Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:45 pm GMT

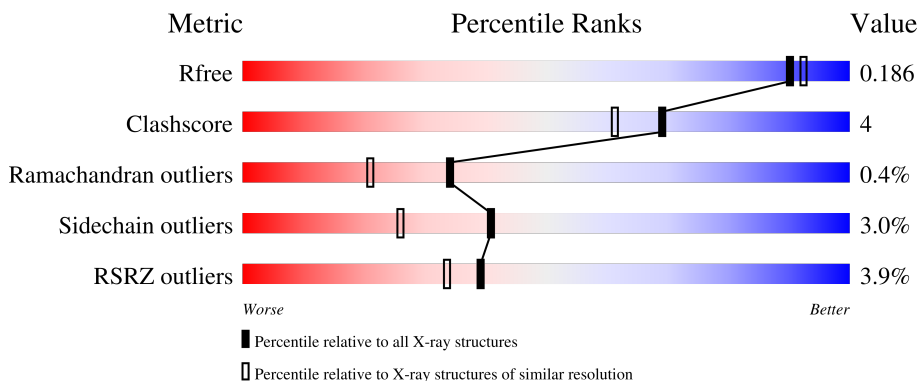|		
PDB ID	:	6H7Y
Title	:	X-ray structure of human glutamate carboxypeptidase II (GCPII) in complex with a inhibitor RNA 1-79-1
Authors	:	Motlova, L.; Novakova, Z.; Barinka, C.
Deposited on	:	2018-07-31
Resolution	:	1.81 Å(reported)

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 1.81 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	Percentile Ranks	Value
Rfree		0.186
Clashscore		4
Ramachandran outliers		0.4%
Sidechain outliers		3.0%
RSRZ outliers		3.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 <=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	4% / 91% / 7% ·
2	B	2	100%
2	C	2	50% / 50%
3	D	4	100%
4	E	5	100%

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 6760 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	696	Total 6012	C 3845	N 1015	O 1124	S 28	0	65	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
2	B	2	Total 28	C 16	N 2	O 10	0	0	0
2	C	2	Total 28	C 16	N 2	O 10	0	0	0

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

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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
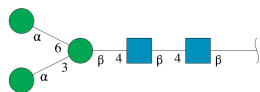
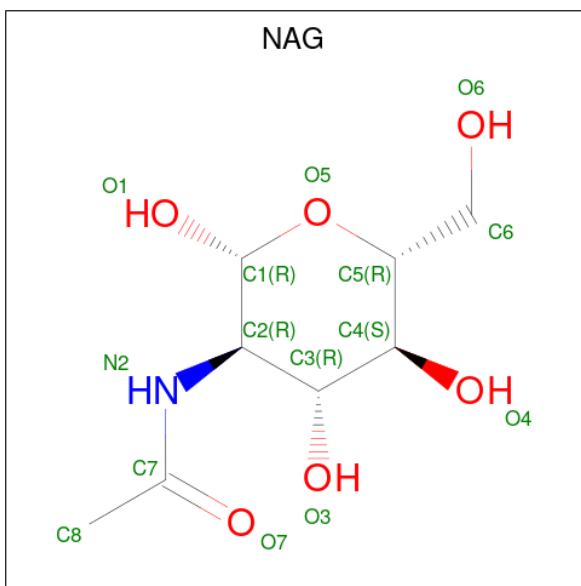| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total Cl 2 2		0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
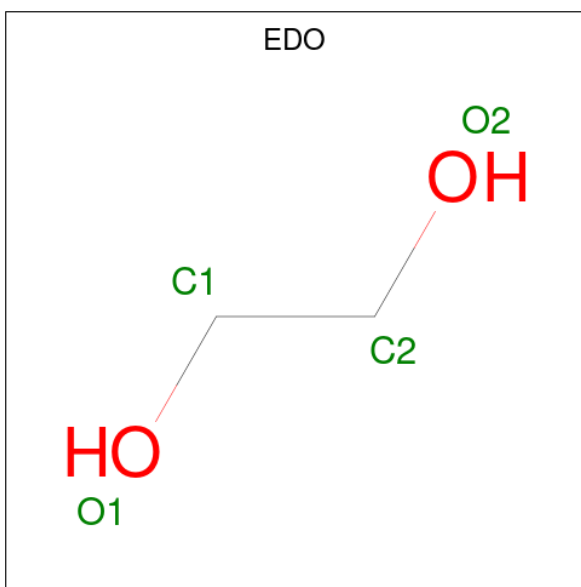
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total C O 4 2 2			0	0
9	A	1	Total C O 4 2 2			0	0
9	A	1	Total C O 4 2 2			0	0
9	A	1	Total C O 4 2 2			0	0
9	A	1	Total C O 4 2 2			0	0
9	A	1	Total C O 4 2 2			0	0

- Molecule 10 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).

TAM
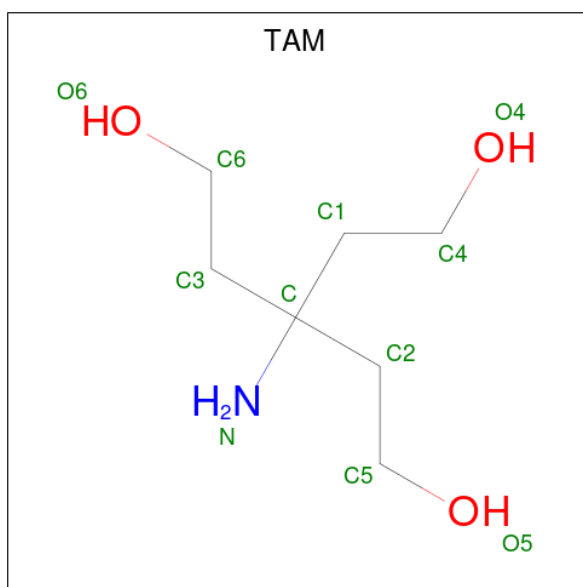
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total 11	C 7	N 1	O 3	0	0
10	A	1	Total 11	C 7	N 1	O 3	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

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

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

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
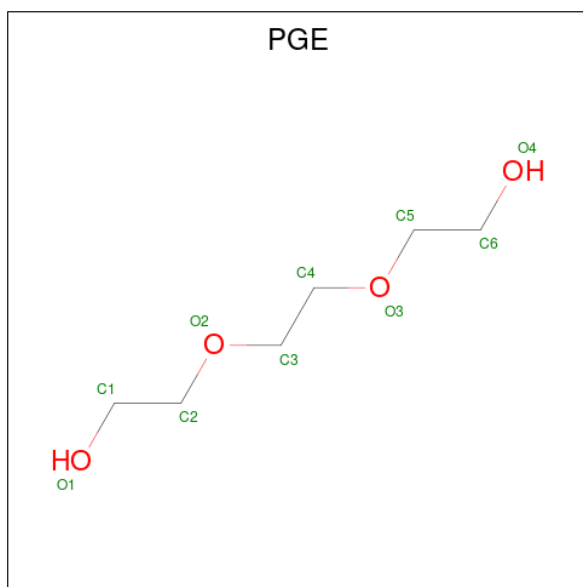
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total 10	C 6	O 4	0	0

- Molecule 13 is (2 {S})-2-[[(2 {S})-6-[(4-fluorophenyl)amino]-1-oxidanyl-1,6-bis(oxidan ylidene)hexan-2-yl]carbamoylamino]pentanedioic acid (three-letter code: FVZ) (formula: $C_{18}H_{22}FN_3O_8$).

