



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:29 PM BST

PDB ID : 6H7Z
Title : X-ray structure of human glutamate carboxypeptidase II (GCP II) in complex with a inhibitor RNA 2-65-1
Authors : Motlova, L.; Novakova, Z.; Barinka, C.
Deposited on : 2018-07-31
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

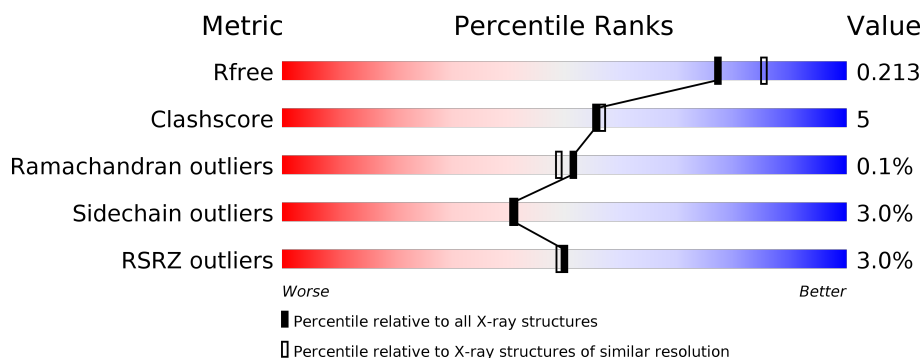
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



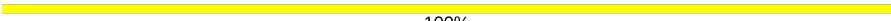
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	707	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>100%</div> </div>
3	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	5	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	827	-	-	-	X
10	EDO	A	828	-	-	-	X
2	NAG	C	2	-	-	-	X
2	NAG	E	2	-	-	-	X
9	PEG	A	831	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 6893 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 Glutamate carboxypeptidase 2.

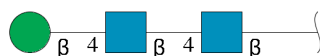
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	68	0
			6033	3860	1018	1129	26			

- 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

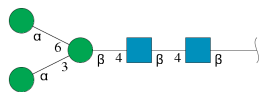
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(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
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



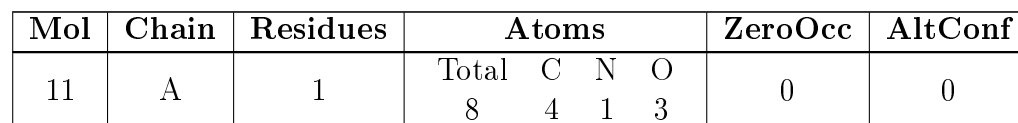
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



- # FWW

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	F	N	O	0	0
			31	18	1	4	8		

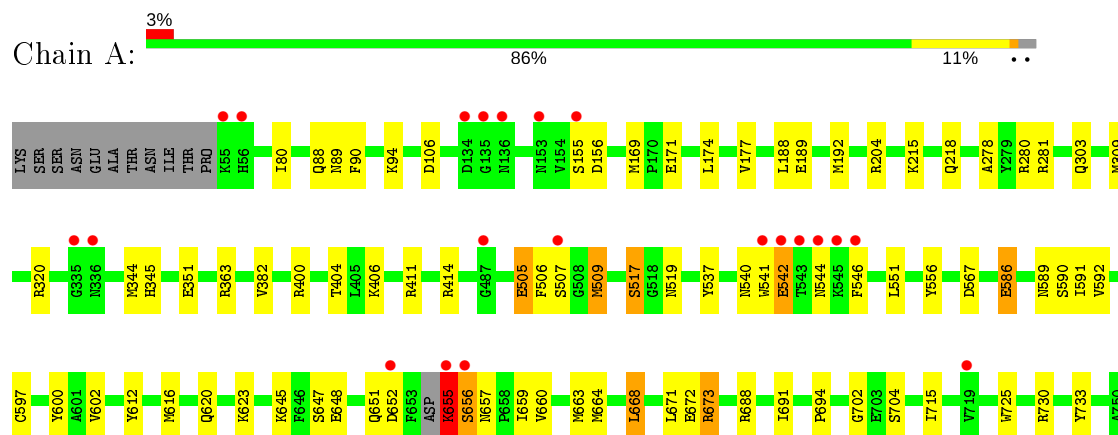
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- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	546	Total 546	O 546	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: Glutamate carboxypeptidase 2



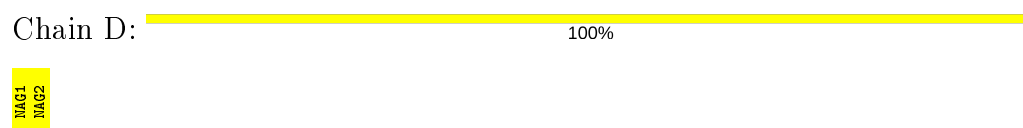
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain F:  100%

MAG1
MAG2
BMA3

- Molecule 4: 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 G:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.22Å 130.39Å 158.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.00) 99.8 (30.80-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.170 , 0.206 0.180 , 0.213	Depositor DCC
R_{free} test set	3589 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6893	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: ZN, BMA, NAG, CL, CA, EDO, FVW, TRS, PEG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	2/6248 (0.0%)	0.86	6/8445 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	GLU	CD-OE2	5.39	1.31	1.25
1	A	517	SER	CA-CB	-5.37	1.44	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	730	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	673	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	733	TYR	CB-CG-CD1	5.80	124.48	121.00
1	A	567	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	204	ARG	NE-CZ-NH2	-5.21	117.70	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	411	ARG	Sidechain
1	A	414	ARG	Sidechain
1	A	655[A]	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6033	0	5859	62	0
2	B	28	0	25	1	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	F	39	0	34	0	0
4	G	61	0	52	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	14	0	13	0	0
9	A	21	0	30	1	0
10	A	24	0	36	3	0
11	A	8	0	12	0	0
12	A	31	0	0	0	0
13	A	546	0	0	7	0
All	All	6893	0	6136	64	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 5.

