



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 12:27 PM EST

PDB ID : 7UNZ  
Title : Crystal structure of H2 nanobody in complex with PfCSS  
Authors : Scally, S.W.; Cowman, A.F.  
Deposited on : 2022-04-12  
Resolution : 2.03 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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	:	2.31.2
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)	:	2.31.2

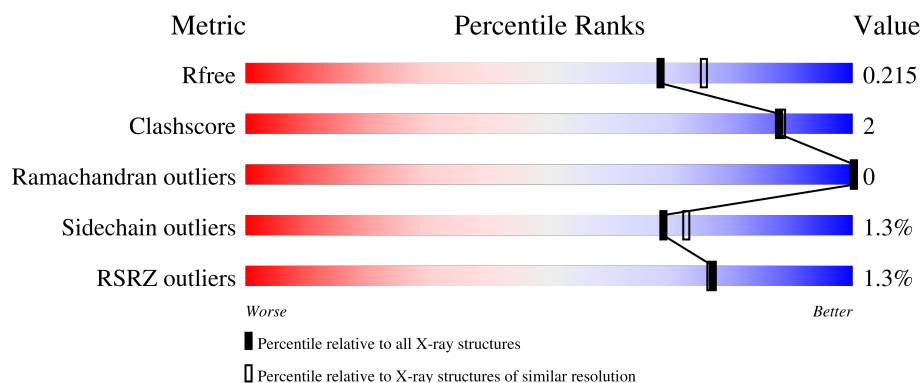
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

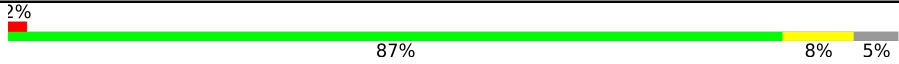
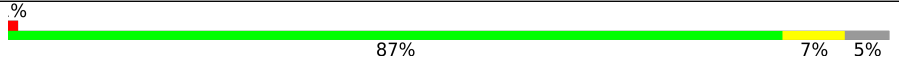
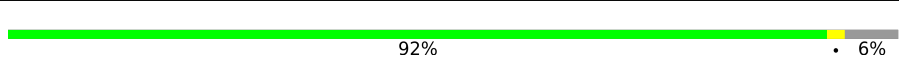
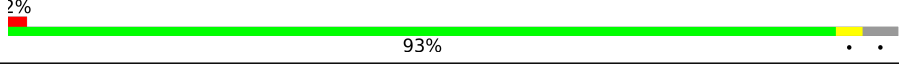

The reported resolution of this entry is 2.03 Å.

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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	279	
1	D	279	
2	A	126	
2	C	126	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	G	2	 100%
3	I	2	 100%
4	H	3	 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
5	NAG	B	301	-	-	-	X
5	NAG	D	301	-	-	-	X
7	EDO	B	306	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6948 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 Cysteine-rich small secreted protein CSS, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	266	Total	C	N	O	S	0	6	0
			2208	1425	359	412	12			
1	D	264	Total	C	N	O	S	0	7	0
			2182	1410	351	409	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	GLY	-	expression tag	UNP Q8IM47
B	20	THR	-	expression tag	UNP Q8IM47
B	263	ALA	THR	engineered mutation	UNP Q8IM47
B	291	LEU	-	expression tag	UNP Q8IM47
B	292	GLU	-	expression tag	UNP Q8IM47
B	293	ASN	-	expression tag	UNP Q8IM47
B	294	LEU	-	expression tag	UNP Q8IM47
B	295	TYR	-	expression tag	UNP Q8IM47
B	296	PHE	-	expression tag	UNP Q8IM47
B	297	GLN	-	expression tag	UNP Q8IM47
D	19	GLY	-	expression tag	UNP Q8IM47
D	20	THR	-	expression tag	UNP Q8IM47
D	263	ALA	THR	engineered mutation	UNP Q8IM47
D	291	LEU	-	expression tag	UNP Q8IM47
D	292	GLU	-	expression tag	UNP Q8IM47
D	293	ASN	-	expression tag	UNP Q8IM47
D	294	LEU	-	expression tag	UNP Q8IM47
D	295	TYR	-	expression tag	UNP Q8IM47
D	296	PHE	-	expression tag	UNP Q8IM47
D	297	GLN	-	expression tag	UNP Q8IM47

- Molecule 2 is a protein called H2 Nanobody.

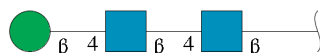
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			896	549	160	183	4			
2	A	119	Total	C	N	O	S	0	0	0
			880	540	156	180	4			

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



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

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



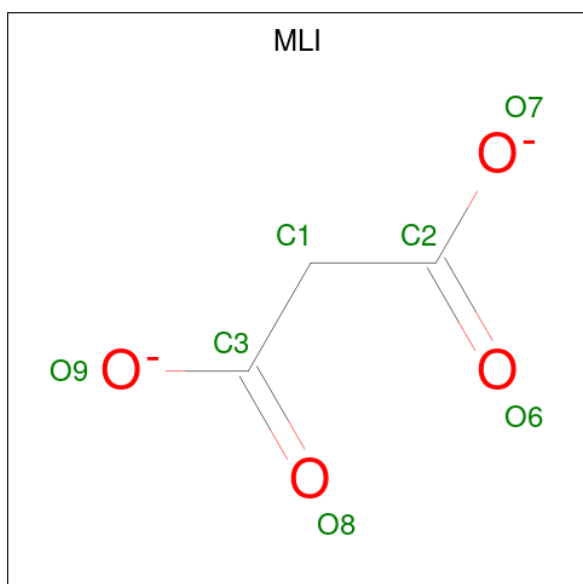
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



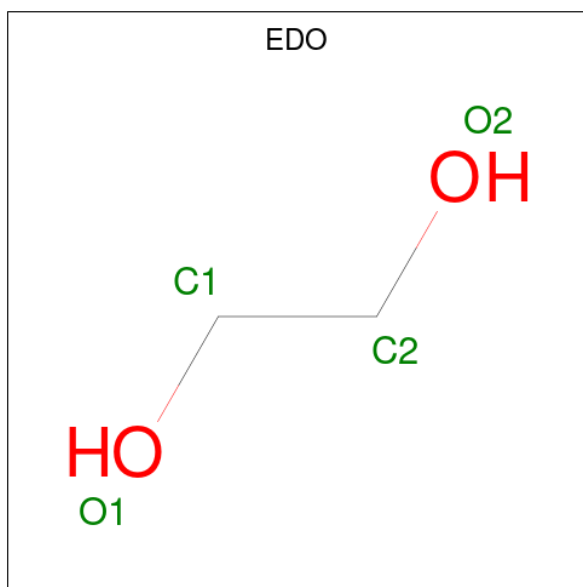
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	3	4		
6	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

