



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:46 AM UTC

PDB ID : 6MDT / pdb_00006mdt
Title : Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P63 space group
Authors : Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on : 2018-09-05
Resolution : 3.82 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:

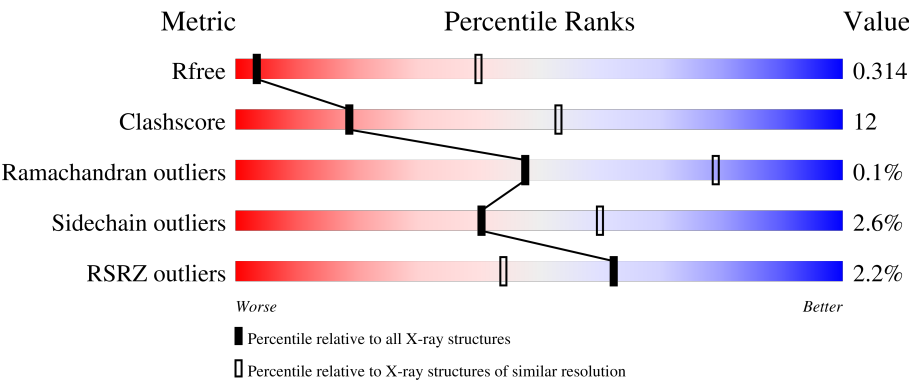
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 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.



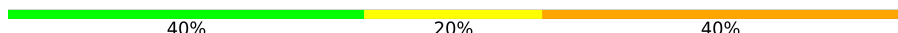
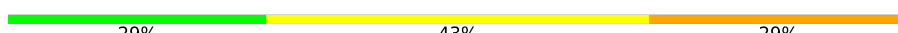
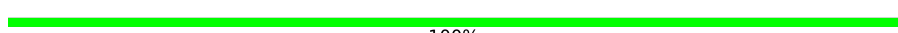
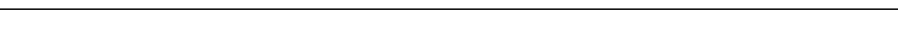
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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	3% 71%16%..11%
2	G	482	2% 67%26%.6%
3	D	243	2% 79%19%.
4	E	216	% 83%14%..
5	H	236	4% 66%31%..

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Mol	Chain	Length	Quality of chain
6	L	214	% 
7	A	5	
7	I	5	
7	K	5	
7	Q	5	
8	C	7	
9	F	2	
10	J	3	
10	M	3	
10	O	3	
10	S	3	
11	N	4	
11	P	4	
12	R	4	
13	T	9	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 12314 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	136	Total	C	N	O	S	0	0	0
			1077	688	181	201	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UES2

- Molecule 2 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	455	Total	C	N	O	S	0	0	0
			3562	2237	628	671	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UF58

- Molecule 3 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 4 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

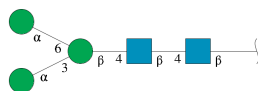
- Molecule 5 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

- Molecule 6 is a protein called PGT124 Fab light chain.

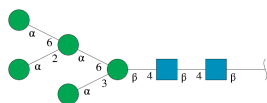
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 is an oligosaccharide called 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.



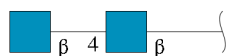
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	I	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	K	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	Q	5	Total	C	N	O		0	0	0
			61	34	2	25				

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]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.



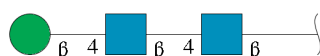
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

- Molecule 9 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
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



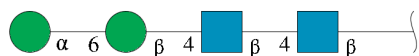
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 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.



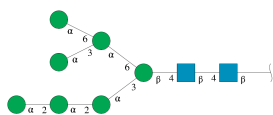
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
11	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called 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.



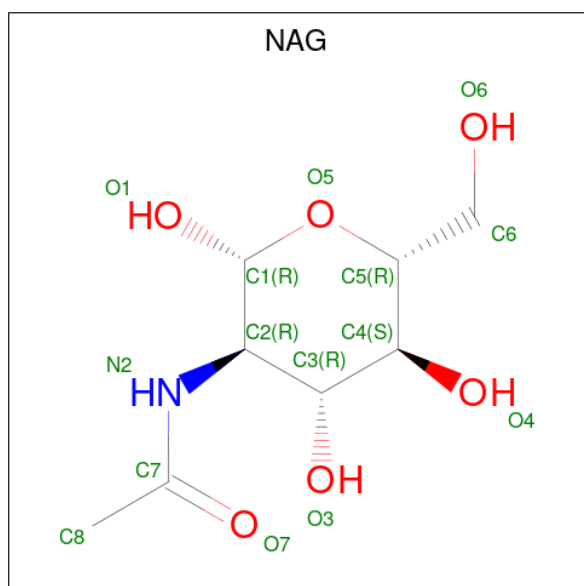
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
13	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



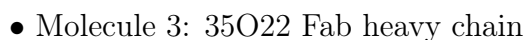
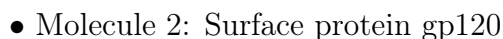
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		

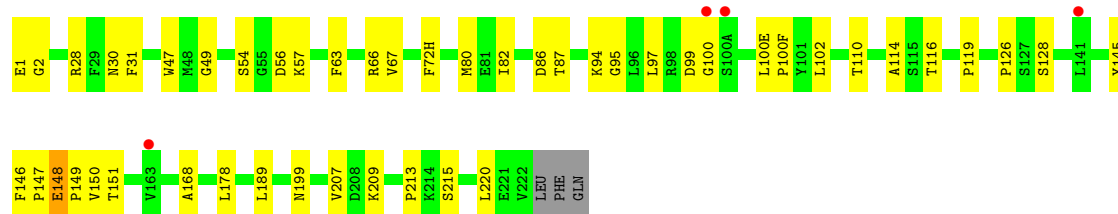
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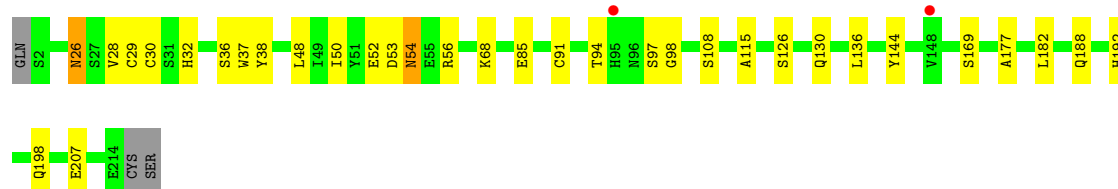
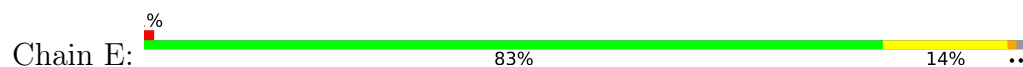
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: Transmembrane protein gp41

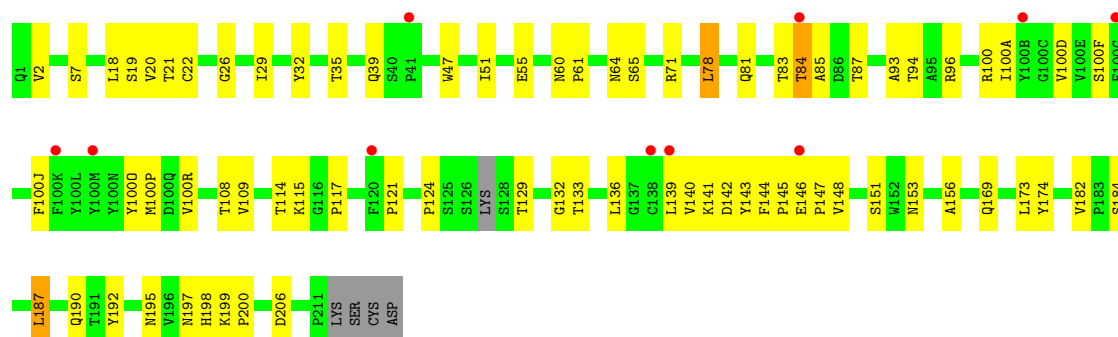




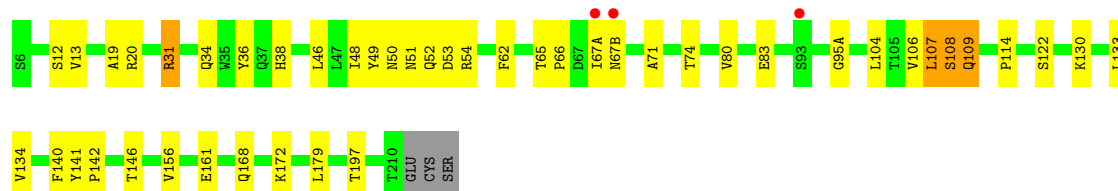
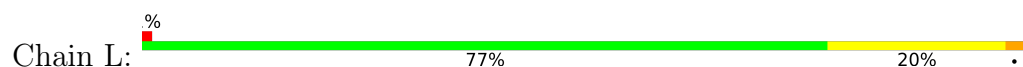
- Molecule 4: 35O22 Fab light chain



- Molecule 5: PGT124 Fab heavy chain



- Molecule 6: PGT124 Fab light chain



- Molecule 7: 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





- Molecule 7: 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 I: 60% 20% 20%



- Molecule 7: 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: 40% 20% 40%



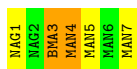
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 40% 40% 20%



- Molecule 8: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]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

Chain C: 29% 43% 29%



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

Chain F: 100%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 33% 33% 33%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 33% 33% 33%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 33% 67%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 67% 33%



- Molecule 11: 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 N: 75% 25%



- Molecule 11: 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 P: 50% 50%

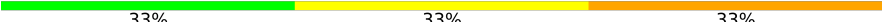


- Molecule 12: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 50% 50%



- Molecule 13: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain T:  33% 33% 33%

MAG1
MAG2
BR13
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	129.34Å 129.34Å 313.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.96 – 3.82 41.96 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.96-3.82) 99.8 (41.96-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.76Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.294 , 0.311 0.300 , 0.314	Depositor DCC
R_{free} test set	1359 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.177 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: MAN, BMA, NAG

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	0.19	0/1096	0.39	0/1487
2	G	0.21	0/3637	0.44	1/4946 (0.0%)
3	D	0.08	0/1860	0.26	0/2533
4	E	0.10	0/1659	0.30	1/2269 (0.0%)
5	H	0.20	0/1797	0.59	5/2453 (0.2%)
6	L	0.26	1/1644 (0.1%)	0.52	5/2246 (0.2%)
All	All	0.19	1/11693 (0.0%)	0.43	12/15934 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	108	SER	CA-C	8.75	1.64	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	109	GLN	N-CA-C	-12.28	94.60	110.07
5	H	85	ALA	N-CA-C	-8.80	101.37	112.90
6	L	108	SER	CA-C-O	8.15	131.00	121.54
6	L	108	SER	CB-CA-C	-7.68	100.59	111.80
5	H	85	ALA	N-CA-CB	7.44	121.50	110.33
6	L	107	LEU	N-CA-C	7.03	120.78	110.59
5	H	65	SER	N-CA-C	6.96	118.95	111.36
5	H	83	THR	N-CA-C	-6.95	99.31	109.18
6	L	108	SER	N-CA-C	6.70	120.66	111.54
4	E	54	ASN	N-CA-C	6.13	117.96	111.28
2	G	412	GLN	N-CA-C	5.93	117.42	111.07
5	H	84	THR	CB-CA-C	-5.71	99.79	110.36

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	1077	0	1066	25	0
2	G	3562	0	3486	109	0
3	D	1813	0	1781	33	0
4	E	1615	0	1544	21	0
5	H	1754	0	1719	72	0
6	L	1601	0	1544	33	0
7	A	61	0	52	4	0
7	I	61	0	52	1	0
7	K	61	0	52	3	0
7	Q	61	0	52	3	0
8	C	83	0	70	6	0
9	F	28	0	25	0	0
10	J	39	0	34	2	0
10	M	39	0	34	3	0
10	O	39	0	34	2	0
10	S	39	0	34	1	0
11	N	50	0	43	0	0
11	P	50	0	43	1	0
12	R	50	0	43	5	0
13	T	105	0	86	11	0
14	B	42	0	39	1	0
14	G	84	0	78	1	0
All	All	12314	0	11911	288	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 12.