All (64) 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:215[B]:LYS:NZ	13:A:903:HOH:O	1.76	1.15
1:A:659[A]:ILE:HG22	1:A:663[A]:MET:CE	1.93	0.97
1:A:659[A]:ILE:O	1:A:663[A]:MET:HG3	1.78	0.83
1:A:659[A]:ILE:HG22	1:A:663[A]:MET:HE2	1.73	0.71
1:A:655[A]:LYS:HZ2	1:A:657[A]:ASN:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659[A]:ILE:HG22	1:A:663[A]:MET:HE1	1.76	0.66
1:A:602:VAL:HG22	9:A:831:PEG:H21	1.77	0.64
1:A:620[B]:GLN:HE22	1:A:623:LYS:NZ	1.97	0.62
1:A:89[B]:ASN:ND2	13:A:905:HOH:O	2.25	0.61
1:A:540:ASN:OD1	1:A:542:GLU:HB2	2.02	0.60
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.83	0.59
1:A:278:ALA:HB3	1:A:280[B]:ARG:NH2	2.18	0.58
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.93	0.56
1:A:177:VAL:HG12	1:A:188[A]:LEU:HD11	1.87	0.55
1:A:400:ARG:O	1:A:404:THR:HG23	2.07	0.55
1:A:702:GLY:H	10:A:825:EDO:C2	2.20	0.54
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.48	0.54
1:A:188[B]:LEU:HA	1:A:192[B]:MET:CE	2.38	0.53
1:A:647[B]:SER:O	1:A:651[B]:GLN:HG2	2.08	0.53
1:A:645[B]:LYS:HE3	13:A:1023:HOH:O	2.09	0.53
1:A:591[B]:ILE:HG21	1:A:655[B]:LYS:HD2	1.91	0.52
1:A:656[A]:SER:OG	1:A:656[A]:SER:O	2.26	0.52
1:A:155:SER:O	1:A:156:ASP:HB2	2.08	0.52
1:A:597[B]:CYS:SG	1:A:668[B]:LEU:HD23	2.50	0.51
1:A:177:VAL:HG12	1:A:188[A]:LEU:CD1	2.42	0.50
1:A:188[B]:LEU:HA	1:A:192[B]:MET:HE2	1.93	0.50
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.94	0.50
1:A:188[B]:LEU:HD12	1:A:192[B]:MET:HE3	1.94	0.50
1:A:659[A]:ILE:HG22	1:A:663[A]:MET:SD	2.50	0.49
13:A:1163:HOH:O	2:C:1:NAG:H83	2.11	0.49
1:A:659[A]:ILE:CG2	1:A:663[A]:MET:HE1	2.41	0.49
1:A:188[B]:LEU:CD1	1:A:192[B]:MET:HE3	2.42	0.49
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.95	0.49
1:A:90:PHE:CE2	1:A:94[A]:LYS:HE2	2.49	0.48
1:A:171[B]:GLU:O	1:A:171[B]:GLU:HG3	2.14	0.47
1:A:169[B]:MET:HG2	1:A:345:HIS:HA	1.96	0.47
1:A:169[B]:MET:HA	1:A:344:MET:O	2.15	0.47
1:A:659[A]:ILE:N	1:A:659[A]:ILE:HD13	2.30	0.46
1:A:106:ASP:OD1	1:A:406:LYS:HE3	2.16	0.46
1:A:620[B]:GLN:HE22	1:A:623:LYS:HZ2	1.62	0.45
1:A:648:GLU:O	1:A:651[A]:GLN:HG2	2.15	0.45
1:A:586[B]:GLU:CD	1:A:590[B]:SER:OG	2.54	0.45
1:A:648:GLU:O	1:A:652[A]:ASP:HB2	2.16	0.45
13:A:914:HOH:O	2:B:1:NAG:N2	2.35	0.45
1:A:612:TYR:CZ	1:A:616[A]:MET:HG3	2.51	0.45
1:A:281:ARG:HH21	10:A:823:EDO:H21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659[A]:ILE:C	1:A:663[A]:MET:HE2	2.38	0.44
1:A:505:GLU:HB2	1:A:506:PHE:CE2	2.52	0.44
1:A:660[A]:VAL:O	1:A:664[A]:MET:HG3	2.16	0.44
1:A:363[A]:ARG:HD2	13:A:1125:HOH:O	2.17	0.43
1:A:597[B]:CYS:SG	1:A:668[B]:LEU:CD2	3.07	0.43
1:A:620[B]:GLN:HE22	1:A:623:LYS:HZ3	1.64	0.43
1:A:541:TRP:N	1:A:541:TRP:CD1	2.86	0.43
1:A:281:ARG:NH2	10:A:823:EDO:H21	2.34	0.42
1:A:80:ILE:HD12	1:A:88:GLN:HG2	2.01	0.42
1:A:174[A]:LEU:HD23	1:A:309[A]:MET:SD	2.60	0.42
1:A:715:ILE:HD13	1:A:725:TRP:CE2	2.55	0.41
1:A:659[A]:ILE:O	1:A:663[A]:MET:HE2	2.20	0.41
1:A:655[A]:LYS:NZ	1:A:657[A]:ASN:HB2	2.31	0.41
1:A:591[B]:ILE:HG22	1:A:592:VAL:HG23	2.03	0.41
1:A:691:ILE:O	1:A:704:SER:HA	2.20	0.41
1:A:544:ASN:HB3	1:A:546:PHE:CE2	2.56	0.40
1:A:616[B]:MET:O	1:A:616[B]:MET:CG	2.69	0.40
1:A:688[A]:ARG:NH1	13:A:906:HOH:O	2.26	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	757/707 (107%)	734 (97%)	22 (3%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	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	660/603 (110%)	634 (96%)	26 (4%)	32	30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	218[A]	GLN
1	A	218[B]	GLN
1	A	303	GLN
1	A	320	ARG
1	A	351[A]	GLU
1	A	351[B]	GLU
1	A	505	GLU
1	A	507[A]	SER
1	A	507[B]	SER
1	A	509	MET
1	A	519	ASN
1	A	537	TYR
1	A	542	GLU
1	A	586[A]	GLU
1	A	586[B]	GLU
1	A	589[A]	ASN
1	A	589[B]	ASN
1	A	600	TYR
1	A	655[A]	LYS
1	A	655[B]	LYS
1	A	656[A]	SER
1	A	656[B]	SER
1	A	668[A]	LEU
1	A	668[B]	LEU
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

16 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	B	1	1,2	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
2	NAG	B	2	2	14,14,15	0.85	0	17,19,21	1.48	2 (11%)
2	NAG	C	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	2.76	8 (47%)
2	NAG	C	2	2	14,14,15	0.80	1 (7%)	17,19,21	1.03	0
2	NAG	D	1	1,2	14,14,15	0.92	1 (7%)	17,19,21	1.44	3 (17%)
2	NAG	D	2	2	14,14,15	0.79	0	17,19,21	1.47	3 (17%)
2	NAG	E	1	1,2	14,14,15	0.95	0	17,19,21	2.04	5 (29%)
2	NAG	E	2	2	14,14,15	0.82	0	17,19,21	1.50	3 (17%)
3	NAG	F	1	1,3	14,14,15	1.08	1 (7%)	17,19,21	1.43	3 (17%)
3	NAG	F	2	3	14,14,15	0.68	0	17,19,21	1.45	3 (17%)
3	BMA	F	3	3	11,11,12	0.68	0	15,15,17	1.89	3 (20%)
4	NAG	G	1	1,4	14,14,15	0.86	0	17,19,21	1.57	5 (29%)
4	NAG	G	2	4	14,14,15	0.87	0	17,19,21	1.68	4 (23%)
4	BMA	G	3	4	11,11,12	0.82	0	15,15,17	0.95	1 (6%)
4	MAN	G	4	4	11,11,12	0.73	0	15,15,17	1.38	3 (20%)
4	MAN	G	5	4	11,11,12	0.82	0	15,15,17	1.26	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C6-C5	2.78	1.61	1.51
3	F	1	NAG	O7-C7	2.56	1.29	1.23
2	C	2	NAG	C1-C2	2.29	1.55	1.52
2	D	1	NAG	C4-C5	2.02	1.57	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C6	7.71	119.30	107.20
2	E	1	NAG	C1-O5-C5	6.19	120.58	112.19
3	F	3	BMA	C3-C4-C5	5.14	119.41	110.24
2	C	1	NAG	O6-C6-C5	4.92	128.18	111.29
4	G	1	NAG	C1-O5-C5	3.81	117.36	112.19
2	B	2	NAG	C2-N2-C7	3.80	128.32	122.90
2	E	2	NAG	C4-C3-C2	3.35	115.93	111.02
3	F	2	NAG	C8-C7-N2	3.32	121.73	116.10
4	G	2	NAG	C4-C3-C2	-3.15	106.41	111.02
2	D	1	NAG	C2-N2-C7	3.14	127.37	122.90
2	D	2	NAG	O4-C4-C5	3.07	116.91	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	O5-C1-C2	-2.99	106.57	111.29
3	F	1	NAG	O5-C5-C6	2.97	111.87	107.20
2	D	2	NAG	C3-C4-C5	-2.96	104.96	110.24
3	F	3	BMA	C2-C3-C4	2.91	115.93	110.89
2	C	1	NAG	C8-C7-N2	2.85	120.93	116.10
2	B	2	NAG	C4-C3-C2	2.84	115.18	111.02
3	F	1	NAG	C2-N2-C7	2.82	126.92	122.90
2	C	1	NAG	O4-C4-C3	-2.78	103.92	110.35
2	B	1	NAG	O5-C5-C6	2.77	111.55	107.20
2	C	1	NAG	C1-C2-N2	-2.73	105.83	110.49
4	G	4	MAN	O3-C3-C2	2.67	115.11	109.99
2	E	1	NAG	O3-C3-C4	-2.59	104.35	110.35
2	B	1	NAG	O4-C4-C3	-2.58	104.38	110.35
2	C	1	NAG	O5-C5-C4	-2.55	104.62	110.83
2	E	1	NAG	O5-C5-C6	2.54	111.18	107.20
4	G	1	NAG	O5-C1-C2	-2.54	107.28	111.29
2	D	2	NAG	C1-O5-C5	2.53	115.62	112.19
4	G	1	NAG	O5-C5-C6	2.53	111.17	107.20
2	E	2	NAG	O5-C5-C6	2.45	111.04	107.20
4	G	2	NAG	O5-C5-C4	-2.39	105.00	110.83
2	D	1	NAG	O3-C3-C2	-2.30	104.71	109.47
4	G	5	MAN	C6-C5-C4	2.29	118.37	113.00
3	F	2	NAG	O7-C7-N2	-2.28	117.76	121.95
2	E	1	NAG	O5-C1-C2	-2.27	107.70	111.29
2	C	1	NAG	C1-O5-C5	2.20	115.18	112.19
3	F	3	BMA	O5-C1-C2	-2.18	107.41	110.77
3	F	2	NAG	C4-C3-C2	-2.18	107.83	111.02
2	C	1	NAG	C6-C5-C4	2.17	118.08	113.00
3	F	1	NAG	O4-C4-C3	-2.16	105.35	110.35
4	G	4	MAN	O5-C5-C6	2.15	110.57	107.20
4	G	2	NAG	O3-C3-C4	2.12	115.25	110.35
4	G	1	NAG	O4-C4-C5	-2.10	104.08	109.30
4	G	4	MAN	O4-C4-C5	2.09	114.49	109.30
4	G	1	NAG	C6-C5-C4	-2.06	108.18	113.00
2	D	1	NAG	C4-C3-C2	2.04	114.01	111.02
2	E	2	NAG	C6-C5-C4	2.04	117.78	113.00
4	G	3	BMA	O6-C6-C5	-2.03	104.32	111.29
2	E	1	NAG	O4-C4-C3	-2.03	105.66	110.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

