



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:03 AM UTC

PDB ID : 6D8D / pdb_00006d8d
Title : The crystal structure of hemagglutinin from A/Hong Kong/125/2017 influenza virus in complex with LSTb
Authors : Yang, H.; Stevens, J.
Deposited on : 2018-04-26
Resolution : 3.55 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

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>.

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

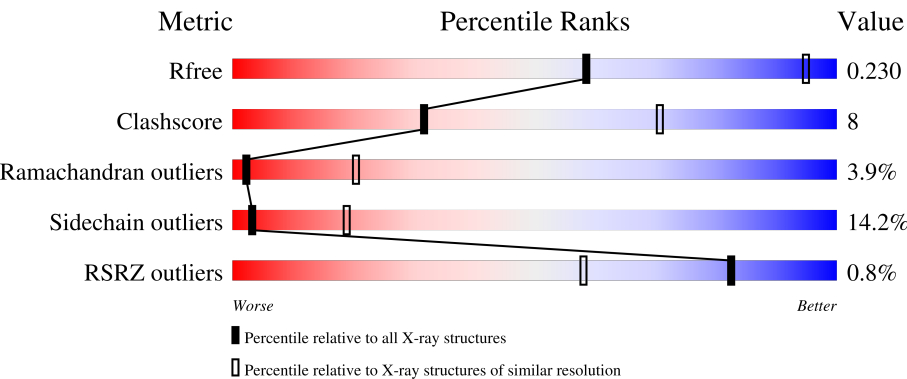
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.55 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}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	321	64%29%5% ..
1	C	321	% 64%28%6% ..
1	E	321	% 64%28%5% ..
2	B	221	53%20%.23%
2	D	221	% 51%23%.23%

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Mol	Chain	Length	Quality of chain
2	F	221	% 52%21%23%
3	G	3	100%
3	H	3	100%
4	I	2	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11670 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.

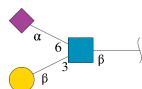
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	C	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	E	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	D	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	F	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O		0	0	0
			45	25	2	18				
3	H	3	Total	C	N	O		0	0	0
			45	25	2	18				

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



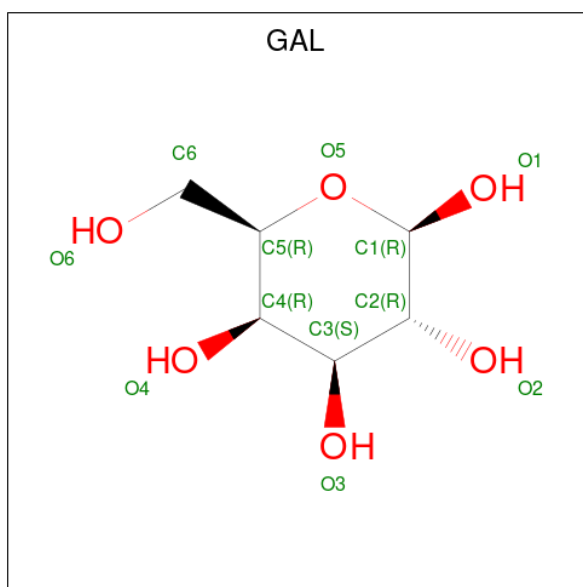
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



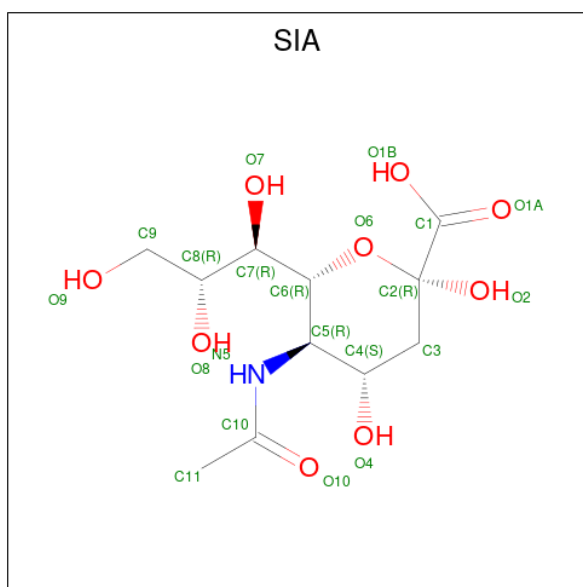
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	E	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).

