



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 01:39 PM BST

PDB ID : 4JUH  
Title : Crystal structure of 1918 pandemic influenza virus hemagglutinin mutant D225G complexed with avian receptor analogue LSTa  
Authors : Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.  
Deposited on : 2013-03-24  
Resolution : 2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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

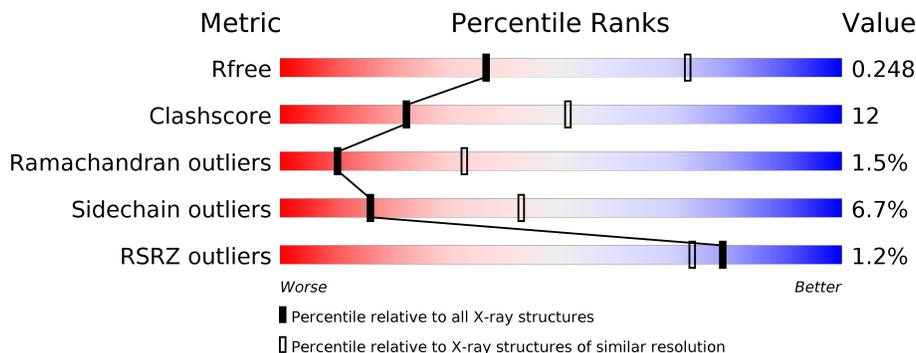
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	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 on 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	324	
1	C	324	
1	E	324	
2	B	170	
2	D	170	
2	F	170	

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Mol	Chain	Length	Quality of chain
3	G	2	 50% 50%
3	I	2	 50% 50%
3	J	2	 50% 50%
4	H	3	 33% 67%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11875 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
			Total	C	N	O	S			
1	A	324	2512	1584	434	483	11	0	0	0
1	C	324	2512	1584	434	483	11	0	0	0
1	E	324	2512	1584	434	483	11	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLY	ASP	engineered mutation	UNP Q9WFX3
A	326	ALA	-	expression tag	UNP Q9WFX3
A	327	ARG	-	expression tag	UNP Q9WFX3
C	225	GLY	ASP	engineered mutation	UNP Q9WFX3
C	326	ALA	-	expression tag	UNP Q9WFX3
C	327	ARG	-	expression tag	UNP Q9WFX3
E	225	GLY	ASP	engineered mutation	UNP Q9WFX3
E	326	ALA	-	expression tag	UNP Q9WFX3
E	327	ARG	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin.

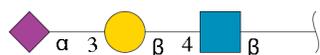
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	170	1368	855	236	271	6	0	0	0
2	D	164	1317	825	225	261	6	0	0	0
2	F	165	1326	830	226	264	6	0	0	0

- 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	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			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(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
			45	25	2	18			

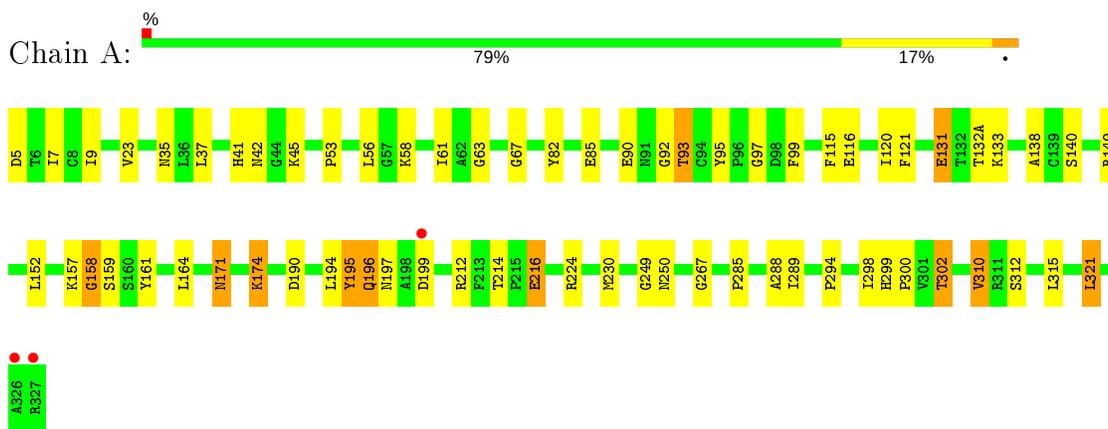
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	23	Total	O	0	0
			23	23		
5	C	51	Total	O	0	0
			51	51		
5	D	9	Total	O	0	0
			9	9		
5	E	46	Total	O	0	0
			46	46		
5	F	17	Total	O	0	0
			17	17		

