Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2020 – 10:23 AM BST

PDB ID	:	6TVF
Title	:	Crystal structure of the haemagglutinin from a H10N7 seal influenza virus isolated in Germany in complex with human receptor analogue, 6'-SLN
Authors	:	Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on	:	2020-01-09
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

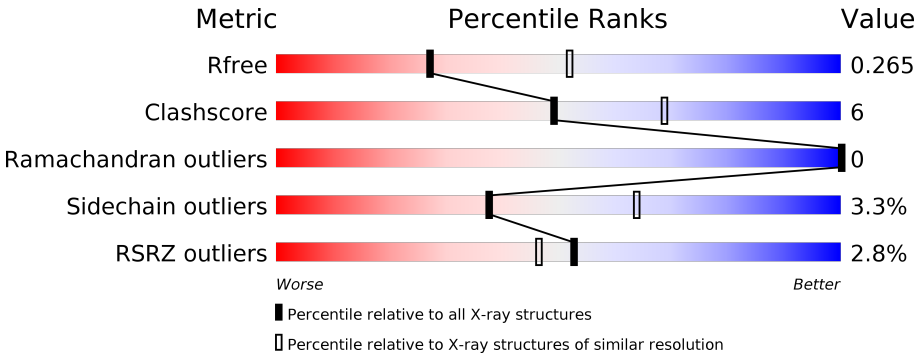
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	325	88% 9%
1	C	325	% 90% 8%
1	E	325	4% 85% 12%
1	G	325	12% 79% 18%
1	I	325	6% 84% 14%
1	K	325	88% 9%

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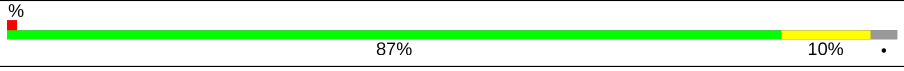
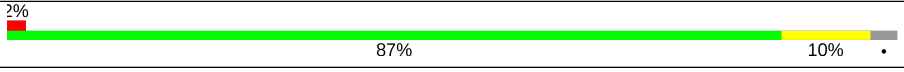
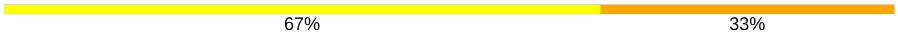
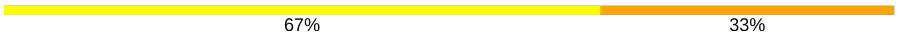
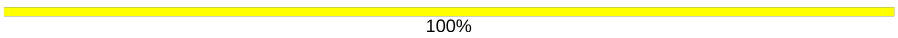
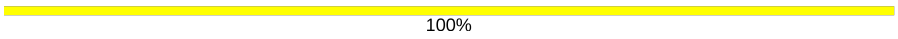
Mol	Chain	Length	Quality of chain
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	M	3	
3	P	3	
3	R	3	
3	U	3	
4	N	2	
5	O	2	
5	Q	2	
5	S	2	
5	T	2	
5	V	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23705 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	1	0
			2448	1517	443	472	16			
1	C	320	Total	C	N	O	S	0	1	0
			2442	1514	440	472	16			
1	E	320	Total	C	N	O	S	0	1	0
			2442	1514	440	472	16			
1	G	320	Total	C	N	O	S	0	0	0
			2410	1489	439	466	16			
1	I	320	Total	C	N	O	S	0	1	0
			2442	1514	440	472	16			
1	K	318	Total	C	N	O	S	0	0	0
			2428	1505	441	466	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	219	GLN	LEU	conflict	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	219	GLN	LEU	conflict	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
E	219	GLN	LEU	conflict	UNP A0A0A7HR51
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
G	219	GLN	LEU	conflict	UNP A0A0A7HR51
I	-1	ASP	-	expression tag	UNP A0A0A7HR51
I	0	PRO	-	expression tag	UNP A0A0A7HR51
I	219	GLN	LEU	conflict	UNP A0A0A7HR51
K	-1	ASP	-	expression tag	UNP A0A0A7HR51
K	0	PRO	-	expression tag	UNP A0A0A7HR51

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Chain	Residue	Modelled	Actual	Comment	Reference
K	219	GLN	LEU	conflict	UNP A0A0A7HR51

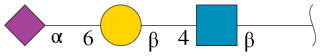
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	H	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	J	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	L	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			

There are 6 discrepancies between the modelled and reference sequences:

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

- 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	0	0	0
			46	25	2	19			
3	P	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	R	3	Total	C	N	O	0	0	0
			46	25	2	19			

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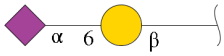
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	U	3	Total C N O 46 25 2 19	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	N	2	Total C N O 32 17 1 14	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
5	Q	2	Total C N O 28 16 2 10	0	0	0
5	S	2	Total C N O 28 16 2 10	0	0	0
5	T	2	Total C N O 28 16 2 10	0	0	0
5	V	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

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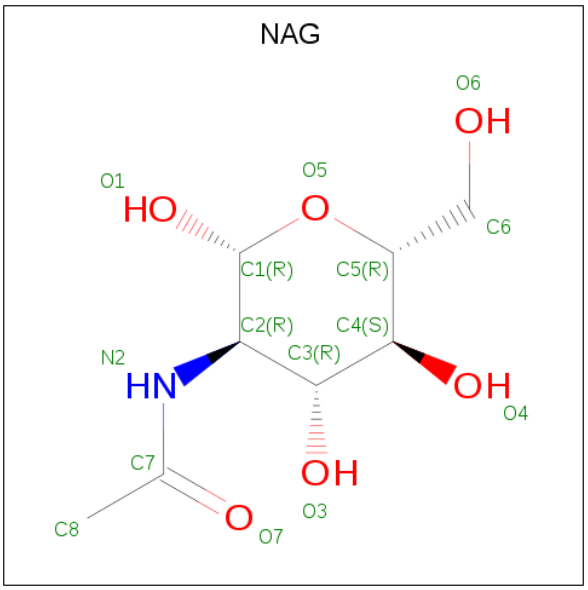
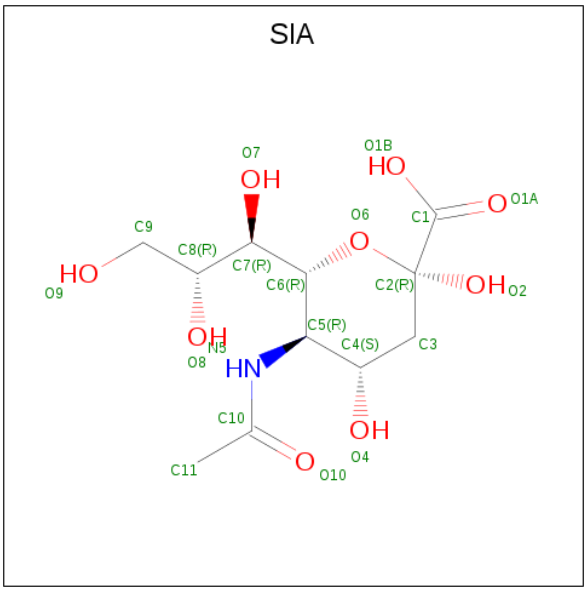
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total Ca 1 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	L	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	1	Total C N O 21 11 1 9	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	34	Total O 34 34	0	0
9	B	22	Total O 22 22	0	0
9	C	45	Total O 45 45	0	0
9	D	38	Total O 38 38	0	0
9	E	24	Total O 24 24	0	0
9	F	28	Total O 28 28	0	0
9	G	12	Total O 12 12	0	0
9	H	28	Total O 28 28	0	0
9	I	7	Total O 7 7	0	0
9	J	20	Total O 20 20	0	0
9	K	79	Total O 79 79	0	0

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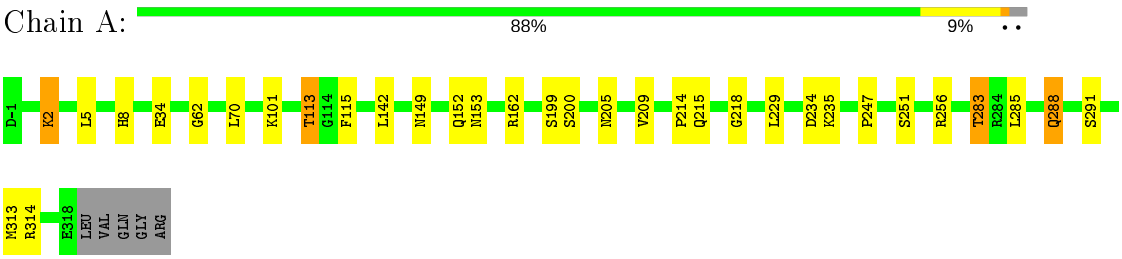
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	33	Total O 33 33	0	0

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.

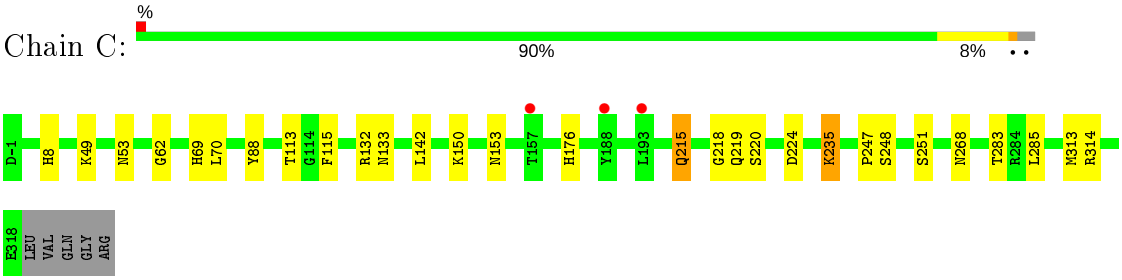
- Molecule 1: Hemagglutinin HA1

Chain A:



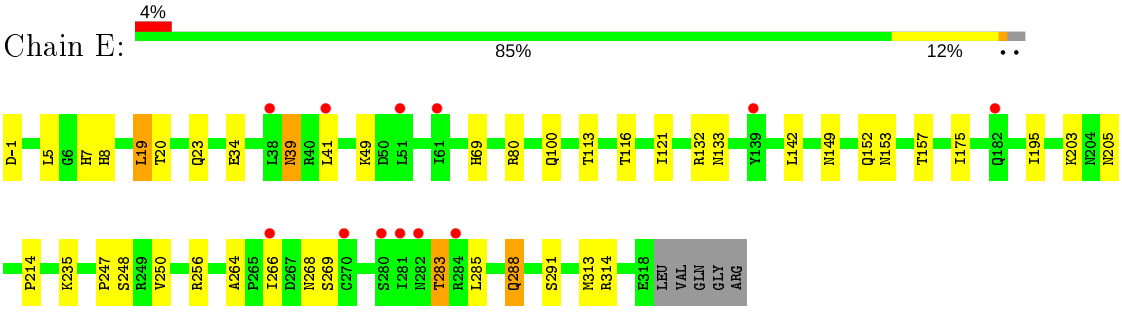
- Molecule 1: Hemagglutinin HA1

Chain C:



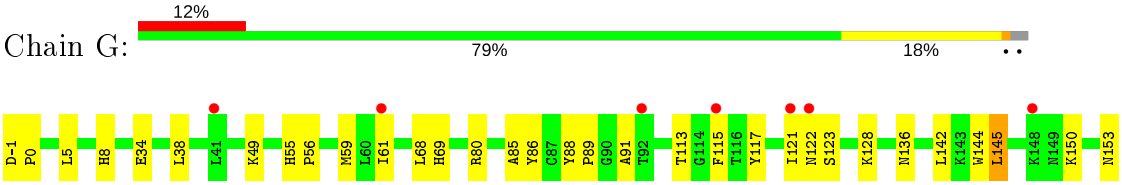
- Molecule 1: Hemagglutinin HA1

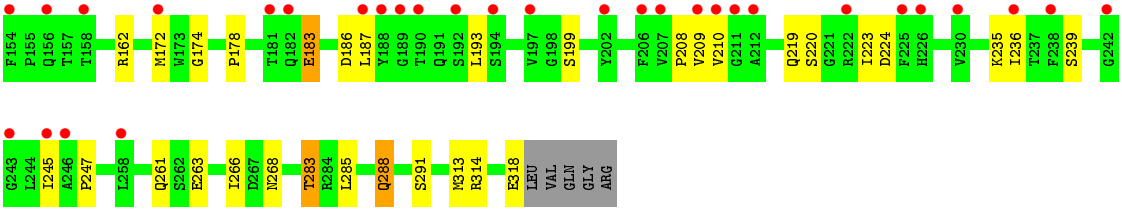
Chain E:



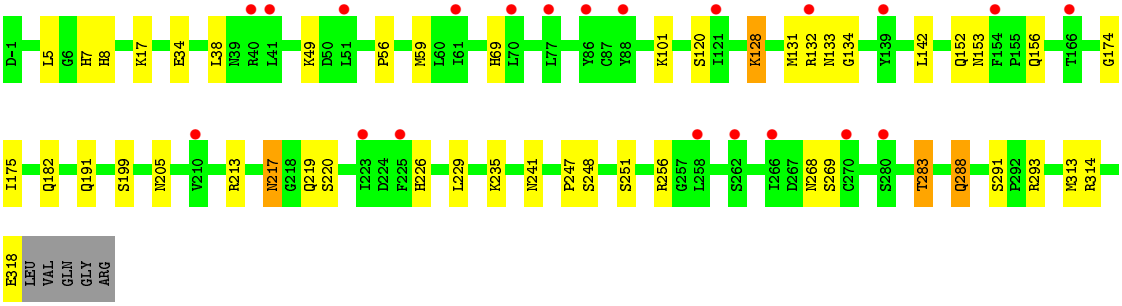
- Molecule 1: Hemagglutinin HA1

Chain G:

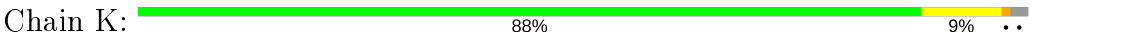


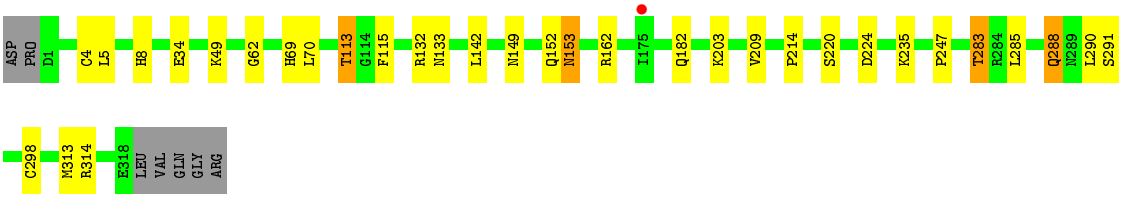


• Molecule 1: Hemagglutinin HA1

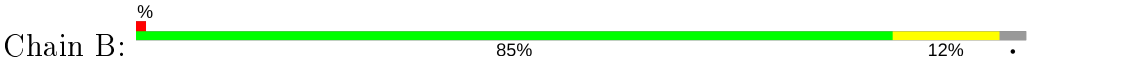


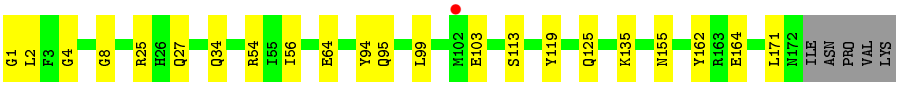
• Molecule 1: Hemagglutinin HA1



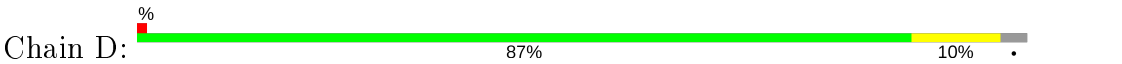


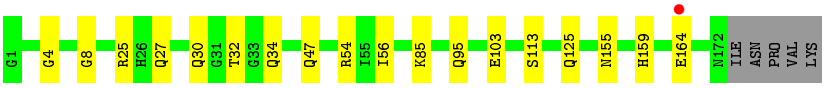
• Molecule 2: Hemagglutinin HA2





• Molecule 2: Hemagglutinin HA2

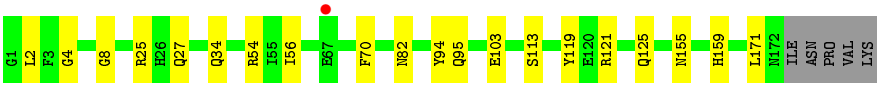




• Molecule 2: Hemagglutinin HA2

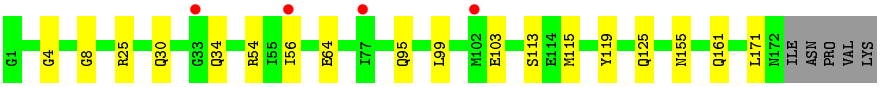
• Molecule 2: Hemagglutinin HA2

Chain H:



• Molecule 2: Hemagglutinin HA2

Chain J:



