



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 09:48 AM EDT

PDB ID : 4KDO  
Title : Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus in complex with human receptor analog LSTc  
Authors : Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.  
Deposited on : 2013-04-25  
Resolution : 2.40 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.

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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
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

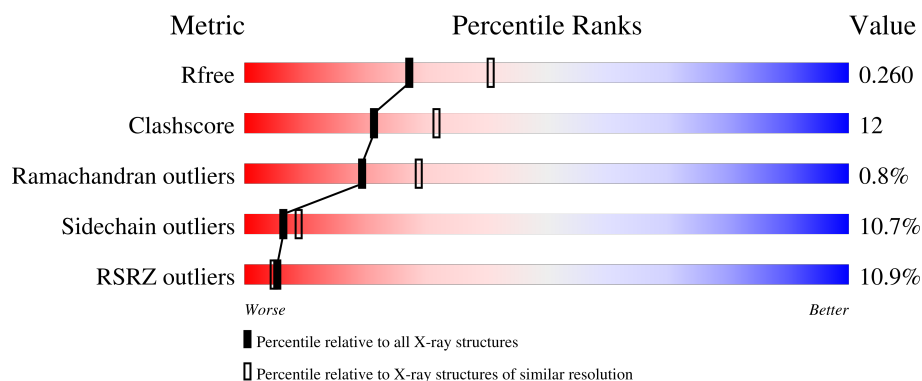
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.




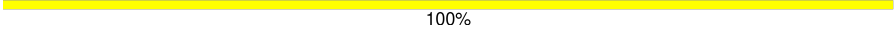
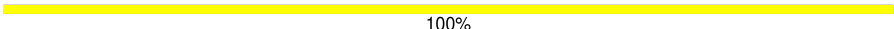

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	322	<div> <div>4%</div> <div>69%</div> <div>25%</div> <div>6%</div> </div>
1	C	322	<div> <div>5%</div> <div>70%</div> <div>24%</div> <div>7%</div> </div>
1	E	322	<div> <div>6%</div> <div>70%</div> <div>23%</div> <div>7%</div> </div>
2	B	175	<div> <div>21%</div> <div>72%</div> <div>23%</div> <div>5%</div> </div>
2	D	175	<div> <div>28%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	175	 17% 73% 24%
3	G	2	 100%
3	H	2	 50% 50%
3	J	2	 100%
4	I	3	 33% 67%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12373 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	A	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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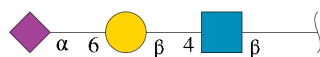
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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



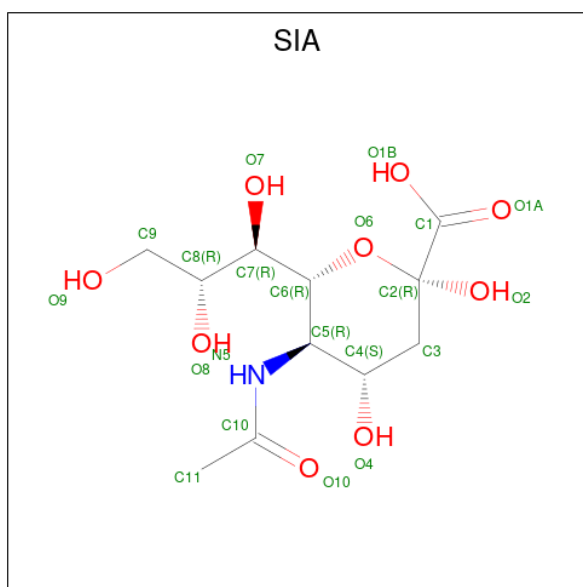
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

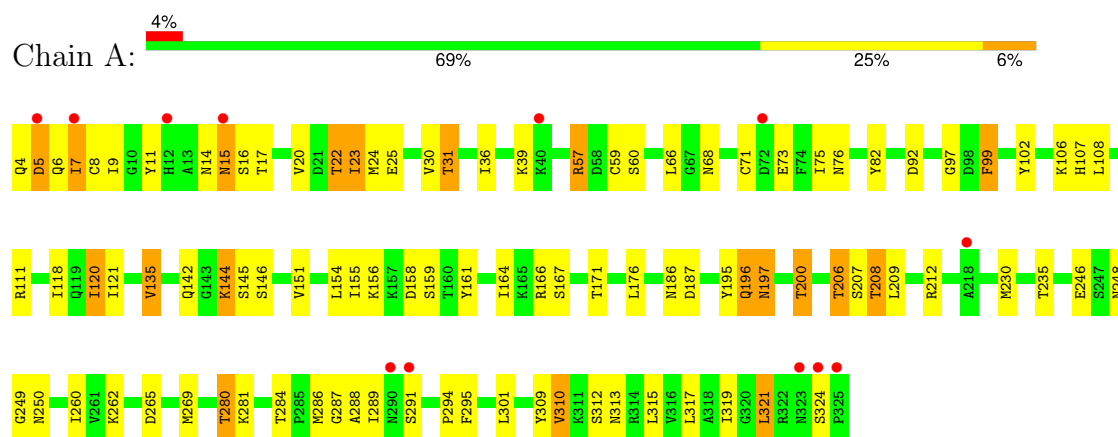
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	80	Total 80	O 80	0	0
7	C	80	Total 80	O 80	0	0
7	E	64	Total 64	O 64	0	0
7	B	24	Total 24	O 24	0	0
7	D	22	Total 22	O 22	0	0
7	F	13	Total 13	O 13	0	0

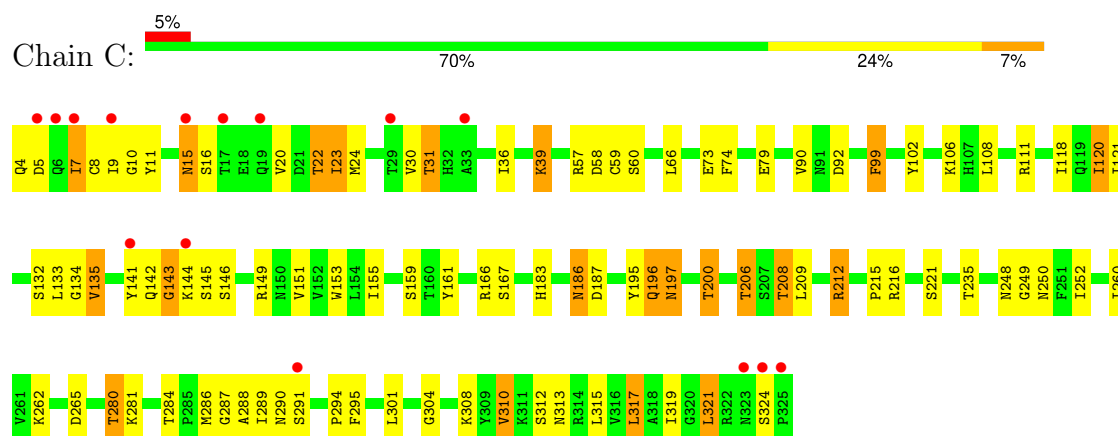
### 3 Residue-property plots [i](#)

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.