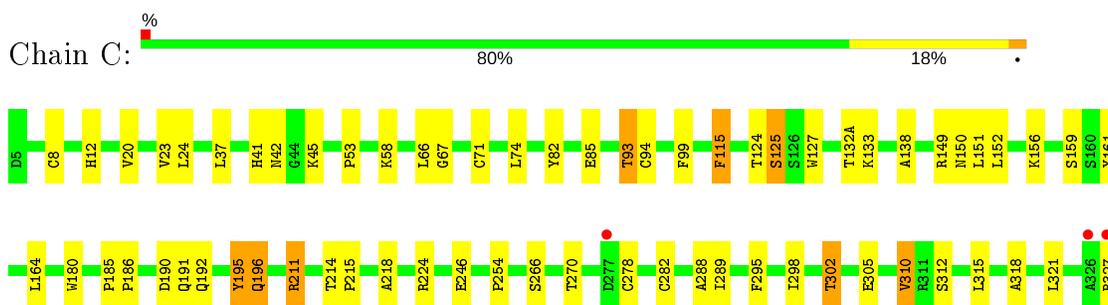
### 3 Residue-property plots [i](#)

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.

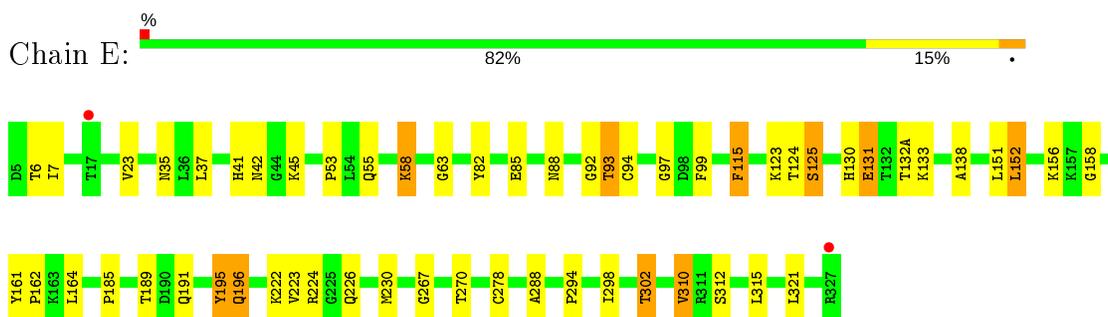
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin



MAC1  
MAC2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%

MAC1  
GAL2  
SIA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.99Å 243.19Å 72.21Å 90.00° 119.62° 90.00°	Depositor
Resolution (Å)	38.40 – 2.81 38.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.40-2.81) 99.4 (38.40-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.201 , 0.246 0.201 , 0.248	Depositor DCC
$R_{free}$ test set	2670 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.021 for -h-l,-k,l 0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: SIA, GAL, 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	0.28	0/2576	0.51	3/3508 (0.1%)
1	C	0.26	0/2576	0.50	3/3508 (0.1%)
1	E	0.27	0/2576	0.49	3/3508 (0.1%)
2	B	0.49	0/1395	0.62	4/1878 (0.2%)
2	D	0.37	0/1344	0.52	2/1811 (0.1%)
2	F	0.28	0/1353	0.51	2/1823 (0.1%)
All	All	0.32	0/11820	0.52	17/16036 (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
2	B	0	1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	525	HIS	CB-CA-C	-13.48	83.43	110.40
1	A	196	GLN	CB-CA-C	-12.30	85.79	110.40
1	E	196	GLN	CB-CA-C	-11.95	86.50	110.40
1	C	195	TYR	CB-CA-C	10.68	131.77	110.40
1	C	196	GLN	CB-CA-C	-9.32	91.76	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	663	SER	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	2512	0	2440	55	0
1	C	2512	0	2440	44	0
1	E	2512	0	2440	41	0
2	B	1368	0	1285	63	0
2	D	1317	0	1231	48	0
2	F	1326	0	1237	40	0
3	G	28	0	25	1	0
3	I	28	0	25	1	0
3	J	28	0	25	1	0
4	H	45	0	38	1	0
5	A	53	0	0	0	0
5	B	23	0	0	1	0
5	C	51	0	0	0	0
5	D	9	0	0	2	0
5	E	46	0	0	1	0
5	F	17	0	0	0	0
All	All	11875	0	11186	265	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 12.

The worst 5 of 265 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:D:663:SER:HA	2:D:664:GLU:CB	1.56	1.31
1:A:131:GLU:OE1	1:A:133:LYS:HD2	1.28	1.29
2:F:526:HIS:HE1	2:F:532:SER:C	1.44	1.21
2:D:663:SER:HA	2:D:664:GLU:HB2	1.12	1.11
2:D:662:TYR:O	2:D:663:SER:HB3	1.45	1.10

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	322/324 (99%)	311 (97%)	10 (3%)	1 (0%)	41	72
1	C	322/324 (99%)	302 (94%)	19 (6%)	1 (0%)	41	72
1	E	322/324 (99%)	304 (94%)	16 (5%)	2 (1%)	25	56
2	B	168/170 (99%)	150 (89%)	14 (8%)	4 (2%)	6	20
2	D	162/170 (95%)	137 (85%)	17 (10%)	8 (5%)	2	7
2	F	163/170 (96%)	141 (86%)	16 (10%)	6 (4%)	3	11
All	All	1459/1482 (98%)	1345 (92%)	92 (6%)	22 (2%)	10	33