FVZ
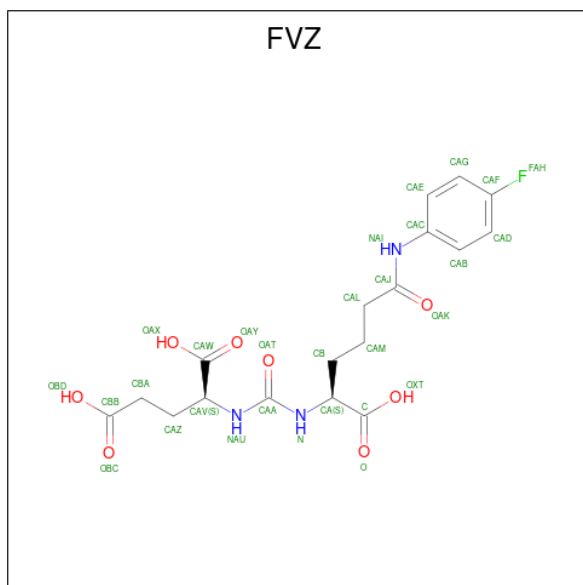
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
13	A	1	30	18	1	3	8	0	0

• Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	427	427	427	0	0

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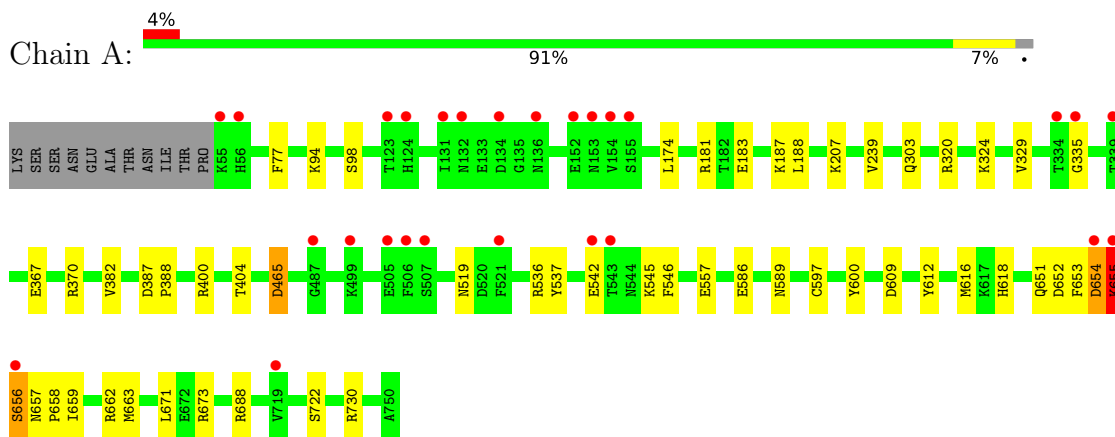
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
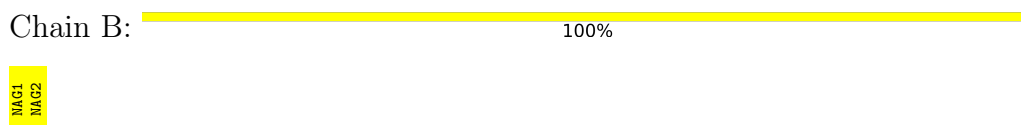
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
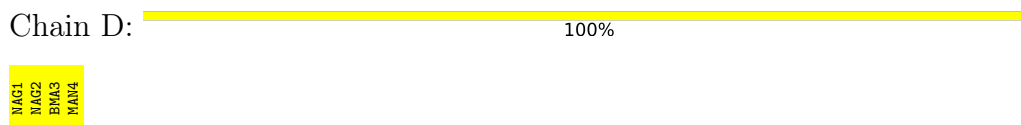
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain E: 100%

NAG1 NAG2 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	102.26Å 131.38Å 159.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 1.81 47.26 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.26-1.81) 98.7 (47.26-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.150 , 0.178 0.164 , 0.186	Depositor DCC
R_{free} test set	2099 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6760	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, CA, BMA, TAM, PGE, EDO, ZN, FVZ, PEG, CL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.87	2/6238 (0.0%)	0.83	7/8433 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	GLU	CD-OE1	6.95	1.33	1.25
1	A	557	GLU	CB-CG	-5.59	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	465	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	730	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	77	PHE	CB-CG-CD1	5.44	124.61	120.80
1	A	536	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	370	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	609	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	654[A]	ASP	Peptide

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	6012	0	5843	46	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	D	50	0	43	0	0
4	E	61	0	52	0	0
5	A	42	0	39	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
9	A	24	0	36	0	0
10	A	22	0	34	1	0
11	A	21	0	30	0	0
12	A	10	0	13	0	0
13	A	30	0	0	0	0
14	A	427	0	0	3	0
All	All	6760	0	6140	47	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 4.

All (47) 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:655[B]:LYS:CD	1:A:656[B]:SER:H	1.18	1.55
1:A:655[B]:LYS:HD2	1:A:656[B]:SER:N	1.04	1.35
1:A:655[B]:LYS:HD2	1:A:656[B]:SER:CA	1.83	1.06
1:A:654[B]:ASP:O	1:A:655[B]:LYS:CB	1.95	1.05
1:A:654[B]:ASP:O	1:A:655[B]:LYS:HB3	1.24	1.04
1:A:655[B]:LYS:CD	1:A:656[B]:SER:HB3	1.87	1.03
1:A:653[A]:PHE:O	1:A:654[A]:ASP:O	1.87	0.92
1:A:655[B]:LYS:HE2	1:A:656[B]:SER:OG	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655[B]:LYS:CD	1:A:656[B]:SER:CB	2.50	0.90
1:A:655[B]:LYS:HD3	1:A:656[B]:SER:HB3	1.57	0.85
1:A:655[B]:LYS:HD2	1:A:656[B]:SER:CB	2.11	0.80
1:A:207[A]:LYS:HD3	1:A:546:PHE:HB3	1.64	0.79
1:A:655[B]:LYS:CG	1:A:656[B]:SER:H	1.95	0.75
1:A:652[A]:ASP:O	1:A:654[A]:ASP:N	2.24	0.71
1:A:655[B]:LYS:CD	1:A:656[B]:SER:N	1.98	0.71
1:A:652[A]:ASP:C	1:A:654[A]:ASP:H	1.93	0.71
1:A:655[B]:LYS:CE	1:A:656[B]:SER:CB	2.68	0.71
1:A:655[B]:LYS:CE	1:A:656[B]:SER:HB3	2.24	0.67
1:A:207[A]:LYS:HE2	1:A:546:PHE:CG	2.30	0.66
1:A:651[B]:GLN:NE2	1:A:652[B]:ASP:OD1	2.29	0.65
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.85	0.64
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.37	0.63
1:A:652[A]:ASP:C	1:A:654[A]:ASP:N	2.50	0.63
1:A:655[B]:LYS:CE	1:A:656[B]:SER:OG	2.45	0.63
1:A:181:ARG:HD3	1:A:207[B]:LYS:HG2	1.81	0.62
1:A:654[B]:ASP:OD1	1:A:655[B]:LYS:HG3	2.00	0.62
1:A:655[B]:LYS:HE2	1:A:656[B]:SER:CB	2.31	0.60
1:A:400:ARG:O	1:A:404:THR:HG23	2.01	0.59
1:A:207[A]:LYS:HE2	1:A:546:PHE:CD2	2.39	0.58
1:A:654[B]:ASP:O	1:A:655[B]:LYS:CG	2.51	0.57
1:A:618:HIS:HD2	14:A:1104:HOH:O	1.87	0.57
1:A:688[B]:ARG:NH1	14:A:902:HOH:O	1.92	0.54
1:A:207[B]:LYS:O	1:A:207[B]:LYS:HG3	2.10	0.52
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.41	0.52
1:A:652[A]:ASP:O	1:A:653[A]:PHE:C	2.45	0.51
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.12	0.49
1:A:320[B]:ARG:HH11	1:A:320[B]:ARG:HB3	1.78	0.49
1:A:320[B]:ARG:HB3	1:A:320[B]:ARG:NH1	2.28	0.48
1:A:656[B]:SER:O	1:A:658[B]:PRO:HD3	2.14	0.48
10:A:827:TAM:C4	14:A:909:HOH:O	2.62	0.47
1:A:659[A]:ILE:N	1:A:659[A]:ILE:HD13	2.30	0.47
1:A:655[B]:LYS:C	1:A:657[B]:ASN:H	2.18	0.46
1:A:586[A]:GLU:OE1	1:A:586[A]:GLU:HA	2.19	0.42
1:A:188:LEU:HD11	1:A:329:VAL:CG1	2.50	0.41
1:A:612:TYR:CZ	1:A:616[B]:MET:HG3	2.56	0.41
1:A:387:ASP:HA	1:A:388:PRO:HA	1.95	0.41
1:A:653[B]:PHE:CD1	1:A:654[B]:ASP:N	2.89	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	760/707 (108%)	730 (96%)	26 (3%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	655[A]	LYS
1	A	655[B]	LYS
1	A	335	GLY
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	659/603 (109%)	633 (96%)	26 (4%)	32	17

