WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 27, 2024 – 09:10 PM EDT

PDB ID	:	6MEJ
Title	:	Crystal structure of Hepatitis C virus envelope glycoprotein E2 ectodomain in complex with human antibodies HEPC3 and HEPC46
Authors	:	Flyak, A.I.; Bjorkman, P.J.
Deposited on	:	2018-09-06
Resolution	:	2.80 Å(reported)

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

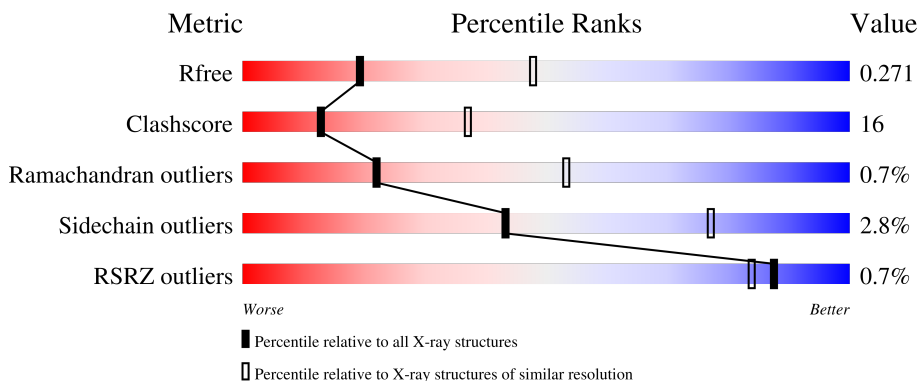|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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		0.271
Clashscore		16
Ramachandran outliers		0.7%
Sidechain outliers		2.8%
RSRZ outliers		0.7%

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	230	65% / 27% / · 7%
2	B	217	68% / 29% / ··
3	C	262	3% (poor fit); 52% / 35% / · 11%
4	H	241	68% / 24% / · 7%
5	L	214	68% / 30% / ·

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Mol	Chain	Length	Quality of chain
6	D	5	60% 40%
7	E	4	75% 25%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 8500 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 antibody HEPC46 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total 1610	C 1013	N 275	O 315	S 7	0	0	0

- Molecule 2 is a protein called antibody HEPC46 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total 1577	C 988	N 264	O 321	S 4	0	0	0

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	234	Total 1830	C 1162	N 325	O 324	S 19	0	0	0

- Molecule 4 is a protein called antibody HEPC3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	225	Total 1680	C 1056	N 282	O 334	S 8	0	0	0

- Molecule 5 is a protein called antibody HEPC3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	213	Total 1636	C 1017	N 281	O 333	S 5	0	0	0

