



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 8SPI / pdb_00008spi
Title : Crystal structure of chimeric omicron RBD (strain XBB.1.5) complexed with human ACE2
Authors : Zhang, W.; Shi, K.; Aihara, H.; Li, F.
Deposited on : 2023-05-03
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

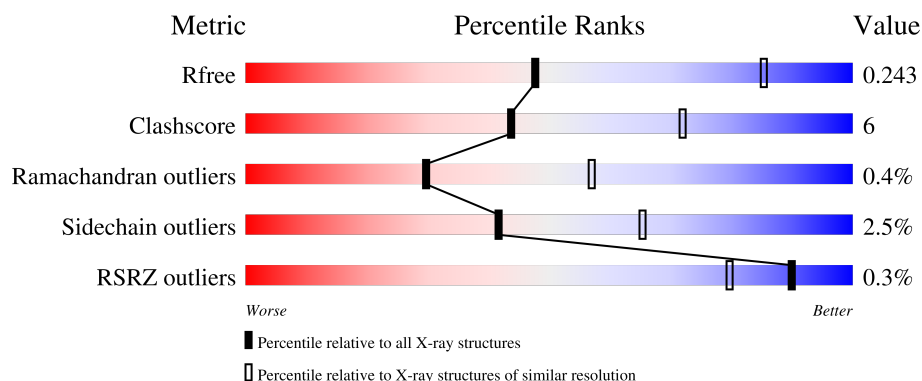
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

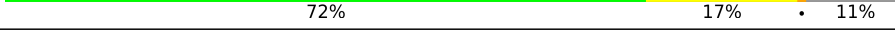
The reported resolution of this entry is 3.06 Å.

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.



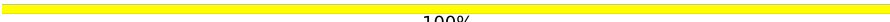
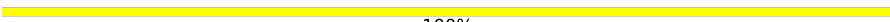
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	597	
1	B	597	
2	E	217	
2	F	217	
3	C	2	

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	I	2	 100%
3	M	2	 50%50%
4	D	3	 100%
4	G	3	 100%
5	J	4	 50%50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13107 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	B	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

- Molecule 2 is a protein called Spike protein S1.

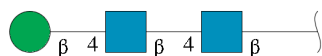
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	192	Total	C	N	O	S	0	0	0
			1514	974	251	280	9			
2	F	194	Total	C	N	O	S	0	0	0
			1527	980	253	285	9			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
5	J	4	Total	C	N	O	0	0	0
			53	30	3	20			

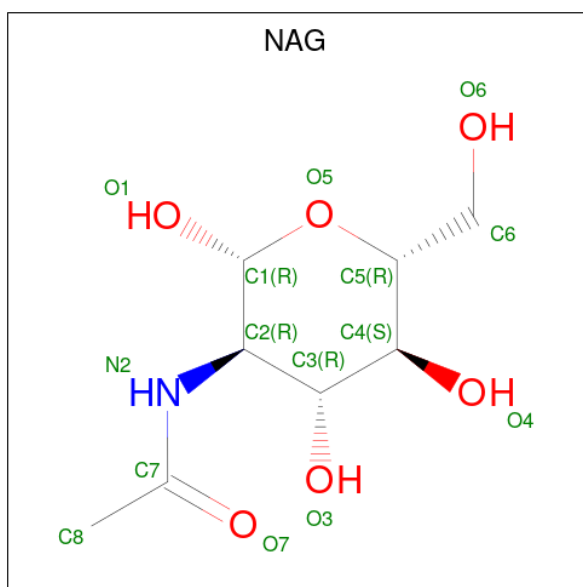
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

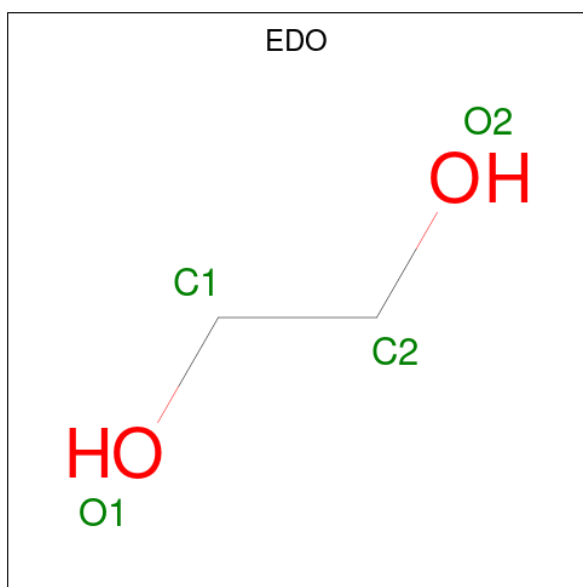
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

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



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

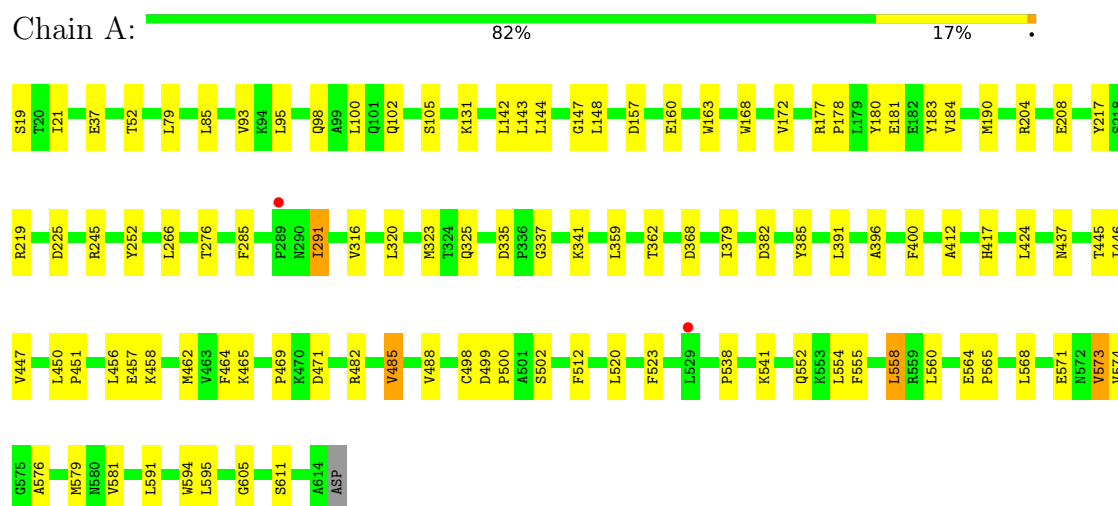
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	B	1	Total	O	0	0
			1	1		
10	E	1	Total	O	0	0
			1	1		

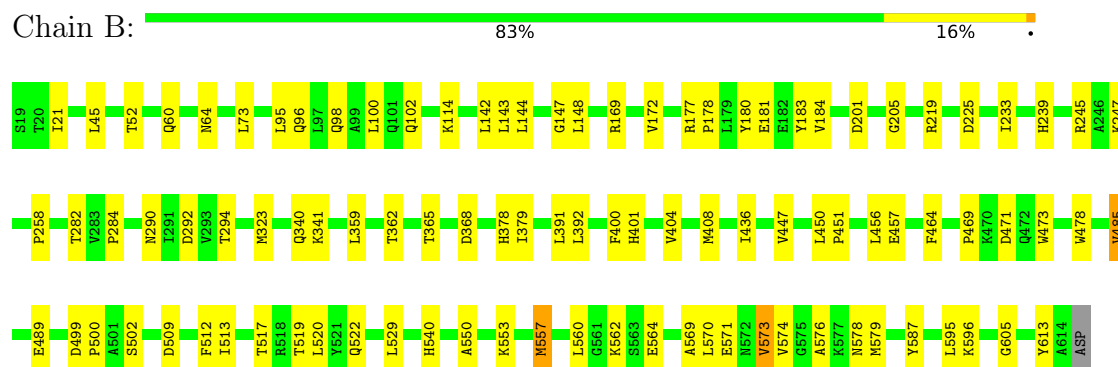
3 Residue-property plots

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

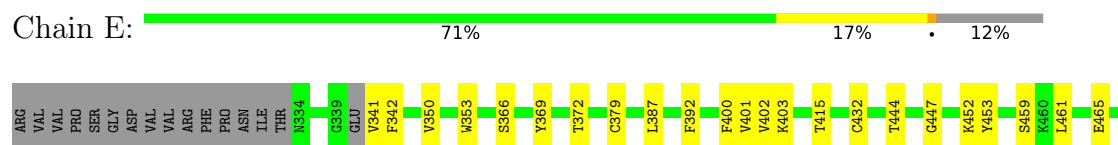
• Molecule 1: Angiotensin-converting enzyme 2



• Molecule 1: Angiotensin-converting enzyme 2



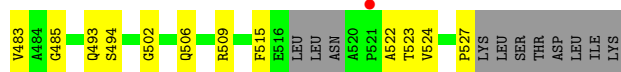
• Molecule 2: Spike protein S1





- Molecule 2: Spike protein S1

Chain F: 72% 17% 11%



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

Chain C: 50% 50%



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

Chain H: 100%



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

Chain I: 100%



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

Chain M: 50% 50%



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

Chain D: 100%



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

Chain G:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.36Å 116.20Å 108.77Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	77.85 – 3.06 77.85 – 3.06	Depositor EDS
% Data completeness (in resolution range)	67.4 (77.85-3.06) 67.7 (77.85-3.06)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.243 0.190 , 0.243	Depositor DCC
R_{free} test set	1276 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13107	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: BMA, ZN, CL, NAG, EDO

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	0.10	0/4999	0.23	0/6792
1	B	0.09	0/4999	0.23	0/6792
2	E	0.21	0/1556	0.29	0/2115
2	F	0.16	0/1570	0.28	0/2136
All	All	0.12	0/13124	0.25	0/17835

There are no bond length outliers.