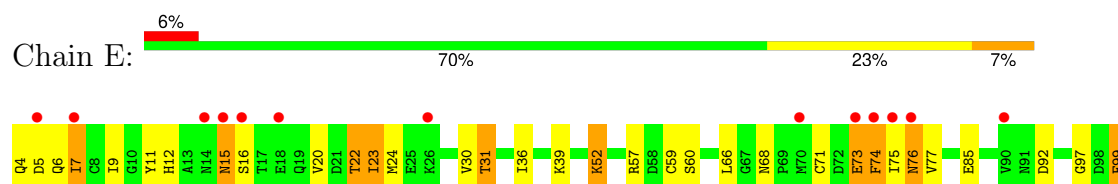
#### • Molecule 1: Hemagglutinin



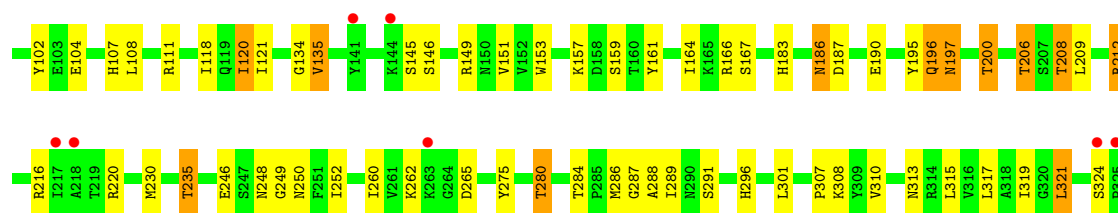
#### • Molecule 1: Hemagglutinin



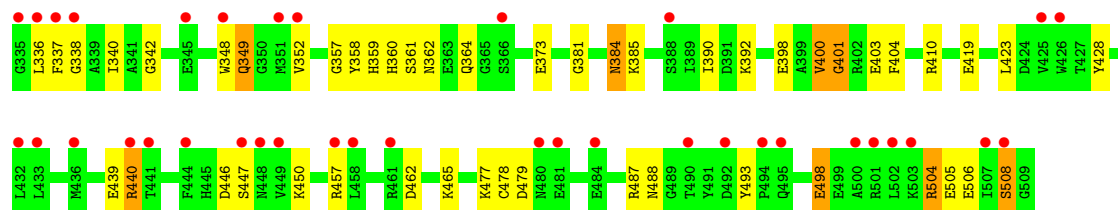
#### • Molecule 1: Hemagglutinin



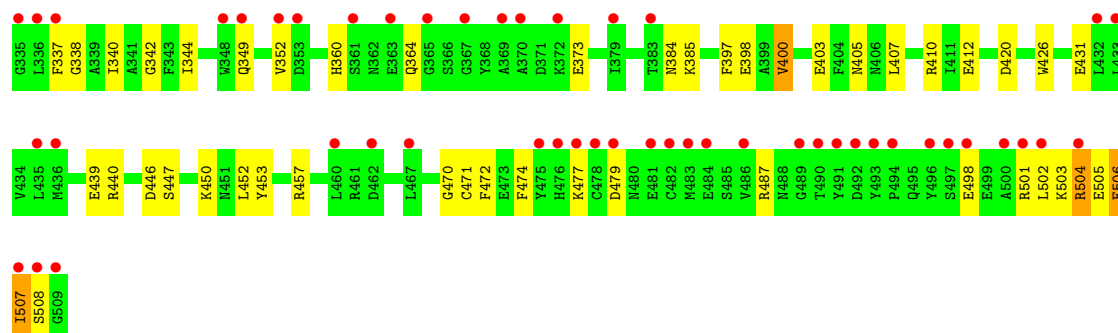
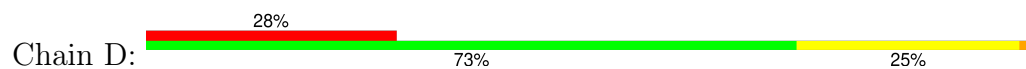




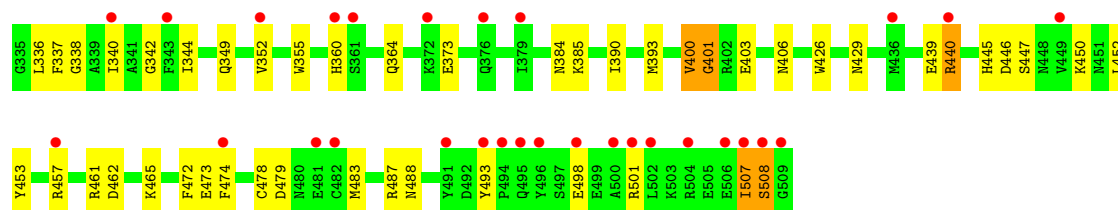
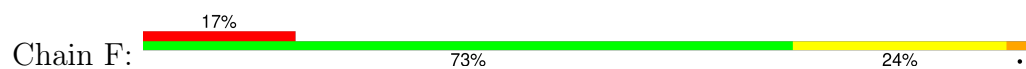
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• 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

Chain H:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

MAG1  
GAL2  
SIA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.26Å 245.91Å 69.57Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	34.18 – 2.40 34.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.18-2.40) 97.2 (34.18-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.237 , 0.269 0.229 , 0.260	Depositor DCC
$R_{free}$ test set	3969 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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, SIA, GAL

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	0.61	0/2621	0.82	9/3558 (0.3%)
1	C	0.59	0/2621	0.98	10/3558 (0.3%)
1	E	0.58	0/2621	0.88	10/3558 (0.3%)
2	B	0.51	0/1443	0.62	0/1939
2	D	0.51	0/1443	0.59	0/1939
2	F	0.54	1/1443 (0.1%)	0.56	0/1939
All	All	0.57	1/12192 (0.0%)	0.80	29/16491 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	ASN	CG-ND2	-6.90	1.15	1.32

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH1	-18.41	111.10	120.30
1	C	57	ARG	NE-CZ-NH2	17.42	129.01	120.30
1	C	212	ARG	NE-CZ-NH1	-16.97	111.81	120.30
1	C	212	ARG	NE-CZ-NH2	16.17	128.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ARG	NE-CZ-NH1	-11.93	114.34	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ILE	Peptide
1	C	143	GLY	Peptide
1	C	4	GLN	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	2559	0	2514	73	1
1	C	2559	0	2513	70	2
1	E	2559	0	2514	79	1
2	B	1416	0	1319	48	0
2	D	1416	0	1319	40	0
2	F	1416	0	1319	52	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
4	I	46	0	40	2	0
5	A	21	0	18	0	0
6	C	14	0	13	0	0
7	A	80	0	0	6	0
7	B	24	0	0	4	0
7	C	80	0	0	10	0
7	D	22	0	0	3	0
7	E	64	0	0	11	0
7	F	13	0	0	3	0
All	All	12373	0	11644	285	2