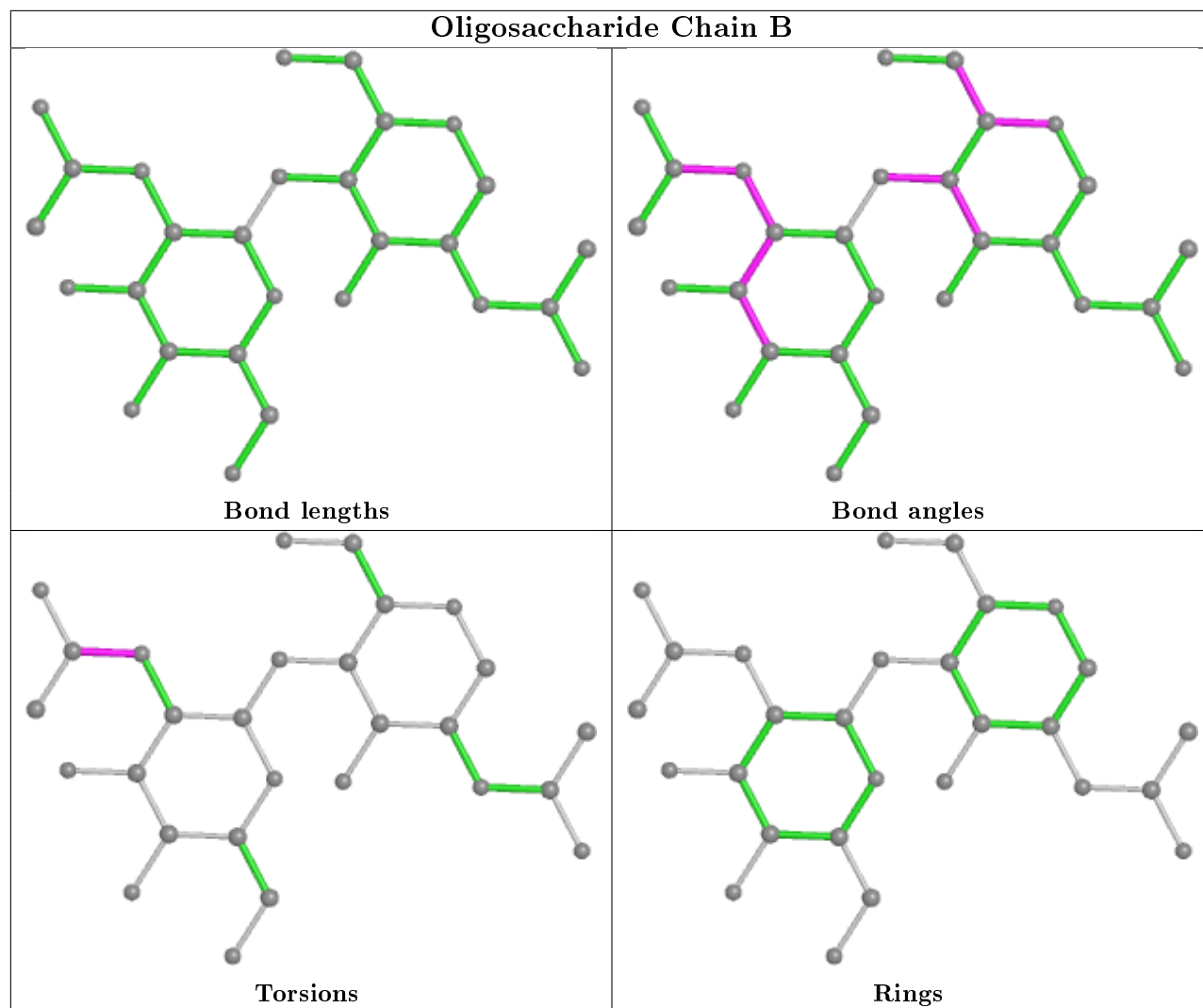
Mol	Chain	Res	Type	Atoms
4	G	5	MAN	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

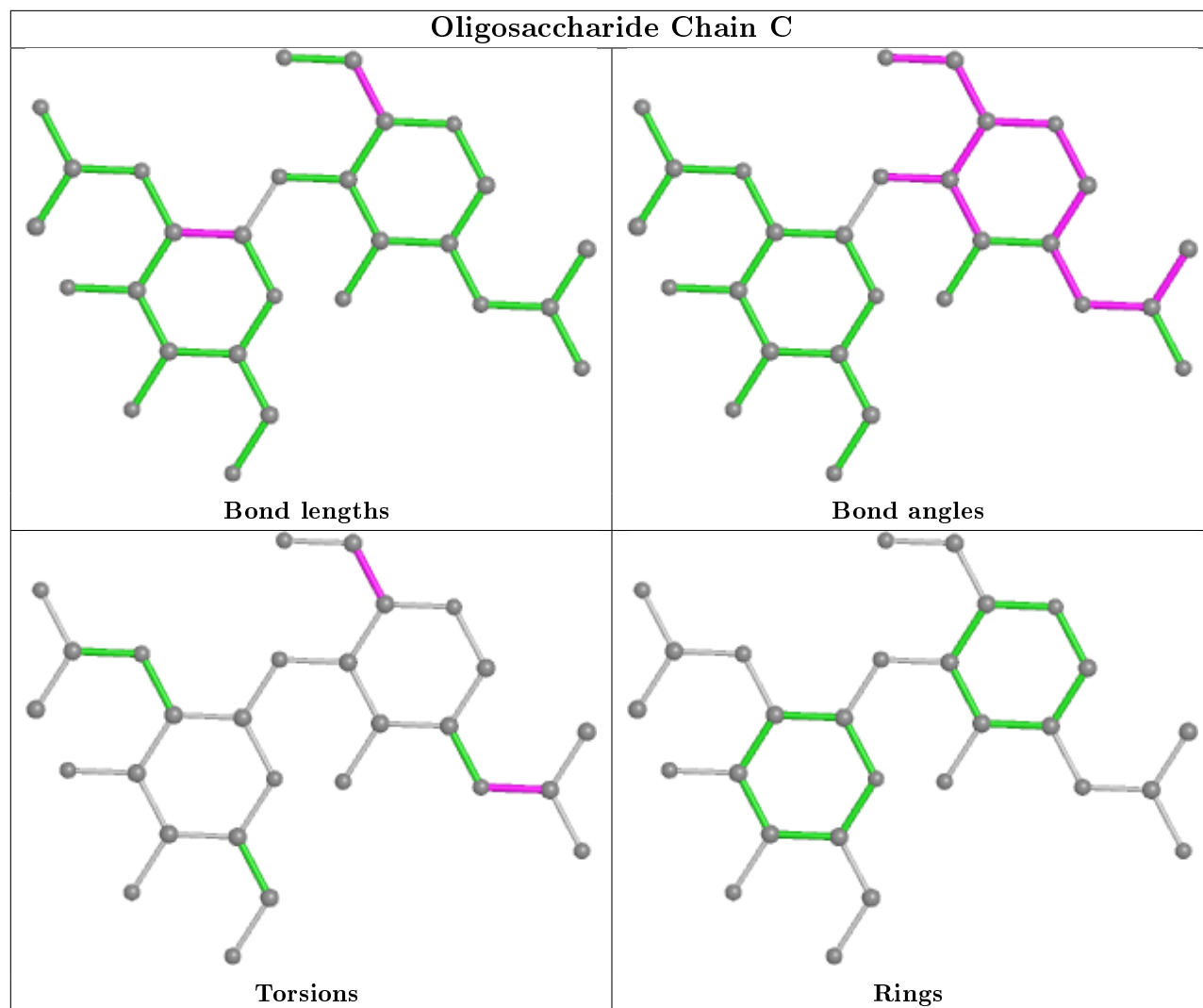
There are no ring outliers.