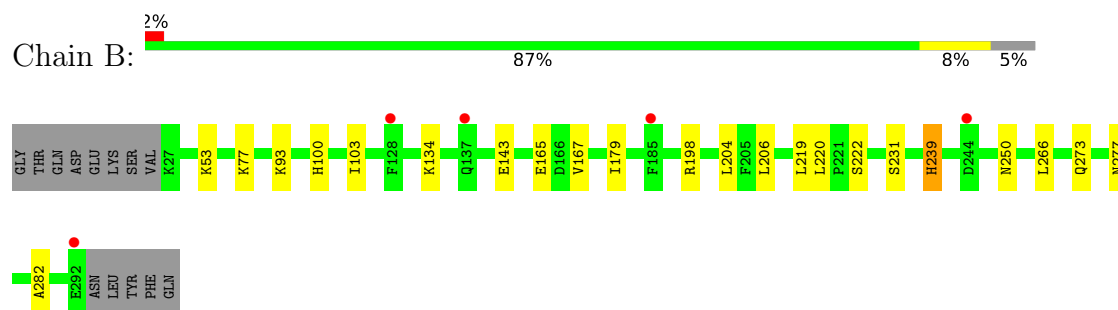
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	155	Total 155	O 155	0	0
8	D	162	Total 162	O 162	0	0
8	C	101	Total 101	O 101	0	0
8	A	93	Total 93	O 93	0	0



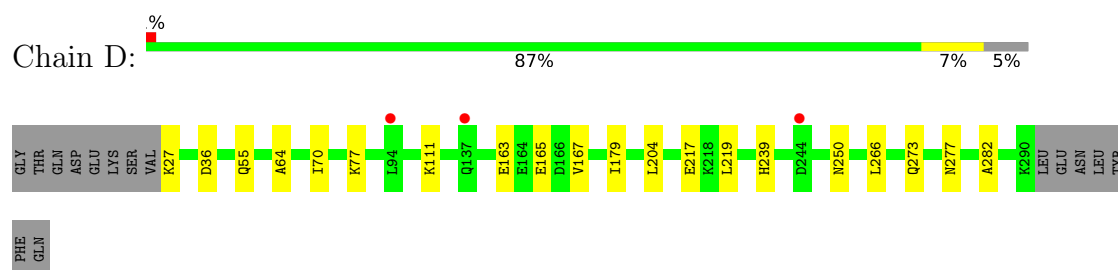
### 3 Residue-property plots [i](#)

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.

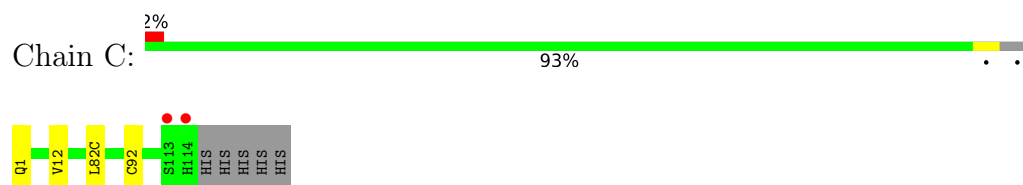
- Molecule 1: Cysteine-rich small secreted protein CSS, putative



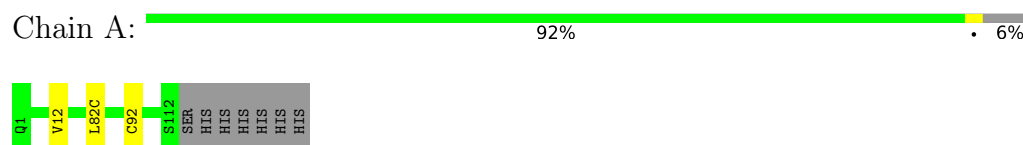
- Molecule 1: Cysteine-rich small secreted protein CSS, putative



- Molecule 2: H2 Nanobody



- Molecule 2: H2 Nanobody



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

Chain E:  50% 50%

HA01  
HA02

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

Chain F:  100%

HA01  
HA02

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

Chain G:  100%

HA01  
HA02

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

Chain I:  100%

HA01  
HA02

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

Chain H:  100%

HA01  
HA02  
BHA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.97Å 190.43Å 56.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.75 – 2.03 48.99 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.75-2.03) 93.6 (48.99-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.185 , 0.217 0.184 , 0.215	Depositor DCC
$R_{free}$ test set	2000 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4979e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, BMA, EDO, MLI, CSD

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	B	0.26	0/2253	0.48	1/3037 (0.0%)
1	D	0.26	0/2238	0.47	0/3018
2	A	0.27	0/894	0.53	0/1211
2	C	0.26	0/911	0.52	0/1234
All	All	0.26	0/6296	0.49	1/8500 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CB-CG-CD2	-6.24	100.40	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2208	0	2198	14	0
1	D	2182	0	2176	9	0
2	A	880	0	847	1	0
2	C	896	0	859	2	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	0	0
3	I	28	0	25	0	0
4	H	39	0	34	0	0
5	B	28	0	26	0	0
5	D	42	0	39	0	0
6	B	7	0	2	1	0
6	D	7	0	2	0	0
7	A	12	0	18	0	0
7	B	20	0	30	2	0
7	D	4	0	6	0	0
8	A	93	0	0	0	0
8	B	155	0	0	0	0
8	C	101	0	0	1	0
8	D	162	0	0	1	0
All	All	6948	0	6337	25	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 2.