There are no bond angle outliers.

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	4862	0	4634	56	0
1	B	4862	0	4633	59	0
2	E	1514	0	1443	18	0
2	F	1527	0	1453	21	0
3	C	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
3	M	28	0	25	2	0
4	D	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	39	0	34	0	0
5	J	53	0	46	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
8	A	28	0	26	0	0
8	B	42	0	39	0	0
8	E	14	0	13	1	0
9	B	8	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
All	All	13107	0	12467	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:NH1	7:B:702:CL:CL	2.53	0.78
1:A:131:LYS:HG2	1:A:143:LEU:HB3	1.66	0.78
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.71	0.71
1:A:276:THR:HG1	1:A:445:THR:HG1	1.36	0.66
2:E:521:PRO:O	2:E:523:THR:N	2.29	0.66
2:F:393:SER:HA	2:F:522:ALA:HA	1.78	0.66
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.79	0.64
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.79	0.64
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.78	0.64
1:B:245:ARG:NH2	1:B:605:GLY:O	2.24	0.63
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.32	0.63
1:B:245:ARG:NH1	1:B:258:PRO:O	2.33	0.61
1:A:245:ARG:NH2	1:A:605:GLY:O	2.34	0.61
1:A:19:SER:N	2:E:477:ASN:HD21	2.00	0.60
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.35	0.60
2:F:360:ASN:HA	2:F:523:THR:HB	1.83	0.59
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.67	0.59
1:B:52:THR:O	1:B:340:GLN:NE2	2.35	0.58
2:F:395:VAL:HG23	2:F:524:VAL:HG21	1.84	0.58
2:F:461:LEU:HD22	2:F:465:GLU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:HH11	1:B:499:ASP:HB3	1.69	0.57
1:B:553:LYS:NZ	1:B:573:VAL:O	2.37	0.57
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.87	0.56
1:A:565:PRO:HD2	1:A:568:LEU:HD13	1.87	0.56
1:B:560:LEU:HD13	1:B:564:GLU:HG3	1.86	0.56
3:M:2:NAG:H83	3:M:2:NAG:H3	1.89	0.55
1:B:290:ASN:HD21	1:B:292:ASP:HB3	1.71	0.54
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.90	0.54
1:B:205:GLY:HA2	1:B:219:ARG:HG2	1.90	0.54
1:A:571:GLU:HA	1:A:576:ALA:H	1.73	0.53
2:F:360:ASN:OD1	2:F:360:ASN:N	2.41	0.53
1:B:142:LEU:HD22	1:B:147:GLY:HA3	1.91	0.53
1:B:499:ASP:O	1:B:502:SER:OG	2.22	0.52
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.91	0.52
1:B:52:THR:HG22	1:B:359:LEU:HD13	1.93	0.51
1:A:382:ASP:OD1	1:A:385:TYR:OH	2.26	0.51
3:I:1:NAG:H62	3:I:2:NAG:N2	2.25	0.51
2:E:461:LEU:HD22	2:E:465:GLU:HB3	1.92	0.50
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.93	0.50
1:B:571:GLU:HA	1:B:576:ALA:H	1.76	0.50
1:A:499:ASP:O	1:A:502:SER:OG	2.25	0.50
2:F:454:ARG:HD3	2:F:457:ARG:HD2	1.93	0.50
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.93	0.49
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.94	0.49
1:B:225:ASP:OD2	1:B:578:ASN:ND2	2.42	0.49
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.24	0.49
1:B:60:GLN:O	1:B:64:ASN:ND2	2.41	0.49
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.95	0.48
1:A:100:LEU:HG	1:A:391:LEU:HD21	1.95	0.48
1:B:557:MET:HE3	1:B:569:ALA:HB1	1.95	0.48
2:E:452:LYS:HA	2:E:494:SER:HA	1.93	0.48
1:A:208:GLU:OE1	1:A:219:ARG:NH1	2.46	0.48
1:B:100:LEU:HG	1:B:391:LEU:HD21	1.94	0.48
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.95	0.48
1:A:555:PHE:HA	1:A:558:LEU:HD22	1.96	0.47
1:A:591:LEU:O	1:A:595:LEU:HD23	2.14	0.47
1:B:450:LEU:HD21	1:B:519:THR:HG21	1.95	0.47
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.95	0.47
1:B:201:ASP:OD2	1:B:219:ARG:NH1	2.47	0.47
1:B:478:TRP:CD2	1:B:489:GLU:HB3	2.49	0.47
1:B:517:THR:HA	1:B:579:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:HIS:CE1	1:B:596:LYS:HG2	2.50	0.47
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.50	0.47
1:A:560:LEU:HD11	1:A:564:GLU:HG3	1.97	0.47
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.97	0.47
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.96	0.46
1:A:594:TRP:HE3	1:A:595:LEU:HD22	1.81	0.46
1:B:169:ARG:NH1	1:B:499:ASP:HB3	2.29	0.46
1:A:451:PRO:HB2	1:A:485:VAL:HG13	1.98	0.46
1:B:96:GLN:HB3	1:B:391:LEU:HD13	1.96	0.46
1:B:247:LYS:HB2	1:B:282:THR:HG22	1.98	0.46
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.98	0.45
1:B:177:ARG:HB3	1:B:178:PRO:HD3	1.98	0.45
1:B:177:ARG:NH2	1:B:473:TRP:HB2	2.32	0.45
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.97	0.45
2:F:366:SER:O	2:F:370:ASN:HB2	2.15	0.45
1:B:294:THR:HG23	1:B:365:THR:HA	1.99	0.45
1:A:142:LEU:HD12	1:A:147:GLY:C	2.42	0.45
1:A:412:ALA:HA	1:A:417:HIS:CD2	2.52	0.45
1:B:529:LEU:HB3	1:B:550:ALA:HB1	1.99	0.45
1:B:143:LEU:HD23	1:B:143:LEU:H	1.82	0.45
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.98	0.44
2:E:379:CYS:HA	2:E:432:CYS:HA	1.98	0.44
1:A:291:ILE:HG23	1:A:424:LEU:HD22	2.00	0.44
1:A:362:THR:HG23	1:A:368:ASP:HB3	1.99	0.44
1:B:290:ASN:ND2	1:B:292:ASP:HB3	2.31	0.44
1:B:573:VAL:HG13	1:B:574:VAL:HG13	1.98	0.44
2:E:366:SER:HA	2:E:369:TYR:CE2	2.52	0.44
1:B:98:GLN:O	1:B:102:GLN:HG3	2.18	0.44
2:F:364:ASP:H	2:F:527:PRO:HD2	1.81	0.44
2:F:502:GLY:O	2:F:506:GLN:HG3	2.18	0.44
1:B:404:VAL:O	1:B:408:MET:HG2	2.18	0.44
2:F:452:LYS:HA	2:F:494:SER:HA	2.00	0.44
1:A:316:VAL:HA	1:A:320:LEU:O	2.18	0.44
2:F:458:LYS:HD2	2:F:458:LYS:H	1.82	0.44
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.99	0.43
1:A:252:TYR:CZ	1:A:266:LEU:HD22	2.53	0.43
1:A:396:ALA:HB3	1:A:400:PHE:CD1	2.53	0.43
1:B:184:VAL:HG22	1:B:464:PHE:HE1	1.83	0.43
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.53	0.43
2:E:392:PHE:O	2:E:523:THR:N	2.51	0.43
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.00	0.43
2:F:472:ILE:HG13	2:F:482:GLY:CA	2.49	0.43
2:E:444:THR:HG23	2:E:447:GLY:H	1.83	0.43
1:B:233:ILE:HD13	1:B:450:LEU:HD13	2.00	0.43
1:B:362:THR:HG23	1:B:368:ASP:HB3	2.01	0.43
1:A:285:PHE:O	1:A:437:ASN:ND2	2.48	0.43
1:A:204:ARG:HH22	1:A:465:LYS:NZ	2.17	0.42
1:A:482:ARG:HH21	1:A:611:SER:HB3	1.83	0.42
2:E:342:PHE:HB2	8:E:601:NAG:H82	2.01	0.42
1:A:98:GLN:O	1:A:102:GLN:HG3	2.20	0.42
1:A:554:LEU:HG	1:A:558:LEU:HD21	2.00	0.42
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.20	0.42
2:F:392:PHE:CD1	2:F:515:PHE:HB3	2.55	0.42
1:A:143:LEU:H	1:A:143:LEU:HD23	1.84	0.42
3:M:1:NAG:H61	3:M:2:NAG:O5	2.19	0.42
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.85	0.42
1:A:488:VAL:HG21	1:A:611:SER:HA	2.01	0.42
1:B:378:HIS:CE1	1:B:401:HIS:HB3	2.54	0.42
2:E:403:LYS:HB2	2:E:495:TYR:CE1	2.55	0.42
1:B:284:PRO:HG2	1:B:436:ILE:HG22	2.01	0.42
1:B:595:LEU:HD23	1:B:595:LEU:HA	1.93	0.42
1:B:114:LYS:HD3	1:B:114:LYS:HA	1.83	0.42
1:B:451:PRO:HB2	1:B:485:VAL:HG13	2.02	0.42
2:F:350:VAL:HG22	2:F:422:ASN:HB3	2.01	0.42
1:A:499:ASP:N	1:A:500:PRO:HD2	2.35	0.41
2:E:353:TRP:H	2:E:353:TRP:CD1	2.38	0.41
2:E:526:GLY:N	2:E:527:PRO:HD3	2.35	0.41
2:F:362:VAL:HB	2:F:527:PRO:HG3	2.02	0.41
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.55	0.41
1:A:21:ILE:H	1:A:21:ILE:HD12	1.84	0.41
2:F:347:PHE:CD1	2:F:509:ARG:HD3	2.55	0.41
1:A:142:LEU:HD21	1:A:163:TRP:HH2	1.84	0.41
1:B:450:LEU:HB2	1:B:451:PRO:HD3	2.01	0.41
2:F:472:ILE:HG13	2:F:482:GLY:HA2	2.01	0.41
1:B:499:ASP:N	1:B:500:PRO:HD2	2.36	0.41
1:A:341:LYS:HA	1:A:341:LYS:HD2	1.79	0.41
1:B:183:TYR:OH	1:B:509:ASP:OD1	2.38	0.41
1:A:142:LEU:HB2	1:A:147:GLY:HA3	2.03	0.41
1:A:458:LYS:NZ	1:A:462:MET:HE3	2.36	0.41
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.20	0.41
2:E:502:GLY:O	2:E:506:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.92	0.41
1:B:96:GLN:HG2	1:B:392:LEU:HD13	2.03	0.41
1:B:519:THR:O	1:B:522:GLN:HG2	2.20	0.41
2:E:453:TYR:CZ	2:E:493:GLN:HB3	2.56	0.41
2:F:431:GLY:HA2	2:F:515:PHE:CE2	2.56	0.41
1:A:105:SER:HA	1:A:190:MET:HG3	2.02	0.41
1:A:335:ASP:C	1:A:337:GLY:H	2.28	0.41
2:E:403:LYS:HD2	2:E:505:HIS:ND1	2.36	0.40
1:B:400:PHE:O	1:B:404:VAL:HG23	2.22	0.40
2:E:350:VAL:HA	2:E:400:PHE:HB2	2.04	0.40
1:B:570:LEU:O	1:B:574:VAL:HG22	2.21	0.40
2:E:497:PHE:CD2	2:E:507:PRO:HB3	2.56	0.40
2:F:365:TYR:HD2	2:F:388:ASN:HA	1.87	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	594/597 (100%)	575 (97%)	18 (3%)	1 (0%)	43	70
1	B	594/597 (100%)	574 (97%)	19 (3%)	1 (0%)	43	70
2	E	186/217 (86%)	164 (88%)	20 (11%)	2 (1%)	11	34
2	F	190/217 (88%)	170 (90%)	18 (10%)	2 (1%)	11	34
All	All	1564/1628 (96%)	1483 (95%)	75 (5%)	6 (0%)	30	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	613	TYR
2	F	485	GLY