All (288) 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)
2:G:413:ASN:HD21	12:R:1:NAG:C1	1.51	1.24
5:H:29:ILE:HB	5:H:71:ARG:HD2	1.20	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:413:ASN:ND2	12:R:1:NAG:C1	2.09	1.15
5:H:35:THR:HG21	5:H:100(P):MET:HE2	1.30	1.06
5:H:29:ILE:HD13	5:H:71:ARG:HE	1.20	1.01
5:H:94:THR:HG22	5:H:100(R):VAL:HB	1.43	0.99
2:G:332:ASN:HD21	13:T:1:NAG:C1	1.79	0.95
2:G:266:ALA:H	2:G:287:GLN:HE21	0.96	0.95
3:D:54:SER:HB2	8:C:5:MAN:H62	1.50	0.94
5:H:29:ILE:CB	5:H:71:ARG:HD2	1.98	0.94
2:G:389:PRO:HB3	7:Q:1:NAG:H62	1.47	0.93
5:H:29:ILE:HB	5:H:71:ARG:CD	1.98	0.92
6:L:20:ARG:HG2	6:L:74:THR:HG22	1.52	0.91
6:L:80:VAL:HG12	6:L:109:GLN:NE2	1.86	0.89
2:G:266:ALA:N	2:G:287:GLN:HE21	1.71	0.88
2:G:332:ASN:ND2	13:T:1:NAG:C1	2.40	0.84
2:G:266:ALA:H	2:G:287:GLN:NE2	1.76	0.83
5:H:100(D):VAL:HG22	13:T:1:NAG:H5	1.57	0.83
3:D:126:PRO:HB2	3:D:215:SER:HB2	1.60	0.82
2:G:295:ASN:HD22	10:M:1:NAG:H83	1.44	0.82
2:G:264:SER:OG	2:G:482:GLU:OE1	1.97	0.81
3:D:97:LEU:HD21	7:A:1:NAG:H82	1.63	0.80
5:H:94:THR:CG2	5:H:100(R):VAL:HB	2.12	0.79
2:G:360:ILE:HG21	2:G:395:TRP:HD1	1.47	0.77
2:G:134:VAL:HG21	2:G:154:MET:HG3	1.67	0.77
2:G:38:VAL:HG12	2:G:496:ILE:HG22	1.69	0.74
5:H:100(D):VAL:CG2	13:T:1:NAG:H5	2.17	0.74
5:H:29:ILE:HD13	5:H:71:ARG:NE	2.00	0.74
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.70	0.73
2:G:135:ASN:N	2:G:135:ASN:OD1	2.22	0.73
5:H:35:THR:HG21	5:H:100(P):MET:CE	2.15	0.72
2:G:427:TRP:HD1	2:G:475:MET:HG2	1.55	0.71
5:H:29:ILE:CD1	5:H:71:ARG:HE	2.00	0.70
5:H:20:VAL:HG12	5:H:21:THR:N	2.06	0.70
3:D:168:ALA:HA	3:D:178:LEU:HB3	1.72	0.70
5:H:141:LYS:HZ1	6:L:130:LYS:HD2	1.56	0.70
5:H:148:VAL:HG22	5:H:198:HIS:HD2	1.56	0.69
5:H:199:LYS:HB2	5:H:200:PRO:HD3	1.74	0.69
2:G:121:LYS:HA	2:G:202:THR:HA	1.76	0.68
2:G:360:ILE:HG12	2:G:394:THR:HA	1.76	0.68
2:G:363:HIS:CD2	2:G:364:SER:HB3	2.29	0.67
6:L:80:VAL:HG12	6:L:109:GLN:HE21	1.57	0.67
4:E:136:LEU:HD12	4:E:182:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:142:ASP:HB2	5:H:173:LEU:HB2	1.78	0.66
3:D:150:VAL:HG11	3:D:178:LEU:HD21	1.78	0.66
2:G:219:ALA:O	2:G:246:GLN:NE2	2.29	0.66
6:L:141:TYR:HB3	6:L:142:PRO:HD3	1.78	0.66
7:I:2:NAG:H3	7:I:2:NAG:H83	1.77	0.66
5:H:132:GLY:O	5:H:184:SER:N	2.28	0.65
2:G:264:SER:O	2:G:287:GLN:NE2	2.29	0.65
3:D:146:PHE:HB3	3:D:147:PRO:HD3	1.79	0.65
5:H:195:ASN:ND2	5:H:206:ASP:OD2	2.30	0.65
4:E:50:ILE:HG23	4:E:53:ASP:O	1.96	0.65
2:G:202:THR:HB	2:G:432:LYS:HE2	1.79	0.65
5:H:197:ASN:OD1	5:H:198:HIS:N	2.31	0.64
5:H:84:THR:HA	5:H:109:VAL:HB	1.81	0.63
1:B:616:ASN:HD22	14:B:701:NAG:C7	2.11	0.63
5:H:87:THR:O	5:H:87:THR:HG23	1.99	0.62
4:E:115:ALA:HB3	4:E:144:TYR:H	1.65	0.62
1:B:578:ALA:HB1	2:G:220:PRO:HB3	1.82	0.62
6:L:54:ARG:NH2	6:L:62:PHE:O	2.29	0.62
2:G:137:ASN:HB3	6:L:95(A):GLY:HA2	1.82	0.61
2:G:304:ARG:HB3	2:G:440:ARG:HH11	1.64	0.61
3:D:128:SER:HB2	3:D:220:LEU:HB2	1.82	0.61
2:G:201:ILE:HD11	2:G:435:TYR:HB2	1.83	0.61
5:H:22:CYS:HB3	5:H:78:LEU:HG	1.82	0.61
2:G:266:ALA:N	2:G:287:GLN:NE2	2.42	0.60
2:G:359:ILE:HG23	2:G:465:THR:HG21	1.83	0.60
4:E:26:ASN:HA	4:E:29:CYS:HB2	1.83	0.60
2:G:270:ILE:HG13	2:G:348:LYS:HG3	1.82	0.60
2:G:389:PRO:HD2	2:G:416:LEU:HD22	1.83	0.60
1:B:585:ARG:NH2	2:G:491:ILE:O	2.34	0.59
1:B:608:VAL:N	1:B:650:GLN:OE1	2.36	0.59
2:G:392:ASN:HD21	7:Q:1:NAG:H83	1.68	0.59
6:L:83:GLU:HB2	6:L:106:VAL:HG23	1.85	0.59
2:G:262:ASN:HD21	7:K:1:NAG:C1	2.16	0.58
2:G:361:PHE:HB3	2:G:468:PHE:HB2	1.84	0.58
5:H:20:VAL:CG1	5:H:21:THR:N	2.66	0.58
6:L:83:GLU:HG3	6:L:104:LEU:O	2.02	0.58
5:H:169:GLN:HG3	6:L:161:GLU:HG3	1.86	0.58
2:G:393:SER:HA	2:G:406:TYR:HD2	1.68	0.58
2:G:280:ASN:HD22	2:G:458:GLY:HA2	1.68	0.58
3:D:148:GLU:N	3:D:149:PRO:HD2	2.19	0.58
1:B:607:ASN:OD1	1:B:607:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ASP:OD1	2:G:57:ASP:N	2.37	0.57
5:H:100(D):VAL:HG22	13:T:1:NAG:C5	2.32	0.57
6:L:66:PRO:HB2	13:T:5:MAN:O3	2.04	0.57
5:H:124:PRO:HG3	5:H:136:LEU:HB3	1.85	0.57
2:G:407:PRO:HG2	2:G:410:GLY:HA3	1.87	0.57
5:H:141:LYS:HG2	5:H:142:ASP:H	1.70	0.57
3:D:66:ARG:NH2	3:D:86:ASP:OD2	2.38	0.56
1:B:528:SER:OG	8:C:1:NAG:O7	2.21	0.56
2:G:463:ASN:H	2:G:463:ASN:HD22	1.52	0.56
1:B:523:LEU:HD11	2:G:491:ILE:HD11	1.88	0.56
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.69	0.56
2:G:190:ASN:OD1	2:G:190:ASN:N	2.38	0.56
4:E:29:CYS:SG	4:E:30:CYS:N	2.78	0.56
5:H:84:THR:O	5:H:87:THR:HG22	2.05	0.56
2:G:360:ILE:HG21	2:G:395:TRP:CD1	2.35	0.56
1:B:607:ASN:OD1	1:B:650:GLN:NE2	2.39	0.56
3:D:168:ALA:HB2	3:D:178:LEU:HD23	1.87	0.55
2:G:413:ASN:HD22	12:R:1:NAG:C1	2.15	0.55
1:B:610:TRP:HB3	2:G:34:LYS:HB2	1.89	0.55
3:D:1:GLU:HG3	7:A:2:NAG:O7	2.06	0.55
5:H:19:SER:O	5:H:20:VAL:HG23	2.07	0.54
5:H:20:VAL:CG1	5:H:21:THR:H	2.20	0.54
5:H:94:THR:HG23	5:H:94:THR:O	2.07	0.54
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.90	0.54
6:L:12:SER:HB3	6:L:107:LEU:HD11	1.88	0.54
2:G:447:SER:OG	7:K:1:NAG:N2	2.36	0.53
12:R:2:NAG:H3	12:R:2:NAG:H83	1.90	0.53
2:G:200:VAL:HG23	2:G:432:LYS:HG3	1.91	0.53
4:E:29:CYS:HB3	4:E:32:HIS:CE1	2.44	0.53
5:H:29:ILE:CG2	5:H:71:ARG:HD2	2.38	0.53
5:H:144:PHE:H	5:H:145:PRO:HD2	1.74	0.53
8:C:3:BMA:H2	8:C:7:MAN:H5	1.91	0.53
3:D:87:THR:HG23	3:D:110:THR:HA	1.89	0.53
5:H:20:VAL:HG12	5:H:21:THR:H	1.71	0.53
5:H:184:SER:HA	5:H:187:LEU:HB2	1.90	0.52
4:E:54:ASN:OD1	4:E:54:ASN:N	2.39	0.52
3:D:151:THR:OG1	3:D:199:ASN:O	2.25	0.52
5:H:129:THR:OG1	5:H:133:THR:OG1	2.00	0.52
1:B:644:THR:O	1:B:648:VAL:HG12	2.09	0.52
2:G:455:THR:N	2:G:469:ARG:O	2.42	0.52
3:D:99:ASP:OD1	3:D:100:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:134:VAL:HG11	2:G:154:MET:HE3	1.92	0.52
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.45	0.52
2:G:463:ASN:ND2	2:G:463:ASN:O	2.43	0.52
3:D:31:PHE:HA	8:C:1:NAG:O6	2.09	0.52
2:G:151:THR:OG1	2:G:152:GLY:N	2.42	0.52
5:H:87:THR:OG1	5:H:108:THR:HA	2.10	0.51
3:D:2:GLY:N	7:A:2:NAG:H82	2.26	0.51
4:E:37:TRP:HB2	4:E:50:ILE:HB	1.92	0.51
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.45	0.51
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.92	0.51
13:T:4:MAN:O4	13:T:4:MAN:O6	2.29	0.51
2:G:444:ARG:NH2	12:R:2:NAG:O7	2.44	0.51
1:B:544:LEU:HD21	2:G:493:PRO:HG3	1.93	0.51
2:G:167:ASP:OD1	2:G:168:LYS:N	2.44	0.51
2:G:199:SER:OG	2:G:431:GLY:O	2.26	0.51
6:L:46:LEU:O	6:L:46:LEU:HD12	2.10	0.51
6:L:48:ILE:HG12	6:L:54:ARG:HG2	1.93	0.51
2:G:112:TRP:CD2	2:G:427:TRP:HH2	2.29	0.50
1:B:617:LYS:HE3	1:B:626:MET:HE1	1.93	0.50
5:H:87:THR:O	5:H:87:THR:CG2	2.59	0.50
6:L:50:ASN:HB3	6:L:53:ASP:HB2	1.93	0.50
5:H:114:THR:HG23	5:H:145:PRO:HG3	1.94	0.50
2:G:363:HIS:HD2	2:G:364:SER:HB3	1.74	0.50
2:G:411:GLU:O	7:Q:2:NAG:H81	2.12	0.50
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.93	0.50
5:H:100(D):VAL:HA	13:T:2:NAG:O7	2.12	0.50
6:L:13:VAL:HG11	6:L:19:ALA:HB2	1.93	0.50
6:L:51:ASN:HB3	6:L:52:GLN:OE1	2.12	0.50
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.77	0.49
2:G:349:LEU:O	2:G:353:PHE:HB2	2.12	0.49
5:H:19:SER:O	5:H:20:VAL:CG2	2.61	0.49
2:G:93:PHE:CD2	2:G:228:CYS:HB2	2.48	0.49
2:G:112:TRP:CG	2:G:427:TRP:HH2	2.31	0.49
5:H:61:PRO:HA	5:H:64:ASN:HB2	1.95	0.49
2:G:388:THR:HB	2:G:389:PRO:HD3	1.94	0.49
3:D:30:ASN:O	8:C:1:NAG:O6	2.31	0.49
4:E:30:CYS:HB3	4:E:68:LYS:HD2	1.93	0.49
1:B:515:LEU:HD23	1:B:515:LEU:H	1.78	0.48
1:B:625:ASN:HD22	7:A:1:NAG:C1	2.26	0.48
2:G:391:PHE:CE2	2:G:470:PRO:HG3	2.48	0.48
6:L:107:LEU:O	6:L:108:SER:OG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:93:PHE:CE2	2:G:228:CYS:HB2	2.48	0.48
2:G:120:VAL:O	2:G:203:GLN:N	2.42	0.48
5:H:7:SER:O	5:H:20:VAL:HG13	2.13	0.48
5:H:100(A):ILE:HG23	5:H:100(J):PHE:HB3	1.95	0.48
5:H:143:TYR:O	5:H:174:TYR:N	2.35	0.48
6:L:67(A):ILE:HG22	13:T:5:MAN:H2	1.95	0.48
6:L:168:GLN:HG2	6:L:172:LYS:O	2.13	0.48
1:B:610:TRP:CE3	2:G:498:PRO:HB3	2.49	0.48
2:G:98:ASN:ND2	2:G:486:TYR:O	2.47	0.48
4:E:198:GLN:HG2	4:E:207:GLU:HG3	1.95	0.48
5:H:60:ASN:O	5:H:64:ASN:N	2.47	0.48
5:H:100(D):VAL:HG12	5:H:100(F):SER:H	1.78	0.48
2:G:229:ASN:CG	10:J:1:NAG:H62	2.39	0.48
2:G:265:LEU:HD11	2:G:291:ALA:HB2	1.96	0.48
5:H:144:PHE:N	5:H:145:PRO:HD2	2.29	0.48
2:G:105:HIS:CG	2:G:476:ARG:HG2	2.48	0.48
4:E:36:SER:OG	4:E:91:CYS:HB3	2.14	0.48
5:H:139:LEU:HD23	5:H:140:VAL:N	2.29	0.47
3:D:94:LYS:HB3	3:D:102:LEU:HB2	1.96	0.47
11:P:3:BMA:O2	11:P:4:MAN:C1	2.63	0.47
2:G:293:GLU:OE2	10:S:1:NAG:H61	2.15	0.47
2:G:276:ASN:HB3	2:G:282:LYS:HG3	1.96	0.47
5:H:121:PRO:O	6:L:122:SER:HB3	2.15	0.47
6:L:36:TYR:CE1	6:L:46:LEU:HB3	2.50	0.47
2:G:67:ASN:OD1	2:G:209:SER:OG	2.31	0.47
2:G:216:HIS:ND1	2:G:248:THR:O	2.45	0.47
5:H:143:TYR:CZ	5:H:148:VAL:HG21	2.50	0.47
2:G:230:SER:HB2	2:G:233:PHE:HB2	1.96	0.47
5:H:35:THR:OG1	5:H:47:TRP:NE1	2.44	0.47
7:K:3:BMA:H2	7:K:4:MAN:H5	1.97	0.47
2:G:223:PHE:CE2	2:G:490:LYS:HB3	2.50	0.46
4:E:50:ILE:HD13	4:E:56:ARG:HA	1.98	0.46
1:B:607:ASN:H	1:B:650:GLN:CD	2.24	0.46
2:G:156:ASN:OD1	2:G:157:CYS:N	2.49	0.46
4:E:188:GLN:O	4:E:192:HIS:ND1	2.48	0.46
10:O:2:NAG:O7	10:O:2:NAG:O3	2.30	0.46
3:D:47:TRP:CH2	4:E:98:GLY:HA3	2.51	0.46
3:D:114:ALA:HB3	3:D:146:PHE:CZ	2.51	0.46
3:D:207:VAL:HG12	3:D:209:LYS:HG2	1.97	0.46
10:O:2:NAG:H4	10:O:3:BMA:H2	1.73	0.45
5:H:146:GLU:N	5:H:147:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:279:ASP:HB3	2:G:282:LYS:HG2	1.97	0.45
5:H:94:THR:CG2	5:H:94:THR:O	2.64	0.45
5:H:2:VAL:HA	5:H:26:GLY:HA3	1.98	0.45
3:D:56:ASP:OD1	3:D:57:LYS:N	2.49	0.45
6:L:67(A):ILE:HG13	6:L:67(B):ASN:H	1.82	0.45
2:G:280:ASN:ND2	2:G:458:GLY:HA2	2.32	0.45
2:G:363:HIS:HA	2:G:470:PRO:HD2	1.99	0.45
5:H:143:TYR:CE1	5:H:174:TYR:HB2	2.52	0.45
5:H:18:LEU:O	5:H:81:GLN:HA	2.16	0.45
6:L:31:ARG:NH1	6:L:51:ASN:ND2	2.65	0.45
2:G:274:SER:HB3	2:G:277:ILE:HG12	1.98	0.44
2:G:203:GLN:HE22	2:G:318:TYR:HD2	1.65	0.44
5:H:100:ARG:HH12	13:T:5:MAN:C6	2.31	0.44
3:D:116:THR:HG23	3:D:147:PRO:HG2	2.00	0.44
4:E:38:TYR:CZ	4:E:48:LEU:HD13	2.52	0.44
5:H:182:VAL:HG21	5:H:192:TYR:HE2	1.82	0.44
10:M:1:NAG:H61	10:M:2:NAG:C7	2.48	0.44
1:B:525:ALA:HB1	1:B:528:SER:HB2	1.98	0.44
3:D:189:LEU:HD22	3:D:213:PRO:HB2	1.99	0.44
3:D:94:LYS:HG2	3:D:95:GLY:N	2.31	0.44
2:G:384:TYR:OH	2:G:424:ILE:HD13	2.17	0.44
2:G:192:ARG:NH2	14:G:602:NAG:O5	2.50	0.44
2:G:385:CYS:HA	2:G:418:CYS:HA	2.00	0.44
5:H:117:PRO:HB3	5:H:143:TYR:HD2	1.83	0.44
5:H:51:ILE:HD11	5:H:55:GLU:HA	1.99	0.44
5:H:142:ASP:OD1	5:H:142:ASP:N	2.51	0.43
2:G:332:ASN:HB3	10:M:1:NAG:H81	2.00	0.43
4:E:85:GLU:HG3	4:E:108:SER:HA	2.00	0.43
6:L:31:ARG:HH12	6:L:51:ASN:ND2	2.16	0.43
2:G:195:ASN:HD21	2:G:201:ILE:HD12	1.82	0.43
5:H:19:SER:C	5:H:20:VAL:HG23	2.43	0.43
1:B:641:HIS:O	1:B:644:THR:OG1	2.34	0.43
6:L:156:VAL:HG11	6:L:179:LEU:HD11	2.00	0.43
2:G:160:ASN:OD1	2:G:160:ASN:N	2.51	0.43
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.53	0.43
4:E:169:SER:O	4:E:177:ALA:N	2.44	0.43
1:B:596:TRP:CE2	1:B:646:LEU:HD23	2.54	0.43
2:G:55:ALA:N	2:G:216:HIS:O	2.52	0.43
2:G:363:HIS:CE1	2:G:388:THR:HG23	2.54	0.43
1:B:606:THR:HG21	1:B:646:LEU:HD11	2.00	0.42
2:G:363:HIS:HE1	2:G:388:THR:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:117:PRO:HB3	5:H:143:TYR:CD2	2.54	0.42
5:H:29:ILE:HB	5:H:71:ARG:NE	2.32	0.42
5:H:153:ASN:HB2	5:H:156:ALA:HB3	2.01	0.42
2:G:101:VAL:HG13	2:G:479:TRP:HB2	2.00	0.42
2:G:359:ILE:HG12	2:G:465:THR:HB	2.01	0.42
2:G:359:ILE:HG13	2:G:466:GLU:O	2.20	0.42
4:E:126:SER:O	4:E:130:GLN:HG3	2.19	0.42
5:H:96:ARG:HD2	5:H:100(O):TYR:OH	2.20	0.42
6:L:141:TYR:CB	6:L:142:PRO:HD3	2.48	0.42
2:G:338:TRP:HE1	2:G:342:LEU:HD12	1.84	0.42
2:G:50:THR:HG22	2:G:488:VAL:HG21	2.01	0.42
2:G:70:ALA:HB3	2:G:213:ILE:HG22	2.02	0.42
2:G:229:ASN:ND2	10:J:1:NAG:H62	2.35	0.42
6:L:114:PRO:HB3	6:L:140:PHE:HB3	2.02	0.42
1:B:597:GLY:N	1:B:651:ILE:HG12	2.35	0.42
2:G:184:LEU:HG	2:G:190:ASN:HB2	2.02	0.42
2:G:304:ARG:HB3	2:G:440:ARG:NH1	2.34	0.42
6:L:133:LEU:HB2	6:L:179:LEU:HB3	2.02	0.42
3:D:56:ASP:OD2	8:C:4:MAN:O4	2.38	0.41
2:G:505:VAL:O	2:G:507:GLN:HG3	2.21	0.41
4:E:94:THR:OG1	4:E:97:SER:HB3	2.19	0.41
2:G:496:ILE:H	2:G:496:ILE:HG13	1.63	0.41
3:D:63:PHE:HB3	3:D:67:VAL:CG2	2.49	0.41
13:T:5:MAN:H2	13:T:6:MAN:H2	1.87	0.41
2:G:121:LYS:HE2	2:G:121:LYS:HB3	1.88	0.41
3:D:80:MET:HE3	3:D:82:ILE:HD13	2.03	0.41
3:D:148:GLU:N	3:D:149:PRO:CD	2.83	0.41
5:H:93:ALA:HB1	5:H:100(P):MET:HB3	2.01	0.41
6:L:146:THR:OG1	6:L:197:THR:HB	2.21	0.41
3:D:28:ARG:HG2	3:D:72(H):PHE:O	2.20	0.41
4:E:37:TRP:HD1	4:E:50:ILE:HG21	1.85	0.41
5:H:182:VAL:HG11	5:H:192:TYR:CE2	2.56	0.41
5:H:151:SER:OG	5:H:195:ASN:HB2	2.20	0.40
2:G:231:LYS:HD3	2:G:231:LYS:HA	1.90	0.40
4:E:52:GLU:O	4:E:53:ASP:HB2	2.22	0.40
5:H:39:GLN:OE1	6:L:38:HIS:NE2	2.54	0.40
2:G:257:THR:OG1	2:G:375:SER:OG	2.30	0.40
6:L:65:THR:OG1	6:L:71:ALA:HA	2.21	0.40
1:B:601:LYS:HE2	1:B:604:CYS:HB3	2.03	0.40
3:D:100(E):LEU:HD12	3:D:100(F):PRO:HD2	2.03	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	B	132/153 (86%)	120 (91%)	11 (8%)	1 (1%)	16	49
2	G	447/482 (93%)	411 (92%)	36 (8%)	0	100	100
3	D	238/243 (98%)	229 (96%)	9 (4%)	0	100	100
4	E	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
5	H	227/236 (96%)	215 (95%)	12 (5%)	0	100	100
6	L	209/214 (98%)	191 (91%)	18 (9%)	0	100	100
All	All	1464/1544 (95%)	1363 (93%)	100 (7%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	651	ILE