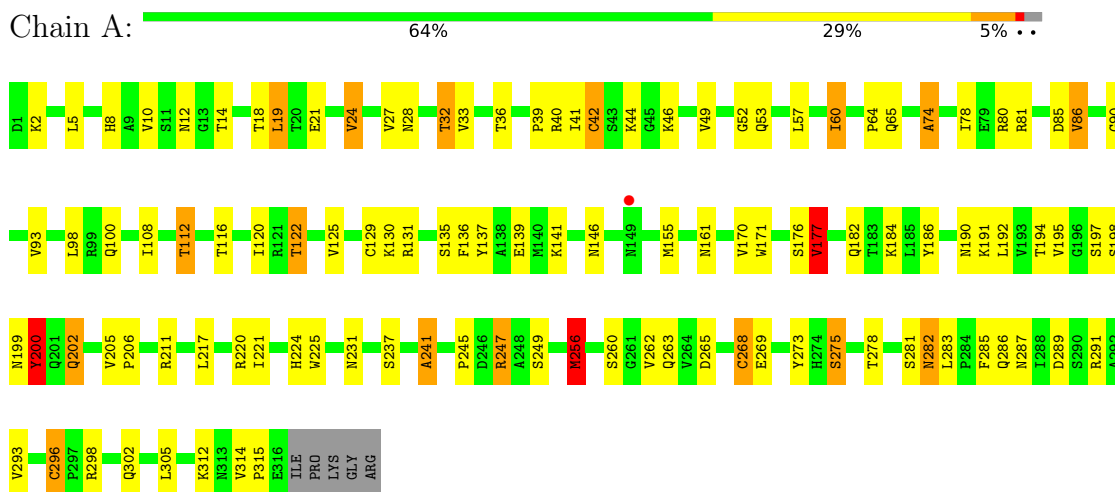


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			20	11	1	8		

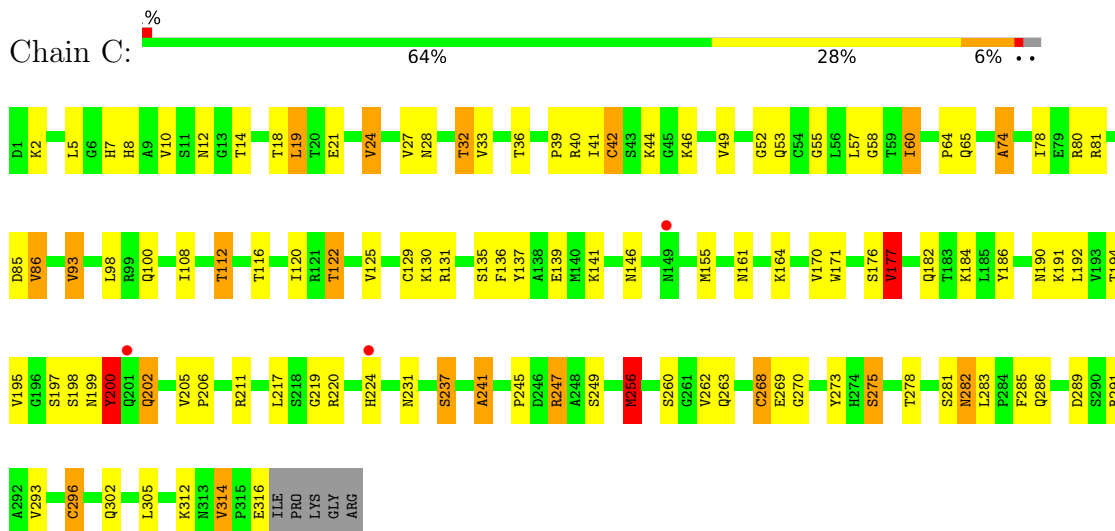
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded 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 HA1 chain

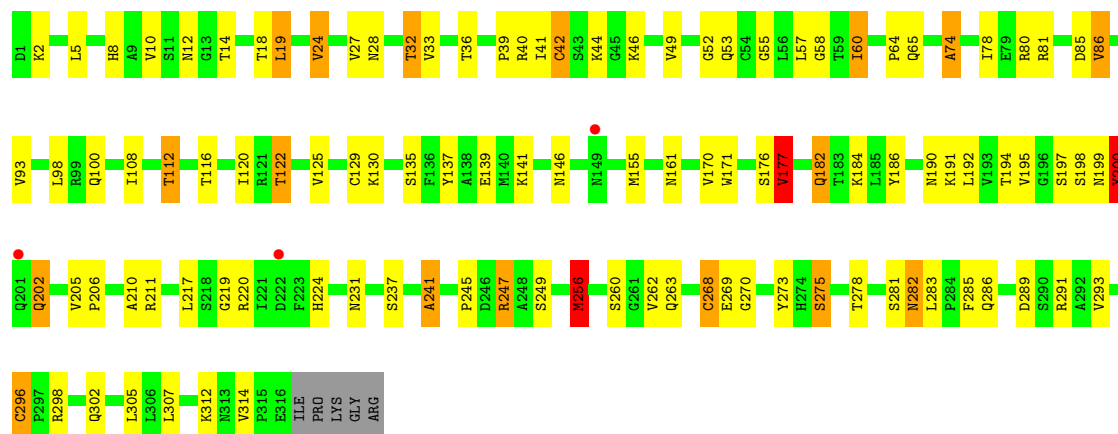


• Molecule 1: Hemagglutinin HA1 chain



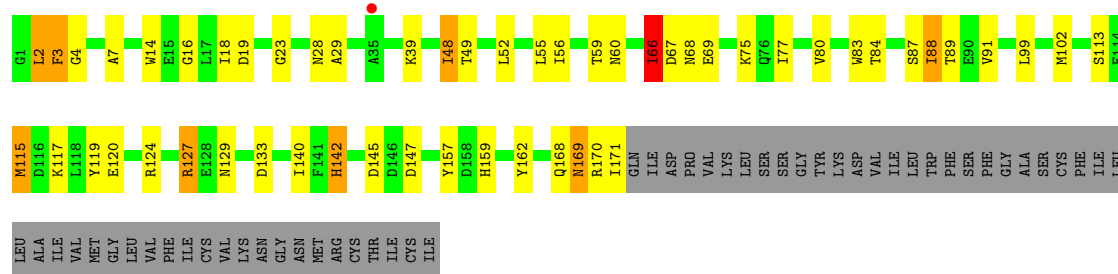
• Molecule 1: Hemagglutinin HA1 chain





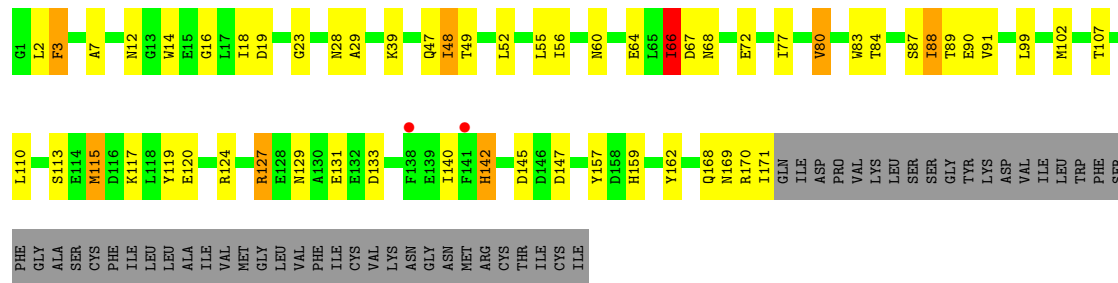
• Molecule 2: Hemagglutinin HA2 chain

Chain B: 53% 20% • 23%



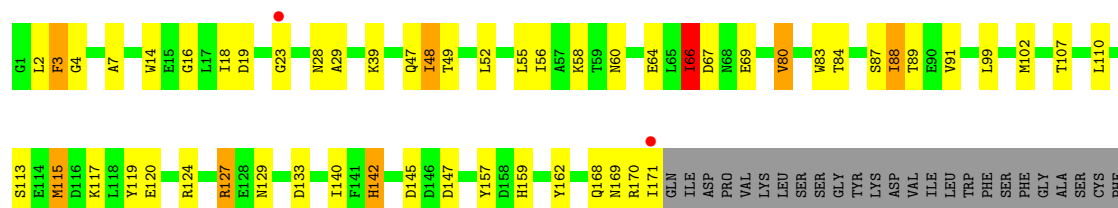
• Molecule 2: Hemagglutinin HA2 chain

Chain D: 51% 23% • 23%



• Molecule 2: Hemagglutinin HA2 chain

Chain F: 52% 21% • 23%



ILE
LEU
LEU
ALA
ILE
VAL
MET
GLY
LEU
VAL
PHE
ILE
CYS
VAL
LYS
ASN
GLY
ASN
MET
ARG
CYS
THR
ILE
CYS
ILE

- Molecule 3: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
GAL2
SIA3

- Molecule 3: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
GAL2
SIA3

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

Chain I:  100%

MAG1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.57Å 117.87Å 119.86Å 90.00° 124.21° 90.00°	Depositor
Resolution (Å)	50.01 – 3.55 50.01 – 3.55	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.01-3.55) 91.9 (50.01-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.260 (Not available) , 0.230	Depositor DCC
R_{free} test set	1297 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.000 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.000 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.000 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.000 for $-h+k-l, -l, -k$ 0.000 for $-h-k-l, l, k$ 0.000 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.000 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.398 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.390 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.000 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11670	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

¹Intensities estimated from amplitudes.