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 285 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:C:7:ILE:HG22	2:D:472:PHE:HB2	1.39	1.04
2:D:398:GLU:OE2	7:D:617:HOH:O	1.81	0.99
1:A:8:CYS:N	2:B:359:HIS:O	2.03	0.91
1:C:206:THR:HG22	1:C:208:THR:H	1.35	0.90
1:E:5:ASP:O	2:F:474:PHE:N	2.02	0.90

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:O	1:C:132:SER:OG[1_556]	2.10	0.10
1:C:58:ASP:OD2	1:E:73:GLU:OE1[1_655]	2.14	0.06

## 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	320/322 (99%)	300 (94%)	18 (6%)	2 (1%)	25	36
1	C	320/322 (99%)	301 (94%)	18 (6%)	1 (0%)	41	55
1	E	320/322 (99%)	302 (94%)	16 (5%)	2 (1%)	25	36
2	B	173/175 (99%)	160 (92%)	9 (5%)	4 (2%)	6	7
2	D	173/175 (99%)	162 (94%)	9 (5%)	2 (1%)	13	19
2	F	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	36
All	All	1479/1491 (99%)	1389 (94%)	78 (5%)	12 (1%)	19	29

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASN

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Mol	Chain	Res	Type
1	E	74	PHE
2	B	504	ARG
2	B	508	SER
2	D	505	GLU

### 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	290/290 (100%)	257 (89%)	33 (11%)	5	7
1	C	290/290 (100%)	254 (88%)	36 (12%)	4	5
1	E	290/290 (100%)	255 (88%)	35 (12%)	5	6
2	B	149/149 (100%)	137 (92%)	12 (8%)	11	18
2	D	149/149 (100%)	136 (91%)	13 (9%)	10	15
2	F	149/149 (100%)	137 (92%)	12 (8%)	11	18
All	All	1317/1317 (100%)	1176 (89%)	141 (11%)	6	9

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	498	GLU
2	D	384	ASN
2	F	352	VAL
1	C	151	VAL
1	C	135	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	495	GLN
2	F	360	HIS
2	F	495	GLN
2	F	396	GLN

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Mol	Chain	Res	Type
2	B	396	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 ⓘ

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	0.65	0	17,19,21	1.09	2 (11%)
3	NAG	G	2	3	14,14,15	0.66	0	17,19,21	1.63	3 (17%)
3	NAG	H	1	1,3	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	1.02	0
4	NAG	I	1	4	15,15,15	0.40	0	21,21,21	1.54	3 (14%)
4	GAL	I	2	4	11,11,12	1.05	1 (9%)	15,15,17	1.27	1 (6%)
4	SIA	I	3	4	20,20,21	3.50	9 (45%)	21,28,31	3.53	7 (33%)
3	NAG	J	1	1,3	14,14,15	0.51	0	17,19,21	1.19	2 (11%)
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	1.47	2 (11%)

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	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4	-	2/6/26/26	0/1/1/1
4	GAL	I	2	4	-	2/2/19/22	0/1/1/1
4	SIA	I	3	4	-	0/18/34/38	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	SIA	C7-C6	-10.12	1.40	1.52
4	I	3	SIA	C3-C4	-6.67	1.40	1.52
4	I	3	SIA	C4-C5	-5.26	1.48	1.53
4	I	3	SIA	O4-C4	4.29	1.52	1.43
4	I	3	SIA	C3-C2	-3.97	1.46	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	SIA	O6-C2-C3	-11.54	95.04	110.56
4	I	3	SIA	O6-C2-C1	8.15	123.11	107.72
3	G	2	NAG	O5-C1-C2	-4.93	103.66	111.29
3	J	2	NAG	C2-N2-C7	-4.58	116.76	122.90
4	I	1	NAG	C1-O5-C5	4.10	121.59	113.65

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

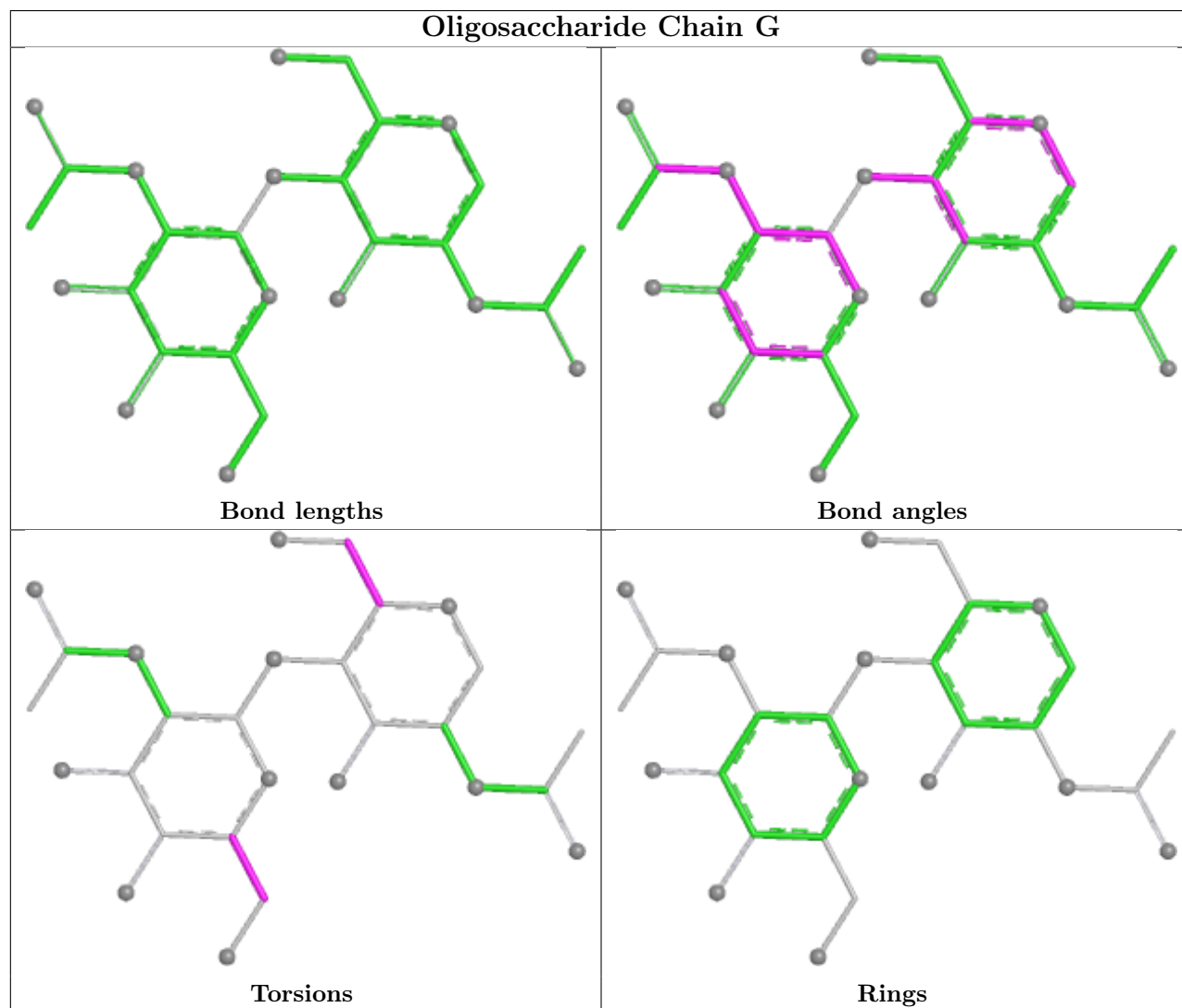
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
4	I	2	GAL	O5-C5-C6-O6
4	I	2	GAL	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2

