wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 06:53 PM EDT

PDB ID	:	4JTV
Title	:	Crystal structure of 2009 pandemic influenza virus hemagglutinin complexed with human receptor analogue LSTc
Authors	:	Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.
Deposited on	:	2013-03-24
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

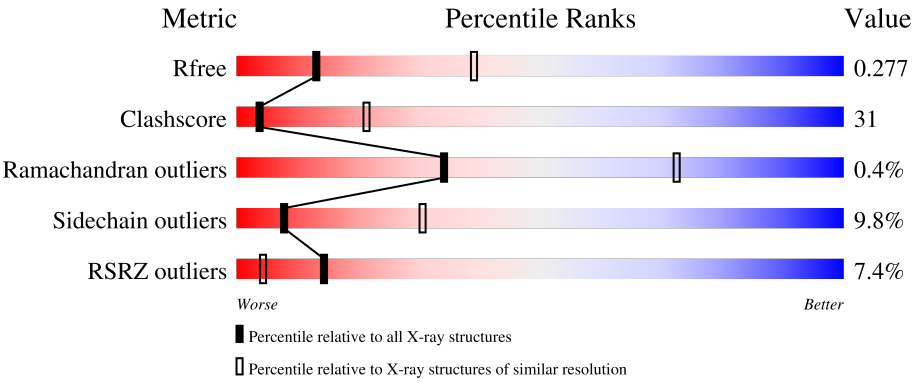
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 >=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 <=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	3% 48% 45% 7%
1	C	321	6% 52% 40% 7%
1	E	321	2% 56% 38% 5%
1	G	321	5% 60% 36%
1	I	321	3% 52% 40% 7%

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Mol	Chain	Length	Quality of chain
1	K	321	6% 55% 40%
2	B	162	9% 59% 36% 6%
2	D	162	9% 60% 34% 6%
2	F	162	17% 66% 28% 5%
2	H	162	10% 61% 35%
2	J	162	2% 62% 35%
2	L	162	35% 51% 43% 6%
3	M	3	67% 33%
3	Q	3	67% 33%
3	R	3	67% 33%
4	N	4	75% 25%
4	P	4	75% 25%
5	O	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	G	601	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23528 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.

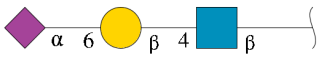
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	C	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	E	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	G	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	I	321	Total	C	N	O	S	0	0	0
			2510	1587	433	479	11			
1	K	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	D	162	Total	C	N	O	S	0	0	0
			1300	818	219	257	6			
2	F	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			
2	H	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	J	162	Total	C	N	O	S	0	0	0
			1300	818	219	257	6			
2	L	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	M	3	Total C N O 45 25 2 18	0	0	0
3	Q	3	Total C N O 45 25 2 18	0	0	0
3	R	3	Total C N O 45 25 2 18	0	0	0

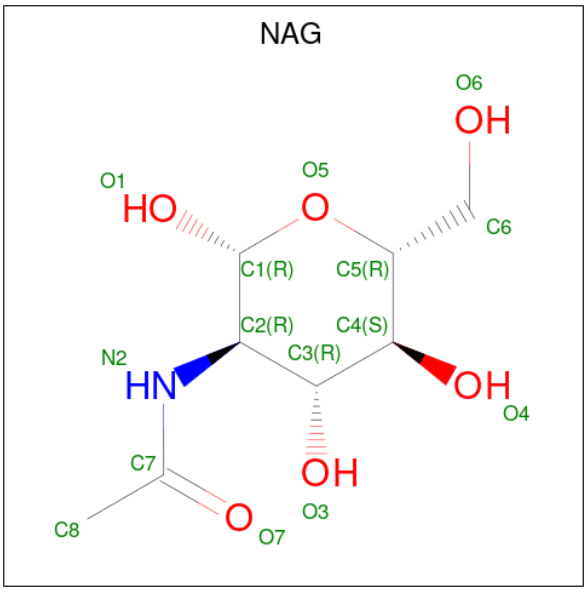
- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	N	4	Total C N O 56 31 2 23	0	0	0
4	P	4	Total C N O 56 31 2 23	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

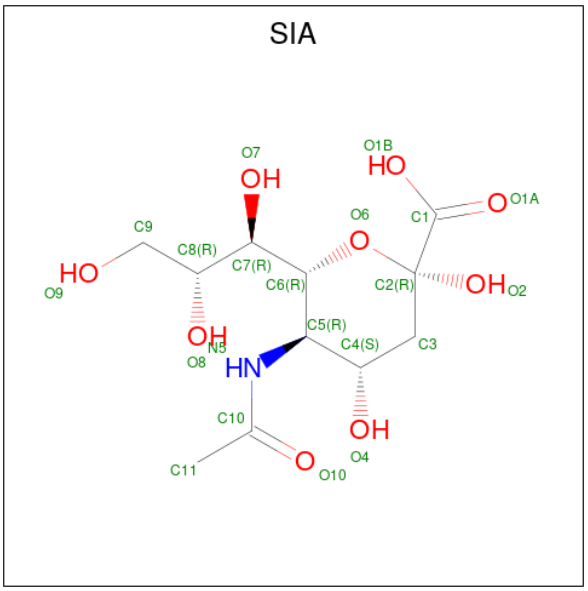
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	O	2	Total C N O 28 16 2 10	0	0	0

- 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	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0
6	G	1	Total C N O 14 8 1 5	0	0

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	40	Total O 40 40	0	0
8	B	13	Total O 13 13	0	0
8	C	29	Total O 29 29	0	0
8	D	13	Total O 13 13	0	0
8	E	31	Total O 31 31	0	0
8	F	7	Total O 7 7	0	0
8	G	19	Total O 19 19	0	0
8	H	13	Total O 13 13	0	0
8	I	35	Total O 35 35	0	0
8	J	18	Total O 18 18	0	0
8	K	25	Total O 25 25	0	0

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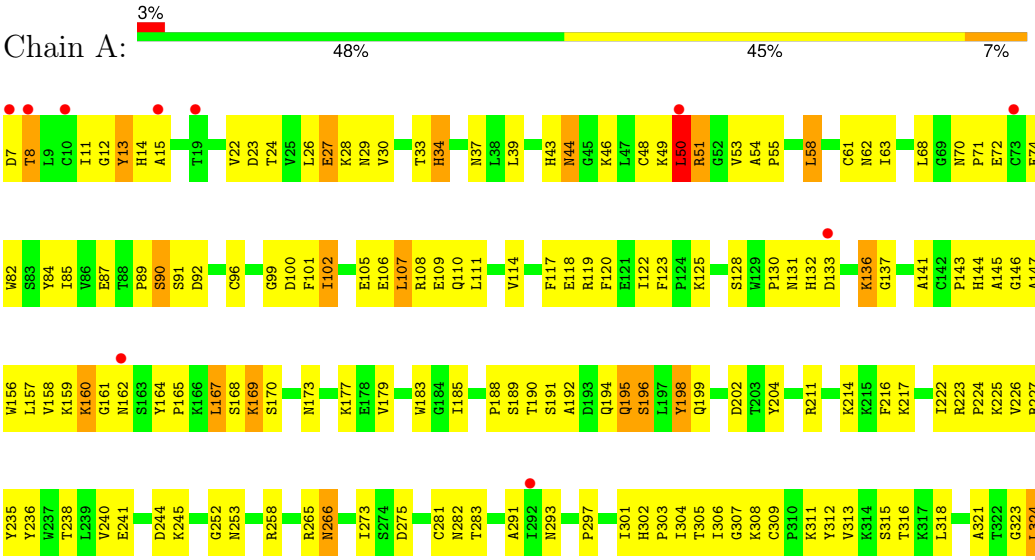
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	31	Total	O	0	0
			31	31		

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.

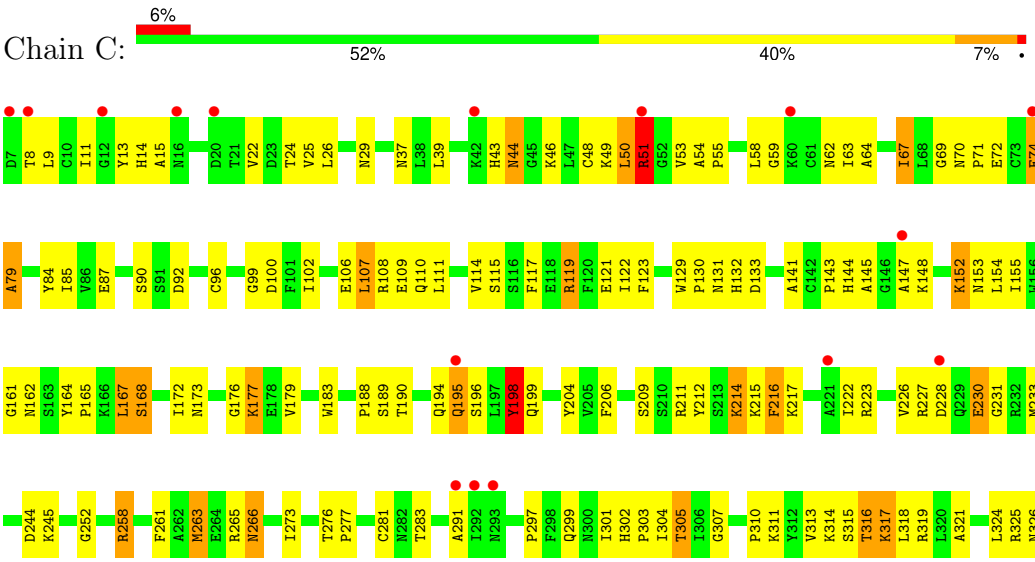
• Molecule 1: Hemagglutinin

Chain A:



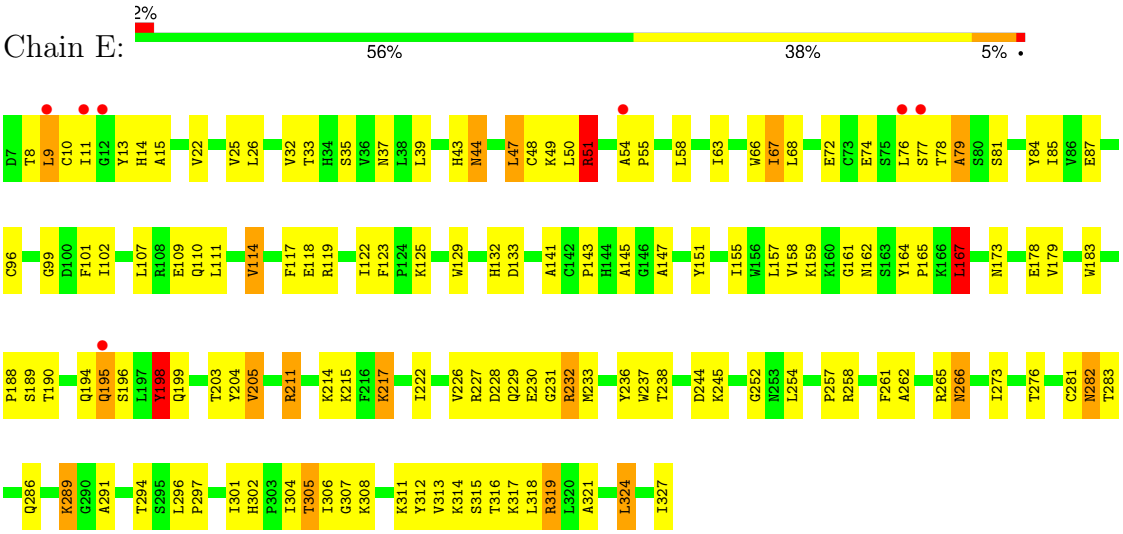
• Molecule 1: Hemagglutinin

Chain C:



