



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 10:27 PM EDT

PDB ID : 6TWS  
Title : Crystal structure of the haemagglutinin mutant (Gln226Leu, Gly228Ser) from an H10N7 seal influenza virus isolated in Germany with 2mM EDTA  
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.  
Deposited on : 2020-01-13  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	2.37.1
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)	:	2.37.1

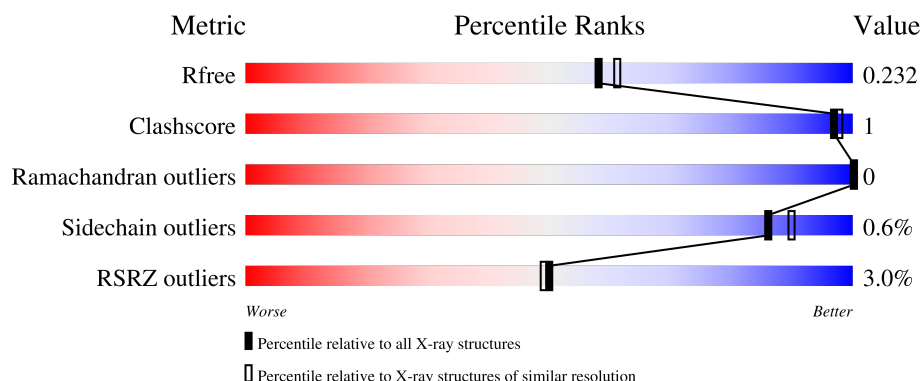
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	325	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div>
1	C	325	<div> <div></div> <div>97%</div> <div></div> </div> <div>..</div>
1	G	325	<div> <div>11%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div>..</div> </div>
2	B	177	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div>.</div> </div>
2	D	177	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	177	<div><div></div><div>94%</div><div></div></div>
3	E	2	<div><div></div><div>100%</div><div></div></div>
3	F	2	<div><div></div><div>100%</div><div></div></div>
3	I	2	<div><div></div><div>100%</div><div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12800 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	320	Total	C	N	O	S	0	0	0
			2439	1513	442	468	16			
1	A	320	Total	C	N	O	S	0	1	0
			2455	1522	445	472	16			
1	C	320	Total	C	N	O	S	0	0	0
			2447	1518	443	470	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
G	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	221	SER	GLY	engineered mutation	UNP A0A0A7HR51

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			

There are 3 discrepancies between the modelled and reference sequences:

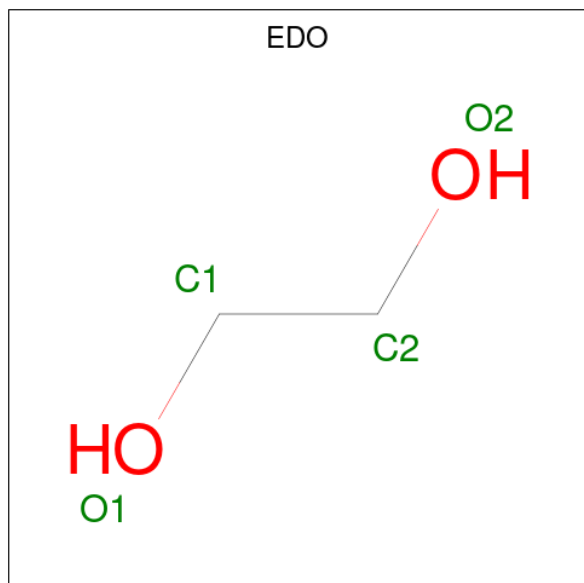
Chain	Residue	Modelled	Actual	Comment	Reference
H	177	LYS	-	expression tag	UNP A0A0A7HR51
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51

- 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	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	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	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

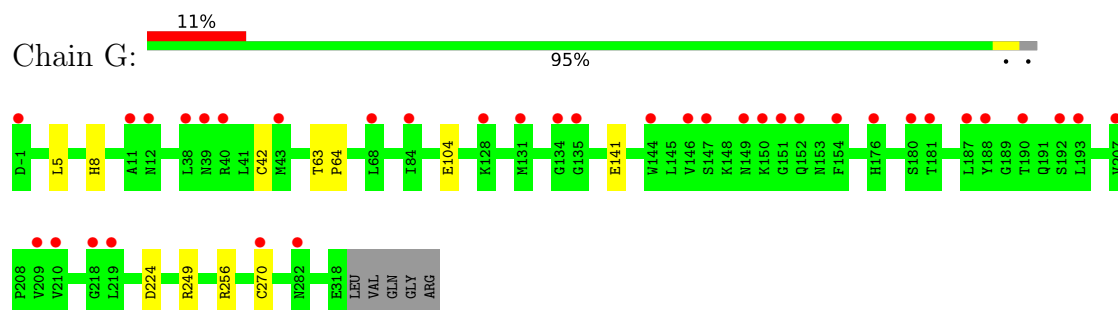
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	135	Total	O	0	0
			135	135		
6	H	137	Total	O	0	0
			137	137		
6	A	243	Total	O	0	0
			243	243		
6	B	179	Total	O	0	0
			179	179		
6	C	262	Total	O	0	0
			262	262		
6	D	145	Total	O	0	0
			145	145		

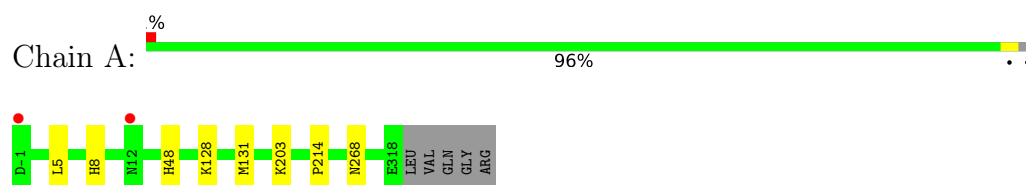
### 3 Residue-property plots [i](#)

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.

