



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 02:26 pm GMT

PDB ID : 8BBX
Title : Structure of prolyl endoprotease from *Aspergillus niger* CBS 109712 in space group C222(1)
Authors : Pijning, T.; Vujicic-Zagar, A.; Van der Laan, J.M.; De Jong, R.M.; Dijkstra, B.W.
Deposited on : 2022-10-14
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

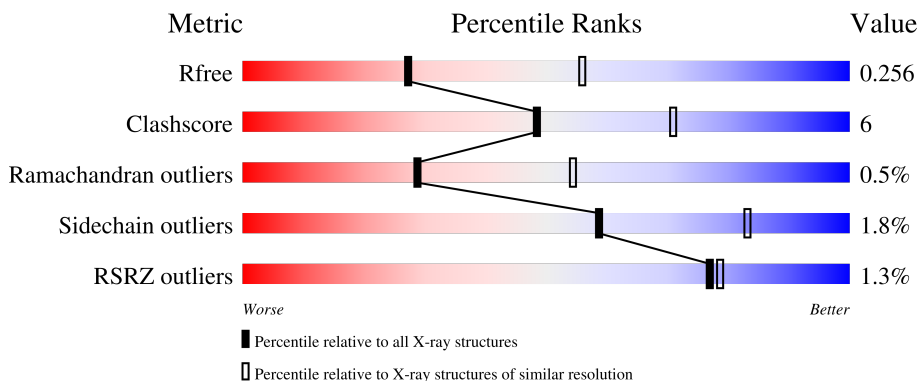
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



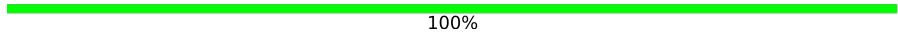

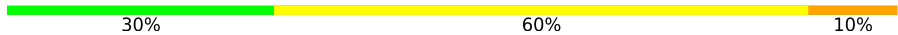
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	485	 83% 16% .
1	B	485	 2% 82% 16% .
2	C	2	 100%
2	E	2	 100%
2	F	2	 100%

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Mol	Chain	Length	Quality of chain
2	G	2	 50% 50%
2	H	2	 100%
2	I	2	 50% 50%
2	K	2	 50% 50%
3	D	10	 30% 60% 10%
4	J	9	 78% 22%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8119 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 Endoprotease endo-Pro.

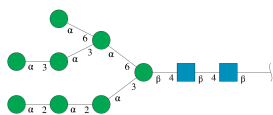
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	Total 3834	C 2462	N 607	O 753	S 12	0	0	0
1	B	484	Total 3839	C 2465	N 608	O 754	S 12	0	0	0

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



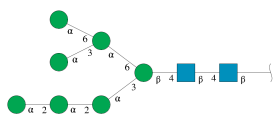
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	Total 28	C 16	N 2	O 10	0	0	0
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0	0
2	H	2	Total 28	C 16	N 2	O 10	0	0	0
2	I	2	Total 28	C 16	N 2	O 10	0	0	0
2	K	2	Total 28	C 16	N 2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

- Molecule 3 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-(1-3)-[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.



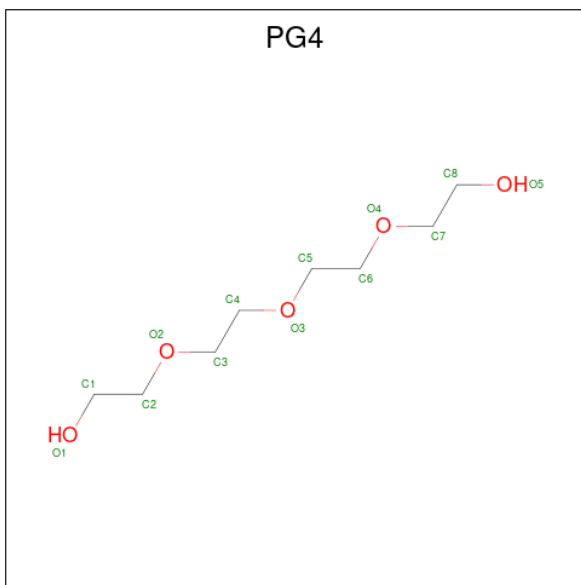
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	10	116	64	2	50	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	J	9	105	58	2	45	0	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	13	8	5	0	0

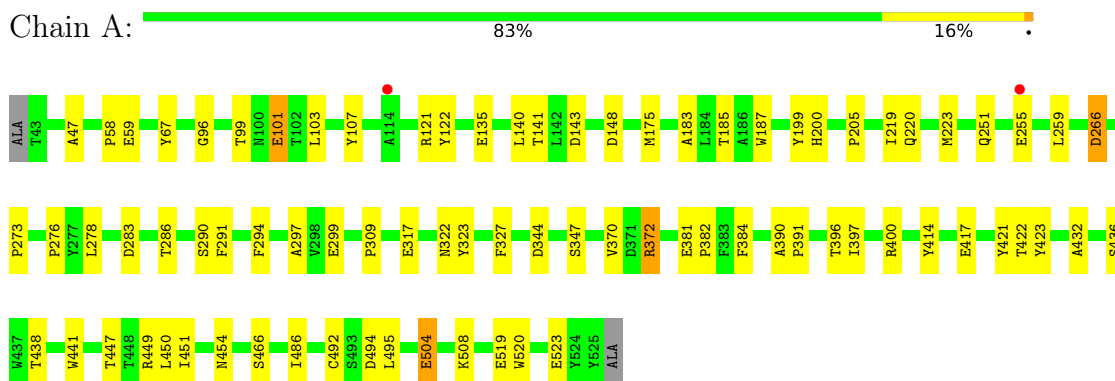
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	8	Total O 8 8	0	0

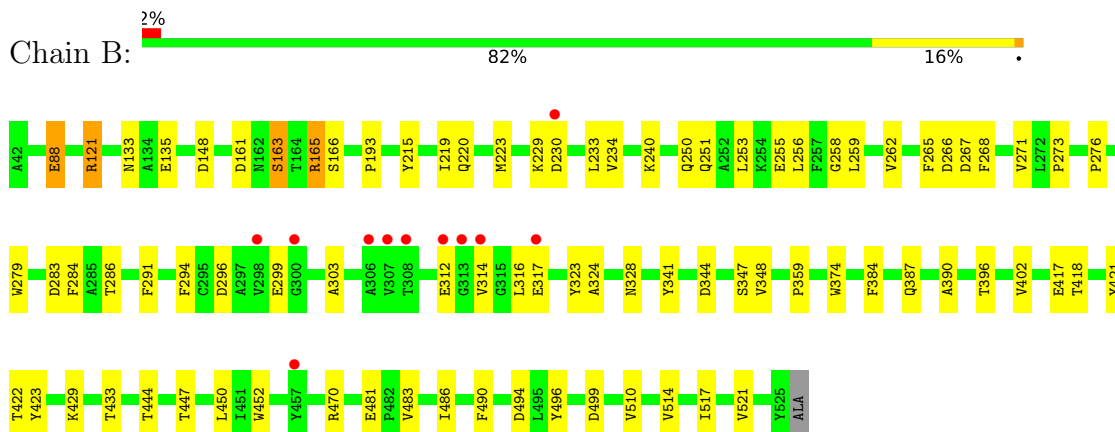
3 Residue-property plots [i](#)

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.

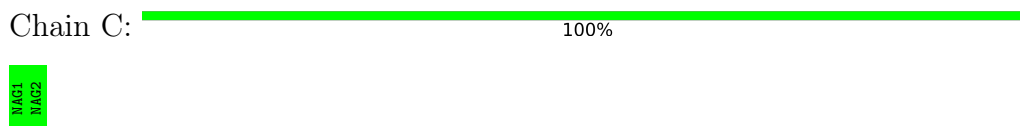
- Molecule 1: Endoprotease endo-Pro



- Molecule 1: Endoprotease endo-Pro



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




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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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

Chain D:  30% 60% 10%



- Molecule 4: 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

Chain J:

78%

22%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.17Å 156.21Å 193.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.70 49.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.39-2.70) 99.7 (49.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.255 0.204 , 0.256	Depositor DCC
R_{free} test set	2144 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, MAN, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	1/3964 (0.0%)	0.68	4/5431 (0.1%)
1	B	0.52	1/3969 (0.0%)	0.64	3/5438 (0.1%)
All	All	0.54	2/7933 (0.0%)	0.66	7/10869 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	TRP	CB-CG	-5.55	1.40	1.50
1	B	317	GLU	CG-CD	5.08	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLU	CA-CB-CG	-10.98	89.25	113.40
1	B	121	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	59	GLU	CA-CB-CG	-6.70	98.67	113.40
1	B	121	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	193	PRO	C-N-CA	-5.58	110.58	122.30
1	A	58	PRO	C-N-CA	5.46	135.35	121.70
1	A	372	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3834	0	3485	44	0
1	B	3839	0	3489	47	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
3	D	116	0	97	1	0
4	J	105	0	88	3	0
5	B	13	0	18	1	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
All	All	8119	0	7352	92	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 6.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:HG23	1:A:101:GLU:H	1.32	0.90
1:A:96:GLY:O	1:A:99:THR:HG22	1.76	0.85
1:B:444:THR:HG21	1:B:470:ARG:HH21	1.44	0.83
1:B:121:ARG:HD2	1:B:148:ASP:OD2	1.80	0.80
1:B:444:THR:HG21	1:B:470:ARG:NH2	1.96	0.80
1:B:344:ASP:HB3	1:B:347:SER:HB2	1.66	0.77
1:A:422:THR:HG22	1:A:423:TYR:H	1.51	0.76
1:A:99:THR:HG23	1:A:101:GLU:N	2.05	0.70
1:A:344:ASP:HB3	1:A:347:SER:HB2	1.74	0.70
1:A:121:ARG:HD2	1:A:148:ASP:OD2	1.93	0.69
1:A:183:ALA:HB2	1:A:205:PRO:HD2	1.75	0.68
1:B:429:LYS:HD2	1:B:433:THR:HG21	1.76	0.68
1:A:492:CYS:HB3	1:A:495:LEU:HD12	1.77	0.65
1:B:341:TYR:CD2	1:B:359:PRO:HB2	2.33	0.63
1:A:283:ASP:HB3	1:A:286:THR:HG23	1.81	0.62
1:B:283:ASP:HB3	1:B:286:THR:HG23	1.83	0.61
1:B:390:ALA:HB3	1:B:396:THR:HB	1.84	0.59
1:B:299:GLU:OE2	1:B:314:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PRO:O	1:A:400:ARG:NH1	2.37	0.57
1:A:297:ALA:O	1:A:322:ASN:HB3	2.05	0.57
1:A:223:MET:HG3	1:A:291:PHE:HZ	1.70	0.56
1:B:259:LEU:O	1:B:262:VAL:HG22	2.05	0.56
1:B:233:LEU:HB3	1:B:316:LEU:HD13	1.88	0.55
1:A:219:ILE:O	1:A:223:MET:HB2	2.06	0.55
1:B:230:ASP:O	1:B:234:VAL:HG23	2.07	0.54
1:B:88:GLU:HG2	1:B:374:TRP:CE3	2.42	0.54
1:B:258:GLY:HA3	1:B:328:ASN:OD1	2.09	0.53
1:A:447:THR:HG23	1:A:450:LEU:HB3	1.92	0.52
1:B:133:ASN:HB2	1:B:418:THR:HG21	1.91	0.52
1:B:233:LEU:HB3	1:B:316:LEU:CD1	2.39	0.52
1:B:452:TRP:HB2	1:B:483:VAL:HG23	1.92	0.52
1:A:422:THR:HG22	1:A:423:TYR:N	2.23	0.51
1:A:317:GLU:H	1:A:317:GLU:CD	2.14	0.51
1:B:229:LYS:NZ	1:B:312:GLU:HG3	2.25	0.51
1:A:432:ALA:O	1:A:436:SER:HB3	2.10	0.51
1:B:163:SER:OG	1:B:165:ARG:HG2	2.11	0.51
1:A:141:THR:HG22	1:A:143:ASP:H	1.76	0.51
1:A:200:HIS:CD2	1:A:451:ILE:HG23	2.47	0.50
1:B:135:GLU:HG3	1:B:421:TYR:CE2	2.46	0.50
1:A:370:VAL:HG11	1:A:414:TYR:HE1	1.75	0.50
1:B:251:GLN:O	1:B:255:GLU:HG3	2.11	0.49
1:A:251:GLN:O	1:A:255:GLU:HG3	2.13	0.49
1:B:215:TYR:CG	1:B:387:GLN:HG2	2.48	0.49
1:A:449:ARG:HG2	1:A:520:TRP:CD2	2.48	0.48
1:A:47:ALA:HB3	1:A:67:TYR:CZ	2.49	0.48
1:A:390:ALA:HB3	1:A:396:THR:HB	1.96	0.47
1:B:486:ILE:HD11	1:B:494:ASP:HB3	1.96	0.47
1:B:303:ALA:HB1	4:J:9:MAN:H5	1.96	0.47
1:B:447:THR:HG21	1:B:481:GLU:HG3	1.96	0.47
1:A:278:LEU:HD22	1:A:290:SER:HB2	1.97	0.47
1:B:88:GLU:H	1:B:88:GLU:CD	2.17	0.46
1:B:490:PHE:HZ	4:J:4:MAN:H62	1.81	0.46
1:A:121:ARG:HG3	1:A:122:TYR:HD1	1.80	0.46
1:B:262:VAL:HG21	1:B:268:PHE:HB2	1.98	0.46
3:D:10:MAN:O3	3:D:10:MAN:H62	2.16	0.46
1:B:161:ASP:OD1	1:B:163:SER:HB3	2.16	0.46
1:A:122:TYR:CD1	1:A:140:LEU:HD13	2.52	0.44
1:A:187:TRP:CD1	1:A:438:THR:HB	2.52	0.44
1:B:273:PRO:HA	1:B:276:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ILE:HG12	1:B:279:TRP:CD1	2.52	0.44
1:A:220:GLN:HG3	1:A:397:ILE:HG12	2.00	0.43
1:B:496:TYR:CE2	5:B:601:PG4:H71	2.53	0.43
1:A:135:GLU:HG3	1:A:421:TYR:CE1	2.53	0.43
1:B:250:GLN:HG2	1:B:265:PHE:CE1	2.53	0.43
1:B:253:LEU:O	1:B:256:LEU:HB2	2.19	0.43
1:B:296:ASP:OD1	4:J:1:NAG:H61	2.19	0.43
1:B:510:VAL:O	1:B:514:VAL:HG23	2.19	0.43
1:A:381:GLU:N	1:A:382:PRO:HA	2.34	0.43
1:A:504:GLU:H	1:A:504:GLU:CD	2.21	0.43
1:B:291:PHE:O	1:B:294:PHE:HB3	2.18	0.43
1:B:348:VAL:O	1:B:348:VAL:HG12	2.17	0.43
1:B:267:ASP:O	1:B:271:VAL:HG23	2.18	0.43
1:A:103:LEU:HG	1:A:107:TYR:CE2	2.54	0.43
1:A:175:MET:HB3	1:A:185:THR:HG23	2.00	0.42
1:A:299:GLU:HB3	1:A:309:PRO:HG2	2.01	0.42
1:A:454:ASN:OD1	1:A:466:SER:HB2	2.20	0.42
1:A:519:GLU:O	1:A:523:GLU:HG3	2.20	0.42
1:B:256:LEU:O	1:B:324:ALA:HB1	2.20	0.42
1:B:283:ASP:OD1	1:B:284:PHE:N	2.52	0.42
1:B:517:ILE:O	1:B:521:VAL:HG23	2.18	0.42
1:A:422:THR:HG22	1:A:423:TYR:CD1	2.55	0.41
1:A:449:ARG:HA	1:A:520:TRP:CZ2	2.55	0.41
1:B:447:THR:HG23	1:B:450:LEU:HB3	2.02	0.41
1:B:223:MET:HE3	1:B:223:MET:HB3	1.78	0.41
1:B:422:THR:HB	1:B:423:TYR:H	1.69	0.41
1:A:273:PRO:HA	1:A:276:PRO:HD2	2.02	0.41
1:B:240:LYS:HD3	1:B:240:LYS:HA	1.72	0.41
1:A:121:ARG:O	1:A:122:TYR:HB2	2.21	0.41
1:A:259:LEU:HD11	1:A:327:PHE:CE2	2.55	0.41
1:A:486:ILE:HD11	1:A:494:ASP:HB3	2.04	0.40
1:A:185:THR:HG22	1:A:199:TYR:HB3	2.04	0.40
1:B:496:TYR:O	1:B:499:ASP:HB2	2.21	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	A	481/485 (99%)	461 (96%)	18 (4%)	2 (0%)	34	60
1	B	482/485 (99%)	464 (96%)	15 (3%)	3 (1%)	25	50
All	All	963/970 (99%)	925 (96%)	33 (3%)	5 (0%)	29	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	PHE
1	B	266	ASP
1	B	384	PHE
1	A	266	ASP
1	B	402	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/396 (100%)	389 (98%)	7 (2%)	59	83
1	B	396/396 (100%)	389 (98%)	7 (2%)	59	83
All	All	792/792 (100%)	778 (98%)	14 (2%)	59	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	ASP

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Mol	Chain	Res	Type
1	A	294	PHE
1	A	323	TYR
1	A	372	ARG
1	A	417	GLU
1	A	504	GLU
1	A	508	LYS
1	B	88	GLU
1	B	163	SER
1	B	165	ARG
1	B	166	SER
1	B	220	GLN
1	B	323	TYR
1	B	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	322	ASN

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](#)