²Theoretical 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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GAL, SIA, 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	1.16	6/2462 (0.2%)	1.23	11/3329 (0.3%)
1	C	1.16	5/2462 (0.2%)	1.24	11/3329 (0.3%)
1	E	1.16	6/2462 (0.2%)	1.23	11/3329 (0.3%)
2	B	1.13	1/1413 (0.1%)	1.26	9/1903 (0.5%)
2	D	1.14	1/1413 (0.1%)	1.26	12/1903 (0.6%)
2	F	1.14	1/1413 (0.1%)	1.26	10/1903 (0.5%)
All	All	1.15	20/11625 (0.2%)	1.24	64/15696 (0.4%)

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	1
1	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	6

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	268	CYS	CB-SG	-6.97	1.58	1.81
2	F	66	ILE	N-CA	6.84	1.53	1.46
2	D	66	ILE	N-CA	6.30	1.52	1.46
2	B	66	ILE	N-CA	6.15	1.52	1.46
1	E	177	VAL	CA-C	5.82	1.60	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	74	ALA	N-CA-C	7.77	120.67	108.79
1	A	74	ALA	N-CA-C	7.73	120.61	108.79
1	C	74	ALA	N-CA-C	7.60	120.42	108.79
1	C	289	ASP	N-CA-C	-7.45	96.28	108.41
1	A	289	ASP	N-CA-C	-7.31	96.50	108.41

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Peptide
2	B	66	ILE	Peptide
1	C	122	THR	Peptide
2	D	66	ILE	Peptide
1	E	122	THR	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	2416	0	2382	41	0
1	C	2416	0	2382	48	0
1	E	2416	0	2382	44	0
2	B	1389	0	1300	26	0
2	D	1389	0	1300	28	0
2	F	1389	0	1300	30	0
3	G	45	0	38	0	0
3	H	45	0	38	0	0
4	I	25	0	20	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	1	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	12	0	12	0	0
6	E	12	0	12	0	0
7	E	20	0	17	0	0
All	All	11670	0	11273	185	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 8.

The worst 5 of 185 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:A:256:MET:HA	1:A:256:MET:HE3	1.69	0.74
1:E:256:MET:HA	1:E:256:MET:HE3	1.69	0.73
1:C:256:MET:HE3	1:C:256:MET:HA	1.69	0.73
1:E:139:GLU:OE1	1:E:247:ARG:HD3	1.93	0.69
1:A:139:GLU:OE1	1:A:247:ARG:HD3	1.93	0.68

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	314/321 (98%)	268 (85%)	35 (11%)	11 (4%)	3	23
1	C	314/321 (98%)	268 (85%)	36 (12%)	10 (3%)	3	24
1	E	314/321 (98%)	268 (85%)	36 (12%)	10 (3%)	3	24
2	B	169/221 (76%)	140 (83%)	20 (12%)	9 (5%)	1	14
2	D	169/221 (76%)	140 (83%)	20 (12%)	9 (5%)	1	14
2	F	169/221 (76%)	140 (83%)	21 (12%)	8 (5%)	2	17
All	All	1449/1626 (89%)	1224 (84%)	168 (12%)	57 (4%)	2	20

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ALA
2	B	127	ARG
2	B	142	HIS
2	D	29	ALA
2	D	127	ARG

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	267/271 (98%)	222 (83%)	45 (17%)	2	13
1	C	267/271 (98%)	224 (84%)	43 (16%)	2	14
1	E	267/271 (98%)	222 (83%)	45 (17%)	2	13
2	B	145/189 (77%)	129 (89%)	16 (11%)	6	27
2	D	145/189 (77%)	131 (90%)	14 (10%)	8	31
2	F	145/189 (77%)	132 (91%)	13 (9%)	9	33
All	All	1236/1380 (90%)	1060 (86%)	176 (14%)	3	19

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	133	ASP
1	E	182	GLN
1	E	10	VAL
1	E	85	ASP
1	E	237	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	263	GLN
2	D	159	HIS

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Mol	Chain	Res	Type
2	F	154	ASN
2	D	154	ASN
1	E	8	HIS

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 ⓘ

8 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	3	14,14,15	1.30	2 (14%)	17,19,21	2.58	6 (35%)
3	GAL	G	2	3	11,11,12	0.74	0	15,15,17	1.32	3 (20%)
3	SIA	G	3	3	20,20,21	1.38	3 (15%)	21,28,31	1.94	8 (38%)
3	NAG	H	1	3	14,14,15	1.31	2 (14%)	17,19,21	2.58	6 (35%)
3	GAL	H	2	3	11,11,12	0.73	0	15,15,17	1.32	3 (20%)
3	SIA	H	3	3	20,20,21	1.37	3 (15%)	21,28,31	1.95	8 (38%)
4	NAG	I	1	4	14,14,15	1.28	2 (14%)	17,19,21	2.65	5 (29%)
4	GAL	I	2	4	11,11,12	0.61	0	15,15,17	1.27	2 (13%)

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	SIA	C7-C6	3.52	1.57	1.52
3	H	3	SIA	C7-C6	3.46	1.57	1.52
4	I	1	NAG	O6-C6	2.73	1.53	1.42
3	H	1	NAG	C3-C2	2.23	1.57	1.52
3	H	3	SIA	C8-C7	2.21	1.57	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O3-C3-C4	7.49	128.02	110.38
3	H	1	NAG	O3-C3-C2	7.46	124.89	109.40
3	G	1	NAG	O3-C3-C2	7.45	124.88	109.40
4	I	1	NAG	C4-C3-C2	4.32	117.35	111.02
3	H	3	SIA	C6-C5-N5	3.95	117.20	110.91