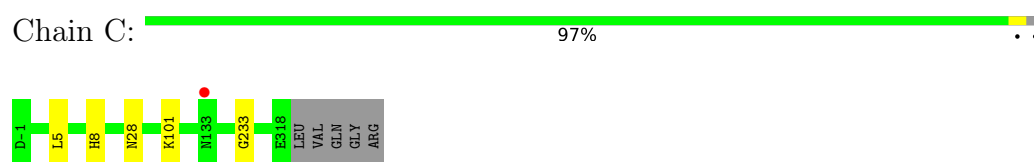
- Molecule 1: Hemagglutinin



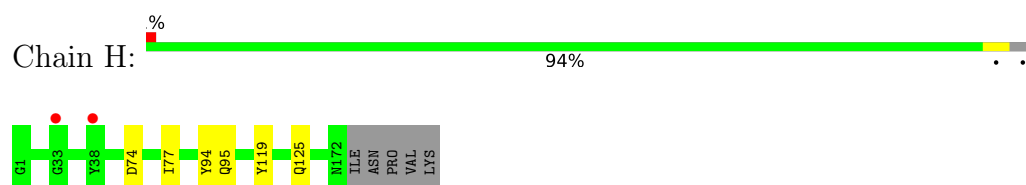
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin HA2



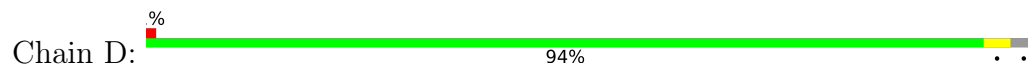
- Molecule 2: Hemagglutinin HA2







• Molecule 2: Hemagglutinin HA2



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.15Å 215.60Å 72.87Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	61.41 – 2.00 61.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (61.41-2.00) 98.8 (61.41-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.209 , 0.231 0.210 , 0.232	Depositor DCC
$R_{free}$ test set	6523 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.975	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.9	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	0.95	EDS
Total number of atoms	12800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.64	0/2505	0.71	0/3394
1	C	0.63	0/2497	0.72	0/3383
1	G	0.65	0/2489	0.72	0/3374
2	B	0.64	0/1411	0.68	0/1903
2	D	0.64	0/1411	0.68	0/1903
2	H	0.65	0/1411	0.68	0/1903
All	All	0.64	0/11724	0.70	0/15860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2455	0	2415	5	0
1	C	2447	0	2409	3	0
1	G	2439	0	2397	6	0
2	B	1386	0	1290	6	0
2	D	1386	0	1291	5	0
2	H	1386	0	1291	4	0
3	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	0	0
3	I	28	0	25	0	0
4	A	20	0	30	0	0
4	B	8	0	12	0	0
4	C	36	0	54	0	0
4	D	8	0	12	0	0
4	G	12	0	18	0	0
4	H	4	0	6	0	0
5	B	14	0	13	0	0
5	C	14	0	13	1	0
6	A	243	0	0	0	0
6	B	179	0	0	0	0
6	C	262	0	0	0	0
6	D	145	0	0	0	0
6	G	135	0	0	0	0
6	H	137	0	0	0	0
All	All	12800	0	11326	20	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 1.