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

Mol	Chain	Res	Type
1	A	94[A]	LYS
1	A	94[B]	LYS
1	A	98[A]	SER
1	A	98[B]	SER
1	A	98[C]	SER
1	A	174	LEU
1	A	187	LYS

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Mol	Chain	Res	Type
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	303	GLN
1	A	324	LYS
1	A	465	ASP
1	A	519	ASN
1	A	537	TYR
1	A	542	GLU
1	A	545	LYS
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	673	ARG
1	A	722[A]	SER
1	A	722[B]	SER

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

Mol	Chain	Res	Type
1	A	475	HIS

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 ⓘ

13 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	2,1	14,14,15	0.46	0	17,19,21	1.27	2 (11%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	1.67	2 (11%)
2	NAG	C	1	2,1	14,14,15	0.81	0	17,19,21	1.04	0
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.77	0	17,19,21	1.27	2 (11%)
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	1.42	3 (17%)
3	BMA	D	3	3	11,11,12	0.76	0	15,15,17	1.40	2 (13%)
3	MAN	D	4	3	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.58	0	17,19,21	1.35	2 (11%)
4	NAG	E	2	4	14,14,15	0.72	0	17,19,21	1.46	2 (11%)
4	BMA	E	3	4	11,11,12	0.89	0	15,15,17	1.10	1 (6%)
4	MAN	E	4	4	11,11,12	0.69	0	15,15,17	1.17	1 (6%)
4	MAN	E	5	4	11,11,12	0.76	0	15,15,17	1.37	3 (20%)

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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C2-N2-C7	4.26	128.97	122.90
3	D	3	BMA	O5-C5-C6	3.69	112.99	107.20
4	E	1	NAG	C1-O5-C5	3.58	117.05	112.19
3	D	2	NAG	C8-C7-N2	3.47	121.97	116.10
3	D	1	NAG	C2-N2-C7	3.18	127.43	122.90
4	E	2	NAG	O4-C4-C5	-3.00	101.86	109.30
3	D	4	MAN	O5-C5-C6	2.77	111.55	107.20
2	B	1	NAG	O5-C5-C6	2.69	111.43	107.20
2	B	1	NAG	O5-C1-C2	-2.68	107.06	111.29
2	B	2	NAG	C8-C7-N2	2.63	120.56	116.10
4	E	1	NAG	O5-C1-C2	-2.61	107.17	111.29
3	D	4	MAN	O5-C1-C2	-2.54	106.86	110.77
3	D	2	NAG	O7-C7-N2	-2.44	117.47	121.95
4	E	3	BMA	C2-C3-C4	-2.44	106.68	110.89
4	E	2	NAG	C8-C7-N2	2.41	120.18	116.10
4	E	5	MAN	O3-C3-C2	-2.37	105.46	109.99
4	E	5	MAN	O5-C5-C6	2.30	110.82	107.20
4	E	5	MAN	O5-C5-C4	-2.30	105.24	110.83
3	D	2	NAG	C4-C3-C2	-2.29	107.66	111.02
4	E	4	MAN	O3-C3-C2	2.29	114.37	109.99
3	D	1	NAG	O4-C4-C3	-2.28	105.07	110.35
2	C	2	NAG	O5-C5-C6	2.21	110.67	107.20
3	D	3	BMA	C3-C4-C5	2.10	113.99	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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| Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