- Molecule 6 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-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.
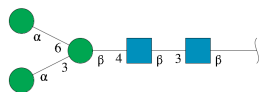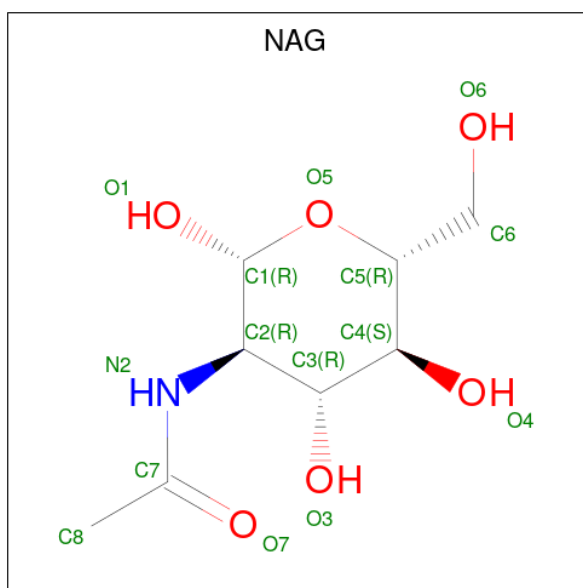
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	D	5	61	34	2	25	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	E	4	50	28	2	20	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	C	1	Total 14	C 8	N 1	O 5	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 ac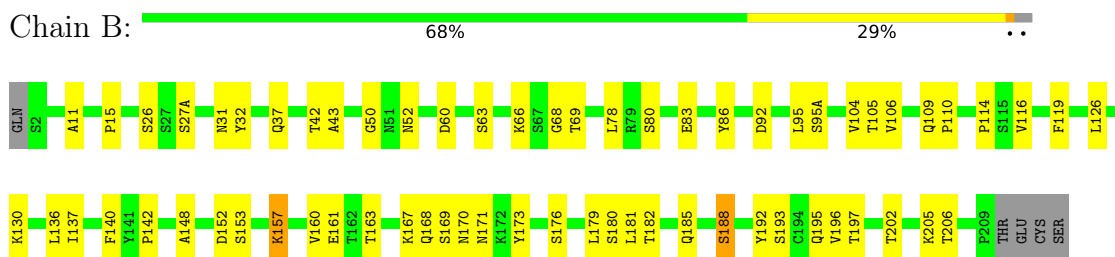cording to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
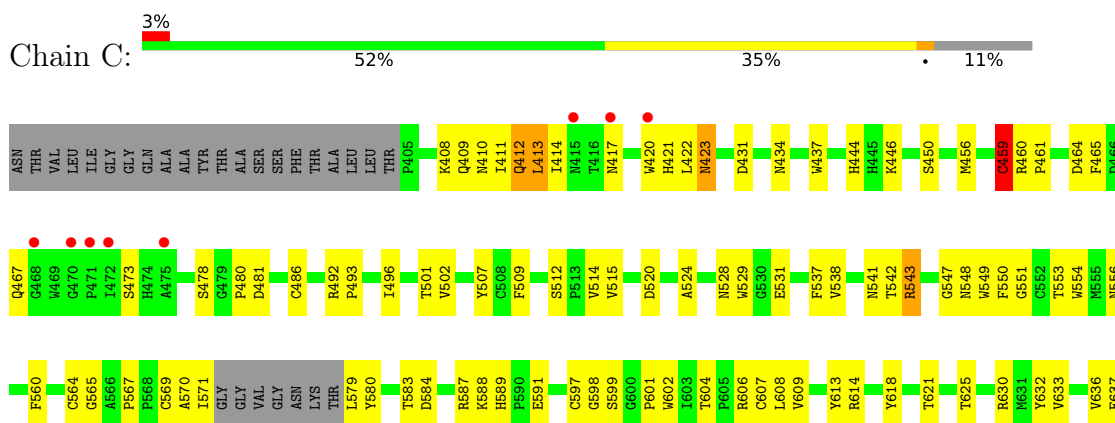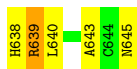
• Molecule 1: antibody HEPC46 Heavy Chain
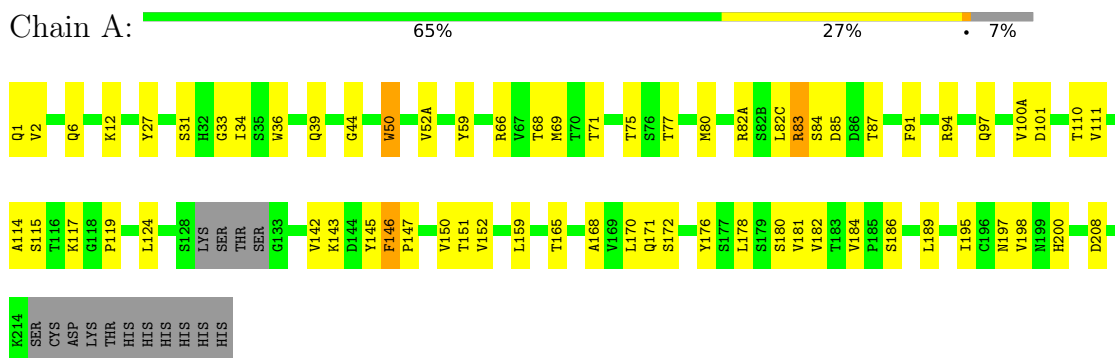
Chain A:

• Molecule 2: antibody HEPC46 Light Chain

Chain B:

• Molecule 3: E2 glycoprotein

Chain C:

H638 R639 L640 A643 C644 N645

• Molecule 4: antibody HEPC3 Heavy Chain

Chain H:

68%   24%   7%

Q1 V2 Q3 L4 K13 V18 K19 C22 E33 I34 T35 W36 A40 Q43 T52 E56 Q61 Q64 G65 R66 V67 D72 E73 S74 T78 Y79 M80 E81 L82 L82C R83 P84 E85 Y91 R94 D95 G96 R100D N100G W100H F100I D101 P102

V111 S112 S113 P119 L124 S128 LYS SER T131 L138 Y145 E148 P149 V150 T151 V152 S153 W154 F166 P167 A168 L178 V184 P185 C196 N197 V198 N199 V211 K214 S215 CYS ASP LYS THR ALA GLY TRP SER HIS PRO GLN PHE GLU LYS
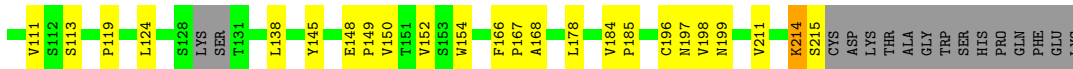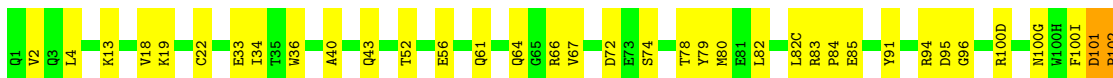
• Molecule 5: antibody HEPC3 Light Chain

Chain L:

68%   30%

D1 Q6 L11 S12 A13 S14 R18 V19 T20 I21 T22 C23 N28 I29 N30 N31 Y32 W35 Q37 V46 L47 I48 L54 Q55 V58 S63 G68 L73 T74 I75 S76 S77 L78 Q79 P80 F83 C88 Q89 Q90 S91 H92 S93 T94 T97

Q100 G101 T102 E105 I106 K107 R108 T109 V110 F118 L125 P141 K149 V150 D151 L154 G157 N158 S159 Q160 E161 S162 V163 S171 L175 S176 S177 T178 L179 T180 K183 A184 D185 K188 V191 C194 E195 E213 CYS
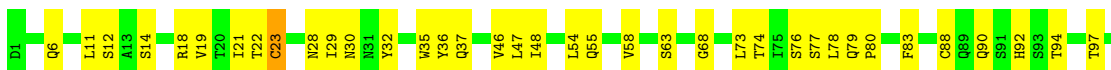
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

60%   40%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain E:

75%   25%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.44Å 76.64Å 118.26Å 90.00° 106.33° 90.00°	Depositor
Resolution (Å)	78.27 – 2.80 78.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.27-2.80) 99.7 (78.27-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.271 0.198 , 0.271	Depositor DCC
R_{free} test set	1806 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8500	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.52	1/1647 (0.1%)	0.64	0/2245
2	B	0.46	0/1620	0.63	0/2216
3	C	0.56	1/1899 (0.1%)	0.75	2/2602 (0.1%)
4	H	0.48	0/1720	0.66	1/2345 (0.0%)
5	L	0.50	1/1669 (0.1%)	0.70	1/2265 (0.0%)
All	All	0.50	3/8555 (0.0%)	0.68	4/11673 (0.0%)

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
3	C	0	1
4	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	564	CYS	CB-SG	-7.36	1.69	1.82
1	A	50	TRP	CB-CG	-5.81	1.39	1.50
5	L	23	CYS	CB-SG	-5.35	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	543	ARG	NE-CZ-NH1	-8.56	116.02	120.30
4	H	101	ASP	C-N-CD	-5.91	107.59	120.60
3	C	459	CYS	CA-CB-SG	-5.45	104.18	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	154	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	409	GLN	Peptide
4	H	101	ASP	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	1610	0	1582	49	0
2	B	1577	0	1509	47	1
3	C	1830	0	1695	88	0
4	H	1680	0	1638	45	0
5	L	1636	0	1589	58	1
6	D	61	0	52	1	0
7	E	50	0	43	1	0
8	C	56	0	52	1	0
All	All	8500	0	8160	274	1

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 16.