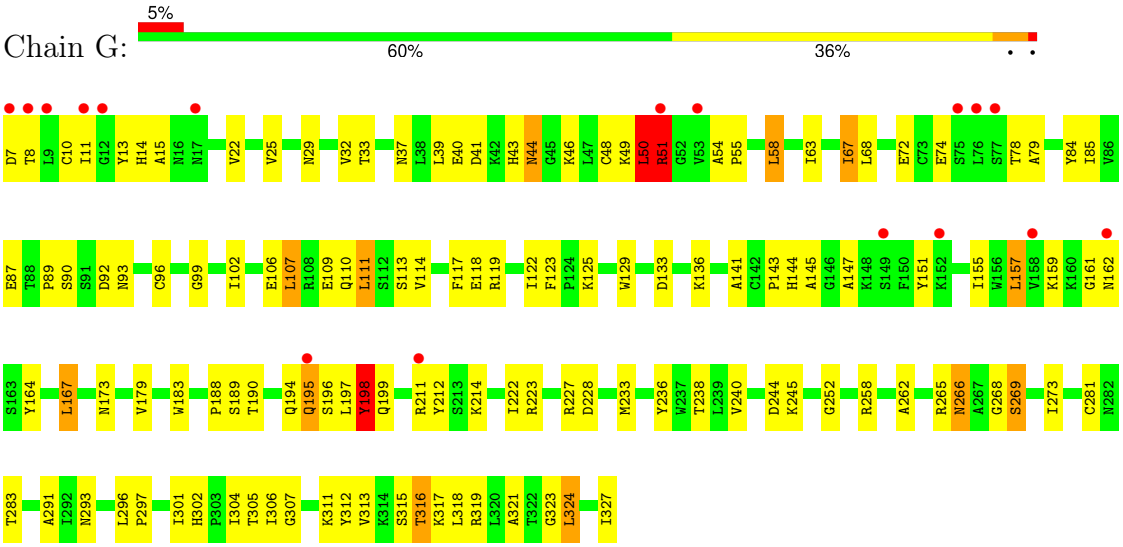
• Molecule 1: Hemagglutinin

Chain E:



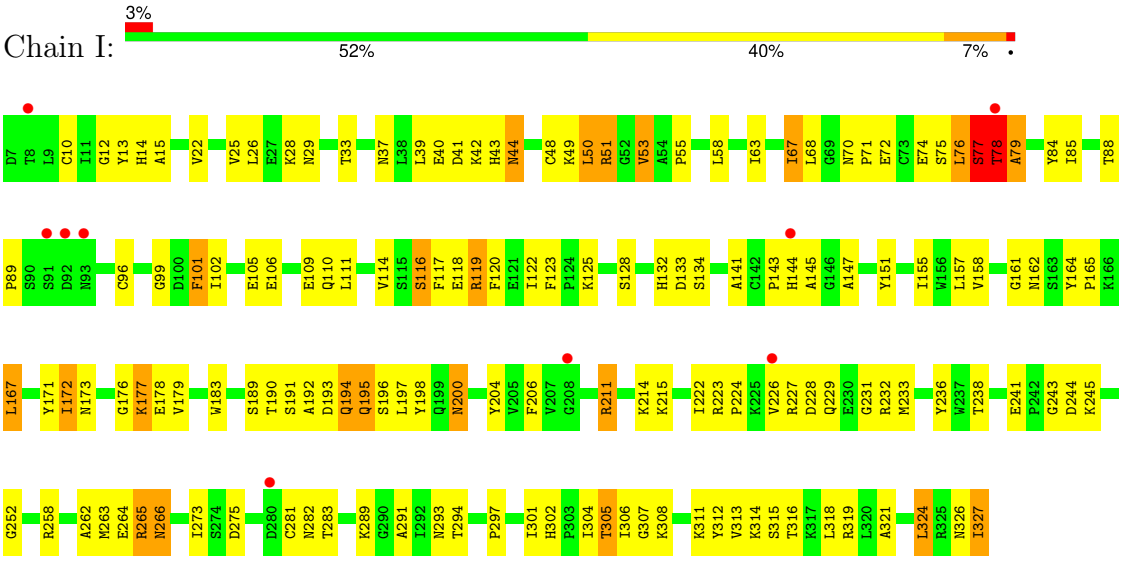
• Molecule 1: Hemagglutinin

Chain G:



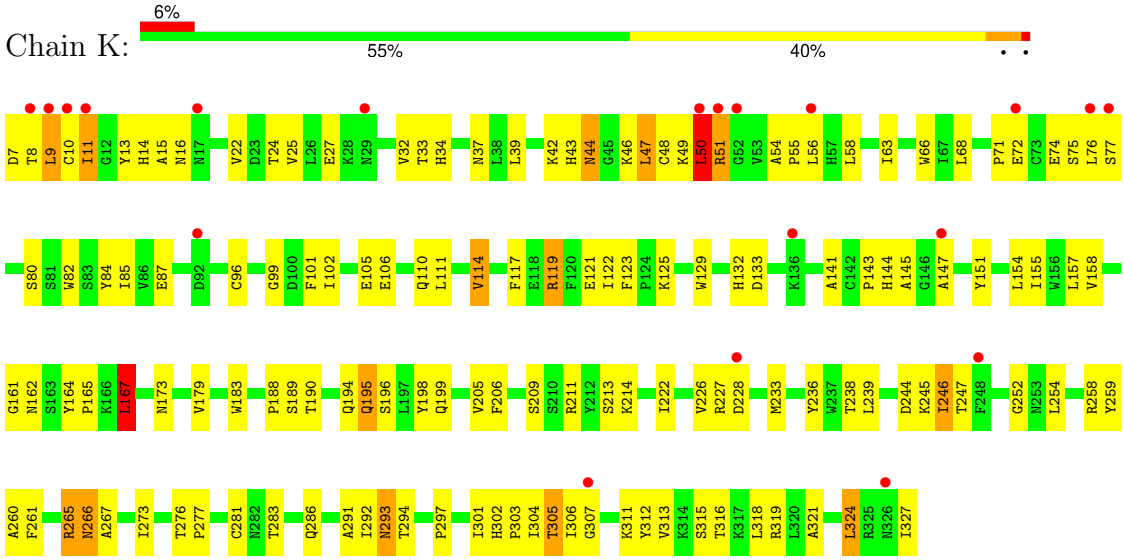
• Molecule 1: Hemagglutinin

Chain I:



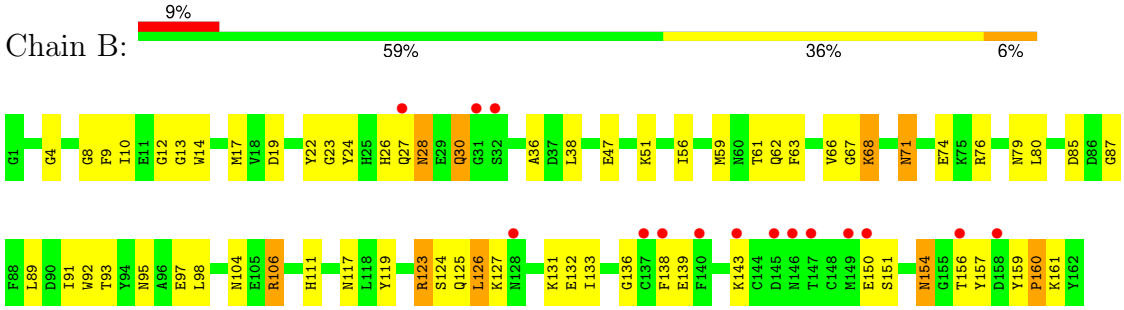
• Molecule 1: Hemagglutinin

Chain K:



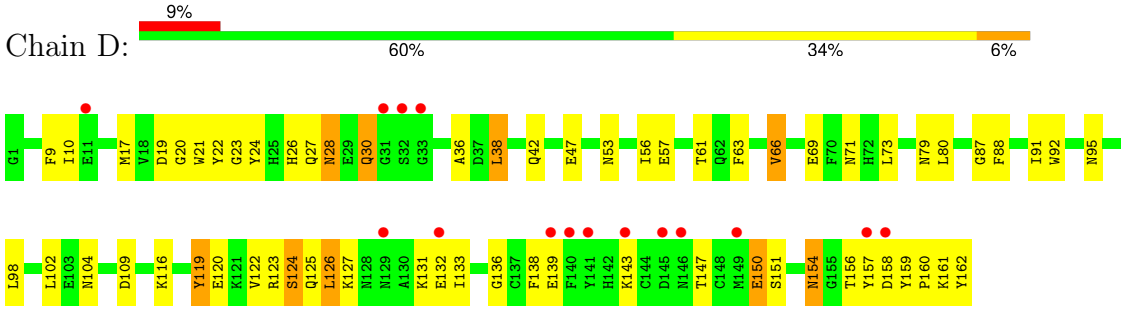
• Molecule 2: Hemagglutinin

Chain B:



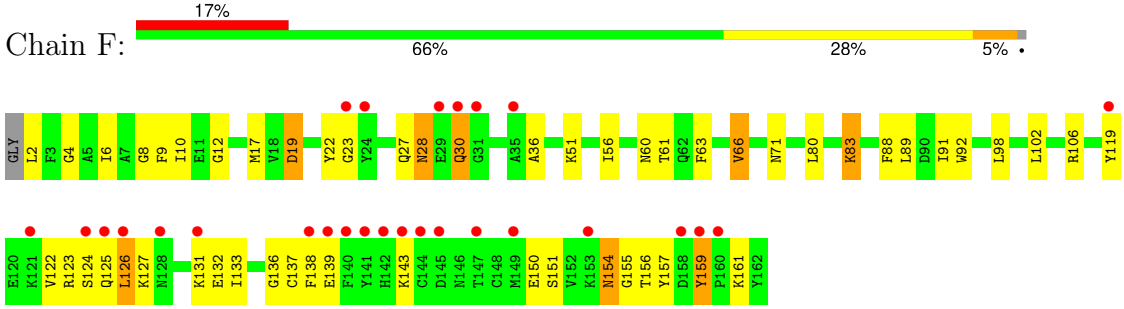
• Molecule 2: Hemagglutinin

Chain D:



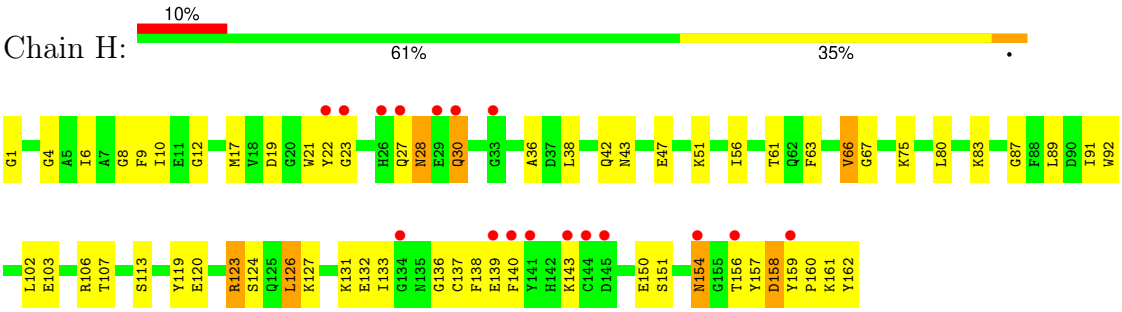
• Molecule 2: Hemagglutinin

Chain F:



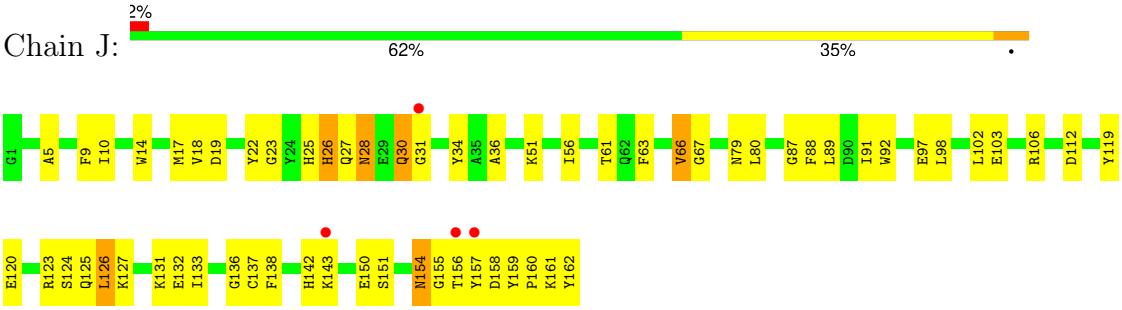
• Molecule 2: Hemagglutinin

Chain H:



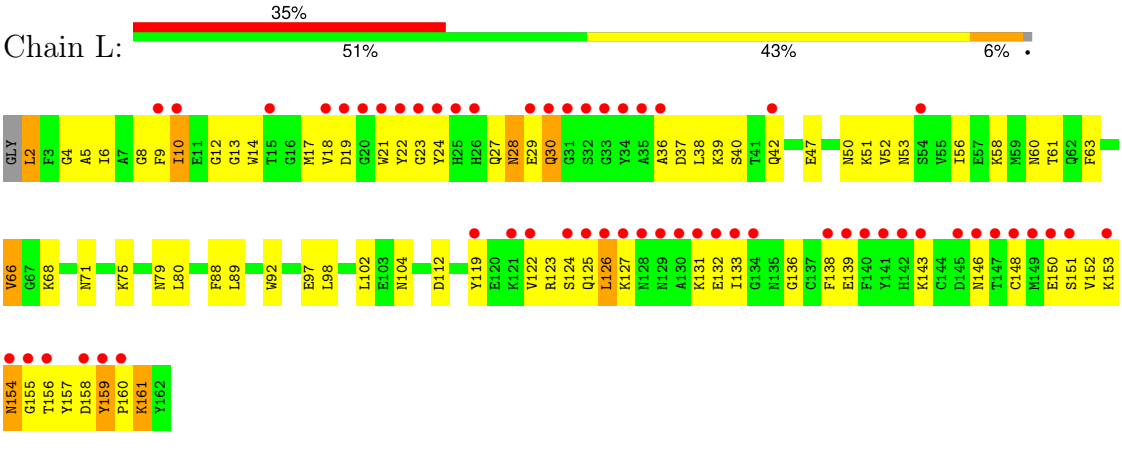
• Molecule 2: Hemagglutinin

Chain J:



• Molecule 2: Hemagglutinin

Chain L:

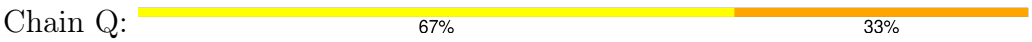


• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

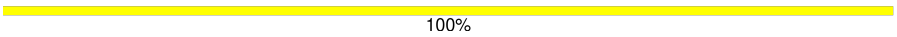
Chain N:

• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain P:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.72Å 117.32Å 117.39Å 61.78° 81.82° 77.42°	Depositor
Resolution (Å)	38.39 – 3.00 49.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (38.39-3.00) 87.5 (49.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.224 , 0.275 0.229 , 0.277	Depositor DCC
R_{free} test set	2711 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23528	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG, 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	0.57	0/2568	0.75	5/3488 (0.1%)
1	C	0.55	0/2572	0.69	8/3493 (0.2%)
1	E	0.39	0/2572	0.58	4/3493 (0.1%)
1	G	0.33	0/2568	0.77	9/3488 (0.3%)
1	I	0.47	0/2573	0.63	3/3495 (0.1%)
1	K	0.33	0/2572	0.63	5/3493 (0.1%)
2	B	0.48	0/1333	0.54	1/1797 (0.1%)
2	D	0.38	0/1328	0.45	0/1791
2	F	0.26	0/1330	0.46	0/1794
2	H	0.26	0/1333	0.49	1/1797 (0.1%)
2	J	0.43	0/1328	0.48	0/1791
2	L	0.26	0/1330	0.53	1/1794 (0.1%)
All	All	0.42	0/23407	0.62	37/31714 (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
1	I	0	1

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	119	ARG	NE-CZ-NH1	-16.56	112.02	120.30
1	A	119	ARG	NE-CZ-NH2	16.50	128.55	120.30
1	A	119	ARG	NE-CZ-NH1	-16.32	112.14	120.30
1	G	119	ARG	NE-CZ-NH2	15.97	128.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	212	TYR	N-CA-CB	11.91	132.04	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	77	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	2505	0	2444	227	0
1	C	2509	0	2451	186	0
1	E	2509	0	2451	159	4
1	G	2505	0	2445	137	0
1	I	2510	0	2456	183	0
1	K	2509	0	2452	188	0
2	B	1305	0	1228	97	0
2	D	1300	0	1216	81	0
2	F	1302	0	1226	65	0
2	H	1305	0	1228	73	0
2	J	1300	0	1216	89	0
2	L	1302	0	1226	126	4
3	M	45	0	38	4	0
3	Q	45	0	38	3	0
3	R	45	0	38	0	0
4	N	56	0	47	1	0
4	P	56	0	47	2	0
5	O	28	0	25	3	0
6	A	56	0	52	6	0
6	C	14	0	13	2	0
6	G	28	0	26	5	0
7	G	20	0	17	1	0
8	A	40	0	0	59	0
8	B	13	0	0	11	0
8	C	29	0	0	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	13	0	0	6	0
8	E	31	0	0	27	0
8	F	7	0	0	6	0
8	G	19	0	0	22	0
8	H	13	0	0	22	0
8	I	35	0	0	32	0
8	J	18	0	0	22	0
8	K	25	0	0	47	0
8	L	31	0	0	48	0
All	All	23528	0	22380	1414	4

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 31.

The worst 5 of 1414 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:11:ILE:HD13	2:D:24:TYR:CD2	1.53	1.42
1:I:190:THR:HG21	1:I:193:ASP:OD1	1.24	1.35
1:K:106:GLU:HB3	8:K:915:HOH:O	1.20	1.34
2:L:19:ASP:HA	8:L:228:HOH:O	1.33	1.28
1:A:8:THR:HG22	2:B:138:PHE:O	1.18	1.27

All (4) 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:E:119:ARG:NH2	2:L:38:LEU:CD2[1_565]	1.96	0.24
1:E:79:ALA:N	2:L:150:GLU:OE2[1_565]	2.01	0.19
1:E:258:ARG:NH2	2:L:42:GLN:OE1[1_565]	2.04	0.16
1:E:81:SER:OG	2:L:146:ASN:OD1[1_565]	2.12	0.08

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	319/321 (99%)	295 (92%)	23 (7%)	1 (0%)	41 76
1	C	319/321 (99%)	296 (93%)	19 (6%)	4 (1%)	12 45
1	E	319/321 (99%)	295 (92%)	23 (7%)	1 (0%)	41 76
1	G	319/321 (99%)	292 (92%)	27 (8%)	0	100 100
1	I	319/321 (99%)	291 (91%)	26 (8%)	2 (1%)	25 64
1	K	319/321 (99%)	290 (91%)	29 (9%)	0	100 100
2	B	160/162 (99%)	146 (91%)	13 (8%)	1 (1%)	25 64
2	D	160/162 (99%)	143 (89%)	16 (10%)	1 (1%)	25 64
2	F	159/162 (98%)	145 (91%)	14 (9%)	0	100 100
2	H	160/162 (99%)	146 (91%)	14 (9%)	0	100 100
2	J	160/162 (99%)	144 (90%)	16 (10%)	0	100 100
2	L	159/162 (98%)	145 (91%)	13 (8%)	1 (1%)	25 64
All	All	2872/2898 (99%)	2628 (92%)	233 (8%)	11 (0%)	34 72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	160	PRO
1	A	146	GLY
1	C	77	SER
1	C	78	THR
1	C	161	GLY

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	281/282 (100%)	248 (88%)	33 (12%)	5 22
1	C	282/282 (100%)	248 (88%)	34 (12%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	282/282 (100%)	254 (90%)	28 (10%)	8 30
1	G	281/282 (100%)	258 (92%)	23 (8%)	11 39
1	I	282/282 (100%)	247 (88%)	35 (12%)	4 20
1	K	282/282 (100%)	255 (90%)	27 (10%)	8 32
2	B	139/139 (100%)	128 (92%)	11 (8%)	12 41
2	D	138/139 (99%)	125 (91%)	13 (9%)	8 32
2	F	139/139 (100%)	126 (91%)	13 (9%)	8 32
2	H	139/139 (100%)	130 (94%)	9 (6%)	17 50
2	J	138/139 (99%)	128 (93%)	10 (7%)	14 45
2	L	139/139 (100%)	128 (92%)	11 (8%)	12 41
All	All	2522/2526 (100%)	2275 (90%)	247 (10%)	8 30

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	305	THR
1	K	167	LEU
1	G	195	GLN
1	K	111	LEU
2	L	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	J	28	ASN
2	H	146	ASN
1	I	194	GLN
2	J	146	ASN

5.3.3 RNA

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)

19 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	M	1	3	14,14,15	0.60	0	17,19,21	0.96	0
3	GAL	M	2	3	11,11,12	0.62	0	15,15,17	0.78	0
3	SIA	M	3	3	20,20,21	0.73	0	21,28,31	3.60	2 (9%)
4	GAL	N	1	4	11,11,12	0.70	0	15,15,17	0.91	1 (6%)
4	NAG	N	2	4	14,14,15	0.58	0	17,19,21	1.27	2 (11%)
4	GAL	N	3	4	11,11,12	0.57	0	15,15,17	0.93	1 (6%)
4	SIA	N	4	4	20,20,21	0.66	0	21,28,31	3.85	2 (9%)
5	NAG	O	1	5,1	14,14,15	0.57	0	17,19,21	0.75	0
5	NAG	O	2	5	14,14,15	0.45	0	17,19,21	0.78	0
4	GAL	P	1	4	11,11,12	0.63	0	15,15,17	0.54	0
4	NAG	P	2	4	14,14,15	0.61	0	17,19,21	0.76	0
4	GAL	P	3	4	11,11,12	0.68	0	15,15,17	0.75	0
4	SIA	P	4	4	20,20,21	0.74	0	21,28,31	3.33	2 (9%)
3	NAG	Q	1	3	14,14,15	0.49	0	17,19,21	0.69	0
3	GAL	Q	2	3	11,11,12	0.71	0	15,15,17	1.11	2 (13%)
3	SIA	Q	3	3	20,20,21	0.63	0	21,28,31	3.53	3 (14%)
3	NAG	R	1	3	14,14,15	0.51	0	17,19,21	0.67	0
3	GAL	R	2	3	11,11,12	0.60	0	15,15,17	0.78	0
3	SIA	R	3	3	20,20,21	0.62	0	21,28,31	3.57	3 (14%)