• Molecule 2: Hemagglutinin HA2

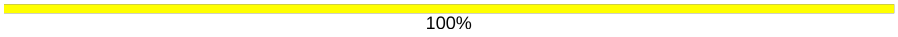
Chain L:

• 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 P:

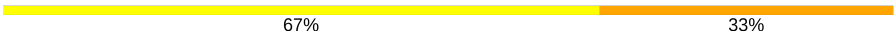


• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain U:

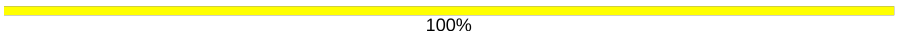


• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain N:

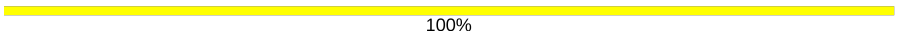
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



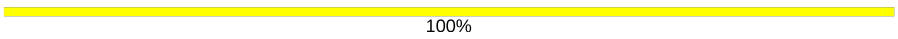
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



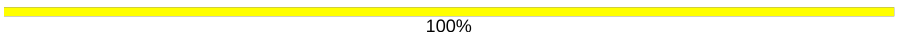
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:



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

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.81Å 214.14Å 158.39Å 90.00° 101.07° 90.00°	Depositor
Resolution (Å)	68.52 – 2.60 64.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (68.52-2.60) 99.0 (64.53-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.239 , 0.276 0.233 , 0.265	Depositor DCC
R_{free} test set	7071 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23705	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1961e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CA, GAL, NAG, SIA

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	0.65	0/2501	0.76	0/3389
1	C	0.68	0/2495	0.77	0/3382
1	E	0.65	0/2495	0.77	0/3382
1	G	0.67	0/2456	0.81	0/3327
1	I	0.68	0/2495	0.77	0/3382
1	K	0.65	0/2477	0.76	0/3355
2	B	0.64	0/1411	0.73	0/1903
2	D	0.64	0/1408	0.74	0/1900
2	F	0.63	0/1408	0.73	0/1900
2	H	0.62	0/1408	0.74	0/1900
2	J	0.64	0/1408	0.74	0/1900
2	L	0.65	0/1408	0.74	0/1900
All	All	0.65	0/23370	0.76	0/31620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2448	0	2400	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2442	0	2389	18	0
1	E	2442	0	2389	32	0
1	G	2410	0	2352	52	0
1	I	2442	0	2389	33	0
1	K	2428	0	2385	27	0
2	B	1386	0	1290	22	0
2	D	1383	0	1282	18	0
2	F	1383	0	1282	28	0
2	H	1383	0	1283	18	0
2	J	1383	0	1282	23	0
2	L	1383	0	1281	22	0
3	M	46	0	40	1	0
3	P	46	0	40	0	0
3	R	46	0	40	4	0
3	U	46	0	40	1	0
4	N	32	0	28	1	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	V	28	0	25	0	0
6	A	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
7	B	28	0	26	0	0
7	L	14	0	13	1	0
8	I	21	0	18	2	0
9	A	34	0	0	1	0
9	B	22	0	0	2	0
9	C	45	0	0	2	0
9	D	38	0	0	4	0
9	E	24	0	0	1	0
9	F	28	0	0	0	0
9	G	12	0	0	0	0
9	H	28	0	0	1	0
9	I	7	0	0	0	0
9	J	20	0	0	2	0
9	K	79	0	0	3	0
9	L	33	0	0	0	0
All	All	23705	0	22374	269	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 6.

All (269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:GLN:HE22	2:J:95:GLN:HE21	1.14	0.90
2:F:95:GLN:HE21	2:L:95:GLN:HE21	1.20	0.88
2:F:25:ARG:HE	2:F:34:GLN:HE21	1.22	0.87
1:I:34:GLU:OE1	1:I:283:THR:HG21	1.76	0.85
2:B:95:GLN:HE21	2:J:95:GLN:HE21	1.22	0.84
2:B:95:GLN:HE21	2:J:95:GLN:NE2	1.76	0.83
2:B:25:ARG:HE	2:B:34:GLN:HE21	1.23	0.83
1:G:123:SER:HA	1:G:145:LEU:HB3	1.60	0.82
1:G:150:LYS:HD3	1:G:186:ASP:HB3	1.61	0.82
2:J:25:ARG:HE	2:J:34:GLN:HE21	1.23	0.82
2:D:25:ARG:HE	2:D:34:GLN:HE21	1.23	0.82
2:H:25:ARG:HE	2:H:34:GLN:HE21	1.24	0.82
1:G:150:LYS:HD3	1:G:186:ASP:CB	2.12	0.79
1:E:116:THR:HA	9:E:503:HOH:O	1.83	0.78
1:C:53:ASN:HB3	9:C:536:HOH:O	1.83	0.78
2:L:25:ARG:HH21	2:L:34:GLN:NE2	1.83	0.77
2:B:95:GLN:NE2	2:J:95:GLN:NE2	2.33	0.76
1:G:199:SER:HB3	1:G:236:ILE:HD12	1.67	0.76
1:G:174:GLY:CA	1:G:245:ILE:HG22	2.15	0.76
1:E:41:LEU:CD1	1:E:264:ALA:HB3	2.16	0.75
1:G:61:ILE:HG23	1:G:172:MET:CE	2.16	0.75
2:F:95:GLN:NE2	2:L:95:GLN:NE2	2.35	0.75
1:G:89:PRO:HG3	1:G:219:GLN:HB2	1.70	0.74
2:F:95:GLN:NE2	2:L:95:GLN:HE21	1.86	0.73
1:E:7:HIS:HB3	2:F:115:MET:CE	2.19	0.72
2:L:150:GLU:OE1	7:L:203:NAG:H82	1.90	0.72
2:D:95:GLN:HE22	2:F:95:GLN:HE21	1.35	0.72
1:E:20:THR:HG22	2:F:105:GLN:HE22	1.53	0.72
1:I:156:GLN:NE2	1:I:241:ASN:HB3	2.04	0.71
2:J:125:GLN:HG2	9:J:302:HOH:O	1.88	0.71
1:I:7:HIS:HB3	2:J:115:MET:CE	2.21	0.70
1:G:144:TRP:CA	1:G:245:ILE:HD11	2.22	0.70
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.25	0.69
1:I:217:ASN:HD22	1:I:217:ASN:N	1.90	0.69
2:L:54:ARG:NH2	2:L:103:GLU:OE2	2.26	0.69
1:G:193:LEU:CB	1:G:208:PRO:HG2	2.23	0.68
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.24	0.68
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.26	0.67
2:F:142:HIS:HE1	2:F:157:TYR:OH	1.78	0.67
1:G:38:LEU:HD12	1:G:38:LEU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:GLY:HA3	1:G:245:ILE:HG22	1.77	0.66
2:H:54:ARG:NH2	2:H:103:GLU:OE2	2.26	0.66
1:A:314:ARG:NH1	9:A:502:HOH:O	2.29	0.65
2:F:95:GLN:HE21	2:L:95:GLN:NE2	1.90	0.65
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.28	0.65
1:I:38:LEU:N	1:I:38:LEU:HD12	2.10	0.65
2:F:121:ARG:HD3	2:F:155:ASN:ND2	2.11	0.65
1:G:91:ALA:O	1:G:224:ASP:HA	1.96	0.65
1:G:88:TYR:CD2	1:G:89:PRO:HD2	2.33	0.64
2:H:121:ARG:HD3	2:H:155:ASN:ND2	2.13	0.64
2:H:95:GLN:NE2	2:J:95:GLN:HE21	1.93	0.64
1:K:113:THR:HG21	1:K:247:PRO:O	1.98	0.64
1:I:153:ASN:HD21	1:I:191:GLN:H	1.47	0.62
1:A:113:THR:HG21	1:A:247:PRO:O	1.99	0.62
1:G:144:TRP:HA	1:G:245:ILE:HD11	1.80	0.62
1:E:235:LYS:HG3	1:K:214:PRO:HG3	1.81	0.62
2:H:95:GLN:HE22	2:J:95:GLN:NE2	1.92	0.61
1:C:113:THR:HG21	1:C:247:PRO:O	2.01	0.61
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.65	0.61
1:I:120:SER:HB2	1:I:152:GLN:HE22	1.65	0.61
3:R:1:NAG:H82	3:R:1:NAG:H1	1.82	0.61
1:G:61:ILE:CG2	1:G:172:MET:CE	2.79	0.60
1:G:178:PRO:HB3	1:G:183:GLU:HG3	1.84	0.60
1:G:56:PRO:O	1:G:59:MET:HG2	2.02	0.60
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.67	0.60
1:I:56:PRO:O	1:I:59:MET:HG2	2.02	0.60
2:D:32:THR:HG23	9:D:302:HOH:O	2.03	0.58
1:K:288:GLN:HE21	1:K:291:SER:H	1.51	0.58
1:A:256:ARG:NH2	2:B:64:GLU:OE2	2.37	0.58
1:E:205:ASN:HB2	1:K:209:VAL:HG23	1.86	0.58
1:A:288:GLN:HE21	1:A:291:SER:H	1.52	0.57
1:I:156:GLN:HE22	1:I:241:ASN:HB3	1.67	0.57
1:I:175:ILE:HD12	1:I:175:ILE:N	2.19	0.57
2:D:47:GLN:HA	1:E:20:THR:OG1	2.05	0.57
1:G:288:GLN:HE21	1:G:291:SER:H	1.52	0.57
1:E:288:GLN:HE21	1:E:291:SER:H	1.52	0.57
1:G:288:GLN:NE2	1:G:291:SER:H	2.03	0.56
1:I:288:GLN:HE21	1:I:291:SER:H	1.52	0.56
2:L:51:LYS:HE3	2:L:103:GLU:OE1	2.05	0.56
1:G:144:TRP:HA	1:G:245:ILE:CD1	2.34	0.56
1:A:34:GLU:OE1	1:A:283:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:LYS:HE3	1:I:69:HIS:ND1	2.20	0.56
1:K:288:GLN:NE2	1:K:291:SER:H	2.04	0.56
2:F:142:HIS:CE1	2:F:157:TYR:OH	2.57	0.56
1:K:34:GLU:OE1	1:K:283:THR:HG23	2.05	0.56
1:E:288:GLN:NE2	1:E:291:SER:H	2.04	0.56
1:E:256:ARG:NH2	2:F:64:GLU:OE2	2.39	0.55
1:G:61:ILE:HG23	1:G:172:MET:HE2	1.88	0.55
1:A:288:GLN:NE2	1:A:291:SER:H	2.04	0.55
1:I:128:LYS:HE3	1:I:128:LYS:O	2.07	0.55
1:I:288:GLN:NE2	1:I:291:SER:H	2.04	0.55
1:G:113:THR:HG21	1:G:247:PRO:O	2.07	0.55
1:I:174:GLY:C	1:I:175:ILE:HD12	2.26	0.55
1:A:149:ASN:HD22	1:A:152:GLN:HE22	1.55	0.54
8:I:401:SIA:O6	8:I:401:SIA:O8	2.26	0.54
1:G:34:GLU:OE1	1:G:283:THR:HG23	2.08	0.54
1:G:144:TRP:CB	1:G:245:ILE:HD11	2.38	0.54
1:E:41:LEU:HD11	1:E:264:ALA:HB3	1.88	0.54
1:G:283:THR:HG22	1:G:285:LEU:HG	1.90	0.53
1:G:219:GLN:NE2	3:R:2:GAL:H4	2.23	0.53
1:C:62:GLY:HA2	1:C:70:LEU:HD21	1.91	0.53
1:E:49:LYS:HE3	1:E:69:HIS:ND1	2.24	0.53
1:E:175:ILE:HD12	1:E:195:ILE:HD13	1.91	0.53
2:D:95:GLN:HE22	2:F:95:GLN:HG2	1.73	0.52
1:A:283:THR:HG22	1:A:285:LEU:HG	1.91	0.52
3:U:1:NAG:H83	3:U:1:NAG:H3	1.91	0.52
1:A:209:VAL:HG23	1:I:205:ASN:CG	2.30	0.52
1:C:88:TYR:CE2	1:C:219:GLN:HG2	2.44	0.52
2:D:95:GLN:HE22	2:F:95:GLN:NE2	2.05	0.52
1:K:113:THR:HG23	1:K:115:PHE:H	1.75	0.52
1:E:34:GLU:OE1	1:E:283:THR:HG23	2.10	0.52
1:I:182:GLN:N	1:I:182:GLN:OE1	2.43	0.52
1:E:149:ASN:O	1:E:152:GLN:HB3	2.09	0.51
1:K:298:CYS:HB2	9:K:525:HOH:O	2.10	0.51
1:G:174:GLY:N	1:G:245:ILE:HG22	2.25	0.51
1:C:113:THR:HG23	1:C:115:PHE:H	1.76	0.51
1:G:55:HIS:HB3	1:G:85:ALA:HA	1.93	0.51
1:G:178:PRO:HD2	1:G:210:VAL:HG12	1.92	0.51
1:E:7:HIS:HB3	2:F:115:MET:HE2	1.91	0.51
2:F:56:ILE:HG22	2:F:56:ILE:O	2.11	0.51
1:E:121:ILE:HD11	1:E:157:THR:HG21	1.93	0.51
2:D:95:GLN:NE2	2:F:95:GLN:HE21	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:LEU:HD13	2:L:119:TYR:HA	1.92	0.50
1:E:283:THR:HG22	1:E:285:LEU:HG	1.92	0.50
1:A:5:LEU:HD13	2:B:119:TYR:HA	1.92	0.50
2:D:95:GLN:NE2	2:F:95:GLN:HG2	2.26	0.50
1:G:34:GLU:OE1	1:G:283:THR:CG2	2.59	0.50
1:A:62:GLY:HA2	1:A:70:LEU:HD21	1.94	0.50
2:D:56:ILE:O	2:D:56:ILE:HG22	2.12	0.50
2:B:56:ILE:HG22	2:B:56:ILE:O	2.12	0.50
1:I:256:ARG:NH2	2:J:64:GLU:OE2	2.45	0.50
2:B:171:LEU:HD11	2:H:171:LEU:HD22	1.93	0.50
1:A:2:LYS:HG2	2:B:27:GLN:HG2	1.94	0.50
2:F:125:GLN:NE2	2:F:155:ASN:HA	2.27	0.50
1:G:5:LEU:HD13	2:H:119:TYR:HA	1.93	0.50
1:K:283:THR:HG22	1:K:285:LEU:HG	1.94	0.50
1:K:34:GLU:OE1	1:K:283:THR:CG2	2.59	0.50
1:A:34:GLU:OE1	1:A:283:THR:CG2	2.59	0.49
1:A:113:THR:HG23	1:A:115:PHE:H	1.77	0.49
2:J:56:ILE:HG22	2:J:56:ILE:O	2.12	0.49
1:K:62:GLY:HA2	1:K:70:LEU:HD21	1.94	0.49
2:L:51:LYS:HE2	2:L:107:THR:OG1	2.13	0.49
2:H:125:GLN:NE2	2:H:155:ASN:HA	2.28	0.49
2:H:56:ILE:O	2:H:56:ILE:HG22	2.12	0.49
2:B:125:GLN:NE2	2:B:155:ASN:HA	2.28	0.49
1:E:121:ILE:CD1	1:E:157:THR:HG21	2.42	0.49
1:G:123:SER:CA	1:G:145:LEU:HB3	2.38	0.49
2:L:125:GLN:NE2	2:L:155:ASN:HA	2.28	0.49
2:D:125:GLN:NE2	2:D:155:ASN:HA	2.28	0.49
2:J:125:GLN:NE2	2:J:155:ASN:HA	2.27	0.49
1:E:34:GLU:OE1	1:E:283:THR:CG2	2.61	0.49
2:B:1:GLY:N	9:B:303:HOH:O	2.45	0.49
1:I:7:HIS:HB3	2:J:115:MET:HE2	1.93	0.49
1:I:5:LEU:HD13	2:J:119:TYR:HA	1.95	0.48
1:A:149:ASN:HD22	1:A:152:GLN:NE2	2.11	0.48
1:E:113:THR:HG22	1:E:250:VAL:HG13	1.94	0.48
1:K:49:LYS:HE3	1:K:69:HIS:ND1	2.28	0.48
2:L:56:ILE:O	2:L:56:ILE:HG22	2.14	0.48
1:I:101:LYS:HE2	1:I:229:LEU:HD11	1.96	0.48
1:G:61:ILE:CG2	1:G:172:MET:HE3	2.42	0.48
1:C:215:GLN:HG2	1:C:218:GLY:C	2.34	0.48
1:C:215:GLN:HE21	1:C:218:GLY:HA2	1.78	0.48
1:C:49:LYS:HE3	1:C:69:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:ARG:HH21	2:L:34:GLN:HE22	1.57	0.48
1:C:314:ARG:NH1	9:C:503:HOH:O	2.45	0.47
1:G:113:THR:HG23	1:G:115:PHE:H	1.78	0.47
1:G:49:LYS:HE3	1:G:69:HIS:ND1	2.30	0.47
1:I:34:GLU:OE1	1:I:283:THR:CG2	2.56	0.47
2:L:4:GLY:O	2:L:8:GLY:HA3	2.14	0.47
1:K:162:ARG:HG3	1:K:235:LYS:HG2	1.97	0.47
1:C:224[A]:ASP:OD2	1:K:203:LYS:HD2	2.15	0.47
2:D:54:ARG:HD2	9:D:326:HOH:O	2.15	0.47
1:E:142:LEU:HD23	1:E:247:PRO:HA	1.97	0.47
1:I:219:GLN:HE22	8:I:401:SIA:C1	2.28	0.47
2:F:4:GLY:O	2:F:8:GLY:HA3	2.15	0.47
2:B:4:GLY:O	2:B:8:GLY:HA3	2.15	0.47
2:J:4:GLY:O	2:J:8:GLY:HA3	2.15	0.47
1:A:214:PRO:HG3	1:I:235:LYS:HG3	1.96	0.47
2:B:162:TYR:HA	9:B:309:HOH:O	2.15	0.47
1:I:132:ARG:HG2	1:I:133:ASN:HD22	1.79	0.47
1:K:132:ARG:HG2	1:K:133:ASN:HD22	1.80	0.47
1:G:150:LYS:C	1:G:150:LYS:HD2	2.35	0.46
2:D:4:GLY:O	2:D:8:GLY:HA3	2.15	0.46
1:E:5:LEU:HD13	2:F:119:TYR:HA	1.96	0.46
2:H:4:GLY:O	2:H:8:GLY:HA3	2.15	0.46
1:I:131:MET:CE	1:I:134:GLY:O	2.63	0.46
1:K:142:LEU:HD23	1:K:247:PRO:HA	1.96	0.46
1:K:5:LEU:HD21	2:L:24:PHE:CE2	2.50	0.46
1:C:132:ARG:HG2	1:C:133:ASN:HD22	1.80	0.46
1:C:88:TYR:CZ	1:C:219:GLN:HG2	2.51	0.46
1:E:132:ARG:HG2	1:E:133:ASN:HD22	1.81	0.46
1:A:205:ASN:HB2	1:G:209:VAL:CG2	2.47	0.45
1:G:142:LEU:HD23	1:G:247:PRO:HA	1.98	0.45
1:A:142:LEU:HD23	1:A:247:PRO:HA	1.98	0.45
1:C:142:LEU:HD23	1:C:247:PRO:HA	1.98	0.45
1:G:128:LYS:HD3	1:G:136:ASN:OD1	2.15	0.45
1:I:142:LEU:HD23	1:I:247:PRO:HA	1.98	0.45
2:F:25:ARG:HH21	2:F:34:GLN:NE2	2.15	0.45
1:A:313:MET:HG3	1:A:314:ARG:O	2.17	0.45
1:G:117:TYR:CZ	1:G:145:LEU:HD21	2.52	0.45
2:J:25:ARG:HH21	2:J:34:GLN:NE2	2.16	0.44
1:G:123:SER:HA	1:G:145:LEU:CB	2.42	0.44
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.17	0.44
1:I:313:MET:HG3	1:I:314:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:153:ASN:ND2	9:K:509:HOH:O	2.49	0.44
1:A:200:SER:OG	1:A:234:ASP:OD2	2.35	0.44
1:C:313:MET:HG3	1:C:314:ARG:O	2.17	0.44
2:F:25:ARG:HH21	2:F:34:GLN:HE22	1.66	0.44
1:G:38:LEU:CD1	1:G:38:LEU:N	2.81	0.44
1:A:101:LYS:HE2	1:A:229:LEU:HD11	2.00	0.44
2:D:30:GLN:HB2	9:D:321:HOH:O	2.18	0.44
2:B:25:ARG:HH21	2:B:34:GLN:NE2	2.16	0.44
1:E:205:ASN:HB2	1:K:209:VAL:CG2	2.47	0.44
1:E:313:MET:HG3	1:E:314:ARG:O	2.18	0.44
2:J:25:ARG:HD2	9:J:315:HOH:O	2.17	0.44
1:K:313:MET:HG3	1:K:314:ARG:O	2.18	0.44
1:C:176:HIS:CE1	4:N:2:SIA:H91	2.52	0.44
1:I:38:LEU:N	1:I:38:LEU:CD1	2.81	0.43
1:K:182:GLN:HG3	9:K:575:HOH:O	2.17	0.43
1:G:162:ARG:HG3	1:G:235:LYS:HG2	2.01	0.43
1:G:313:MET:HG3	1:G:314:ARG:O	2.18	0.43
1:K:149:ASN:HD22	1:K:152:GLN:NE2	2.17	0.43
2:B:25:ARG:HH21	2:B:34:GLN:HE22	1.67	0.42
1:C:235:LYS:HG3	1:E:214:PRO:HG3	2.00	0.42
2:L:25:ARG:HE	2:L:34:GLN:HE21	1.67	0.42
1:G:219:GLN:HE22	3:R:2:GAL:H4	1.83	0.42
2:H:25:ARG:HH21	2:H:34:GLN:NE2	2.17	0.42
2:J:25:ARG:HH21	2:J:34:GLN:HE22	1.67	0.42
1:G:122:ASN:O	1:G:145:LEU:HA	2.19	0.42
1:A:162:ARG:HG3	1:A:235:LYS:HG2	2.01	0.42
1:C:224[B]:ASP:OD1	1:K:203:LYS:HD2	2.17	0.42
2:D:25:ARG:HH21	2:D:34:GLN:NE2	2.17	0.42
2:D:159:HIS:HD2	9:D:311:HOH:O	2.01	0.42
2:L:133:ASP:HB3	2:L:137:CYS:O	2.20	0.42
3:M:1:NAG:H83	3:M:1:NAG:H3	2.01	0.42
2:B:95:GLN:NE2	2:J:95:GLN:HE22	2.17	0.42
1:I:128:LYS:HE3	1:I:128:LYS:C	2.40	0.42
2:L:164:GLU:CD	2:L:164:GLU:H	2.23	0.42
2:L:133:ASP:OD2	2:L:135:LYS:N	2.46	0.42
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.20	0.41
1:E:41:LEU:N	1:E:41:LEU:HD12	2.35	0.41
2:B:95:GLN:HE21	2:H:95:GLN:NE2	2.19	0.41
1:E:80:ARG:HH21	1:E:266:ILE:HD11	1.85	0.41
1:E:39:ASN:HD22	1:E:39:ASN:N	2.17	0.41
1:G:68:LEU:HD12	1:G:68:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:GLN:HB2	2:L:30:GLN:HE21	1.56	0.41
3:R:1:NAG:C8	3:R:1:NAG:H1	2.48	0.41
1:E:19:LEU:HB2	2:F:105:GLN:HE21	1.86	0.41
1:G:88:TYR:CE1	1:G:223:ILE:HG13	2.55	0.41
2:F:30:GLN:HB2	2:F:30:GLN:HE21	1.58	0.41
2:H:2:LEU:HD23	2:H:2:LEU:HA	1.95	0.41
2:D:25:ARG:HH21	2:D:34:GLN:HE22	1.69	0.41
1:G:80:ARG:HH21	1:G:266:ILE:HD11	1.85	0.41
2:D:85:LYS:HG2	2:F:83:TRP:CH2	2.56	0.41
1:E:203:LYS:CE	1:K:224:ASP:OD2	2.69	0.41
1:G:-1:ASP:HB3	1:G:0:PRO:HD3	2.02	0.41
2:B:171:LEU:HD22	2:J:171:LEU:HD21	2.02	0.41
2:B:2:LEU:HD23	2:B:2:LEU:HA	1.94	0.41
1:C:283:THR:OG1	1:C:285:LEU:HG	2.21	0.40
1:I:175:ILE:HD13	1:I:226:HIS:ND1	2.36	0.40
1:I:7:HIS:HB3	2:J:115:MET:HE1	2.01	0.40
1:K:4:CYS:HA	2:L:137:CYS:HA	2.03	0.40
1:G:174:GLY:H	1:G:245:ILE:HG22	1.85	0.40
2:H:159:HIS:HD2	9:H:311:HOH:O	2.03	0.40
1:K:288:GLN:HG2	1:K:290:LEU:H	1.87	0.40
1:G:261:GLN:HB3	2:H:70:PHE:CE2	2.56	0.40
2:H:82:ASN:HD22	2:H:82:ASN:HA	1.61	0.40
1:I:175:ILE:N	1:I:175:ILE:CD1	2.85	0.40
1:A:215:GLN:HE21	1:A:218:GLY:HA2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/325 (98%)	315 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	319/325 (98%)	317 (99%)	2 (1%)	0	100	100
1	E	319/325 (98%)	316 (99%)	3 (1%)	0	100	100
1	G	318/325 (98%)	316 (99%)	2 (1%)	0	100	100
1	I	319/325 (98%)	317 (99%)	2 (1%)	0	100	100
1	K	316/325 (97%)	311 (98%)	5 (2%)	0	100	100
2	B	170/177 (96%)	167 (98%)	3 (2%)	0	100	100
2	D	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
2	F	170/177 (96%)	167 (98%)	3 (2%)	0	100	100
2	H	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
2	J	170/177 (96%)	167 (98%)	3 (2%)	0	100	100
2	L	170/177 (96%)	166 (98%)	4 (2%)	0	100	100
All	All	2930/3012 (97%)	2891 (99%)	39 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/275 (98%)	263 (97%)	8 (3%)	41	67
1	C	270/275 (98%)	261 (97%)	9 (3%)	38	64
1	E	270/275 (98%)	258 (96%)	12 (4%)	28	53
1	G	263/275 (96%)	249 (95%)	14 (5%)	22	45
1	I	270/275 (98%)	255 (94%)	15 (6%)	21	42
1	K	268/275 (98%)	262 (98%)	6 (2%)	52	76
2	B	146/151 (97%)	143 (98%)	3 (2%)	53	77
2	D	145/151 (96%)	142 (98%)	3 (2%)	53	77
2	F	145/151 (96%)	142 (98%)	3 (2%)	53	77
2	H	145/151 (96%)	143 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	145/151 (96%)	142 (98%)	3 (2%)	53 77
2	L	145/151 (96%)	141 (97%)	4 (3%)	43 69
All	All	2483/2556 (97%)	2401 (97%)	82 (3%)	38 64