33 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.49	0	17,19,21	0.47	0
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	0.52	0
3	NAG	D	1	3,1	14,14,15	0.54	0	17,19,21	0.62	0
3	MAN	D	10	3	11,11,12	2.17	4 (36%)	15,15,17	2.60	8 (53%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	0.58	0
3	BMA	D	3	3	11,11,12	0.95	0	15,15,17	0.65	0
3	MAN	D	4	3	11,11,12	1.27	2 (18%)	15,15,17	1.15	2 (13%)
3	MAN	D	5	3	11,11,12	1.22	1 (9%)	15,15,17	1.22	1 (6%)
3	MAN	D	6	3	11,11,12	1.12	0	15,15,17	1.31	2 (13%)
3	MAN	D	7	3	11,11,12	0.93	1 (9%)	15,15,17	1.11	2 (13%)
3	MAN	D	8	3	11,11,12	1.93	3 (27%)	15,15,17	1.15	2 (13%)
3	MAN	D	9	3	11,11,12	1.95	3 (27%)	15,15,17	1.58	3 (20%)
2	NAG	E	1	2,1	14,14,15	0.34	0	17,19,21	0.42	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.42	0
2	NAG	F	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	0.70	0
2	NAG	F	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.60	0
2	NAG	G	1	2,1	14,14,15	0.36	0	17,19,21	0.55	0
2	NAG	G	2	2	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.51	0	17,19,21	0.58	0
2	NAG	H	2	2	14,14,15	0.41	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	1.43	1 (7%)	17,19,21	0.79	0
2	NAG	I	2	2	14,14,15	0.50	0	17,19,21	0.62	0
4	NAG	J	1	4,1	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	J	2	4	14,14,15	0.42	0	17,19,21	1.00	1 (5%)
4	BMA	J	3	4	11,11,12	1.19	1 (9%)	15,15,17	1.20	0
4	MAN	J	4	4	11,11,12	0.96	0	15,15,17	1.23	2 (13%)
4	MAN	J	5	4	11,11,12	0.83	0	15,15,17	1.17	2 (13%)
4	MAN	J	6	4	11,11,12	0.94	1 (9%)	15,15,17	1.13	1 (6%)
4	MAN	J	7	4	11,11,12	1.57	2 (18%)	15,15,17	1.18	2 (13%)
4	MAN	J	8	4	11,11,12	1.49	2 (18%)	15,15,17	1.35	2 (13%)
4	MAN	J	9	4	11,11,12	1.43	0	15,15,17	1.21	1 (6%)
2	NAG	K	1	2,1	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.47	0	17,19,21	0.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	1/2/19/22	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
4	MAN	J	6	4	-	2/2/19/22	0/1/1/1
4	MAN	J	7	4	-	0/2/19/22	0/1/1/1
4	MAN	J	8	4	-	1/2/19/22	0/1/1/1
4	MAN	J	9	4	-	1/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	10	MAN	C2-C3	-5.26	1.44	1.52
2	I	1	NAG	O5-C1	-5.22	1.35	1.43
3	D	8	MAN	C2-C3	4.03	1.58	1.52
3	D	9	MAN	C2-C3	3.59	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	MAN	O5-C1	-3.58	1.38	1.43
3	D	8	MAN	C1-C2	-3.39	1.44	1.52
3	D	8	MAN	O5-C5	3.36	1.50	1.43
3	D	9	MAN	C1-C2	-3.15	1.45	1.52
3	D	10	MAN	C4-C5	-2.94	1.46	1.53
3	D	9	MAN	O5-C5	2.88	1.49	1.43
3	D	4	MAN	O5-C5	2.84	1.49	1.43
4	J	7	MAN	C4-C5	2.82	1.59	1.53
2	F	2	NAG	C1-C2	2.81	1.56	1.52
4	J	8	MAN	O5-C5	2.78	1.49	1.43
4	J	7	MAN	C4-C3	2.67	1.59	1.52
2	F	1	NAG	O5-C1	-2.56	1.39	1.43
4	J	3	BMA	O5-C5	2.50	1.48	1.43
4	J	8	MAN	C4-C3	2.48	1.58	1.52
3	D	4	MAN	C4-C5	2.29	1.57	1.53
3	D	7	MAN	O5-C1	-2.22	1.40	1.43
3	D	10	MAN	C4-C3	2.21	1.57	1.52
4	J	6	MAN	O5-C1	-2.07	1.40	1.43
3	D	10	MAN	O4-C4	2.04	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	MAN	C1-O5-C5	6.06	120.40	112.19
3	D	10	MAN	C1-C2-C3	-4.08	104.65	109.67
3	D	9	MAN	C1-O5-C5	3.85	117.40	112.19
3	D	6	MAN	C1-O5-C5	3.50	116.94	112.19
3	D	10	MAN	O2-C2-C3	-3.13	103.86	110.14
4	J	8	MAN	C1-C2-C3	-3.10	105.86	109.67
4	J	2	NAG	C1-O5-C5	3.01	116.27	112.19
4	J	8	MAN	C1-O5-C5	2.95	116.19	112.19
3	D	10	MAN	O3-C3-C4	2.87	116.99	110.35
3	D	9	MAN	C1-C2-C3	-2.82	106.20	109.67
4	J	7	MAN	O3-C3-C4	2.74	116.69	110.35
4	J	9	MAN	C1-O5-C5	2.69	115.84	112.19
4	J	4	MAN	O2-C2-C3	-2.58	104.97	110.14
3	D	7	MAN	O2-C2-C3	-2.54	105.04	110.14
3	D	10	MAN	O5-C5-C4	-2.53	104.67	110.83
4	J	4	MAN	C1-O5-C5	2.52	115.61	112.19
4	J	5	MAN	C1-O5-C5	2.45	115.52	112.19
4	J	7	MAN	O2-C2-C3	-2.44	105.25	110.14
3	D	5	MAN	O2-C2-C3	-2.38	105.37	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	MAN	O3-C3-C2	2.37	114.53	109.99
3	D	10	MAN	C2-C3-C4	-2.34	106.84	110.89
3	D	4	MAN	C1-O5-C5	2.33	115.35	112.19
4	J	5	MAN	O2-C2-C3	-2.28	105.58	110.14
3	D	8	MAN	C1-C2-C3	-2.28	106.87	109.67
3	D	10	MAN	O4-C4-C5	-2.27	103.66	109.30
3	D	9	MAN	O3-C3-C2	2.21	114.22	109.99
2	K	2	NAG	C1-O5-C5	2.21	115.18	112.19
3	D	10	MAN	O2-C2-C1	2.16	113.57	109.15
3	D	7	MAN	O2-C2-C1	2.14	113.53	109.15
3	D	4	MAN	O2-C2-C3	-2.11	105.92	110.14
2	G	2	NAG	C1-O5-C5	2.08	115.01	112.19
4	J	6	MAN	C1-C2-C3	-2.07	107.12	109.67
3	D	6	MAN	O2-C2-C1	2.00	113.25	109.15

There are no chirality outliers.

All (23) torsion outliers are listed below:

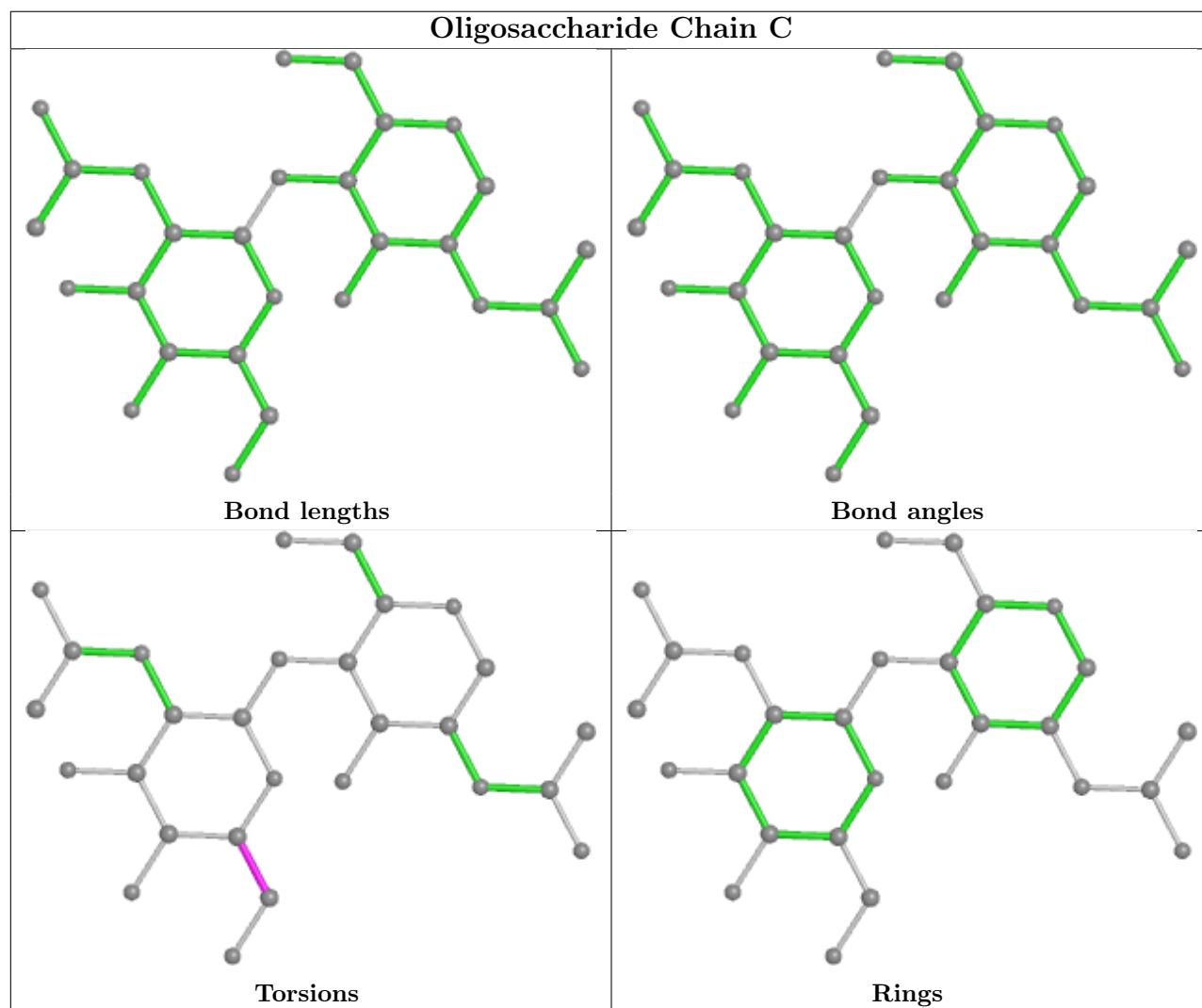
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
4	J	6	MAN	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
4	J	6	MAN	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	8	MAN	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	10	MAN	O5-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
4	J	9	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

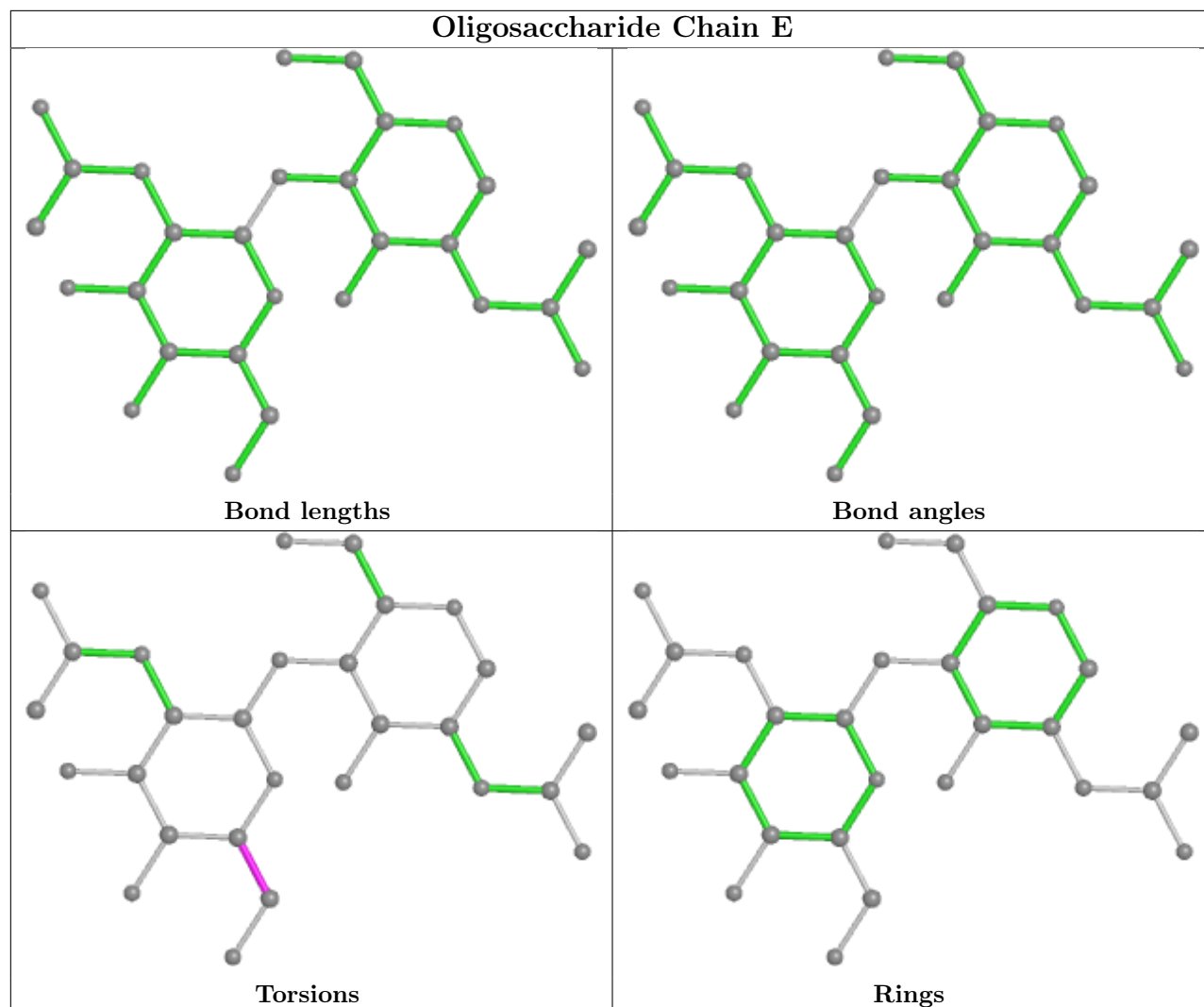
There are no ring outliers.