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	115/130 (88%)	111 (96%)	4 (4%)	32	54
2	G	401/427 (94%)	382 (95%)	19 (5%)	23	48
3	D	203/206 (98%)	202 (100%)	1 (0%)	81	81
4	E	186/189 (98%)	184 (99%)	2 (1%)	65	73
5	H	199/204 (98%)	194 (98%)	5 (2%)	42	61
6	L	177/180 (98%)	175 (99%)	2 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1281/1336 (96%)	1248 (97%)	33 (3%)	40 60

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

Mol	Chain	Res	Type
1	B	607	ASN
1	B	624	ASP
1	B	639	THR
1	B	651	ILE
2	G	54	CYS
2	G	135	ASN
2	G	160	ASN
2	G	188	ILE
2	G	190	ASN
2	G	201	ILE
2	G	264	SER
2	G	326	ILE
2	G	361	PHE
2	G	378	CYS
2	G	408	THR
2	G	411	GLU
2	G	414	ILE
2	G	448	ASN
2	G	463	ASN
2	G	465	THR
2	G	467	THR
2	G	496	ILE
2	G	507	GLN
3	D	148	GLU
4	E	26	ASN
4	E	28	VAL
5	H	32	TYR
5	H	78	LEU
5	H	115	LYS
5	H	187	LEU
5	H	190	GLN
6	L	31	ARG
6	L	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	630	GLN
2	G	92	ASN
2	G	133	ASN
2	G	138	ASN
2	G	262	ASN
2	G	287	GLN
2	G	332	ASN
2	G	363	HIS
2	G	413	ASN
2	G	422	GLN
2	G	463	ASN
3	D	192	GLN
3	D	199	ASN
4	E	201	HIS
6	L	34	GLN
6	L	51	ASN
6	L	109	GLN
6	L	168	GLN
6	L	170	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 ⓘ

62 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	14,14,15	0.58	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	2	7	14,14,15	0.27	0	17,19,21	1.12	1 (5%)
7	BMA	A	3	7	11,11,12	0.59	0	15,15,17	1.50	2 (13%)
7	MAN	A	4	7	11,11,12	0.55	0	15,15,17	0.71	0
7	MAN	A	5	7	11,11,12	0.45	0	15,15,17	0.55	0
8	NAG	C	1	8,2	14,14,15	0.53	0	17,19,21	0.44	0
8	NAG	C	2	8	14,14,15	0.39	0	17,19,21	0.52	0
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	1.18	2 (13%)
8	MAN	C	4	8	11,11,12	0.91	1 (9%)	15,15,17	2.38	5 (33%)
8	MAN	C	5	8	11,11,12	0.52	0	15,15,17	1.09	0
8	MAN	C	6	8	11,11,12	0.28	0	15,15,17	0.69	0
8	MAN	C	7	8	11,11,12	0.26	0	15,15,17	0.72	0
9	NAG	F	1	9,2	14,14,15	0.20	0	17,19,21	0.50	0
9	NAG	F	2	9	14,14,15	0.35	0	17,19,21	0.48	0
7	NAG	I	1	7,2	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	I	2	7	14,14,15	1.23	1 (7%)	17,19,21	1.37	1 (5%)
7	BMA	I	3	7	11,11,12	0.36	0	15,15,17	1.07	1 (6%)
7	MAN	I	4	7	11,11,12	0.44	0	15,15,17	0.77	0
7	MAN	I	5	7	11,11,12	0.36	0	15,15,17	0.71	0
10	NAG	J	1	10,2	14,14,15	0.93	1 (7%)	17,19,21	1.84	5 (29%)
10	NAG	J	2	10	14,14,15	0.98	1 (7%)	17,19,21	0.84	1 (5%)
10	BMA	J	3	10	11,11,12	0.40	0	15,15,17	0.69	0
7	NAG	K	1	7	14,14,15	1.07	1 (7%)	17,19,21	0.52	0
7	NAG	K	2	7	14,14,15	0.14	0	17,19,21	0.49	0
7	BMA	K	3	7	11,11,12	0.43	0	15,15,17	1.06	1 (6%)
7	MAN	K	4	7	11,11,12	0.56	0	15,15,17	0.78	0
7	MAN	K	5	7	11,11,12	0.42	0	15,15,17	0.62	0
10	NAG	M	1	10,2	14,14,15	0.71	0	17,19,21	0.57	0
10	NAG	M	2	10	14,14,15	0.40	0	17,19,21	1.39	3 (17%)
10	BMA	M	3	10	11,11,12	0.38	0	15,15,17	0.69	0
11	NAG	N	1	11,2	14,14,15	0.28	0	17,19,21	0.56	0
11	NAG	N	2	11	14,14,15	0.41	0	17,19,21	0.56	0
11	BMA	N	3	11	11,11,12	0.70	0	15,15,17	1.11	0
11	MAN	N	4	11	11,11,12	0.79	0	15,15,17	1.20	2 (13%)
10	NAG	O	1	10,2	14,14,15	0.44	0	17,19,21	0.57	0
10	NAG	O	2	10	14,14,15	0.57	0	17,19,21	0.48	0
10	BMA	O	3	10	11,11,12	0.62	0	15,15,17	0.72	0
11	NAG	P	1	11,2	14,14,15	0.35	0	17,19,21	0.65	0
11	NAG	P	2	11	14,14,15	0.54	0	17,19,21	0.65	0
11	BMA	P	3	11	11,11,12	0.24	0	15,15,17	0.63	0
11	MAN	P	4	11	11,11,12	0.24	0	15,15,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Q	1	7,2	14,14,15	0.32	0	17,19,21	0.49	0
7	NAG	Q	2	7	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
7	BMA	Q	3	7	11,11,12	0.54	0	15,15,17	1.03	1 (6%)
7	MAN	Q	4	7	11,11,12	0.30	0	15,15,17	0.70	0
7	MAN	Q	5	7	11,11,12	0.32	0	15,15,17	0.67	0
12	NAG	R	1	12	14,14,15	0.68	1 (7%)	17,19,21	0.56	0
12	NAG	R	2	12	14,14,15	0.56	0	17,19,21	1.50	2 (11%)
12	BMA	R	3	12	11,11,12	0.32	0	15,15,17	0.66	0
12	MAN	R	4	12	11,11,12	0.59	0	15,15,17	0.57	0
10	NAG	S	1	10,2	14,14,15	0.32	0	17,19,21	0.52	0
10	NAG	S	2	10	14,14,15	0.39	0	17,19,21	0.61	0
10	BMA	S	3	10	11,11,12	0.41	0	15,15,17	0.71	0
13	NAG	T	1	13	14,14,15	0.49	0	17,19,21	0.62	0
13	NAG	T	2	13	14,14,15	0.91	1 (7%)	17,19,21	0.95	2 (11%)
13	BMA	T	3	13	11,11,12	0.81	0	15,15,17	2.38	5 (33%)
13	MAN	T	4	13	11,11,12	0.36	0	15,15,17	1.44	2 (13%)
13	MAN	T	5	13	11,11,12	0.48	0	15,15,17	1.56	2 (13%)
13	MAN	T	6	13	11,11,12	0.24	0	15,15,17	0.63	0
13	MAN	T	7	13	11,11,12	0.32	0	15,15,17	0.80	0
13	MAN	T	8	13	11,11,12	0.36	0	15,15,17	0.52	0
13	MAN	T	9	13	11,11,12	0.41	0	15,15,17	0.73	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	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	2/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	0/1/1/1
8	MAN	C	6	8	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	C	7	8	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
7	NAG	I	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	5/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	2/2/19/22	0/1/1/1
10	NAG	J	1	10,2	-	3/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,2	-	5/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
11	NAG	N	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	4/6/23/26	0/1/1/1
11	BMA	N	3	11	-	1/2/19/22	0/1/1/1
11	MAN	N	4	11	-	1/2/19/22	0/1/1/1
10	NAG	O	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	BMA	O	3	10	-	1/2/19/22	0/1/1/1
11	NAG	P	1	11,2	-	3/6/23/26	0/1/1/1
11	NAG	P	2	11	-	2/6/23/26	0/1/1/1
11	BMA	P	3	11	-	1/2/19/22	0/1/1/1
11	MAN	P	4	11	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12	-	2/6/23/26	0/1/1/1
12	NAG	R	2	12	-	6/6/23/26	0/1/1/1
12	BMA	R	3	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	R	4	12	-	1/2/19/22	0/1/1/1
10	NAG	S	1	10,2	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	1/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	2/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	0/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	2/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	C1-C2	4.26	1.58	1.52
7	K	1	NAG	O5-C1	-3.87	1.37	1.43
10	J	2	NAG	O5-C1	-3.41	1.38	1.43
10	J	1	NAG	O5-C1	-2.56	1.39	1.43
13	T	2	NAG	O5-C1	-2.42	1.39	1.43
12	R	1	NAG	C1-C2	2.31	1.55	1.52
8	C	4	MAN	O2-C2	2.27	1.48	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	4	MAN	C1-C2-C3	-5.22	102.04	109.64
13	T	3	BMA	O5-C1-C2	4.94	122.57	110.79
13	T	3	BMA	O3-C3-C2	-4.82	100.21	110.05
8	C	4	MAN	O2-C2-C3	4.80	120.10	110.15
12	R	2	NAG	C2-N2-C7	4.74	129.26	122.90
10	J	1	NAG	C1-O5-C5	-4.52	106.13	112.19
7	I	2	NAG	C2-N2-C7	4.29	128.65	122.90
10	M	2	NAG	C1-O5-C5	4.15	117.75	112.19
13	T	5	MAN	O2-C2-C1	-3.60	100.99	109.22
13	T	3	BMA	O5-C5-C4	-3.57	102.14	110.83
13	T	4	MAN	C1-C2-C3	3.57	114.84	109.64
10	J	1	NAG	C2-N2-C7	3.28	127.29	122.90
8	C	4	MAN	O2-C2-C1	3.18	116.50	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	5	MAN	O3-C3-C2	-3.13	103.67	110.05
8	C	4	MAN	C6-C5-C4	-3.09	105.42	113.02
7	Q	2	NAG	C2-N2-C7	2.99	126.90	122.90
7	A	3	BMA	C1-O5-C5	-2.92	108.27	112.19
7	K	3	BMA	O3-C3-C2	-2.88	104.19	110.05
13	T	3	BMA	C1-O5-C5	-2.77	108.47	112.19
12	R	2	NAG	C1-C2-N2	2.69	114.68	110.43
7	I	3	BMA	O5-C5-C6	2.63	112.78	107.66
7	A	2	NAG	C2-N2-C7	2.60	126.38	122.90
10	J	1	NAG	O4-C4-C5	-2.53	103.10	109.32
7	A	3	BMA	O5-C1-C2	-2.48	104.86	110.79
10	J	1	NAG	C1-C2-N2	2.45	114.29	110.43
10	J	2	NAG	C1-O5-C5	2.42	115.42	112.19
10	M	2	NAG	C2-N2-C7	2.40	126.12	122.90
13	T	3	BMA	O2-C2-C1	2.29	114.47	109.22
8	C	3	BMA	C1-O5-C5	-2.25	109.17	112.19
11	N	4	MAN	C1-O5-C5	2.19	115.12	112.19
10	M	2	NAG	C1-C2-N2	2.18	113.86	110.43
13	T	2	NAG	C3-C4-C5	-2.15	106.33	110.23
11	N	4	MAN	C1-C2-C3	2.15	112.77	109.64
7	Q	3	BMA	O5-C5-C6	-2.14	103.51	107.66
8	C	4	MAN	O4-C4-C5	-2.08	104.20	109.32
8	C	3	BMA	C3-C4-C5	-2.08	106.47	110.23
13	T	4	MAN	O2-C2-C1	-2.07	104.48	109.22
10	J	1	NAG	C3-C4-C5	2.02	113.90	110.23
13	T	2	NAG	O4-C4-C5	-2.01	104.38	109.32

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2	NAG	C1-C2-N2-C7
10	J	1	NAG	C1-C2-N2-C7
10	J	1	NAG	C4-C5-C6-O6
11	P	1	NAG	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
8	C	4	MAN	C4-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
13	T	4	MAN	O5-C5-C6-O6
8	C	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	7	MAN	O5-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
11	P	2	NAG	O5-C5-C6-O6
13	T	8	MAN	O5-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
11	P	1	NAG	C4-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
13	T	8	MAN	C4-C5-C6-O6
8	C	5	MAN	O5-C5-C6-O6
11	N	4	MAN	O5-C5-C6-O6
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	Q	1	NAG	C8-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
11	N	2	NAG	C8-C7-N2-C2
11	N	2	NAG	O7-C7-N2-C2
12	R	1	NAG	C8-C7-N2-C2
12	R	1	NAG	O7-C7-N2-C2
12	R	2	NAG	C8-C7-N2-C2
12	R	2	NAG	O7-C7-N2-C2
13	T	1	NAG	C8-C7-N2-C2
13	T	1	NAG	O7-C7-N2-C2
11	N	2	NAG	C4-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
11	P	2	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
11	N	1	NAG	C4-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
11	N	2	NAG	O5-C5-C6-O6
8	C	6	MAN	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
13	T	7	MAN	O5-C5-C6-O6

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

There are no ring outliers.