The worst 5 of 274 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)
3:C:422:LEU:HD12	3:C:529:TRP:CH2	1.84	1.12
4:H:2:VAL:HG23	4:H:102:PRO:HG2	1.48	0.95
1:A:87:THR:HG23	1:A:110:THR:HA	1.49	0.93
3:C:465:PHE:HB3	3:C:588:LYS:HG3	1.52	0.89
5:L:106:ILE:HD11	5:L:171:SER:OG	1.73	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ASP:OD1	5:L:183:LYS:NZ[2_544]	2.13	0.07

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	211/230 (92%)	201 (95%)	9 (4%)	1 (0%)	29	61
2	B	210/217 (97%)	188 (90%)	18 (9%)	4 (2%)	8	26
3	C	230/262 (88%)	202 (88%)	27 (12%)	1 (0%)	34	66
4	H	221/241 (92%)	202 (91%)	18 (8%)	1 (0%)	29	61
5	L	211/214 (99%)	193 (92%)	17 (8%)	1 (0%)	29	61
All	All	1083/1164 (93%)	986 (91%)	89 (8%)	8 (1%)	22	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	102	PRO
5	L	158	ASN
2	B	171	ASN
2	B	188	SER
3	C	412	GLN

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	180/195 (92%)	177 (98%)	3 (2%)	60	87
2	B	176/181 (97%)	172 (98%)	4 (2%)	50	82
3	C	197/216 (91%)	185 (94%)	12 (6%)	18	48
4	H	189/203 (93%)	186 (98%)	3 (2%)	62	88
5	L	187/188 (100%)	183 (98%)	4 (2%)	53	84
All	All	929/983 (94%)	903 (97%)	26 (3%)	43	77

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	492	ARG
3	C	639	ARG
5	L	176	SER
3	C	638	HIS
3	C	640	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	61	GLN
4	H	171	GLN
5	L	28	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 ⓘ

9 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	#$|Z| > 2$
6	NAG	D	1	6,3	14,14,15	0.66	0	17,19,21	2.54	6 (35%)
6	NAG	D	2	6	14,14,15	0.56	0	17,19,21	1.91	5 (29%)
6	BMA	D	3	6	11,11,12	1.08	1 (9%)	15,15,17	1.03	1 (6%)
6	MAN	D	4	6	11,11,12	0.64	0	15,15,17	1.22	2 (13%)
6	MAN	D	5	6	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
7	NAG	E	1	3,7	14,14,15	0.41	0	17,19,21	1.06	1 (5%)
7	NAG	E	2	7	14,14,15	0.44	0	17,19,21	1.22	2 (11%)
7	BMA	E	3	7	11,11,12	1.22	2 (18%)	15,15,17	1.01	0
7	MAN	E	4	7	11,11,12	0.58	0	15,15,17	0.81	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
6	NAG	D	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	3/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	0/2/19/22	0/1/1/1
7	NAG	E	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	4/6/23/26	0/1/1/1
7	BMA	E	3	7	-	1/2/19/22	0/1/1/1
7	MAN	E	4	7	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	3	BMA	C4-C5	2.67	1.58	1.53
7	E	3	BMA	C4-C3	2.50	1.58	1.52
6	D	3	BMA	C1-C2	2.28	1.57	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1	NAG	C1-C2-N2	-6.17	99.94	110.49
6	D	1	NAG	C2-N2-C7	5.01	130.04	122.90
6	D	2	NAG	C2-N2-C7	4.34	129.08	122.90
6	D	1	NAG	O3-C3-C4	-3.07	103.25	110.35
6	D	2	NAG	C4-C3-C2	3.01	115.43	111.02