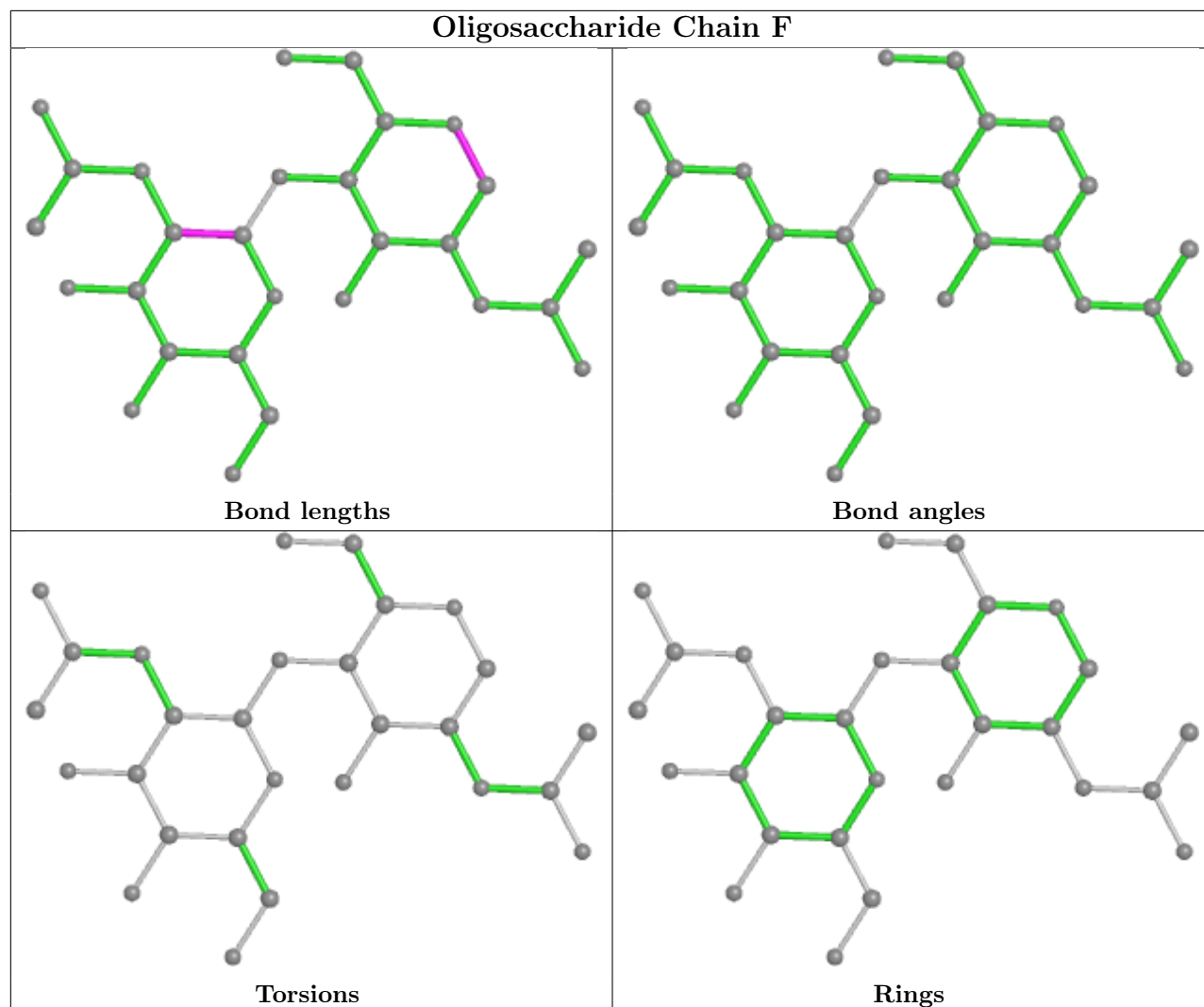
4 monomers are involved in 4 short contacts:

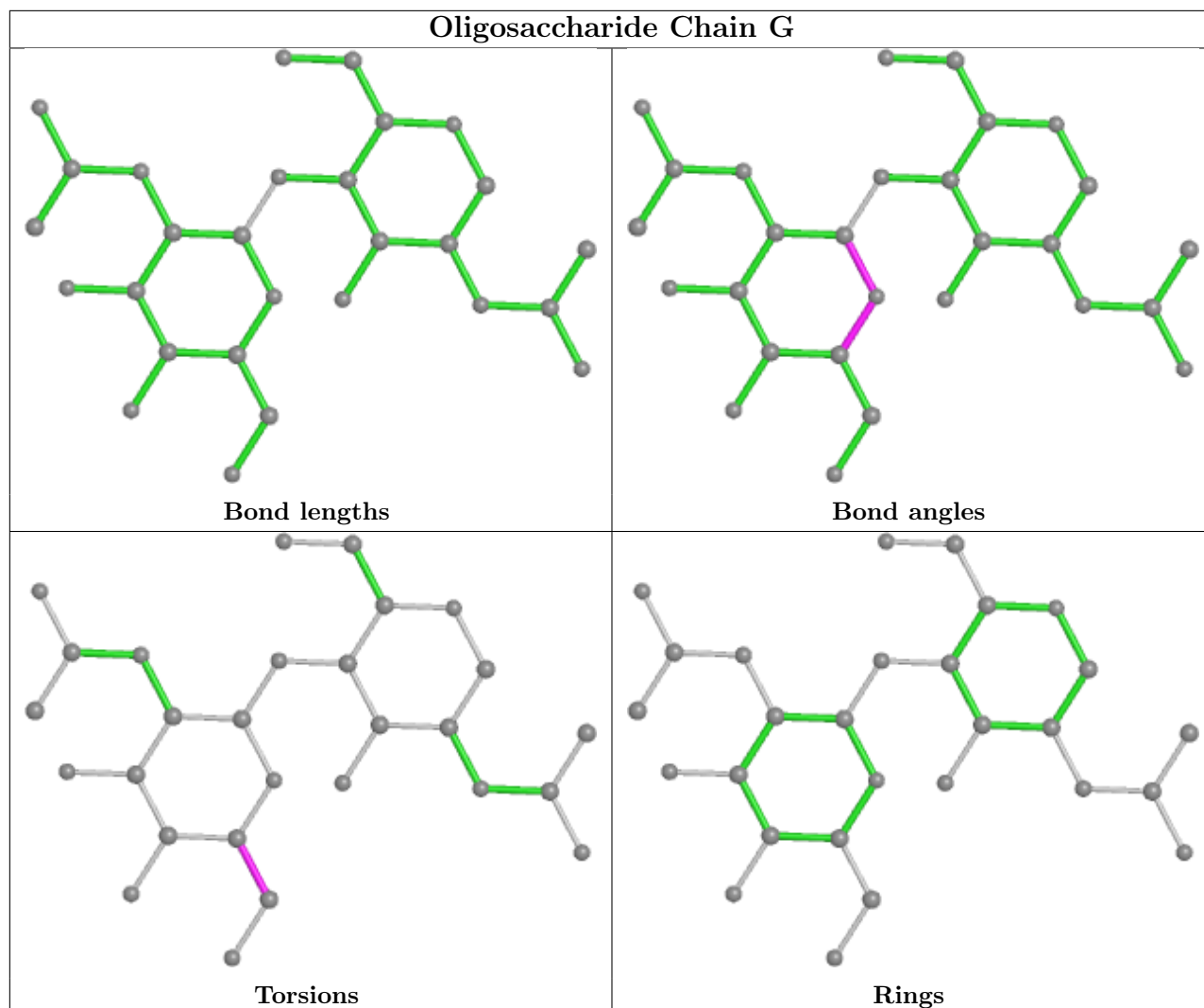
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	10	MAN	1	0
4	J	9	MAN	1	0
4	J	1	NAG	1	0
4	J	4	MAN	1	0