All (25) 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:D:77:LYS:NZ	8:D:401:HOH:O	2.32	0.63
1:B:231:SER:HG	7:B:304:EDO:HO1	1.47	0.59
1:B:167:VAL:HG21	1:B:206:LEU:HD13	1.85	0.58
1:B:134:LYS:HG2	1:B:143[B]:GLU:HG2	1.86	0.58
1:D:36:ASP:OD2	1:D:111:LYS:HE3	2.07	0.55
1:B:219:LEU:HG	1:B:266:LEU:HB3	1.91	0.52
1:B:165:GLU:HB2	1:B:167:VAL:HG12	1.92	0.52
1:B:93:LYS:HE2	1:B:100:HIS:HA	1.92	0.52
1:D:165[B]:GLU:HB2	1:D:167:VAL:HG22	1.93	0.51
1:D:273:GLN:HB3	1:D:277:ASN:HB2	1.93	0.49
1:B:231:SER:OG	7:B:304:EDO:O1	2.25	0.48
1:B:179:ILE:HG21	1:B:282:ALA:HB2	1.96	0.47
2:A:12:VAL:HG11	2:A:82(C):LEU:HD13	1.95	0.47
2:C:12:VAL:HG11	2:C:82(C):LEU:HD13	1.98	0.46
1:B:77:LYS:HB2	1:B:77:LYS:HE3	1.61	0.46
1:B:204:LEU:HD11	1:B:250:ASN:HB3	1.96	0.46
1:B:273:GLN:HB3	1:B:277:ASN:HB2	1.98	0.45
2:C:1:GLN:N	8:C:201:HOH:O	2.45	0.45
1:D:179:ILE:HG21	1:D:282:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HG	1:D:266:LEU:HB3	1.98	0.43
1:D:64:ALA:HB3	1:D:70:ILE:HD11	2.01	0.42
1:B:103:ILE:HB	3:E:1:NAG:H62	2.02	0.42
1:D:204:LEU:HD11	1:D:250:ASN:HB3	2.02	0.42
1:B:53:LYS:H	6:B:303:MLI:H12	1.85	0.41
1:B:239[A]:HIS:CE1	1:D:217:GLU:HB3	2.56	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/279 (96%)	261 (97%)	8 (3%)	0	100	100
1	D	268/279 (96%)	262 (98%)	6 (2%)	0	100	100
2	A	117/126 (93%)	117 (100%)	0	0	100	100
2	C	119/126 (94%)	119 (100%)	0	0	100	100
All	All	773/810 (95%)	759 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	255/261 (98%)	250 (98%)	5 (2%)	55	57
1	D	253/261 (97%)	249 (98%)	4 (2%)	62	66
2	A	93/100 (93%)	92 (99%)	1 (1%)	73	77
2	C	95/100 (95%)	94 (99%)	1 (1%)	73	77
All	All	696/722 (96%)	685 (98%)	11 (2%)	69	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	198[A]	ARG
1	B	198[B]	ARG
1	B	222	SER
1	B	239[A]	HIS
1	B	239[B]	HIS
1	D	27	LYS
1	D	55	GLN
1	D	163	GLU
1	D	239	HIS
2	C	92	CYS
2	A	92	CYS

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

Mol	Chain	Res	Type
1	B	55	GLN
1	B	153	HIS
1	B	241	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSD	D	30	1	3,7,8	0.89	0	1,8,10	0.08	0
1	CSD	B	30	1	3,7,8	0.90	0	1,8,10	0.11	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
1	CSD	D	30	1	-	2/2/6/8	-
1	CSD	B	30	1	-	2/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	30	CSD	CA-CB-SG-OD1
1	D	30	CSD	CA-CB-SG-OD1
1	B	30	CSD	N-CA-CB-SG
1	D	30	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	F	1	3,1	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	G	1	3,1	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	H	1	4,1	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	H	2	4	14,14,15	0.25	0	17,19,21	0.44	0
4	BMA	H	3	4	11,11,12	0.66	0	15,15,17	0.79	0
3	NAG	I	1	3,1	14,14,15	0.37	0	17,19,21	0.51	0
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.40	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6

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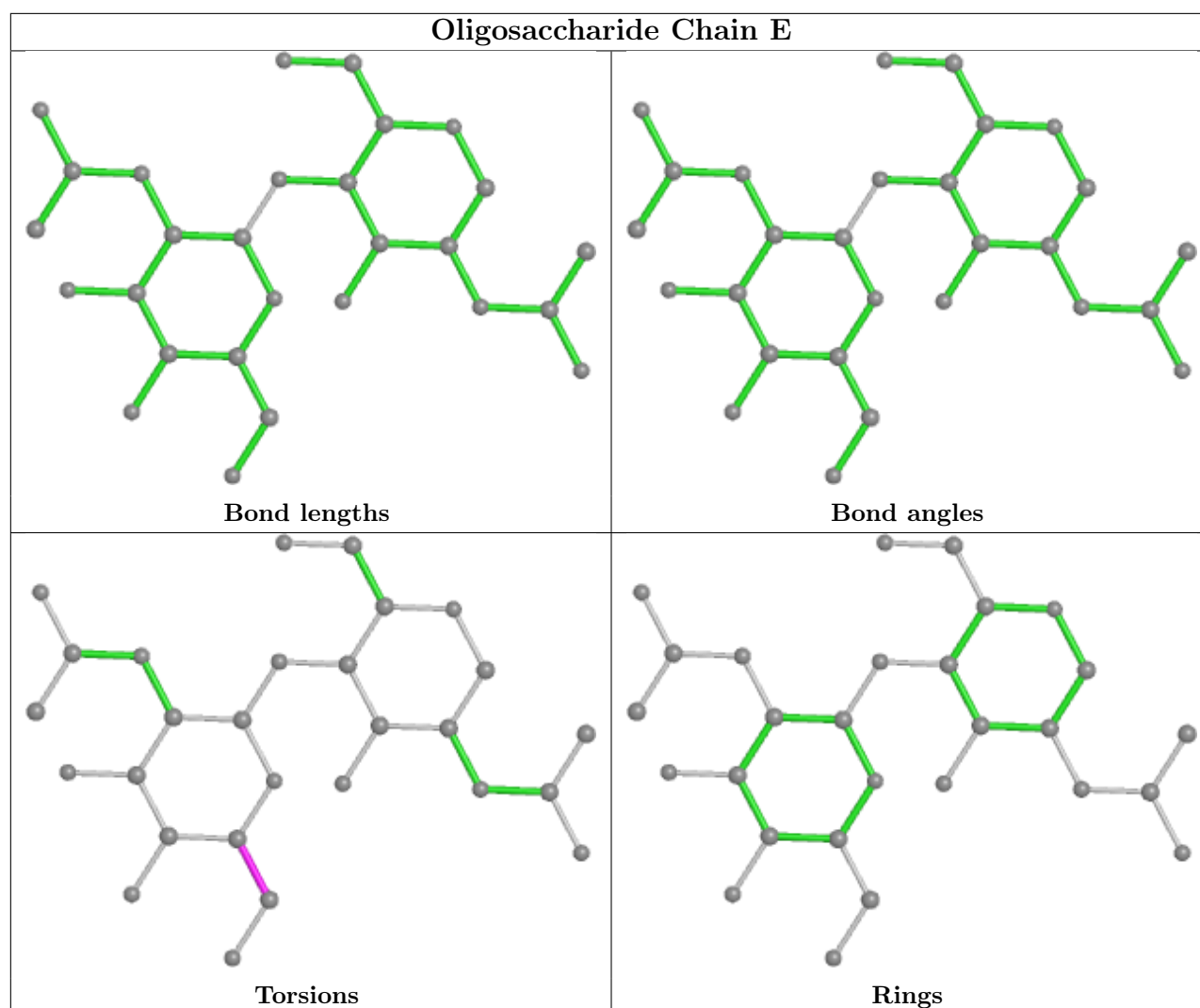
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6