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	M	1	3	-	0/6/23/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	3/18/34/38	0/1/1/1
4	GAL	N	1	4	-	1/2/19/22	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	GAL	N	3	4	-	0/2/19/22	0/1/1/1
4	SIA	N	4	4	-	3/18/34/38	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
4	GAL	P	1	4	-	0/2/19/22	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	GAL	P	3	4	-	0/2/19/22	0/1/1/1
4	SIA	P	4	4	-	3/18/34/38	0/1/1/1
3	NAG	Q	1	3	-	0/6/23/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	2/18/34/38	0/1/1/1
3	NAG	R	1	3	-	0/6/23/26	0/1/1/1
3	GAL	R	2	3	-	2/2/19/22	0/1/1/1
3	SIA	R	3	3	-	4/18/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	4	SIA	O6-C2-C3	-15.23	90.09	110.56
3	M	3	SIA	O6-C2-C3	-13.85	91.93	110.56
3	R	3	SIA	O6-C2-C3	-13.53	92.37	110.56
3	Q	3	SIA	O6-C2-C3	-13.51	92.39	110.56
4	P	4	SIA	O6-C2-C3	-12.98	93.11	110.56

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	2	GAL	C4-C5-C6-O6
3	R	2	GAL	O5-C5-C6-O6
3	M	3	SIA	C11-C10-N5-C5
3	M	3	SIA	O10-C10-N5-C5
3	Q	3	SIA	C11-C10-N5-C5

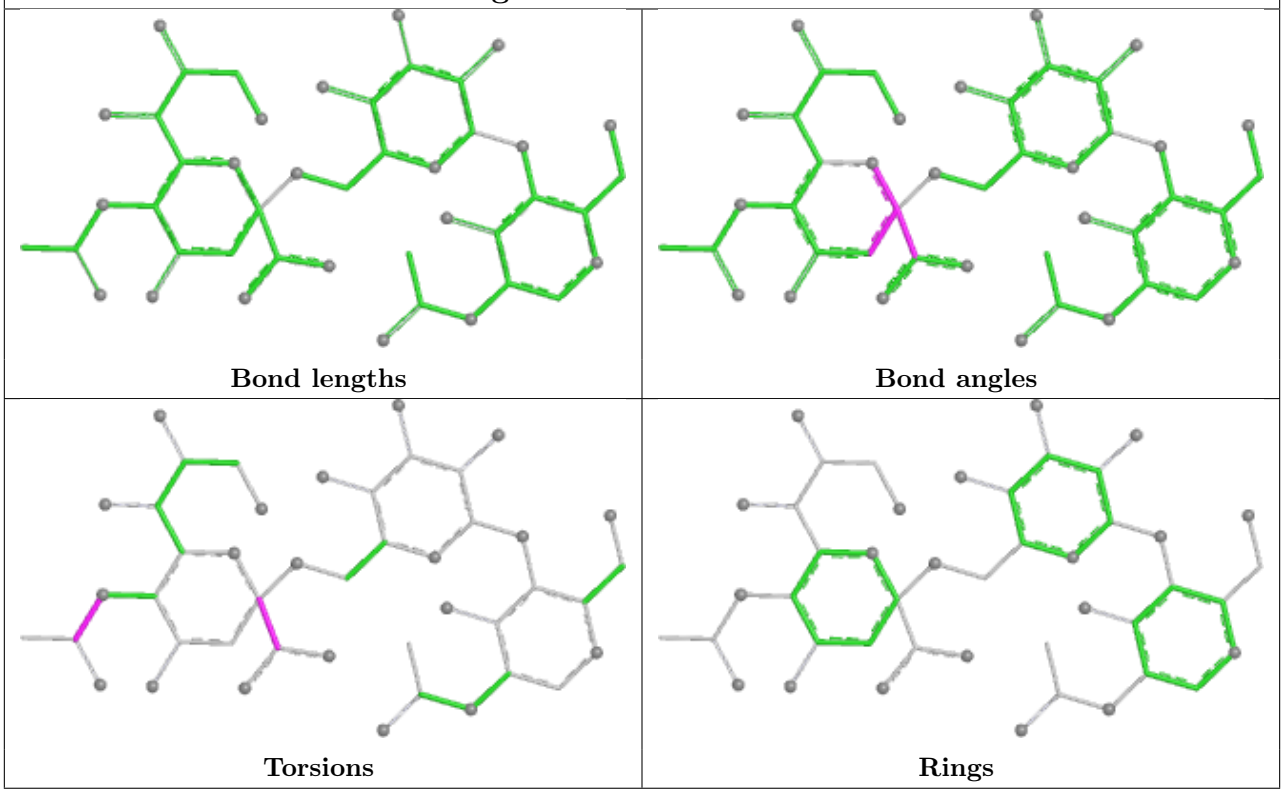
There are no ring outliers.

9 monomers are involved in 13 short contacts:

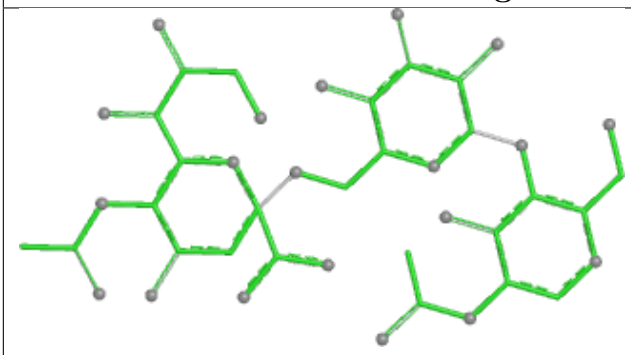
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GAL	1	0
3	Q	1	NAG	1	0
4	P	4	SIA	2	0
5	O	1	NAG	3	0
3	M	1	NAG	2	0
4	N	4	SIA	1	0
3	M	3	SIA	1	0
3	Q	3	SIA	3	0
5	O	2	NAG	1	0