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C3-C2-N2-C7
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
7	E	3	BMA	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	4	MAN	1	0
6	D	1	NAG	1	0
6	D	2	NAG	1	0
7	E	3	BMA	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E
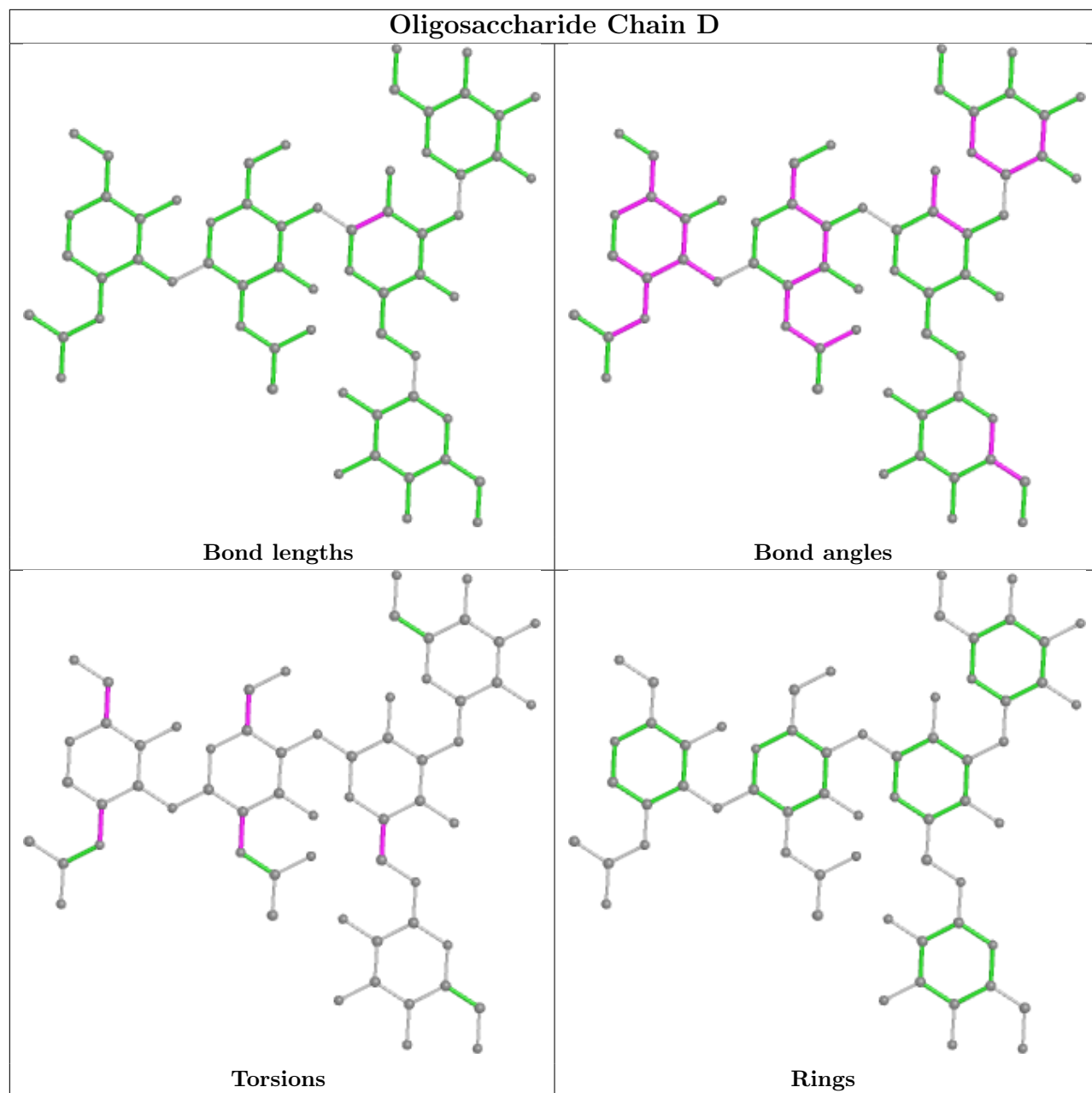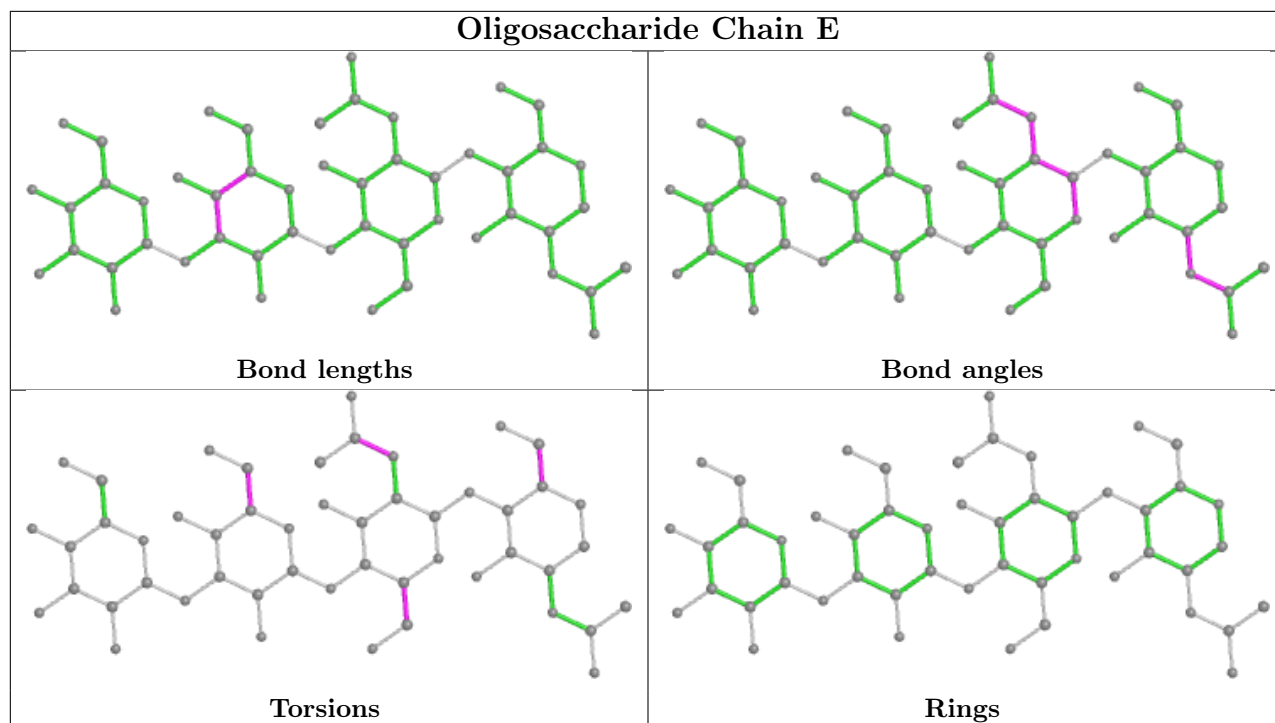
5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
8	NAG	C	4301	3	14,14,15	0.53	0	17,19,21	0.90	0
8	NAG	C	4313	3	14,14,15	0.49	0	17,19,21	1.04	1 (5%)
8	NAG	C	4311	3	14,14,15	0.62	0	17,19,21	1.82	5 (29%)
8	NAG	C	4312	3	14,14,15	0.67	0	17,19,21	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	4301	3	-	6/6/23/26	0/1/1/1
8	NAG	C	4313	3	-	0/6/23/26	0/1/1/1
8	NAG	C	4311	3	-	4/6/23/26	0/1/1/1
8	NAG	C	4312	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4311	NAG	C6-C5-C4	-3.44	104.94	113.00
8	C	4311	NAG	O5-C1-C2	-2.99	106.57	111.29
8	C	4311	NAG	C4-C3-C2	-2.99	106.64	111.02
8	C	4311	NAG	C1-O5-C5	2.49	115.57	112.19
8	C	4311	NAG	O7-C7-N2	2.36	126.30	121.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	4301	NAG	C1-C2-N2-C7
8	C	4301	NAG	C8-C7-N2-C2
8	C	4301	NAG	O7-C7-N2-C2
8	C	4311	NAG	C8-C7-N2-C2
8	C	4311	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	4313	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 ⓘ