All (20) 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)
2:H:94:TYR:OH	2:B:99:LEU:HD22	1.99	0.63
1:C:28:ASN:HD22	5:C:401:NAG:H83	1.68	0.59
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.07	0.53
2:H:95:GLN:HE22	2:D:91:ILE:HG23	1.75	0.51
2:B:94:TYR:OH	2:D:99:LEU:HD22	2.10	0.50
1:A:214:PRO:HG3	1:C:233:GLY:O	2.11	0.50
1:A:5:LEU:HD22	2:B:119:TYR:HA	1.92	0.50
1:A:128:LYS:O	1:A:131:MET:HG2	2.13	0.49
1:G:104:GLU:OE2	2:D:79:ASN:ND2	2.40	0.48
1:C:5:LEU:HD22	2:D:119:TYR:HA	1.95	0.48
1:G:42:CYS:CB	1:G:270:CYS:HG	2.22	0.48
1:G:5:LEU:HD22	2:H:119:TYR:HA	1.98	0.45
2:H:74:ASP:HB3	2:H:77:ILE:HG22	1.99	0.45
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.51	0.45
1:A:48:HIS:HE1	1:A:268:ASN:HD21	1.64	0.44
1:G:63:THR:HG22	1:G:64:PRO:HD2	2.00	0.43
1:G:224:ASP:OD2	1:A:203:LYS:NZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASP:HB3	2:B:77:ILE:HG22	2.01	0.43
2:B:20:GLY:HA3	2:B:36:ALA:HB1	2.00	0.42
2:D:2:LEU:HD23	2:D:2:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/325 (98%)	313 (98%)	6 (2%)	0	100	100
1	C	318/325 (98%)	313 (98%)	5 (2%)	0	100	100
1	G	318/325 (98%)	310 (98%)	8 (2%)	0	100	100
2	B	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
2	D	170/177 (96%)	163 (96%)	7 (4%)	0	100	100
2	H	170/177 (96%)	167 (98%)	3 (2%)	0	100	100
All	All	1465/1506 (97%)	1432 (98%)	33 (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	A	273/276 (99%)	272 (100%)	1 (0%)	91	93
1	C	272/276 (99%)	270 (99%)	2 (1%)	84	88
1	G	270/276 (98%)	268 (99%)	2 (1%)	84	88
2	B	146/151 (97%)	146 (100%)	0	100	100
2	D	146/151 (97%)	145 (99%)	1 (1%)	84	88
2	H	146/151 (97%)	145 (99%)	1 (1%)	84	88
All	All	1253/1281 (98%)	1246 (99%)	7 (1%)	86	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	8	HIS
1	G	256	ARG
2	H	125	GLN
1	A	8	HIS
1	C	8	HIS
1	C	101	LYS
2	D	75	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	205	ASN
1	G	215	GLN
1	G	226	HIS
1	G	303	ASN
2	H	95	GLN
2	H	154	ASN
2	H	161	GLN
1	A	226	HIS
1	A	268	ASN
2	B	95	GLN
2	B	161	GLN

### 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 ⓘ

6 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	3,2	14,14,15	0.30	0	17,19,21	0.88	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.72	0
3	NAG	F	1	3,2	14,14,15	0.31	0	17,19,21	0.78	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	I	1	3,2	14,14,15	0.31	0	17,19,21	0.70	0
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.59	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	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	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.

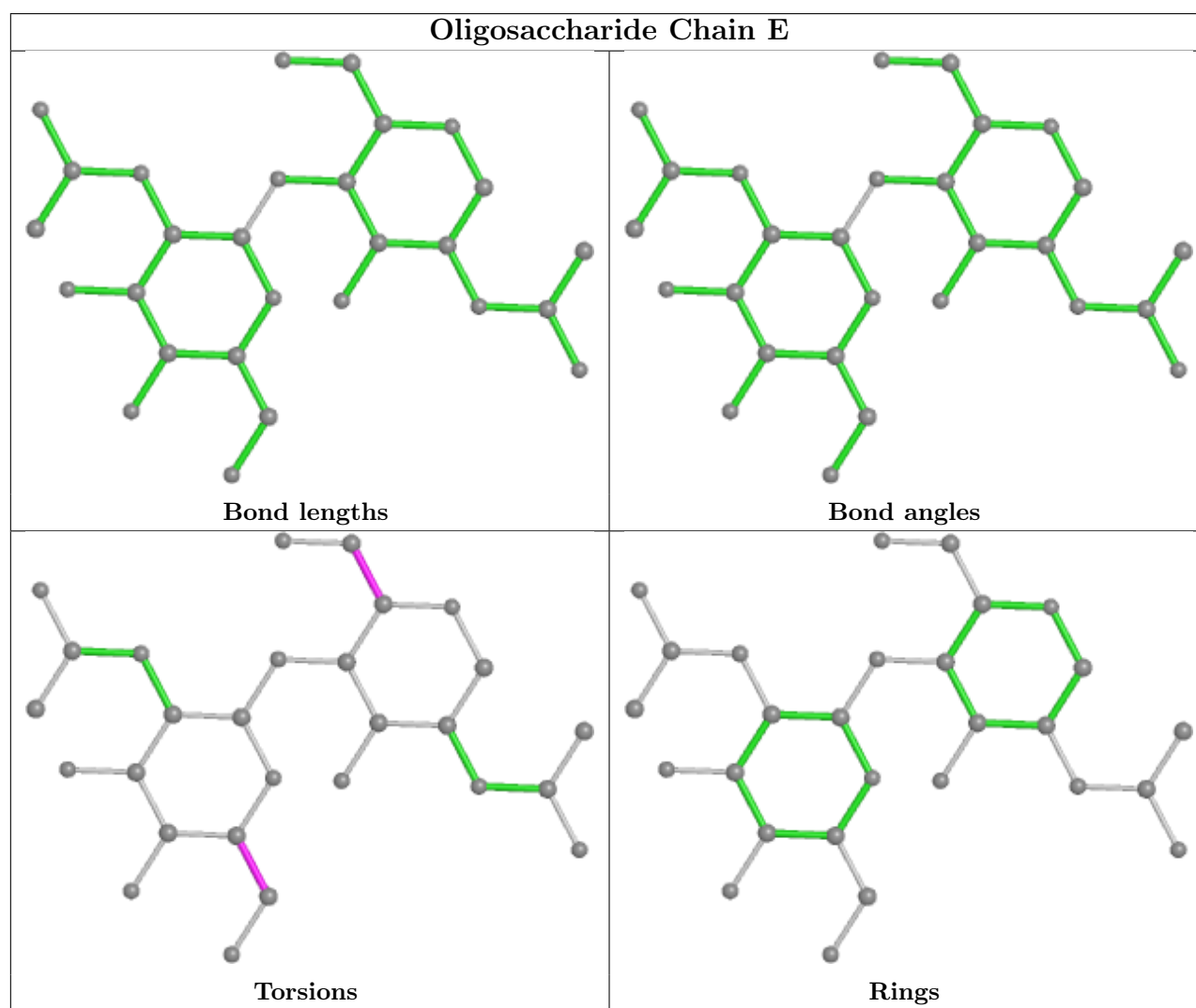
All (8) torsion outliers are listed below:

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

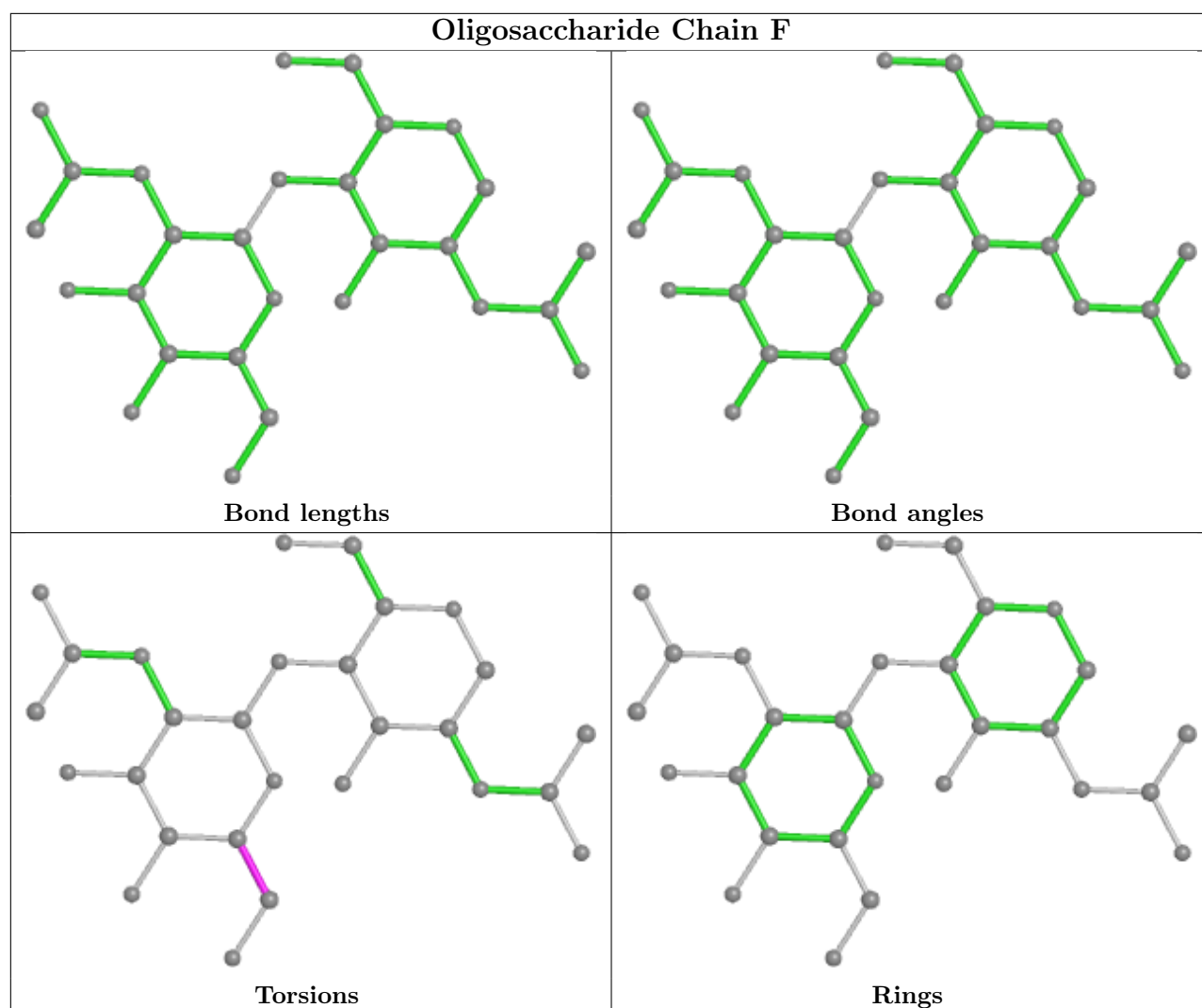
There are no ring outliers.