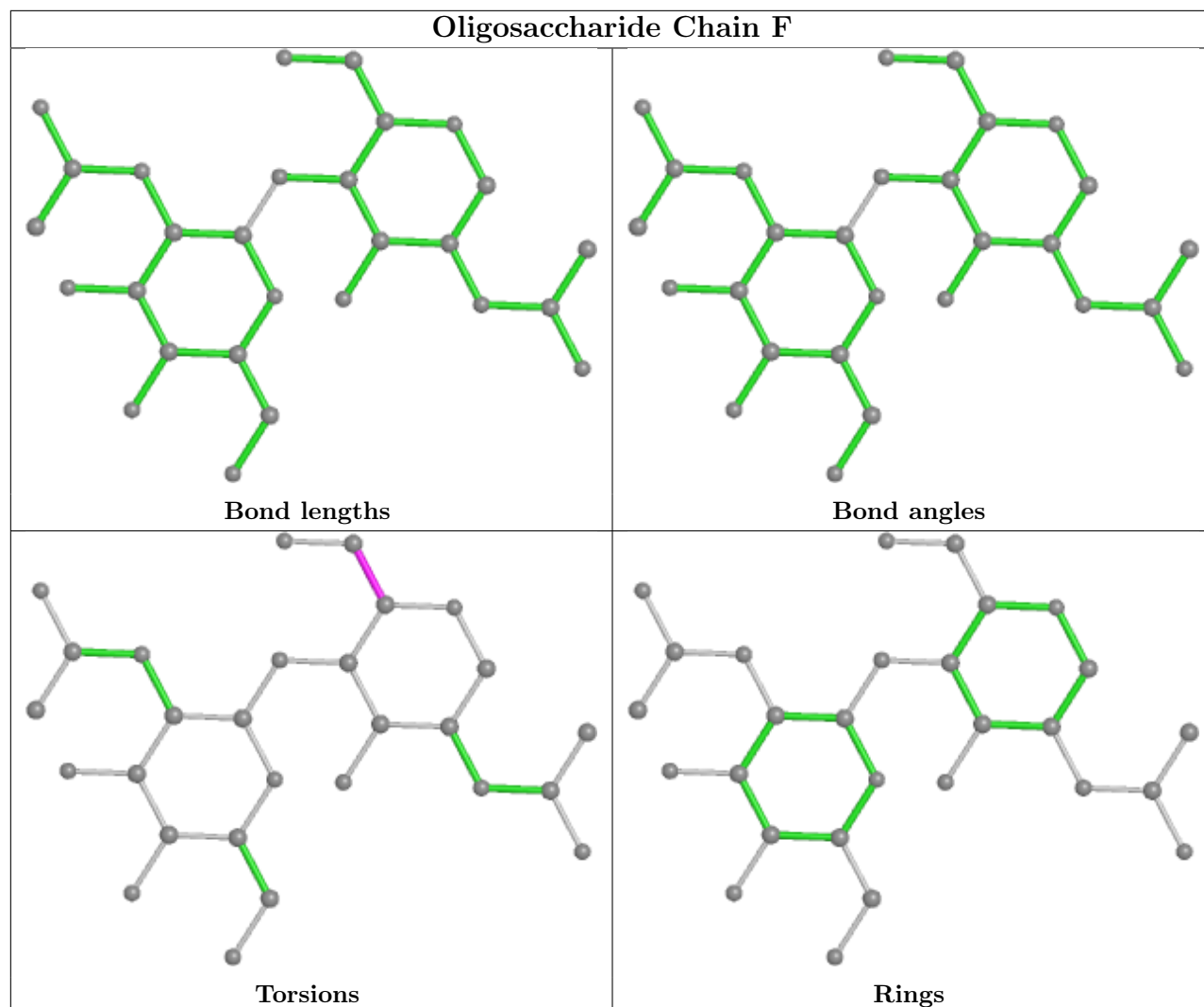
There are no ring outliers.

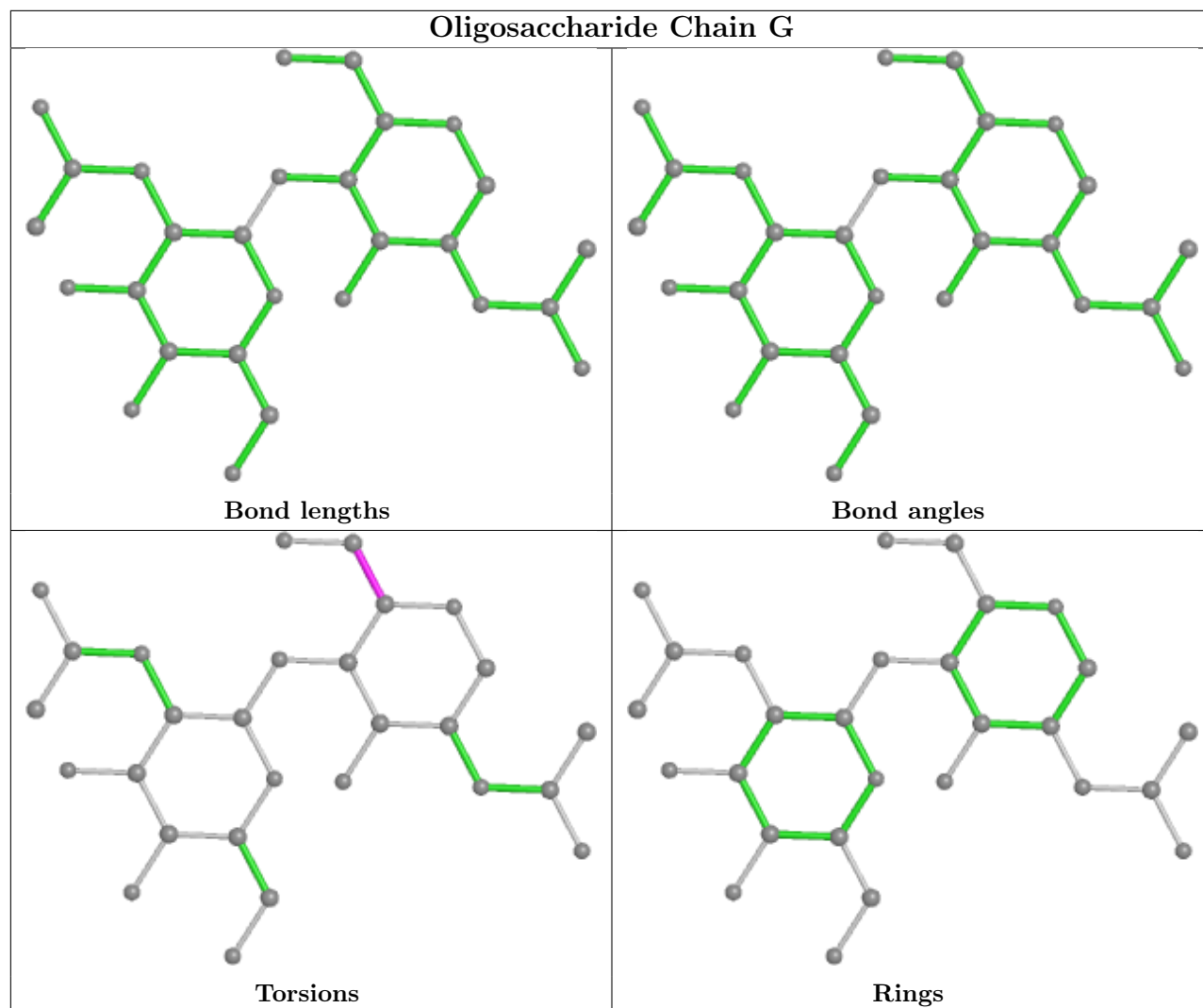
1 monomer is involved in 1 short contact:

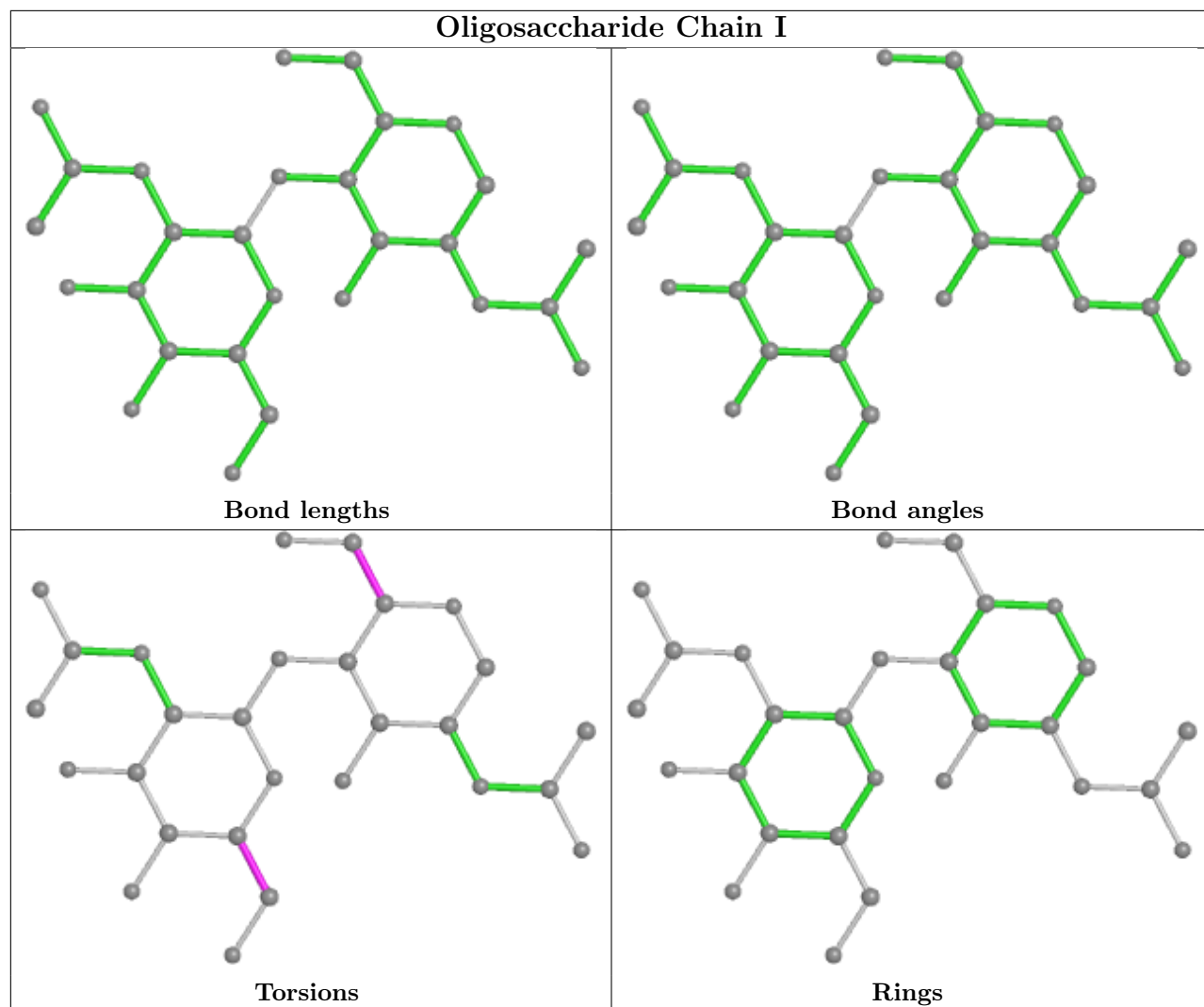
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0

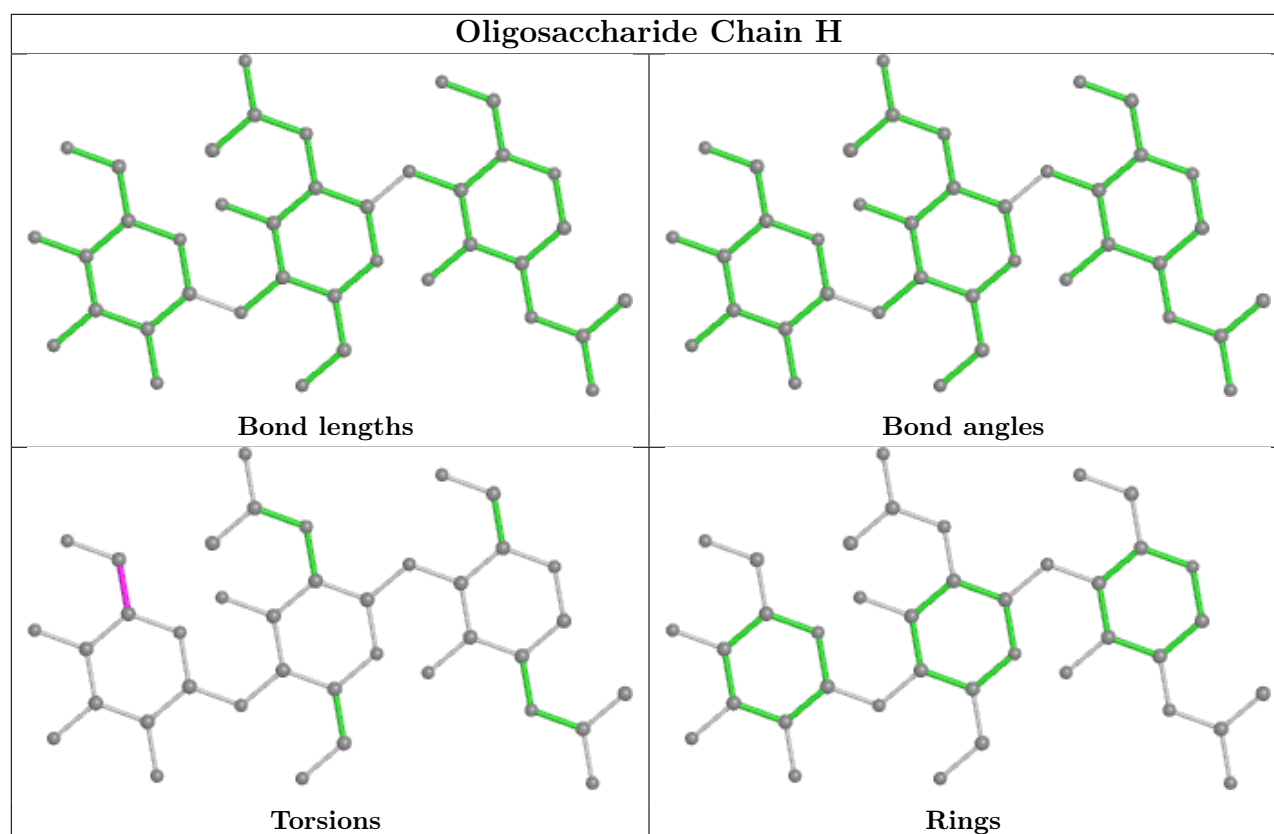
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