| Bond lengths | Bond angles |
| Torsions | Rings |
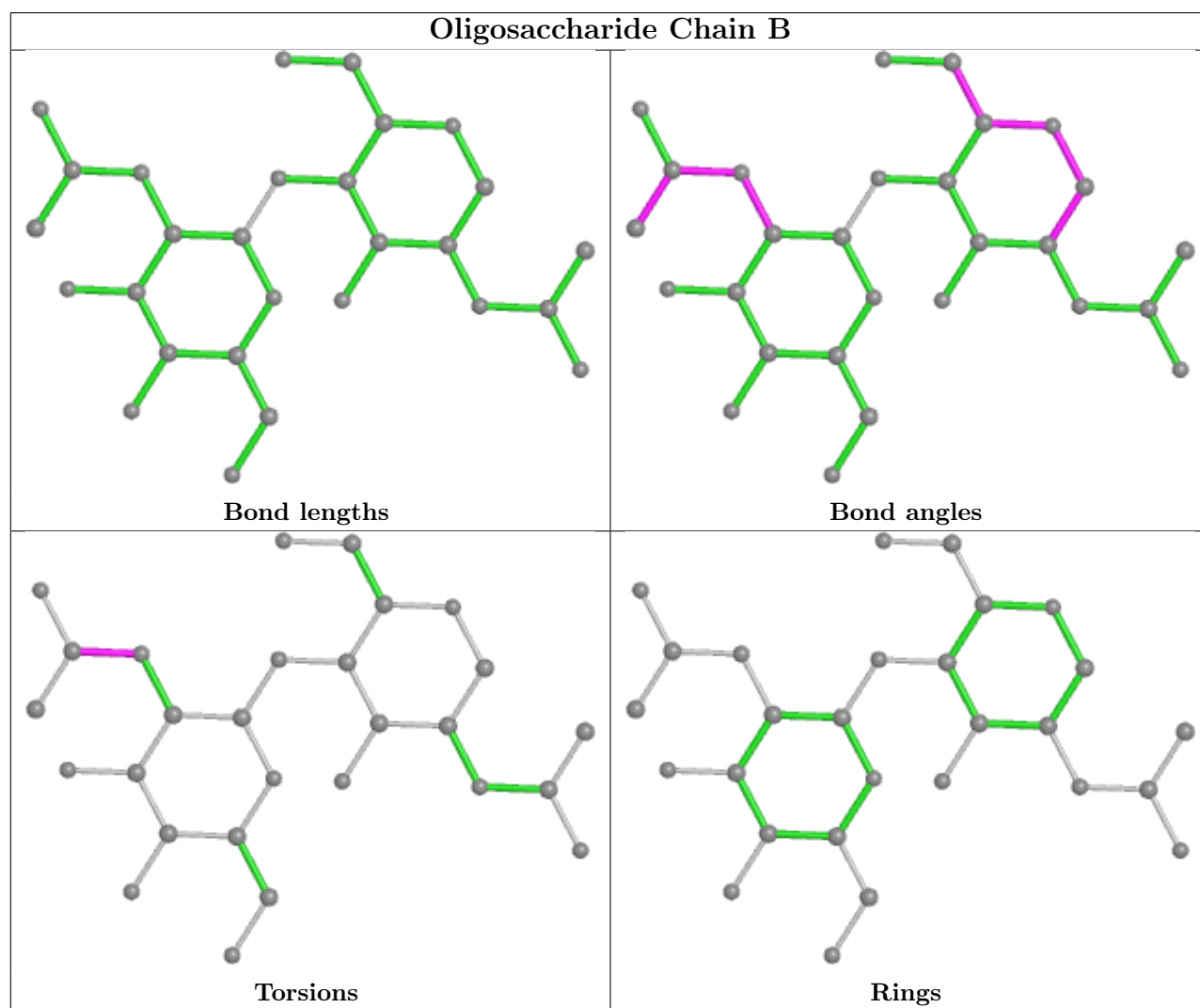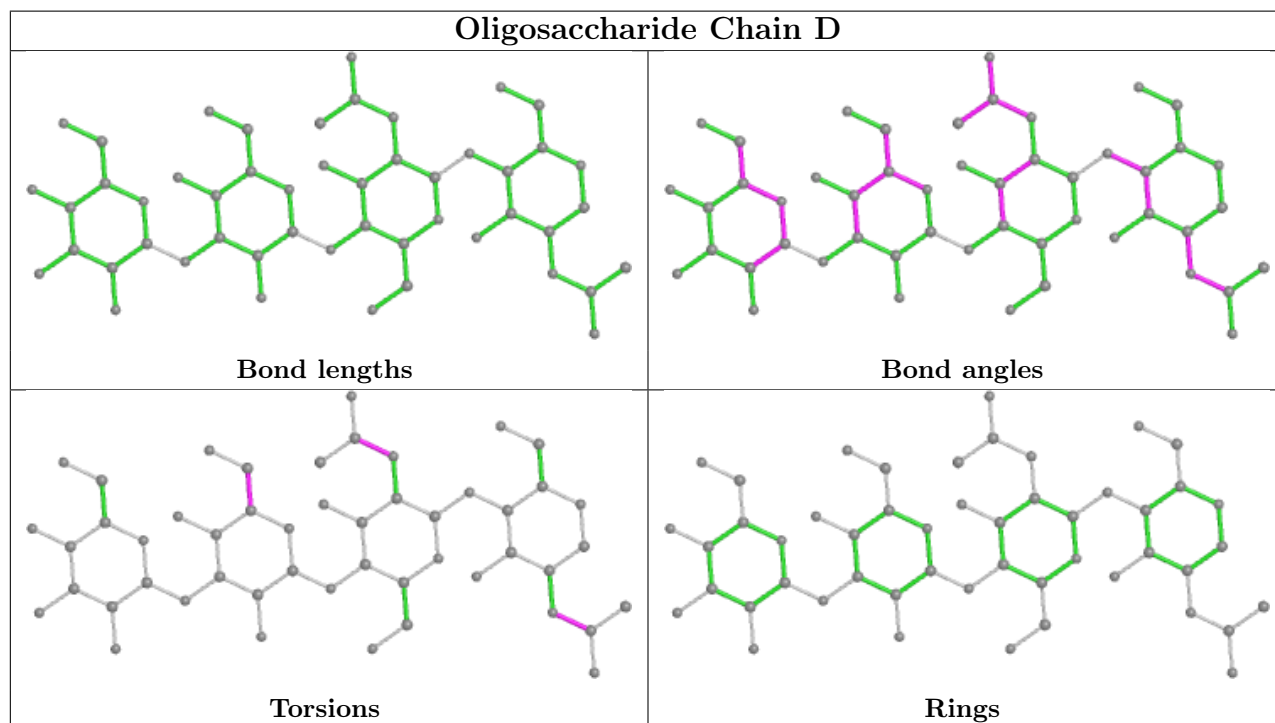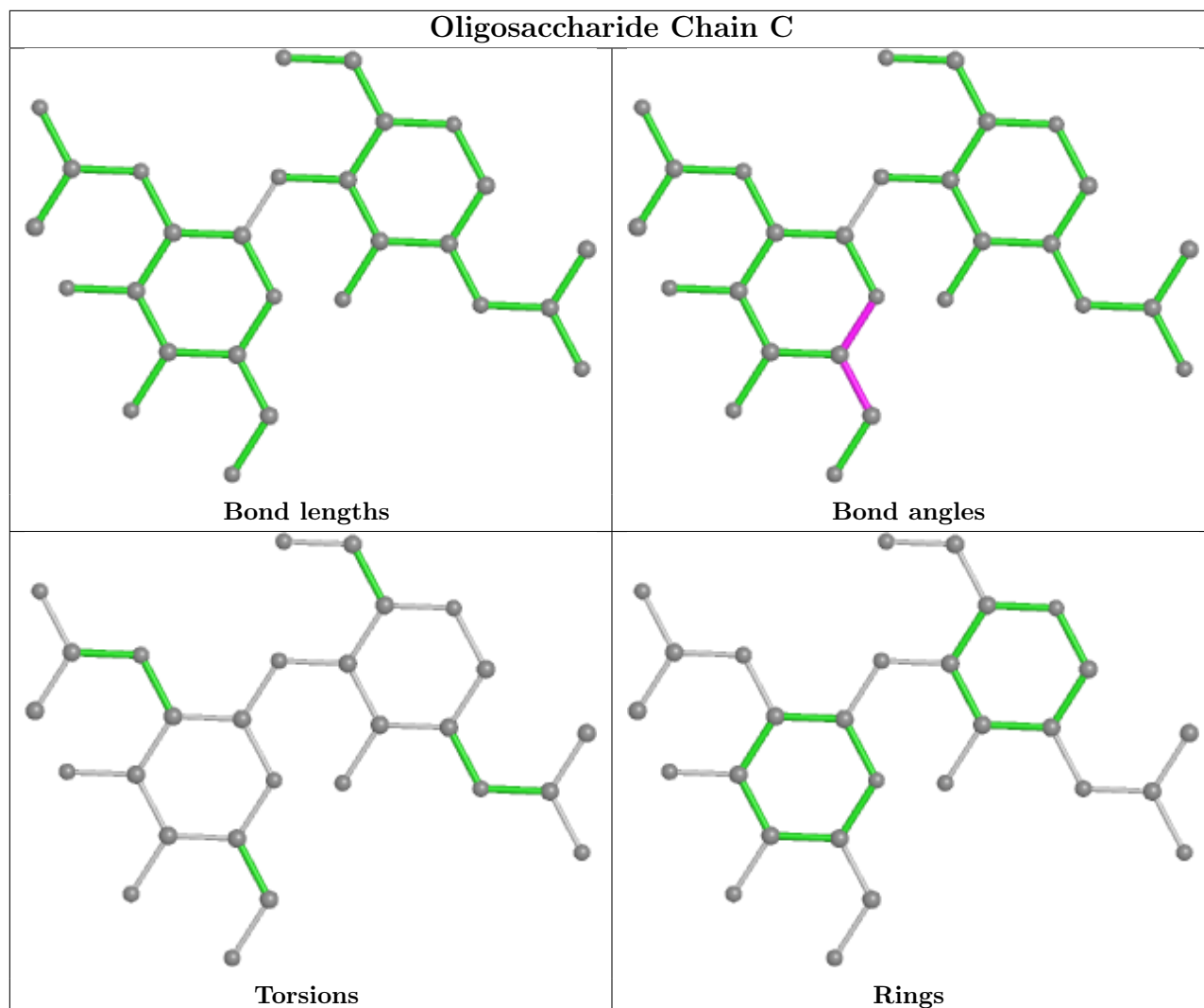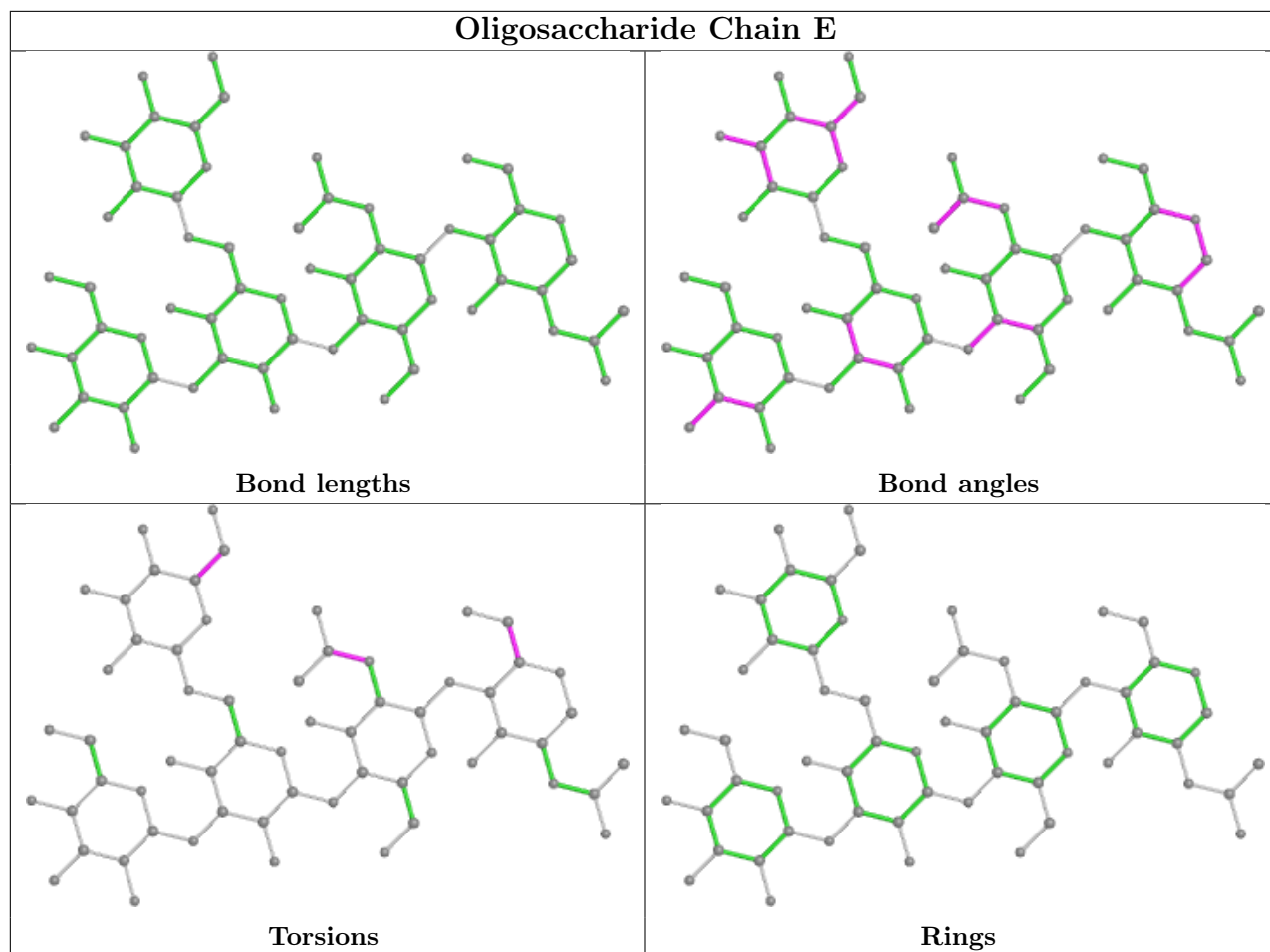
5.6　Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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	#$|Z| > 2$
11	PEG	A	830	-	6,6,6	0.57	0	5,5,5	0.34	0
9	EDO	A	824	-	3,3,3	0.49	0	2,2,2	0.34	0
9	EDO	A	826	-	3,3,3	0.48	0	2,2,2	0.26	0
9	EDO	A	821	-	3,3,3	0.42	0	2,2,2	0.41	0
11	PEG	A	831	-	6,6,6	0.51	0	5,5,5	0.29	0
5	NAG	A	803	1	14,14,15	0.78	0	17,19,21	2.19	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	EDO	A	825	-	3,3,3	0.43	0	2,2,2	0.38	0
12	PGE	A	832	-	9,9,9	1.09	0	8,8,8	2.76	4 (50%)
11	PEG	A	829	-	6,6,6	0.45	0	5,5,5	0.47	0
10	TAM	A	828	-	7,10,10	0.69	0	9,12,12	1.19	1 (11%)
10	TAM	A	827	-	7,10,10	1.22	1 (14%)	9,12,12	1.90	2 (22%)
13	FVZ	A	833	6	30,30,30	1.81	8 (26%)	39,39,39	1.27	3 (7%)
5	NAG	A	806	1	14,14,15	0.69	0	17,19,21	1.99	6 (35%)
9	EDO	A	822	-	3,3,3	0.48	0	2,2,2	0.05	0
5	NAG	A	807	1	14,14,15	0.76	0	17,19,21	2.13	6 (35%)
9	EDO	A	823	-	3,3,3	0.47	0	2,2,2	0.20	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
11	PEG	A	830	-	-	2/4/4/4	-
9	EDO	A	824	-	-	0/1/1/1	-
9	EDO	A	826	-	-	1/1/1/1	-
9	EDO	A	821	-	-	1/1/1/1	-
11	PEG	A	831	-	-	2/4/4/4	-
5	NAG	A	803	1	-	2/6/23/26	0/1/1/1
9	EDO	A	825	-	-	1/1/1/1	-
12	PGE	A	832	-	-	4/7/7/7	-
11	PEG	A	829	-	-	0/4/4/4	-
10	TAM	A	828	-	-	6/12/12/12	-
10	TAM	A	827	-	-	9/12/12/12	-
13	FVZ	A	833	6	-	0/31/31/31	0/1/1/1
5	NAG	A	806	1	-	2/6/23/26	0/1/1/1
9	EDO	A	822	-	-	1/1/1/1	-
5	NAG	A	807	1	-	2/6/23/26	0/1/1/1
9	EDO	A	823	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	833	FVZ	FAH-CAF	5.00	1.48	1.36
13	A	833	FVZ	CAL-CAJ	3.70	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	833	FVZ	OAY-CAW	2.44	1.29	1.22
13	A	833	FVZ	CAZ-CAV	2.42	1.59	1.53
10	A	827	TAM	C1-C4	2.39	1.56	1.52
13	A	833	FVZ	CAC-NAI	-2.21	1.37	1.41
13	A	833	FVZ	CBA-CBB	2.18	1.55	1.50
13	A	833	FVZ	O-C	2.17	1.28	1.22
13	A	833	FVZ	CAD-CAF	2.02	1.41	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	807	NAG	C1-O5-C5	5.47	119.61	112.19
12	A	832	PGE	C5-O3-C4	-5.05	91.39	113.29
5	A	803	NAG	O5-C5-C6	4.82	114.75	107.20
5	A	806	NAG	C1-O5-C5	4.12	117.77	112.19
10	A	827	TAM	C3-C-C1	4.04	117.62	110.50
5	A	806	NAG	C8-C7-N2	3.55	122.11	116.10
10	A	827	TAM	O4-C4-C1	3.52	120.80	111.39
12	A	832	PGE	C3-O2-C2	-3.43	98.41	113.29
5	A	803	NAG	C1-O5-C5	3.41	116.81	112.19
5	A	807	NAG	O5-C5-C6	3.36	112.47	107.20
5	A	806	NAG	O5-C5-C6	3.23	112.27	107.20
5	A	803	NAG	C8-C7-N2	3.14	121.41	116.10
13	A	833	FVZ	CAG-CAF-CAD	-3.07	118.74	122.83
5	A	806	NAG	O5-C1-C2	-2.99	106.56	111.29
5	A	803	NAG	C1-C2-N2	-2.91	105.52	110.49
5	A	807	NAG	O5-C1-C2	-2.90	106.72	111.29
5	A	807	NAG	C4-C3-C2	-2.65	107.13	111.02
12	A	832	PGE	O2-C2-C1	-2.65	98.44	110.07
5	A	803	NAG	C3-C4-C5	2.61	114.89	110.24
10	A	828	TAM	C3-C-C1	2.60	115.09	110.50
12	A	832	PGE	O3-C4-C3	-2.55	98.92	110.39
5	A	807	NAG	C3-C4-C5	-2.17	106.37	110.24
5	A	806	NAG	O7-C7-C8	-2.13	118.10	122.06
13	A	833	FVZ	CAE-CAG-CAF	2.09	120.53	118.36
5	A	803	NAG	C4-C3-C2	2.06	114.03	111.02
5	A	807	NAG	O3-C3-C4	-2.04	105.63	110.35
5	A	806	NAG	C3-C4-C5	-2.03	106.61	110.24
13	A	833	FVZ	CAZ-CAV-NAU	2.02	114.95	110.88
5	A	803	NAG	O6-C6-C5	2.01	118.17	111.29