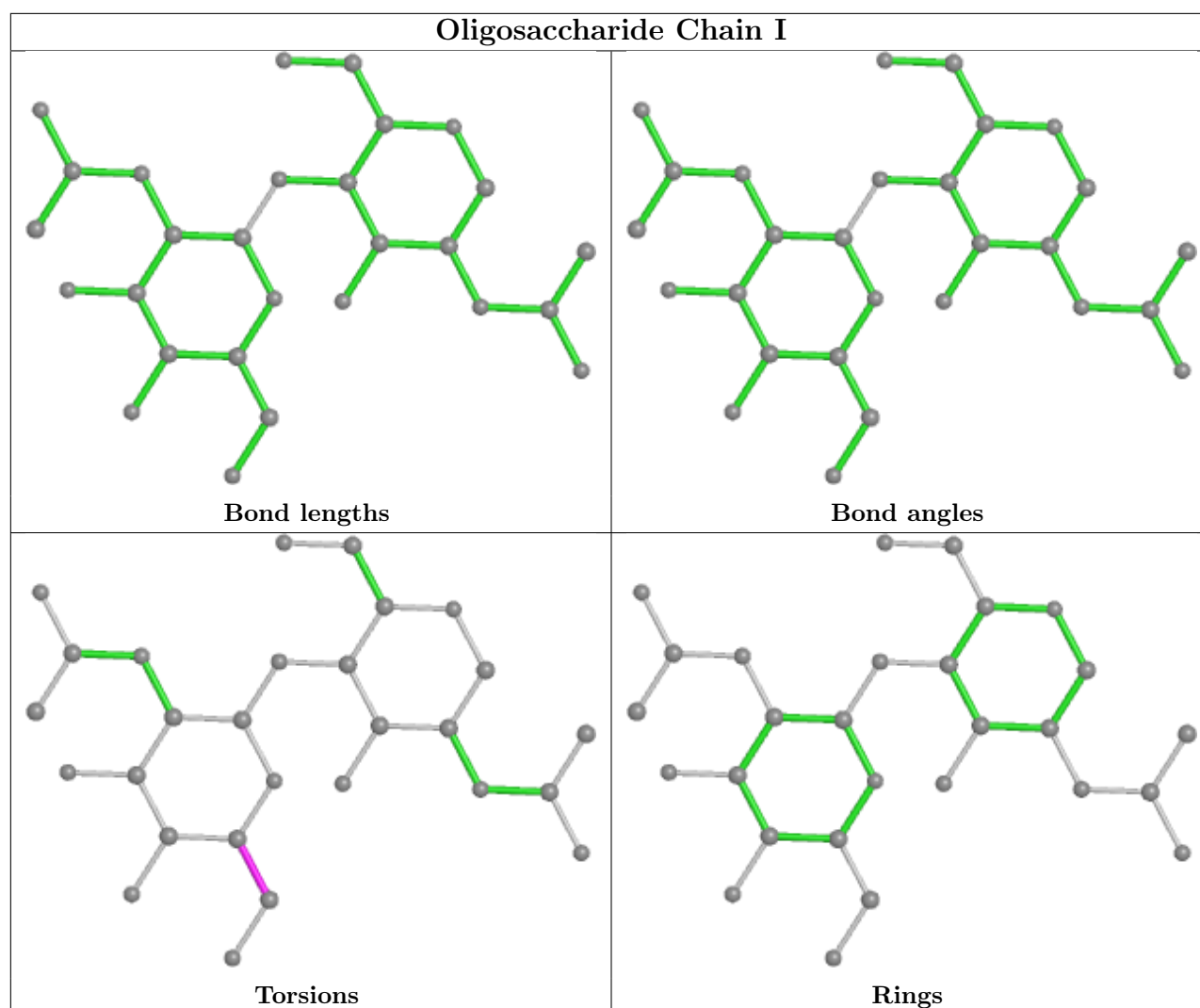
No monomer is involved in short contacts.

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









## 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
4	EDO	C	409	-	3,3,3	0.05	0	2,2,2	0.12	0
4	EDO	G	403	-	3,3,3	0.07	0	2,2,2	0.23	0
4	EDO	G	402	-	3,3,3	0.05	0	2,2,2	0.16	0
4	EDO	C	403	-	3,3,3	0.07	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	408	-	3,3,3	0.16	0	2,2,2	0.07	0
4	EDO	A	402	-	3,3,3	0.04	0	2,2,2	0.13	0
4	EDO	A	403	-	3,3,3	0.07	0	2,2,2	0.22	0
4	EDO	A	405	-	3,3,3	0.04	0	2,2,2	0.06	0
4	EDO	H	203	-	3,3,3	0.06	0	2,2,2	0.19	0
5	NAG	B	205	2	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
4	EDO	A	401	-	3,3,3	0.05	0	2,2,2	0.16	0
4	EDO	C	404	-	3,3,3	0.08	0	2,2,2	0.26	0
4	EDO	C	402	-	3,3,3	0.11	0	2,2,2	0.58	0
4	EDO	B	203	-	3,3,3	0.08	0	2,2,2	0.17	0
4	EDO	D	203	-	3,3,3	0.08	0	2,2,2	0.18	0
4	EDO	B	204	-	3,3,3	0.10	0	2,2,2	0.44	0
4	EDO	C	406	-	3,3,3	0.09	0	2,2,2	0.21	0
5	NAG	C	401	1	14,14,15	0.29	0	17,19,21	1.58	3 (17%)
4	EDO	A	404	-	3,3,3	0.08	0	2,2,2	0.22	0
4	EDO	C	410	-	3,3,3	0.11	0	2,2,2	0.15	0
4	EDO	C	405	-	3,3,3	0.09	0	2,2,2	0.19	0
4	EDO	D	204	-	3,3,3	0.09	0	2,2,2	0.18	0
4	EDO	G	401	-	3,3,3	0.06	0	2,2,2	0.16	0
4	EDO	C	407	-	3,3,3	0.09	0	2,2,2	0.27	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
4	EDO	C	409	-	-	0/1/1/1	-
4	EDO	G	403	-	-	0/1/1/1	-
4	EDO	G	402	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	C	408	-	-	1/1/1/1	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	H	203	-	-	0/1/1/1	-
5	NAG	B	205	2	-	0/6/23/26	0/1/1/1
4	EDO	A	401	-	-	1/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	C	402	-	-	1/1/1/1	-
4	EDO	B	203	-	-	0/1/1/1	-
4	EDO	D	203	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	204	-	-	1/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	C	410	-	-	0/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	D	204	-	-	1/1/1/1	-
4	EDO	G	401	-	-	0/1/1/1	-
4	EDO	C	407	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	NAG	C1-O5-C5	4.22	117.91	112.19
5	C	401	NAG	C8-C7-N2	2.64	120.57	116.10
5	C	401	NAG	C2-N2-C7	2.35	126.26	122.90
5	B	205	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	NAG	C8-C7-N2-C2
5	C	401	NAG	O7-C7-N2-C2
4	B	204	EDO	O1-C1-C2-O2
4	C	407	EDO	O1-C1-C2-O2
4	A	401	EDO	O1-C1-C2-O2
4	C	408	EDO	O1-C1-C2-O2
4	D	204	EDO	O1-C1-C2-O2
4	C	402	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	NAG	1	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