28 monomers are involved in 42 short contacts:

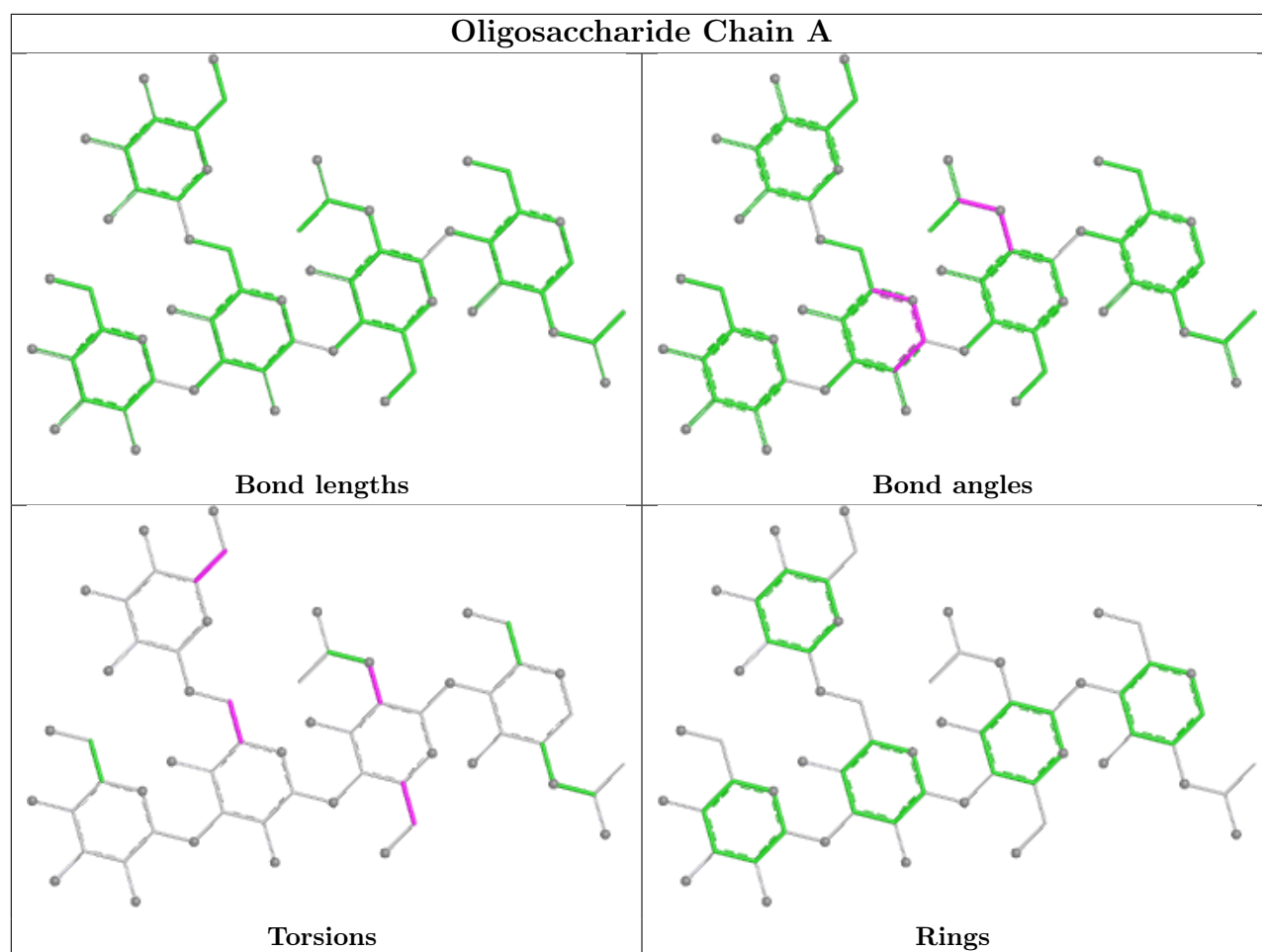
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	2	NAG	2	0

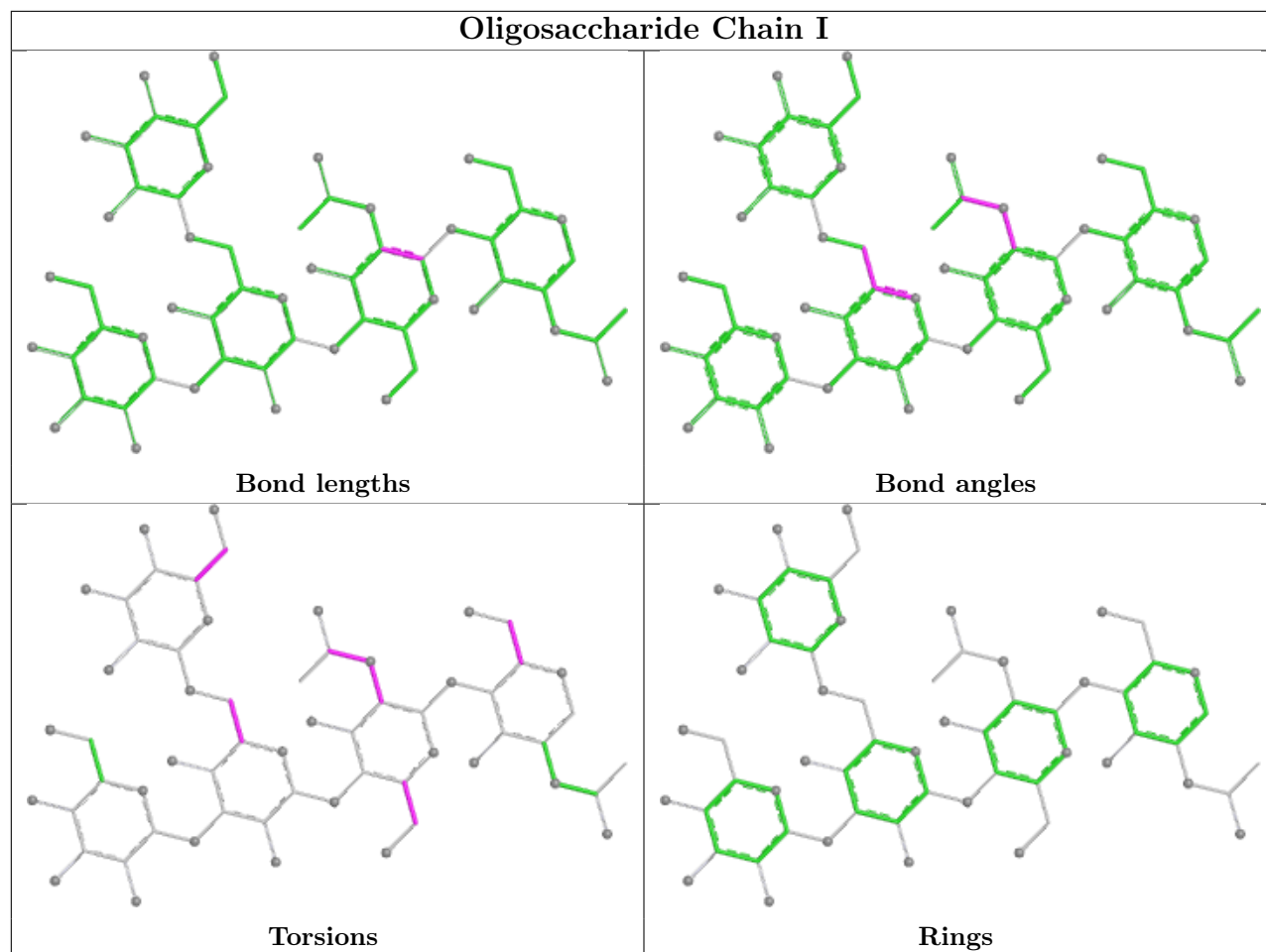
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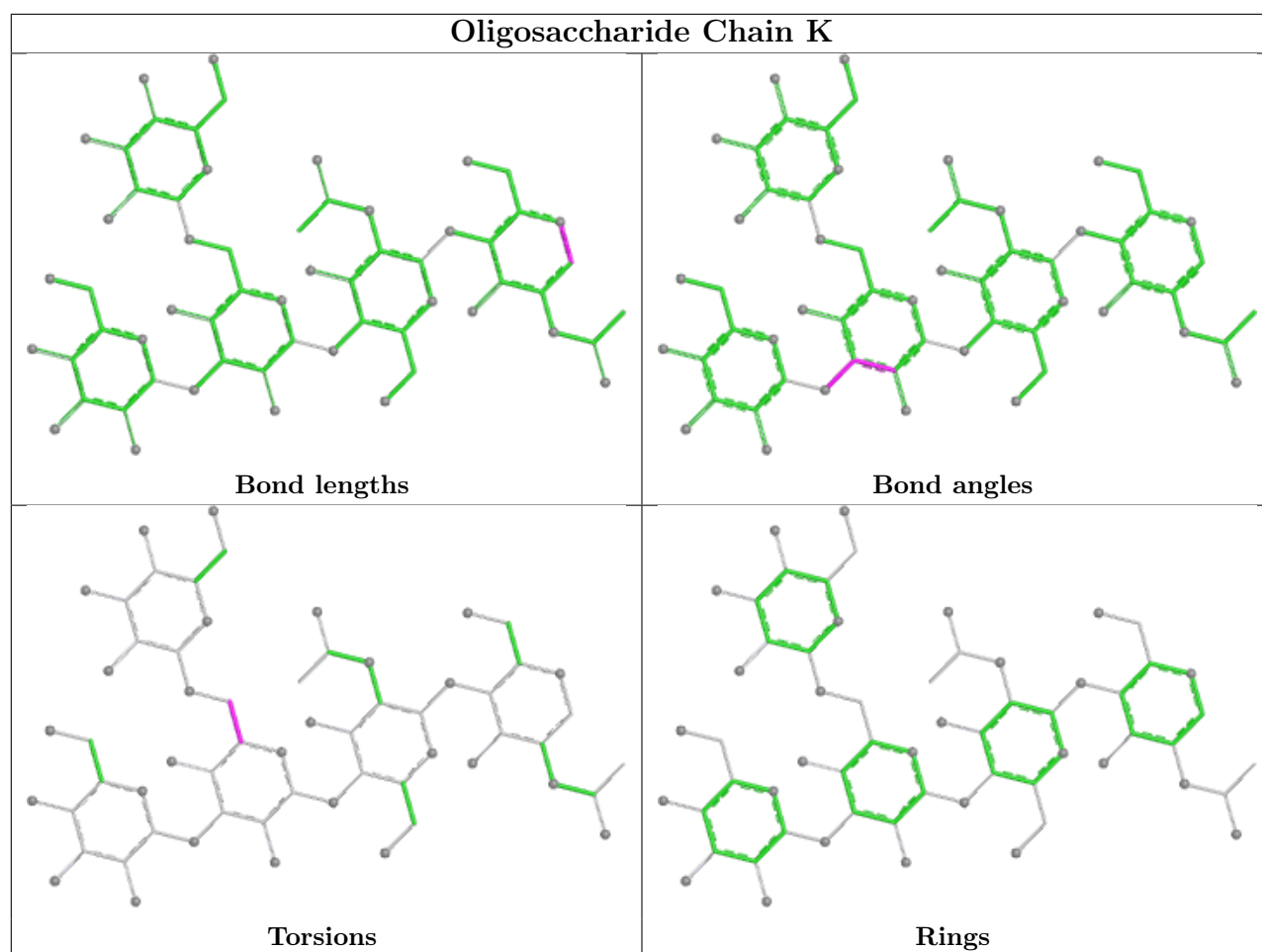
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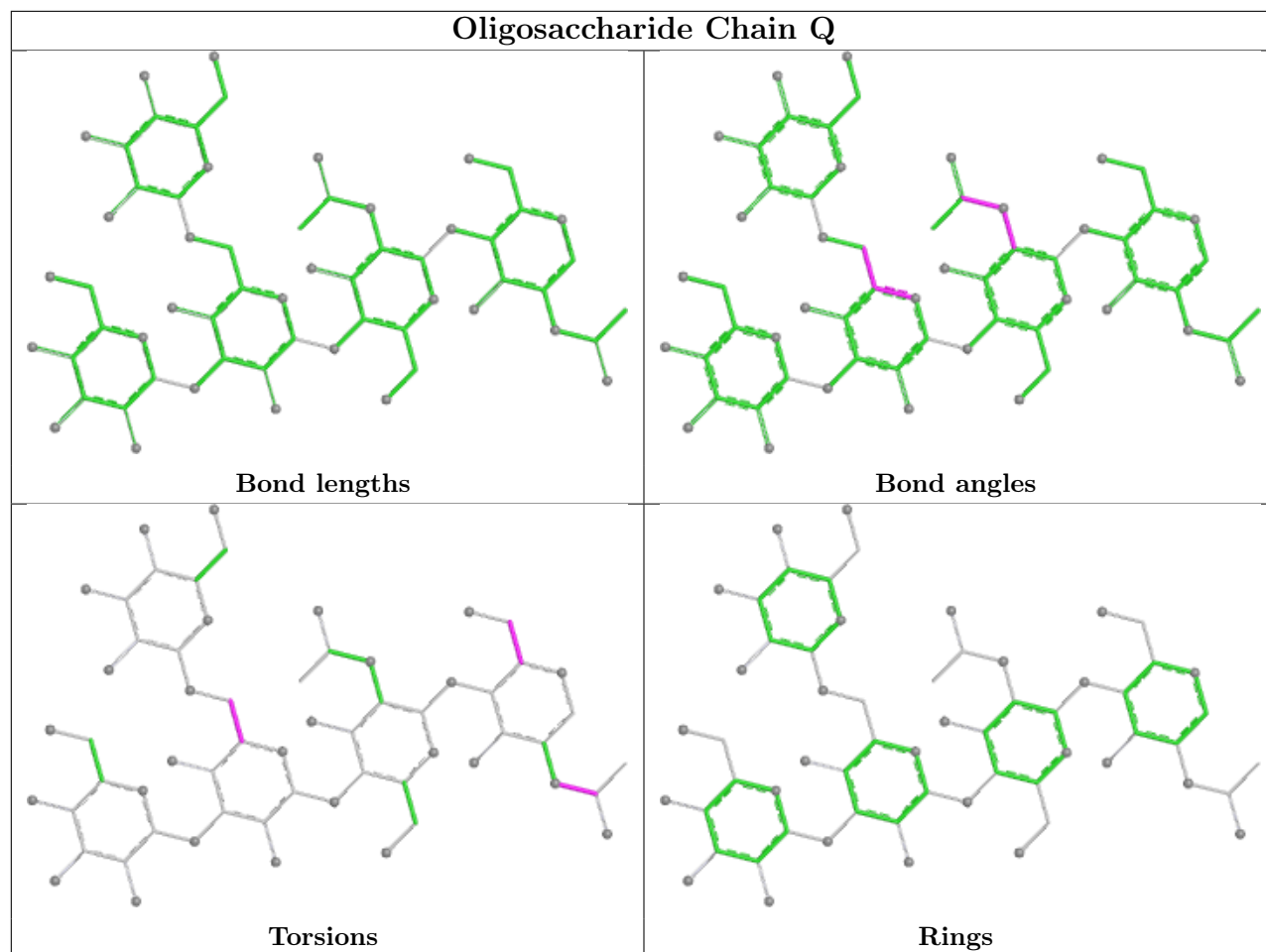
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3	BMA	1	0
8	C	7	MAN	1	0
7	I	2	NAG	1	0
13	T	1	NAG	5	0
10	S	1	NAG	1	0
13	T	2	NAG	1	0
8	C	4	MAN	1	0
12	R	1	NAG	3	0
8	C	5	MAN	1	0
7	Q	2	NAG	1	0
7	K	3	BMA	1	0
8	C	1	NAG	3	0
10	O	2	NAG	2	0
11	P	3	BMA	1	0
7	Q	1	NAG	2	0
7	A	1	NAG	2	0
13	T	5	MAN	4	0
10	J	1	NAG	2	0
10	M	2	NAG	1	0
13	T	6	MAN	1	0
10	O	3	BMA	1	0
7	A	2	NAG	2	0
11	P	4	MAN	1	0
7	K	4	MAN	1	0
10	M	1	NAG	3	0
7	K	1	NAG	2	0
13	T	4	MAN	1	0

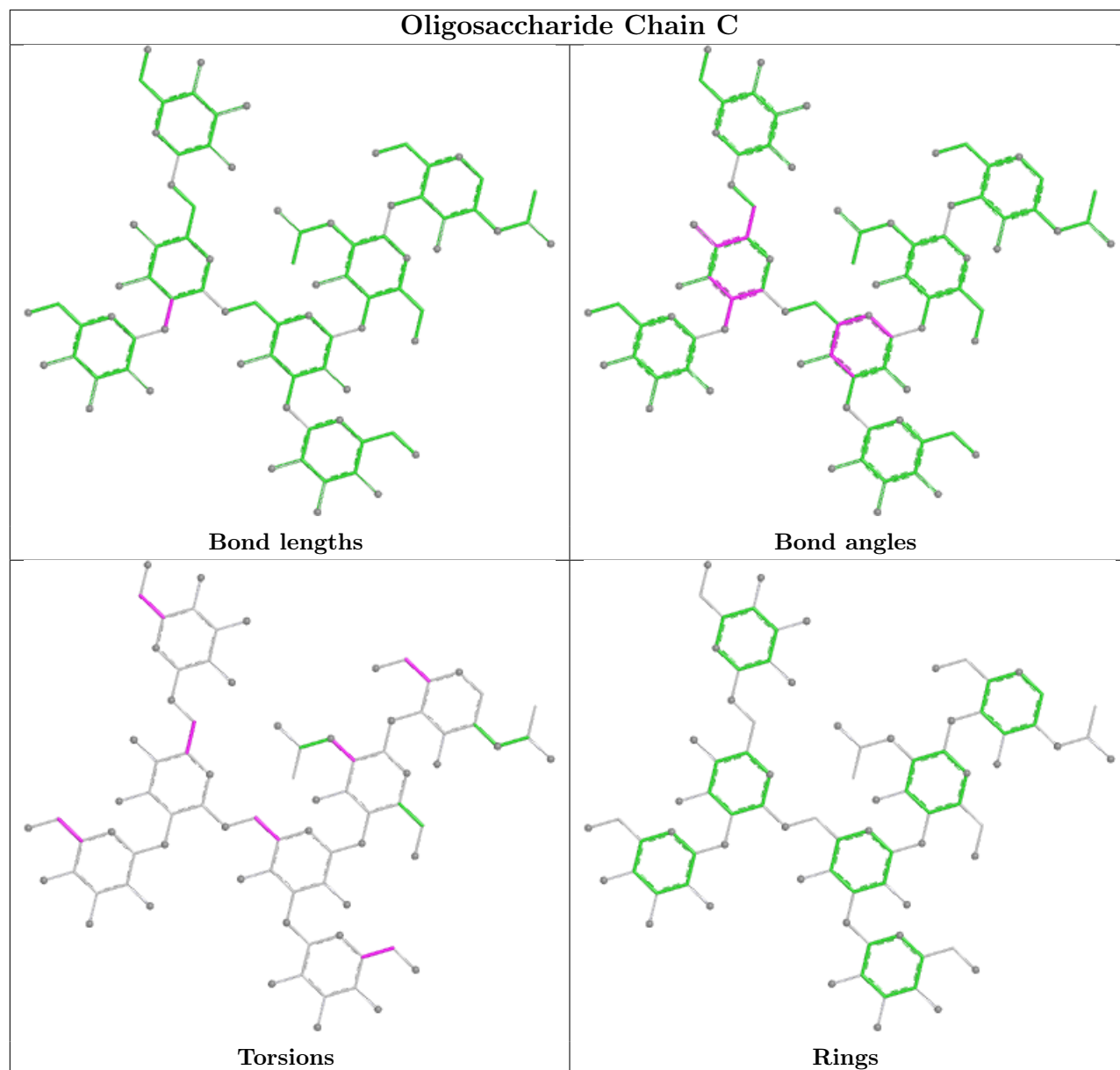
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