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	633	ILE
2	D	657	TYR
2	D	660	PRO
2	D	663	SER
1	E	125	SER

### 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	278/278 (100%)	258 (93%)	20 (7%)	14	38
1	C	278/278 (100%)	264 (95%)	14 (5%)	24	56
1	E	278/278 (100%)	264 (95%)	14 (5%)	24	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	145/145 (100%)	132 (91%)	13 (9%)	9	28
2	D	139/145 (96%)	127 (91%)	12 (9%)	10	30
2	F	140/145 (97%)	129 (92%)	11 (8%)	12	34
All	All	1258/1269 (99%)	1174 (93%)	84 (7%)	16	43

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	115	PHE
2	D	519	ASP
2	F	575	ARG
1	C	152	LEU
1	C	266	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	GLN
2	D	562	GLN
2	F	572	ASN
1	C	250	ASN
2	D	526	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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
3	NAG	G	1	1,3	14,14,15	0.53	0	17,19,21	0.92	1 (5%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.79	0
4	NAG	H	1	4	14,14,15	0.57	0	17,19,21	0.76	0
4	GAL	H	2	4	11,11,12	0.70	0	15,15,17	1.50	2 (13%)
4	SIA	H	3	4	17,20,21	0.28	0	21,28,31	0.52	0
3	NAG	I	1	1,3	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
3	NAG	I	2	3	14,14,15	0.51	0	17,19,21	0.74	0
3	NAG	J	1	1,3	14,14,15	0.49	0	17,19,21	0.84	0
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	0.84	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	G	1	1,3	-	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	-	0/6/23/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/14/34/38	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GAL	C1-C2-C3	4.44	115.13	109.67
4	H	2	GAL	O3-C3-C2	-2.83	104.58	109.99
3	I	1	NAG	C1-O5-C5	2.71	115.86	112.19
3	G	1	NAG	C3-C4-C5	-2.06	106.56	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

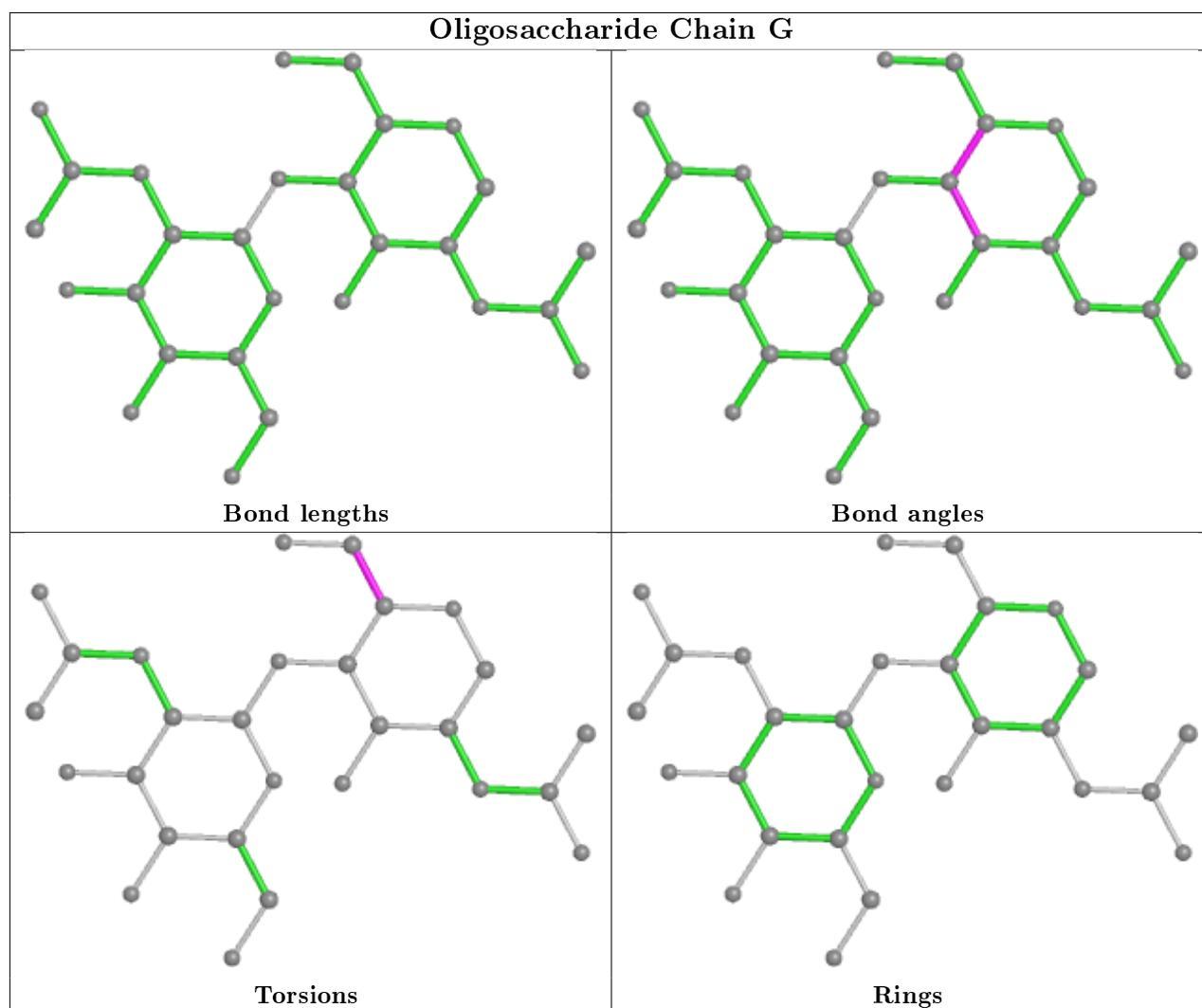
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