### 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, 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	A	320/325 (98%)	-0.16	2 (0%) 89 88	25, 37, 53, 64	0
1	C	320/325 (98%)	-0.20	1 (0%) 94 93	24, 34, 55, 67	0
1	G	320/325 (98%)	0.59	36 (11%) 5 4	29, 48, 82, 101	0
2	B	172/177 (97%)	-0.20	2 (1%) 79 78	23, 32, 47, 78	0
2	D	172/177 (97%)	-0.23	1 (0%) 89 88	23, 35, 52, 86	0
2	H	172/177 (97%)	-0.02	2 (1%) 79 78	24, 38, 52, 71	0
All	All	1476/1506 (98%)	-0.00	44 (2%) 50 49	23, 37, 66, 101	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	149	ASN	5.5
1	G	180	SER	5.3
1	G	187	LEU	5.3
1	G	218	GLY	5.1
1	G	181	THR	5.1
1	G	134	GLY	5.1
1	G	210	VAL	4.8
1	G	190	THR	4.3
1	G	-1	ASP	4.0
1	G	146	VAL	3.9
1	G	152	GLN	3.8
1	G	39	ASN	3.6
1	G	193	LEU	3.6
1	G	135	GLY	3.6
2	D	171	LEU	3.3
1	G	209	VAL	3.2
1	G	40	ARG	3.0
1	G	188	TYR	3.0
1	G	128	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	154	PHE	2.9
1	G	192	SER	2.8
1	G	147	SER	2.7
1	G	282	ASN	2.6
1	G	150	LYS	2.6
2	H	33	GLY	2.4
1	A	12	ASN	2.4
1	G	207	VAL	2.4
1	G	144	TRP	2.4
2	B	172	ASN	2.3
1	G	176	HIS	2.3
2	H	38	TYR	2.3
1	G	11	ALA	2.3
1	G	43	MET	2.3
1	G	12	ASN	2.3
1	C	133	ASN	2.2
1	G	84	ILE	2.2
1	G	131	MET	2.2
1	G	38	LEU	2.2
1	G	68	LEU	2.2
2	B	171	LEU	2.1
1	G	219	LEU	2.0
1	G	270	CYS	2.0
1	G	151	GLY	2.0
1	A	-1	ASP	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, 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.