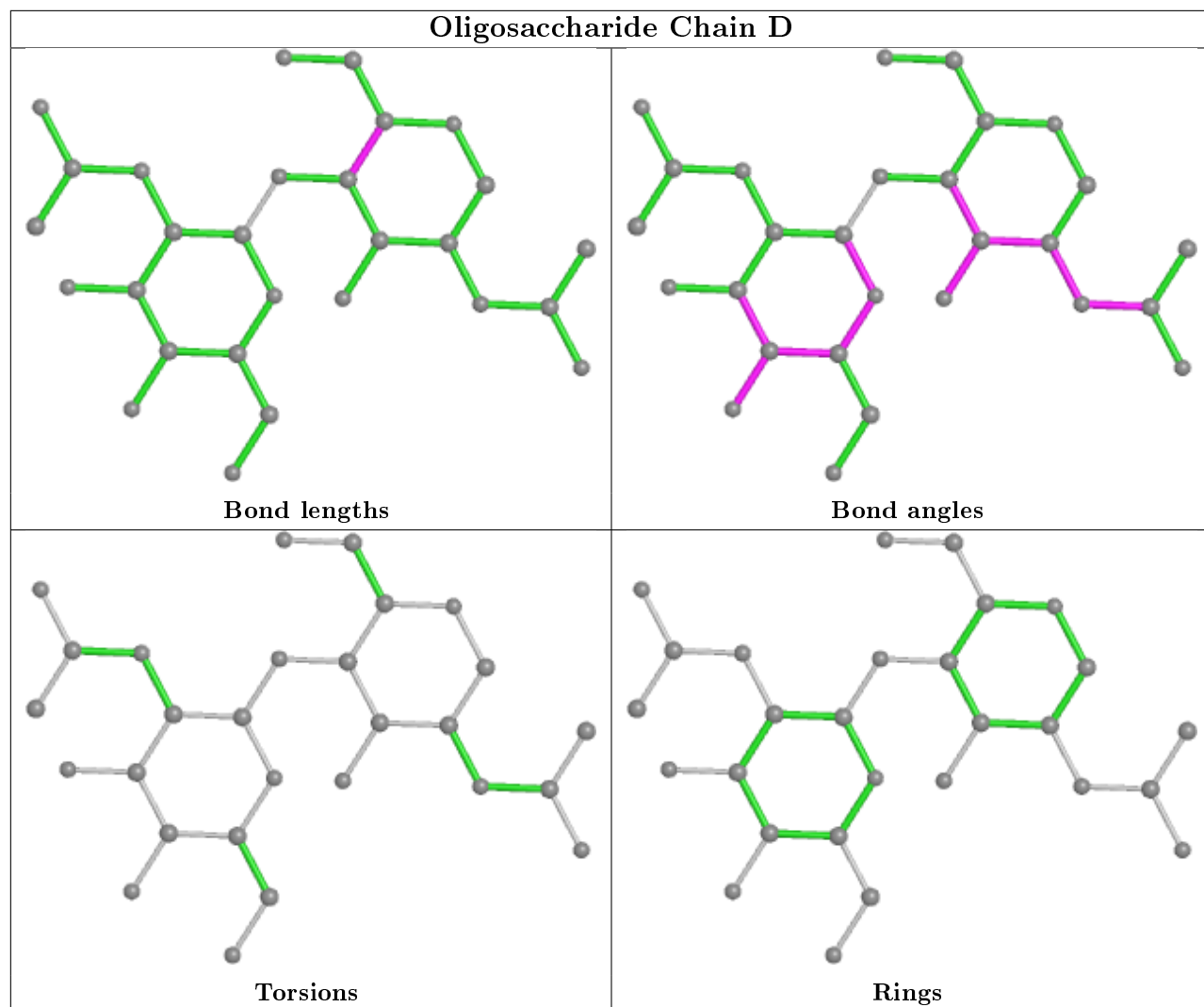
2 monomers are involved in 2 short contacts:

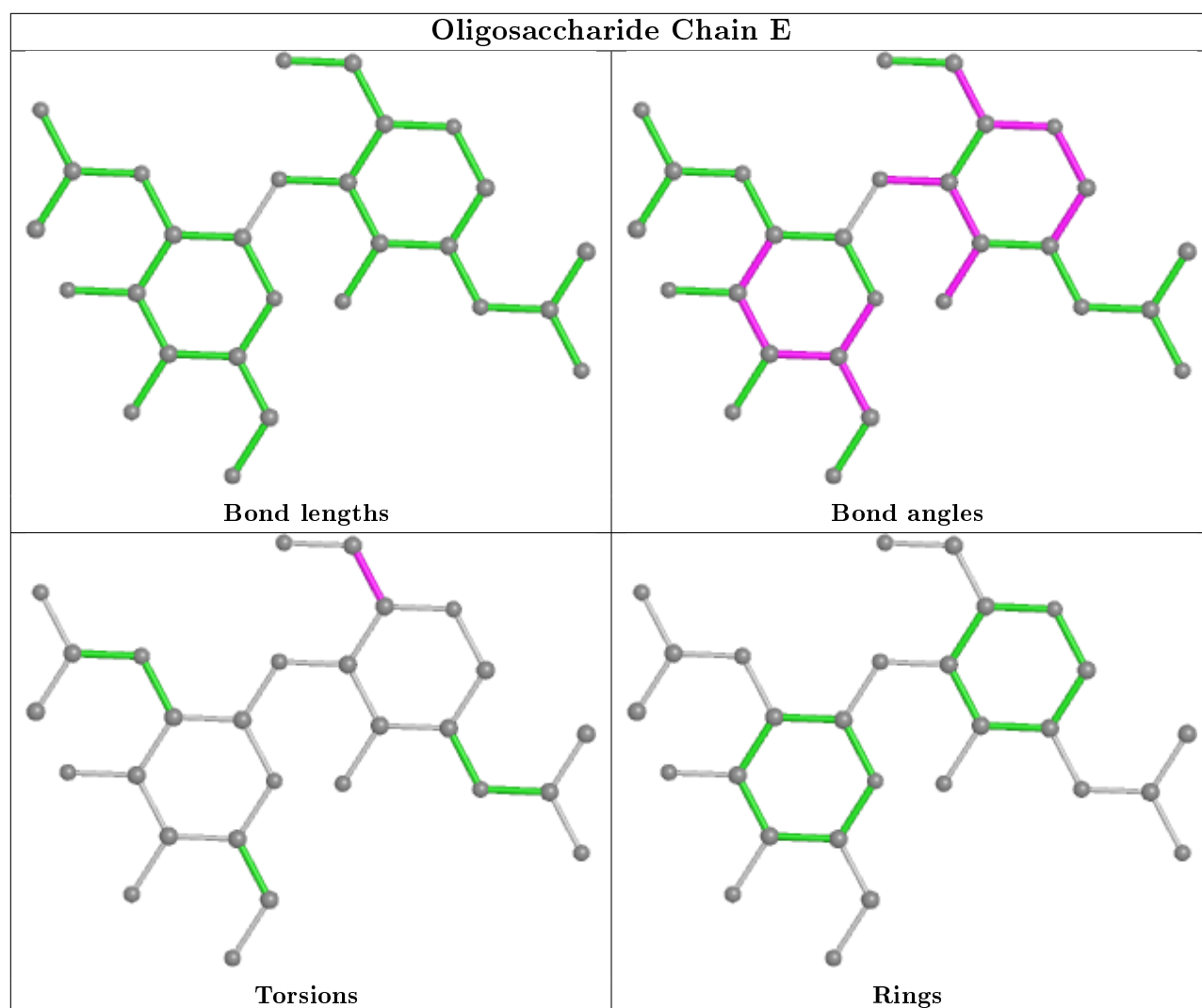
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	C	1	NAG	1	0