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	8	HIS
1	A	113	THR
1	A	153	ASN
1	A	199	SER
1	A	251	SER
1	A	283	THR
1	A	288	GLN
2	B	113	SER
2	B	135	LYS
2	B	164	GLU
1	C	8	HIS
1	C	150	LYS
1	C	153	ASN
1	C	215	GLN
1	C	220	SER
1	C	235	LYS
1	C	248	SER
1	C	251	SER
1	C	268	ASN
2	D	27	GLN
2	D	113	SER
2	D	164	GLU
1	E	-1	ASP
1	E	8	HIS
1	E	19	LEU
1	E	23	GLN
1	E	39	ASN
1	E	100	GLN
1	E	153	ASN
1	E	248	SER
1	E	268	ASN
1	E	269	SER
1	E	283	THR

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Mol	Chain	Res	Type
1	E	288	GLN
2	F	30	GLN
2	F	73	ILE
2	F	113	SER
1	G	8	HIS
1	G	86	TYR
1	G	121	ILE
1	G	145	LEU
1	G	153	ASN
1	G	183	GLU
1	G	187	LEU
1	G	220	SER
1	G	239	SER
1	G	263	GLU
1	G	268	ASN
1	G	283	THR
1	G	288	GLN
1	G	318	GLU
2	H	27	GLN
2	H	113	SER
1	I	8	HIS
1	I	17	LYS
1	I	128	LYS
1	I	199	SER
1	I	213	ARG
1	I	217	ASN
1	I	220	SER
1	I	248	SER
1	I	251	SER
1	I	268	ASN
1	I	269	SER
1	I	283	THR
1	I	288	GLN
1	I	293	ARG
1	I	318	GLU
2	J	30	GLN
2	J	113	SER
2	J	161	GLN
1	K	8	HIS
1	K	113	THR
1	K	153	ASN
1	K	220	SER

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Mol	Chain	Res	Type
1	K	283	THR
1	K	288	GLN
2	L	30	GLN
2	L	113	SER
2	L	133	ASP
2	L	164	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	23	GLN
1	A	152	GLN
1	A	153	ASN
1	A	159	ASN
1	A	176	HIS
1	A	215	GLN
1	A	240	HIS
1	A	288	GLN
1	A	297	GLN
2	B	34	GLN
2	B	79	ASN
2	B	105	GLN
2	B	117	ASN
2	B	125	GLN
1	C	8	HIS
1	C	23	GLN
1	C	133	ASN
1	C	153	ASN
1	C	159	ASN
1	C	176	HIS
1	C	191	GLN
1	C	215	GLN
1	C	219	GLN
1	C	240	HIS
1	C	268	ASN
1	C	297	GLN
2	D	27	GLN
2	D	34	GLN
2	D	95	GLN
2	D	105	GLN
2	D	117	ASN

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Mol	Chain	Res	Type
2	D	125	GLN
1	E	8	HIS
1	E	23	GLN
1	E	39	ASN
1	E	133	ASN
1	E	152	GLN
1	E	153	ASN
1	E	159	ASN
1	E	176	HIS
1	E	185	ASN
1	E	268	ASN
1	E	288	GLN
1	E	297	GLN
2	F	30	GLN
2	F	34	GLN
2	F	95	GLN
2	F	105	GLN
2	F	117	ASN
2	F	125	GLN
2	F	142	HIS
2	F	155	ASN
2	F	161	GLN
1	G	23	GLN
1	G	153	ASN
1	G	176	HIS
1	G	185	ASN
1	G	215	GLN
1	G	219	GLN
1	G	288	GLN
1	G	297	GLN
2	H	27	GLN
2	H	34	GLN
2	H	95	GLN
2	H	105	GLN
2	H	117	ASN
2	H	125	GLN
2	H	155	ASN
2	H	161	GLN
1	I	8	HIS
1	I	23	GLN
1	I	100	GLN
1	I	133	ASN

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Mol	Chain	Res	Type
1	I	152	GLN
1	I	153	ASN
1	I	156	GLN
1	I	159	ASN
1	I	176	HIS
1	I	217	ASN
1	I	219	GLN
1	I	240	HIS
1	I	288	GLN
1	I	297	GLN
2	J	27	GLN
2	J	34	GLN
2	J	95	GLN
2	J	105	GLN
2	J	117	ASN
2	J	125	GLN
1	K	8	HIS
1	K	23	GLN
1	K	133	ASN
1	K	152	GLN
1	K	153	ASN
1	K	159	ASN
1	K	176	HIS
1	K	217	ASN
1	K	240	HIS
1	K	288	GLN
1	K	297	GLN
2	L	27	GLN
2	L	30	GLN
2	L	34	GLN
2	L	117	ASN
2	L	125	GLN
2	L	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