16 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	$\# Z  > 2$
7	EDO	A	201	-	3,3,3	0.46	0	2,2,2	0.34	0
6	MLI	B	303	-	6,6,6	1.31	0	7,7,7	1.27	0
7	EDO	A	203	-	3,3,3	0.45	0	2,2,2	0.41	0
5	NAG	D	301	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	D	302	1	14,14,15	0.28	0	17,19,21	0.39	0
7	EDO	A	202	-	3,3,3	0.43	0	2,2,2	0.39	0
7	EDO	B	304	-	3,3,3	0.44	0	2,2,2	0.34	0
5	NAG	D	304	1	14,14,15	0.20	0	17,19,21	0.33	0
7	EDO	B	308	-	3,3,3	0.48	0	2,2,2	0.30	0
5	NAG	B	302	1	14,14,15	0.17	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	B	305	-	3,3,3	0.47	0	2,2,2	0.34	0
7	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.33	0
5	NAG	B	301	1	14,14,15	0.19	0	17,19,21	0.54	0
6	MLI	D	303	-	6,6,6	1.29	0	7,7,7	1.23	0
7	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.32	0
7	EDO	D	305	-	3,3,3	0.44	0	2,2,2	0.38	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
7	EDO	A	201	-	-	0/1/1/1	-
6	MLI	B	303	-	-	0/4/4/4	-
7	EDO	A	203	-	-	0/1/1/1	-
5	NAG	D	301	1	-	2/6/23/26	0/1/1/1
5	NAG	D	302	1	-	2/6/23/26	0/1/1/1
7	EDO	A	202	-	-	0/1/1/1	-
7	EDO	B	304	-	-	0/1/1/1	-
5	NAG	D	304	1	-	2/6/23/26	0/1/1/1
7	EDO	B	308	-	-	1/1/1/1	-
5	NAG	B	302	1	-	0/6/23/26	0/1/1/1
7	EDO	B	305	-	-	0/1/1/1	-
7	EDO	B	307	-	-	0/1/1/1	-
5	NAG	B	301	1	-	3/6/23/26	0/1/1/1
6	MLI	D	303	-	-	0/4/4/4	-
7	EDO	B	306	-	-	0/1/1/1	-
7	EDO	D	305	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	301	NAG	C4-C5-C6-O6
5	D	301	NAG	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	D	304	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	302	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	D	302	NAG	O5-C5-C6-O6
7	B	308	EDO	O1-C1-C2-O2
7	D	305	EDO	O1-C1-C2-O2
5	D	304	NAG	C4-C5-C6-O6
5	B	301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	MLI	1	0
7	B	304	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	265/279 (94%)	0.30	5 (1%) 66 66	26, 45, 77, 109	0
1	D	263/279 (94%)	0.24	3 (1%) 80 80	26, 43, 71, 114	0
2	A	119/126 (94%)	0.19	0 100 100	26, 43, 68, 80	0
2	C	121/126 (96%)	0.27	2 (1%) 70 69	27, 40, 58, 116	0
All	All	768/810 (94%)	0.26	10 (1%) 77 76	26, 43, 73, 116	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	PHE	2.8
1	B	137	GLN	2.4
1	B	244	ASP	2.2
1	D	137	GLN	2.2
2	C	113	SER	2.2
1	B	292	GLU	2.1
2	C	114	HIS	2.1
1	B	185	PHE	2.1
1	D	244	ASP	2.0
1	D	94	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

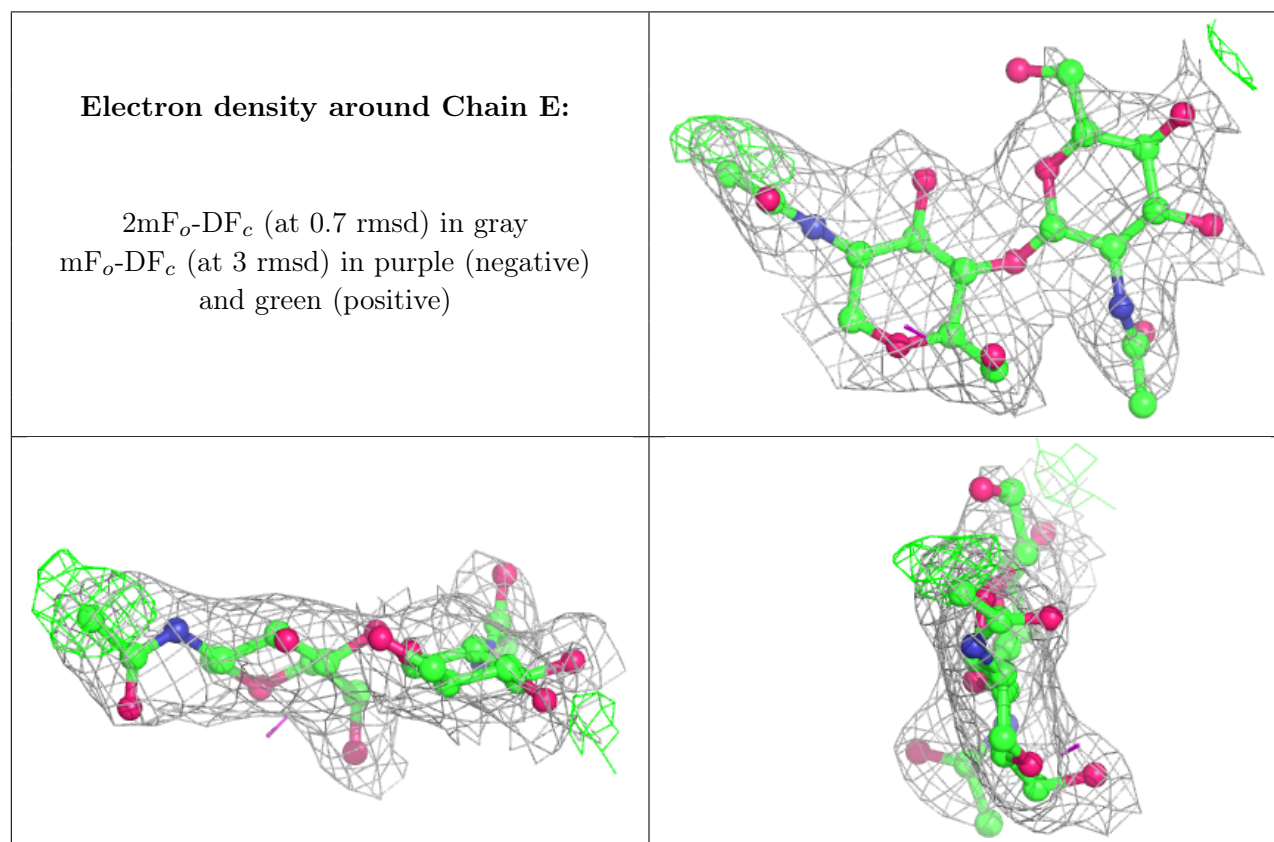
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	D	30	8/9	0.93	0.12	47,49,62,69	0
1	CSD	B	30	8/9	0.96	0.11	48,57,62,73	0