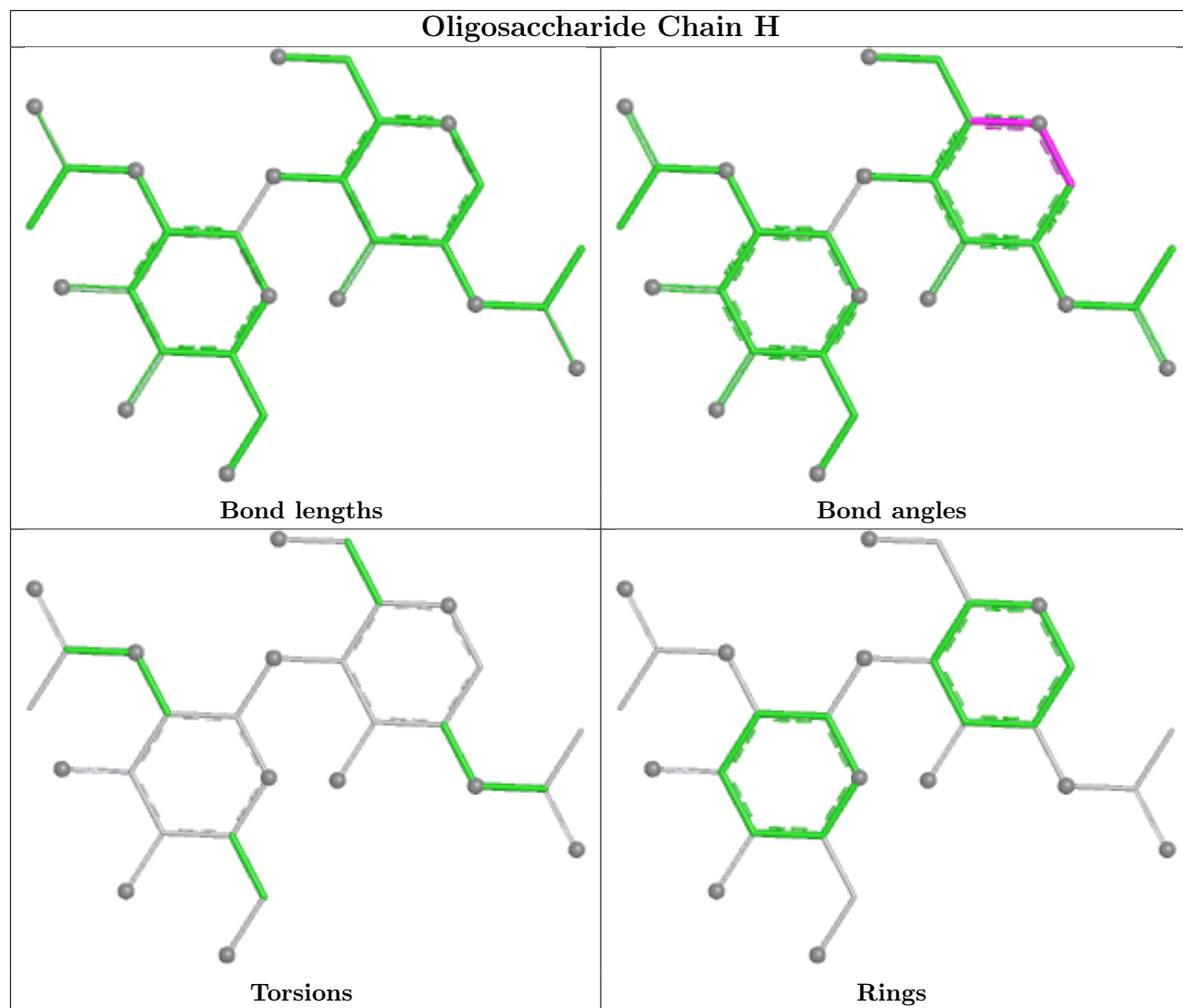
There are no ring outliers.