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Mol	Chain	Res	Type
2	E	459	SER
1	A	291	ILE
2	E	526	GLY
2	F	483	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/527 (100%)	513 (98%)	13 (2%)	42	65
1	B	526/527 (100%)	516 (98%)	10 (2%)	50	69
2	E	165/189 (87%)	158 (96%)	7 (4%)	26	54
2	F	166/189 (88%)	161 (97%)	5 (3%)	36	62
All	All	1383/1432 (97%)	1348 (98%)	35 (2%)	42	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	79	LEU
1	A	85	LEU
1	A	93	VAL
1	A	95	LEU
1	A	172	VAL
1	A	325	GLN
1	A	447	VAL
1	A	485	VAL
1	A	552	GLN
1	A	558	LEU
1	A	573	VAL
1	A	581	VAL
1	B	21	ILE
1	B	45	LEU
1	B	95	LEU
1	B	172	VAL

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Mol	Chain	Res	Type
1	B	341	LYS
1	B	447	VAL
1	B	485	VAL
1	B	557	MET
1	B	562	LYS
1	B	573	VAL
2	E	341	VAL
2	E	372	THR
2	E	387	LEU
2	E	402	VAL
2	E	415	THR
2	E	468	ILE
2	E	493	GLN
2	F	355	ARG
2	F	360	ASN
2	F	458	LYS
2	F	468	ILE
2	F	493	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	76	GLN
1	A	239	HIS
1	A	325	GLN
1	A	599	ASN
1	B	42	GLN
1	B	63	ASN
1	B	76	GLN
1	B	290	ASN
1	B	300	GLN
1	B	325	GLN
1	B	472	GLN
1	B	552	GLN
1	B	556	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 ⓘ

18 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.48	0	17,19,21	0.75	1 (5%)
3	NAG	C	2	3	14,14,15	0.35	0	17,19,21	0.42	0
4	NAG	D	1	4,1	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.45	0
4	BMA	D	3	4	11,11,12	0.64	0	15,15,17	0.72	0
4	NAG	G	1	4,1	14,14,15	0.34	0	17,19,21	0.54	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.73	0
3	NAG	H	1	3,1	14,14,15	0.37	0	17,19,21	1.09	2 (11%)
3	NAG	H	2	3	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.34	0	17,19,21	0.58	0
3	NAG	I	2	3	14,14,15	0.36	0	17,19,21	0.56	0
5	NAG	J	1	5,1	14,14,15	0.33	0	17,19,21	0.49	0
5	NAG	J	2	5	14,14,15	0.24	0	17,19,21	0.43	0
5	BMA	J	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.35	1 (6%)
5	NAG	J	4	5	14,14,15	0.84	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	M	1	3,2	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	M	2	3	14,14,15	0.61	0	17,19,21	1.37	2 (11%)

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
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	NAG	J	4	5	-	4/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	NAG	O5-C1	2.39	1.47	1.43
5	J	3	BMA	C2-C3	2.29	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	C2-N2-C7	4.58	129.03	122.90
5	J	3	BMA	C1-C2-C3	3.72	115.06	109.64
5	J	4	NAG	C1-O5-C5	3.25	116.54	112.19
3	H	1	NAG	O4-C4-C5	2.89	116.45	109.32
3	H	2	NAG	C1-O5-C5	2.83	115.97	112.19
3	H	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	C	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	M	2	NAG	C1-C2-N2	2.25	113.97	110.43

There are no chirality outliers.

All (38) torsion outliers are listed below:

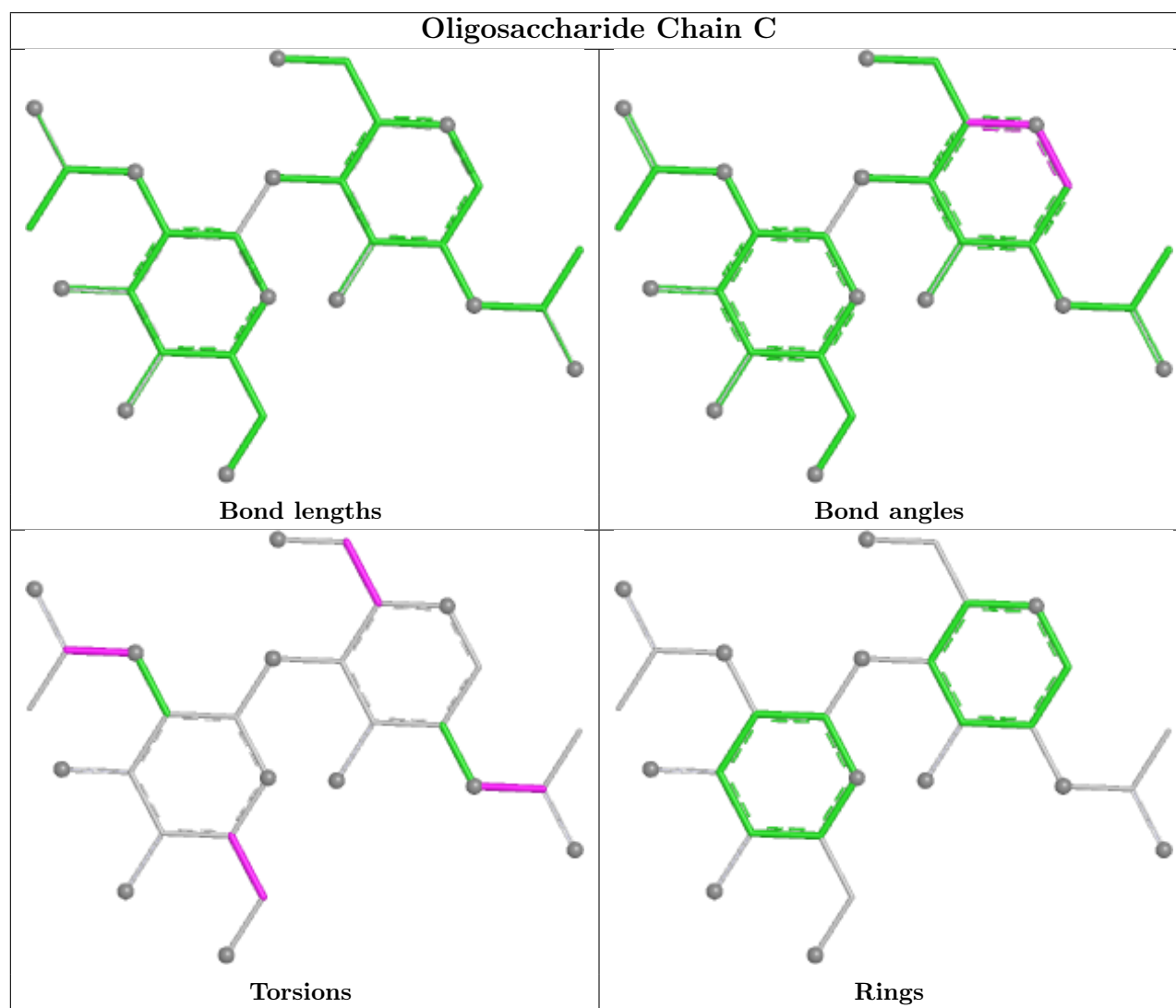
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	J	4	NAG	C8-C7-N2-C2
5	J	4	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
5	J	4	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C3-C2-N2-C7
5	J	4	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6

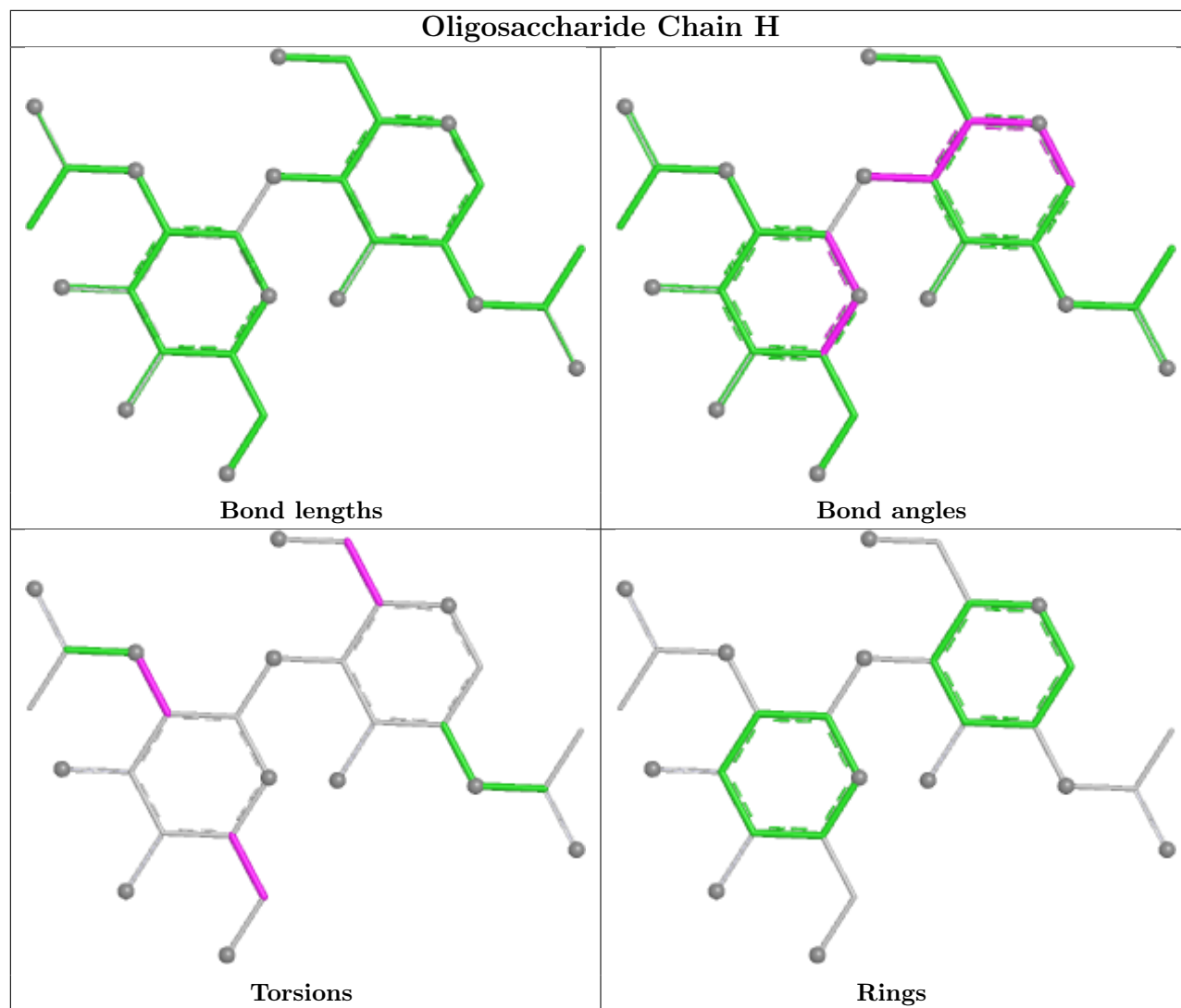
There are no ring outliers.

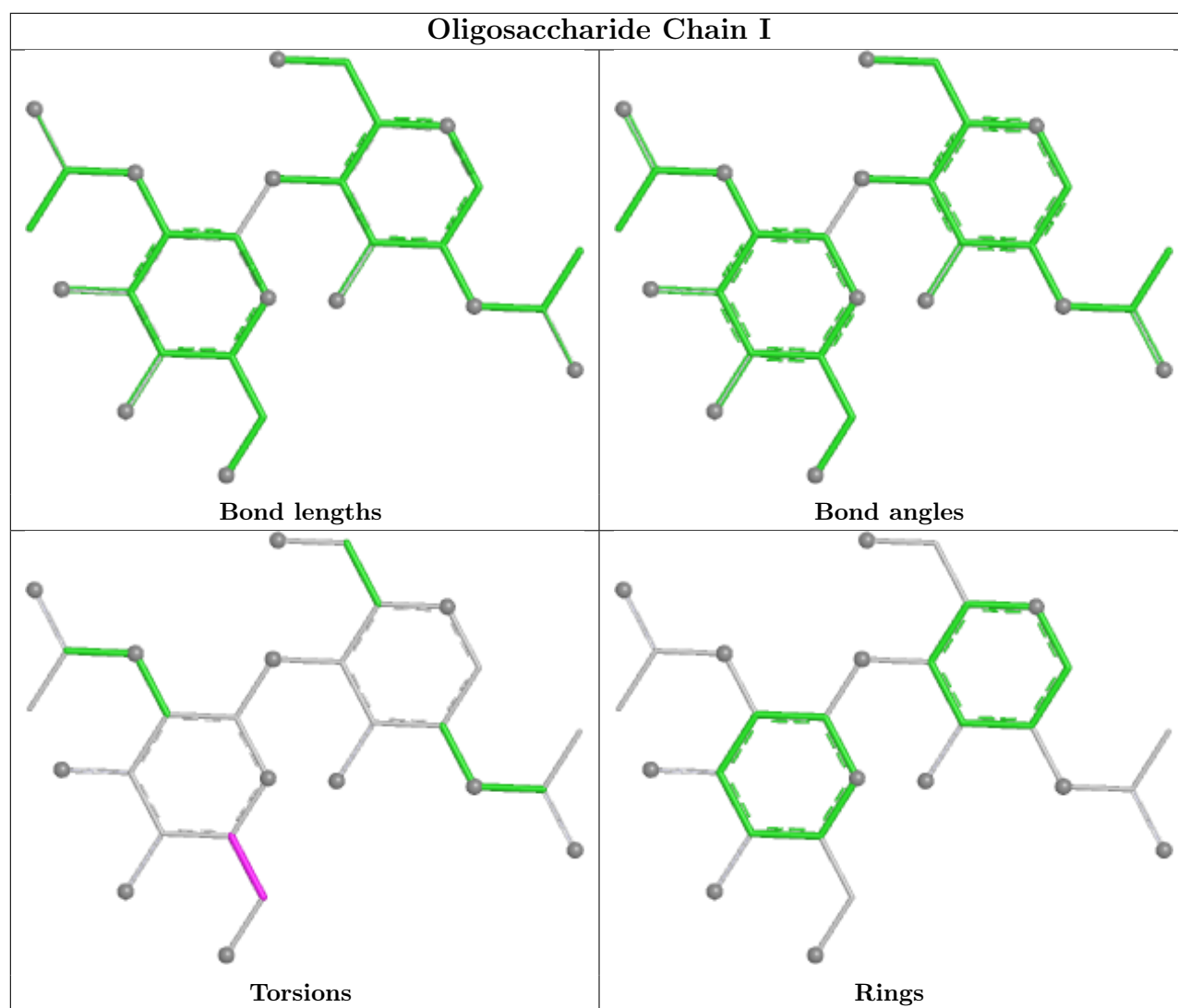
4 monomers are involved in 3 short contacts:

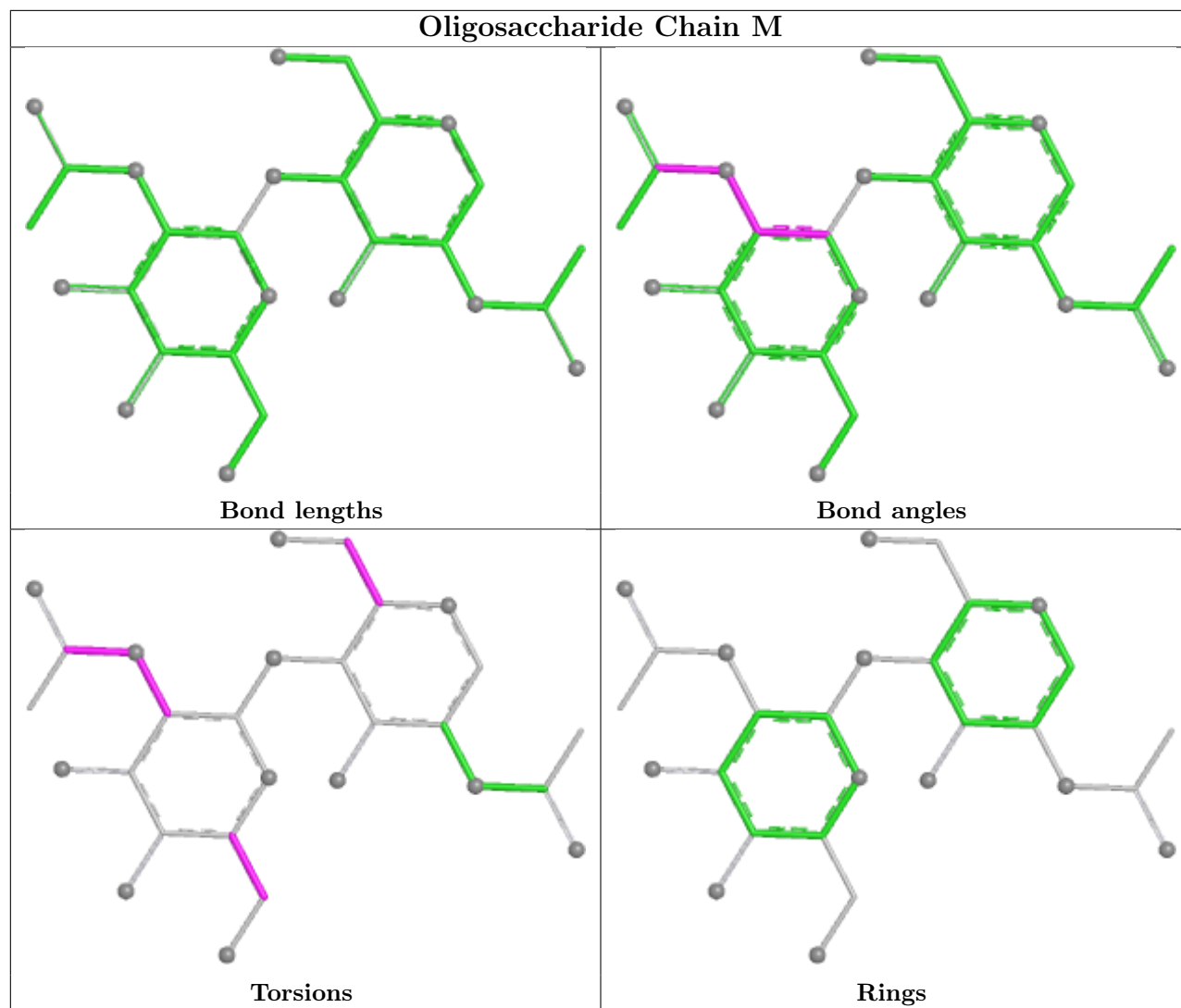
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
3	M	2	NAG	2	0
3	I	1	NAG	1	0
3	M	1	NAG	1	0

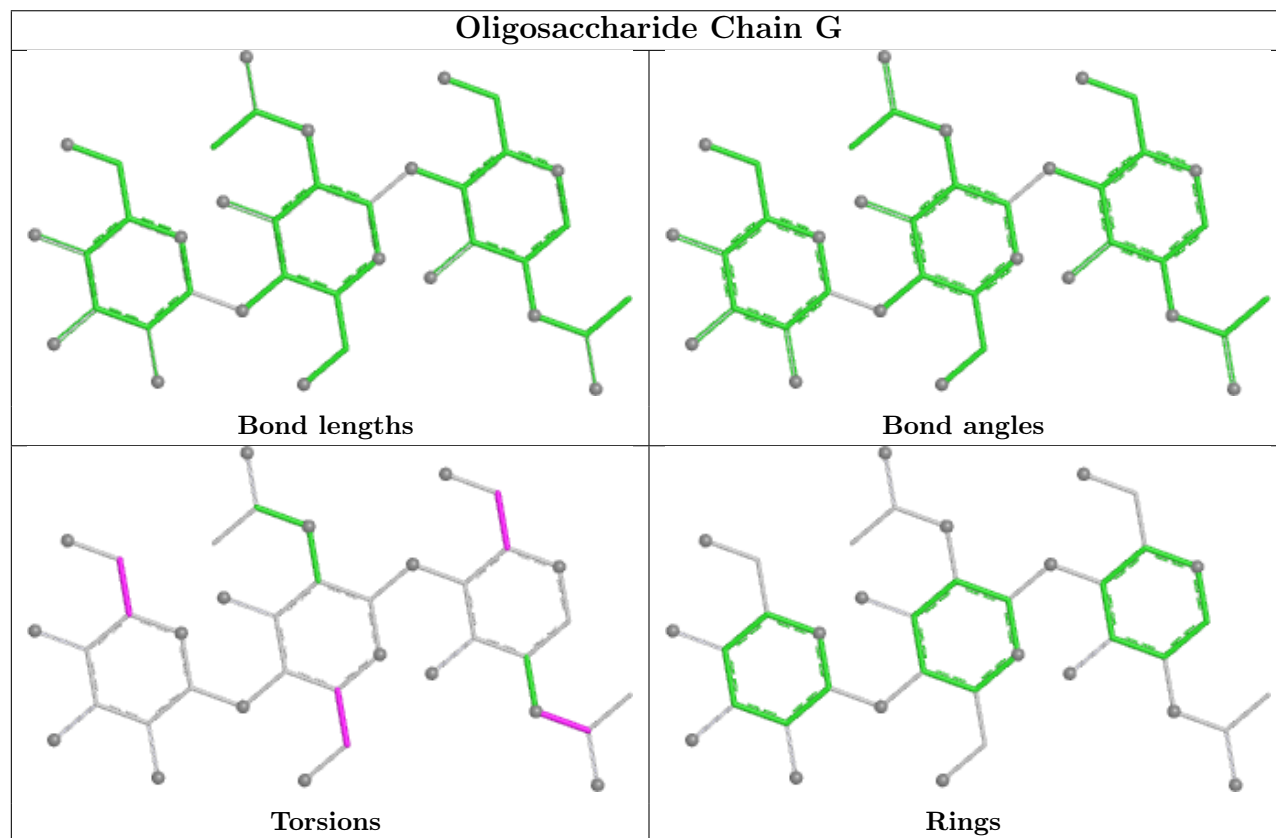
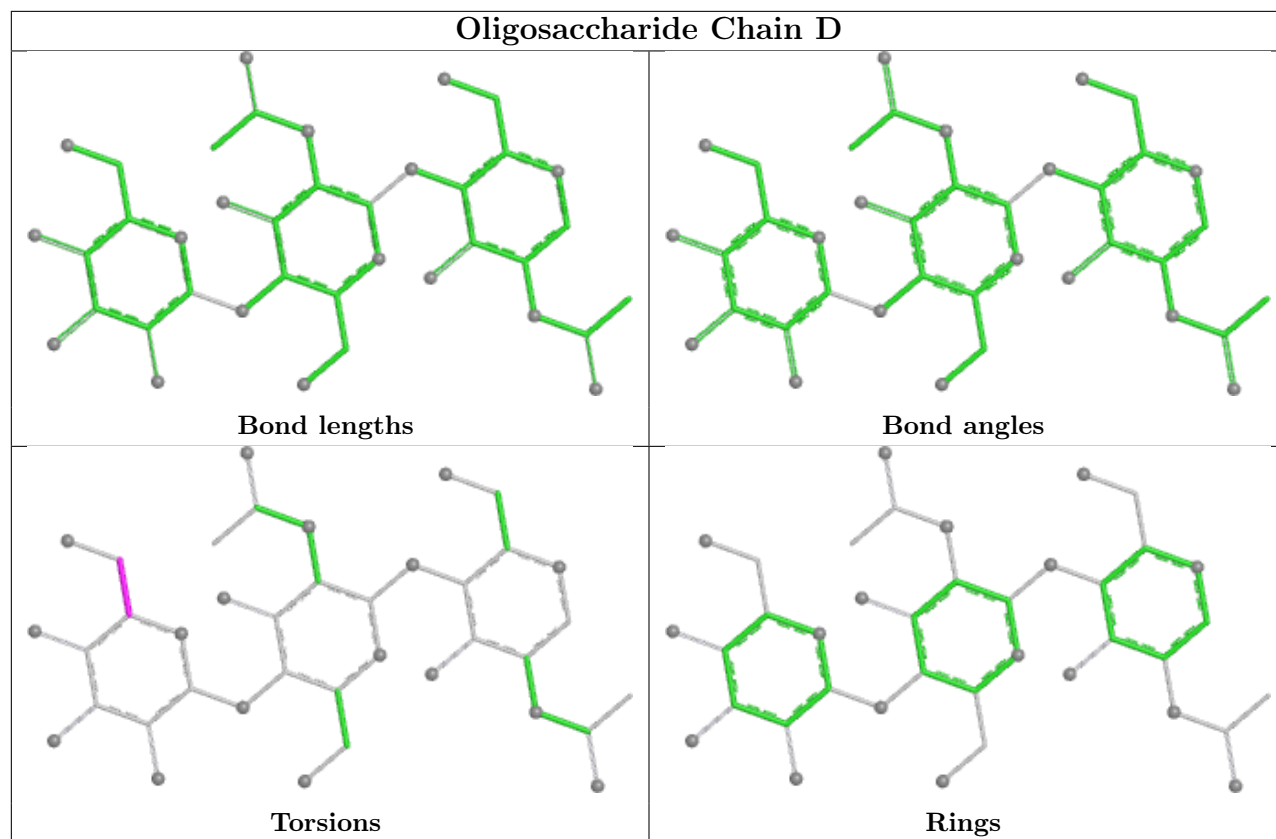
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