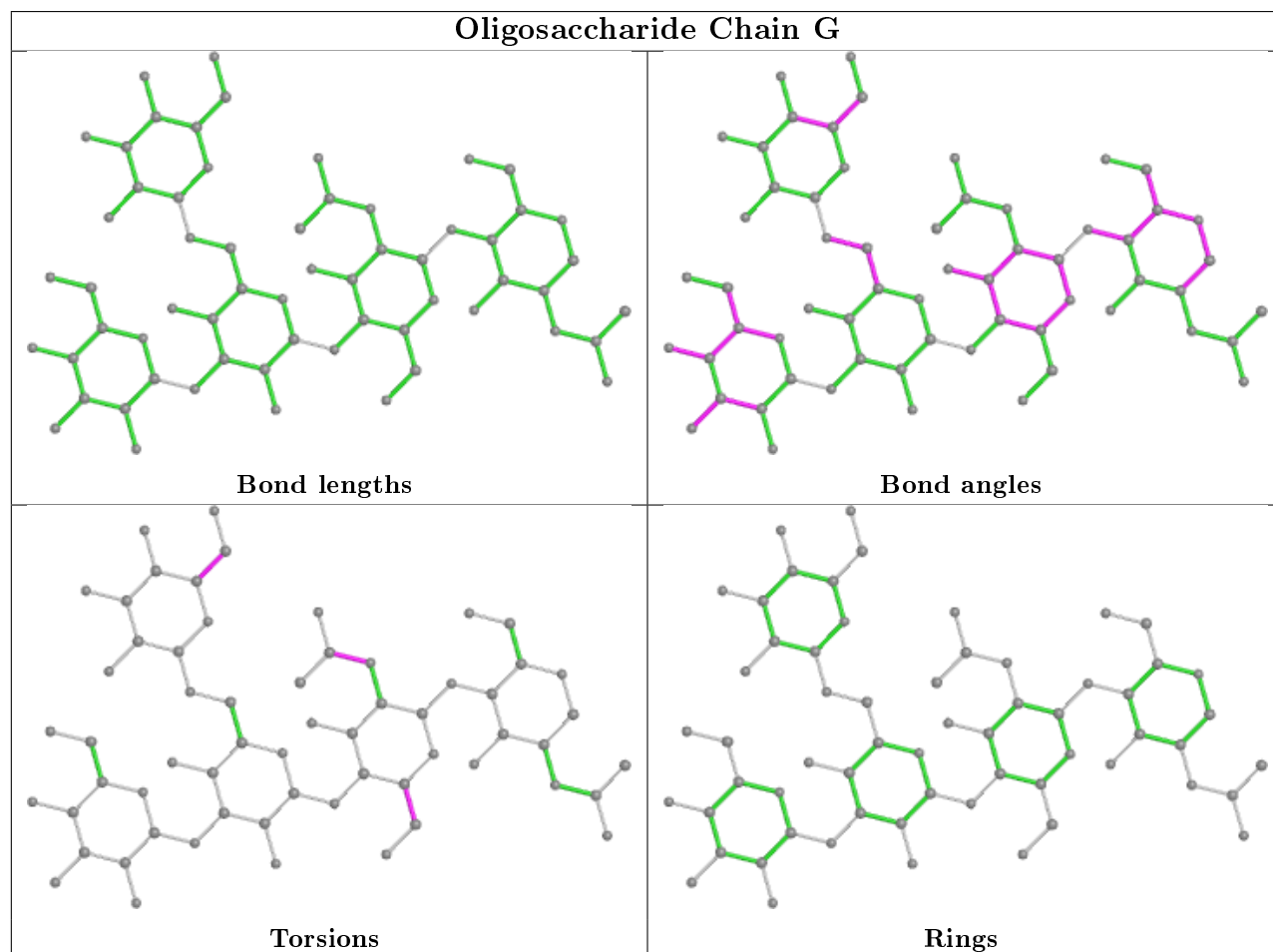
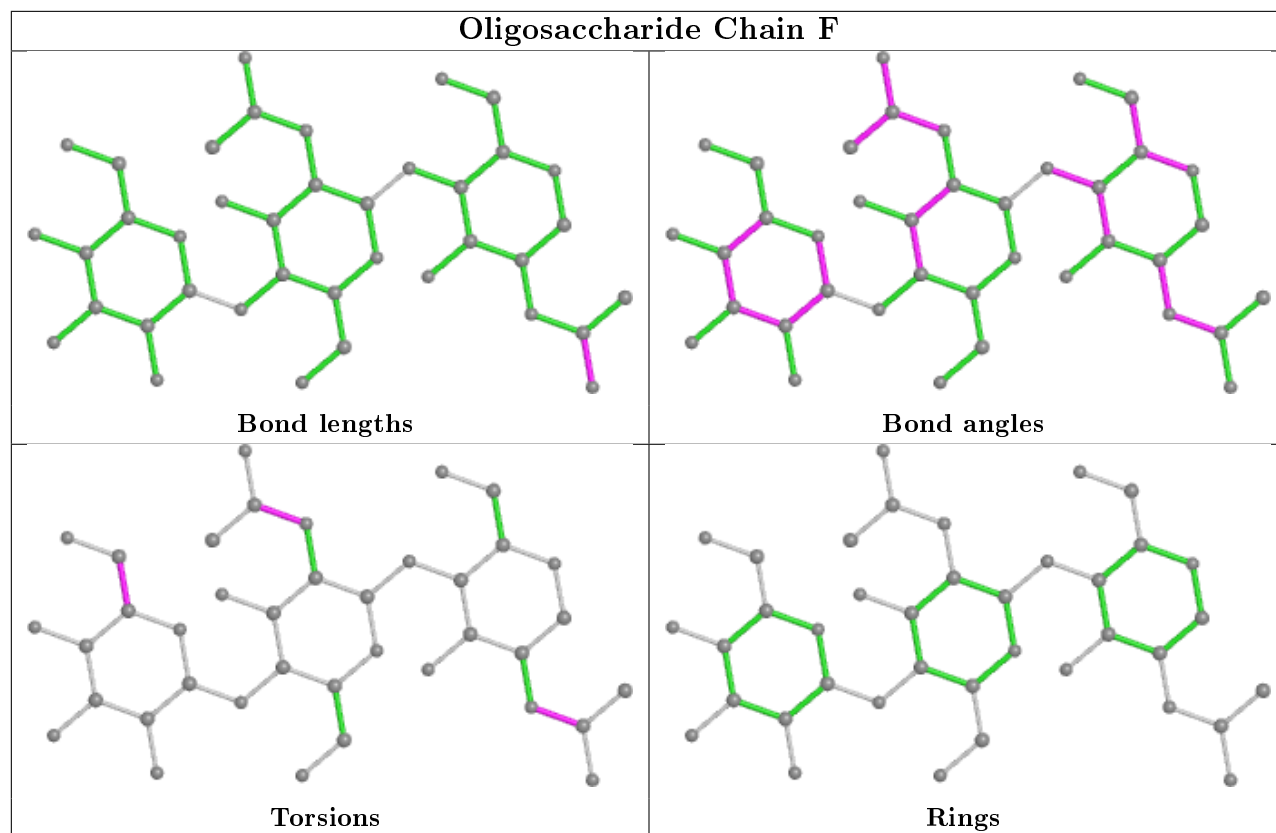
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
10	EDO	A	824	-	3,3,3	0.53	0	2,2,2	0.12	0
10	EDO	A	823	-	3,3,3	0.76	0	2,2,2	0.78	0
9	PEG	A	822	-	6,6,6	0.62	0	5,5,5	0.27	0
10	EDO	A	827	-	3,3,3	0.55	0	2,2,2	0.14	0
9	PEG	A	830	-	6,6,6	0.52	0	5,5,5	0.41	0
10	EDO	A	826	-	3,3,3	0.51	0	2,2,2	0.16	0
9	PEG	A	831	-	6,6,6	0.80	0	5,5,5	0.92	0
12	FVW	A	832	5	22,31,31	2.39	6 (27%)	25,41,41	2.86	5 (20%)
10	EDO	A	828	-	3,3,3	0.65	0	2,2,2	0.49	0
10	EDO	A	825	-	3,3,3	0.66	0	2,2,2	0.28	0
11	TRS	A	829	-	7,7,7	0.38	0	9,9,9	0.55	0
8	NAG	A	811	1	14,14,15	1.15	2 (14%)	17,19,21	3.17	5 (29%)

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
10	EDO	A	824	-	-	0/1/1/1	-
10	EDO	A	823	-	-	1/1/1/1	-
9	PEG	A	822	-	-	1/4/4/4	-
10	EDO	A	827	-	-	1/1/1/1	-
9	PEG	A	830	-	-	2/4/4/4	-
10	EDO	A	826	-	-	1/1/1/1	-
9	PEG	A	831	-	-	1/4/4/4	-
12	FVW	A	832	5	-	3/25/35/35	0/1/1/1
10	EDO	A	828	-	-	1/1/1/1	-
10	EDO	A	825	-	-	1/1/1/1	-
11	TRS	A	829	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	811	1	-	3/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	832	FVW	FAX-CAU	-7.96	1.22	1.35
12	A	832	FVW	CAR-NAQ	-4.19	1.36	1.43
8	A	811	NAG	O5-C1	3.10	1.48	1.43
12	A	832	FVW	CB-CA	3.05	1.57	1.53
12	A	832	FVW	CAU-NAV	2.71	1.33	1.30
12	A	832	FVW	CA-N	-2.61	1.43	1.46
12	A	832	FVW	CAT-CAU	2.34	1.40	1.37
8	A	811	NAG	O5-C5	2.16	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	811	NAG	C1-O5-C5	11.30	127.50	112.19
12	A	832	FVW	CAW-NAV-CAU	9.68	118.91	115.75
12	A	832	FVW	CAT-CAU-NAV	-7.39	122.78	126.83
8	A	811	NAG	C8-C7-N2	3.43	121.91	116.10
12	A	832	FVW	FAX-CAU-NAV	3.28	117.08	114.95
8	A	811	NAG	O5-C5-C6	2.62	111.30	107.20
12	A	832	FVW	CAS-CAT-CAU	2.50	118.21	116.35
8	A	811	NAG	C6-C5-C4	-2.17	107.92	113.00
8	A	811	NAG	O5-C1-C2	-2.16	107.87	111.29
12	A	832	FVW	OA-CAE-N	2.06	126.37	122.62