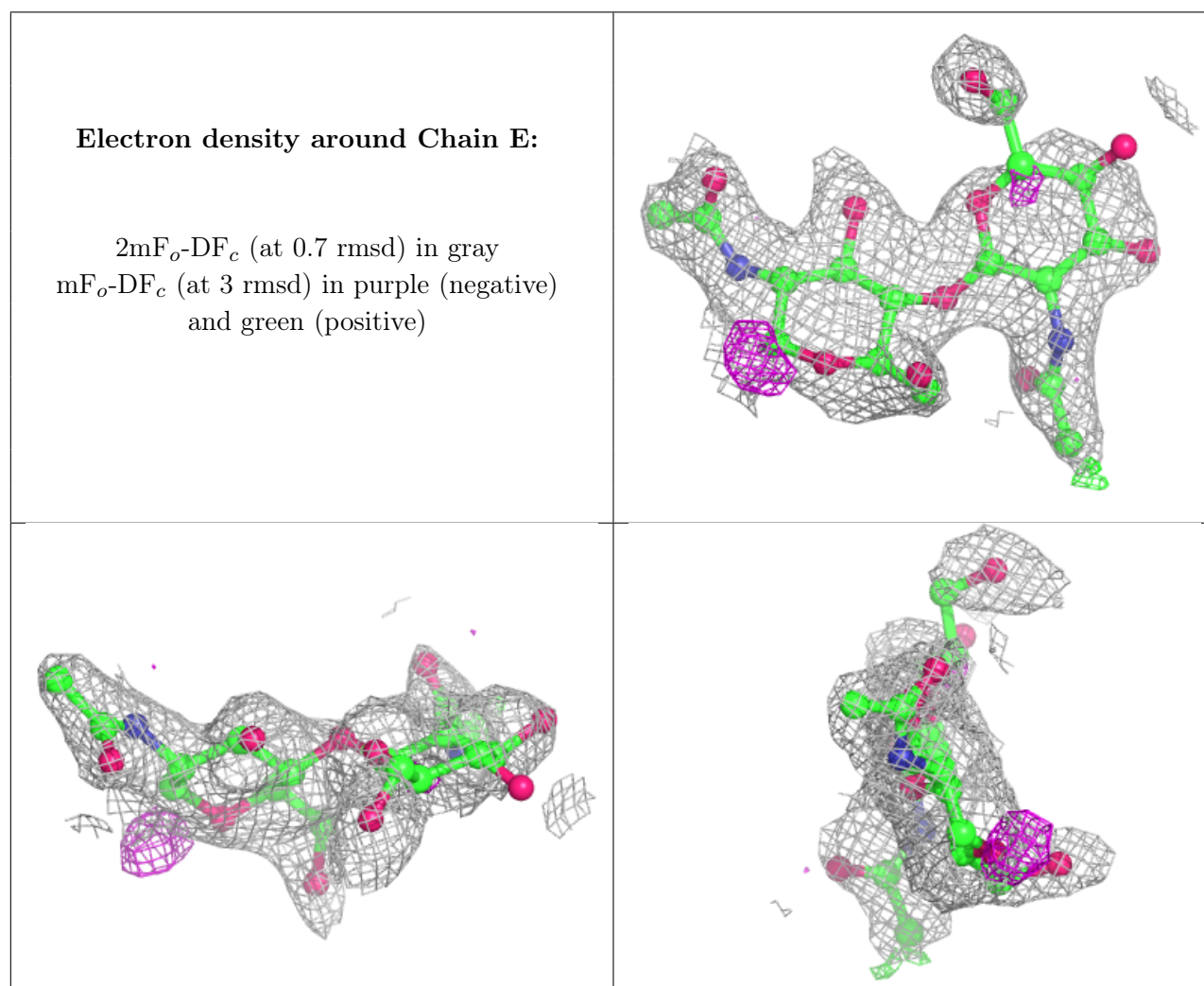
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.69	0.26	73,77,81,81	0
3	NAG	F	2	14/15	0.71	0.35	72,76,84,88	0
3	NAG	I	2	14/15	0.71	0.28	71,76,85,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	1	14/15	0.78	0.18	53,60,63,69	0
3	NAG	I	1	14/15	0.82	0.17	46,53,64,66	0
3	NAG	F	1	14/15	0.85	0.18	47,54,65,68	0

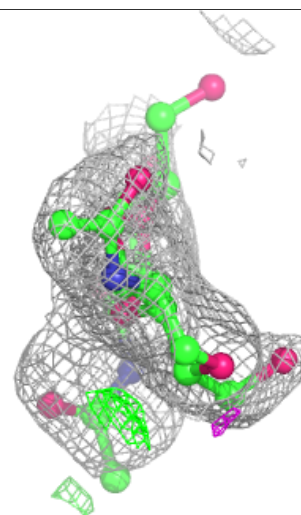
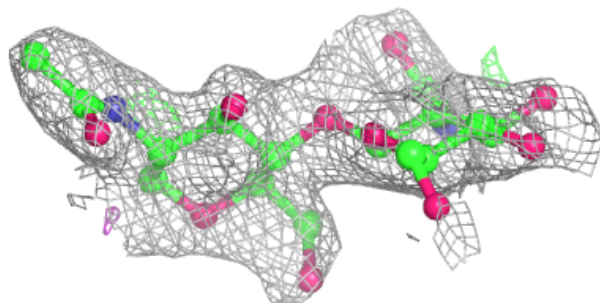
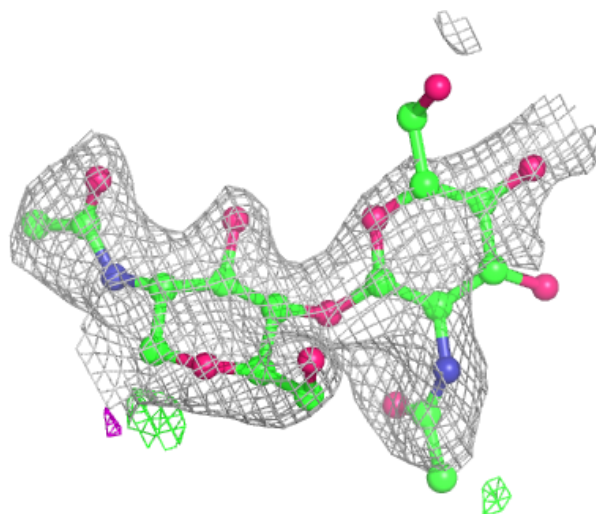
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