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

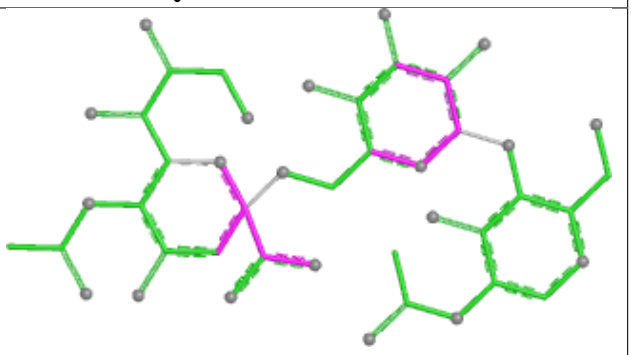
Oligosaccharide Chain M



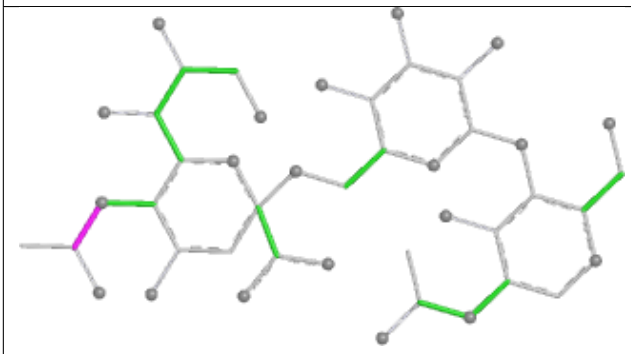
Oligosaccharide Chain Q



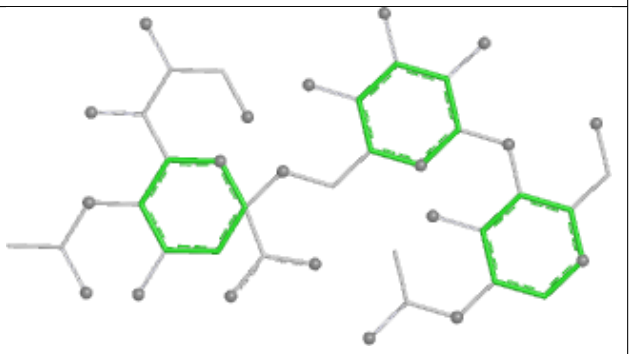
Bond lengths



Bond angles

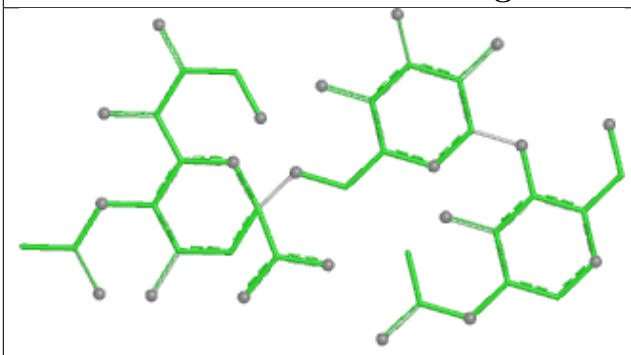


Torsions

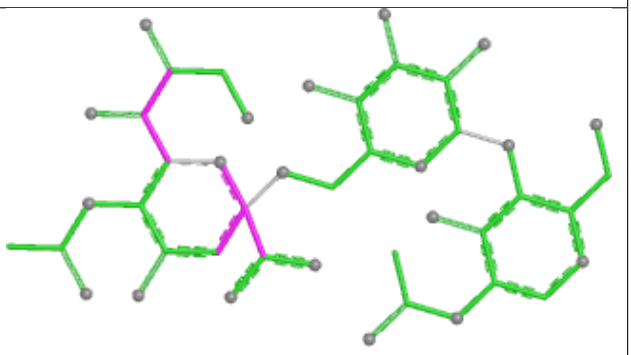


Rings

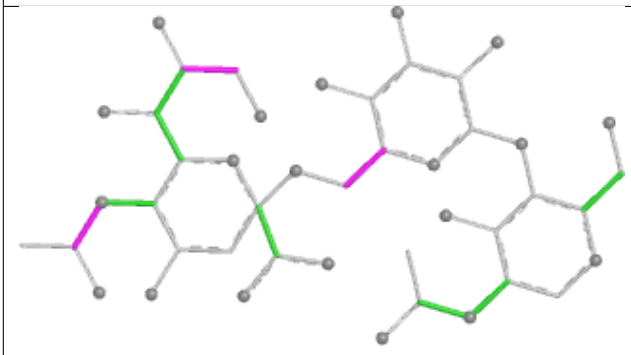
Oligosaccharide Chain R



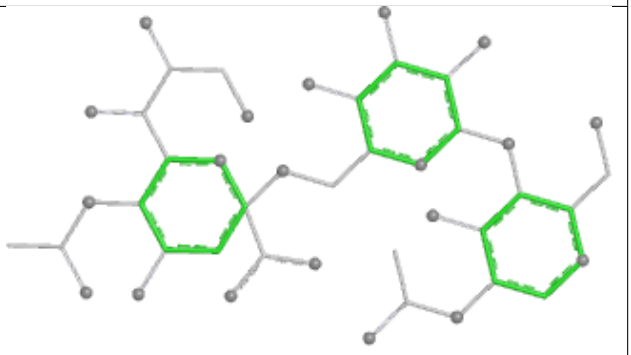
Bond lengths



Bond angles

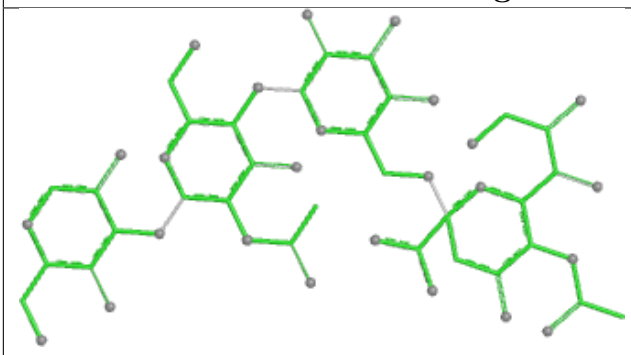


Torsions

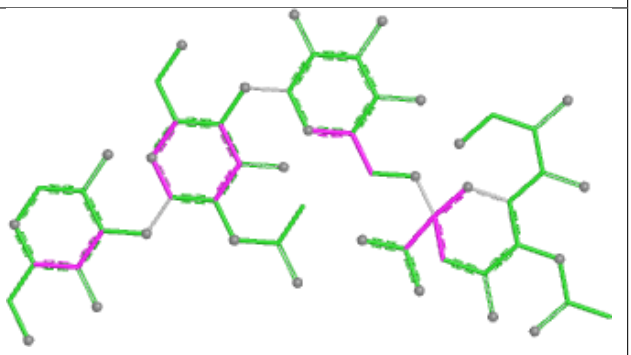


Rings

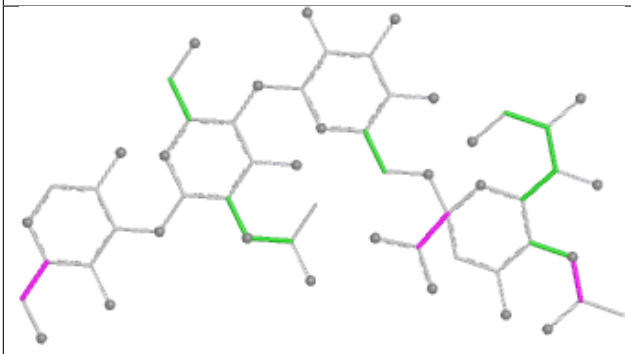
Oligosaccharide Chain N



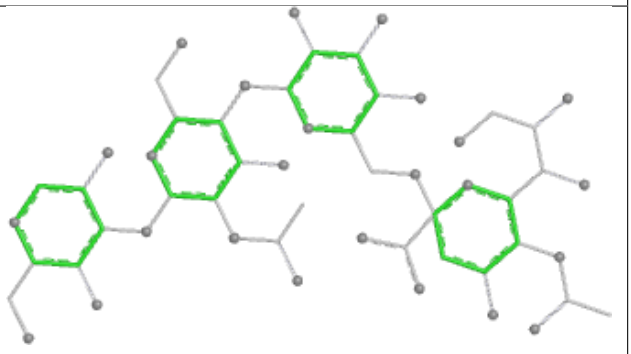
Bond lengths



Bond angles

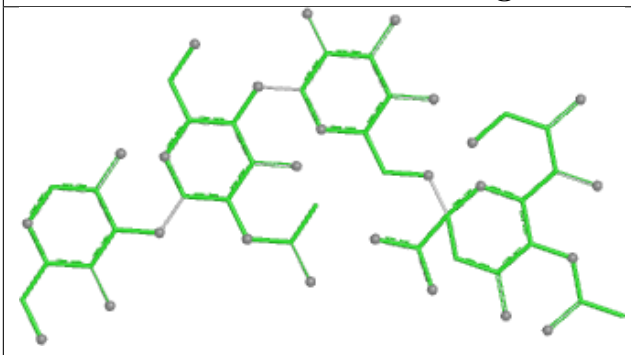


Torsions

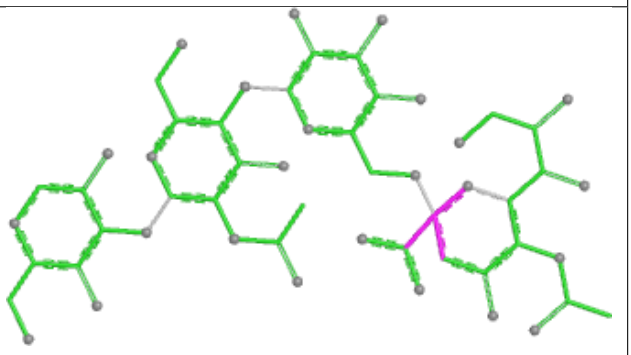


Rings

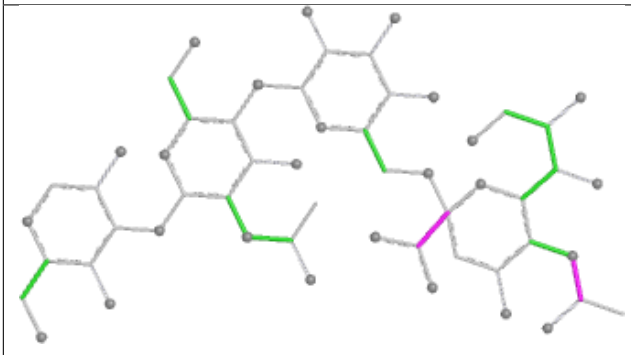
Oligosaccharide Chain P



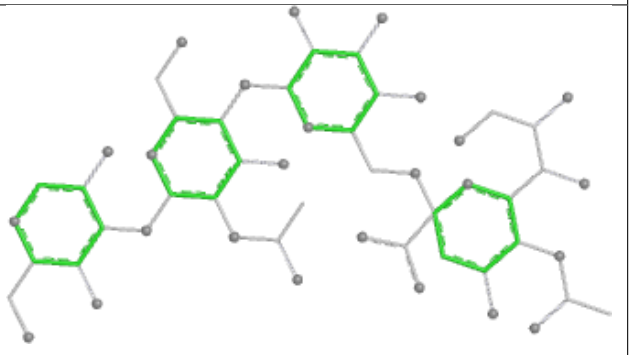
Bond lengths



Bond angles

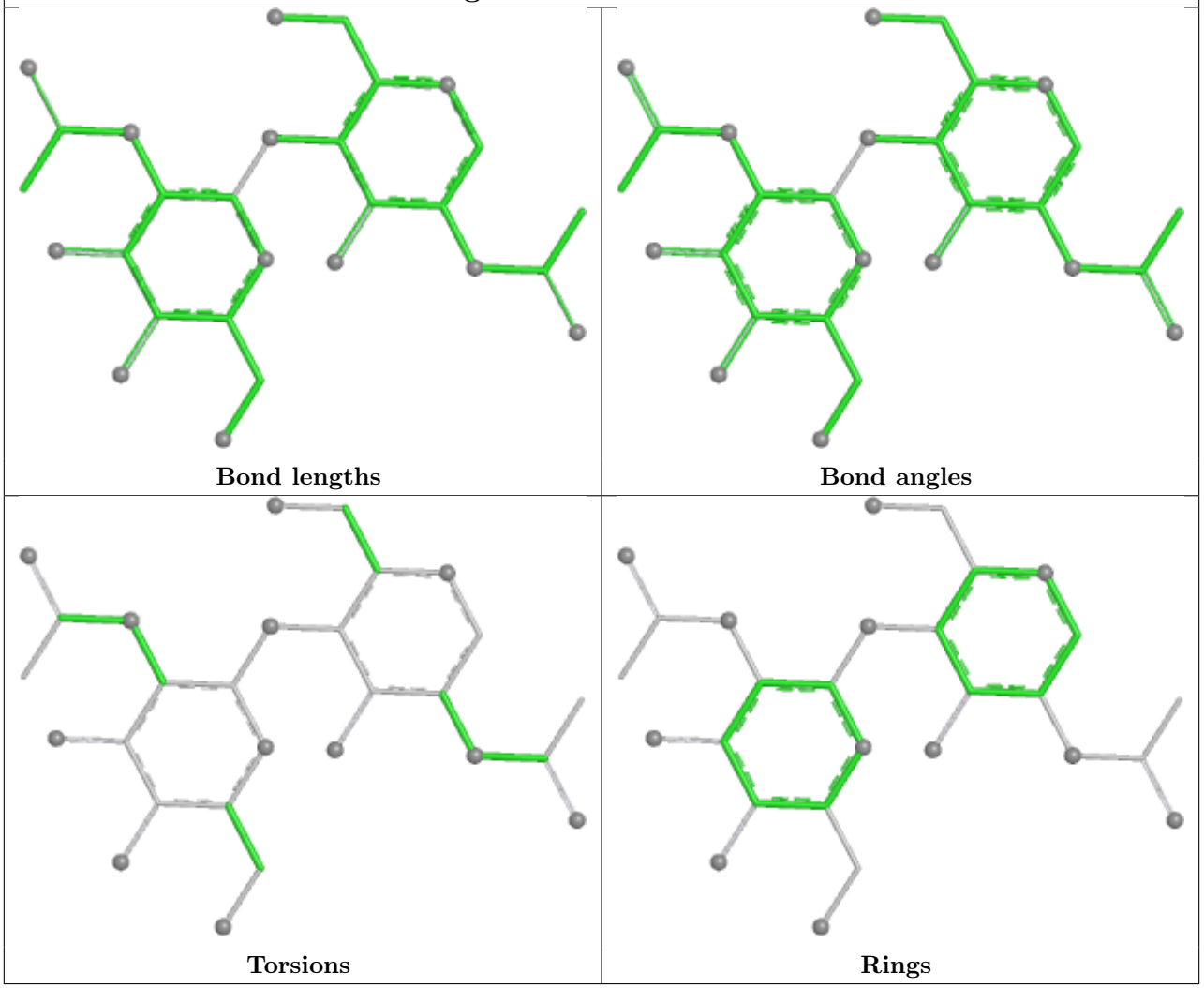


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	NAG	A	603	1	14,14,15	0.53	0	17,19,21	0.56	0
6	NAG	G	602	1	14,14,15	0.77	0	17,19,21	1.72	3 (17%)
6	NAG	A	604	1	14,14,15	0.56	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	602	1	14,14,15	0.55	0	17,19,21	0.61	0
6	NAG	G	601	1	14,14,15	0.29	0	17,19,21	0.56	0
6	NAG	C	601	1	14,14,15	0.46	0	17,19,21	1.04	1 (5%)
7	SIA	G	603	-	20,20,21	0.65	0	21,28,31	1.21	3 (14%)
6	NAG	A	601	1	14,14,15	0.52	0	17,19,21	0.81	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
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	G	602	1	-	1/6/23/26	0/1/1/1
6	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	NAG	A	602	1	-	1/6/23/26	0/1/1/1
6	NAG	G	601	1	-	2/6/23/26	0/1/1/1
6	NAG	C	601	1	-	2/6/23/26	0/1/1/1
7	SIA	G	603	-	-	3/18/34/38	0/1/1/1
6	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	602	NAG	C2-N2-C7	4.30	128.67	122.90
7	G	603	SIA	O6-C2-C3	4.03	115.98	110.56
6	C	601	NAG	C1-O5-C5	3.21	116.49	112.19
6	G	602	NAG	C1-C2-N2	2.66	114.62	110.43
6	G	602	NAG	C4-C3-C2	2.19	114.22	111.02