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	827	TAM	C2-C-C1-C4
10	A	827	TAM	C3-C-C1-C4
10	A	827	TAM	N-C-C1-C4
10	A	827	TAM	C1-C-C2-C5
10	A	827	TAM	N-C-C2-C5
10	A	827	TAM	N-C-C3-C6
10	A	827	TAM	C-C2-C5-O5
10	A	828	TAM	C3-C-C1-C4
10	A	828	TAM	N-C-C1-C4
10	A	828	TAM	C-C2-C5-O5
11	A	831	PEG	O1-C1-C2-O2
5	A	803	NAG	C8-C7-N2-C2
5	A	803	NAG	O7-C7-N2-C2
5	A	806	NAG	C8-C7-N2-C2
5	A	806	NAG	O7-C7-N2-C2
12	A	832	PGE	O2-C3-C4-O3
12	A	832	PGE	O1-C1-C2-O2
12	A	832	PGE	O3-C5-C6-O4
9	A	821	EDO	O1-C1-C2-O2
9	A	825	EDO	O1-C1-C2-O2
5	A	807	NAG	O5-C5-C6-O6
10	A	827	TAM	C1-C-C3-C6
10	A	828	TAM	C2-C-C1-C4
5	A	807	NAG	C4-C5-C6-O6
10	A	828	TAM	C-C1-C4-O4
10	A	828	TAM	C-C3-C6-O6
11	A	831	PEG	O2-C3-C4-O4
11	A	830	PEG	O2-C3-C4-O4
9	A	822	EDO	O1-C1-C2-O2
9	A	823	EDO	O1-C1-C2-O2
11	A	830	PEG	C1-C2-O2-C3
10	A	827	TAM	C2-C-C3-C6
9	A	826	EDO	O1-C1-C2-O2
12	A	832	PGE	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	827	TAM	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 then 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.