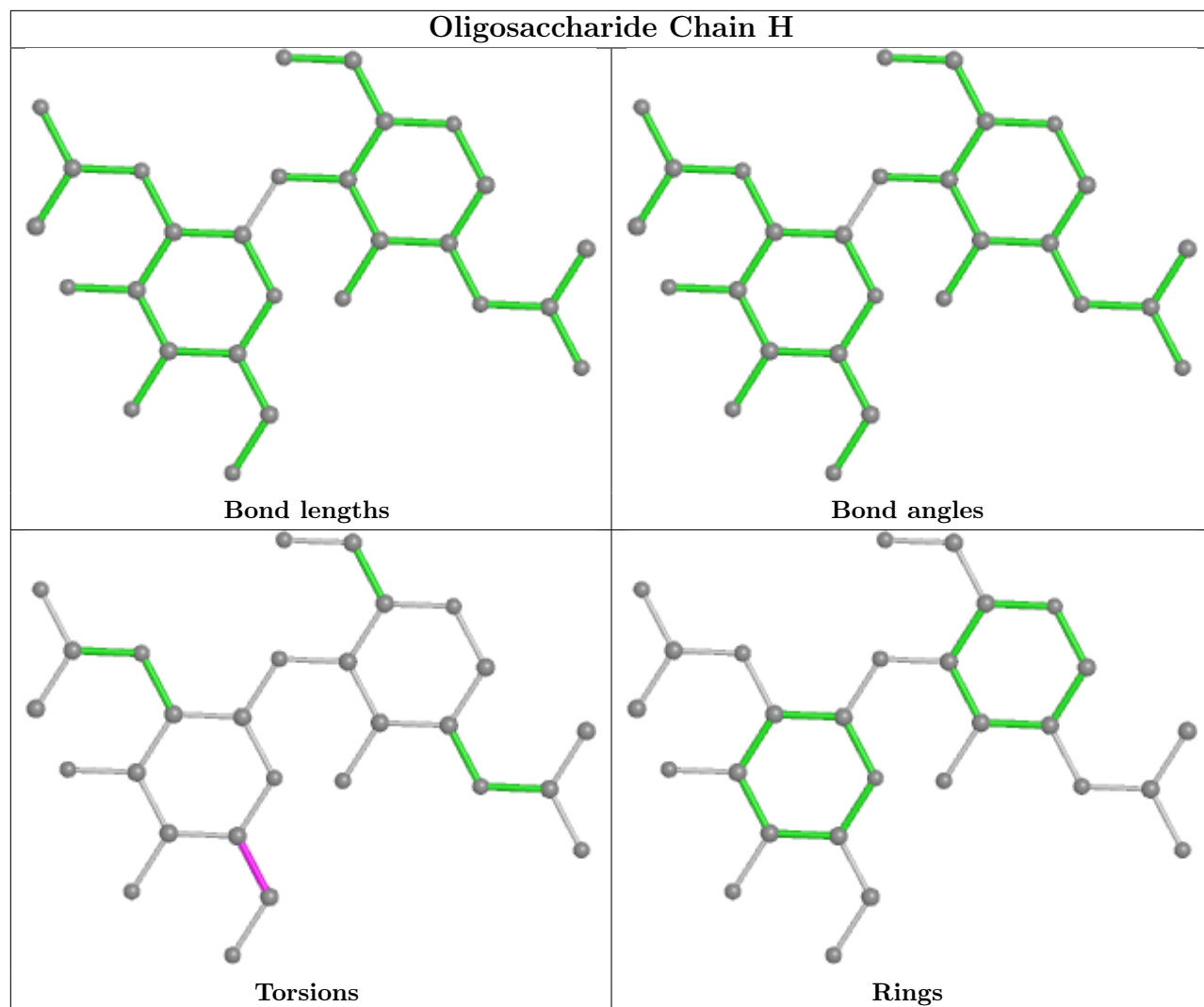
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