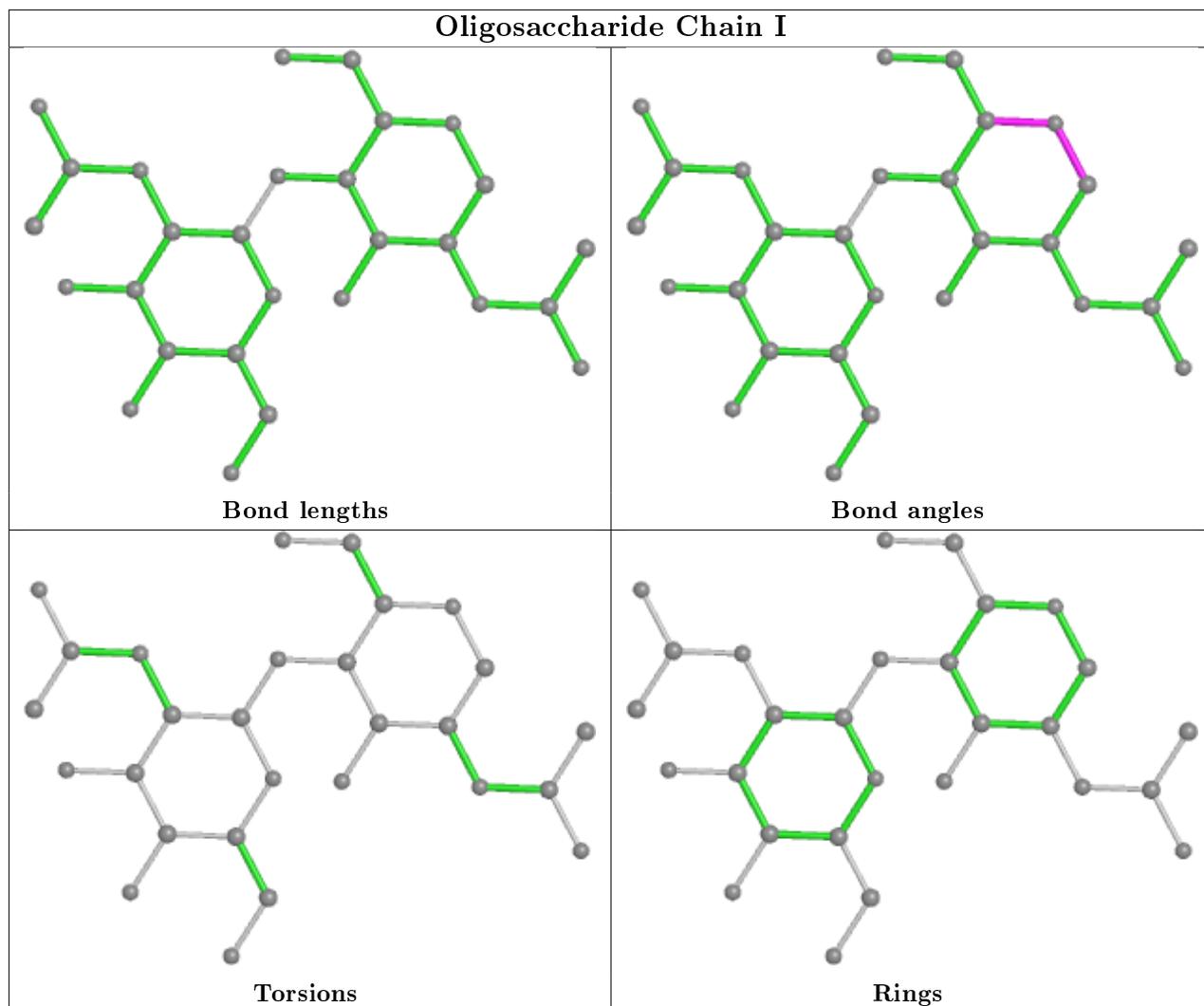
There are no ring outliers.