Ligand FVZ A 833

Bond lengths

Bond angles

Torsions

Rings
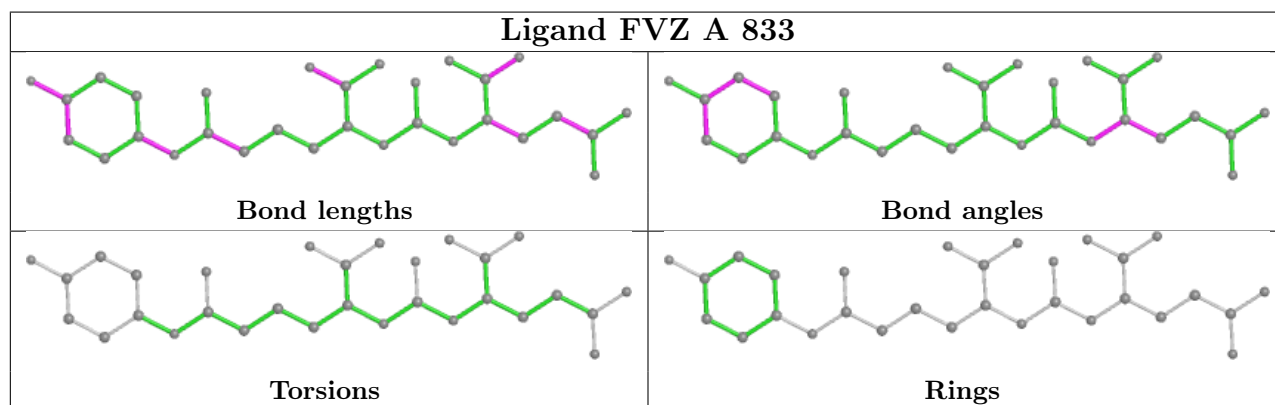
5.7 Other polymers ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	696/707 (98%)	0.09	27 (3%)	39	34	29, 40, 61, 97	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	THR	6.1
1	A	155[A]	SER	4.9
1	A	719[A]	VAL	4.6
1	A	507	SER	3.8
1	A	153	ASN	3.6
1	A	505	GLU	3.3
1	A	335	GLY	3.3
1	A	134	ASP	3.3
1	A	55	LYS	3.2
1	A	506	PHE	3.2
1	A	154	VAL	3.1
1	A	654[A]	ASP	2.8
1	A	124	HIS	2.7
1	A	656[A]	SER	2.6
1	A	542	GLU	2.6
1	A	56	HIS	2.6
1	A	487	GLY	2.5
1	A	123	THR	2.5
1	A	499	LYS	2.4
1	A	136	ASN	2.4
1	A	334	THR	2.4
1	A	339	THR	2.3
1	A	152	GLU	2.2
1	A	521	PHE	2.2
1	A	131	ILE	2.1
1	A	132	ASN	2.1
1	A	655[A]	LYS	2.0