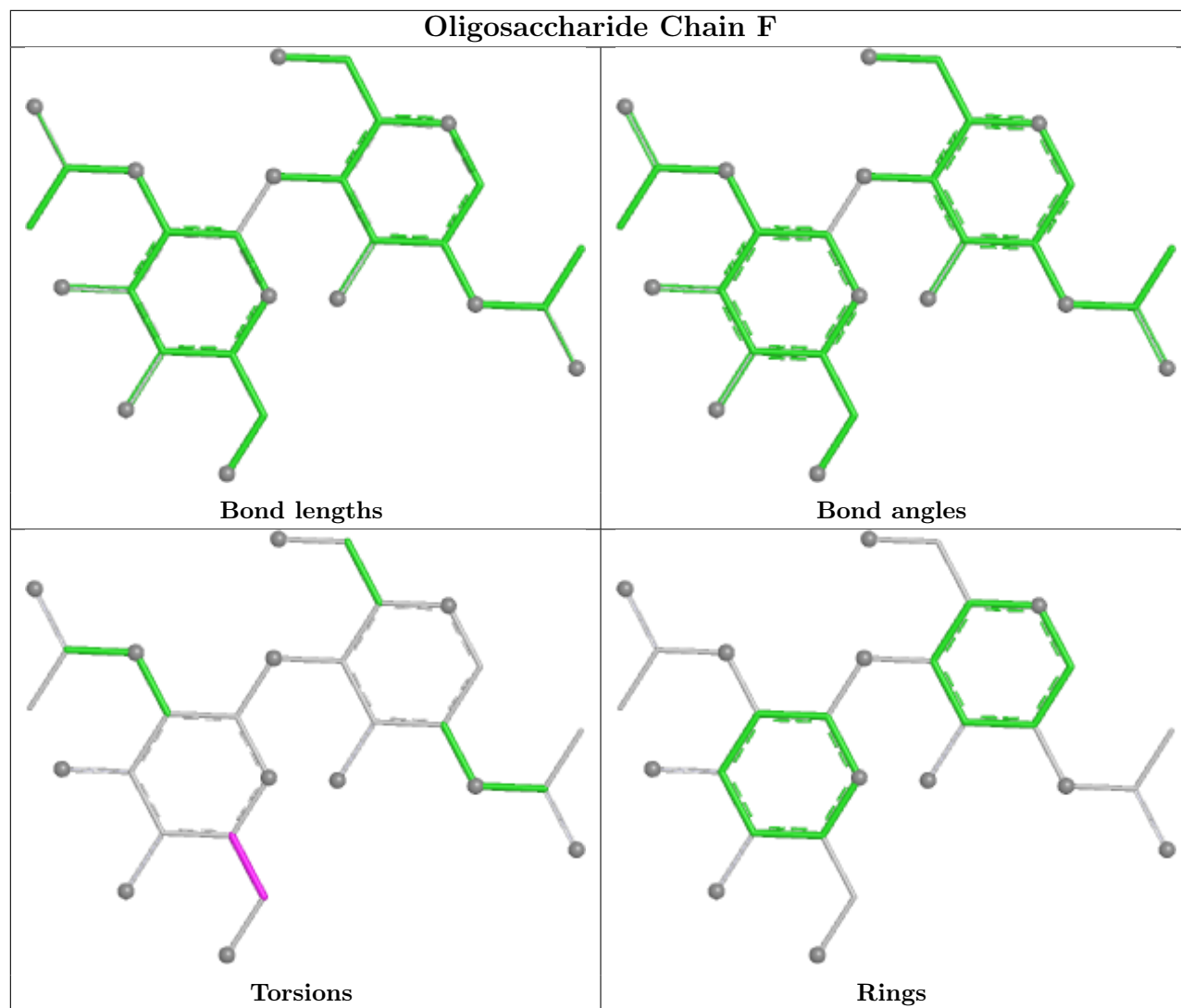


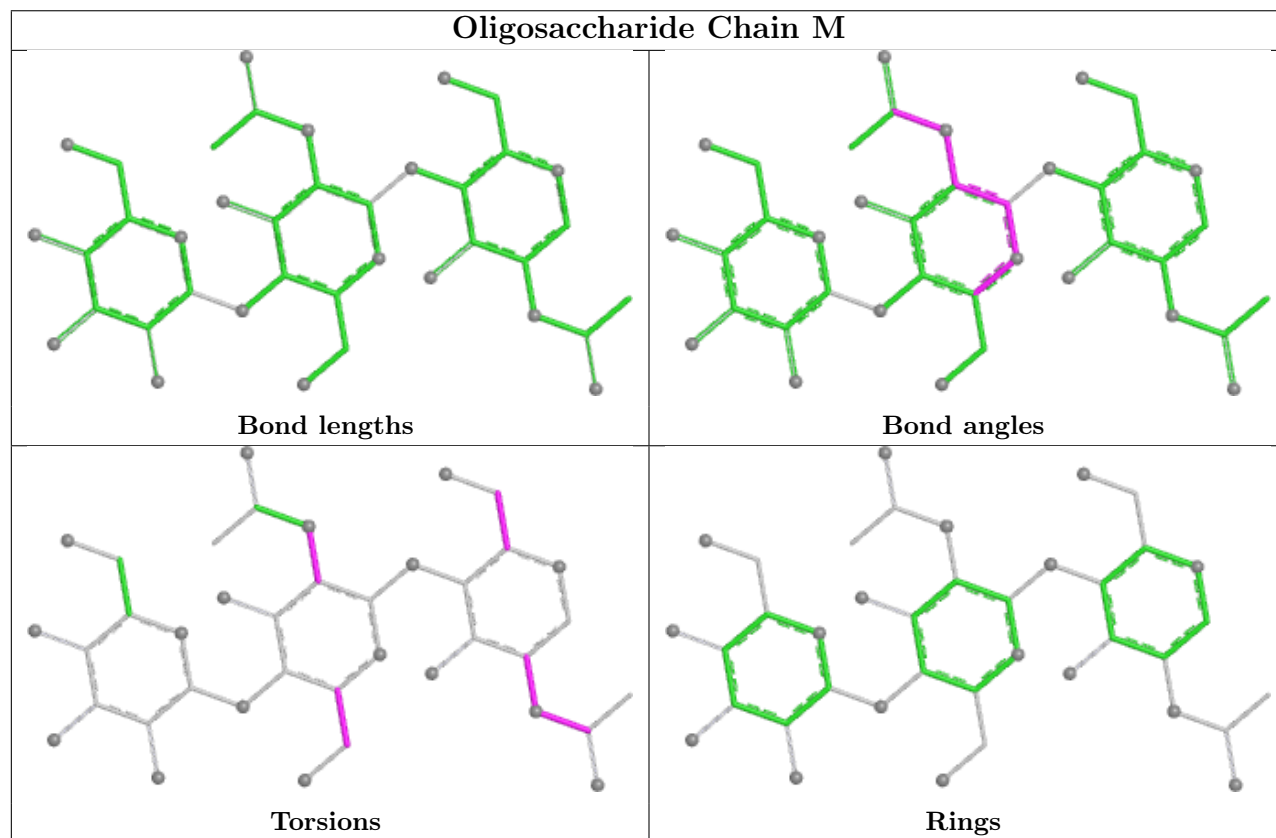
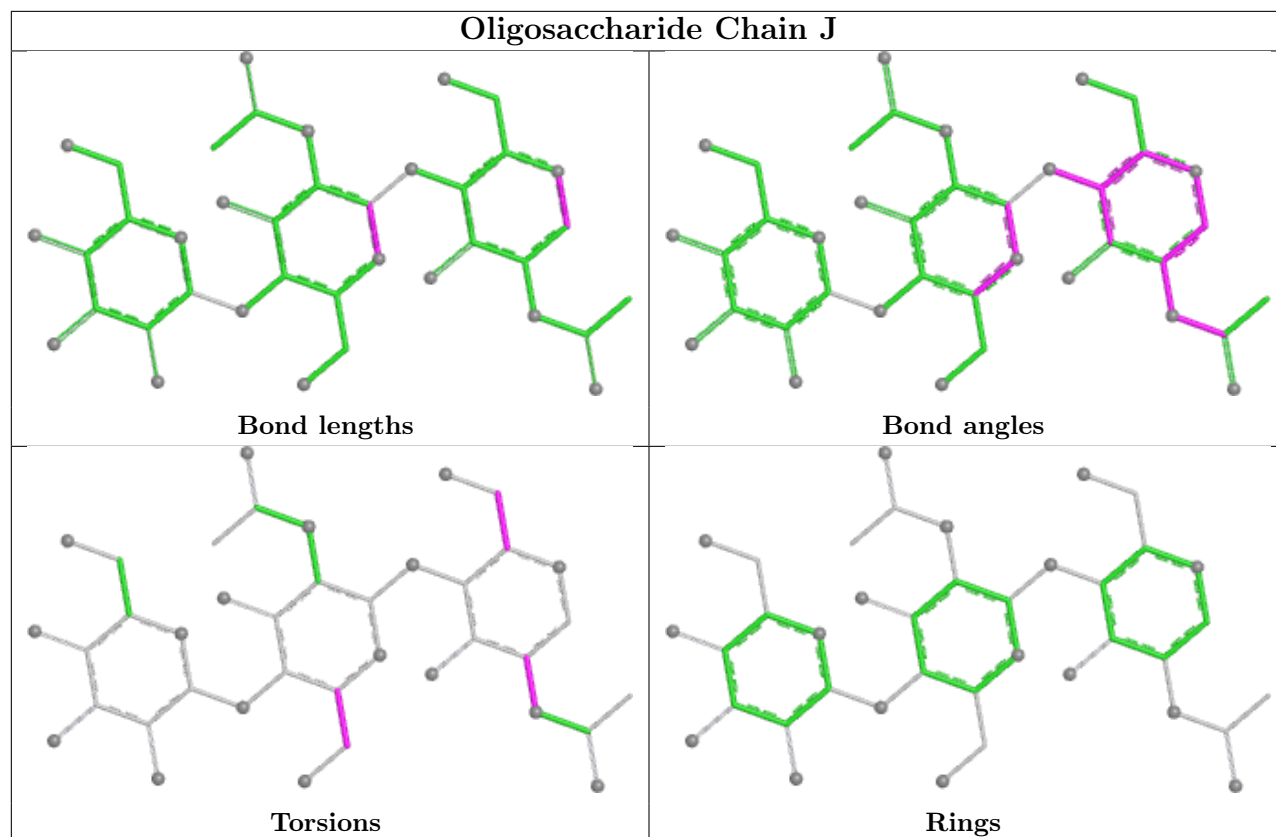


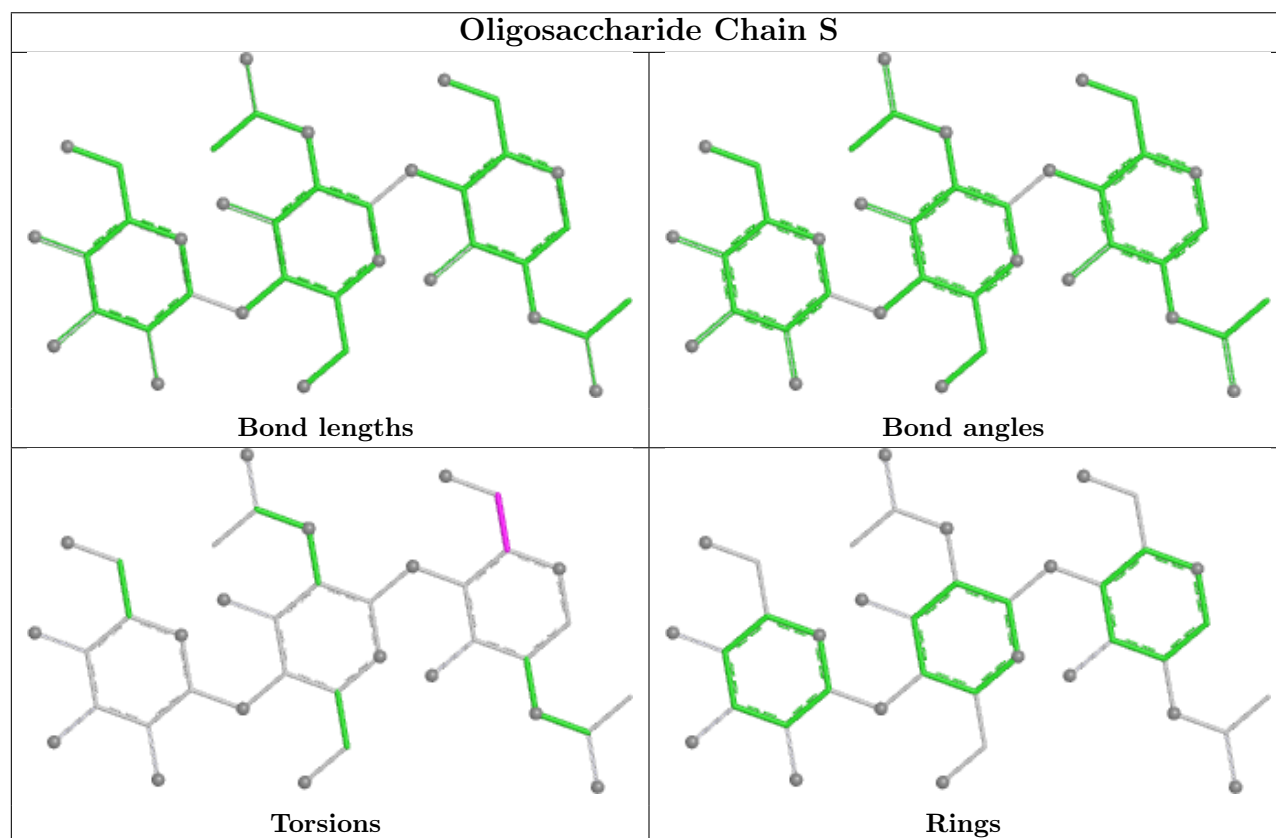
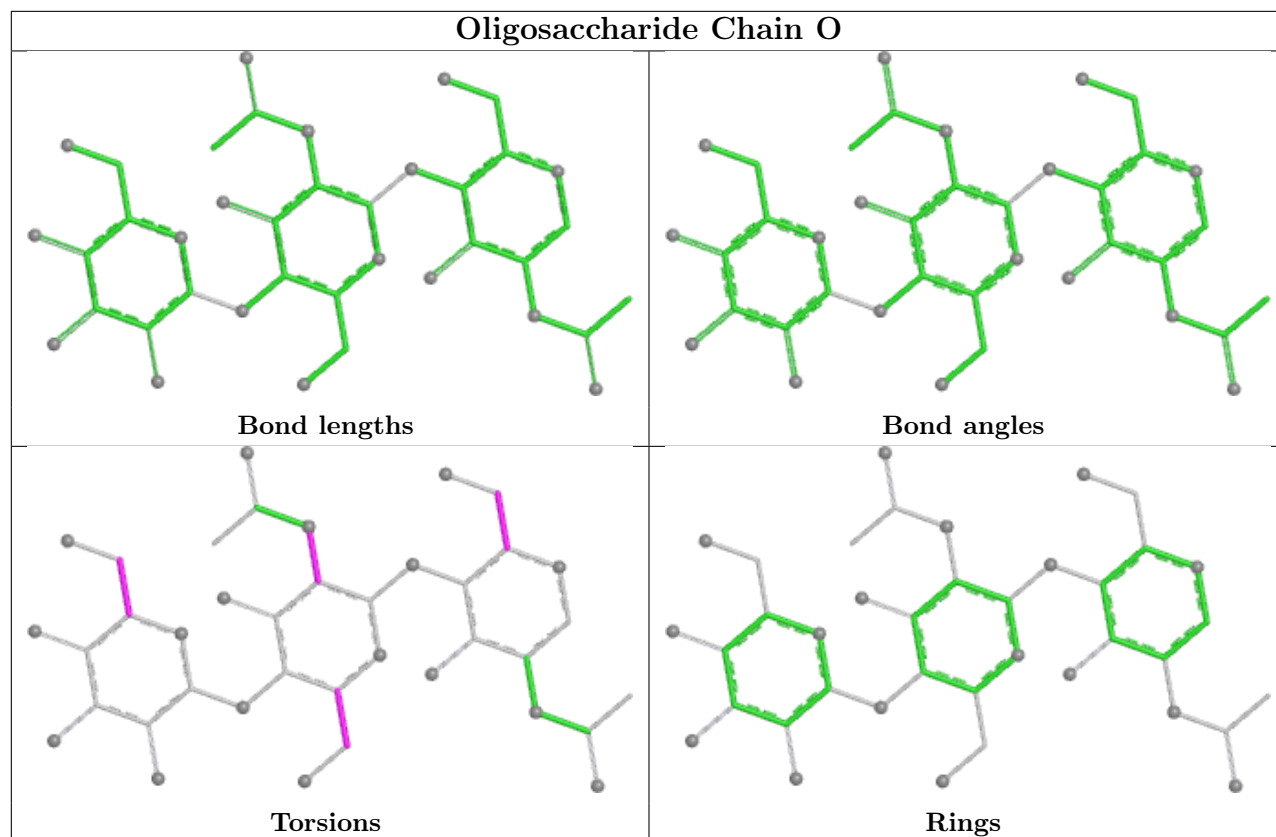