24 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	15,15,15	0.84	0	21,21,21	2.27	7 (33%)
3	GAL	M	2	3	11,11,12	0.43	0	15,15,17	1.34	2 (13%)
3	SIA	M	3	3	17,20,21	0.53	0	21,28,31	1.32	3 (14%)
4	GAL	N	1	4	12,12,12	0.73	0	17,17,17	1.41	3 (17%)
4	SIA	N	2	4	17,20,21	0.53	0	21,28,31	1.24	2 (9%)
5	NAG	O	1	2,5,6	14,14,15	0.58	0	17,19,21	1.82	3 (17%)
5	NAG	O	2	5	14,14,15	0.46	0	17,19,21	1.21	1 (5%)
3	NAG	P	1	3	15,15,15	0.81	0	21,21,21	1.98	3 (14%)
3	GAL	P	2	3	11,11,12	0.62	0	15,15,17	1.62	2 (13%)
3	SIA	P	3	3	17,20,21	0.60	0	21,28,31	1.44	3 (14%)
5	NAG	Q	1	2,5	14,14,15	0.52	0	17,19,21	1.52	3 (17%)
5	NAG	Q	2	5	14,14,15	0.49	0	17,19,21	1.12	1 (5%)
3	NAG	R	1	3	15,15,15	0.51	0	21,21,21	2.18	8 (38%)
3	GAL	R	2	3	11,11,12	0.39	0	15,15,17	1.29	3 (20%)
3	SIA	R	3	3	17,20,21	0.69	0	21,28,31	1.23	3 (14%)
5	NAG	S	1	2,5,6	14,14,15	0.57	0	17,19,21	1.98	4 (23%)
5	NAG	S	2	5	14,14,15	0.40	0	17,19,21	0.90	1 (5%)
5	NAG	T	1	2,5	14,14,15	0.43	0	17,19,21	1.66	1 (5%)
5	NAG	T	2	5	14,14,15	0.35	0	17,19,21	1.35	1 (5%)
3	NAG	U	1	3	15,15,15	0.82	0	21,21,21	1.68	4 (19%)
3	GAL	U	2	3	11,11,12	0.28	0	15,15,17	1.49	3 (20%)
3	SIA	U	3	3	17,20,21	0.49	0	21,28,31	1.38	4 (19%)
5	NAG	V	1	2,5	14,14,15	0.39	0	17,19,21	1.18	2 (11%)
5	NAG	V	2	5	14,14,15	0.52	0	17,19,21	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3	-	6/6/26/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	2/14/34/38	0/1/1/1
4	GAL	N	1	4	-	2/2/22/22	0/1/1/1
4	SIA	N	2	4	-	0/14/34/38	0/1/1/1
5	NAG	O	1	2,5,6	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3	-	2/6/26/26	0/1/1/1
3	GAL	P	2	3	-	1/2/19/22	0/1/1/1
3	SIA	P	3	3	-	0/14/34/38	0/1/1/1
5	NAG	Q	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3	-	4/6/26/26	0/1/1/1
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	1/14/34/38	0/1/1/1
5	NAG	S	1	2,5,6	-	1/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3	-	3/6/26/26	0/1/1/1
3	GAL	U	2	3	-	0/2/19/22	0/1/1/1
3	SIA	U	3	3	-	0/14/34/38	0/1/1/1
5	NAG	V	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	1	NAG	C1-O5-C5	5.83	120.09	112.19
5	S	1	NAG	C1-O5-C5	5.64	119.84	112.19
3	P	1	NAG	O5-C1-C2	5.59	115.13	109.52
3	P	1	NAG	C1-C2-N2	-4.96	104.98	110.73
3	P	2	GAL	C1-C2-C3	4.93	115.72	109.67
3	M	1	NAG	C1-C2-C3	4.92	117.25	110.54
5	O	1	NAG	O5-C5-C6	-4.81	99.66	107.20
5	T	2	NAG	C1-O5-C5	4.55	118.36	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1	NAG	C8-C7-N2	4.46	123.65	116.10
3	U	1	NAG	C2-N2-C7	4.11	133.18	123.18
3	P	3	SIA	C4-C5-N5	-4.10	102.26	110.38
3	R	1	NAG	C1-C2-C3	4.03	116.05	110.54
3	U	1	NAG	C8-C7-N2	3.96	122.81	116.10
3	M	1	NAG	C8-C7-N2	3.87	122.65	116.10
3	M	1	NAG	C2-N2-C7	3.81	132.45	123.18
4	N	2	SIA	C6-O6-C2	3.79	119.45	111.34
3	M	1	NAG	C4-C3-C2	3.69	115.75	110.34
3	R	1	NAG	C4-C3-C2	3.67	115.71	110.34
3	U	3	SIA	C4-C5-N5	-3.66	103.13	110.38
5	Q	1	NAG	O5-C1-C2	-3.59	105.61	111.29
4	N	1	GAL	C3-C4-C5	3.59	116.65	110.24
5	O	1	NAG	C1-O5-C5	3.32	116.68	112.19
3	M	1	NAG	O5-C1-C2	3.20	112.74	109.52
3	M	3	SIA	C4-C5-N5	-3.17	104.09	110.38
3	P	3	SIA	C6-O6-C2	3.13	118.03	111.34
5	Q	1	NAG	C1-O5-C5	3.06	116.34	112.19
3	M	2	GAL	C1-C2-C3	3.06	113.42	109.67
3	M	1	NAG	C3-C4-C5	3.02	115.63	110.24
3	U	1	NAG	C1-C2-C3	3.01	114.65	110.54
3	P	1	NAG	C1-C2-C3	2.97	114.59	110.54
3	R	1	NAG	C2-N2-C7	2.97	130.40	123.18
3	R	1	NAG	C3-C2-N2	-2.84	105.25	110.62
3	R	1	NAG	C3-C4-C5	2.83	115.29	110.24
4	N	2	SIA	C4-C5-N5	-2.80	104.83	110.38
5	Q	2	NAG	C1-O5-C5	2.77	115.94	112.19
5	S	1	NAG	C6-C5-C4	-2.76	106.55	113.00
3	U	3	SIA	C3-C4-C5	-2.66	108.25	111.46
3	U	2	GAL	C3-C4-C5	2.65	114.96	110.24
3	U	2	GAL	O5-C1-C2	-2.62	106.73	110.77
3	R	2	GAL	O5-C1-C2	-2.61	106.75	110.77
4	N	1	GAL	O5-C5-C4	2.60	114.42	109.69
4	N	1	GAL	O5-C1-C2	-2.59	105.66	110.28
3	R	1	NAG	O7-C7-C8	-2.59	117.25	122.06
3	R	3	SIA	C4-C5-N5	-2.52	105.39	110.38
5	Q	1	NAG	C8-C7-N2	-2.38	112.07	116.10
3	U	2	GAL	C1-O5-C5	2.34	115.36	112.19
3	R	3	SIA	C6-O6-C2	2.31	116.28	111.34
3	M	1	NAG	C1-C2-N2	-2.29	108.07	110.73
3	U	3	SIA	C9-C8-C7	-2.28	107.46	112.41
5	O	1	NAG	C1-C2-N2	-2.25	106.64	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	2	GAL	C1-C2-C3	-2.25	106.90	109.67
3	R	2	GAL	O5-C5-C6	2.25	110.73	107.20
3	U	1	NAG	O7-C7-N2	-2.22	117.87	121.95
3	R	3	SIA	C5-N5-C10	2.18	128.49	123.18
5	S	1	NAG	C3-C4-C5	2.18	114.13	110.24
5	V	1	NAG	C2-N2-C7	2.15	125.96	122.90
3	R	1	NAG	O4-C4-C3	-2.15	105.38	110.35
5	S	2	NAG	C1-C2-N2	2.12	114.11	110.49
3	P	3	SIA	C3-C4-C5	-2.10	108.92	111.46
3	M	2	GAL	C1-O5-C5	-2.09	109.35	112.19
3	M	3	SIA	C6-O6-C2	2.08	115.79	111.34
3	M	3	SIA	C5-N5-C10	2.07	128.22	123.18
3	P	2	GAL	O2-C2-C3	-2.07	105.99	110.14
5	O	2	NAG	O4-C4-C5	2.07	114.44	109.30
5	V	1	NAG	O5-C5-C4	-2.05	105.84	110.83
3	U	3	SIA	O6-C2-C3	-2.03	106.31	109.87
5	S	1	NAG	O3-C3-C4	-2.03	105.67	110.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	1	NAG	C1-C2-N2-C7
4	N	1	GAL	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
4	N	1	GAL	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	P	2	GAL	O5-C5-C6-O6
3	M	1	NAG	C3-C2-N2-C7
5	T	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C1-C2-N2-C7
5	T	2	NAG	O5-C5-C6-O6
3	M	3	SIA	C4-C5-N5-C10
3	P	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
5	S	1	NAG	O5-C5-C6-O6
3	M	3	SIA	C6-C5-N5-C10
3	R	3	SIA	C6-C5-N5-C10
3	M	1	NAG	C1-C2-N2-C7

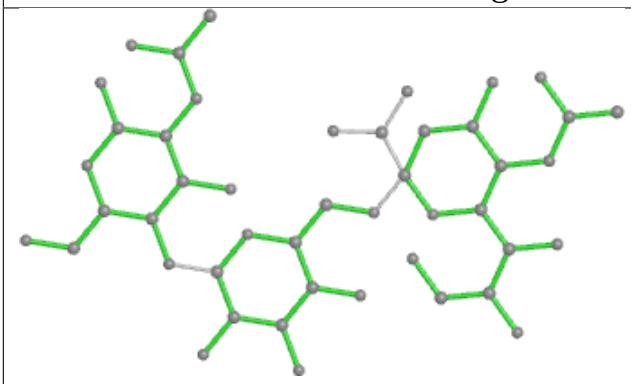
There are no ring outliers.

5 monomers are involved in 7 short contacts:

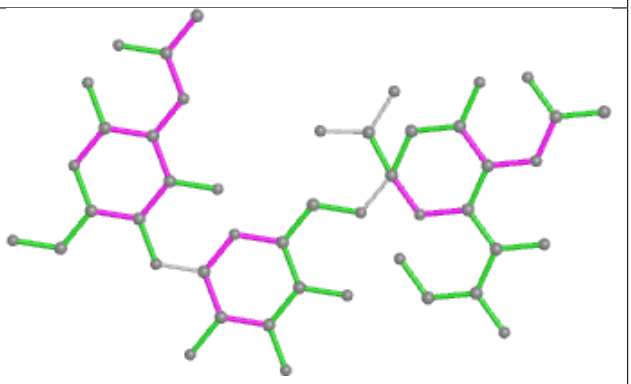
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	2	0
4	N	2	SIA	1	0
3	U	1	NAG	1	0
3	M	1	NAG	1	0
3	R	2	GAL	2	0