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

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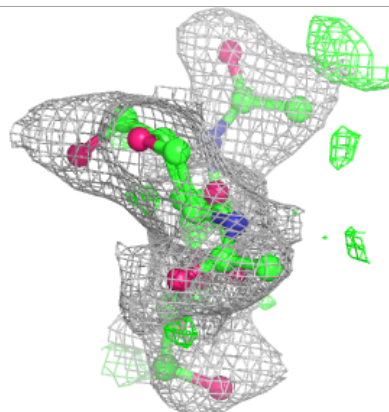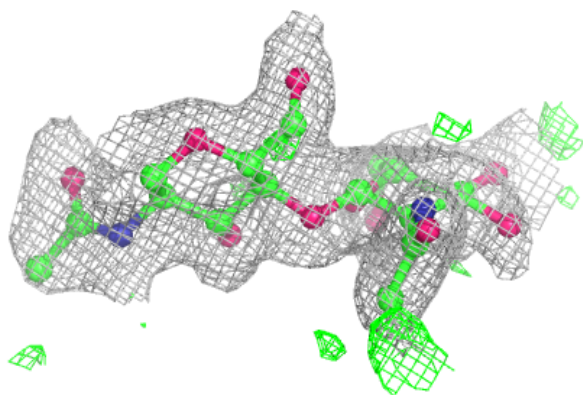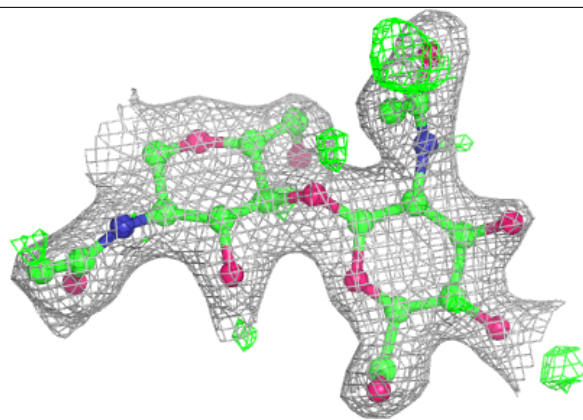
6.3 Carbohydrates ⓘ

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
3	MAN	D	4	11/12	0.71	0.30	82,86,88,89	0
2	NAG	B	2	14/15	0.77	0.31	57,67,73,78	0
4	MAN	E	5	11/12	0.77	0.20	63,74,78,78	0
2	NAG	C	2	14/15	0.81	0.33	70,76,82,89	0
3	BMA	D	3	11/12	0.82	0.26	80,89,93,93	0
2	NAG	C	1	14/15	0.84	0.18	56,57,61,66	0
4	NAG	E	1	14/15	0.90	0.10	36,40,49,58	0
3	NAG	D	2	14/15	0.90	0.15	57,64,75,75	0
4	NAG	E	2	14/15	0.91	0.14	49,52,58,66	0
4	BMA	E	3	11/12	0.93	0.10	49,52,56,60	0
4	MAN	E	4	11/12	0.93	0.09	51,56,59,60	0
3	NAG	D	1	14/15	0.93	0.10	47,49,54,58	0
2	NAG	B	1	14/15	0.94	0.17	47,56,63,65	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)
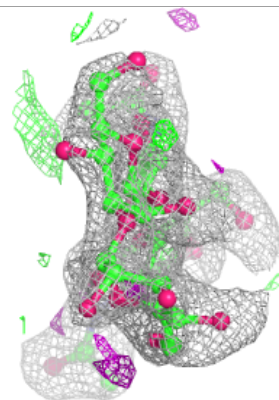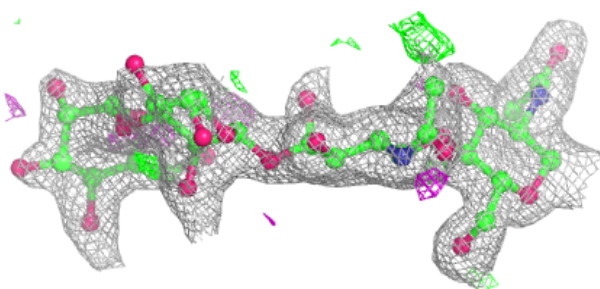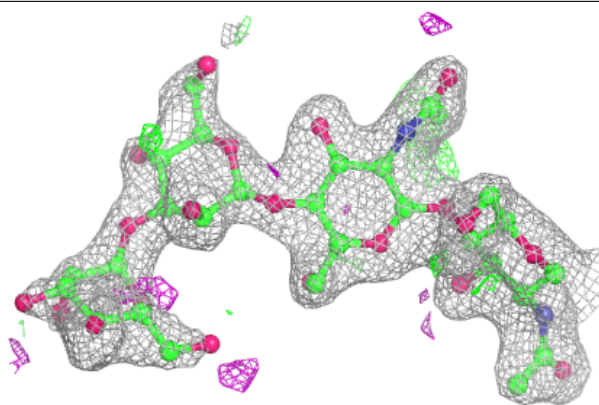and green (positive)

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)
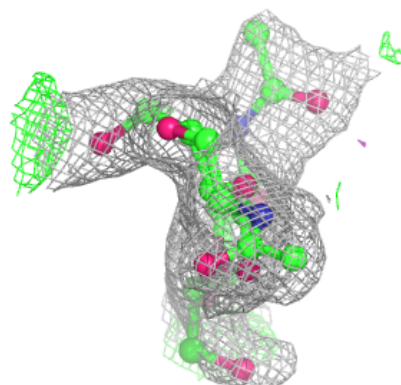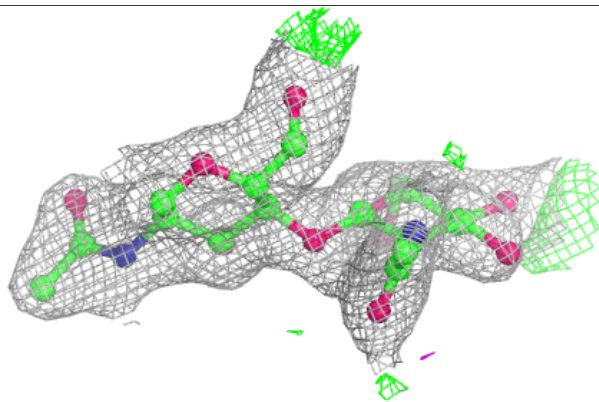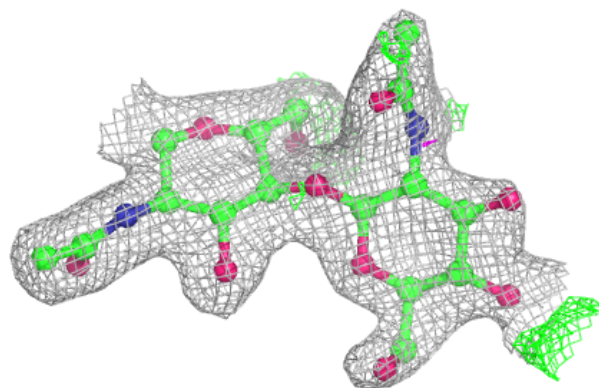
Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
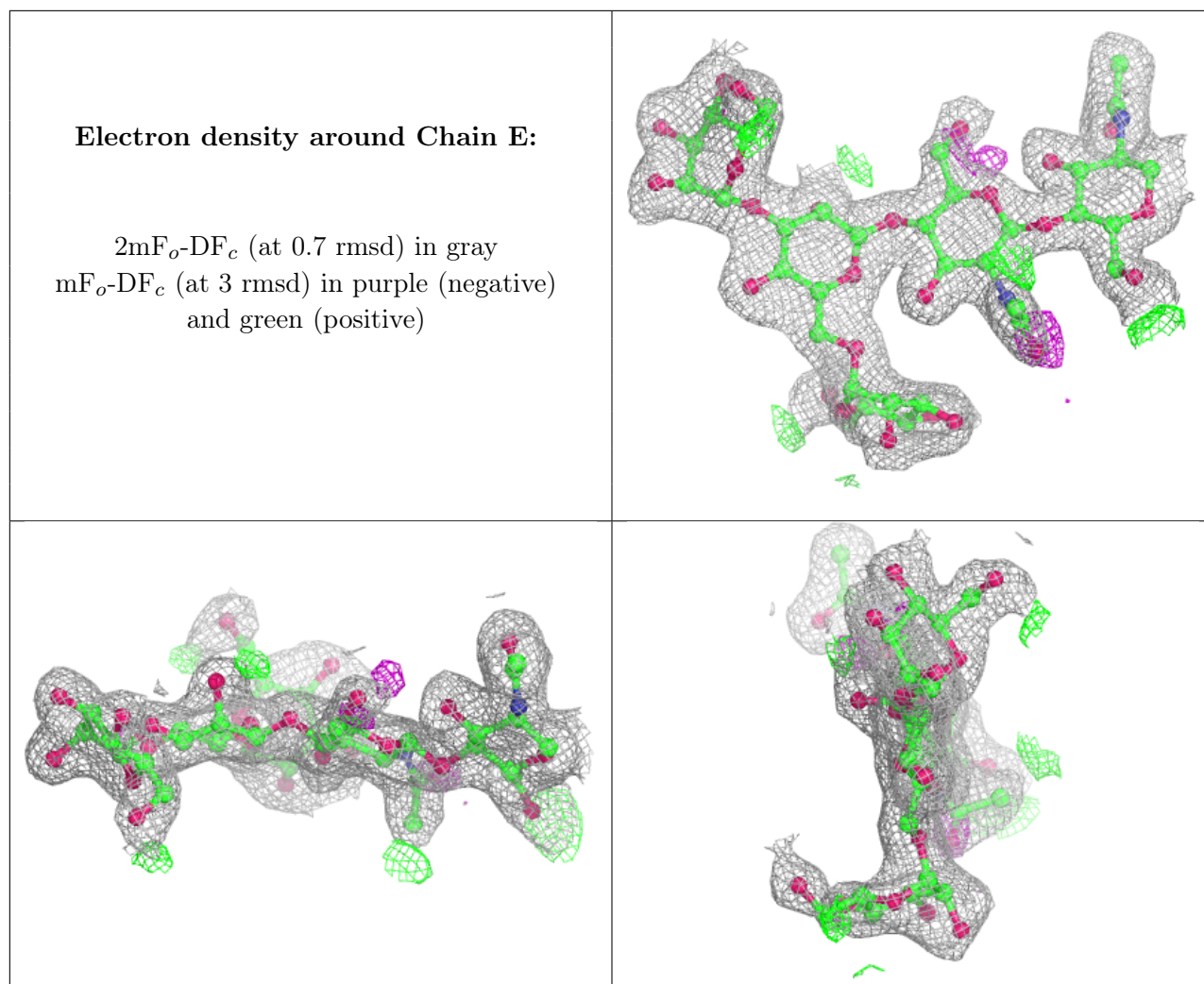
Electron density around Chain E:

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

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.
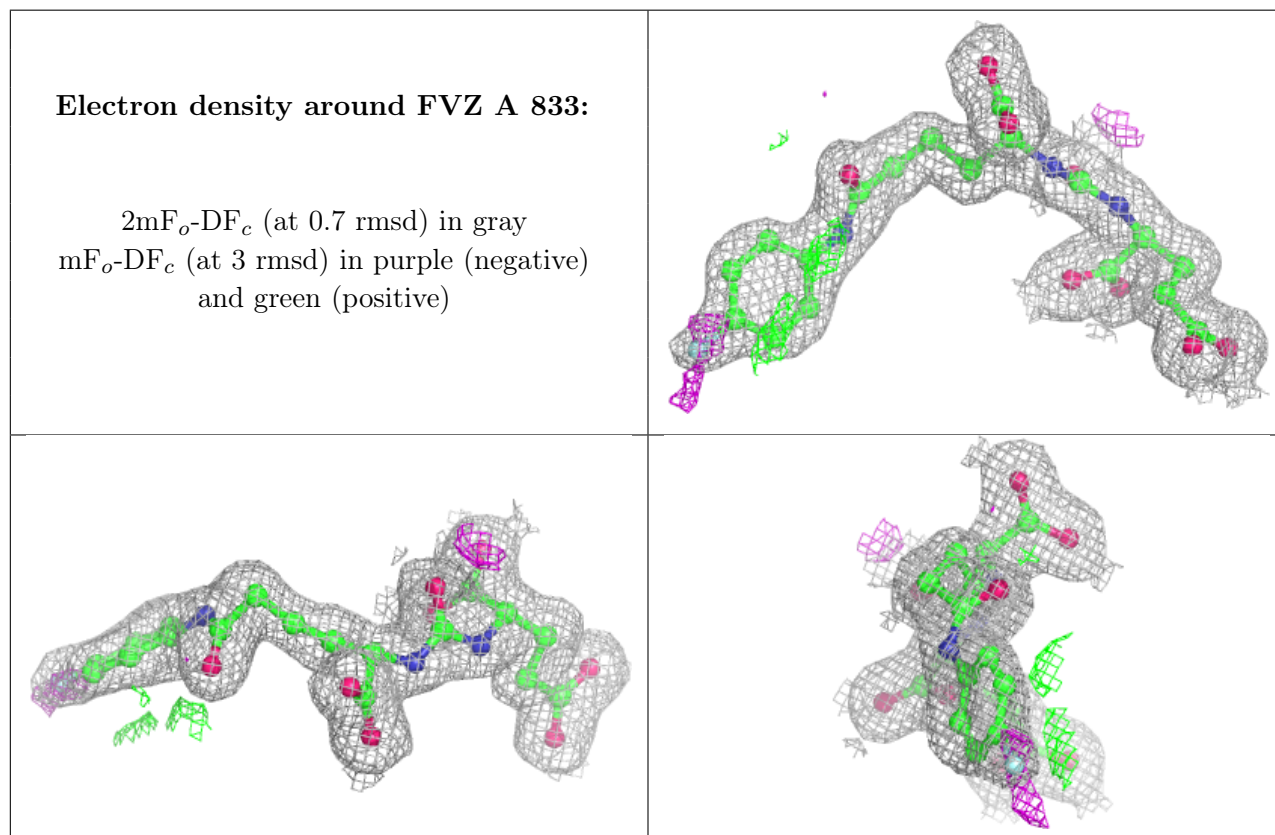
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	PEG	A	830	7/7	0.47	0.27	83,85,92,93	0
9	EDO	A	825	4/4	0.48	0.23	83,86,89,92	0
10	TAM	A	827	11/11	0.56	0.25	52,76,81,82	0
9	EDO	A	822	4/4	0.59	0.25	77,84,85,90	0
9	EDO	A	823	4/4	0.60	0.19	80,80,80,83	0
10	TAM	A	828	11/11	0.65	0.17	66,70,76,79	0
5	NAG	A	803	14/15	0.67	0.27	65,75,89,92	0
5	NAG	A	806	14/15	0.71	0.28	83,90,93,94	0
9	EDO	A	824	4/4	0.74	0.31	86,90,93,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	A	826	4/4	0.78	0.21	90,91,92,93	0
11	PEG	A	831	7/7	0.78	0.15	83,86,87,90	0
5	NAG	A	807	14/15	0.80	0.17	48,67,74,75	0
11	PEG	A	829	7/7	0.86	0.15	65,67,70,72	0
9	EDO	A	821	4/4	0.90	0.40	61,71,72,80	0
12	PGE	A	832	10/10	0.94	0.24	19,27,28,31	10
13	FVZ	A	833	30/30	0.95	0.16	30,34,54,58	0
8	CL	A	834	1/1	0.98	0.19	43,43,43,43	0
7	CA	A	819	1/1	1.00	0.09	31,31,31,31	0
8	CL	A	820	1/1	1.00	0.17	34,34,34,34	0
6	ZN	A	817	1/1	1.00	0.08	33,33,33,33	0
6	ZN	A	818	1/1	1.00	0.10	32,32,32,32	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.

Electron density around FVZ A 833:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.