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	NAG	C1-C2-N2-C7
6	G	602	NAG	C1-C2-N2-C7
6	C	601	NAG	O5-C5-C6-O6
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6

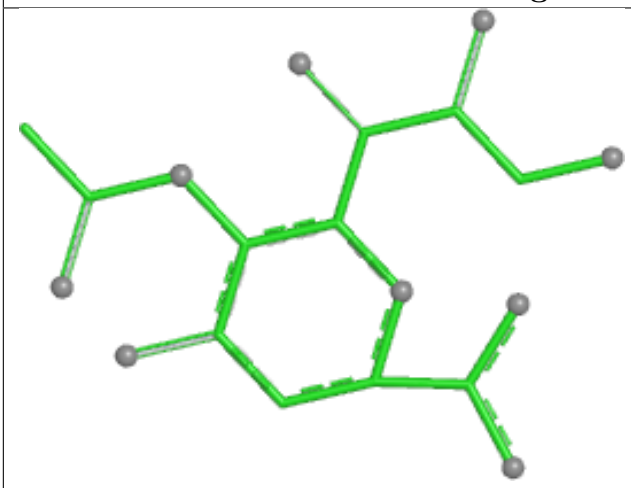
There are no ring outliers.

6 monomers are involved in 14 short contacts:

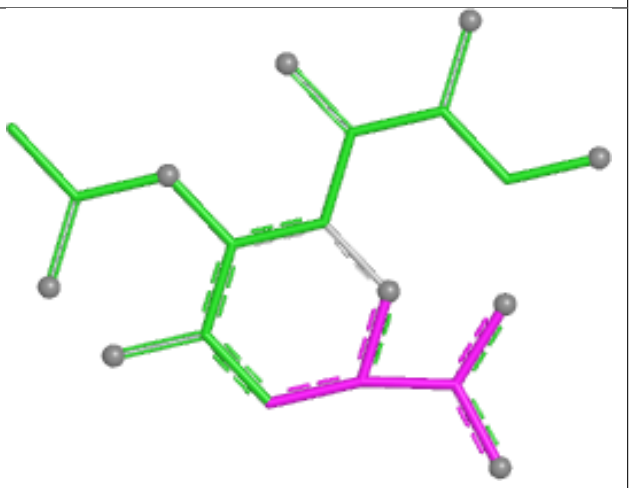
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	NAG	2	0
6	G	602	NAG	4	0
6	A	602	NAG	4	0
6	G	601	NAG	1	0
6	C	601	NAG	2	0
7	G	603	SIA	1	0

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

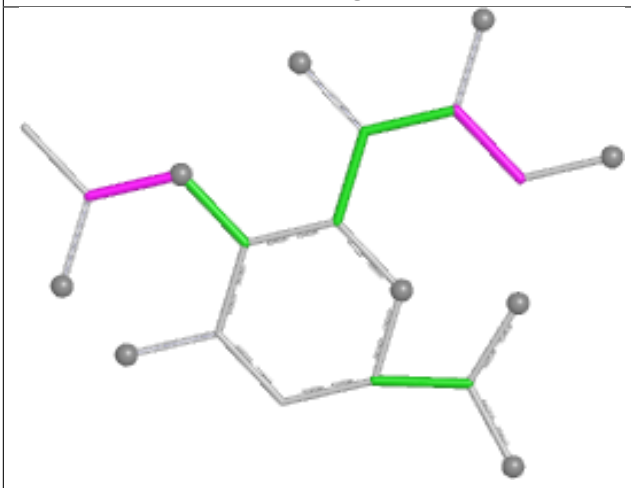
Ligand SIA G 603



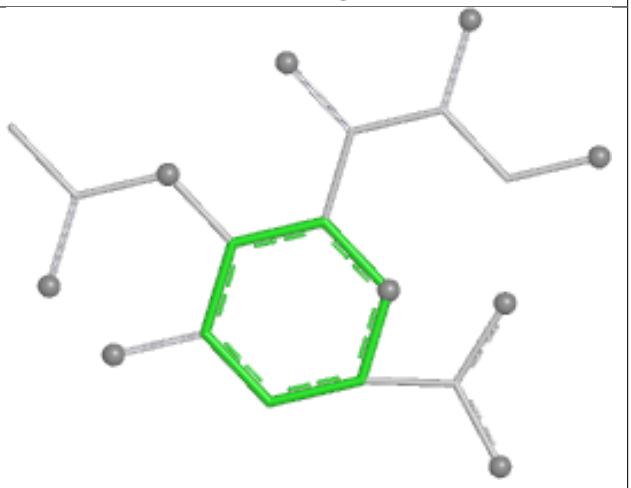
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	321/321 (100%)	0.14	10 (3%) 49 21	35, 69, 111, 154	0
1	C	321/321 (100%)	0.22	18 (5%) 24 8	36, 68, 118, 223	0
1	E	321/321 (100%)	0.15	7 (2%) 62 33	41, 71, 121, 203	0
1	G	321/321 (100%)	0.29	17 (5%) 26 10	39, 76, 124, 154	0
1	I	321/321 (100%)	0.25	9 (2%) 53 25	39, 75, 117, 169	0
1	K	321/321 (100%)	0.48	20 (6%) 20 7	52, 91, 136, 187	0
2	B	162/162 (100%)	0.41	15 (9%) 8 3	35, 84, 142, 180	0
2	D	162/162 (100%)	0.51	15 (9%) 8 3	39, 86, 163, 220	0
2	F	161/162 (99%)	0.72	27 (16%) 1 0	43, 86, 160, 246	0
2	H	162/162 (100%)	0.46	17 (10%) 6 2	40, 85, 149, 181	0
2	J	162/162 (100%)	0.26	4 (2%) 57 29	47, 80, 129, 156	0
2	L	161/162 (99%)	1.82	56 (34%) 0 0	43, 101, 223, 362	0
All	All	2896/2898 (99%)	0.40	215 (7%) 14 4	35, 78, 142, 362	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	129	ASN	11.9
2	L	146	ASN	10.3
2	L	130	ALA	9.2
2	L	147	THR	9.0
2	L	149	MET	8.5

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 (i)

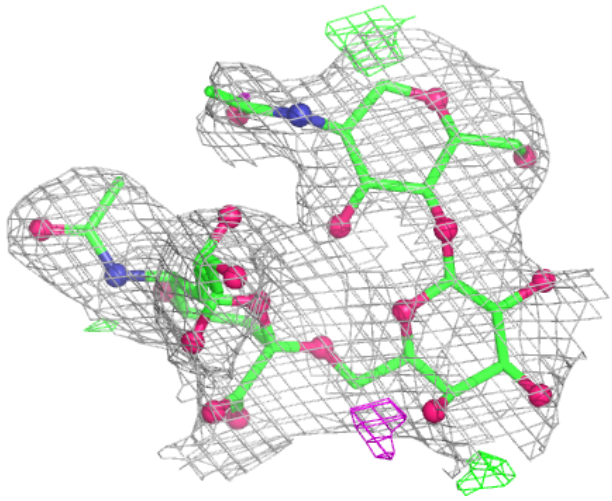
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

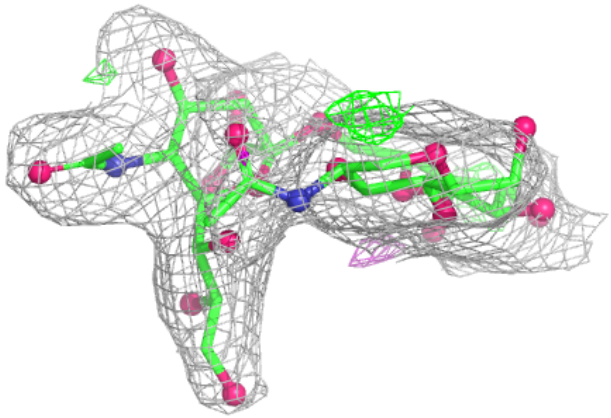
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GAL	N	1	11/12	0.64	0.26	104,129,151,153	0
4	GAL	P	1	11/12	0.75	0.26	110,139,162,174	0
5	NAG	O	2	14/15	0.79	0.34	88,113,132,144	0
3	GAL	R	2	11/12	0.80	0.23	96,131,149,169	0
3	NAG	R	1	14/15	0.83	0.23	110,146,159,172	0
4	NAG	N	2	14/15	0.83	0.25	75,106,127,128	0
3	NAG	M	1	14/15	0.85	0.23	65,80,89,96	0
4	NAG	P	2	14/15	0.86	0.32	120,126,146,147	0
3	NAG	Q	1	14/15	0.86	0.27	111,129,140,142	0
3	GAL	Q	2	11/12	0.87	0.23	61,95,108,114	0
5	NAG	O	1	14/15	0.92	0.16	74,82,98,102	0
4	SIA	P	4	20/21	0.92	0.22	42,65,87,99	0
4	GAL	P	3	11/12	0.93	0.15	78,95,110,122	0
4	SIA	N	4	20/21	0.93	0.20	48,71,90,97	0
3	GAL	M	2	11/12	0.93	0.12	53,93,104,109	0
3	SIA	Q	3	20/21	0.93	0.18	61,77,95,96	0
3	SIA	R	3	20/21	0.94	0.21	64,83,91,91	0
4	GAL	N	3	11/12	0.94	0.17	56,84,92,100	0
3	SIA	M	3	20/21	0.94	0.17	37,53,76,80	0

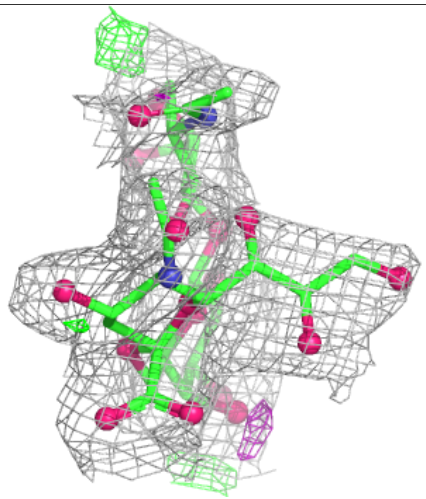
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