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

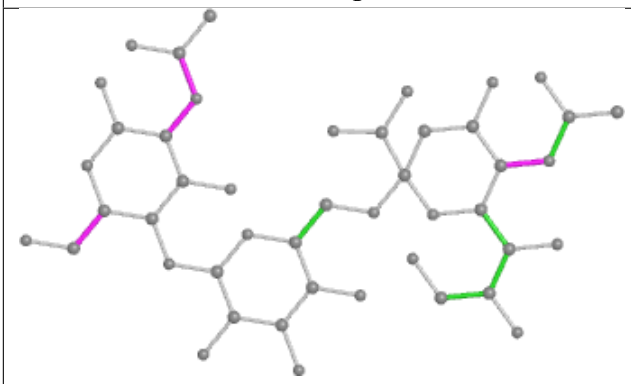
Oligosaccharide Chain M



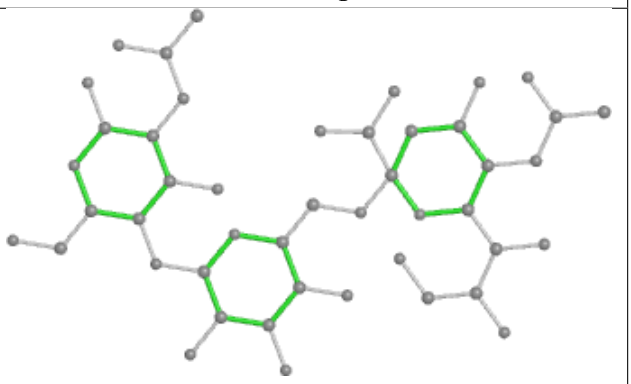
Bond lengths



Bond angles

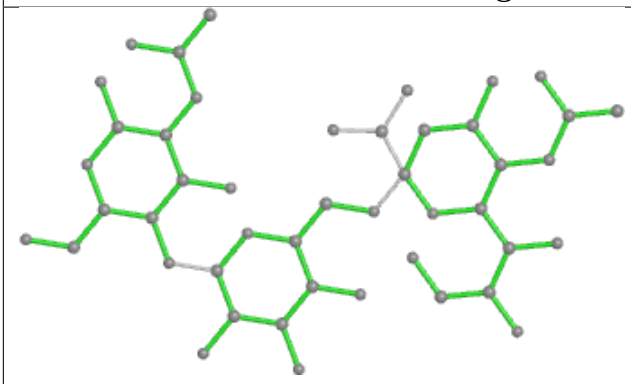


Torsions

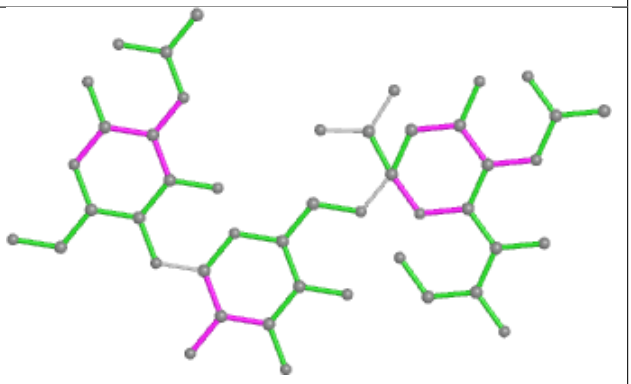


Rings

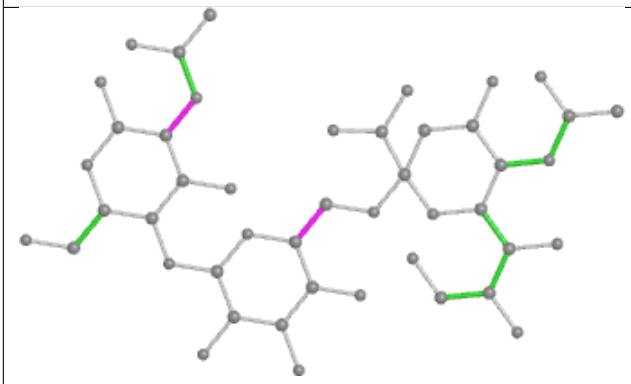
Oligosaccharide Chain P



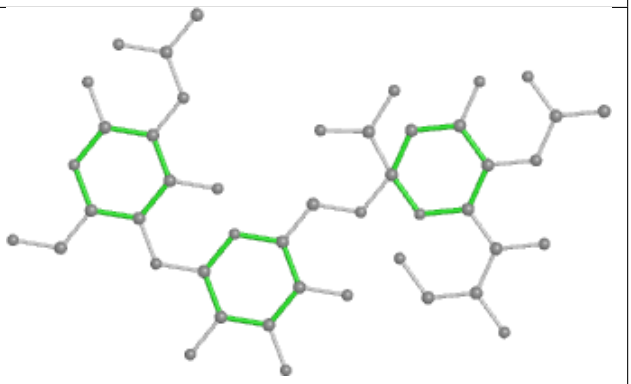
Bond lengths



Bond angles

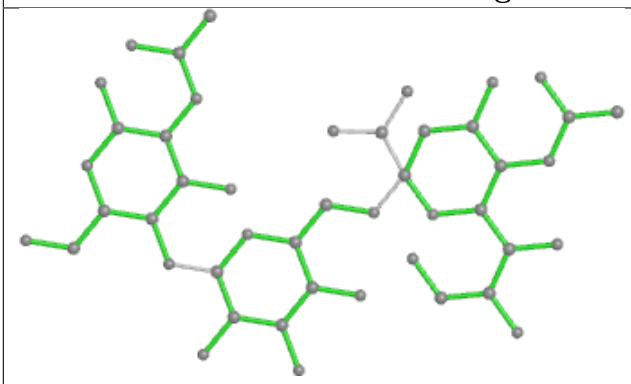


Torsions

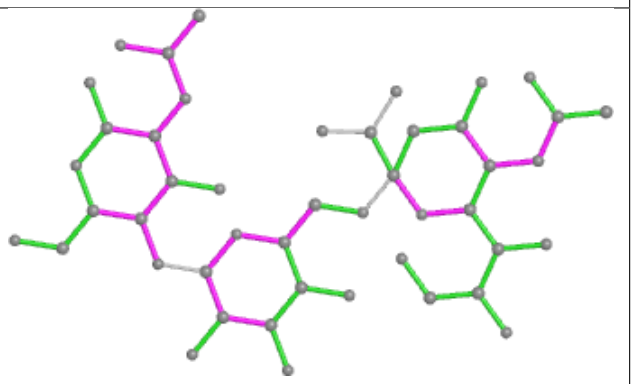


Rings

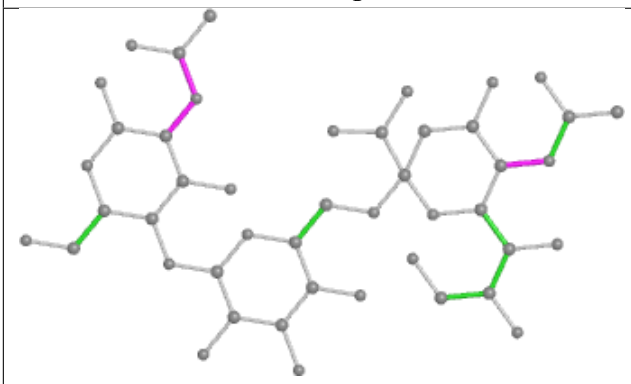
Oligosaccharide Chain R



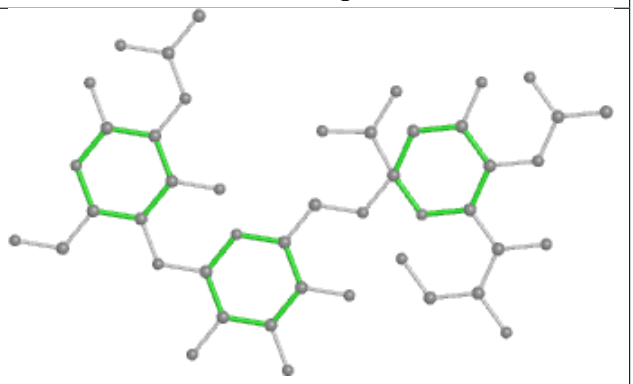
Bond lengths



Bond angles

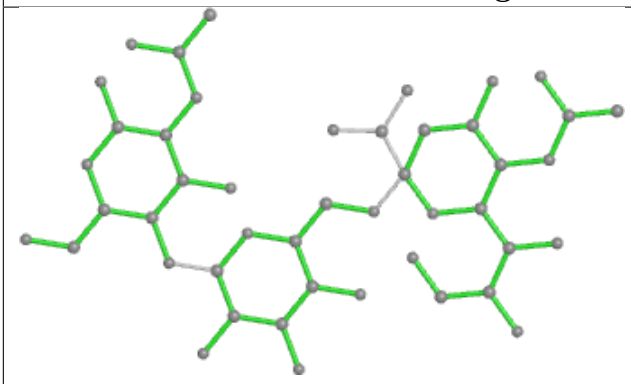


Torsions

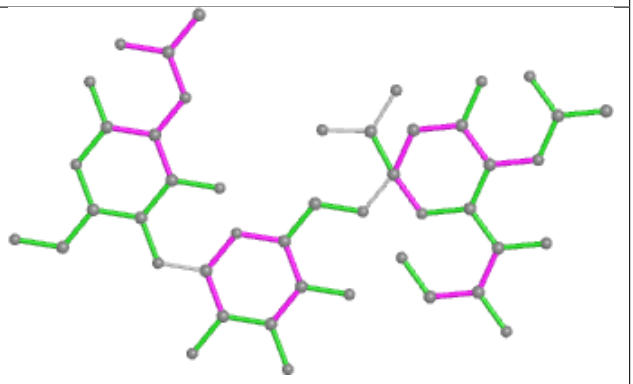


Rings

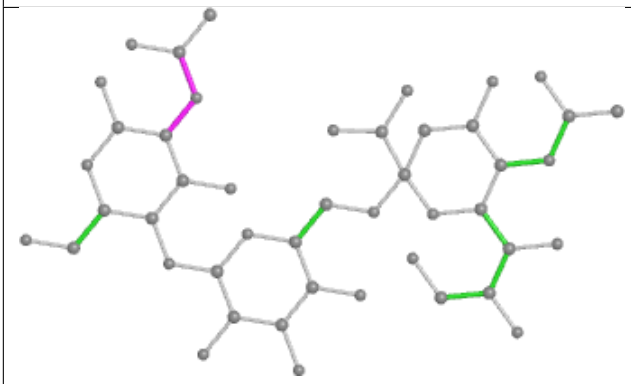
Oligosaccharide Chain U



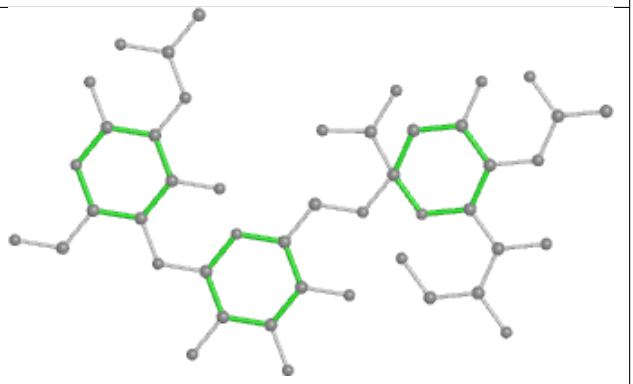
Bond lengths



Bond angles

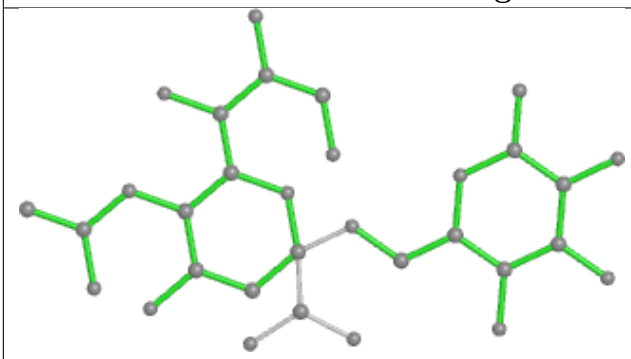


Torsions

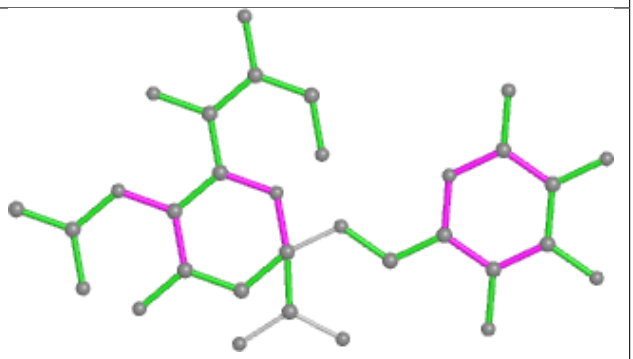


Rings

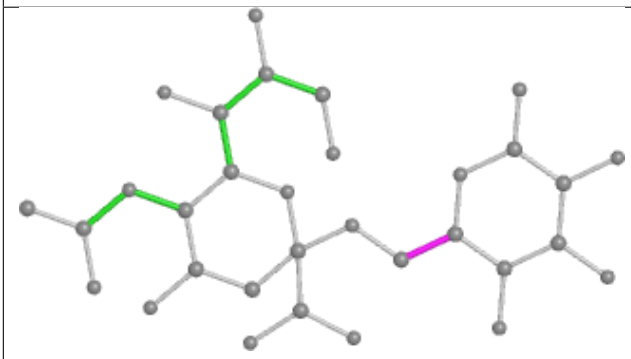
Oligosaccharide Chain N



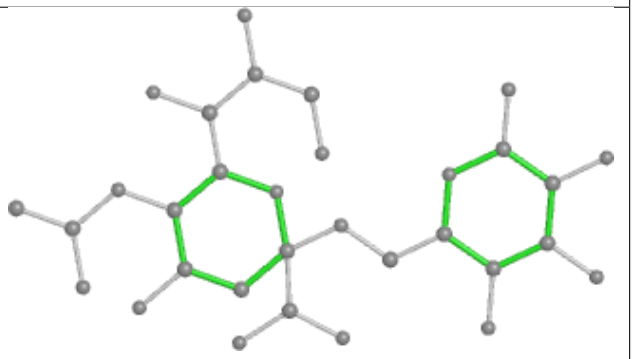
Bond lengths



Bond angles

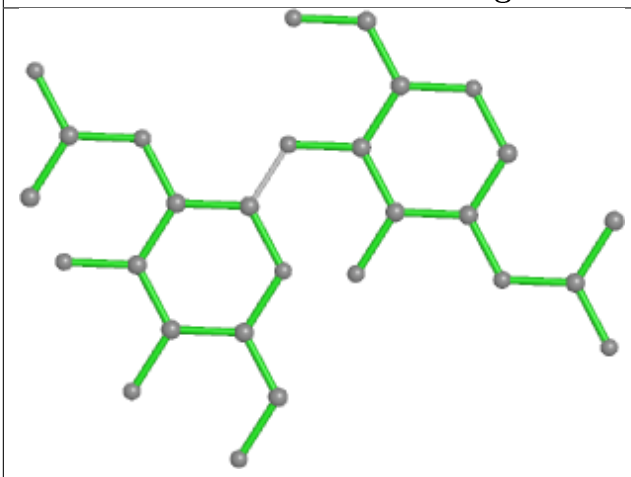


Torsions

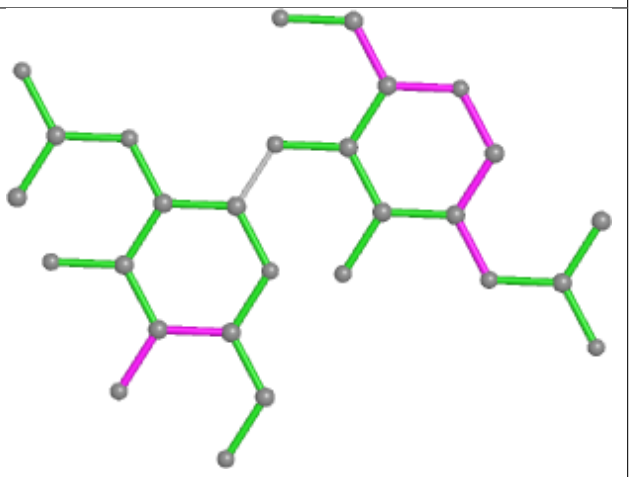


Rings

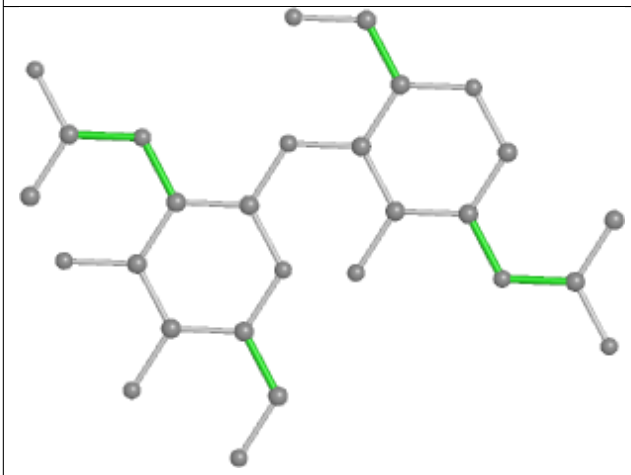
Oligosaccharide Chain O



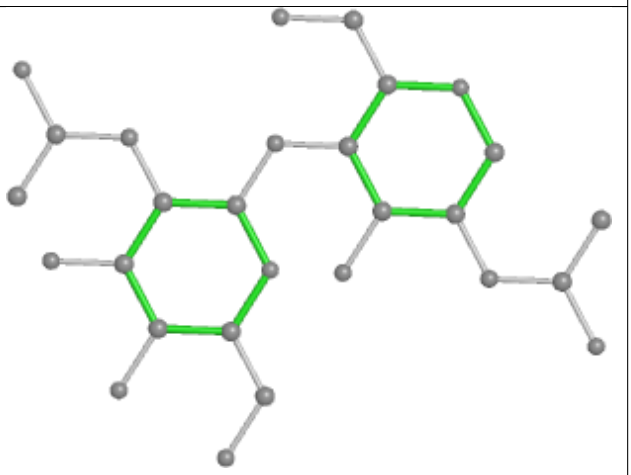
Bond lengths



Bond angles

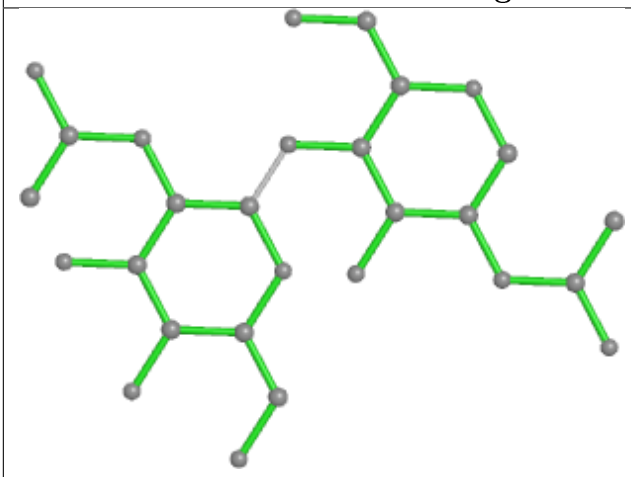


Torsions

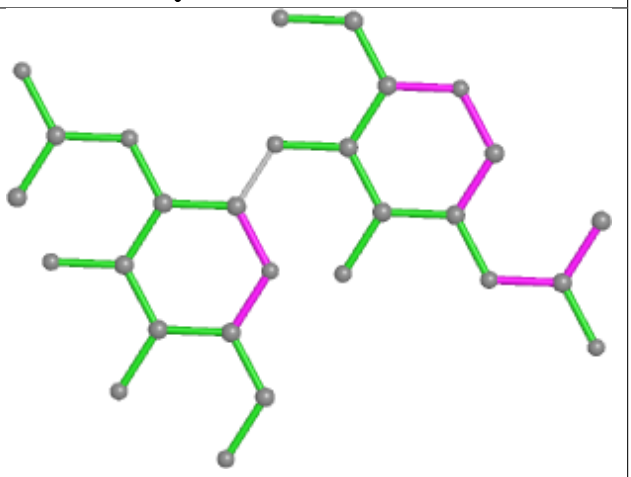


Rings

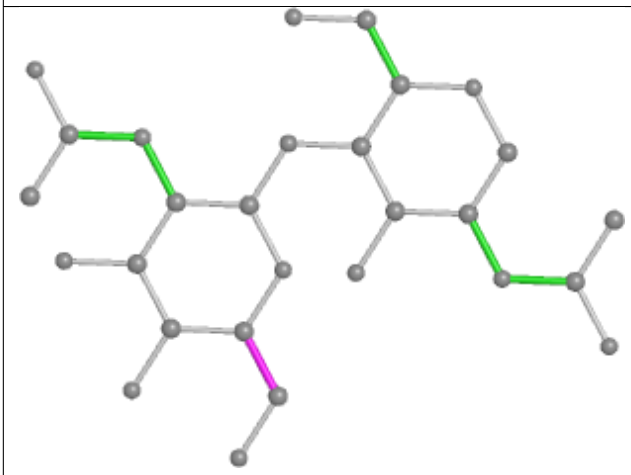
Oligosaccharide Chain Q



Bond lengths



Bond angles



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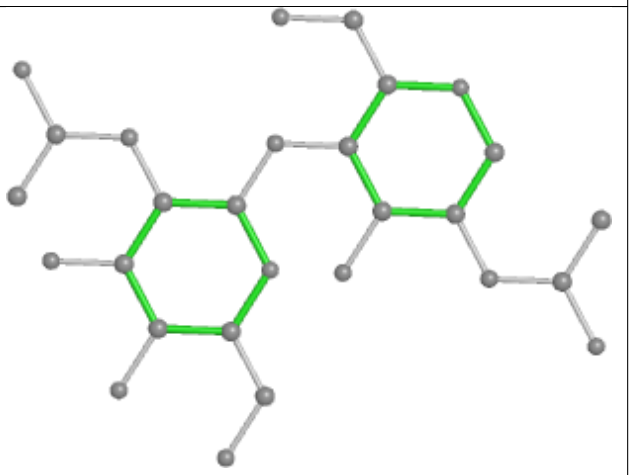
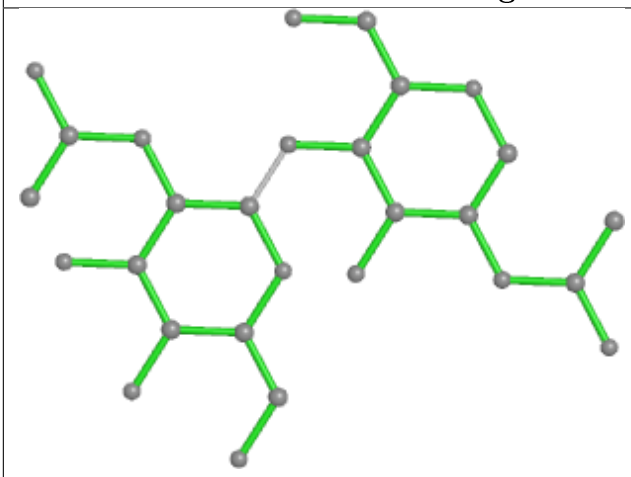
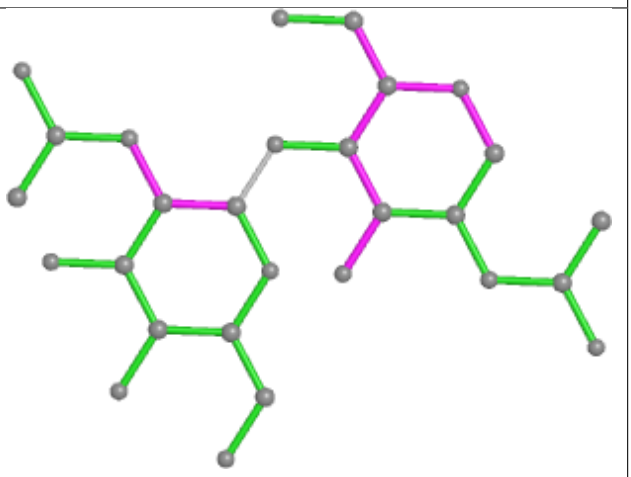