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	215/230 (93%)	-0.17	0	100	100	45, 70, 99, 128	0
2	B	212/217 (97%)	-0.04	0	100	100	42, 77, 106, 136	0
3	C	234/262 (89%)	0.24	8 (3%)	45	35	43, 70, 132, 180	0
4	H	225/241 (93%)	-0.05	0	100	100	40, 63, 94, 140	0
5	L	213/214 (99%)	-0.06	0	100	100	44, 72, 103, 124	0
All	All	1099/1164 (94%)	-0.01	8 (0%)	87	84	40, 70, 108, 180	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	417	ASN	4.6
3	C	468	GLY	4.4
3	C	415	ASN	3.8
3	C	471	PRO	3.0
3	C	472	ILE	2.9

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.
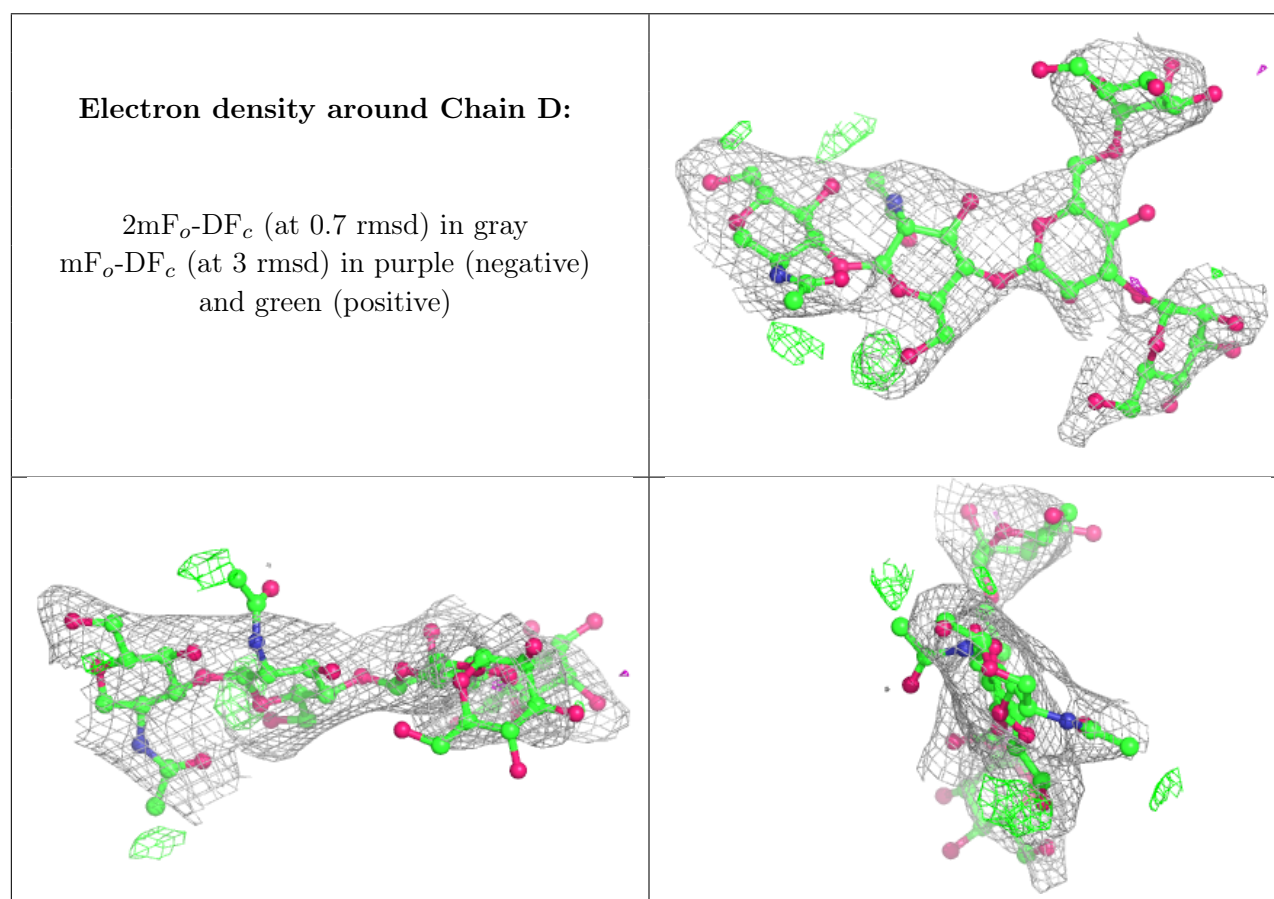
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	D	3	11/12	0.67	0.27	127,136,147,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