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

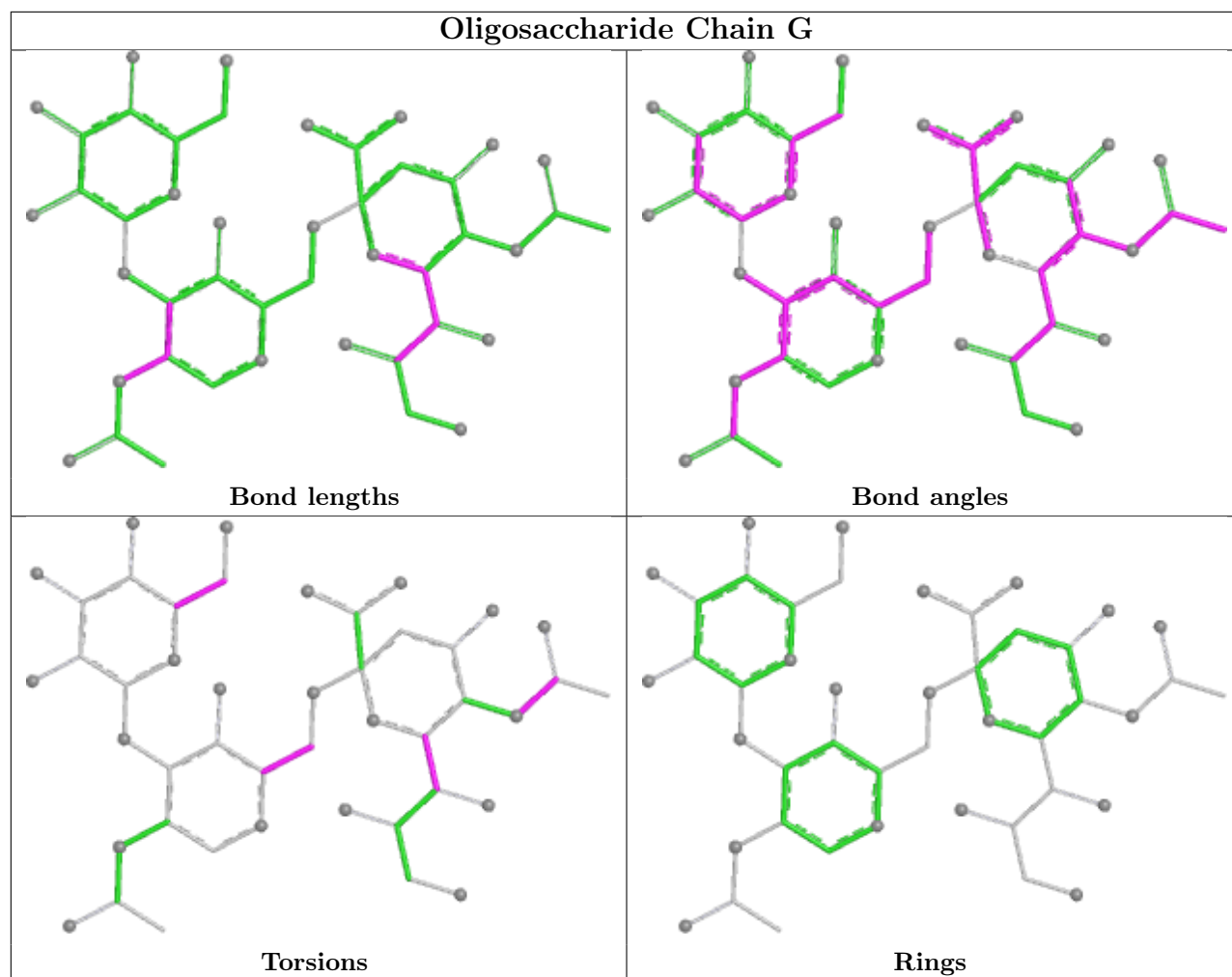
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	G	2	GAL	O5-C5-C6-O6
3	H	2	GAL	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

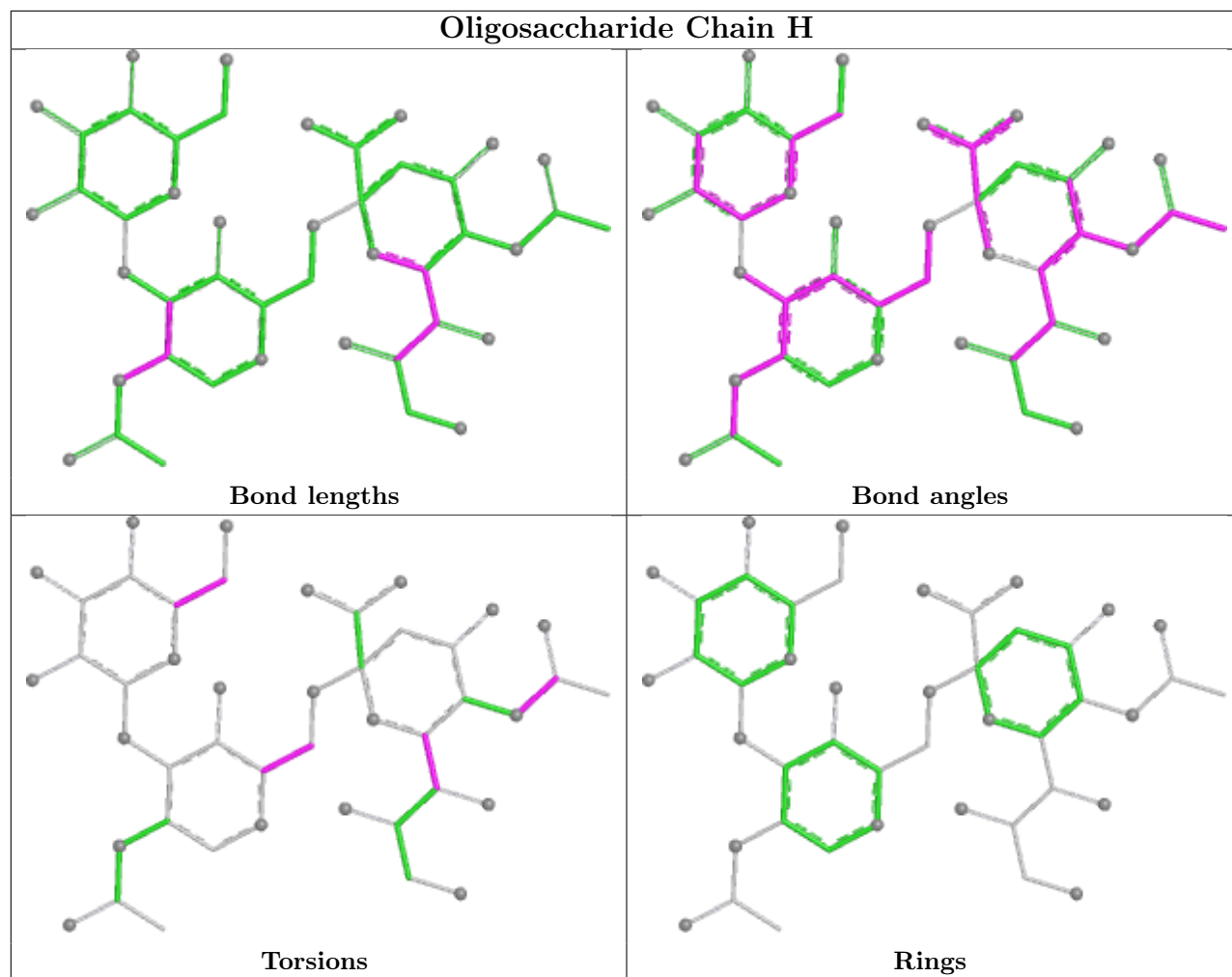
There are no ring outliers.