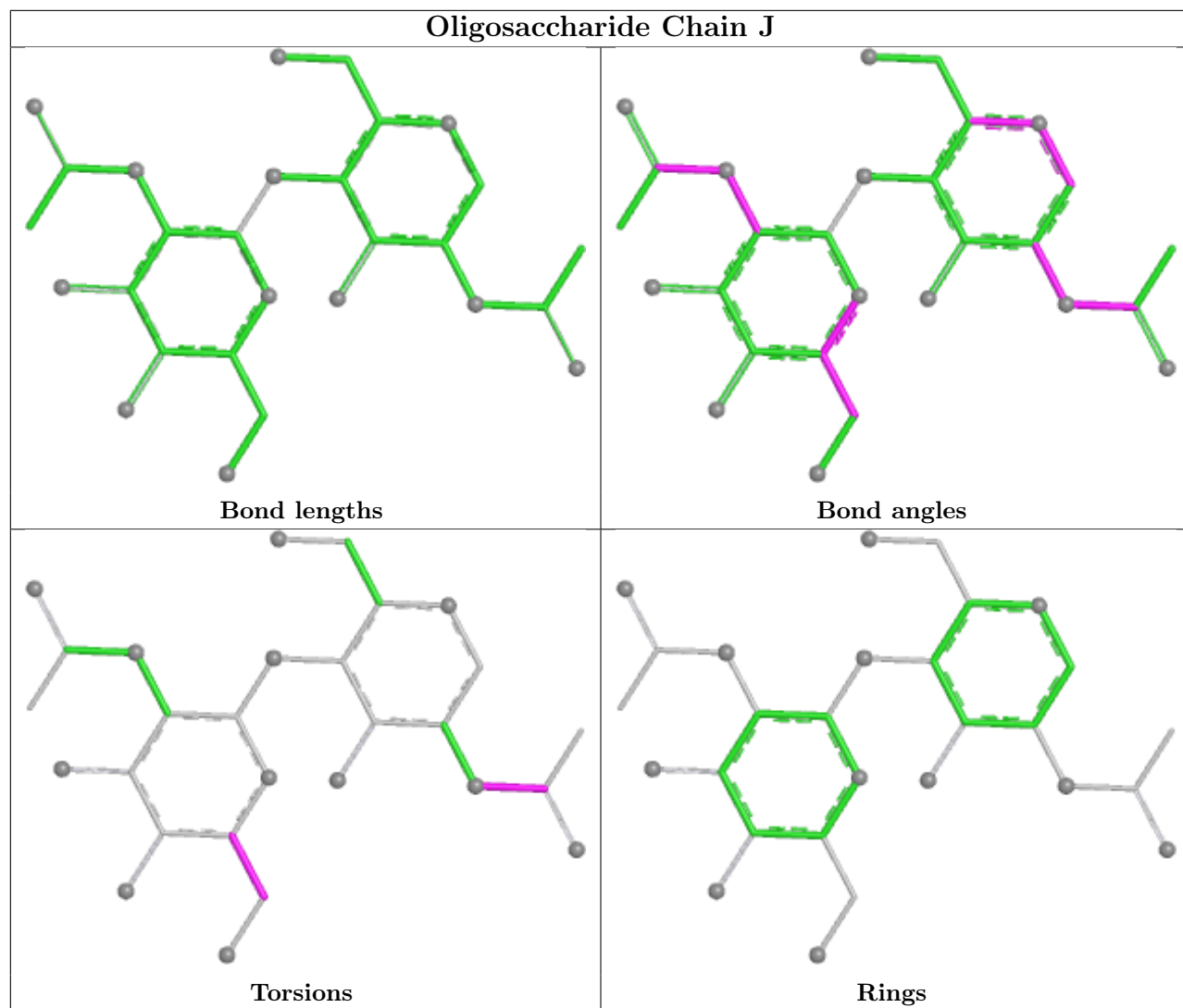
2 monomers are involved in 2 short contacts:

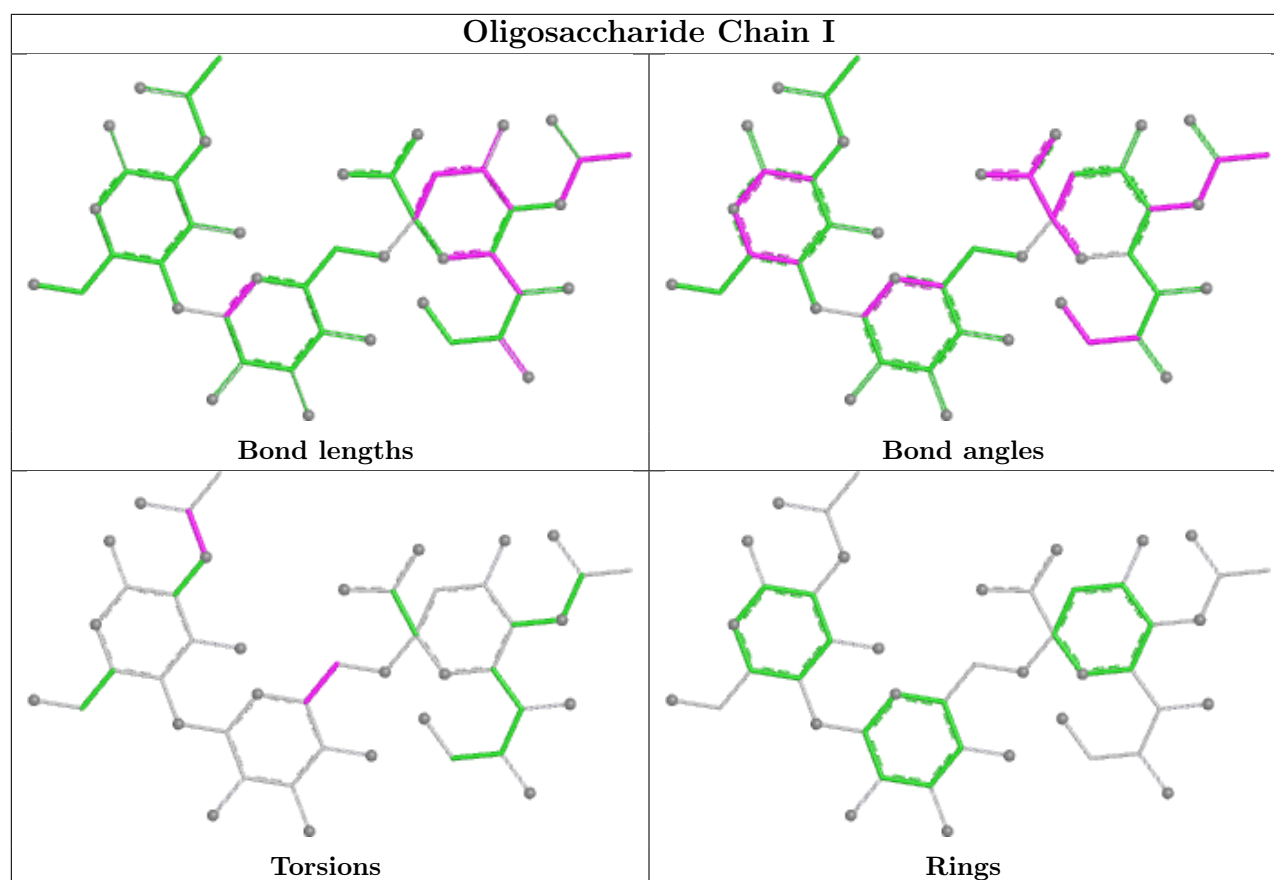
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	GAL	1	0
4	I	3	SIA	1	0

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](#)

2 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$
5	SIA	A	403	-	21,21,21	3.94	8 (38%)	24,31,31	1.97	7 (29%)
6	NAG	C	601	1	14,14,15	0.44	0	17,19,21	1.46	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
5	SIA	A	403	-	-	2/20/38/38	0/1/1/1
6	NAG	C	601	1	-	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	SIA	C7-C6	-9.27	1.41	1.52
5	A	403	SIA	C3-C4	-9.12	1.39	1.53
5	A	403	SIA	C4-C5	-6.88	1.47	1.53
5	A	403	SIA	O6-C6	6.02	1.53	1.44
5	A	403	SIA	O6-C2	4.67	1.47	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C1-O5-C5	5.13	119.06	112.19
5	A	403	SIA	O6-C6-C7	4.76	114.09	106.65
5	A	403	SIA	C6-C5-N5	-4.01	104.50	110.91
5	A	403	SIA	C8-C7-C6	-3.02	107.39	113.05
5	A	403	SIA	O6-C6-C5	-2.71	107.37	109.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