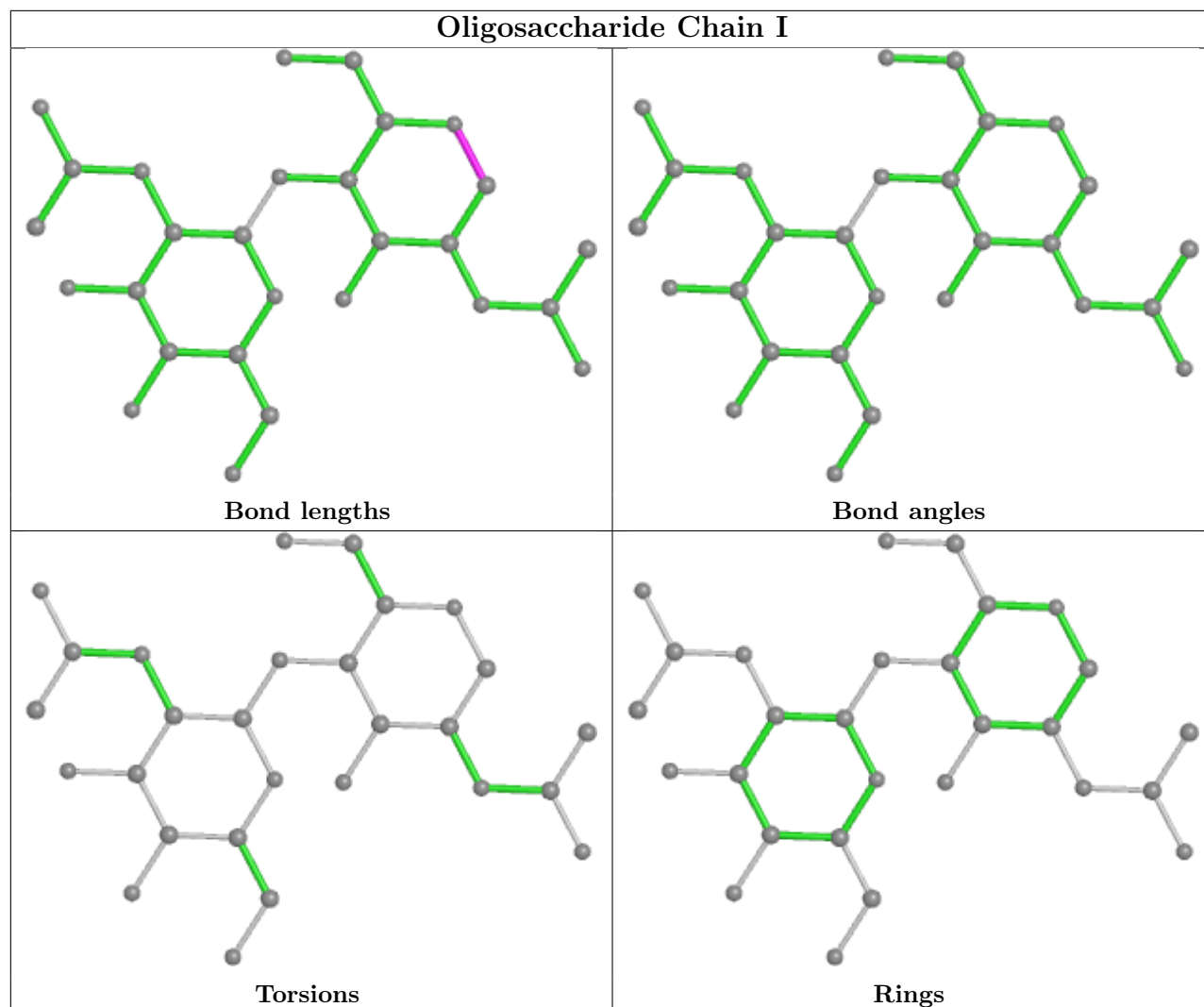


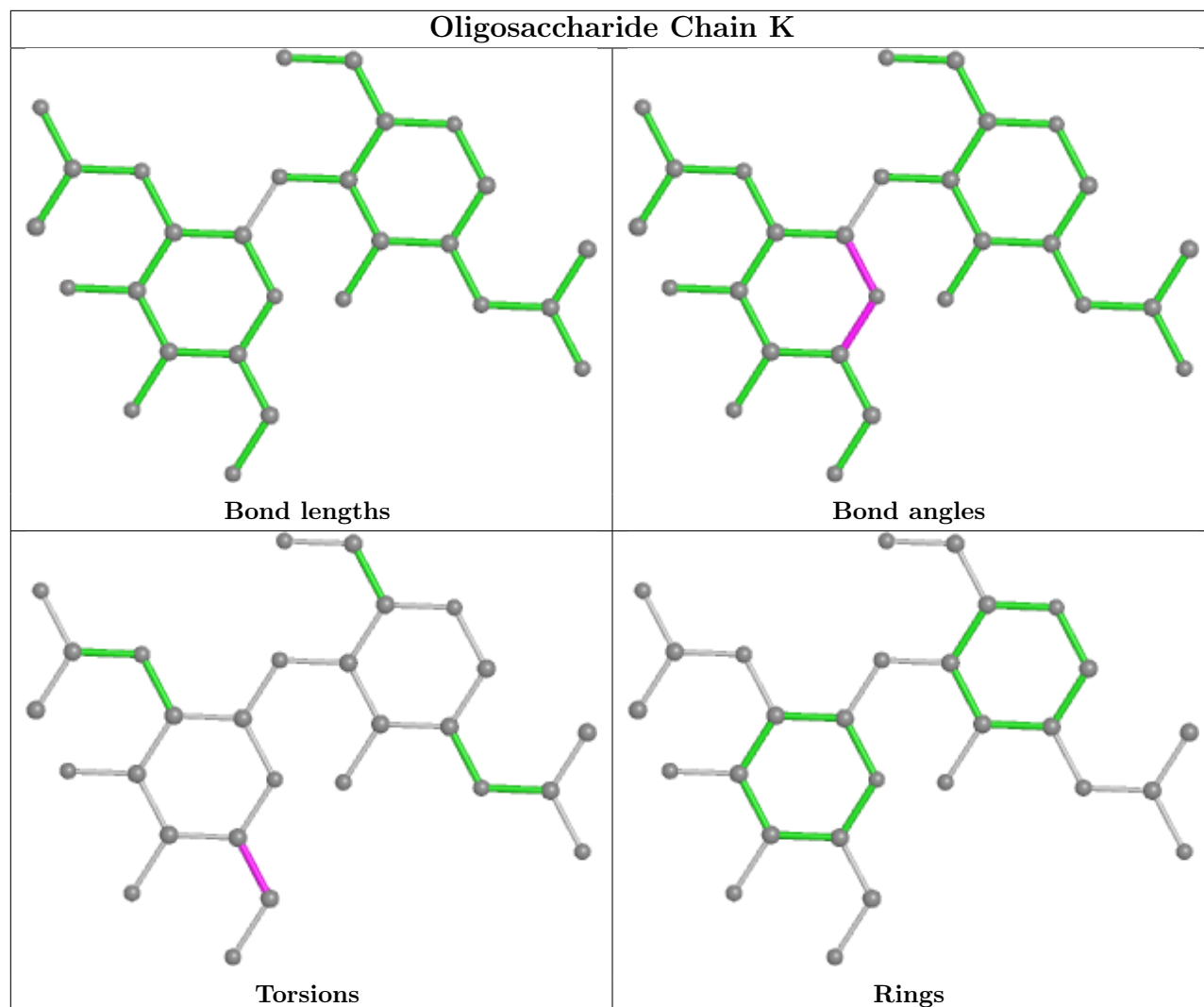


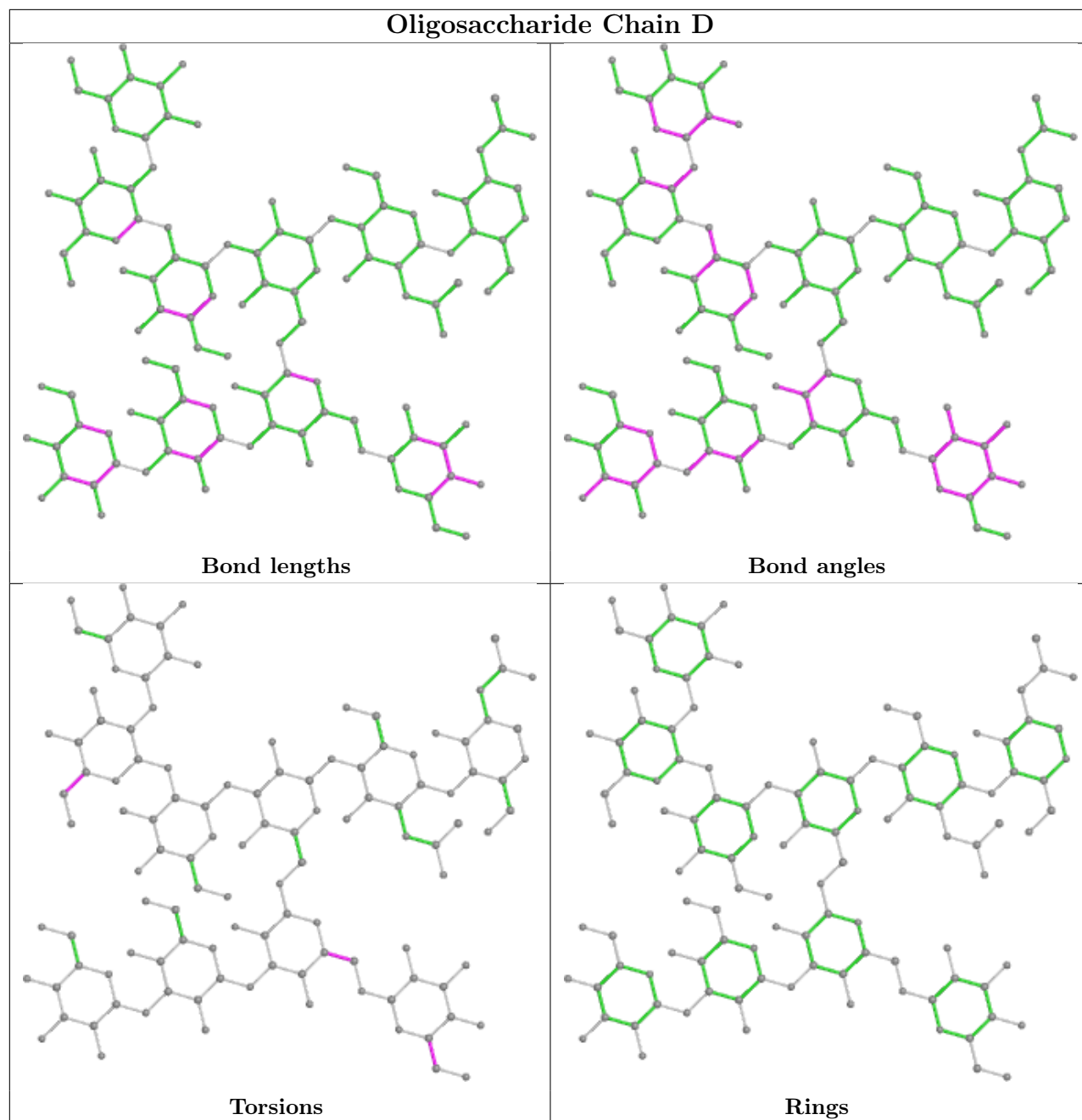


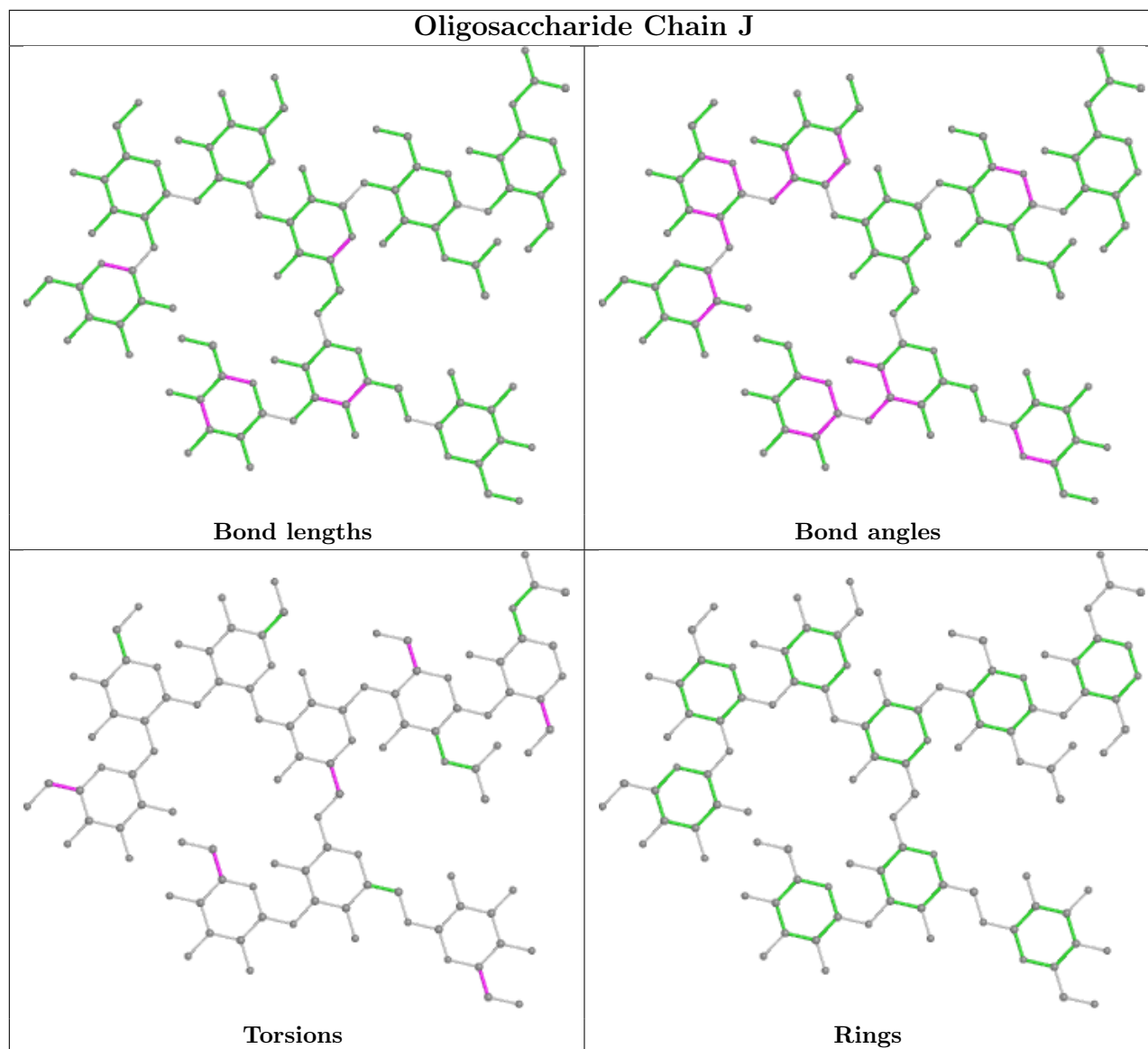












5.6 Ligand geometry [i](#)

1 ligand is 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
5	PG4	B	601	-	12,12,12	0.57	0	11,11,11	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
5	PG4	B	601	-	-	6/10/10/10	-

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
5	B	601	PG4	O2-C3-C4-O3
5	B	601	PG4	O4-C7-C8-O5
5	B	601	PG4	O1-C1-C2-O2
5	B	601	PG4	C6-C5-O3-C4
5	B	601	PG4	C3-C4-O3-C5
5	B	601	PG4	C5-C6-O4-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/485 (99%)	-0.05	2 (0%) 92 93	28, 40, 56, 71	0
1	B	484/485 (99%)	0.04	11 (2%) 60 62	27, 43, 71, 110	0
All	All	967/970 (99%)	-0.01	13 (1%) 77 78	27, 41, 67, 110	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ALA	5.6
1	B	314	VAL	4.3
1	B	307	VAL	4.2
1	B	298	VAL	3.9
1	B	313	GLY	3.5
1	B	300	GLY	2.6
1	B	308	THR	2.5
1	A	255	GLU	2.4
1	B	312	GLU	2.3
1	B	457	TYR	2.3
1	A	114	ALA	2.2
1	B	230	ASP	2.2
1	B	317	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