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	829	TRS	C2-C-C1-O1
11	A	829	TRS	C3-C-C1-O1
11	A	829	TRS	N-C-C1-O1
8	A	811	NAG	C8-C7-N2-C2
8	A	811	NAG	O7-C7-N2-C2
9	A	831	PEG	O1-C1-C2-O2
10	A	828	EDO	O1-C1-C2-O2
10	A	825	EDO	O1-C1-C2-O2
12	A	832	FVW	CB-CAD-CAM-CAO

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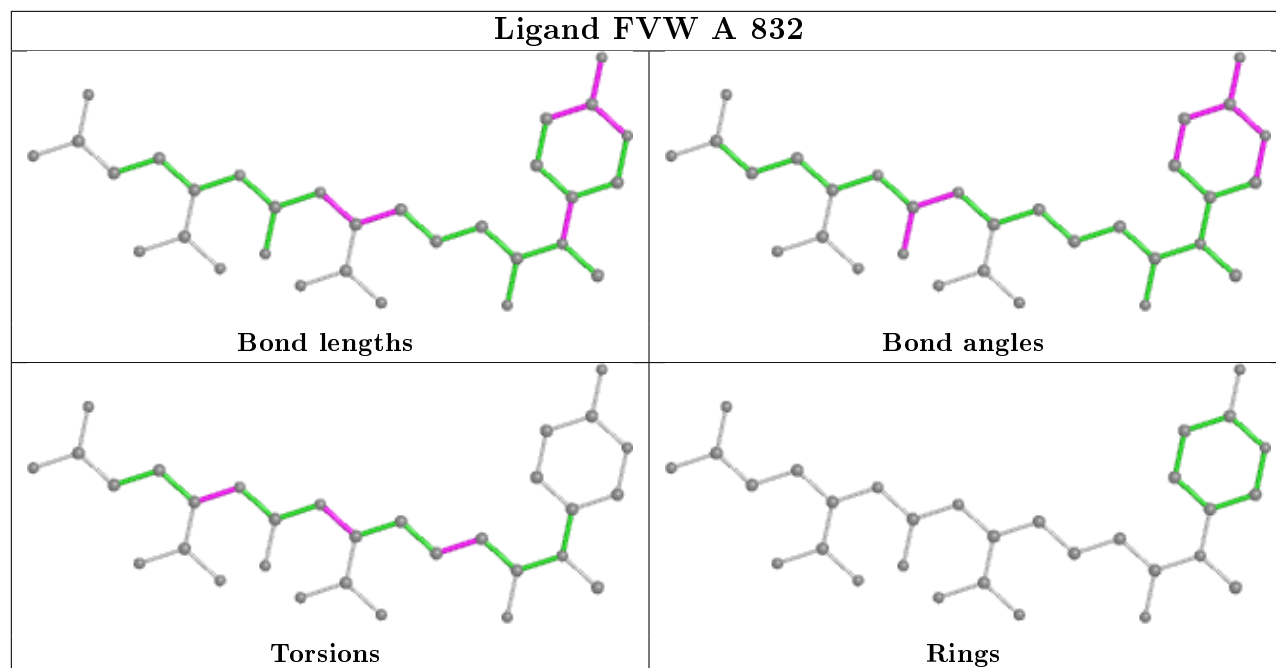
Mol	Chain	Res	Type	Atoms
10	A	827	EDO	O1-C1-C2-O2
12	A	832	FVW	CAJ-CAG-NAF-CAE
10	A	826	EDO	O1-C1-C2-O2
8	A	811	NAG	C4-C5-C6-O6
9	A	822	PEG	C4-C3-O2-C2
12	A	832	FVW	C-CA-N-CAE
9	A	830	PEG	C1-C2-O2-C3
9	A	830	PEG	C4-C3-O2-C2
10	A	823	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	823	EDO	2	0
9	A	831	PEG	1	0
10	A	825	EDO	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	A	695/707 (98%)	-0.28	21 (3%)	50 49	10, 20, 40, 83	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	655[A]	LYS	4.6
1	A	541	TRP	4.5
1	A	543	THR	4.5
1	A	545	LYS	3.8
1	A	544	ASN	3.6
1	A	656[A]	SER	3.5
1	A	335	GLY	3.2
1	A	507[A]	SER	3.0
1	A	542	GLU	2.9
1	A	546	PHE	2.9
1	A	652[A]	ASP	2.9
1	A	134	ASP	2.7
1	A	56	HIS	2.7
1	A	153	ASN	2.6
1	A	719	VAL	2.5
1	A	487	GLY	2.3
1	A	55	LYS	2.3
1	A	135	GLY	2.3
1	A	136	ASN	2.2
1	A	336	ASN	2.2
1	A	155	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

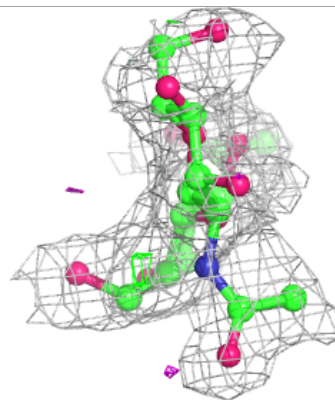
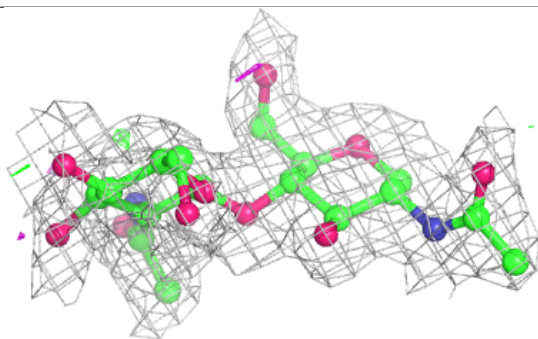
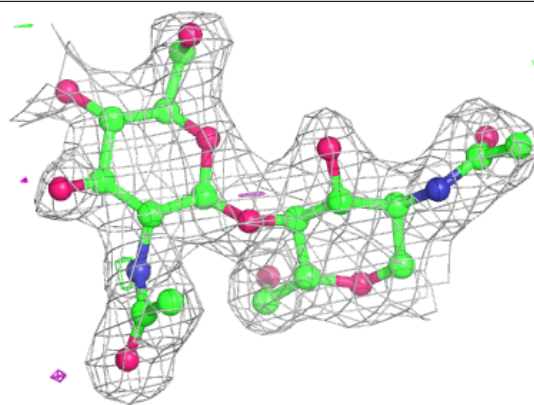
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.59	0.45	71,78,82,85	0
2	NAG	C	1	14/15	0.63	0.28	42,49,57,67	0
2	NAG	C	2	14/15	0.64	0.46	74,76,80,86	0
3	BMA	F	3	11/12	0.66	0.32	59,65,75,82	0
2	NAG	D	2	14/15	0.77	0.35	49,55,62,62	0
2	NAG	B	2	14/15	0.77	0.27	38,45,49,53	0
4	MAN	G	5	11/12	0.78	0.24	53,57,61,63	0
2	NAG	E	1	14/15	0.86	0.19	28,41,49,61	0
4	NAG	G	2	14/15	0.87	0.21	33,36,40,42	0
2	NAG	D	1	14/15	0.92	0.14	35,37,40,45	0
4	MAN	G	4	11/12	0.92	0.15	39,41,43,43	0
4	NAG	G	1	14/15	0.92	0.11	17,23,32,34	0
3	NAG	F	2	14/15	0.93	0.21	37,42,47,53	0
2	NAG	B	1	14/15	0.94	0.10	29,34,36,42	0
4	BMA	G	3	11/12	0.94	0.13	35,39,44,46	0
3	NAG	F	1	14/15	0.95	0.12	26,28,32,32	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.