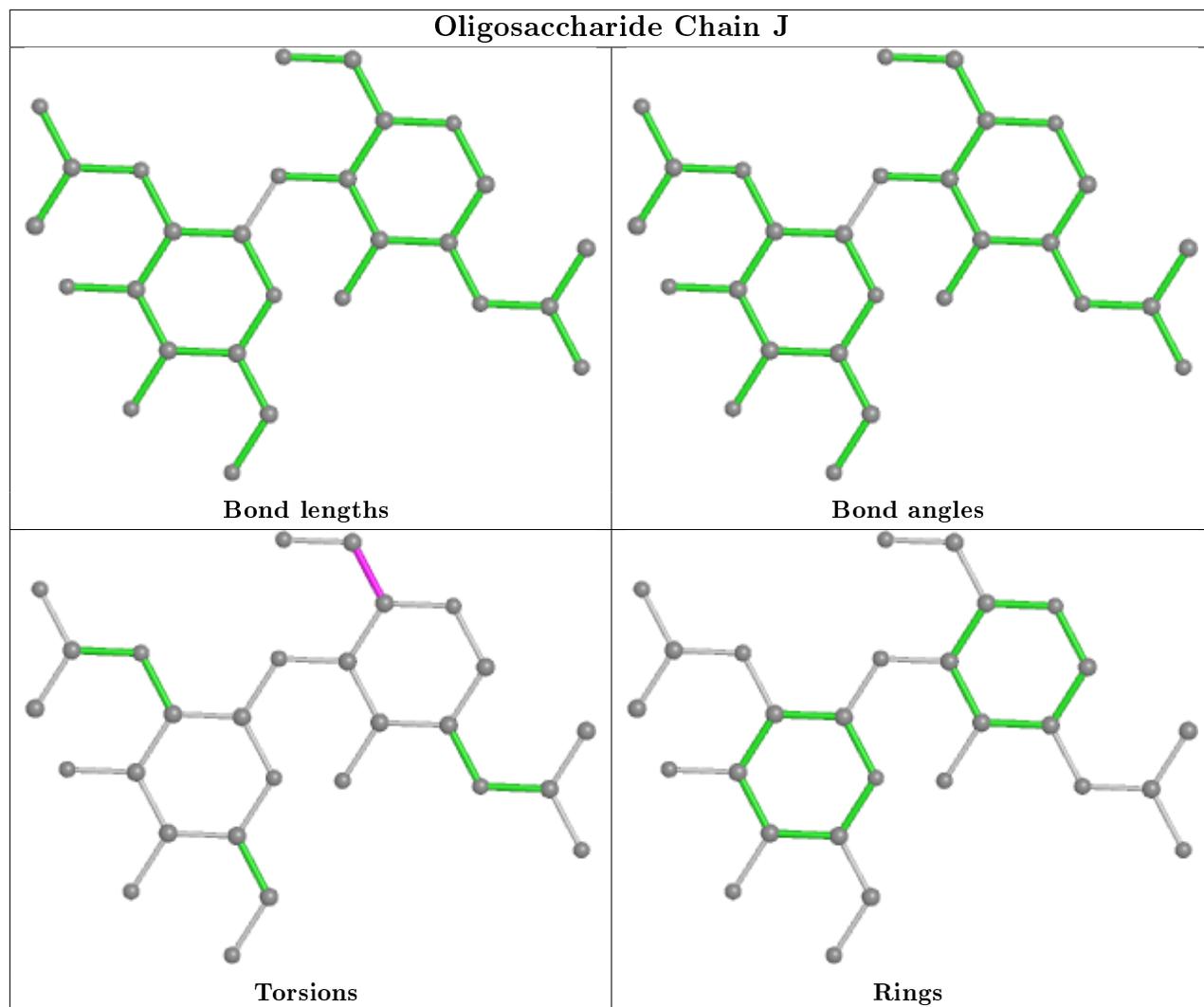
4 monomers are involved in 4 short contacts:

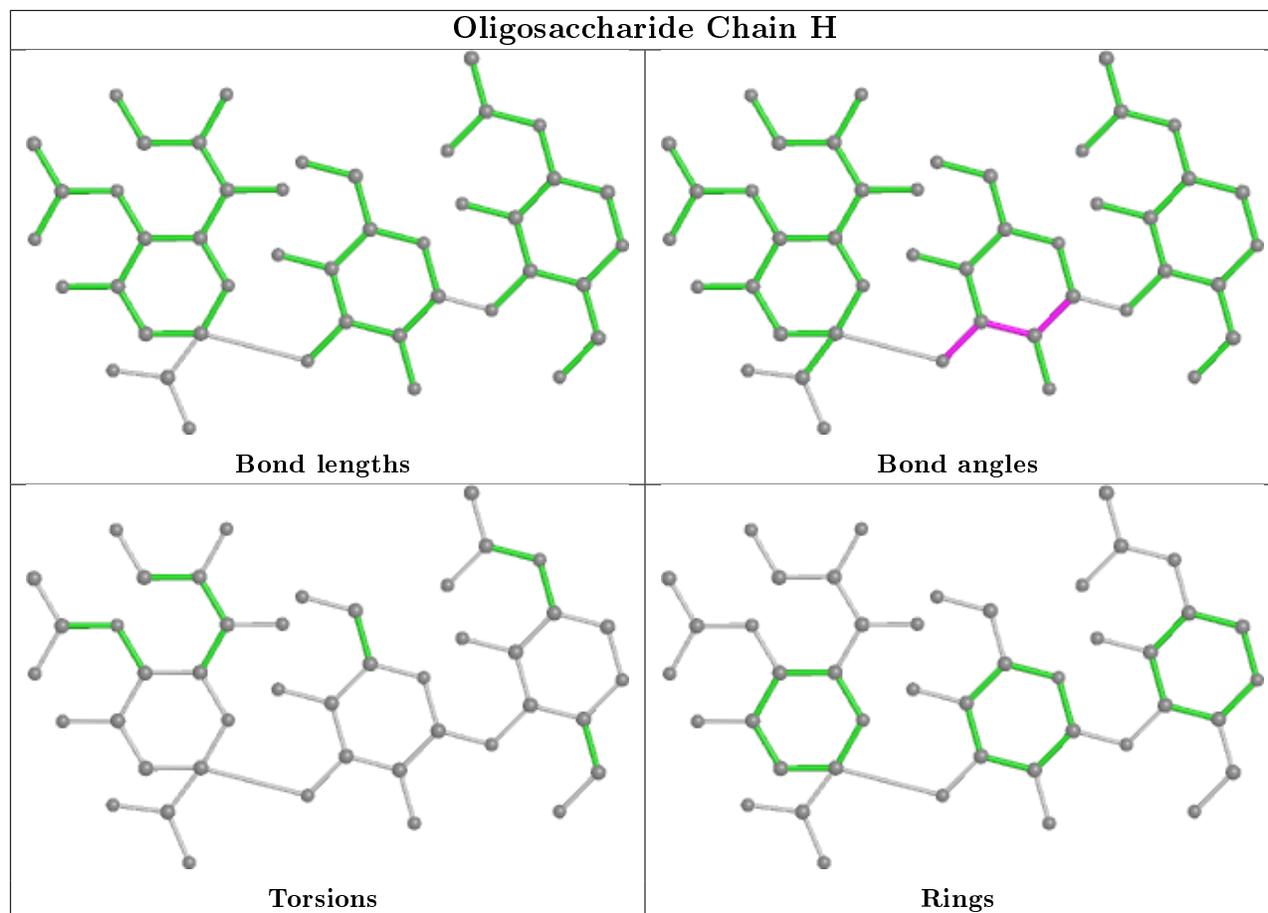
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
4	H	3	SIA	1	0
3	G	1	NAG	1	0
3	I	1	NAG	1	0

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](#)

There are no ligands in this entry.

## 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	A	324/324 (100%)	-0.41	3 (0%) 84 80	21, 42, 72, 178	0
1	C	324/324 (100%)	-0.37	3 (0%) 84 80	22, 50, 78, 188	0
1	E	324/324 (100%)	-0.50	2 (0%) 89 86	22, 43, 74, 165	0
2	B	170/170 (100%)	-0.22	0 100 100	30, 56, 85, 116	0
2	D	164/170 (96%)	0.11	6 (3%) 41 31	33, 69, 113, 144	0
2	F	165/170 (97%)	0.01	3 (1%) 68 61	31, 68, 118, 150	0
All	All	1471/1482 (99%)	-0.29	17 (1%) 79 73	21, 51, 97, 188	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	ARG	8.0
1	C	327	ARG	6.6
1	E	327	ARG	5.1
1	A	326	ALA	3.2
2	D	529	GLU	3.2