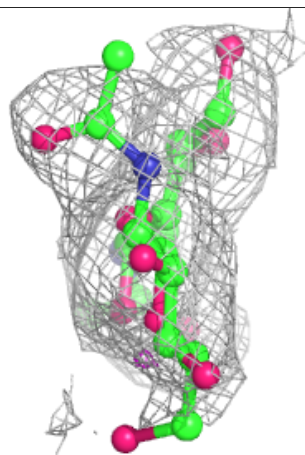
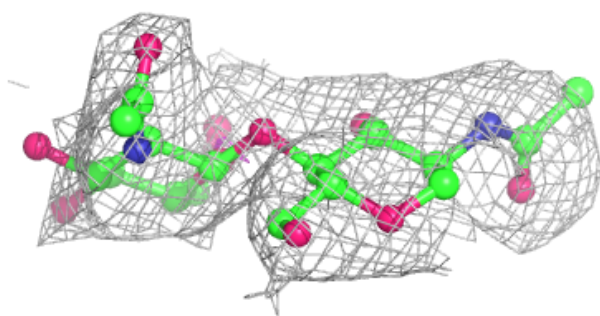
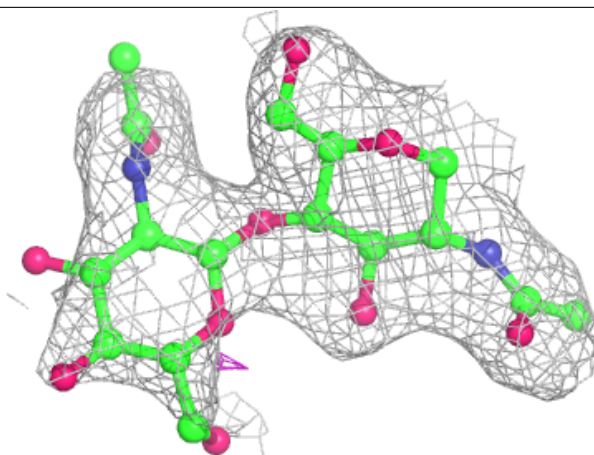
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	J	8	11/12	0.76	0.15	83,97,104,105	0
2	NAG	K	2	14/15	0.80	0.24	77,89,94,97	0
2	NAG	C	2	14/15	0.82	0.47	75,96,101,101	0
3	MAN	D	8	11/12	0.84	0.19	56,61,68,74	0
3	MAN	D	9	11/12	0.85	0.27	51,58,64,65	0
2	NAG	G	2	14/15	0.85	0.20	65,79,88,90	0
2	NAG	E	2	14/15	0.87	0.22	52,73,78,79	0
2	NAG	H	2	14/15	0.87	0.29	74,82,99,101	0
4	MAN	J	9	11/12	0.87	0.14	67,83,90,92	0
3	MAN	D	10	11/12	0.88	0.18	49,56,64,64	0
2	NAG	F	2	14/15	0.89	0.23	47,71,79,85	0
2	NAG	I	1	14/15	0.89	0.21	35,51,61,66	0
2	NAG	K	1	14/15	0.89	0.14	69,83,90,93	0
4	MAN	J	7	11/12	0.90	0.14	73,81,88,93	0
4	NAG	J	2	14/15	0.92	0.21	65,69,81,84	0
2	NAG	I	2	14/15	0.92	0.22	48,72,81,81	0
3	MAN	D	7	11/12	0.93	0.13	45,50,55,56	0
4	BMA	J	3	11/12	0.93	0.25	61,64,77,81	0
4	MAN	J	4	11/12	0.93	0.13	55,58,60,62	0
2	NAG	H	1	14/15	0.93	0.25	50,59,68,74	0
2	NAG	C	1	14/15	0.93	0.22	46,62,80,88	0
2	NAG	F	1	14/15	0.93	0.16	35,46,52,57	0
2	NAG	G	1	14/15	0.94	0.14	51,59,70,70	0
3	MAN	D	6	11/12	0.94	0.15	37,43,47,51	0
4	NAG	J	1	14/15	0.95	0.14	55,62,68,74	0
3	MAN	D	4	11/12	0.95	0.12	35,39,44,46	0
4	MAN	J	5	11/12	0.95	0.15	55,58,67,70	0
4	MAN	J	6	11/12	0.96	0.09	55,59,64,65	0
3	MAN	D	5	11/12	0.97	0.13	37,41,47,54	0
3	NAG	D	1	14/15	0.97	0.14	34,38,43,46	0
2	NAG	E	1	14/15	0.97	0.14	45,55,57,63	0
3	NAG	D	2	14/15	0.98	0.12	32,36,42,48	0
3	BMA	D	3	11/12	0.98	0.13	30,37,42,48	0

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

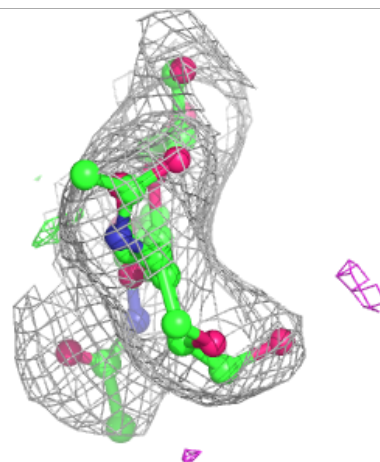
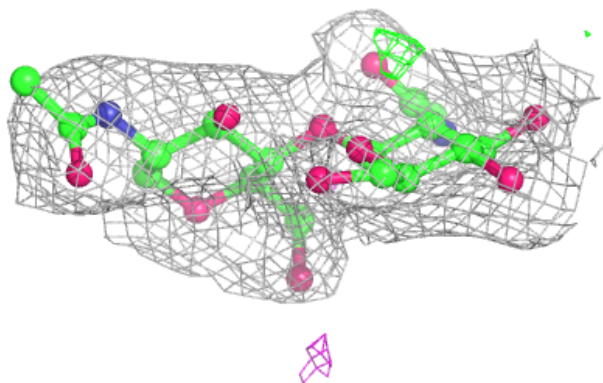
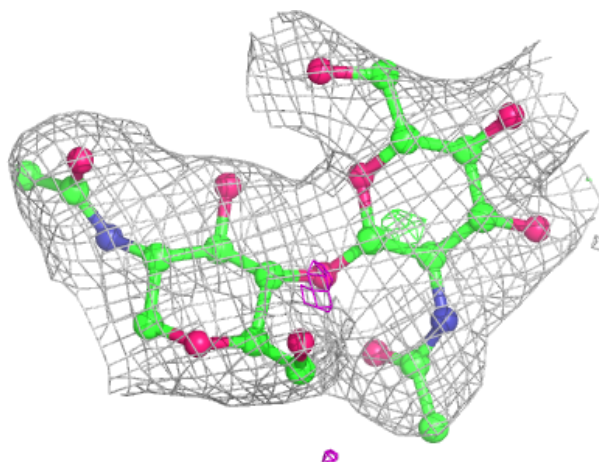
Electron density around Chain C:

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



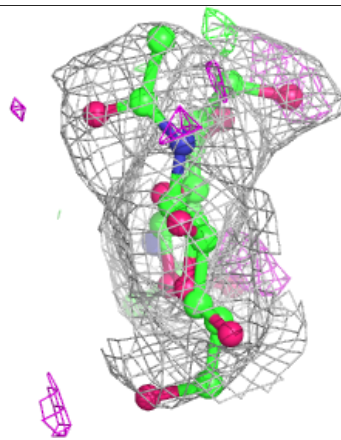
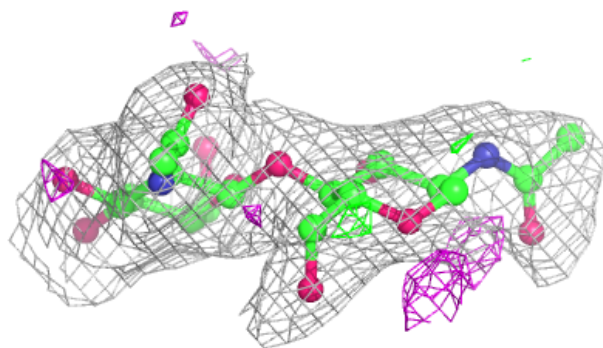
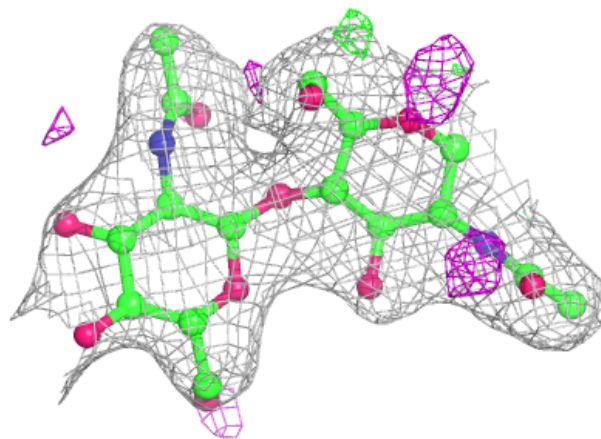
Electron density around Chain E:

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



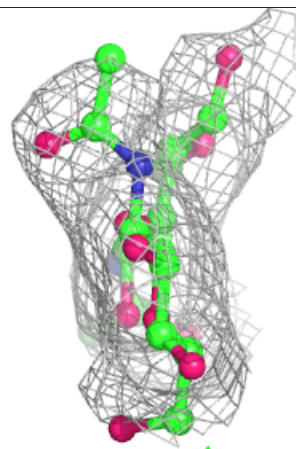
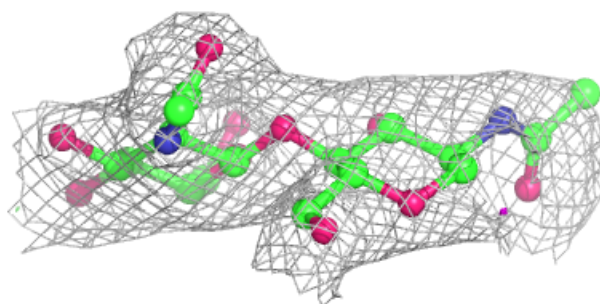
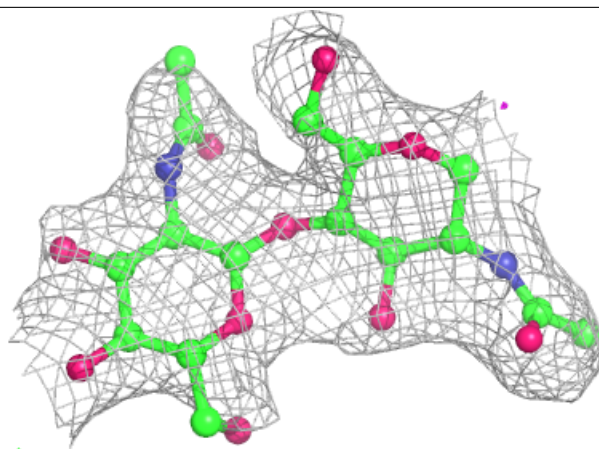
Electron density around Chain F:

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



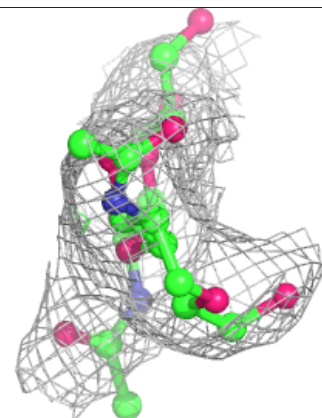
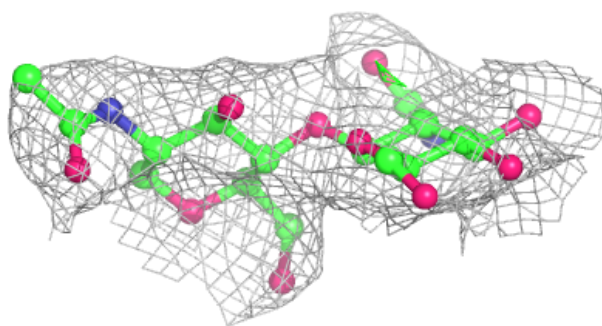
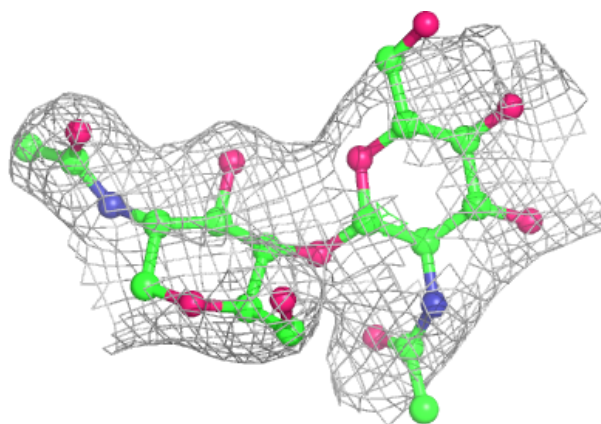
Electron density around Chain G:

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

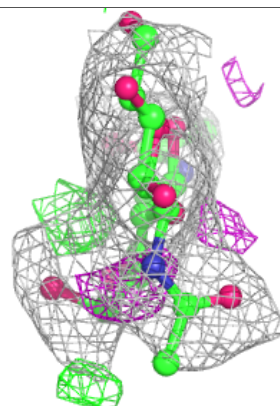
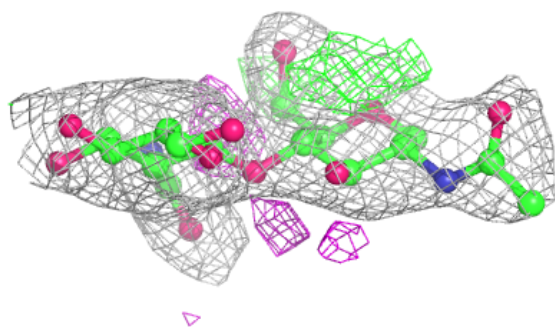
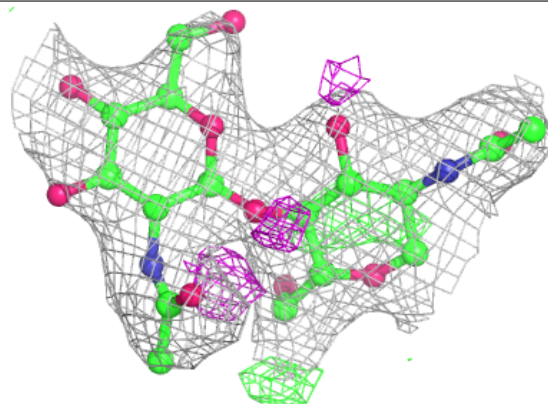


Electron density around Chain H:

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

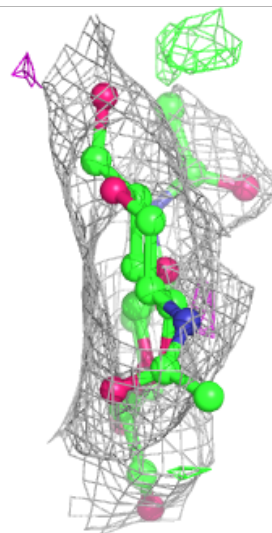
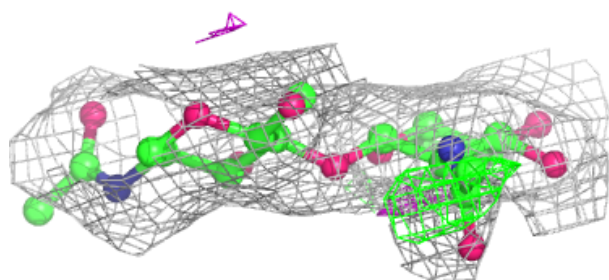
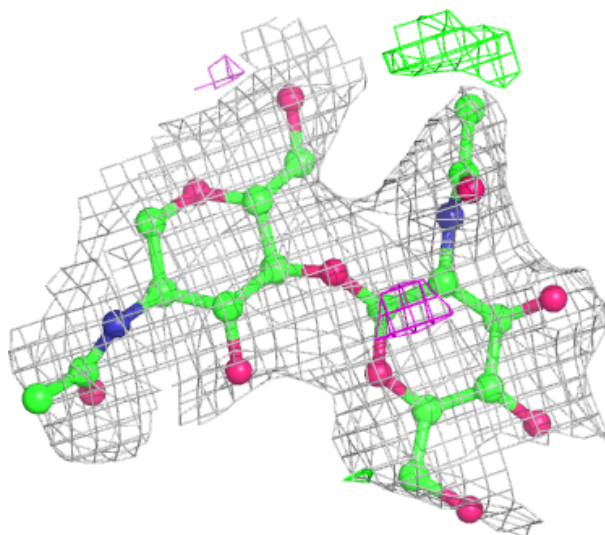
**Electron density around Chain I:**

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



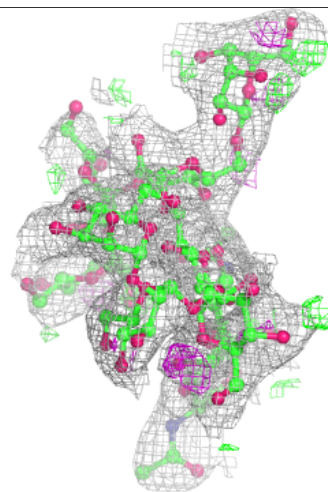
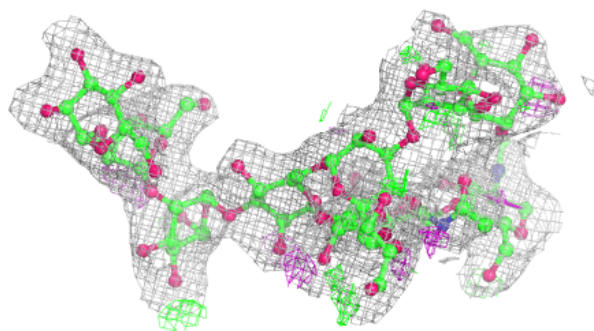
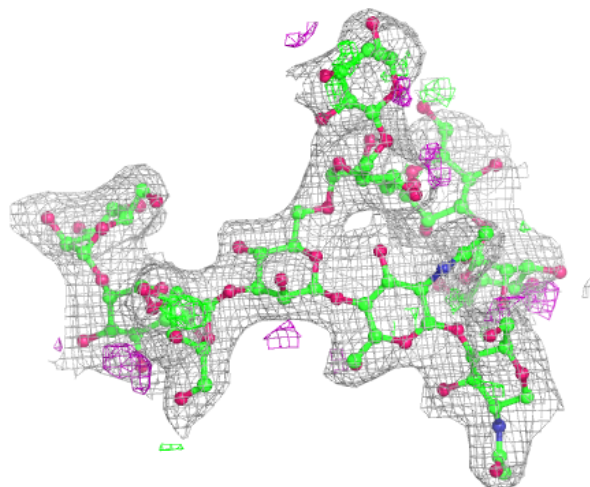
Electron density around Chain K:

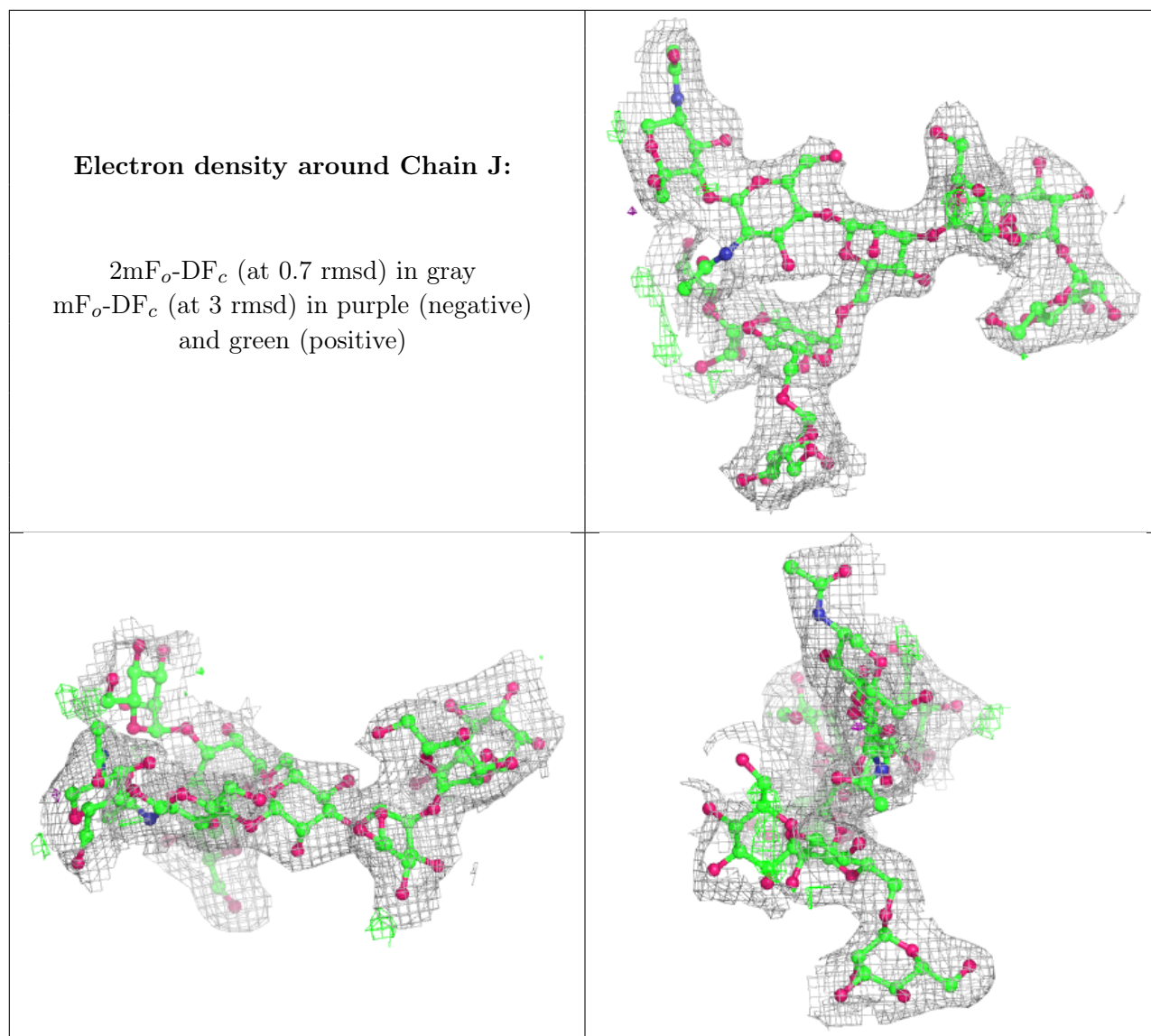
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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
5	PG4	B	601	13/13	0.90	0.31	53,58,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.