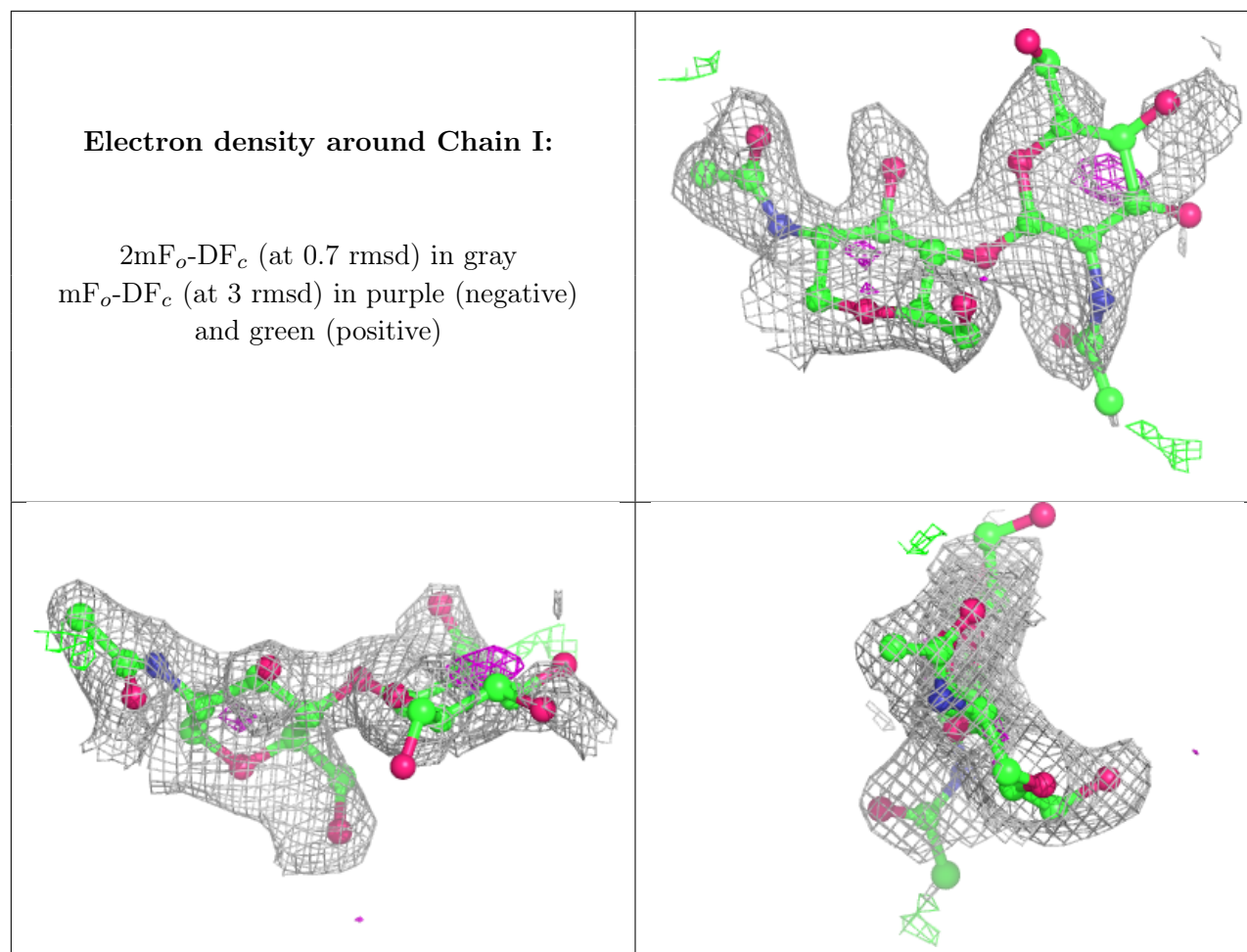




**Electron density around Chain F:**

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





## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	205	14/15	0.68	0.29	77,84,89,96	0
4	EDO	C	407	4/4	0.70	0.14	61,62,62,64	0
4	EDO	C	408	4/4	0.72	0.26	55,59,59,62	0
5	NAG	C	401	14/15	0.73	0.27	53,71,85,85	0
4	EDO	B	204	4/4	0.79	0.20	47,49,50,55	0
4	EDO	C	403	4/4	0.84	0.16	50,51,52,54	0
4	EDO	C	405	4/4	0.85	0.19	62,62,63,63	0
4	EDO	C	410	4/4	0.85	0.15	47,48,50,53	0
4	EDO	A	401	4/4	0.89	0.13	51,52,53,53	0
4	EDO	D	204	4/4	0.89	0.24	51,52,54,61	0
4	EDO	B	203	4/4	0.90	0.16	37,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	404	4/4	0.90	0.15	47,48,48,54	0
4	EDO	A	405	4/4	0.90	0.19	44,52,55,56	0
4	EDO	A	404	4/4	0.91	0.15	33,34,35,35	0
4	EDO	H	203	4/4	0.92	0.14	42,46,48,50	0
4	EDO	C	402	4/4	0.92	0.10	27,33,35,36	0
4	EDO	D	203	4/4	0.92	0.17	39,40,42,46	0
4	EDO	A	403	4/4	0.94	0.12	40,40,41,42	0
4	EDO	A	402	4/4	0.94	0.13	29,30,31,34	0
4	EDO	G	402	4/4	0.95	0.10	41,42,44,47	0
4	EDO	C	409	4/4	0.96	0.12	28,29,30,32	0
4	EDO	G	403	4/4	0.96	0.13	40,41,42,44	0
4	EDO	G	401	4/4	0.97	0.12	32,34,36,37	0
4	EDO	C	406	4/4	0.97	0.15	30,30,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.