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

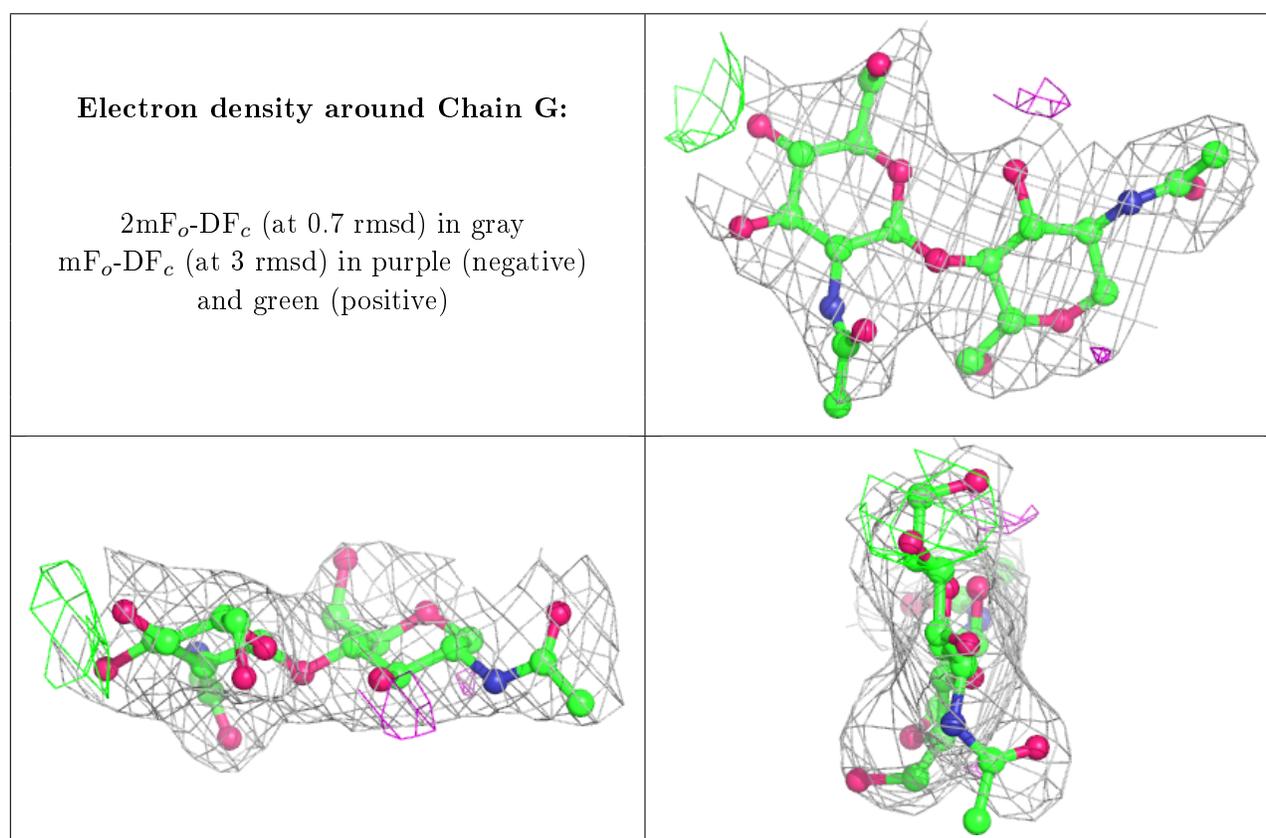
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [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.

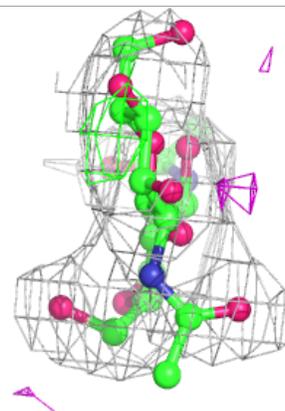
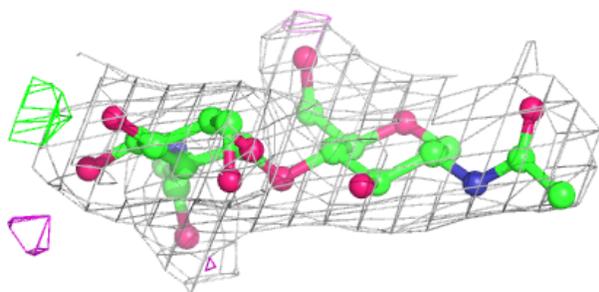
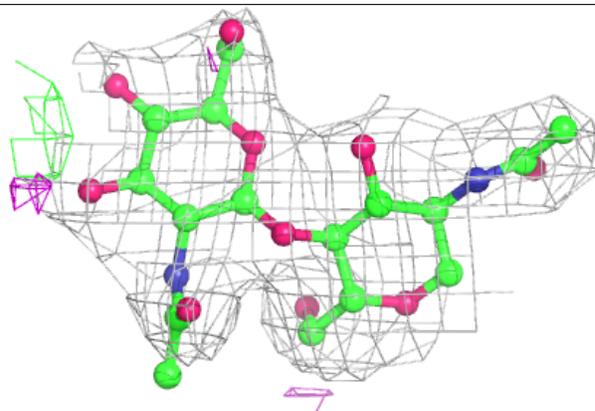
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	1	14/15	0.86	0.20	72,87,110,113	0
3	NAG	G	2	14/15	0.87	0.17	52,63,74,76	0
3	NAG	J	2	14/15	0.92	0.17	70,78,89,90	0
3	NAG	I	2	14/15	0.92	0.15	67,73,82,82	0
4	SIA	H	3	20/21	0.94	0.14	38,41,46,49	0
3	NAG	G	1	14/15	0.95	0.14	32,41,59,64	0
4	GAL	H	2	11/12	0.96	0.13	36,46,54,58	0
3	NAG	J	1	14/15	0.97	0.09	35,44,49,53	0
3	NAG	I	1	14/15	0.97	0.13	42,47,53,55	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.