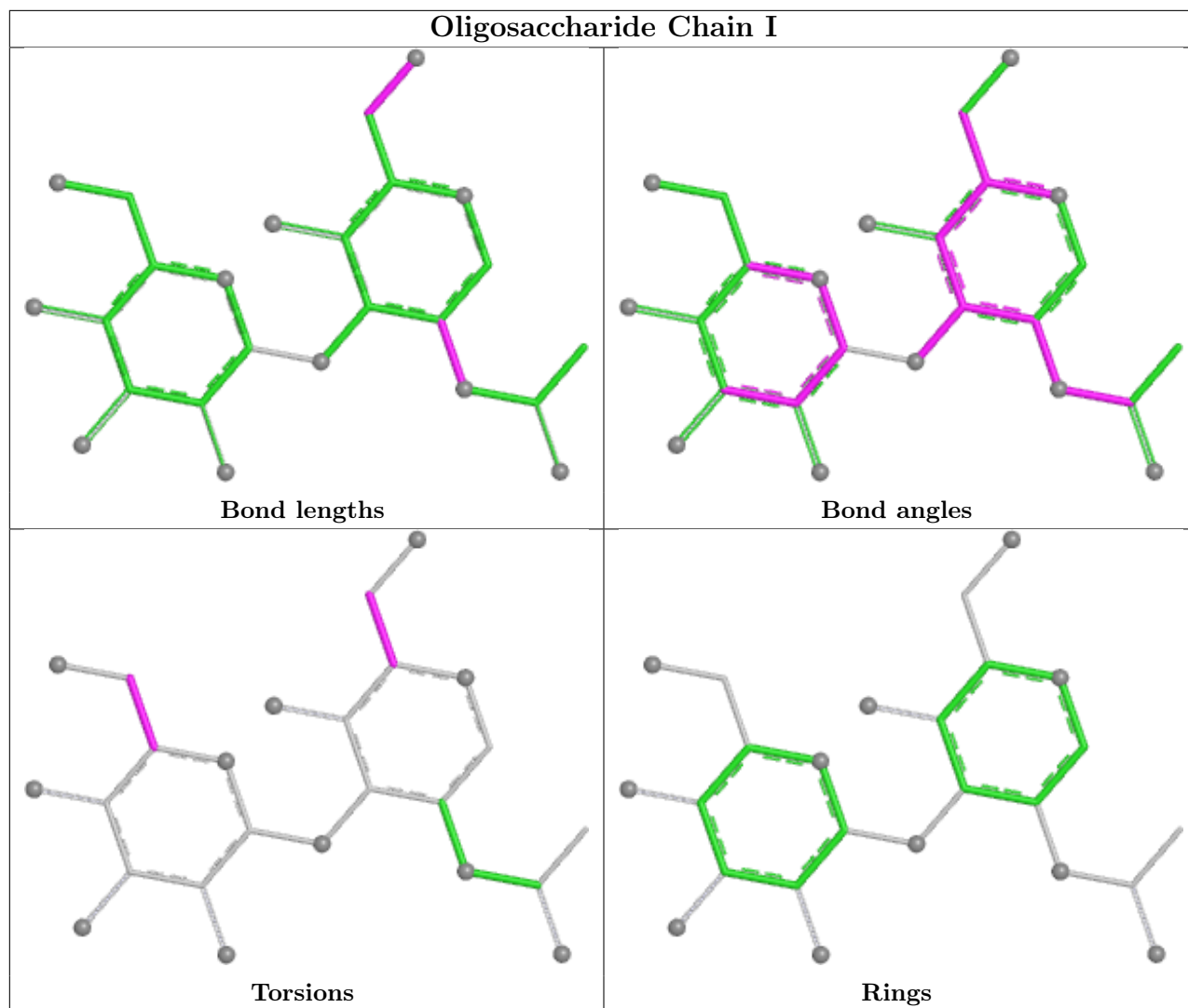
No monomer is involved in short contacts.

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](#)

10 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	NAG	F	301	2	14,14,15	1.80	3 (21%)	17,19,21	3.83	10 (58%)
5	NAG	B	301	2	14,14,15	1.27	1 (7%)	17,19,21	2.69	6 (35%)
6	GAL	E	405	-	12,12,12	0.73	0	17,17,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	401	1	14,14,15	1.10	1 (7%)	17,19,21	2.09	6 (35%)
5	NAG	E	401	1	14,14,15	1.06	1 (7%)	17,19,21	1.73	1 (5%)
5	NAG	A	401	1	14,14,15	1.25	1 (7%)	17,19,21	2.29	5 (29%)
6	GAL	A	405	-	12,12,12	0.82	0	17,17,17	1.17	1 (5%)
5	NAG	D	301	2	14,14,15	1.64	2 (14%)	17,19,21	3.02	9 (52%)
7	SIA	E	402	-	20,20,21	1.58	3 (15%)	21,28,31	2.13	7 (33%)
6	GAL	C	405	-	12,12,12	0.82	0	17,17,17	1.17	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	NAG	F	301	2	-	2/6/23/26	0/1/1/1
5	NAG	B	301	2	-	2/6/23/26	0/1/1/1
6	GAL	E	405	-	-	0/2/22/22	0/1/1/1
5	NAG	C	401	1	-	3/6/23/26	0/1/1/1
5	NAG	E	401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	401	1	-	4/6/23/26	0/1/1/1
6	GAL	A	405	-	-	2/2/22/22	0/1/1/1
5	NAG	D	301	2	-	0/6/23/26	0/1/1/1
7	SIA	E	402	-	-	3/18/34/38	0/1/1/1
6	GAL	C	405	-	-	2/2/22/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	402	SIA	C7-C6	4.43	1.58	1.52
5	F	301	NAG	O5-C1	3.80	1.50	1.43
7	E	402	SIA	O6-C6	3.13	1.48	1.44
5	F	301	NAG	C1-C2	3.10	1.56	1.52
5	D	301	NAG	C1-C2	3.08	1.56	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	NAG	C1-C2-N2	10.55	127.05	110.43
5	B	301	NAG	C1-O5-C5	8.61	123.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	NAG	C1-C2-N2	8.06	123.14	110.43
5	F	301	NAG	C1-O5-C5	6.93	121.47	112.19
5	A	401	NAG	C2-N2-C7	6.84	132.06	122.90