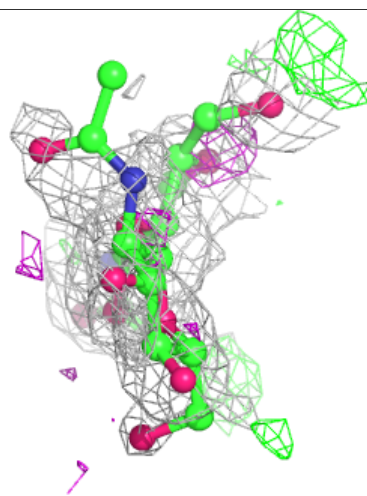
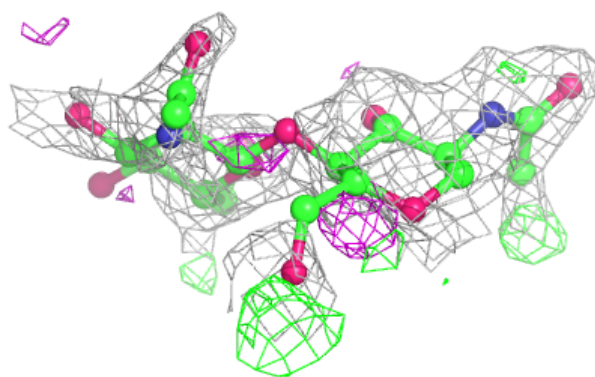
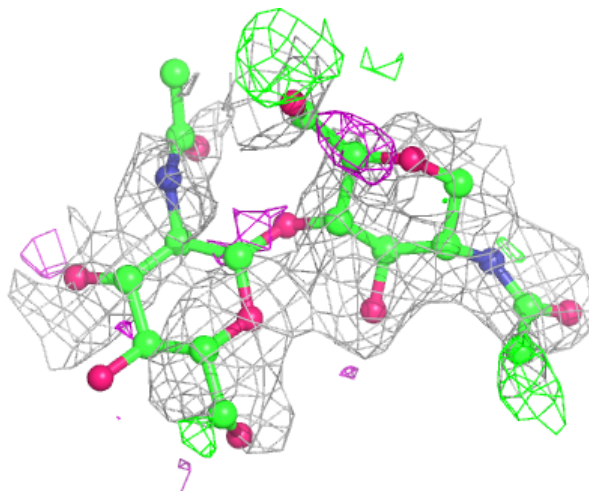
Electron density around Chain B:

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



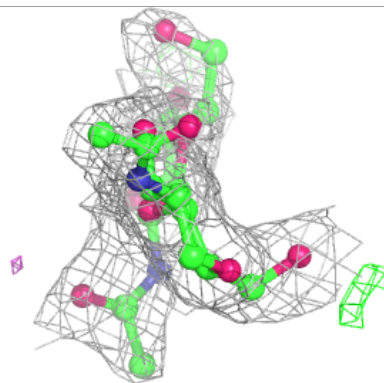
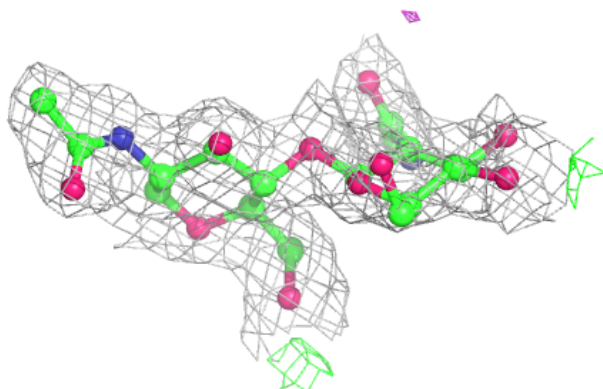
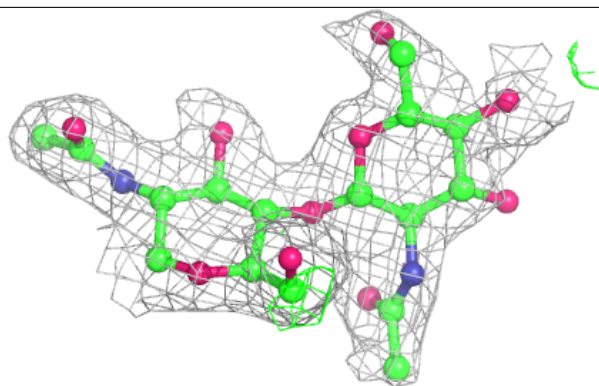
Electron density around Chain C:

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



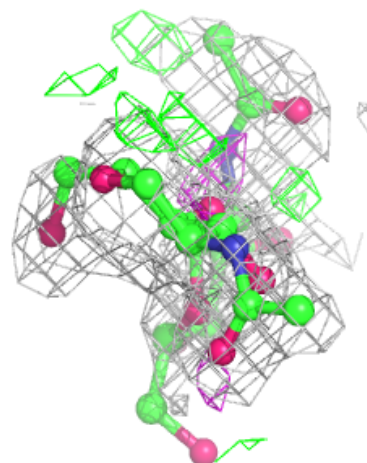
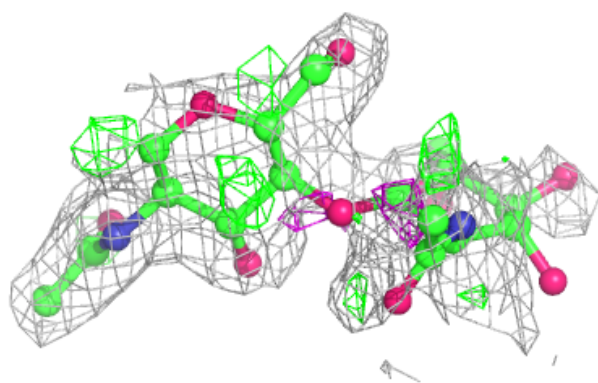
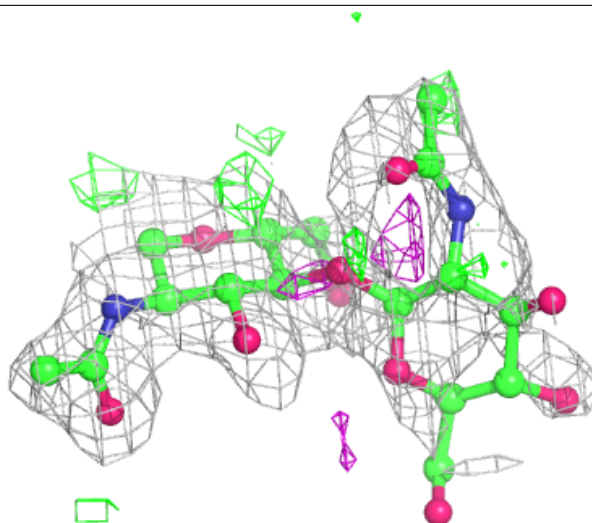
Electron density around Chain D:

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



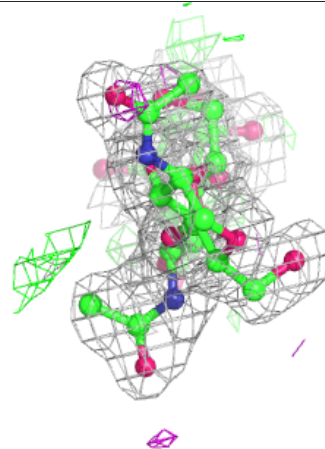
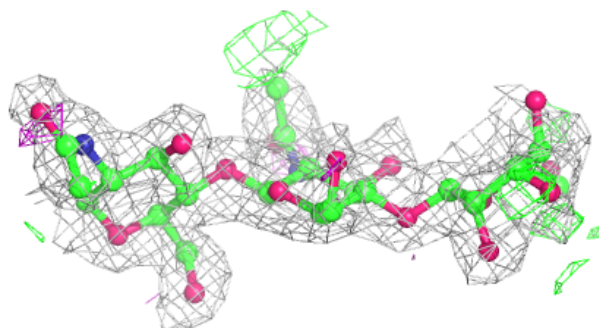
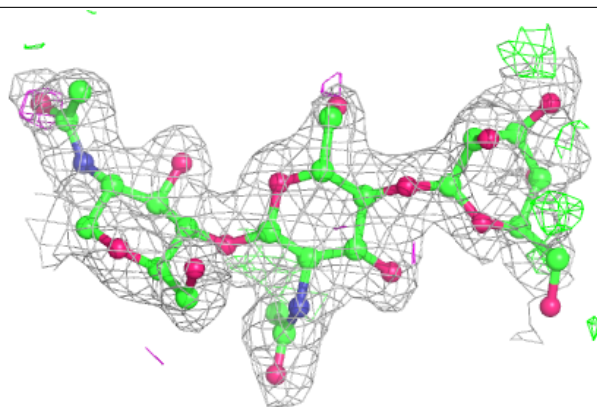
Electron density around Chain E:

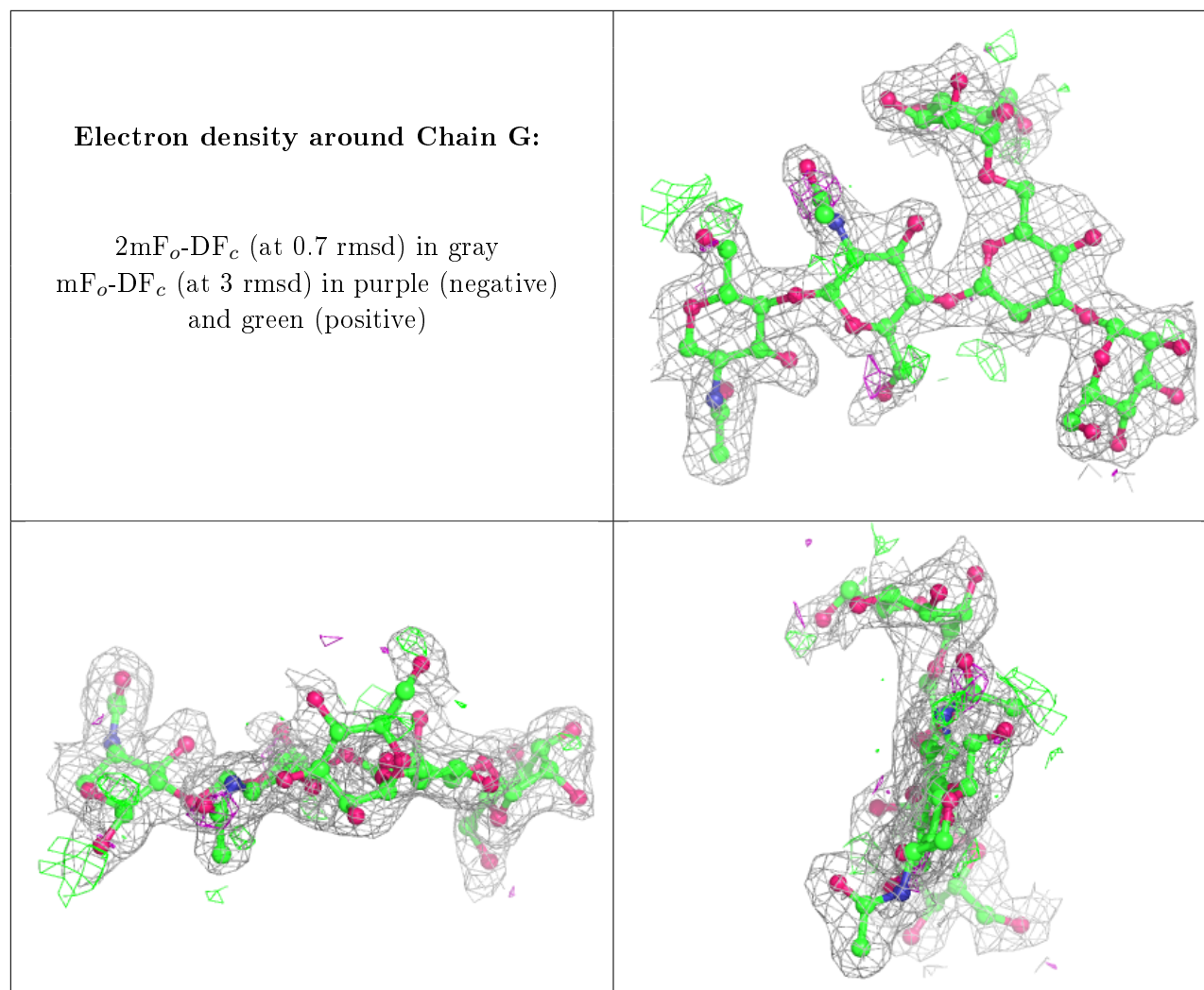
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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.

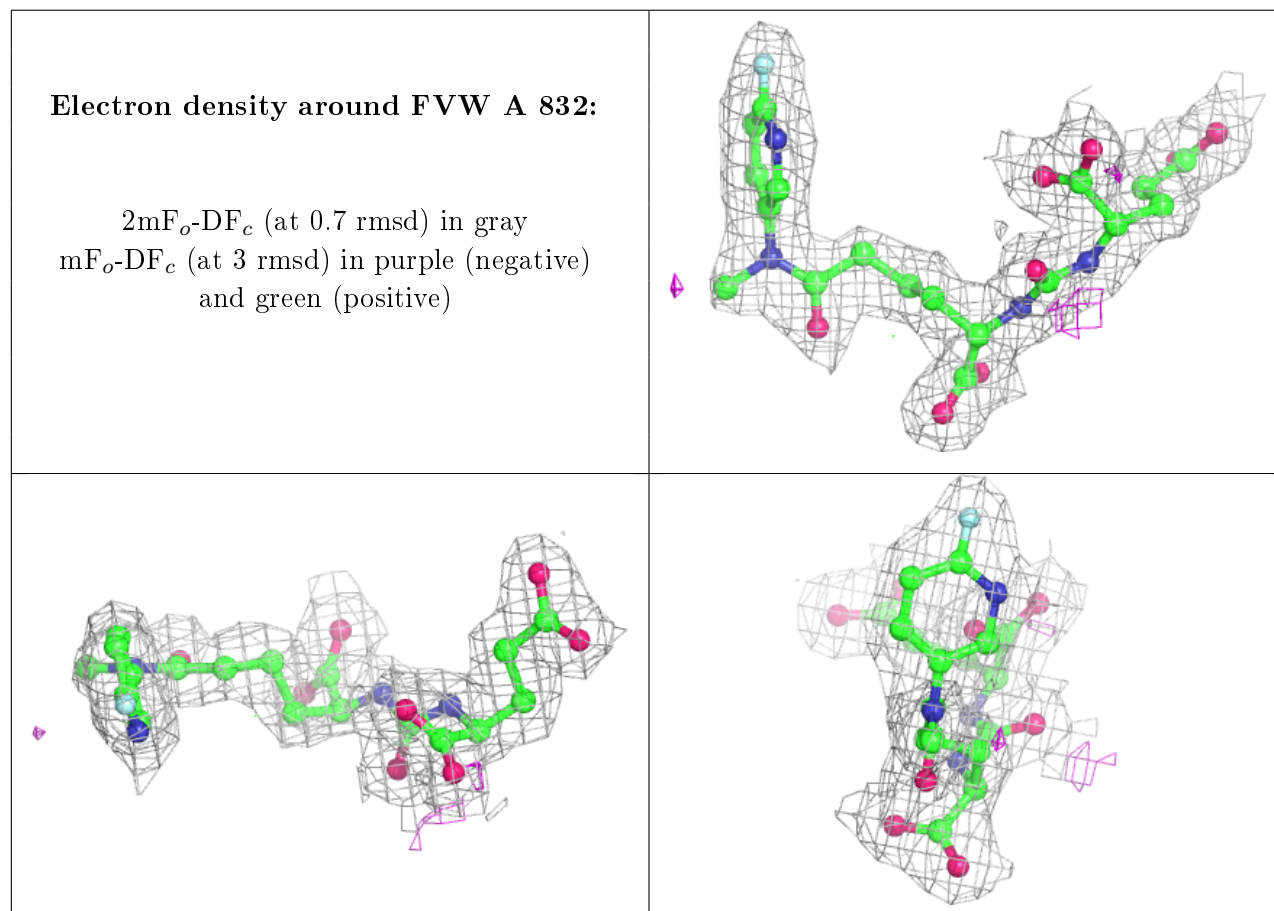
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	EDO	A	828	4/4	0.54	0.43	46,47,49,50	0
10	EDO	A	823	4/4	0.56	0.23	44,47,48,51	0
10	EDO	A	824	4/4	0.65	0.24	57,58,61,62	0
8	NAG	A	811	14/15	0.70	0.20	60,67,72,73	0
9	PEG	A	830	7/7	0.71	0.18	59,60,63,66	0
10	EDO	A	825	4/4	0.71	0.36	43,43,46,47	0
9	PEG	A	831	7/7	0.75	0.52	31,39,40,46	0
11	TRS	A	829	8/8	0.75	0.18	66,70,73,79	0
10	EDO	A	827	4/4	0.78	0.49	63,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	826	4/4	0.79	0.26	45,47,50,52	0
9	PEG	A	822	7/7	0.83	0.16	45,47,50,51	0
12	FVW	A	832	31/31	0.96	0.09	15,19,32,35	0
7	CL	A	804	1/1	0.99	0.05	17,17,17,17	0
6	CA	A	803	1/1	1.00	0.05	11,11,11,11	0
5	ZN	A	802	1/1	1.00	0.03	15,15,15,15	0
5	ZN	A	801	1/1	1.00	0.01	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.