Rings

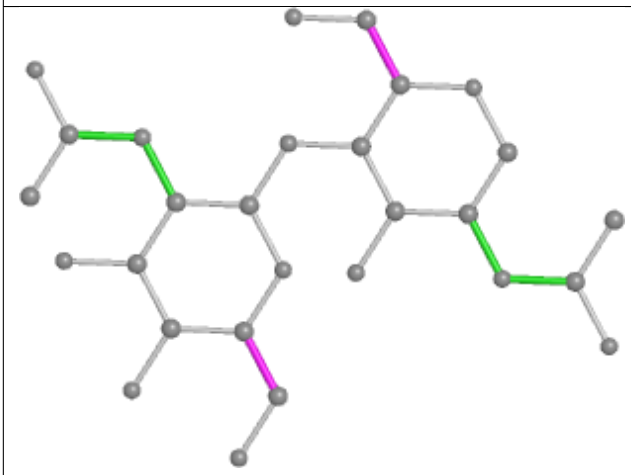
Oligosaccharide Chain S



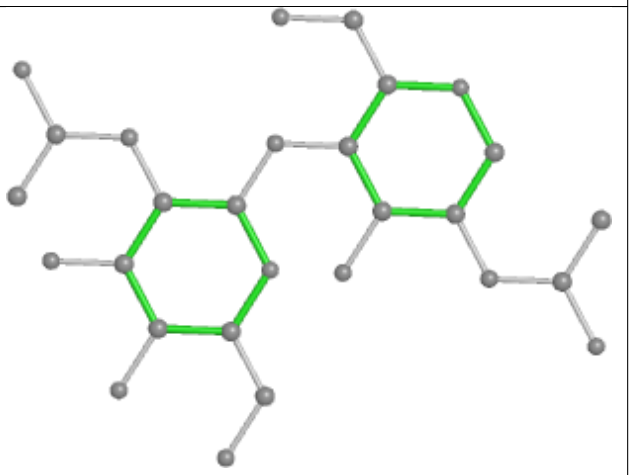
Bond lengths



Bond angles

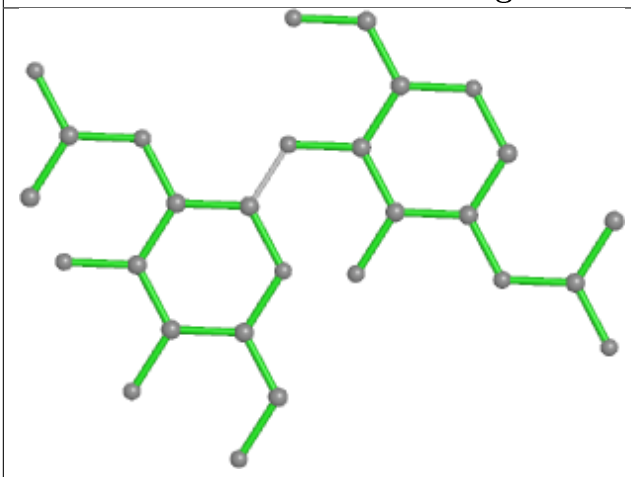


Torsions

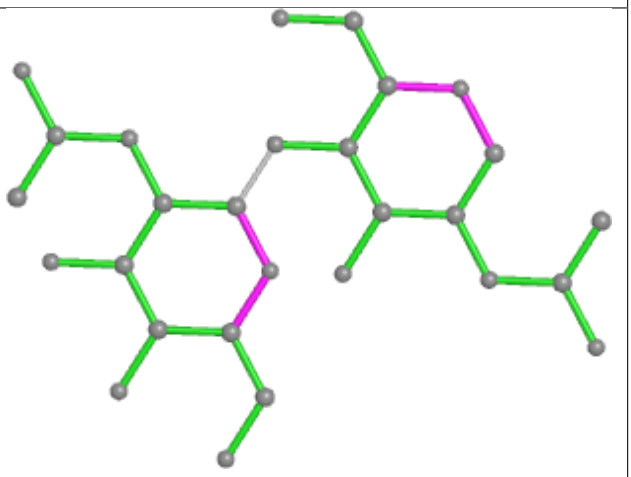


Rings

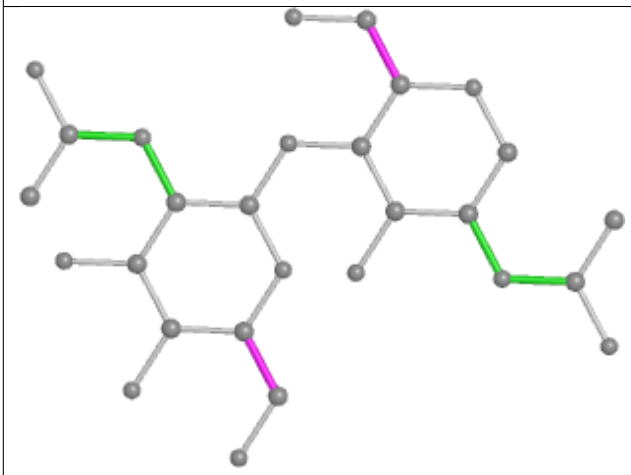
Oligosaccharide Chain T



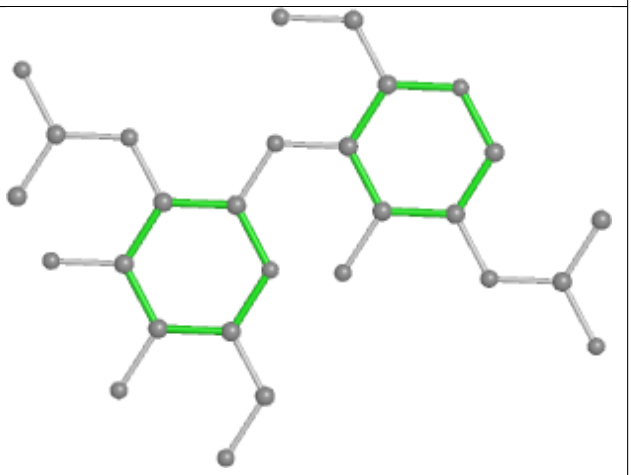
Bond lengths



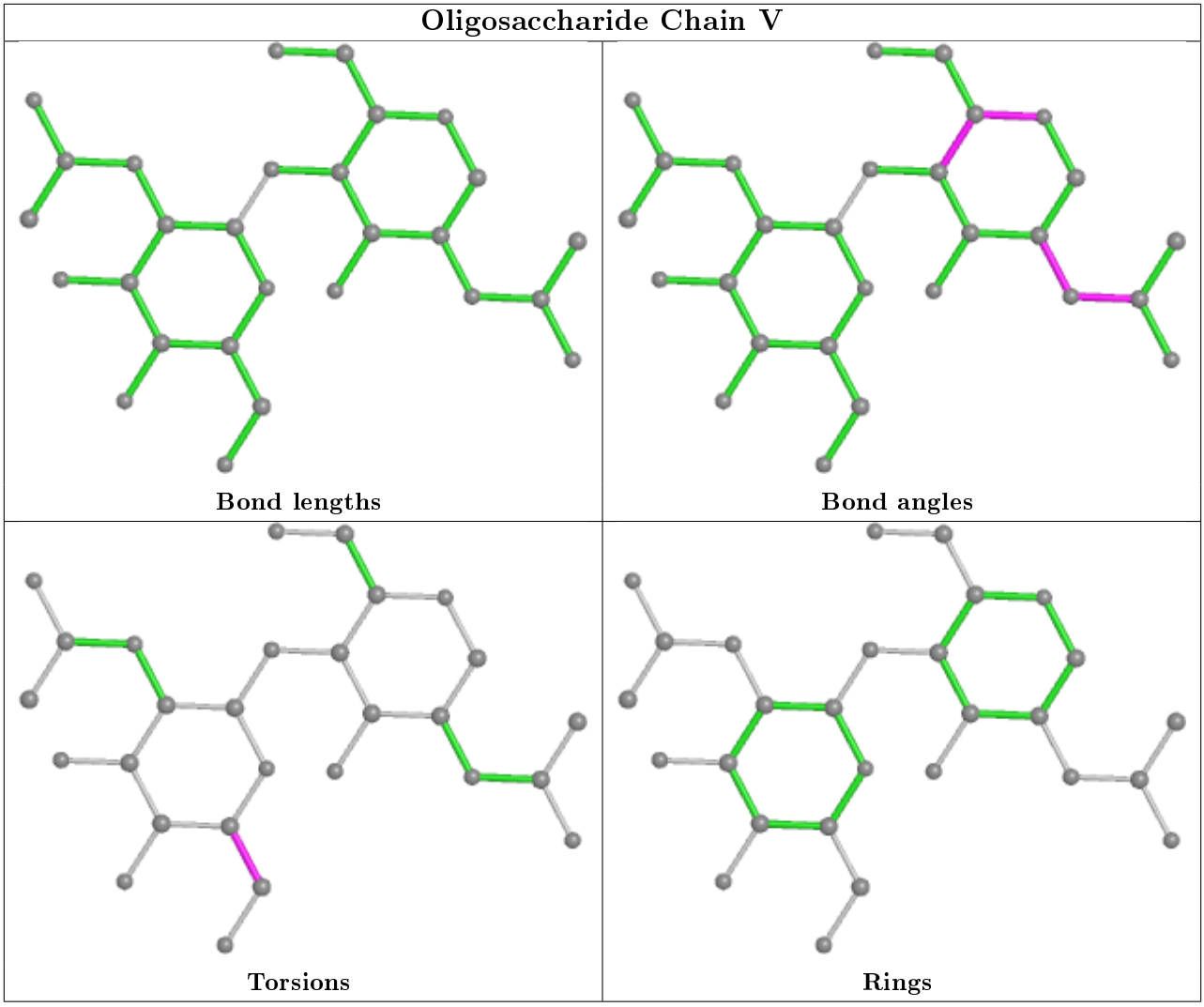
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
7	NAG	L	203	2	14,14,15	0.51	0	17,19,21	1.76	3 (17%)
7	NAG	B	202	2	14,14,15	0.62	1 (7%)	17,19,21	1.35	2 (11%)
8	SIA	I	401	-	18,21,21	0.51	0	21,31,31	0.79	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	201	2,6	14,14,15	0.55	0	17,19,21	1.65	3 (17%)

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
7	NAG	L	203	2	-	2/6/23/26	0/1/1/1
7	NAG	B	202	2	-	2/6/23/26	0/1/1/1
8	SIA	I	401	-	-	6/14/38/38	0/1/1/1
7	NAG	B	201	2,6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	202	NAG	C1-C2	2.02	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	203	NAG	C1-C2-N2	5.12	119.24	110.49
7	B	201	NAG	C1-O5-C5	4.29	118.01	112.19
7	B	201	NAG	O5-C1-C2	-3.58	105.63	111.29
7	L	203	NAG	O5-C1-C2	-3.19	106.25	111.29
7	B	202	NAG	O5-C1-C2	2.99	116.00	111.29
7	B	202	NAG	O5-C5-C6	2.83	111.64	107.20
7	L	203	NAG	C3-C4-C5	2.41	114.53	110.24
8	I	401	SIA	C8-C7-C6	2.05	116.92	113.03
7	B	201	NAG	O4-C4-C5	2.04	114.36	109.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	401	SIA	O8-C8-C9-O9
8	I	401	SIA	C7-C8-C9-O9
7	B	202	NAG	C4-C5-C6-O6
8	I	401	SIA	O7-C7-C8-C9
8	I	401	SIA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	B	202	NAG	O5-C5-C6-O6
7	L	203	NAG	C4-C5-C6-O6
8	I	401	SIA	O7-C7-C8-O8
8	I	401	SIA	C6-C7-C8-O8
7	L	203	NAG	O5-C5-C6-O6
7	B	201	NAG	C4-C5-C6-O6
7	B	201	NAG	O5-C5-C6-O6

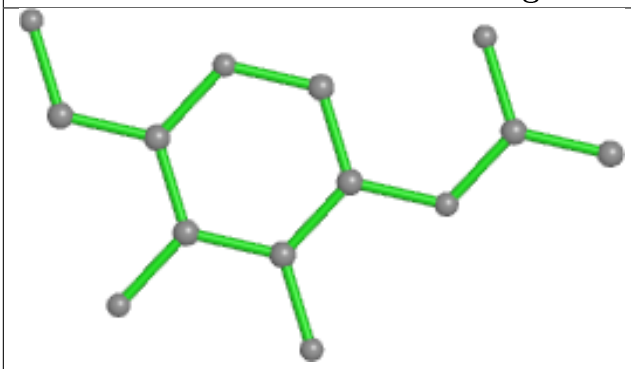
There are no ring outliers.

2 monomers are involved in 3 short contacts:

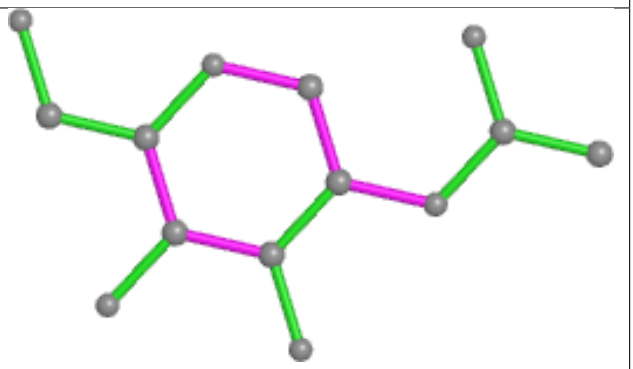
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	203	NAG	1	0
8	I	401	SIA	2	0

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.