6	MAN	D	4	11/12	0.70	0.31	118,140,145,145	0
7	BMA	E	3	11/12	0.74	0.18	126,134,141,143	0
7	MAN	E	4	11/12	0.75	0.25	104,132,139,141	0
6	NAG	D	2	14/15	0.83	0.21	70,87,108,116	0
6	MAN	D	5	11/12	0.90	0.27	117,122,125,126	0
7	NAG	E	2	14/15	0.93	0.14	88,99,102,117	0
6	NAG	D	1	14/15	0.96	0.15	56,67,88,91	0
7	NAG	E	1	14/15	0.97	0.12	31,53,63,72	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.
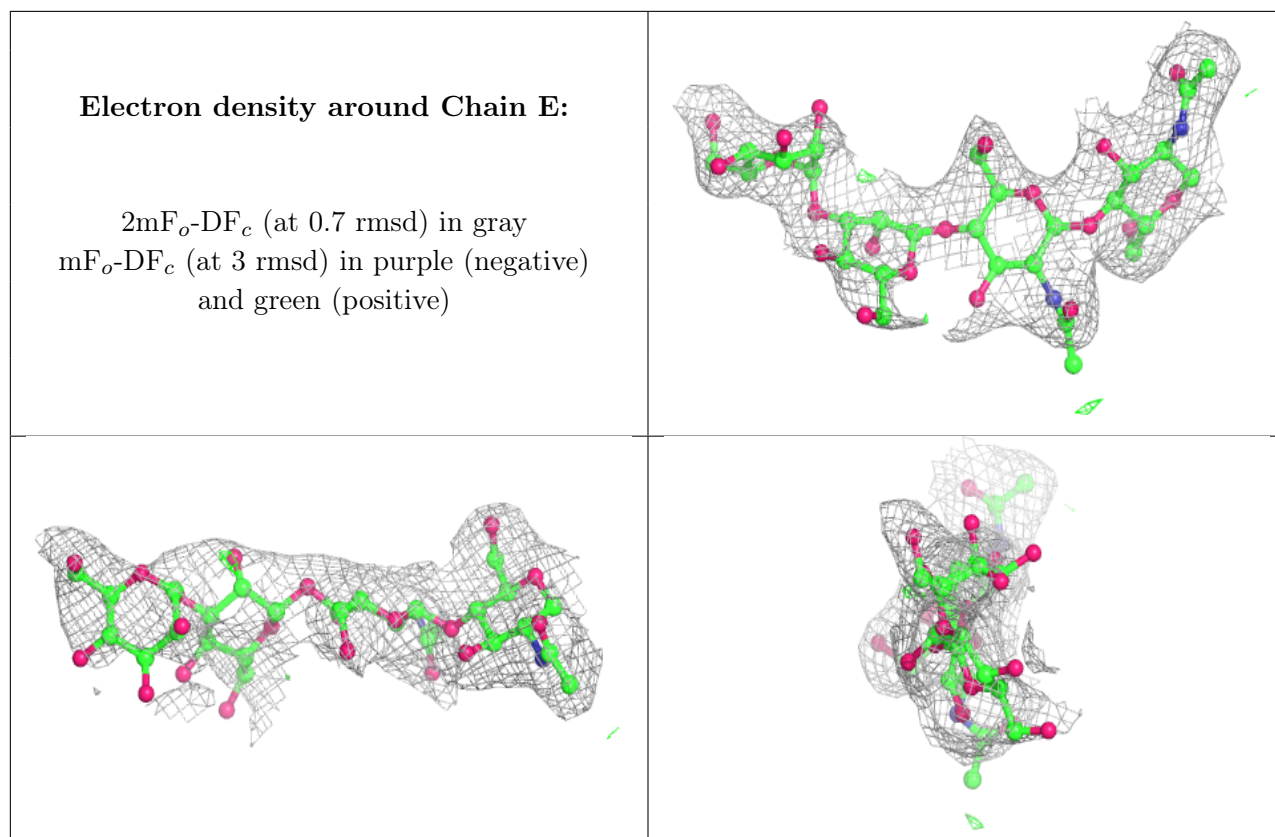
Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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
8	NAG	C	4312	14/15	0.81	0.27	92,101,105,111	0
8	NAG	C	4311	14/15	0.86	0.15	58,76,104,108	0
8	NAG	C	4313	14/15	0.87	0.18	91,107,120,125	0
8	NAG	C	4301	14/15	0.90	0.15	86,92,99,108	0

6.5 Other polymers ⓘ

There are no such residues in this entry.