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

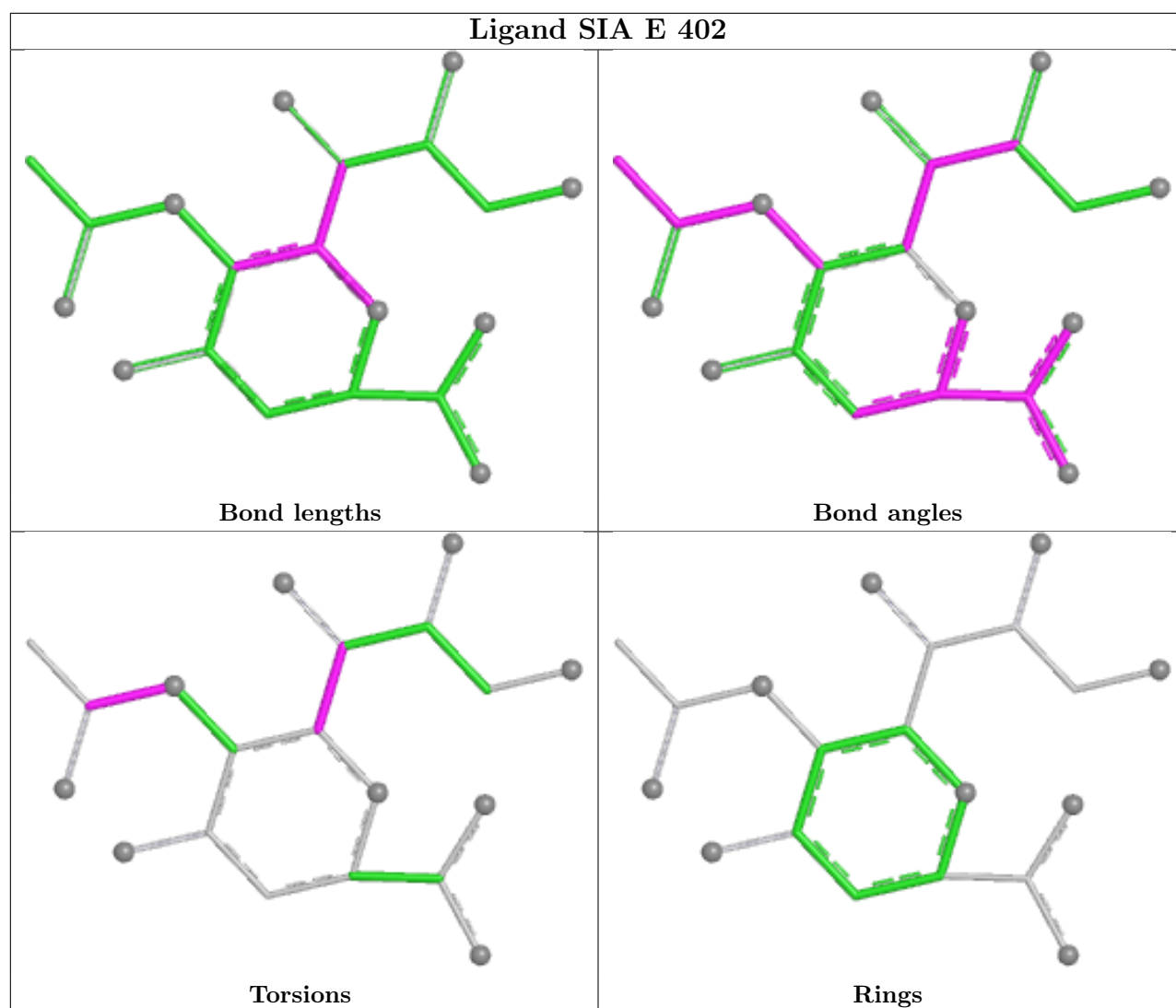
Mol	Chain	Res	Type	Atoms
5	C	401	NAG	C1-C2-N2-C7
7	E	402	SIA	O6-C6-C7-O7
5	F	301	NAG	O5-C5-C6-O6
5	F	301	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	316/321 (98%)	0.01	1 (0%)	90 74	19, 59, 116, 145	1 (0%)
1	C	316/321 (98%)	-0.02	3 (0%)	81 56	18, 60, 112, 145	1 (0%)
1	E	316/321 (98%)	0.02	3 (0%)	81 56	20, 59, 116, 148	1 (0%)
2	B	171/221 (77%)	0.29	1 (0%)	85 63	17, 94, 134, 150	0
2	D	171/221 (77%)	0.28	2 (1%)	76 49	20, 90, 135, 153	0
2	F	171/221 (77%)	0.29	2 (1%)	76 49	22, 95, 134, 157	0
All	All	1461/1626 (89%)	0.10	12 (0%)	82 58	17, 71, 128, 157	3 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	149	ASN	3.2
1	A	149	ASN	2.9
1	C	149	ASN	2.7
2	D	138	PHE	2.6
2	B	35	ALA	2.2