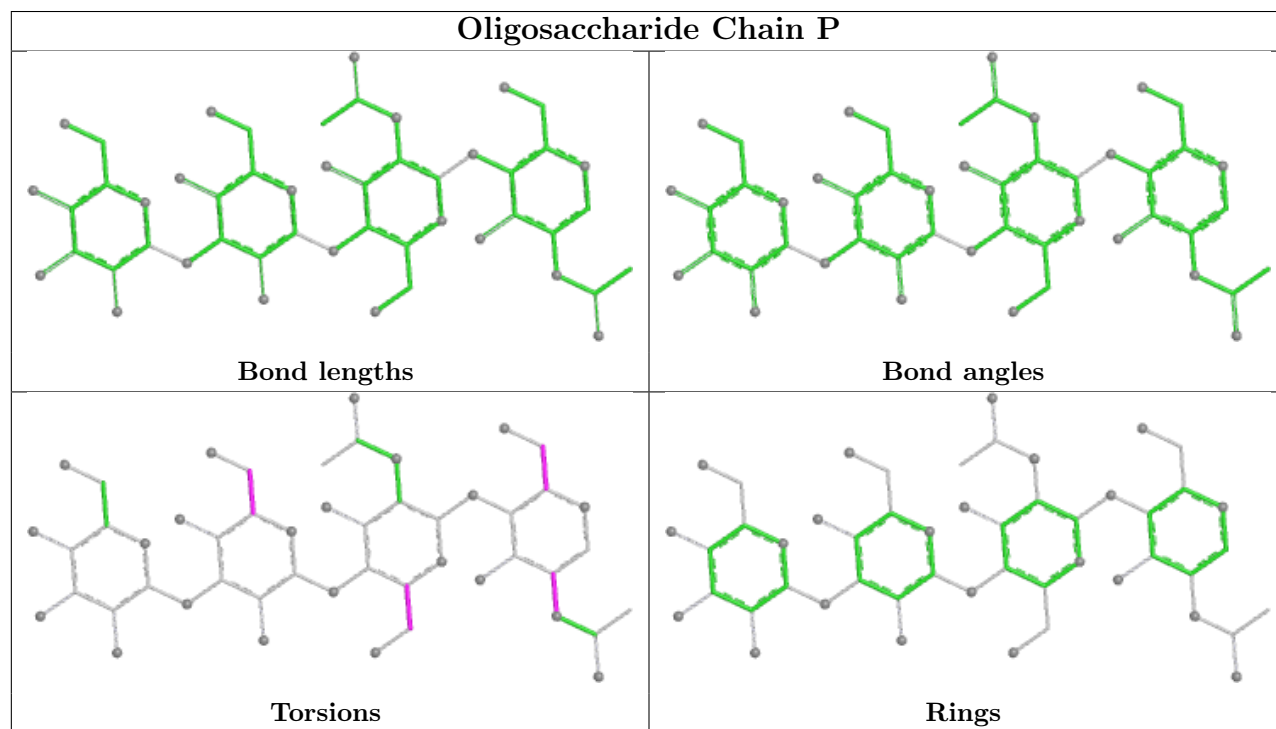
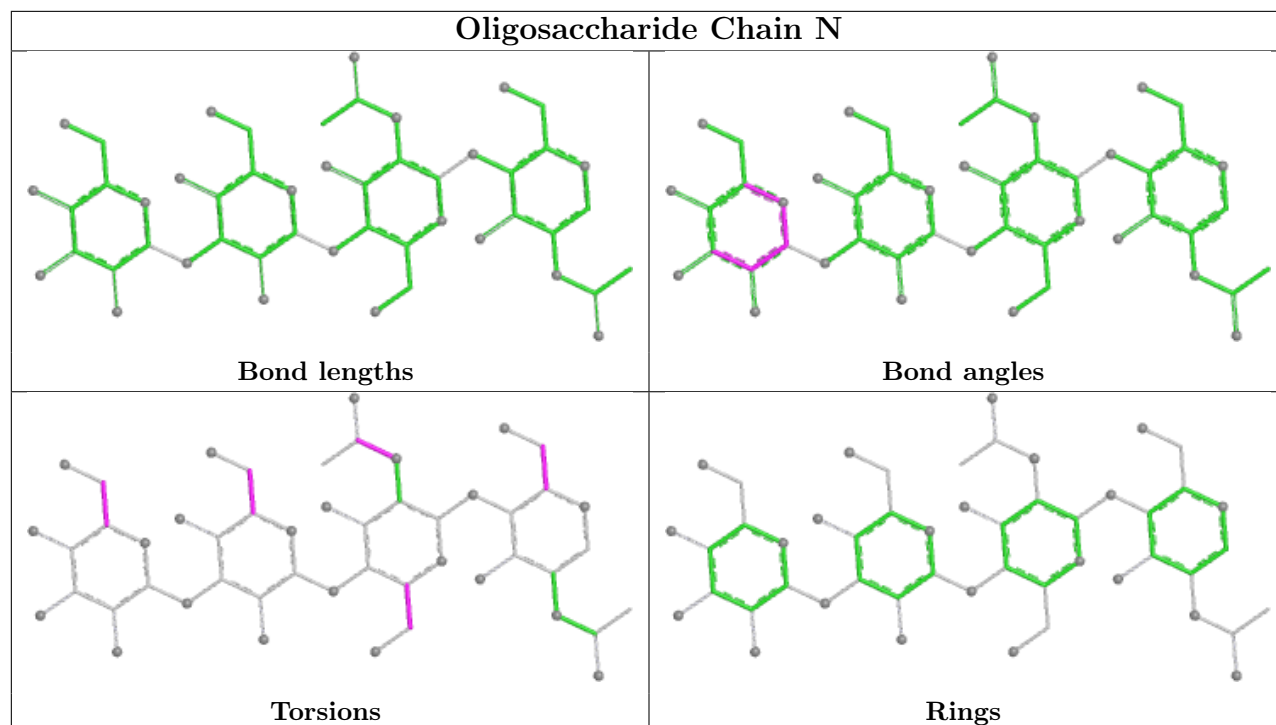


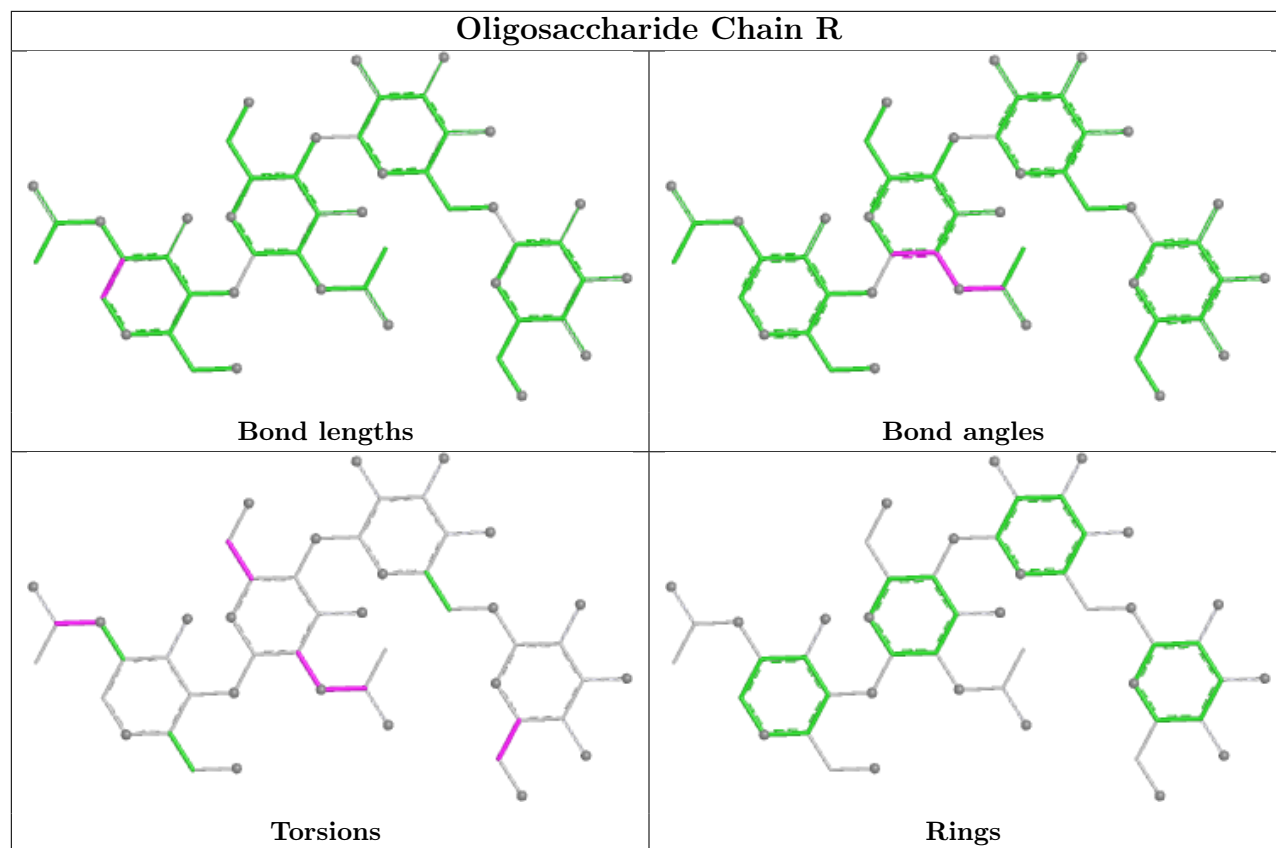


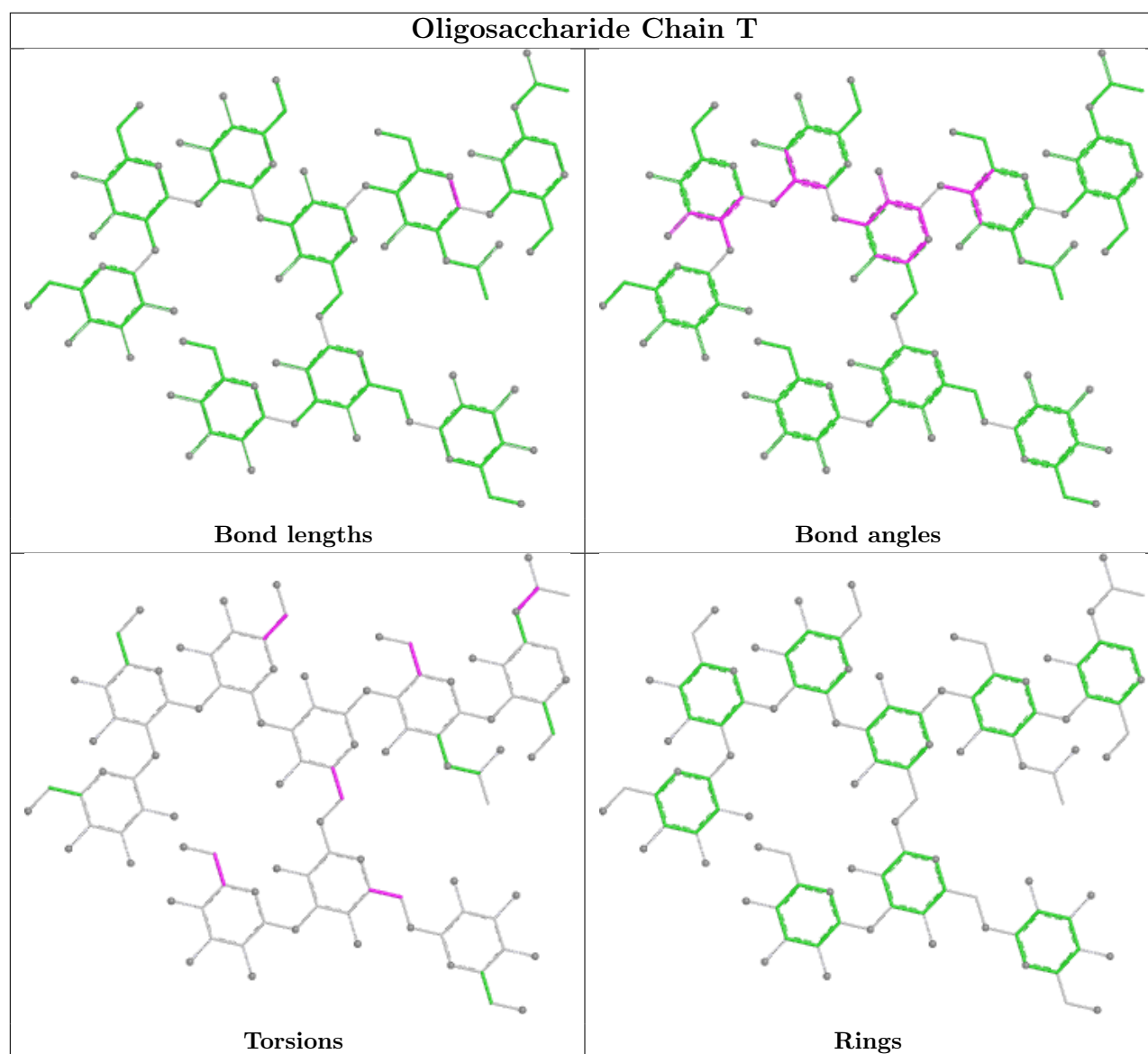












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
14	NAG	G	605	2	14,14,15	0.57	0	17,19,21	0.63	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	G	602	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
14	NAG	B	702	1	14,14,15	0.54	0	17,19,21	0.42	0
14	NAG	G	606	2	14,14,15	0.27	0	17,19,21	0.66	0
14	NAG	G	603	2	14,14,15	0.27	0	17,19,21	0.36	0
14	NAG	G	604	2	14,14,15	0.28	0	17,19,21	0.56	0
14	NAG	B	701	1	14,14,15	0.22	0	17,19,21	0.41	0
14	NAG	G	601	2	14,14,15	0.38	0	17,19,21	0.48	0
14	NAG	B	703	1	14,14,15	0.34	0	17,19,21	0.52	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
14	NAG	G	605	2	-	2/6/23/26	0/1/1/1
14	NAG	G	602	2	-	0/6/23/26	0/1/1/1
14	NAG	B	702	1	-	0/6/23/26	0/1/1/1
14	NAG	G	606	2	-	2/6/23/26	0/1/1/1
14	NAG	G	603	2	-	0/6/23/26	0/1/1/1
14	NAG	G	604	2	-	3/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1
14	NAG	G	601	2	-	4/6/23/26	0/1/1/1
14	NAG	B	703	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	602	NAG	C1-O5-C5	3.47	116.84	112.19
14	G	605	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	606	NAG	O5-C5-C6-O6
14	G	601	NAG	C8-C7-N2-C2
14	G	601	NAG	O7-C7-N2-C2
14	G	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	G	606	NAG	C4-C5-C6-O6
14	G	601	NAG	C4-C5-C6-O6
14	G	604	NAG	C4-C5-C6-O6
14	G	604	NAG	C1-C2-N2-C7
14	G	604	NAG	O5-C5-C6-O6
14	G	605	NAG	O5-C5-C6-O6
14	G	605	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	602	NAG	1	0
14	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

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	136/153 (88%)	0.13	4 (2%)	53	37	46, 87, 150, 168	0
2	G	455/482 (94%)	0.13	9 (1%)	65	45	47, 107, 175, 214	0
3	D	240/243 (98%)	-0.10	4 (1%)	69	48	62, 150, 289, 309	0
4	E	213/216 (98%)	0.01	2 (0%)	81	61	80, 144, 226, 242	0
5	H	231/236 (97%)	0.14	10 (4%)	40	29	56, 129, 176, 198	0
6	L	211/214 (98%)	0.01	3 (1%)	73	52	53, 115, 142, 156	0
All	All	1486/1544 (96%)	0.06	32 (2%)	62	44	46, 117, 219, 309	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	146	GLU	4.1
2	G	70	ALA	3.6
5	H	138	CYS	3.3
1	B	664	ASP	3.3
5	H	120	PHE	3.1
2	G	506	VAL	3.0
5	H	41	PRO	2.9
6	L	67(B)	ASN	2.9
2	G	69	TRP	2.9
6	L	93	SER	2.9
1	B	652	GLN	2.9
5	H	139	LEU	2.7
2	G	247	CYS	2.5
2	G	83	GLU	2.5
2	G	430	VAL	2.4
5	H	100(G)	PHE	2.3
1	B	518	PHE	2.3
4	E	148	VAL	2.3
5	H	100(M)	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
6	L	67(A)	ILE	2.3
2	G	429	GLY	2.3
4	E	95	HIS	2.2
2	G	218	CYS	2.2
5	H	84	THR	2.2
5	H	100(K)	PHE	2.1
2	G	370	GLU	2.1
1	B	520	LEU	2.1
3	D	100	GLY	2.0
3	D	100(A)	SER	2.0
3	D	163	VAL	2.0
5	H	100(B)	TYR	2.0
3	D	141	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	118,118,118,118	0
7	NAG	A	2	14/15	-	-	118,118,118,118	0
7	BMA	A	3	11/12	-	-	118,118,118,118	0
7	MAN	A	4	11/12	-	-	42,42,42,42	0
7	MAN	A	5	11/12	-	-	76,76,76,76	0
10	NAG	S	2	14/15	0.22	0.15	118,118,118,118	0
10	NAG	O	1	14/15	0.32	0.12	118,118,118,118	0
7	BMA	I	3	11/12	-	-	76,76,76,76	0
7	MAN	I	4	11/12	-	-	37,37,37,37	0
7	MAN	I	5	11/12	-	-	76,76,76,76	0
10	BMA	M	3	11/12	0.36	0.13	118,118,118,118	0
10	NAG	J	1	14/15	0.43	0.17	118,118,118,118	0
7	MAN	Q	5	11/12	0.43	0.11	118,118,118,118	0
7	MAN	K	4	11/12	-	-	42,42,42,42	0
7	MAN	K	5	11/12	-	-	76,76,76,76	0