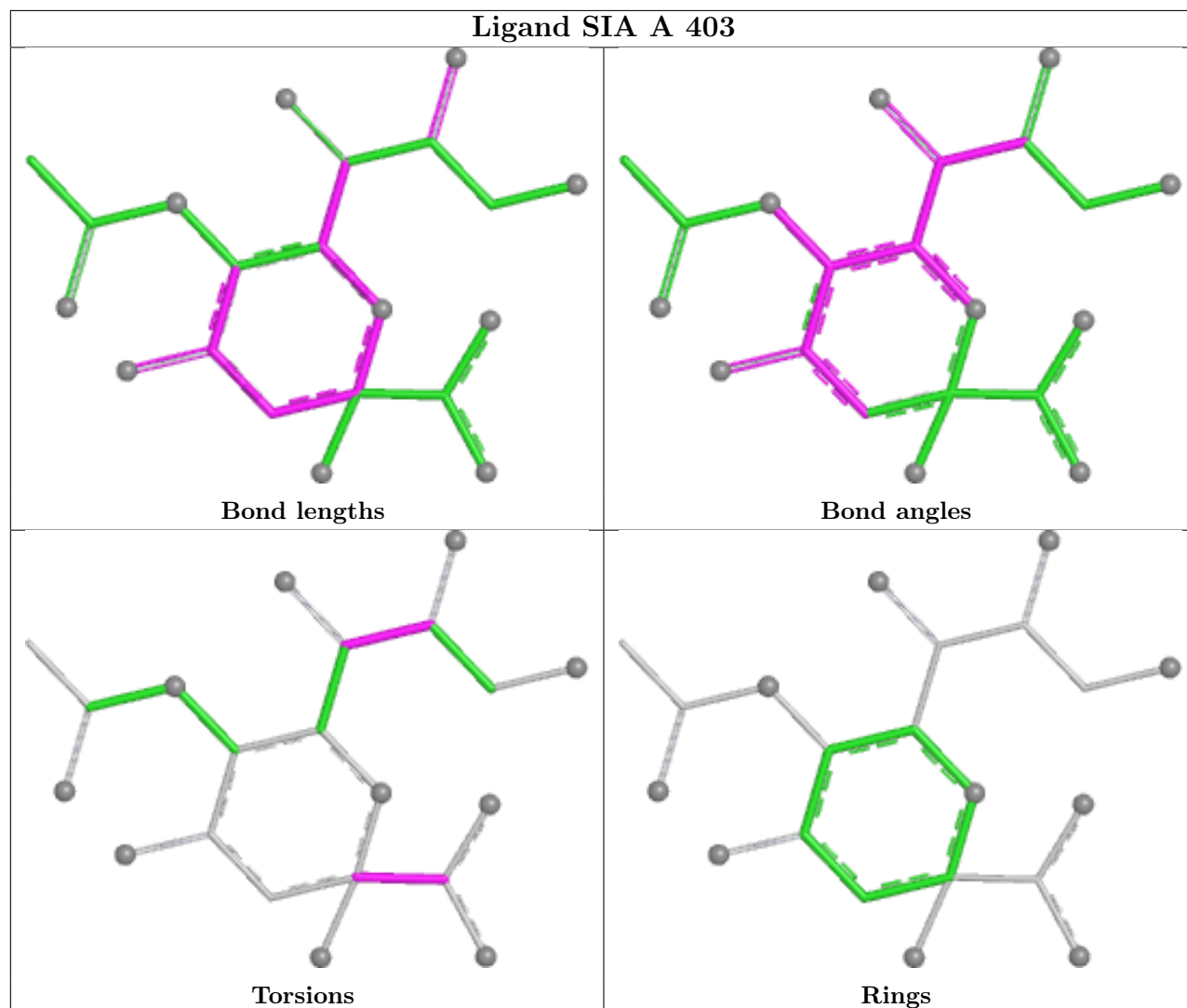
Mol	Chain	Res	Type	Atoms
6	C	601	NAG	O7-C7-N2-C2
6	C	601	NAG	C8-C7-N2-C2
5	A	403	SIA	C6-C7-C8-O8
5	A	403	SIA	O1B-C1-C2-C3

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	322/322 (100%)	0.24	12 (3%) 41 41	24, 48, 89, 162	0
1	C	322/322 (100%)	0.31	15 (4%) 31 30	26, 51, 96, 150	0
1	E	322/322 (100%)	0.46	20 (6%) 20 19	27, 54, 103, 167	0
2	B	175/175 (100%)	1.28	37 (21%) 1 0	34, 78, 126, 170	0
2	D	175/175 (100%)	1.48	49 (28%) 0 0	31, 92, 146, 183	0
2	F	175/175 (100%)	1.00	29 (16%) 1 1	32, 90, 143, 205	0
All	All	1491/1491 (100%)	0.66	162 (10%) 5 5	24, 58, 126, 205	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	PRO	9.4
2	D	509	GLY	8.6
1	E	141	TYR	7.2
2	D	507	ILE	7.0
1	C	141	TYR	6.6

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

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

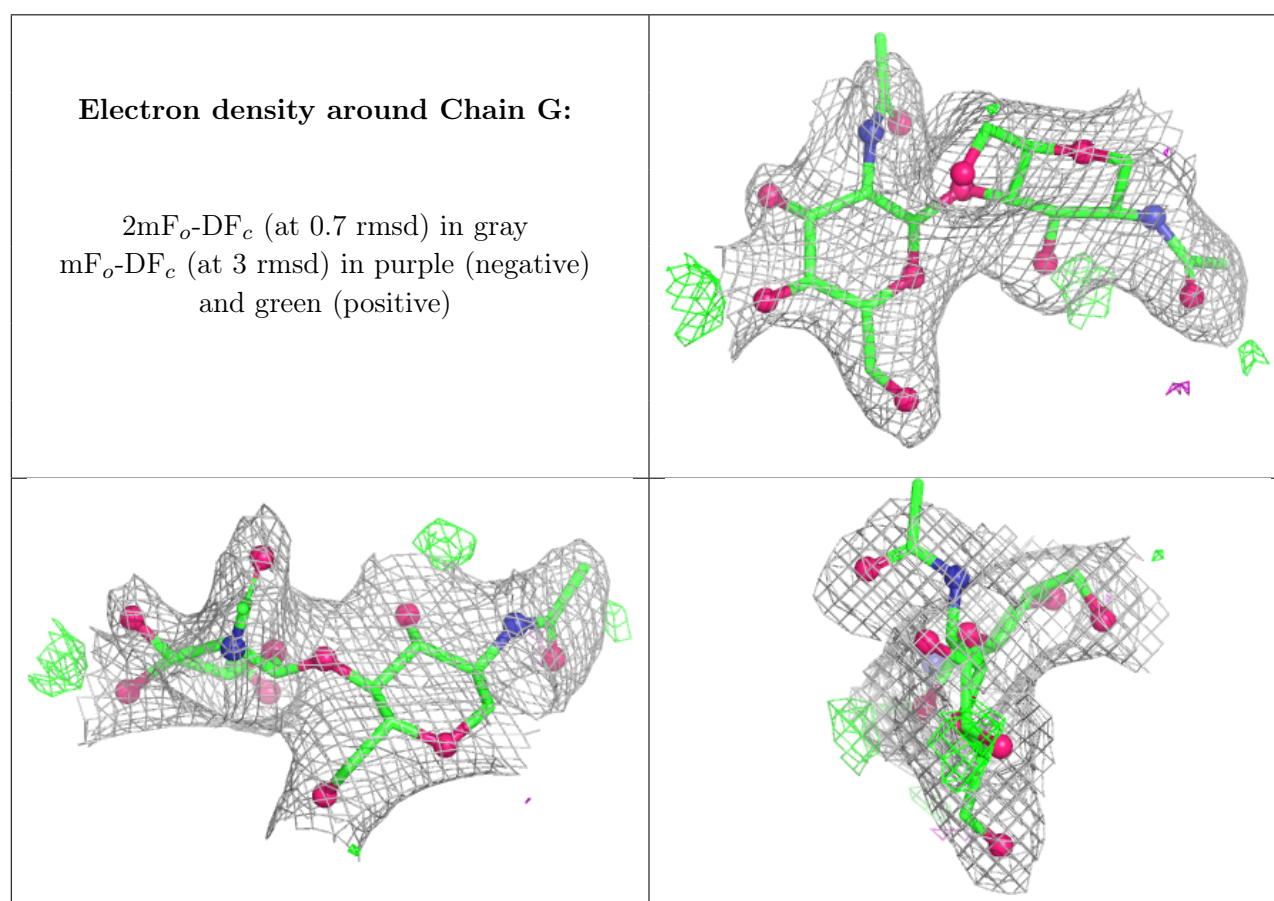
### 6.3 Carbohydrates [i](#)

