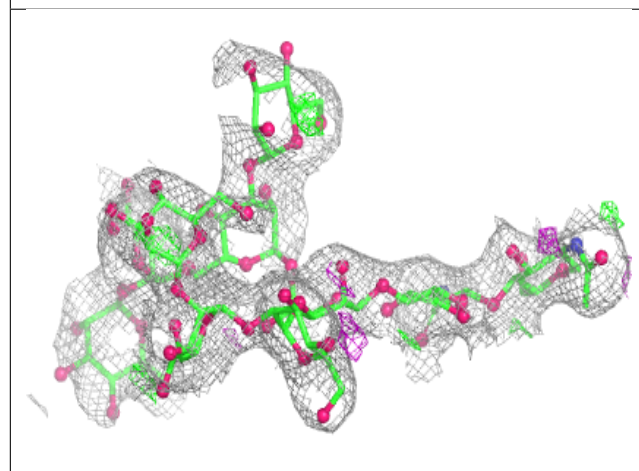
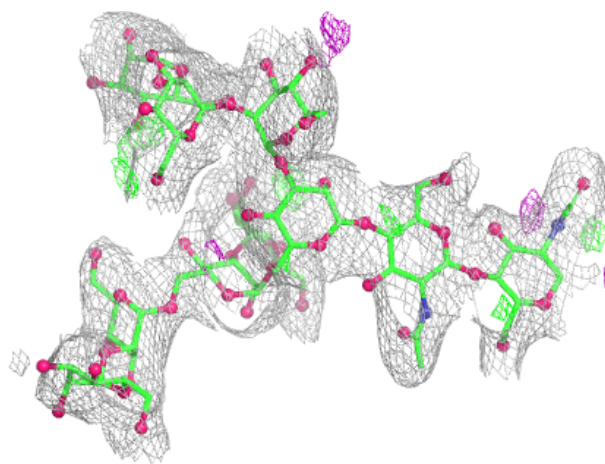
Electron density around Chain O:

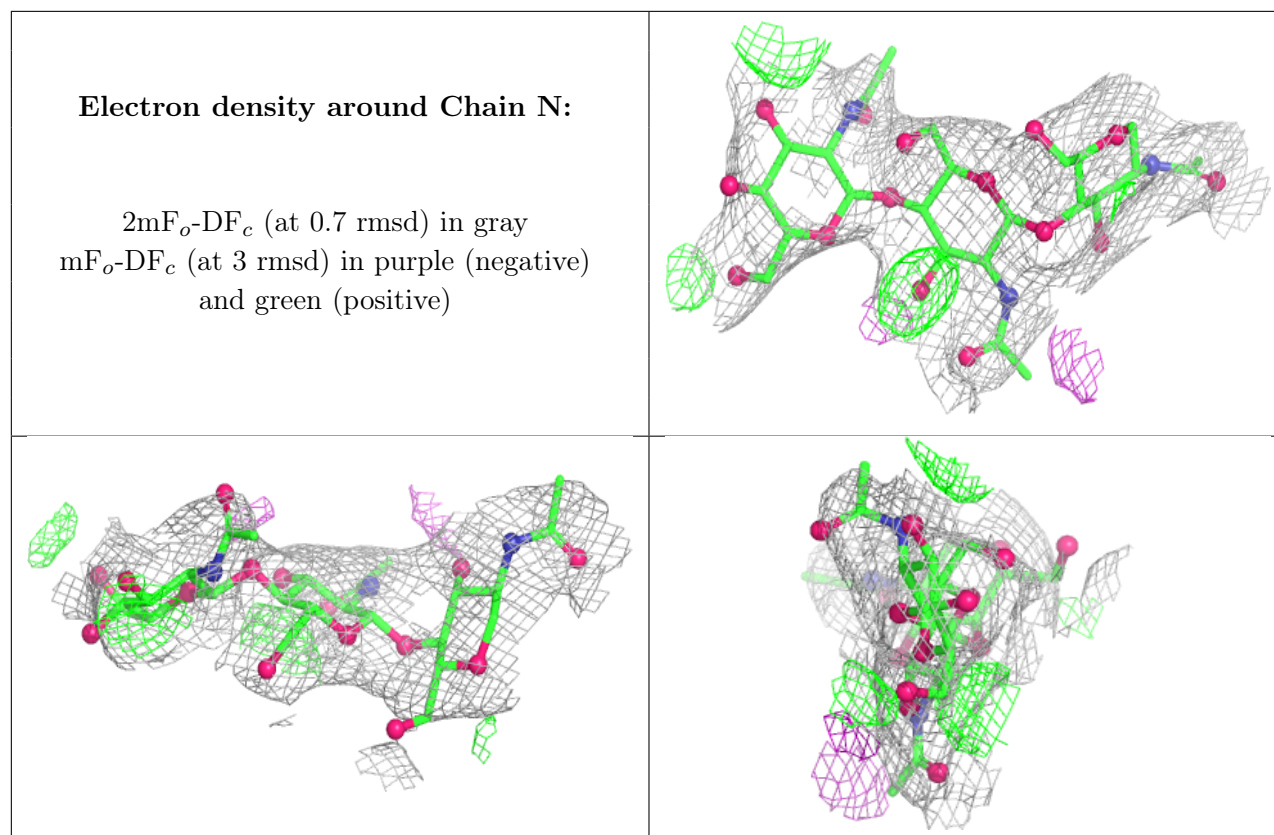
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





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(Å ²)	Q<0.9
12	NAG	G	604	14/15	0.76	0.17	52,88,114,119	0
12	NAG	G	603	14/15	0.83	0.17	53,75,109,110	0
12	NAG	G	602	14/15	0.87	0.14	26,66,86,88	0
12	NAG	G	601	14/15	0.90	0.12	39,50,65,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.