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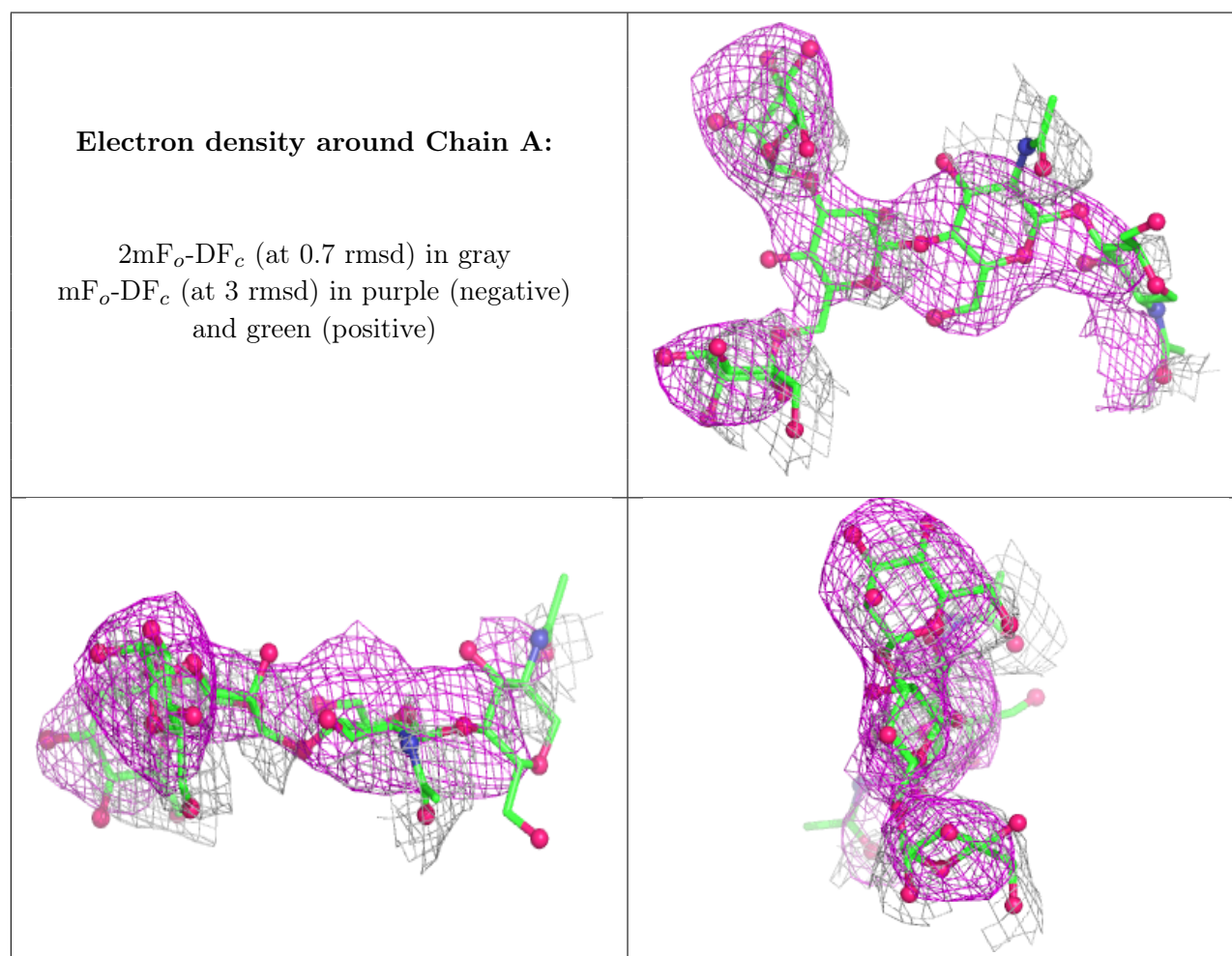
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	M	2	14/15	0.44	0.12	118,118,118,118	0
10	NAG	M	1	14/15	0.48	0.12	118,118,118,118	0
10	BMA	S	3	11/12	0.50	0.12	118,118,118,118	0
13	MAN	T	9	11/12	0.50	0.14	76,76,76,76	0
12	BMA	R	3	11/12	0.53	0.12	118,118,118,118	0
8	NAG	C	1	14/15	-	-	118,118,118,118	0
8	NAG	C	2	14/15	-	-	118,118,118,118	0
8	BMA	C	3	11/12	-	-	118,118,118,118	0
8	MAN	C	4	11/12	-	-	118,118,118,118	0
8	MAN	C	5	11/12	-	-	118,118,118,118	0
8	MAN	C	6	11/12	-	-	118,118,118,118	0
8	MAN	C	7	11/12	-	-	118,118,118,118	0
9	NAG	F	1	14/15	-	-	118,118,118,118	0
9	NAG	F	2	14/15	-	-	118,118,118,118	0
10	NAG	J	2	14/15	0.53	0.12	46,46,46,46	0
7	NAG	I	2	14/15	0.55	0.11	76,76,76,76	0
11	NAG	P	2	14/15	0.55	0.12	118,118,118,118	0
7	NAG	K	1	14/15	0.56	0.16	118,118,118,118	0
7	BMA	Q	3	11/12	0.61	0.10	118,118,118,118	0
10	NAG	S	1	14/15	0.62	0.16	118,118,118,118	0
12	NAG	R	2	14/15	0.62	0.12	118,118,118,118	0
13	MAN	T	8	11/12	0.63	0.11	76,76,76,76	0
13	MAN	T	6	11/12	0.65	0.10	76,76,76,76	0
11	MAN	P	4	11/12	0.66	0.11	76,76,76,76	0
7	MAN	Q	4	11/12	0.66	0.09	118,118,118,118	0
10	NAG	O	2	14/15	0.66	0.09	118,118,118,118	0
12	NAG	R	1	14/15	0.69	0.14	118,118,118,118	0
13	MAN	T	7	11/12	0.70	0.10	76,76,76,76	0
13	NAG	T	1	14/15	0.71	0.14	118,118,118,118	0
11	BMA	P	3	11/12	0.73	0.11	76,76,76,76	0
11	BMA	N	3	11/12	0.73	0.11	76,76,76,76	0
12	MAN	R	4	11/12	0.73	0.12	37,37,37,37	0
7	NAG	Q	1	14/15	0.73	0.11	118,118,118,118	0
11	NAG	P	1	14/15	0.74	0.11	118,118,118,118	0
13	MAN	T	5	11/12	0.76	0.10	76,76,76,76	0
10	BMA	O	3	11/12	0.77	0.12	39,39,39,39	0
13	BMA	T	3	11/12	0.78	0.08	76,76,76,76	0
10	BMA	J	3	11/12	0.79	0.09	46,46,46,46	0
7	NAG	I	1	14/15	0.79	0.14	118,118,118,118	0
13	MAN	T	4	11/12	0.81	0.10	76,76,76,76	0
11	MAN	N	4	11/12	0.81	0.10	42,42,42,42	0
7	BMA	K	3	11/12	0.83	0.11	118,118,118,118	0

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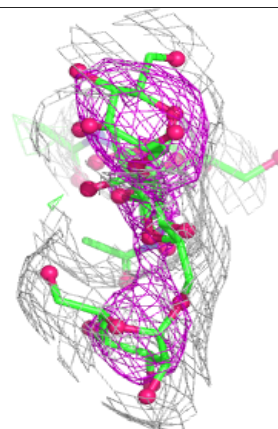
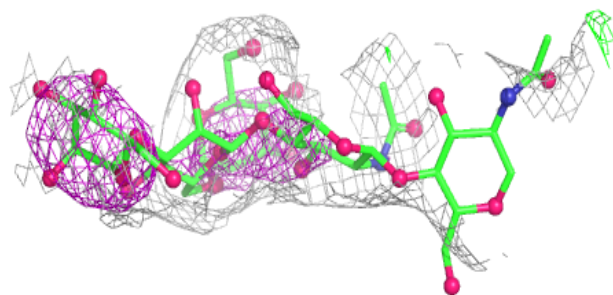
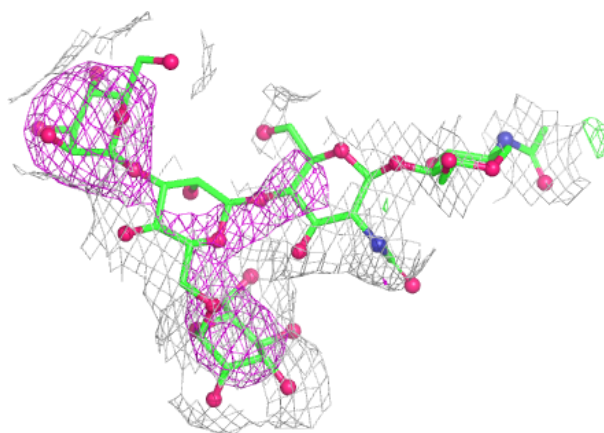
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	NAG	T	2	14/15	0.83	0.12	118,118,118,118	0
11	NAG	N	2	14/15	0.83	0.08	76,76,76,76	0
7	NAG	Q	2	14/15	0.84	0.08	118,118,118,118	0
7	NAG	K	2	14/15	0.87	0.10	118,118,118,118	0
11	NAG	N	1	14/15	0.89	0.14	118,118,118,118	0

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.



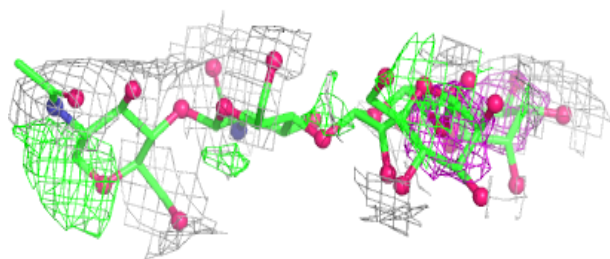
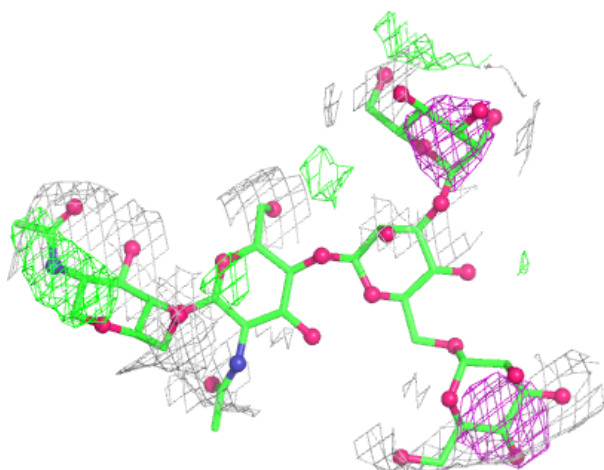
Electron density around Chain I:

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



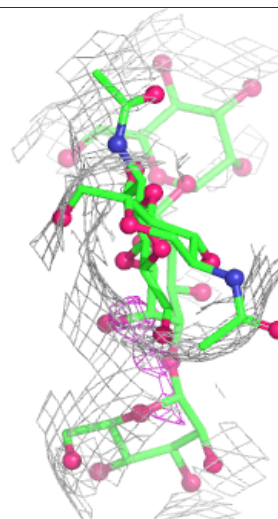
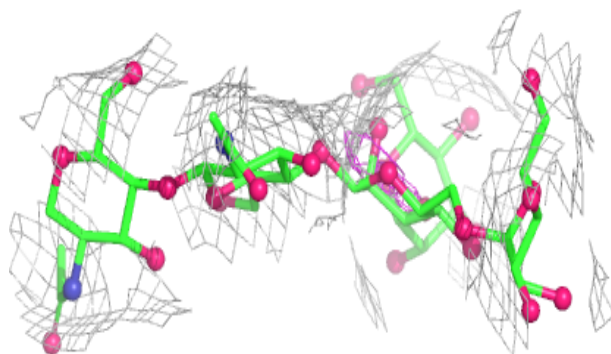
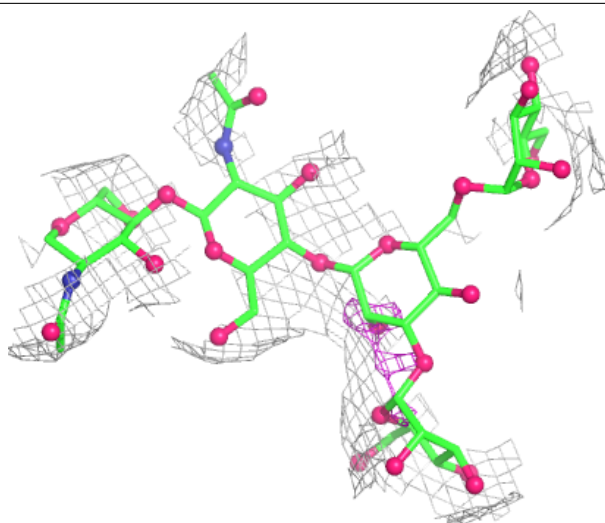
Electron density around Chain K:

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



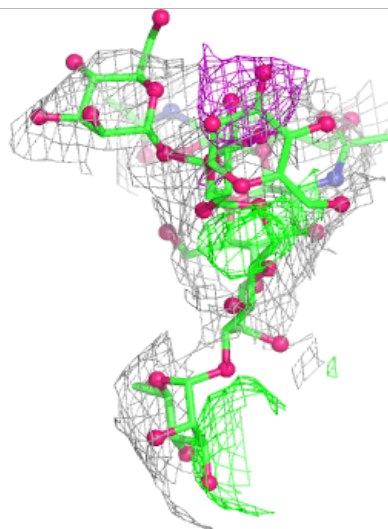
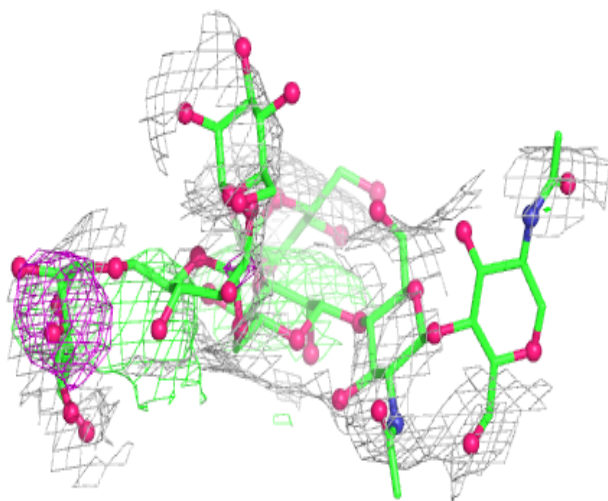
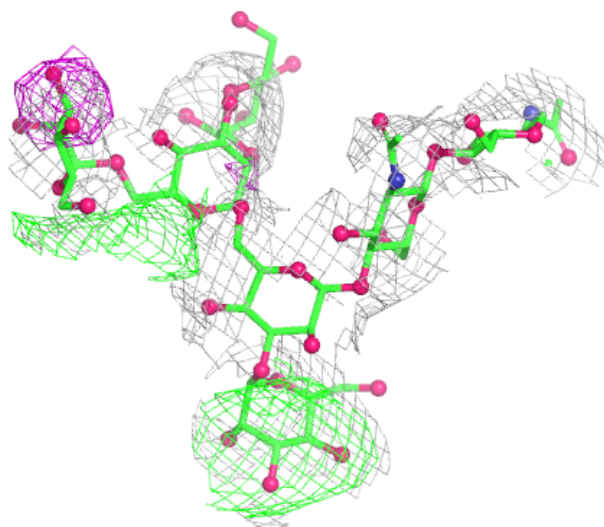
Electron density around Chain Q:

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



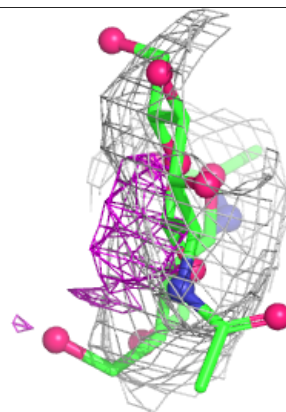
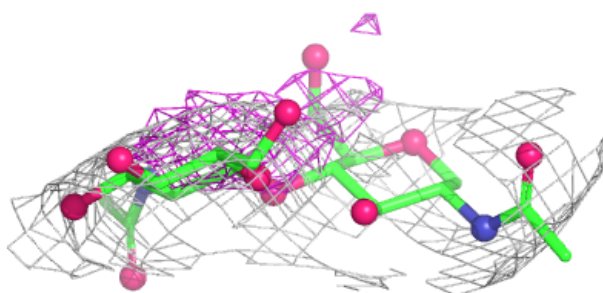
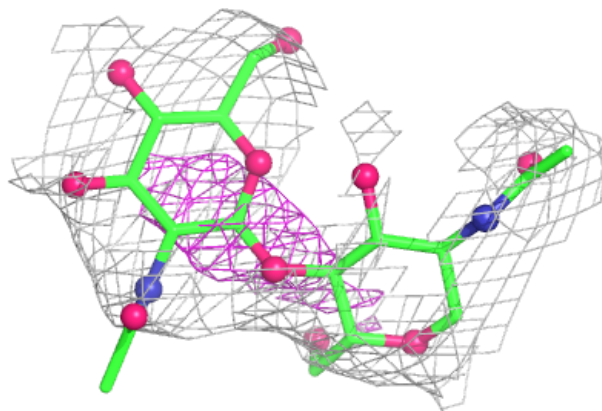
Electron density around Chain C:

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

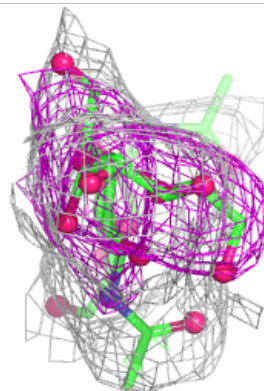
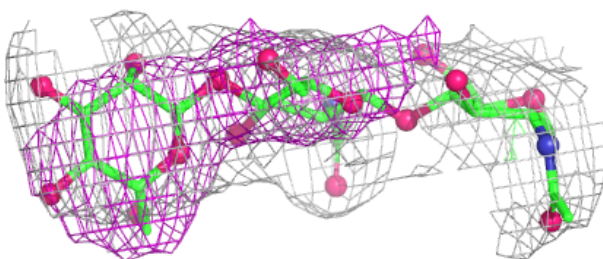
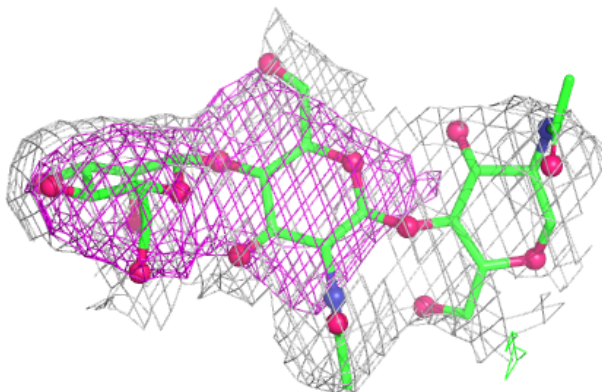


Electron density around Chain F:

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

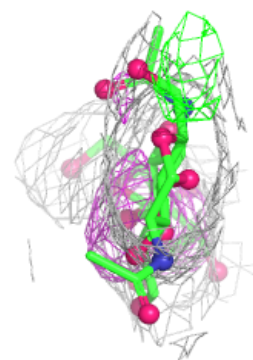
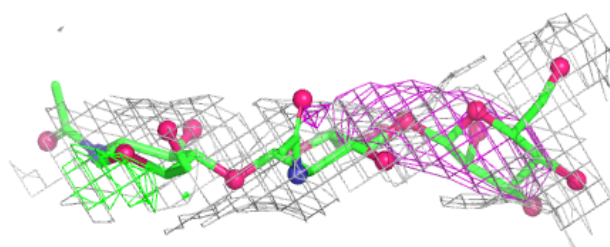
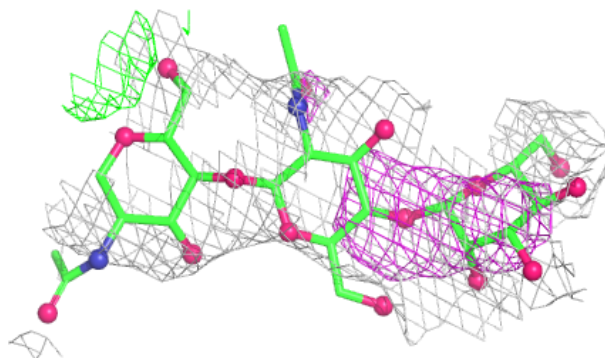
**Electron density around Chain J:**

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

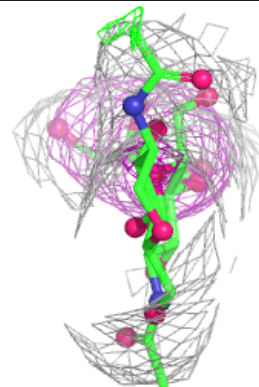
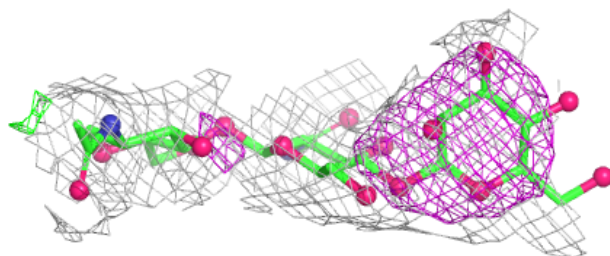
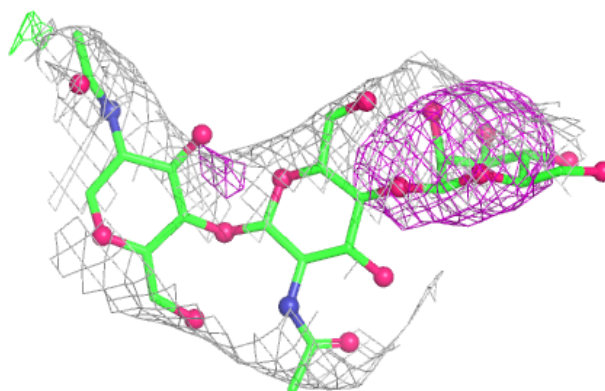


Electron density around Chain M:

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

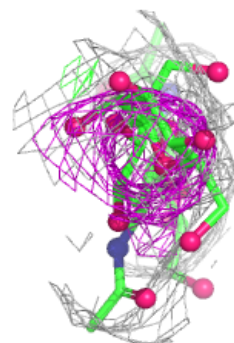
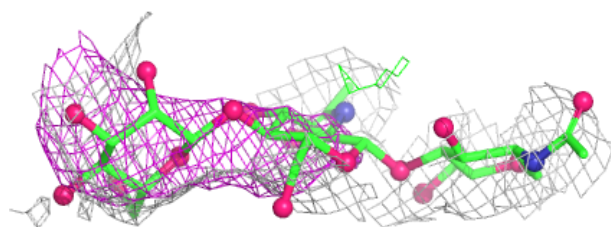
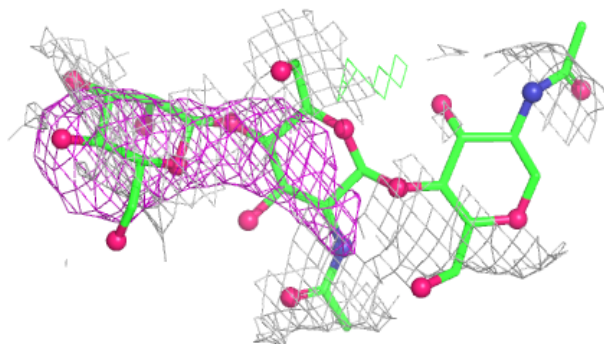
**Electron density around Chain O:**

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

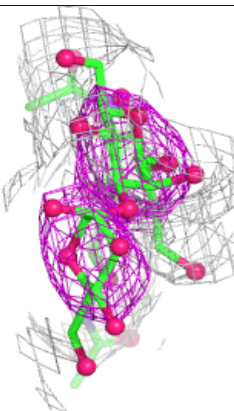
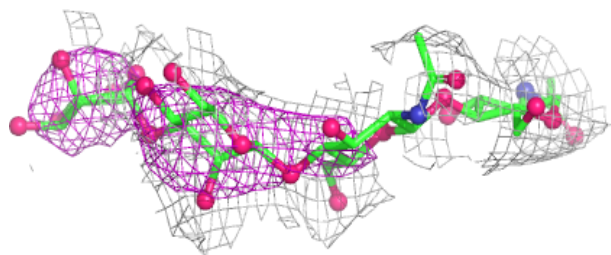
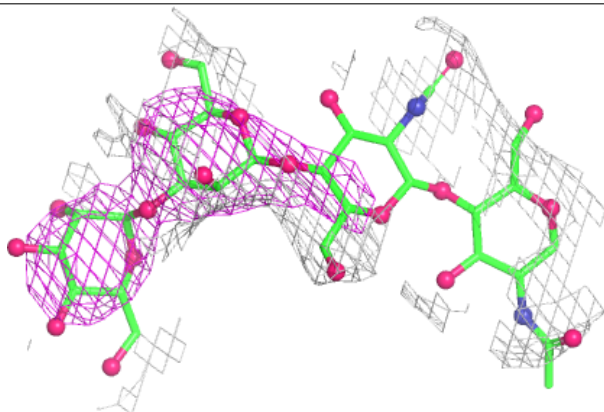


Electron density around Chain S:

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

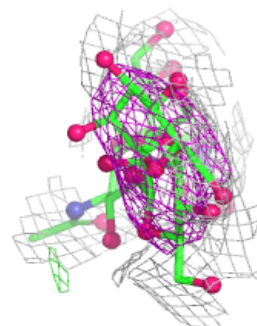
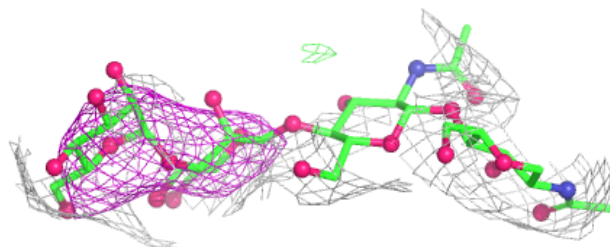
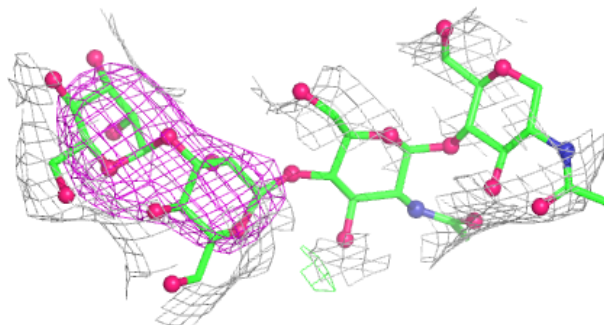
**Electron density around Chain N:**

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

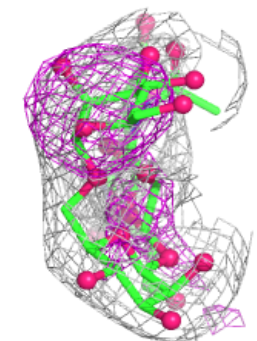
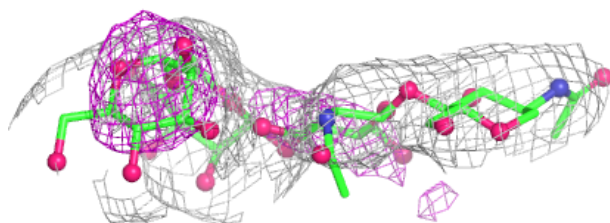
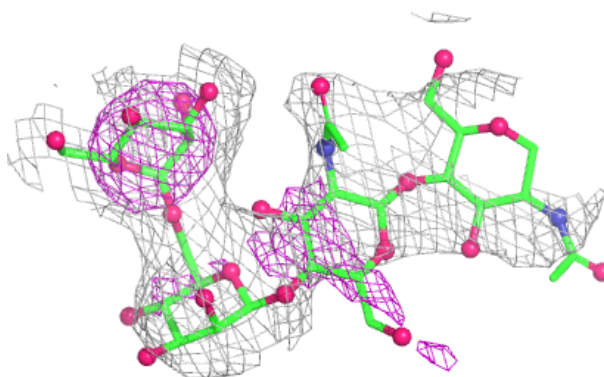


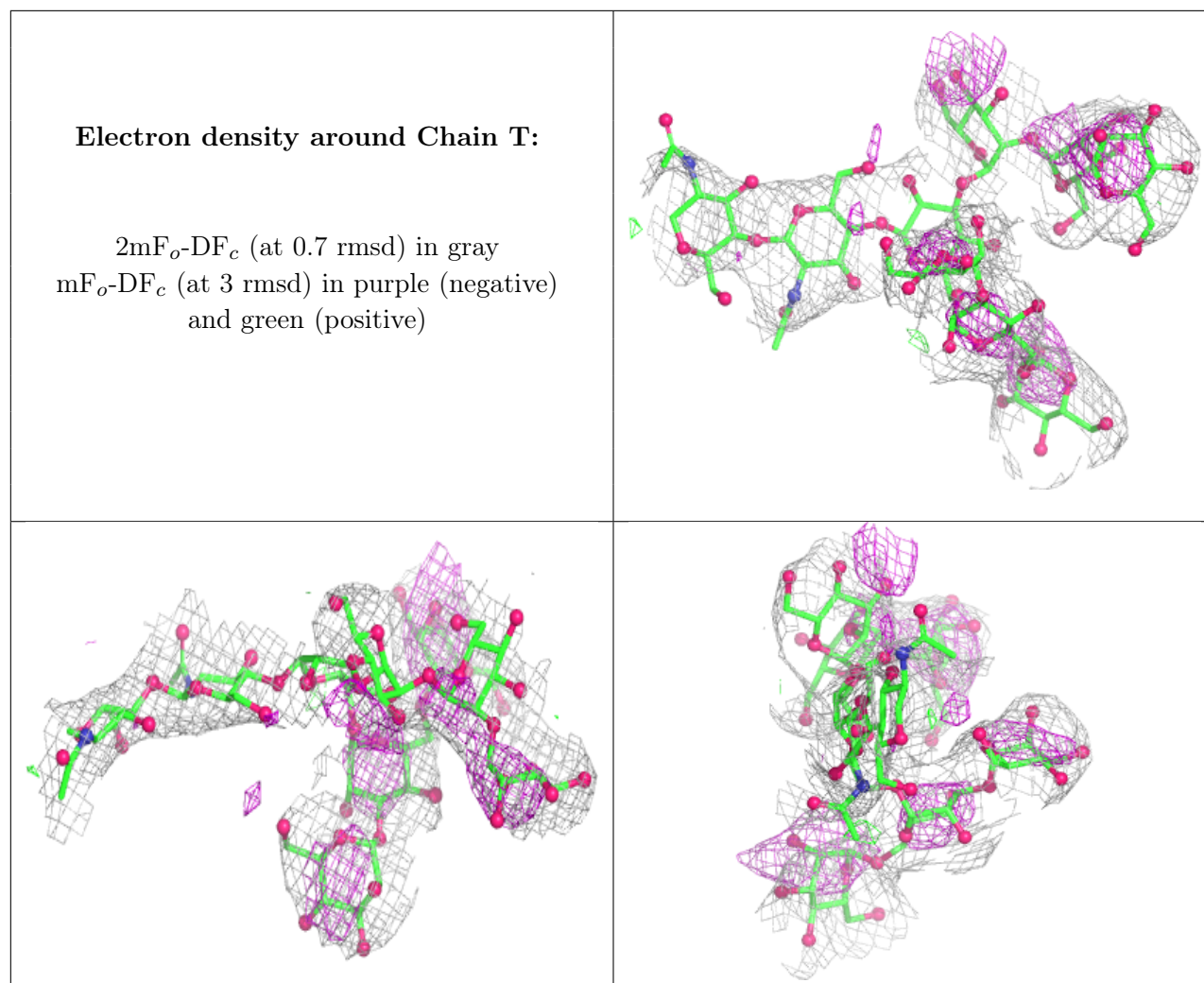
Electron density around Chain P:

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

**Electron density around Chain R:**

$2mF_o-DF_c$ (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
14	NAG	B	701	14/15	0.38	0.14	118,118,118,118	0
14	NAG	G	604	14/15	0.51	0.10	118,118,118,118	0
14	NAG	G	605	14/15	0.55	0.10	118,118,118,118	0
14	NAG	G	601	14/15	0.68	0.09	118,118,118,118	0
14	NAG	G	602	14/15	0.73	0.09	118,118,118,118	0
14	NAG	B	702	14/15	0.75	0.17	37,37,37,37	0
14	NAG	G	603	14/15	0.76	0.09	118,118,118,118	0
14	NAG	B	703	14/15	0.81	0.16	37,37,37,37	0
14	NAG	G	606	14/15	0.86	0.12	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.