### 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, 95<sup>th</sup> 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.

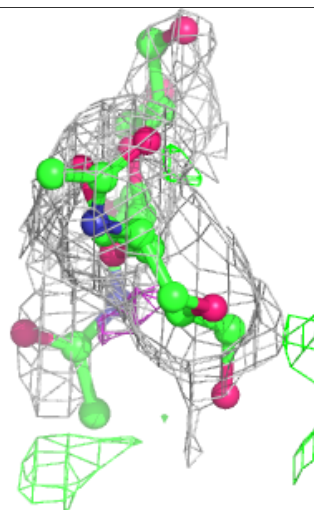
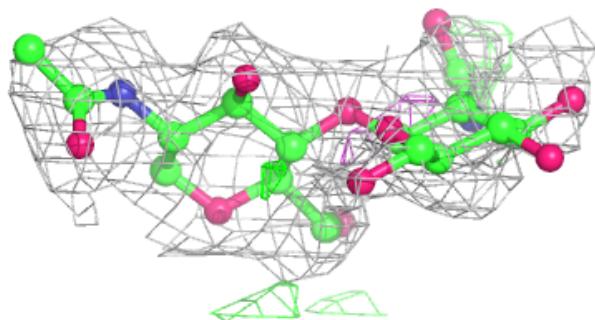
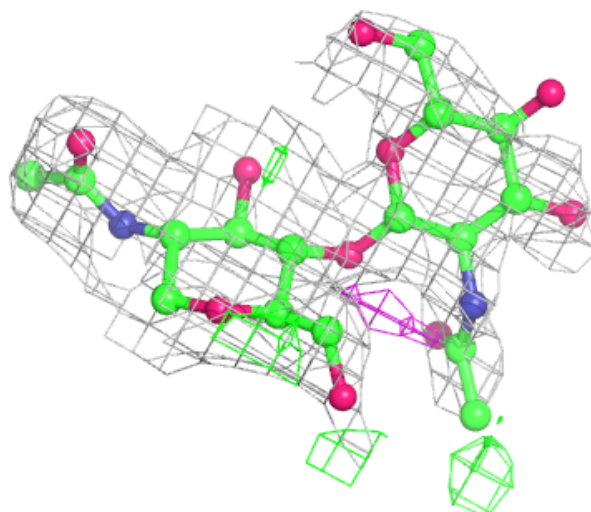
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	H	3	11/12	0.67	0.20	80,91,95,96	0
3	NAG	G	1	14/15	0.68	0.30	64,72,82,89	0
3	NAG	G	2	14/15	0.71	0.29	65,92,96,98	0
3	NAG	I	2	14/15	0.74	0.27	68,93,104,107	0
3	NAG	F	2	14/15	0.74	0.35	81,98,106,107	0
3	NAG	E	2	14/15	0.84	0.27	81,91,101,102	0
4	NAG	H	2	14/15	0.85	0.16	69,75,80,84	0
3	NAG	F	1	14/15	0.86	0.13	68,75,85,92	0
3	NAG	I	1	14/15	0.87	0.20	47,65,78,81	0
3	NAG	E	1	14/15	0.89	0.14	57,65,74,87	0
4	NAG	H	1	14/15	0.91	0.11	52,61,65,74	0

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



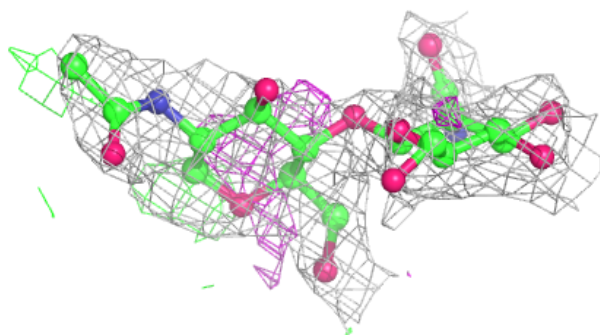
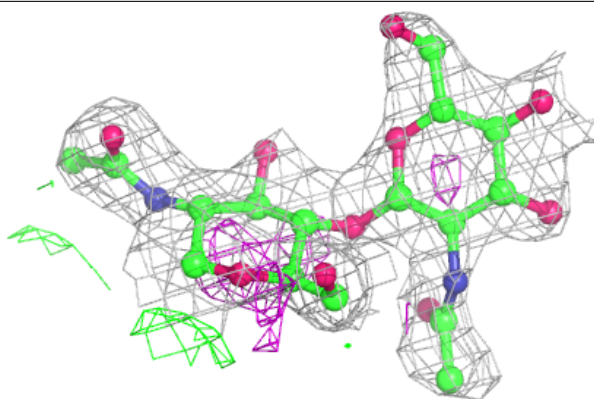
**Electron density around Chain F:**