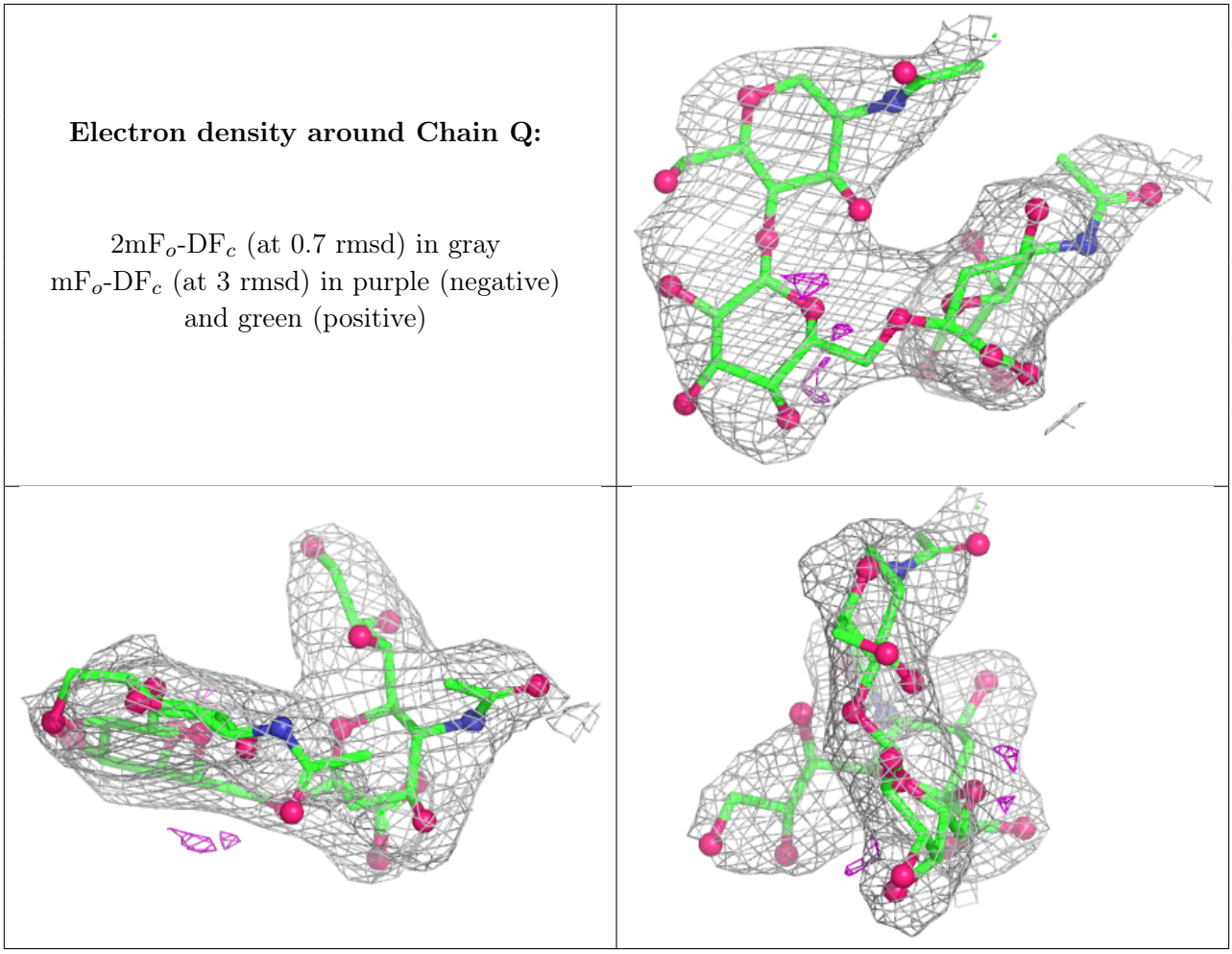






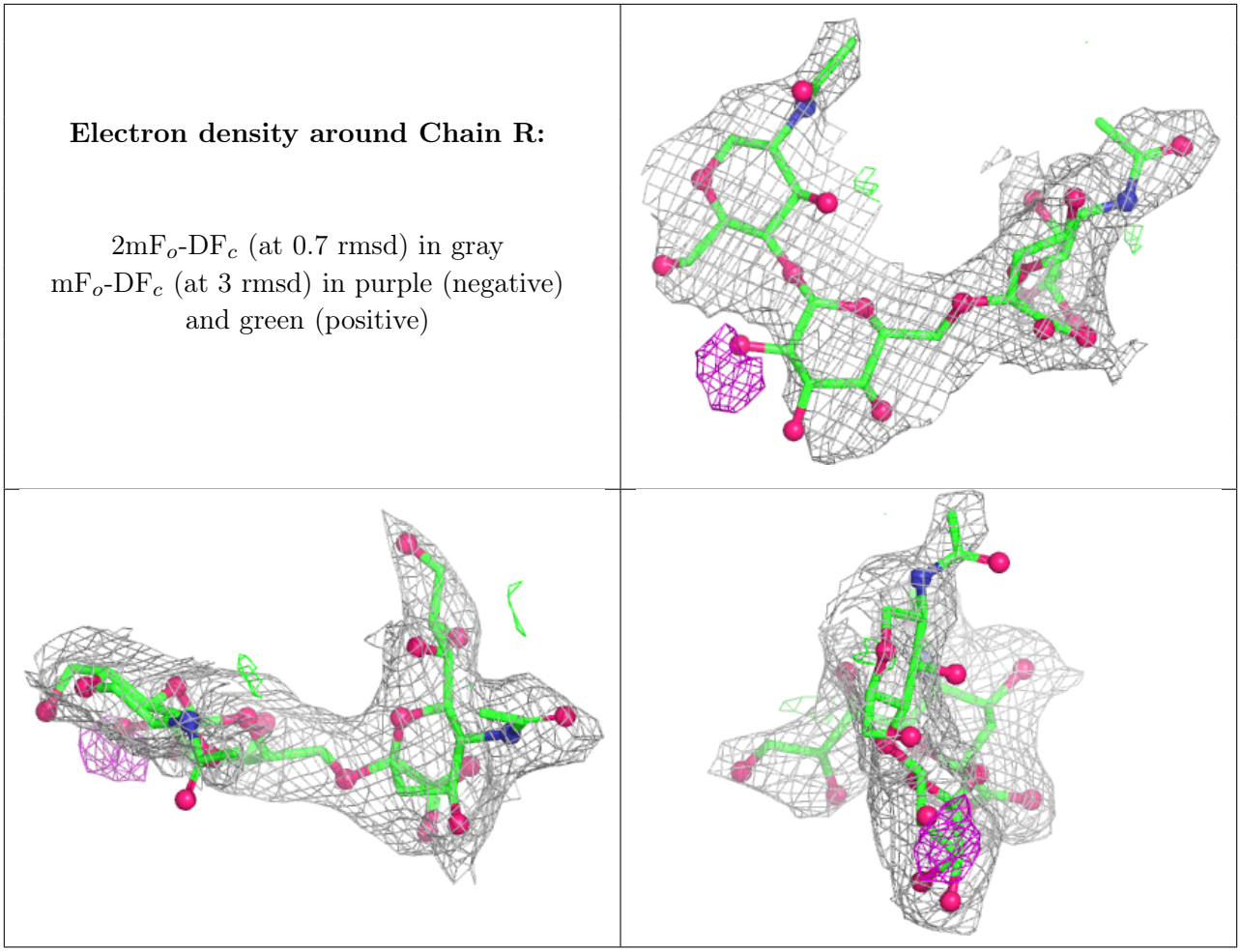
Electron density around Chain Q:

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



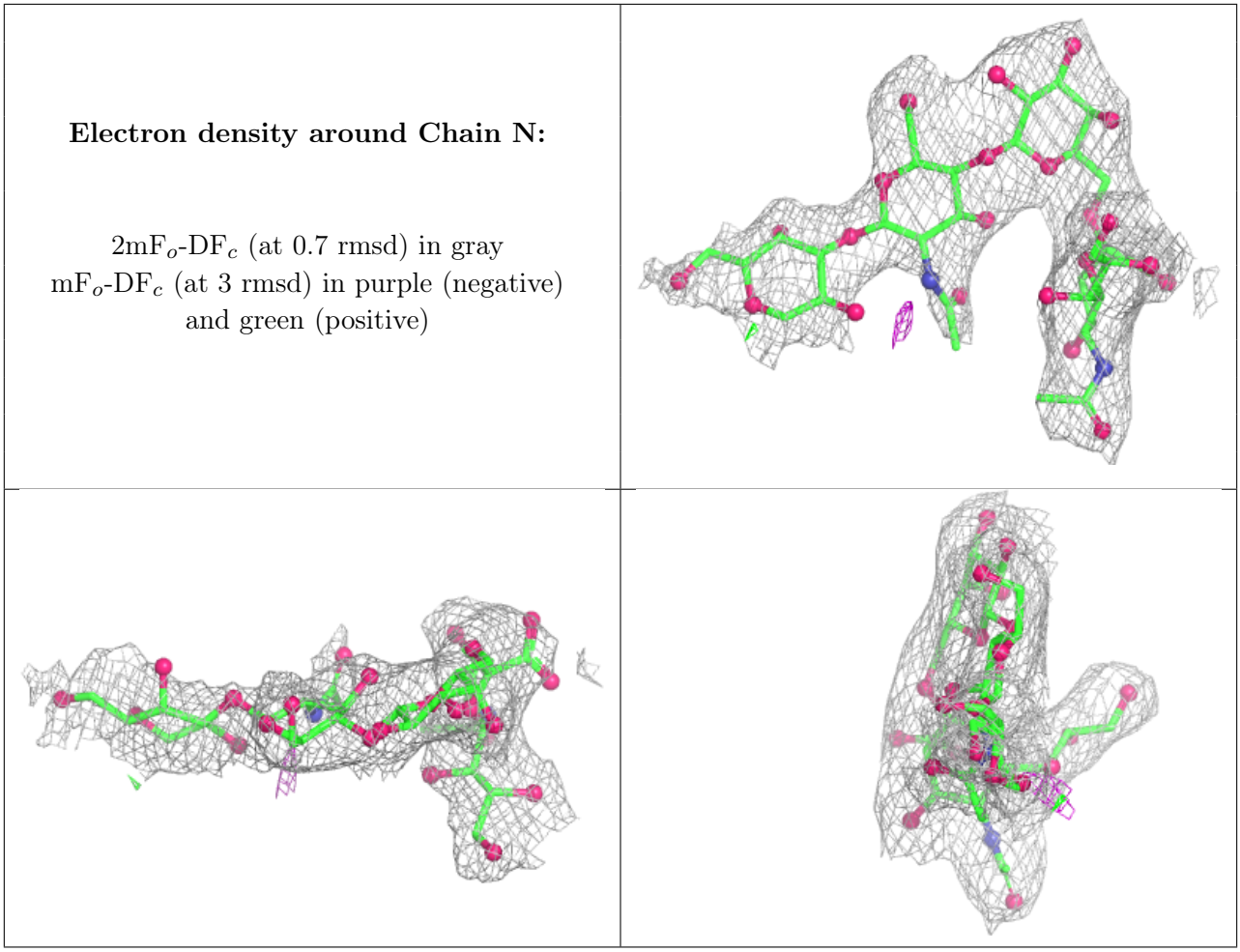
Electron density around Chain R:

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



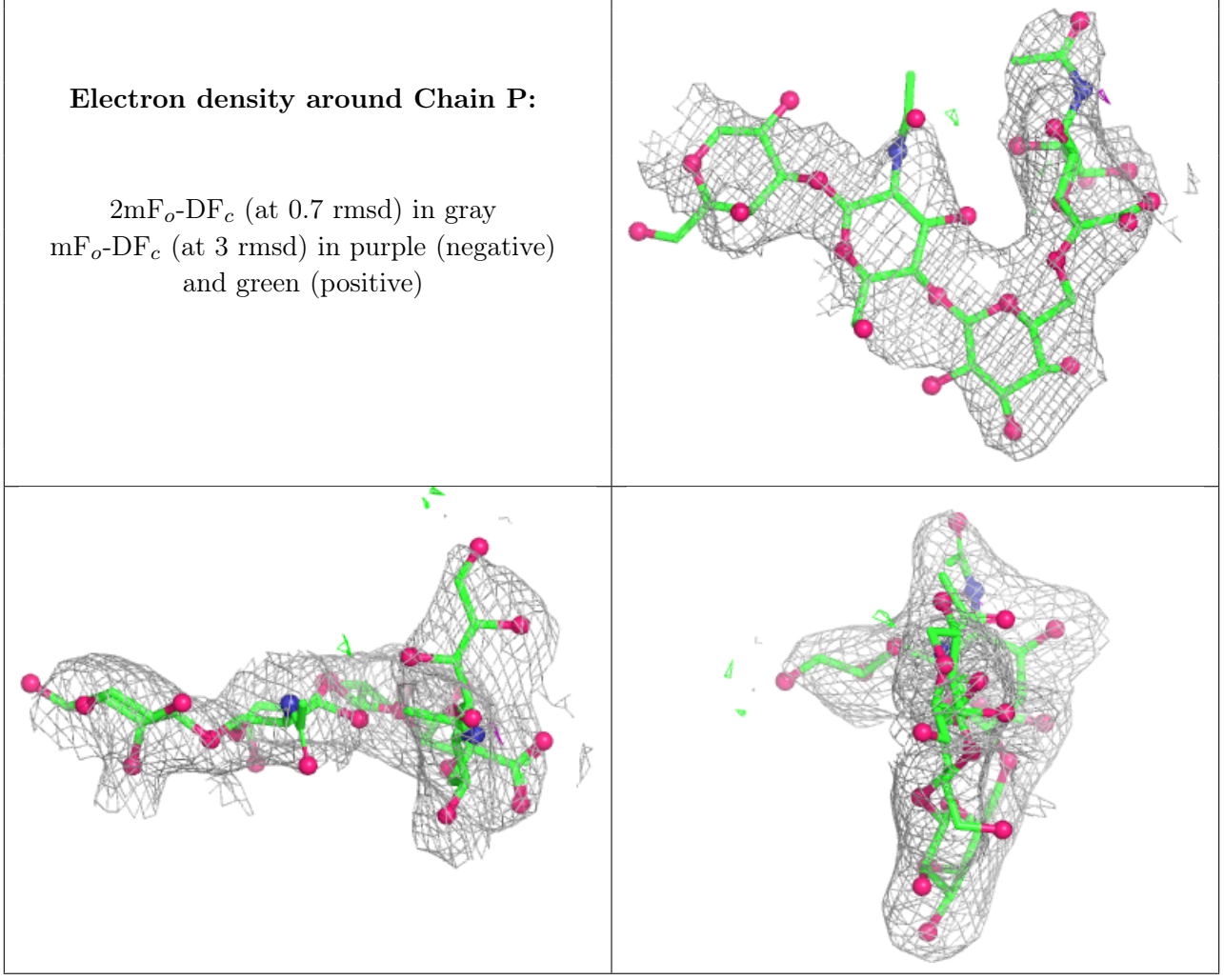
Electron density around Chain N:

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



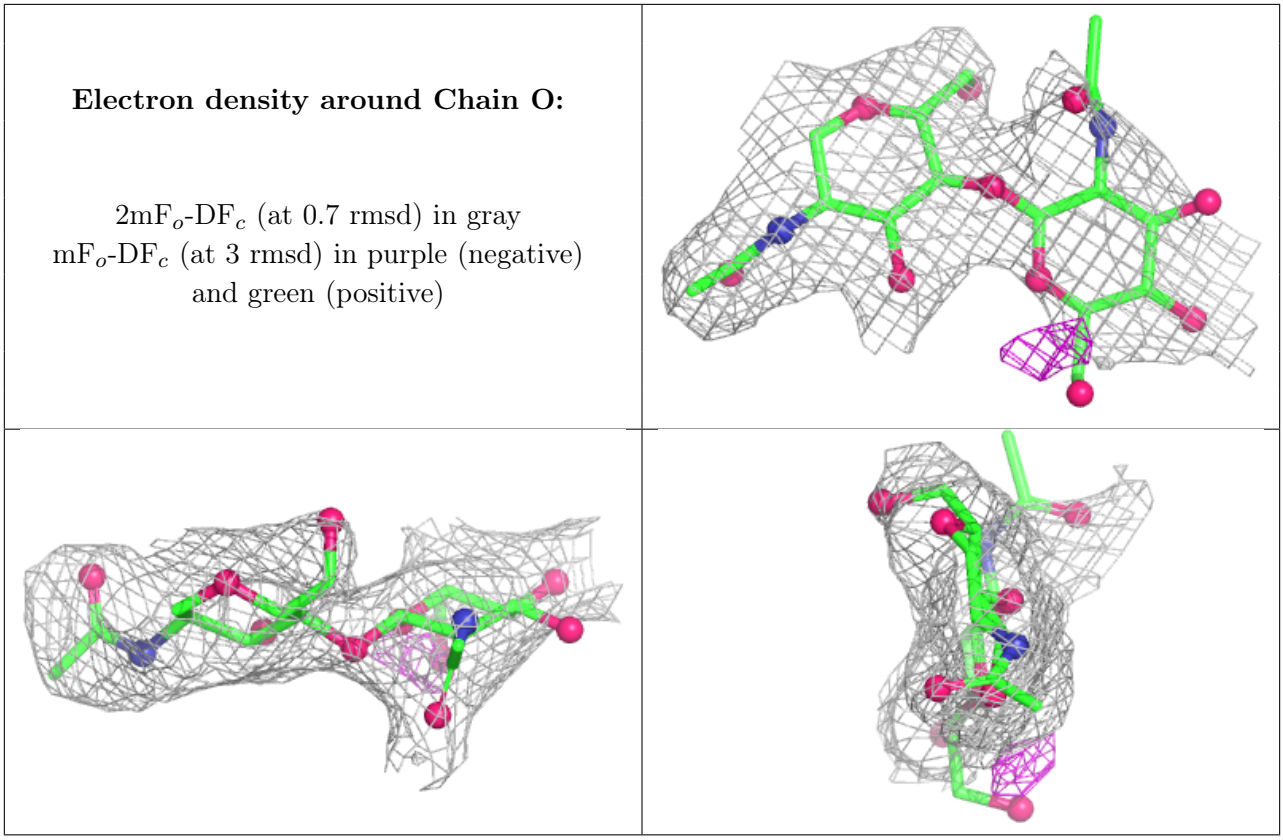
Electron density around Chain P:

$2mF_o$-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 O:

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



6.4 Ligands

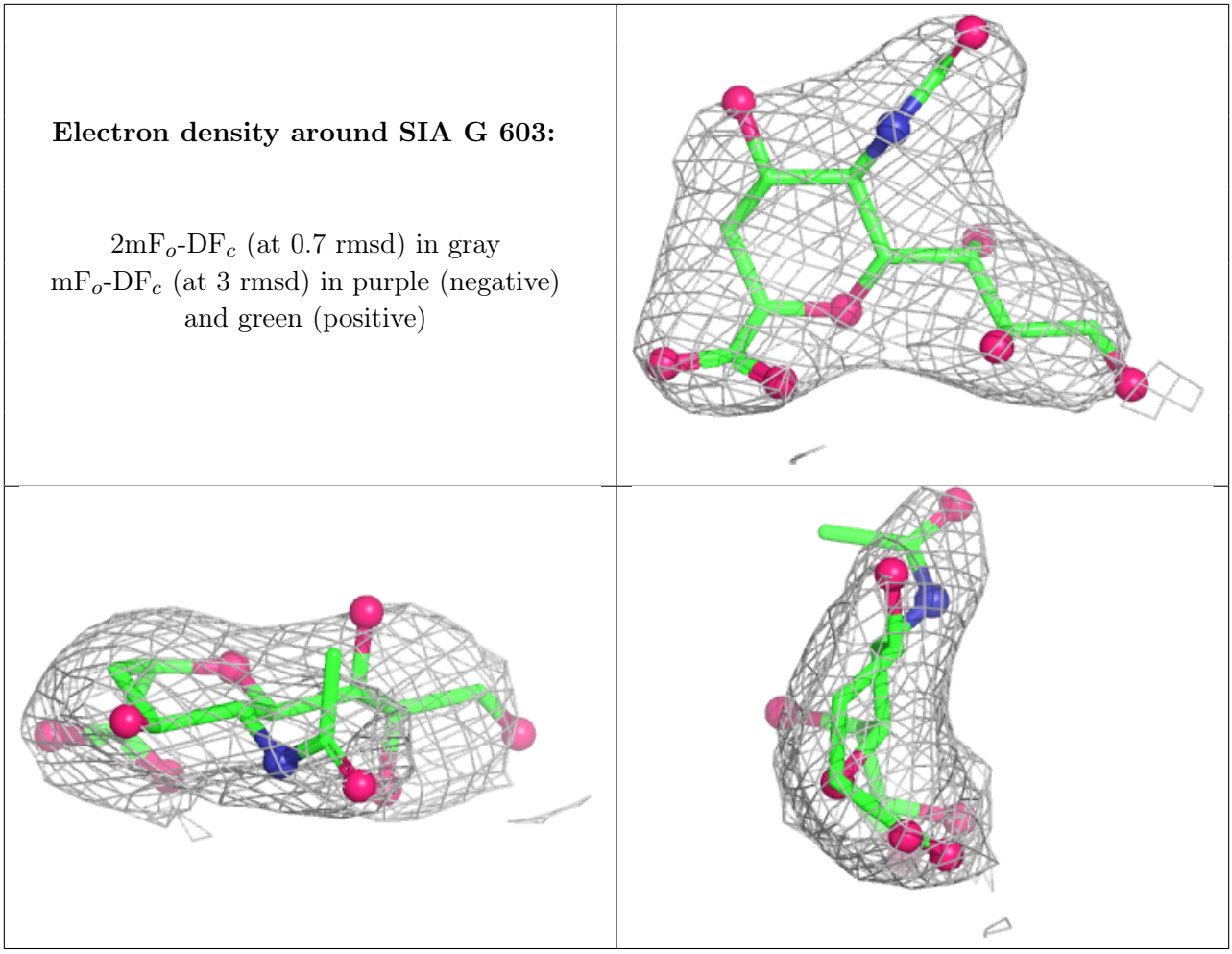
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	G	601	14/15	0.52	0.48	119,147,162,173	0
6	NAG	A	601	14/15	0.67	0.35	142,168,177,178	0
6	NAG	A	602	14/15	0.69	0.30	146,167,182,187	0
6	NAG	A	604	14/15	0.72	0.26	99,145,158,161	0
6	NAG	C	601	14/15	0.81	0.23	70,86,97,103	0
6	NAG	G	602	14/15	0.82	0.28	100,121,147,149	0
6	NAG	A	603	14/15	0.89	0.27	70,102,144,146	0
7	SIA	G	603	20/21	0.89	0.28	65,86,119,122	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 G 603:

$2mF_o$-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.