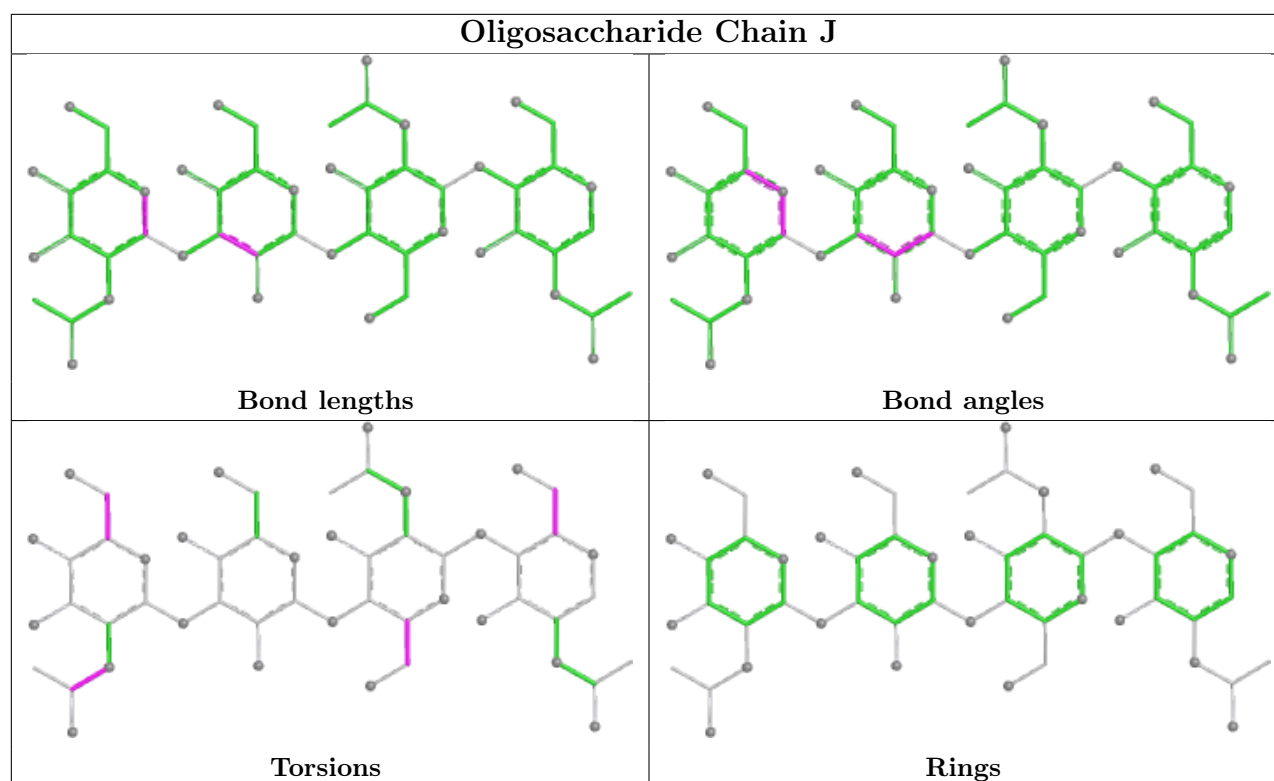












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.36	0
8	NAG	E	601	2	14,14,15	0.26	0	17,19,21	0.44	0
8	NAG	B	707	1	14,14,15	0.30	0	17,19,21	0.48	0
8	NAG	B	706	1	14,14,15	0.38	0	17,19,21	0.51	0
9	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.39	0
8	NAG	A	704	1	14,14,15	0.27	0	17,19,21	0.49	0
8	NAG	B	705	1	14,14,15	0.24	0	17,19,21	0.49	0
8	NAG	A	703	1	14,14,15	0.32	0	17,19,21	0.49	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
9	EDO	B	704	-	-	0/1/1/1	-
8	NAG	E	601	2	-	2/6/23/26	0/1/1/1
8	NAG	B	707	1	-	2/6/23/26	0/1/1/1
8	NAG	B	706	1	-	2/6/23/26	0/1/1/1
9	EDO	B	703	-	-	0/1/1/1	-
8	NAG	A	704	1	-	1/6/23/26	0/1/1/1
8	NAG	B	705	1	-	2/6/23/26	0/1/1/1
8	NAG	A	703	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	705	NAG	O5-C5-C6-O6
8	E	601	NAG	O5-C5-C6-O6
8	B	706	NAG	O5-C5-C6-O6
8	A	703	NAG	O5-C5-C6-O6
8	B	705	NAG	C4-C5-C6-O6
8	B	706	NAG	C4-C5-C6-O6
8	B	707	NAG	O5-C5-C6-O6
8	E	601	NAG	C4-C5-C6-O6
8	A	703	NAG	C4-C5-C6-O6
8	B	707	NAG	C4-C5-C6-O6
8	A	704	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	601	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	596/597 (99%)	-0.16	2 (0%) 90 80	44, 80, 122, 173	0
1	B	596/597 (99%)	-0.28	0 100 100	33, 67, 113, 173	0
2	E	192/217 (88%)	-0.15	1 (0%) 87 72	44, 73, 138, 192	0
2	F	194/217 (89%)	-0.09	1 (0%) 87 72	53, 89, 138, 204	0
All	All	1578/1628 (96%)	-0.20	4 (0%) 90 80	33, 75, 127, 204	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	521	PRO	3.5
1	A	289	PRO	2.7
1	A	529	LEU	2.3
2	E	526	GLY	2.2

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.