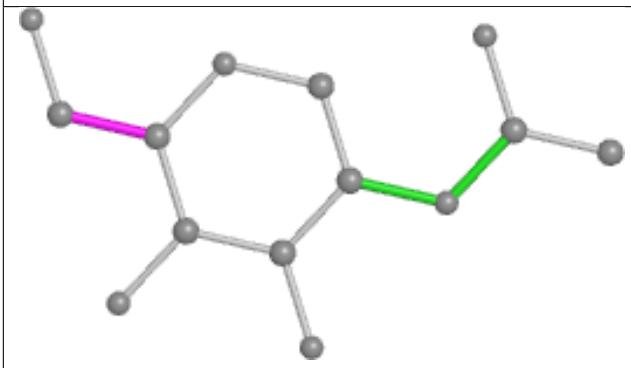
Ligand NAG L 203



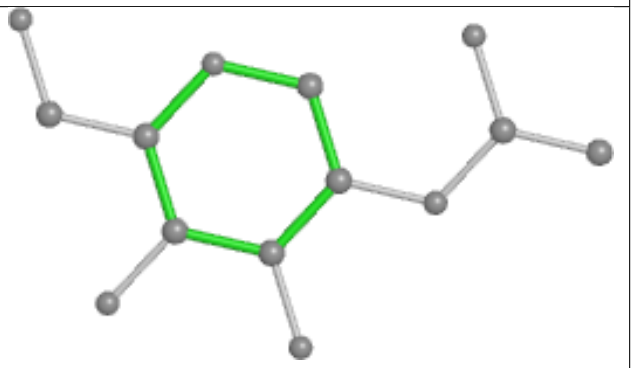
Bond lengths



Bond angles

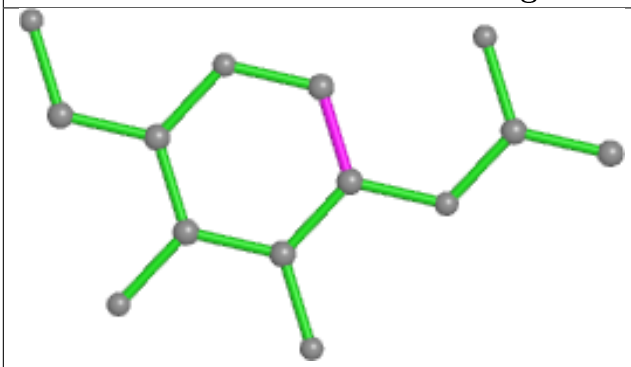


Torsions

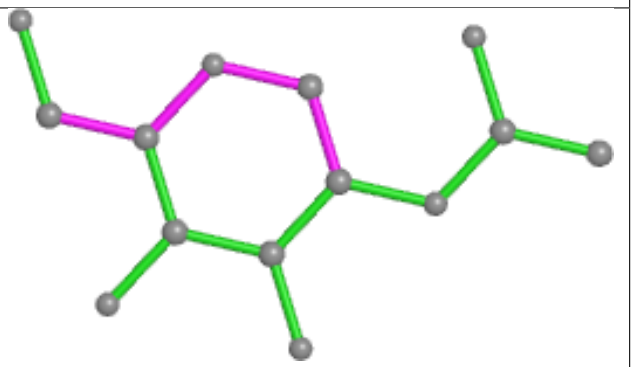


Rings

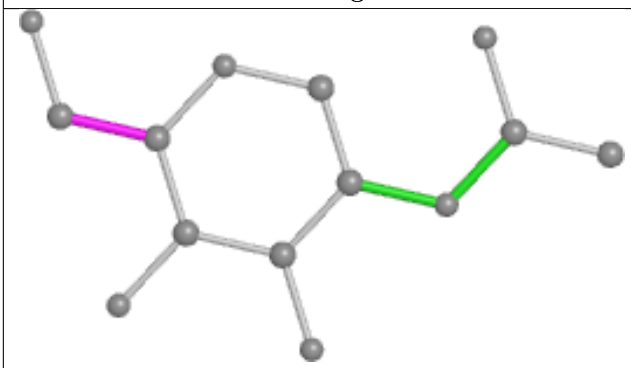
Ligand NAG B 202



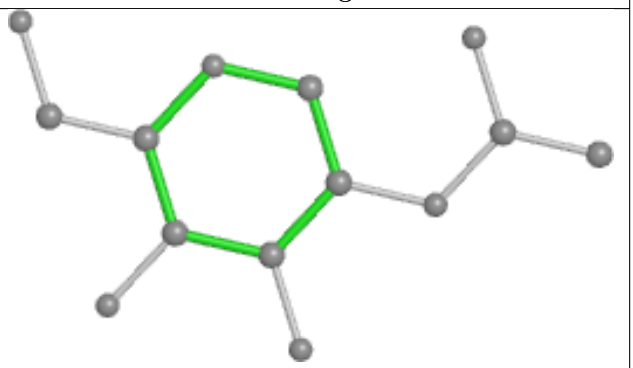
Bond lengths



Bond angles

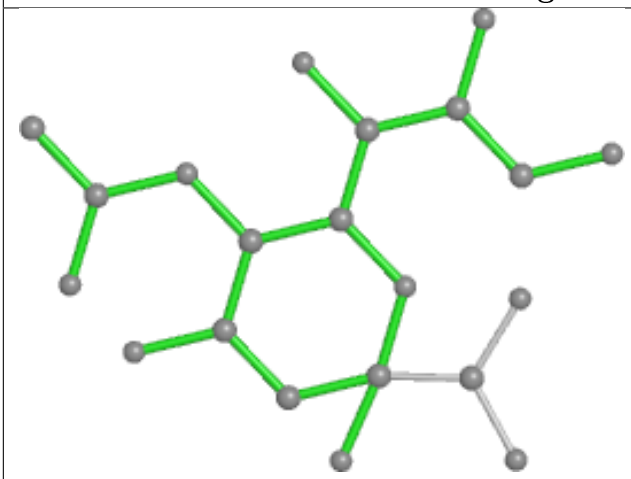


Torsions

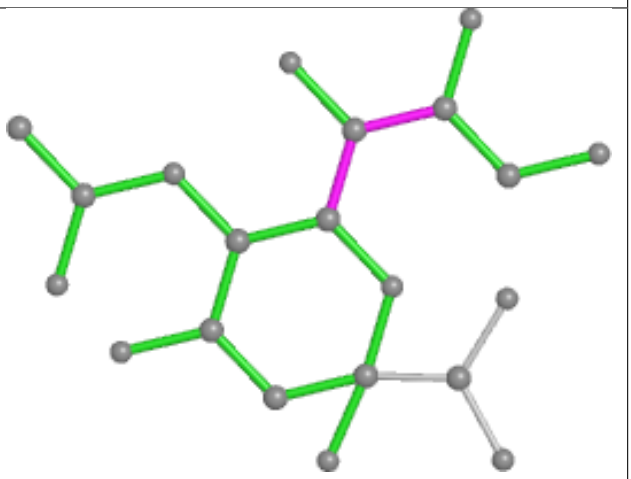


Rings

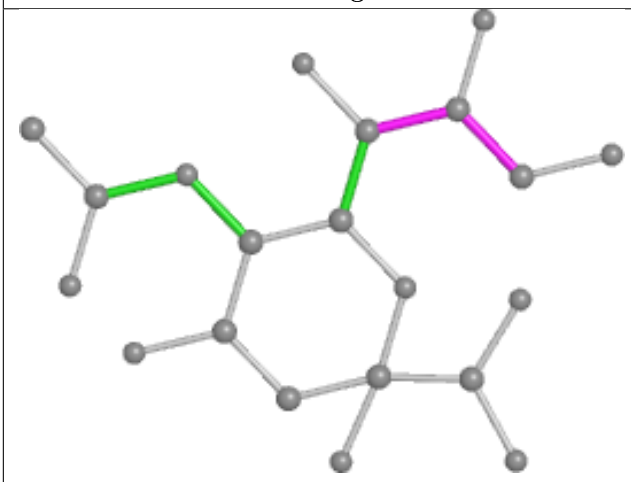
Ligand SIA I 401



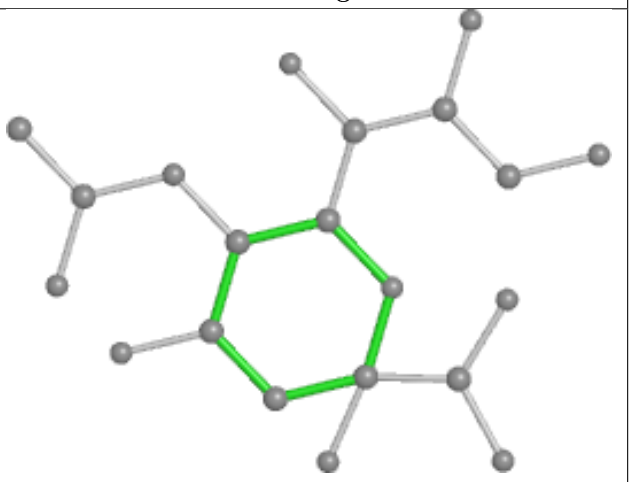
Bond lengths



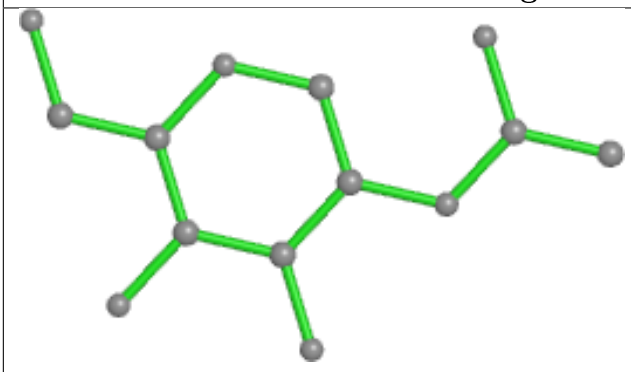
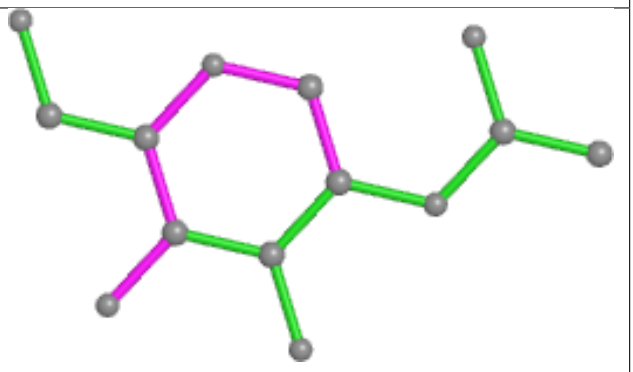
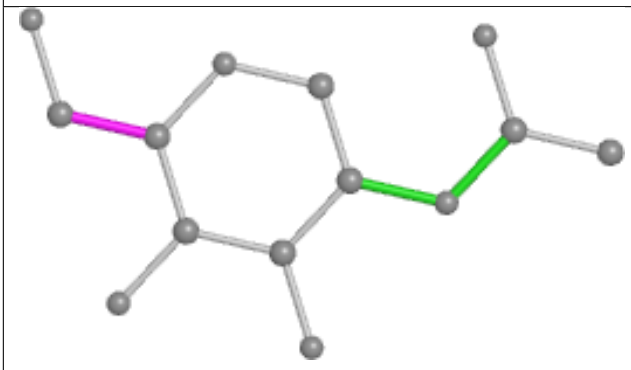
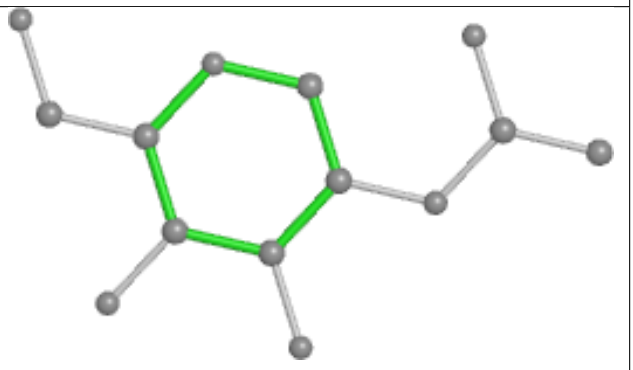
Bond angles



Torsions



Rings

Ligand NAG B 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	320/325 (98%)	-0.03	0 100 100	53, 76, 108, 140	0
1	C	320/325 (98%)	0.19	3 (0%) 84 82	55, 88, 120, 137	0
1	E	320/325 (98%)	0.28	12 (3%) 40 33	67, 98, 129, 146	0
1	G	320/325 (98%)	0.79	38 (11%) 4 3	53, 120, 171, 196	0
1	I	320/325 (98%)	0.44	21 (6%) 18 13	62, 108, 155, 183	0
1	K	318/325 (97%)	-0.02	1 (0%) 94 93	55, 76, 97, 116	0
2	B	172/177 (97%)	-0.01	1 (0%) 89 88	58, 81, 110, 123	0
2	D	172/177 (97%)	0.16	1 (0%) 89 88	52, 75, 99, 119	0
2	F	172/177 (97%)	0.24	0 100 100	55, 84, 112, 131	0
2	H	172/177 (97%)	0.23	1 (0%) 89 88	54, 79, 111, 139	0
2	J	172/177 (97%)	0.32	4 (2%) 60 54	61, 85, 115, 132	0
2	L	172/177 (97%)	-0.05	0 100 100	56, 75, 103, 116	0
All	All	2950/3012 (97%)	0.23	82 (2%) 53 46	52, 86, 140, 196	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	212	ALA	7.9
1	G	210	VAL	7.6
1	G	181	THR	7.3
1	G	211	GLY	6.8
1	G	209	VAL	6.2
1	G	243	GLY	5.9
1	G	158	THR	5.9
1	I	266	ILE	5.5
1	G	122	ASN	5.3
1	G	187	LEU	5.1
1	G	189	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	I	41	LEU	4.9
1	G	156	GLN	4.7
1	G	238	PHE	4.7
1	E	282	ASN	4.6
1	E	266	ILE	4.6
1	C	188	TYR	4.3
2	H	67	GLU	4.3
1	G	225	PHE	4.0
1	I	210	VAL	4.0
1	I	86	TYR	3.9
1	G	188	TYR	3.8
1	G	172	MET	3.8
1	I	225	PHE	3.8
1	G	242	GLY	3.6
1	I	223	ILE	3.3
2	J	33	GLY	3.3
1	G	226	HIS	3.3
1	E	41	LEU	3.3
2	J	77	ILE	3.2
1	I	139	TYR	3.1
1	I	262	SER	3.1
1	G	190	THR	3.1
1	G	222	ARG	3.1
2	D	164	GLU	3.0
1	G	202	TYR	3.0
1	G	192	SER	3.0
1	E	139	TYR	2.8
1	E	284	ARG	2.8
1	G	121	ILE	2.7
1	E	280	SER	2.7
1	I	70	LEU	2.7
1	G	236	ILE	2.7
1	G	92	THR	2.7
1	E	270	CYS	2.6
1	I	61	ILE	2.6
1	I	88	TYR	2.5
1	G	154	PHE	2.5
1	G	41	LEU	2.5
1	G	230	VAL	2.4
1	G	206	PHE	2.4
1	I	270	CYS	2.4
1	G	115	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	40	ARG	2.3
1	I	121	ILE	2.3
1	G	207	VAL	2.2
2	J	56	ILE	2.2
1	E	281	ILE	2.2
1	E	51	LEU	2.2
1	I	77	LEU	2.2
1	G	197	VAL	2.2
1	I	258	LEU	2.2
1	G	246	ALA	2.2
1	G	182	GLN	2.2
1	K	175	ILE	2.2
1	I	51	LEU	2.2
1	I	166	THR	2.2
1	I	154	PHE	2.2
1	C	193	LEU	2.1
1	G	245	ILE	2.1
2	B	102	MET	2.1
1	E	61	ILE	2.1
2	J	102	MET	2.1
1	E	38	LEU	2.1
1	I	132	ARG	2.1
1	E	182	GLN	2.1
1	I	280	SER	2.1
1	G	194	SER	2.0
1	G	148	LYS	2.0
1	G	258	LEU	2.0
1	G	61	ILE	2.0
1	C	157	THR	2.0

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)

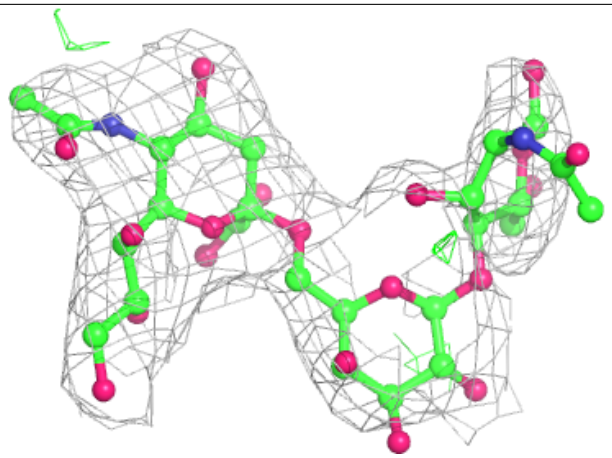
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

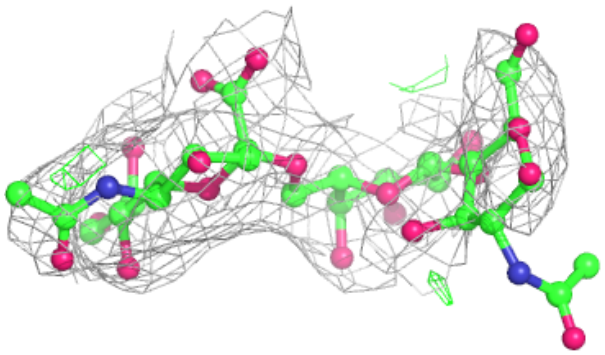
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	M	1	15/15	0.70	0.32	119,133,147,149	15
3	NAG	U	1	15/15	0.76	0.21	108,124,137,138	15
5	NAG	Q	2	14/15	0.78	0.19	118,147,152,155	0
3	GAL	R	2	11/12	0.79	0.15	146,152,158,160	0
3	NAG	R	1	15/15	0.80	0.17	130,142,153,161	15
5	NAG	Q	1	14/15	0.83	0.14	121,135,141,143	0
3	NAG	P	1	15/15	0.85	0.34	104,122,131,141	15
5	NAG	S	2	14/15	0.85	0.22	117,126,134,137	0
5	NAG	T	2	14/15	0.85	0.17	125,142,148,149	0
3	SIA	R	3	20/21	0.86	0.13	87,123,146,147	0
4	GAL	N	1	12/12	0.86	0.11	124,140,153,156	0
5	NAG	O	2	14/15	0.88	0.18	107,113,129,130	0
5	NAG	V	2	14/15	0.89	0.17	122,131,140,148	0
3	GAL	U	2	11/12	0.90	0.15	101,124,129,130	0
5	NAG	T	1	14/15	0.90	0.11	110,119,128,134	0
3	GAL	P	2	11/12	0.90	0.13	97,116,135,138	0
3	GAL	M	2	11/12	0.91	0.11	110,124,133,139	0
5	NAG	S	1	14/15	0.93	0.12	79,94,101,107	0
4	SIA	N	2	20/21	0.93	0.18	93,101,127,138	0
5	NAG	V	1	14/15	0.94	0.13	99,113,126,133	0
5	NAG	O	1	14/15	0.96	0.12	75,84,91,98	0
3	SIA	M	3	20/21	0.96	0.14	61,79,94,95	0
3	SIA	P	3	20/21	0.96	0.18	91,102,120,127	0
3	SIA	U	3	20/21	0.97	0.13	57,70,97,104	0

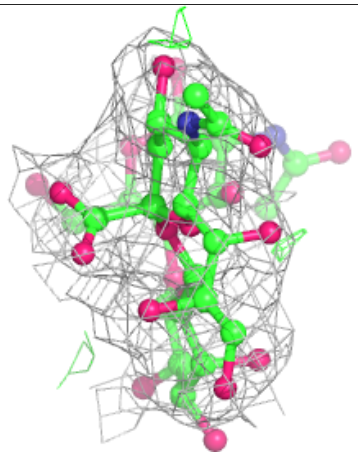
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