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

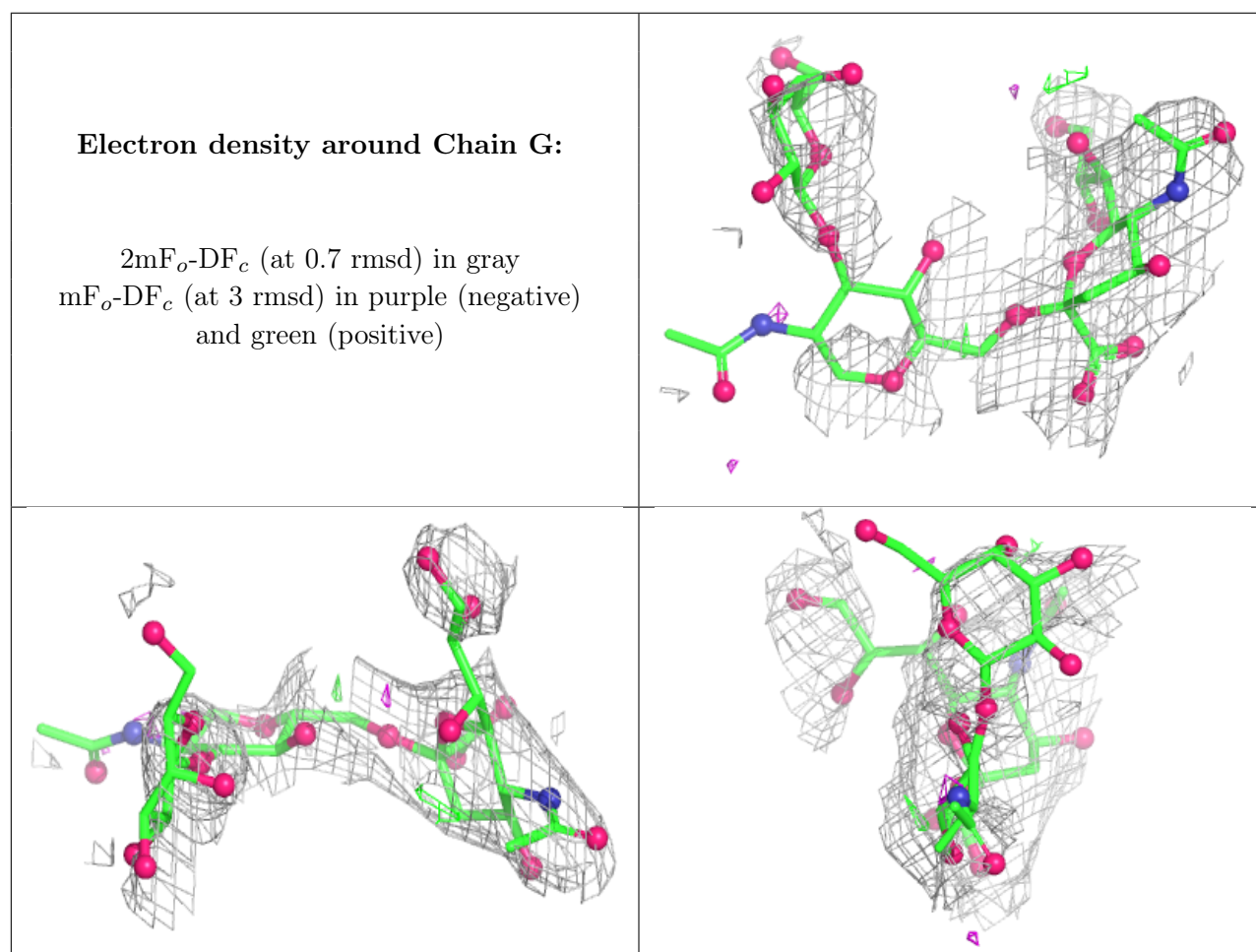
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

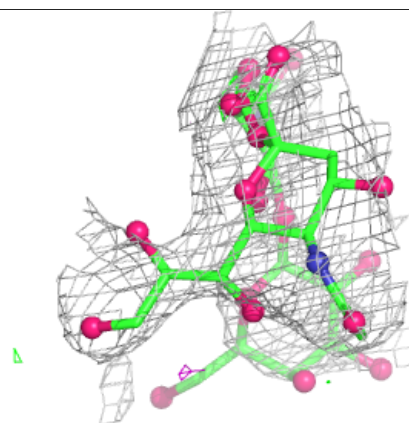
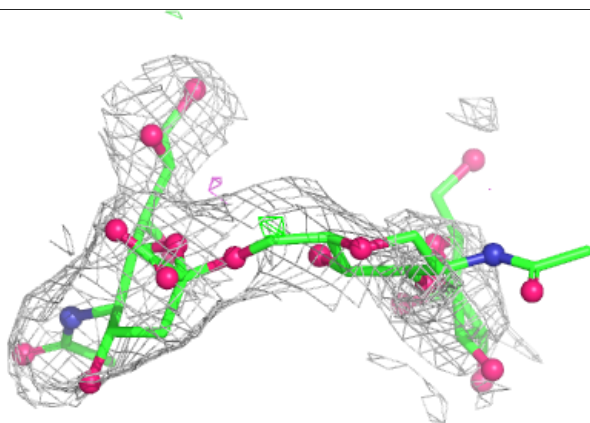
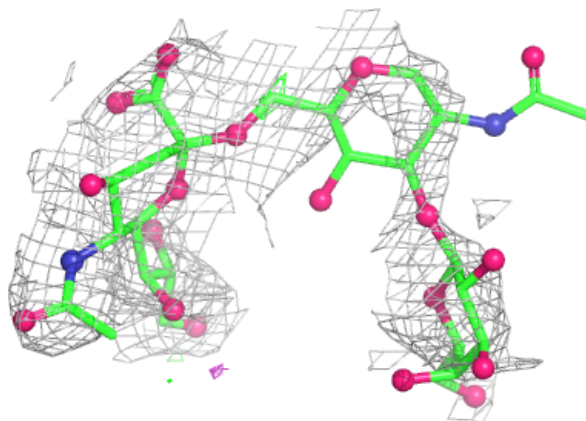
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	1	14/15	0.49	0.19	129,144,153,156	0
4	NAG	I	1	14/15	0.51	0.18	130,142,151,161	0
3	NAG	G	1	14/15	0.53	0.18	129,144,153,156	0
3	GAL	H	2	11/12	0.67	0.15	143,153,154,154	0
4	GAL	I	2	11/12	0.67	0.14	153,161,163,165	0
3	GAL	G	2	11/12	0.68	0.15	143,153,154,154	0
3	SIA	G	3	20/21	0.77	0.14	93,117,127,128	0
3	SIA	H	3	20/21	0.77	0.15	93,117,127,128	0