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.



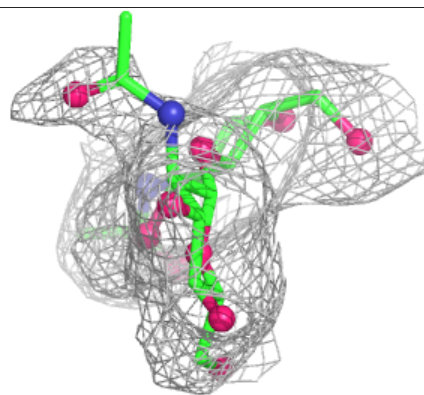
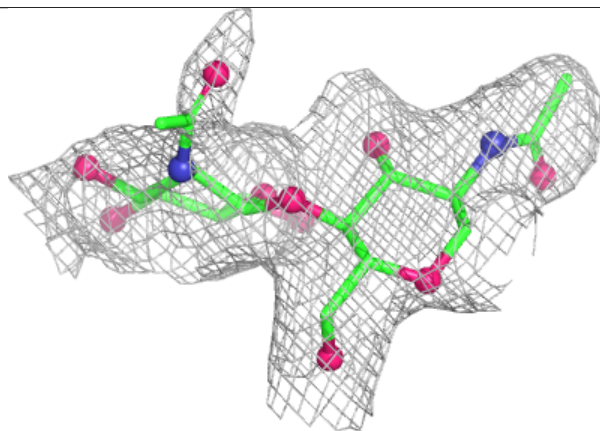
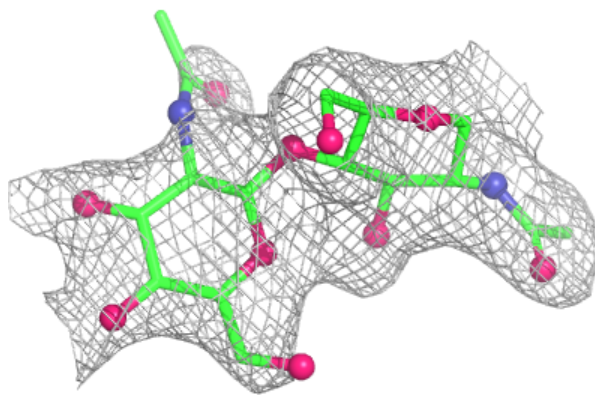
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	I	1	15/15	0.76	0.28	119,129,140,147	0
3	NAG	H	2	14/15	0.84	0.32	86,97,111,112	0
3	NAG	G	2	14/15	0.86	0.28	65,79,88,93	0
3	NAG	H	1	14/15	0.90	0.14	55,68,85,86	0
3	NAG	J	2	14/15	0.91	0.32	85,107,117,122	0
4	GAL	I	2	11/12	0.91	0.11	81,96,111,112	0
3	NAG	J	1	14/15	0.93	0.19	45,58,69,75	0
3	NAG	G	1	14/15	0.93	0.12	37,50,65,67	0
4	SIA	I	3	20/21	0.93	0.15	46,60,74,74	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.



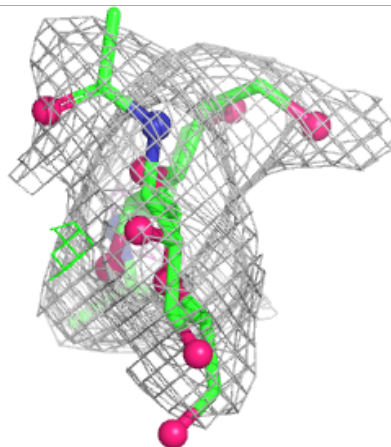
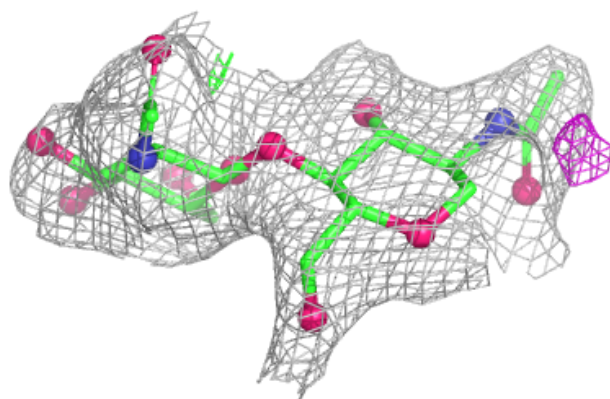
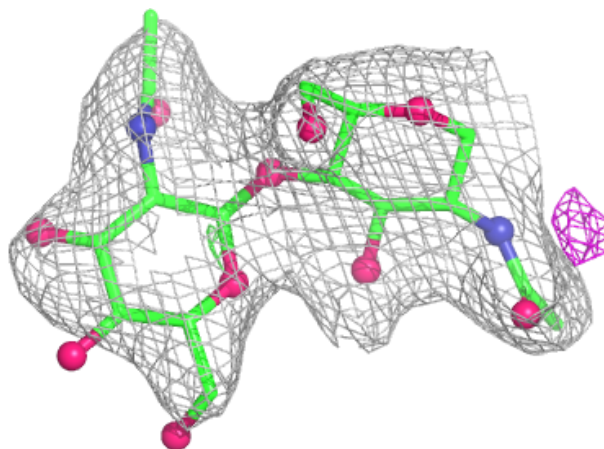
**Electron density around Chain H:**