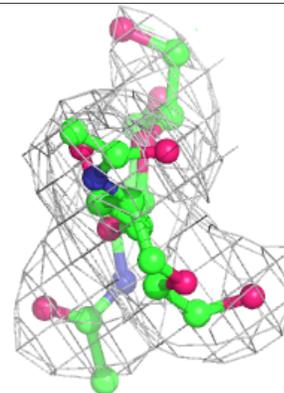
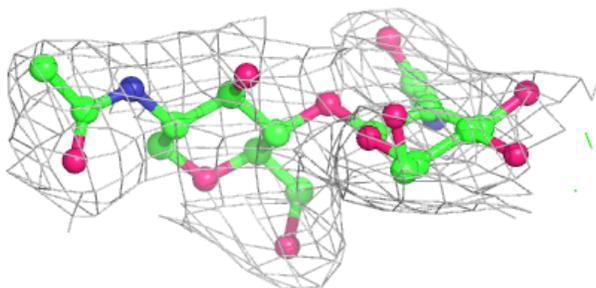
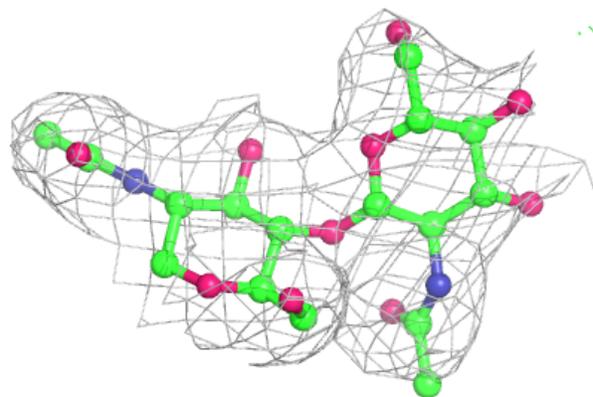


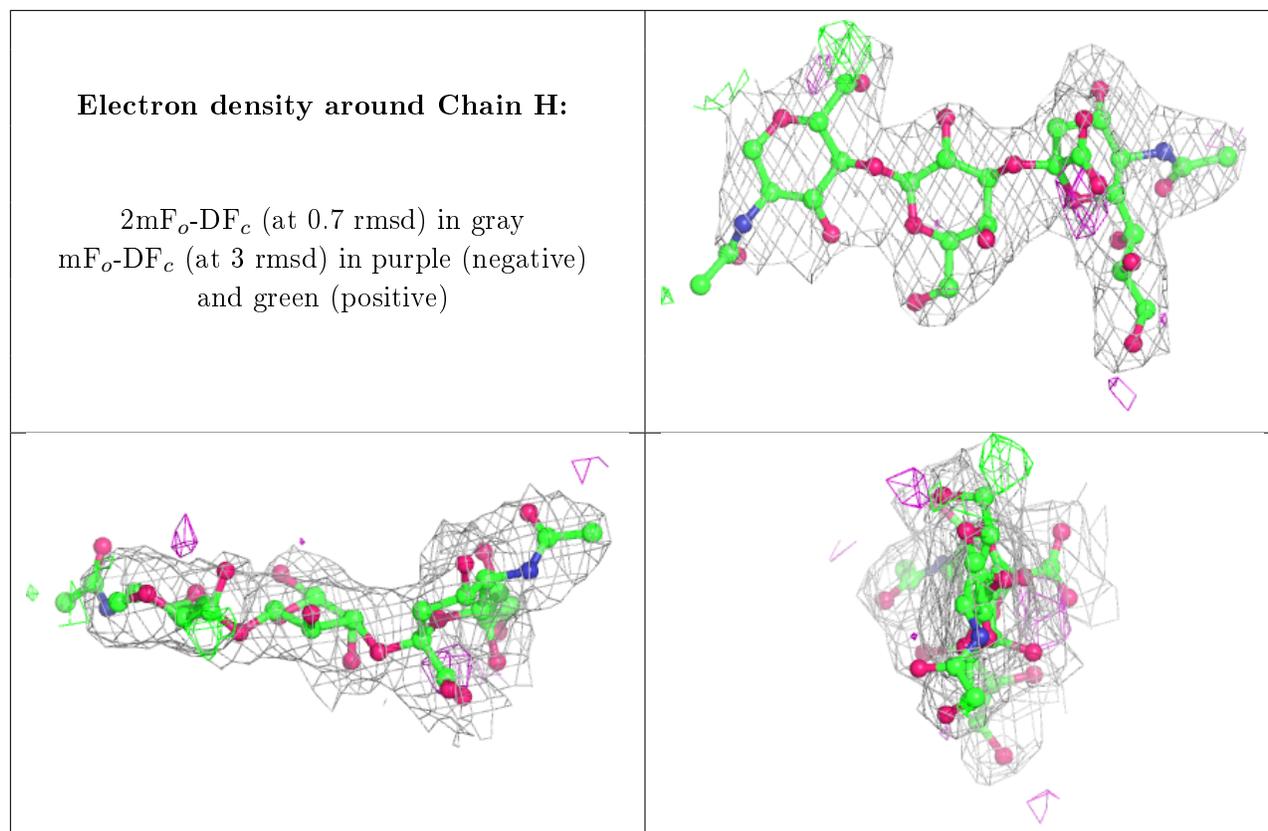
**Electron density around Chain I:**

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

**Electron density around Chain J:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.