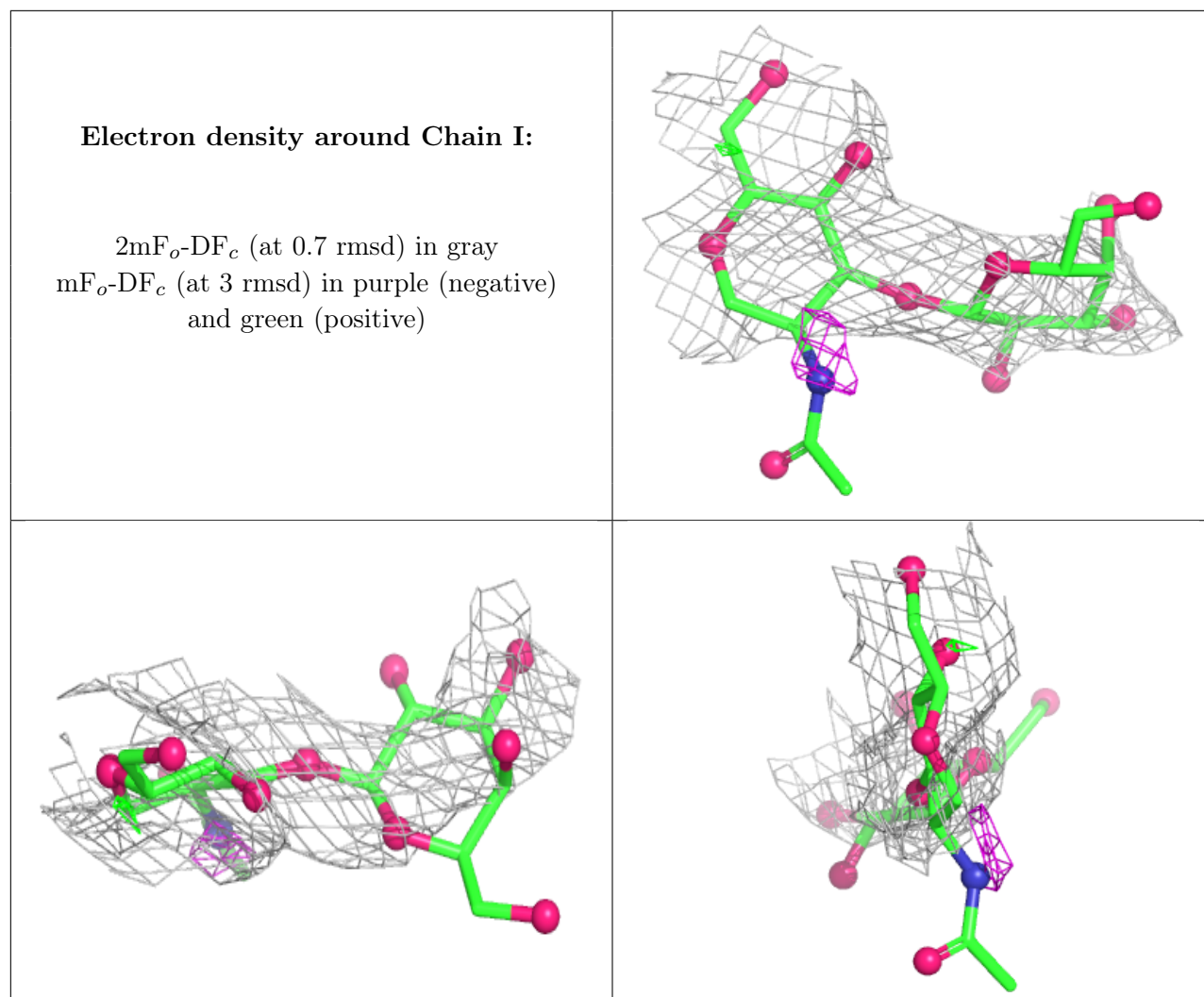
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GAL	C	405	12/12	0.42	0.16	122,133,139,140	0
6	GAL	A	405	12/12	0.55	0.13	122,133,139,140	0
6	GAL	E	405	12/12	0.57	0.13	121,137,142,142	0
5	NAG	A	401	14/15	0.60	0.14	111,124,135,144	0
5	NAG	C	401	14/15	0.66	0.12	115,124,137,137	0
5	NAG	E	401	14/15	0.75	0.11	113,132,143,150	0
7	SIA	E	402	20/21	0.84	0.14	101,121,126,129	0
5	NAG	D	301	14/15	0.87	0.11	50,55,61,65	0
5	NAG	F	301	14/15	0.87	0.11	54,60,63,67	0

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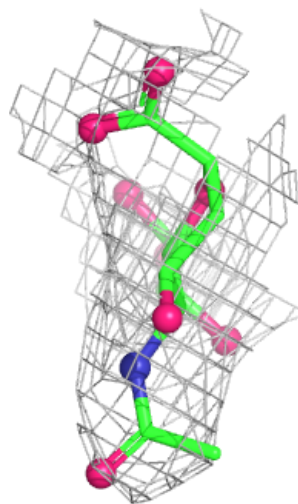
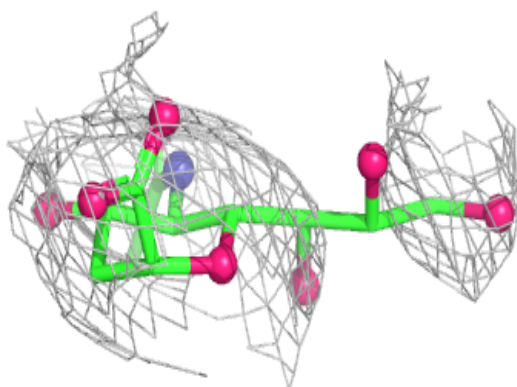
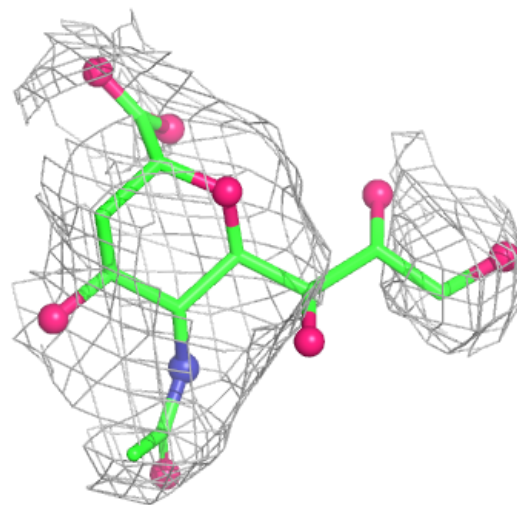
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	301	14/15	0.88	0.11	54,62,69,73	0

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 E 402:

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 ⓘ

There are no such residues in this entry.