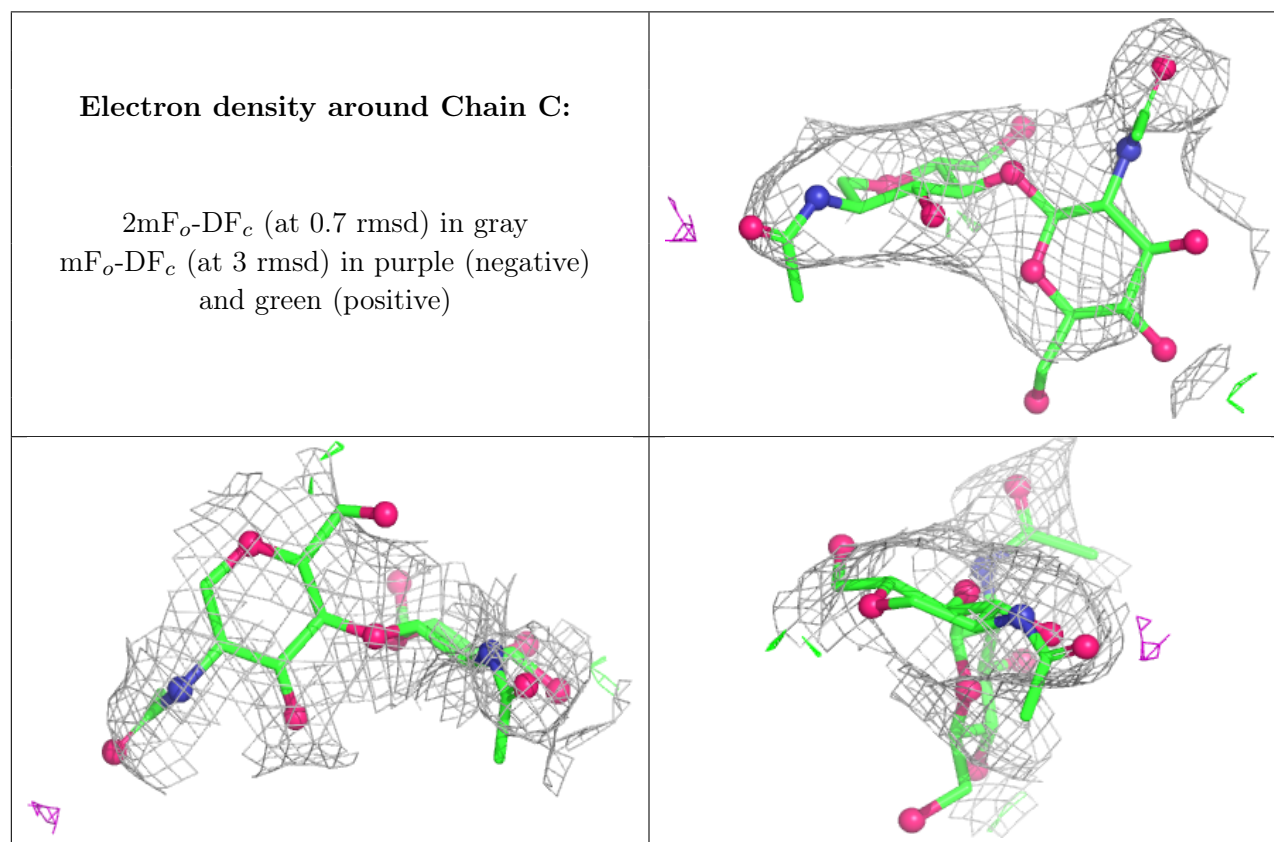
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	94,106,131,133	0
3	NAG	C	2	14/15	-	-	129,147,154,157	0
3	NAG	H	2	14/15	0.40	0.12	104,132,142,152	0

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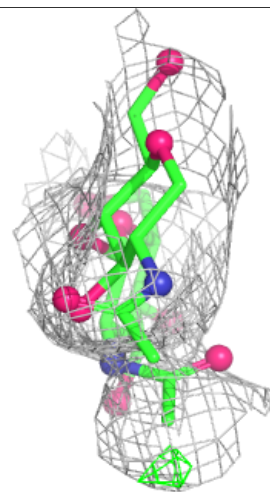
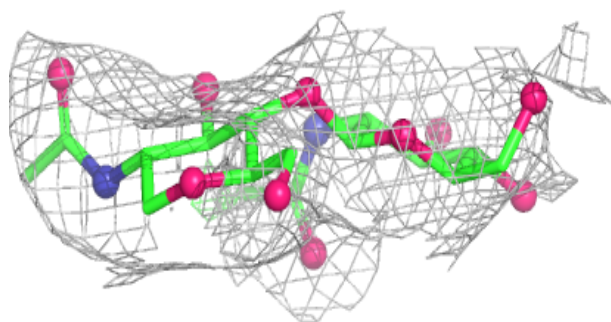
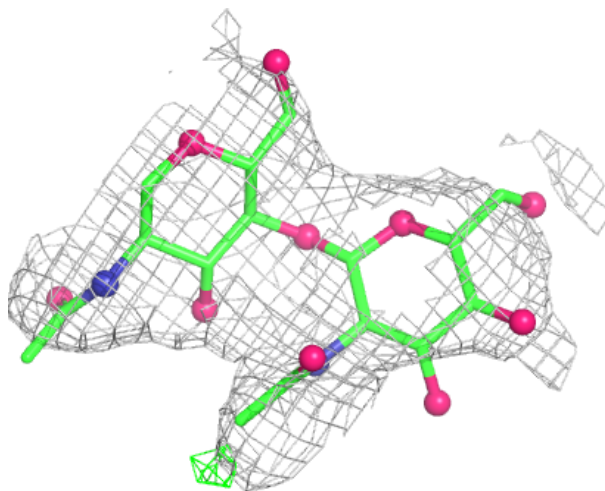
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	G	3	11/12	0.54	0.10	97,125,136,137	0
5	BMA	J	3	11/12	0.62	0.11	85,100,105,113	0
3	NAG	I	2	14/15	0.65	0.12	111,128,135,135	0
3	NAG	M	1	14/15	-	-	88,116,130,135	0
3	NAG	M	2	14/15	-	-	101,127,135,136	0
4	NAG	D	1	14/15	-	-	87,97,100,100	0
4	NAG	D	2	14/15	-	-	86,102,108,114	0
4	BMA	D	3	11/12	-	-	91,107,119,122	0
4	NAG	G	2	14/15	0.74	0.12	109,123,137,148	0
5	NAG	J	2	14/15	0.75	0.11	59,81,92,93	0
5	NAG	J	4	14/15	0.75	0.12	103,126,132,143	0
4	NAG	G	1	14/15	0.81	0.12	97,117,124,124	0
3	NAG	I	1	14/15	0.81	0.10	108,118,130,130	0
3	NAG	H	1	14/15	0.85	0.09	73,90,109,118	0
5	NAG	J	1	14/15	0.87	0.10	41,63,72,74	0

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



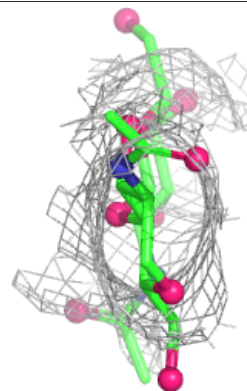
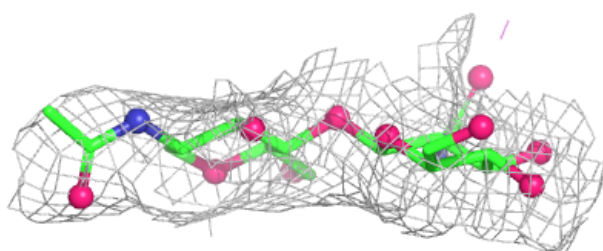
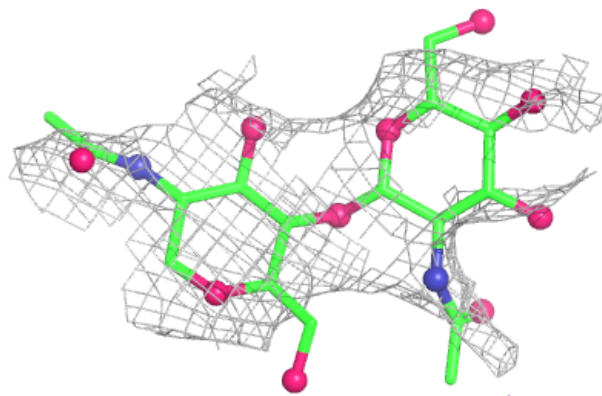
Electron density around Chain H:

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



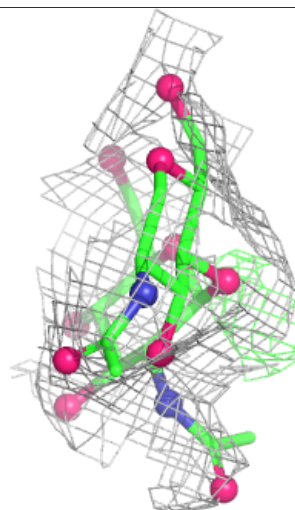
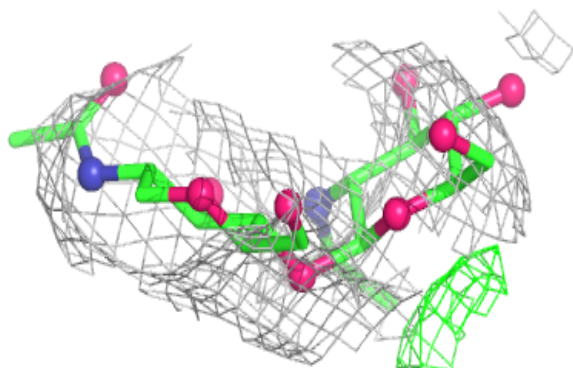
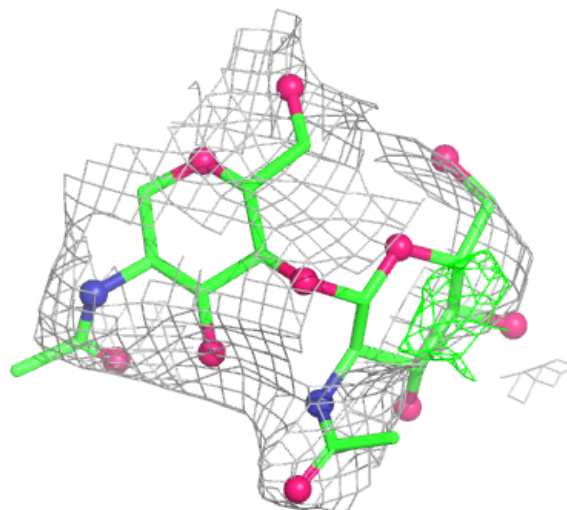
Electron density around Chain I:

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



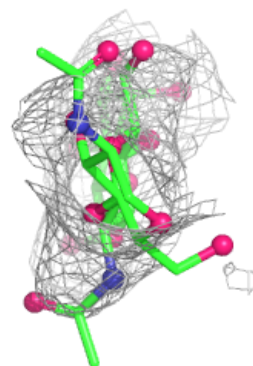
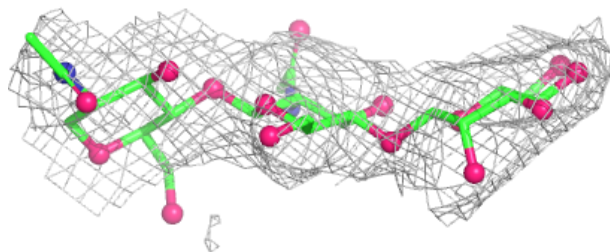
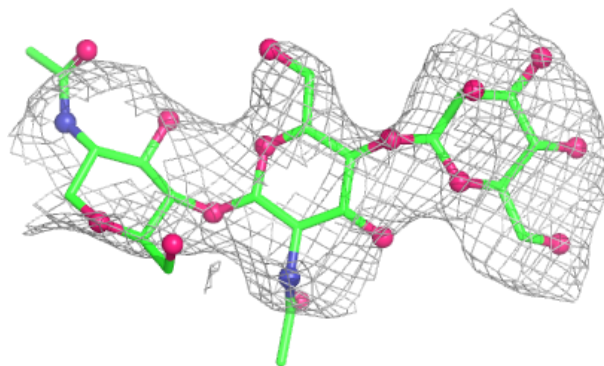
Electron density around Chain M:

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

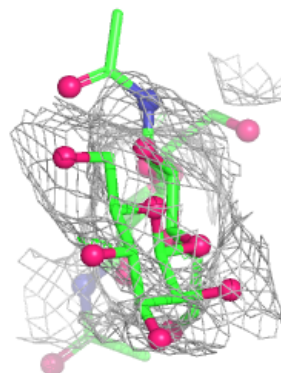
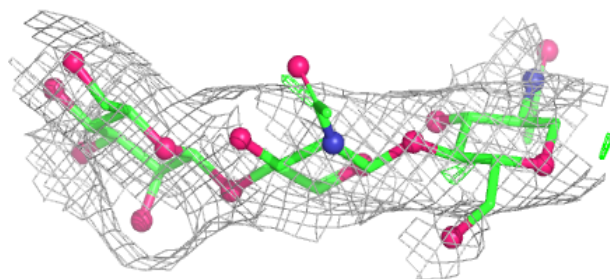
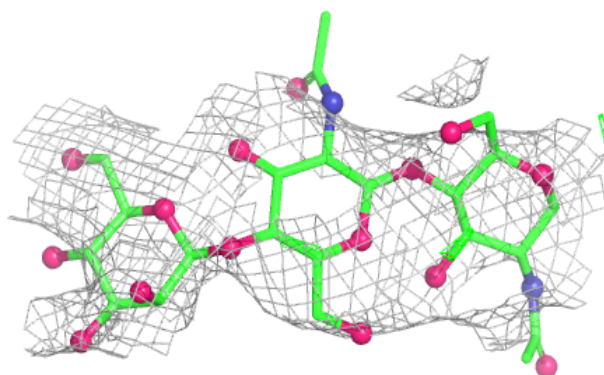


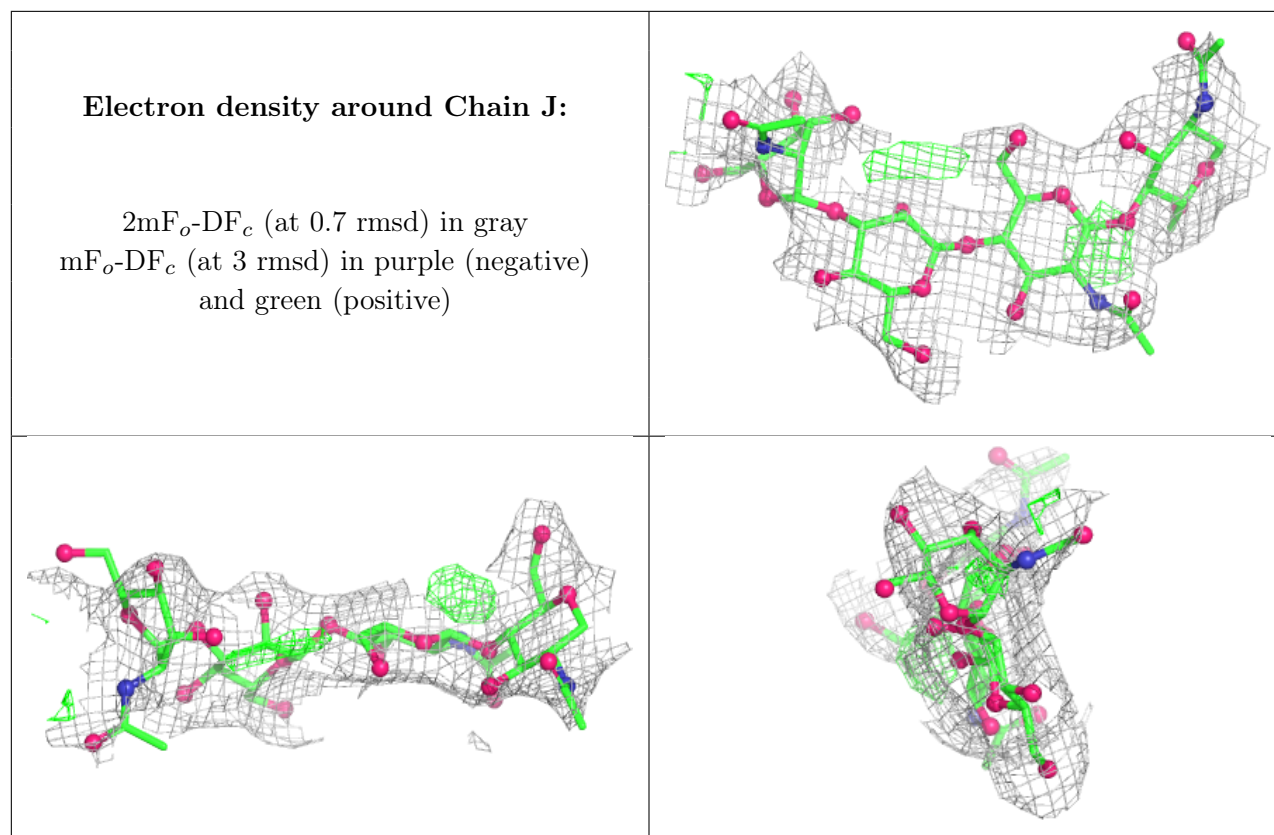
Electron density around Chain D:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

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
8	NAG	B	707	14/15	0.67	0.11	69,88,101,107	0
8	NAG	B	706	14/15	0.69	0.11	103,118,132,135	0
8	NAG	A	704	14/15	0.74	0.10	97,122,129,129	0
8	NAG	E	601	14/15	0.75	0.10	93,116,119,122	0
8	NAG	B	705	14/15	0.81	0.09	83,109,124,127	0
8	NAG	A	703	14/15	0.81	0.11	78,90,97,99	0
9	EDO	B	704	4/4	0.84	0.14	43,54,61,63	0
7	CL	A	702	1/1	0.89	0.32	104,104,104,104	0
9	EDO	B	703	4/4	0.91	0.10	43,49,55,63	0
6	ZN	B	701	1/1	0.95	0.05	92,92,92,92	0
7	CL	B	702	1/1	0.95	0.12	71,71,71,71	0
6	ZN	A	701	1/1	0.97	0.05	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.