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

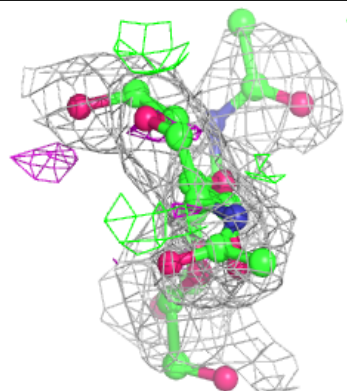
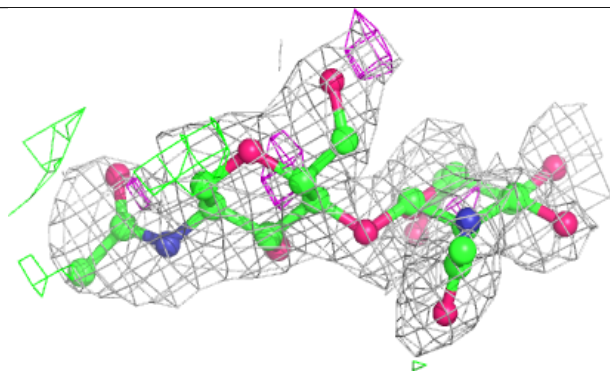
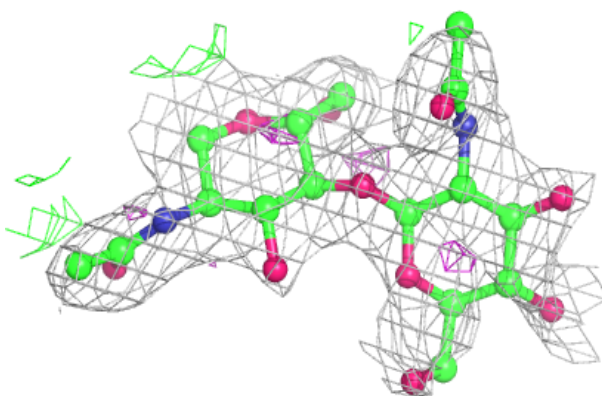


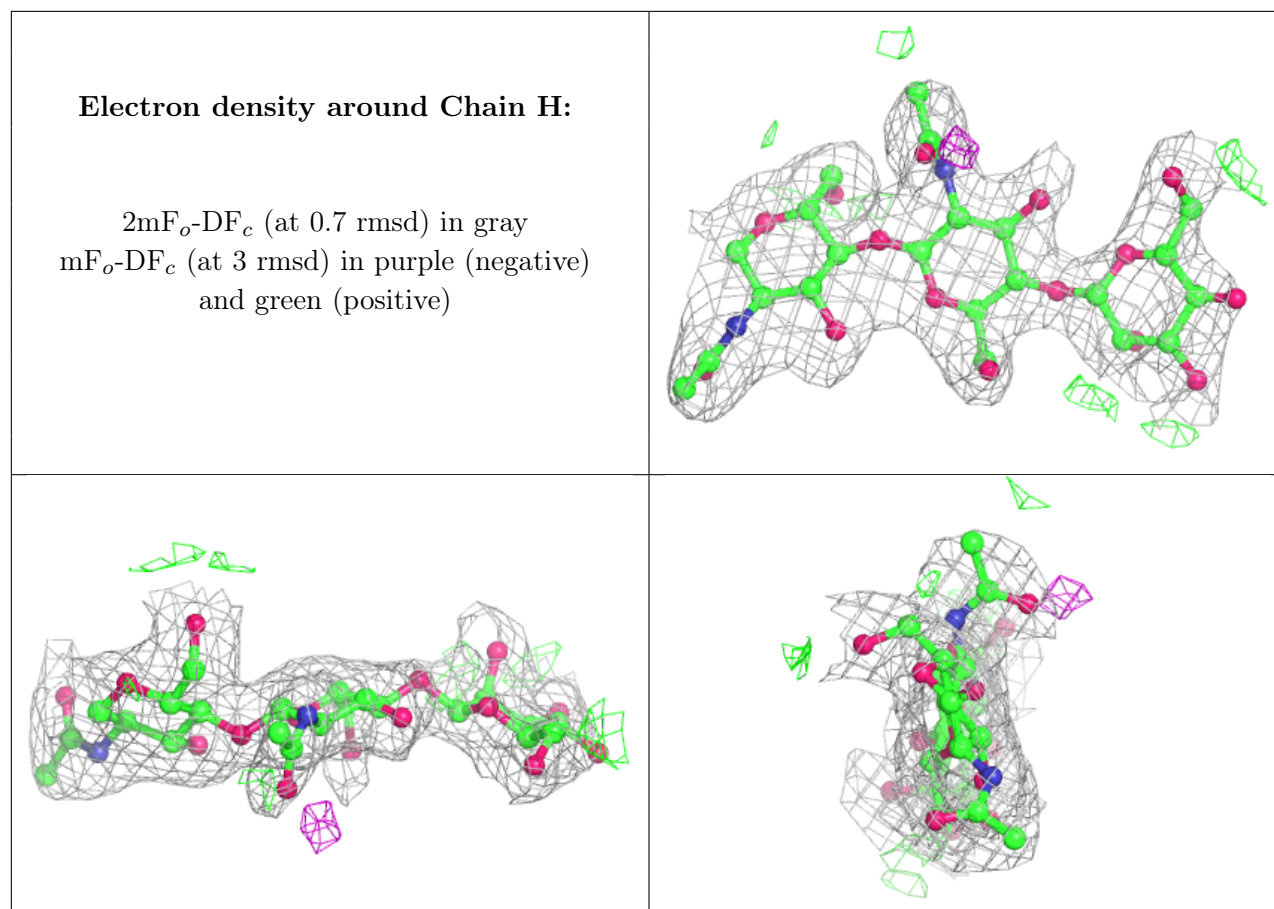
**Electron density around Chain G:**

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

**Electron density around Chain I:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	EDO	A	203	4/4	0.60	0.30	58,61,62,62	0
7	EDO	B	308	4/4	0.61	0.21	70,75,76,79	0
5	NAG	D	304	14/15	0.69	0.35	54,78,91,92	0
7	EDO	B	306	4/4	0.72	0.47	70,74,76,78	0
7	EDO	A	201	4/4	0.75	0.14	57,63,68,73	0
5	NAG	D	302	14/15	0.76	0.23	68,75,83,85	0
5	NAG	B	301	14/15	0.79	0.52	112,118,125,127	0
5	NAG	D	301	14/15	0.79	0.41	82,101,108,111	0
5	NAG	B	302	14/15	0.80	0.17	31,40,55,62	14
6	MLI	B	303	7/7	0.80	0.21	50,70,76,77	0
7	EDO	B	307	4/4	0.87	0.30	57,63,67,70	0
6	MLI	D	303	7/7	0.88	0.12	52,56,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	D	305	4/4	0.88	0.16	61,63,68,77	0
7	EDO	B	304	4/4	0.91	0.35	52,53,54,58	0
7	EDO	B	305	4/4	0.91	0.28	43,43,49,55	0
7	EDO	A	202	4/4	0.94	0.08	72,74,78,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.