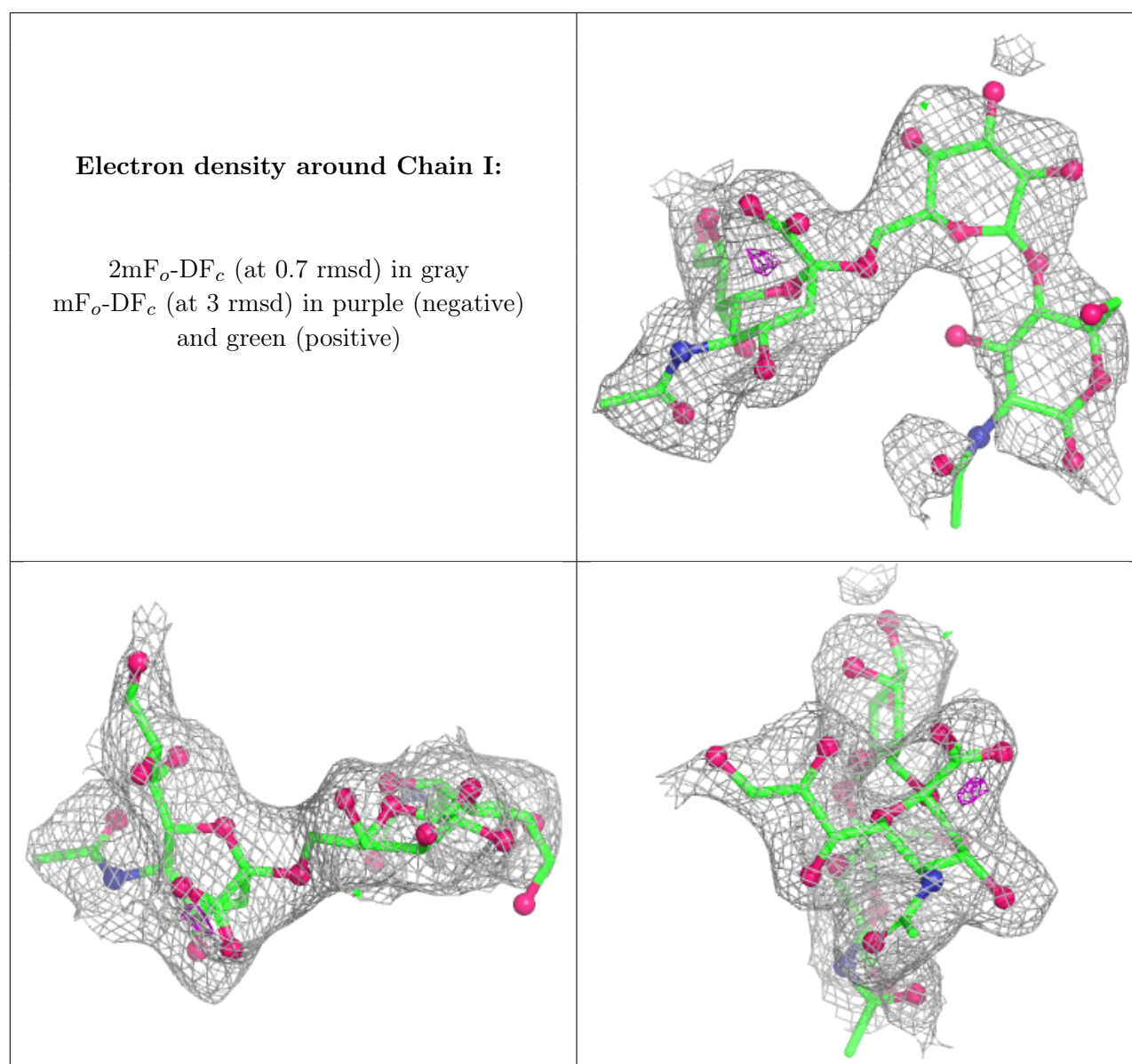
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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](#)

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.

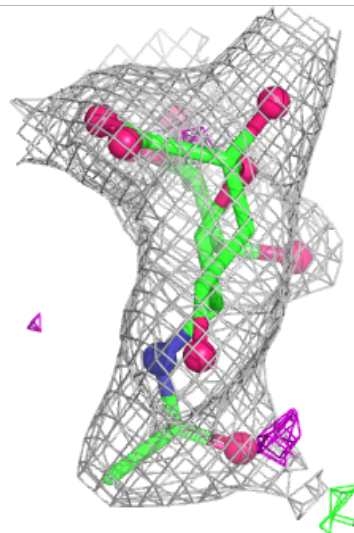
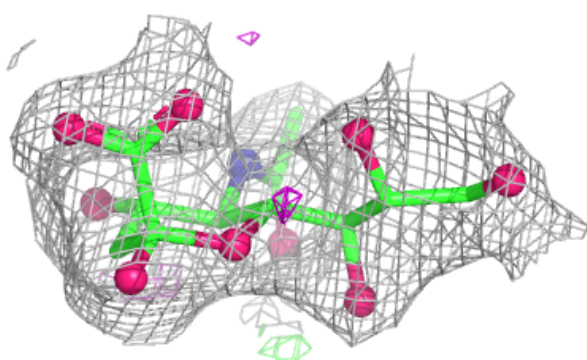
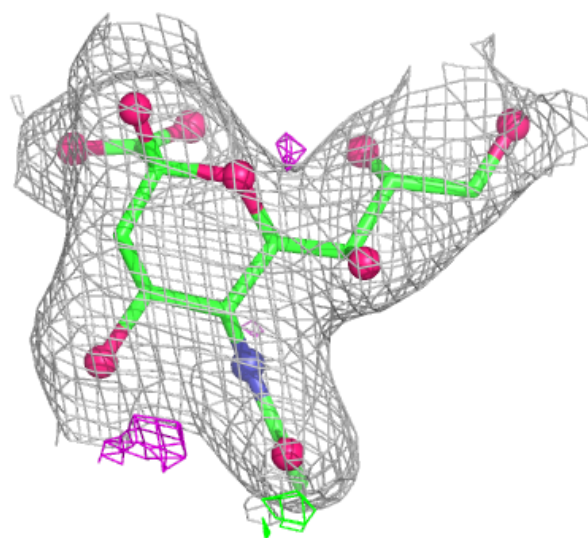
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	C	601	14/15	0.83	0.22	98,114,123,128	0
5	SIA	A	403	21/21	0.91	0.13	51,57,68,69	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

**Electron density around SIA A 403:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.