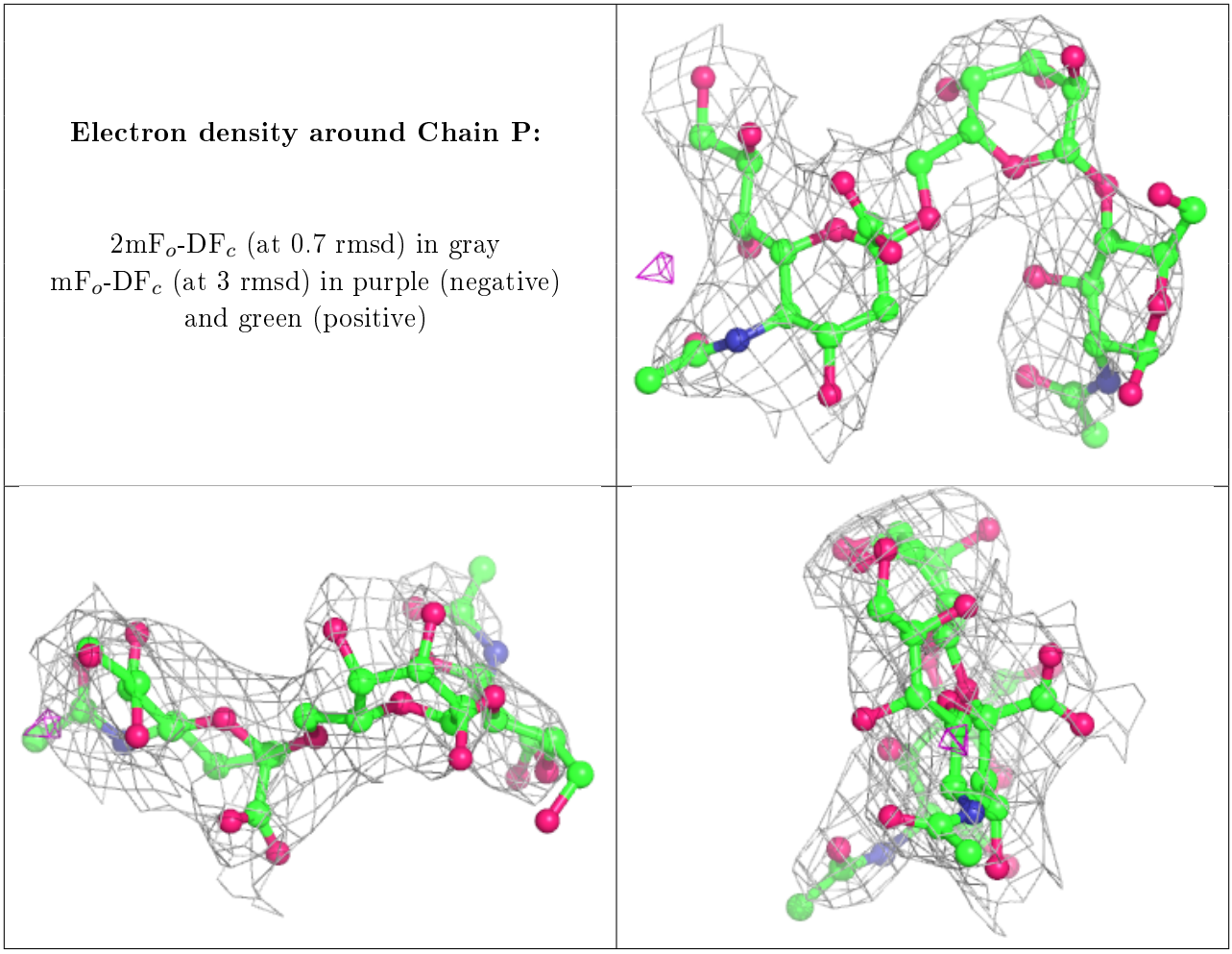






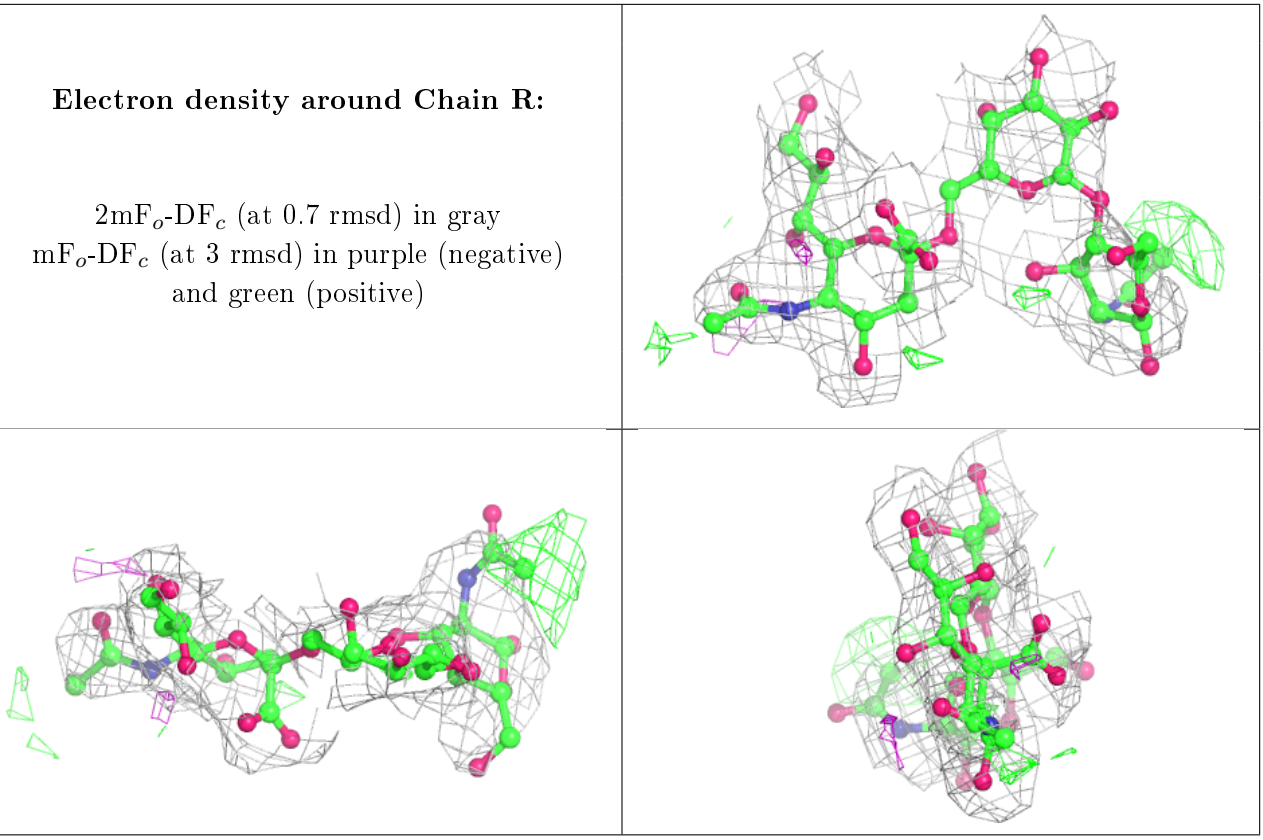
Electron density around Chain P:

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



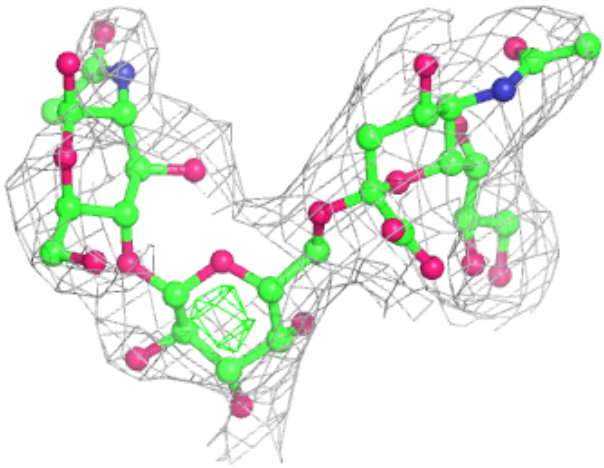
Electron density around Chain R:

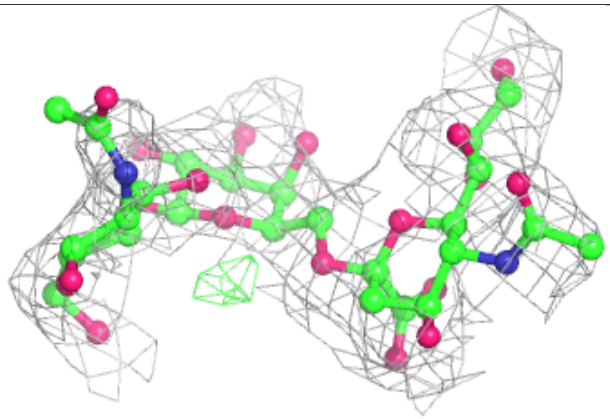
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

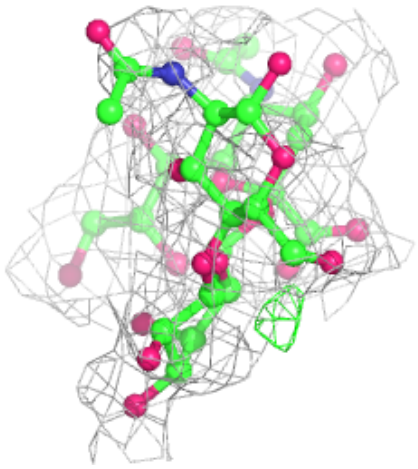


Electron density around Chain U:

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

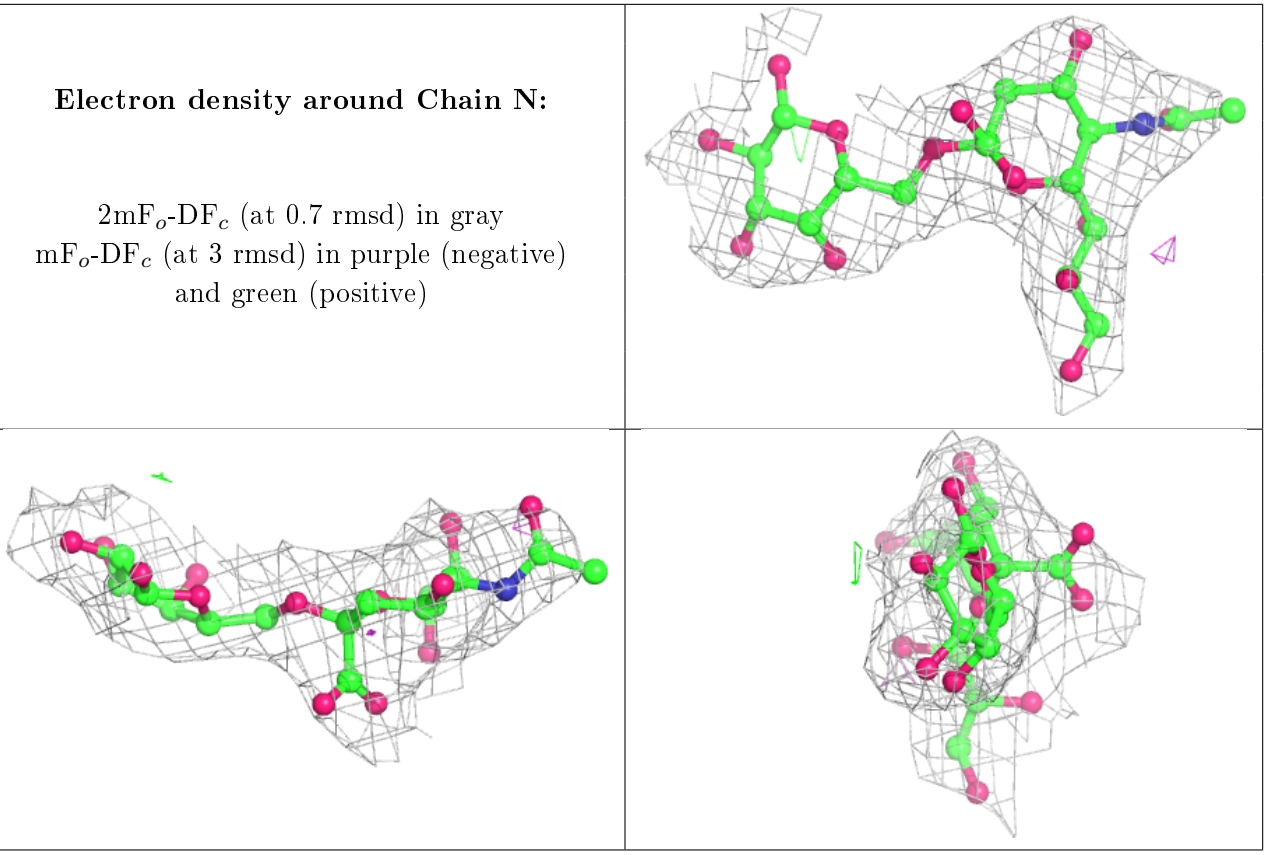






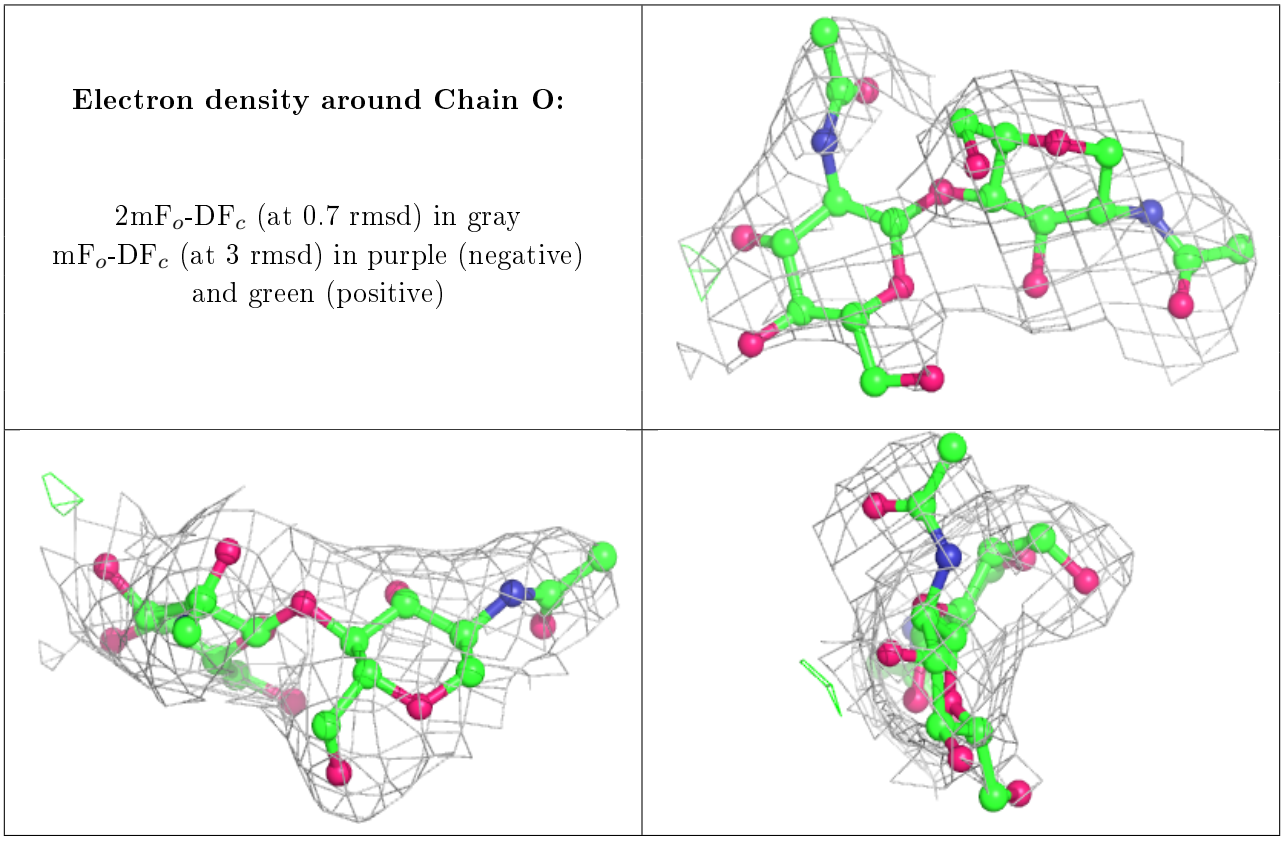
Electron density around Chain N:

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



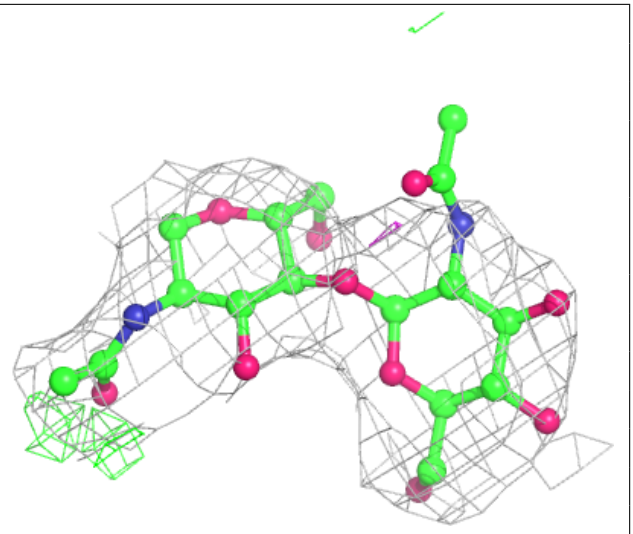
Electron density around Chain O:

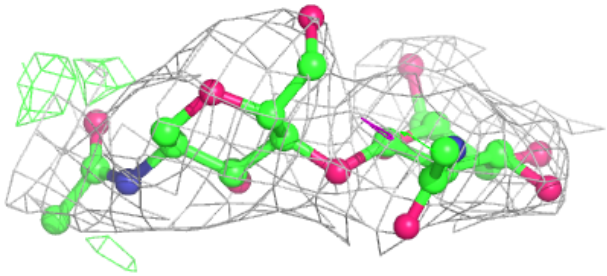
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

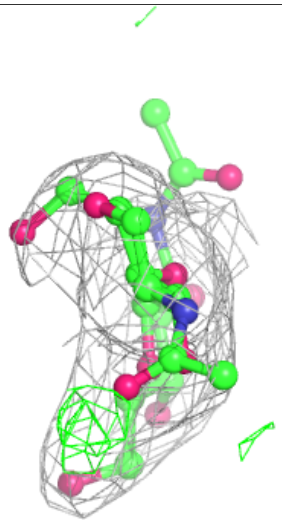


Electron density around Chain Q:

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

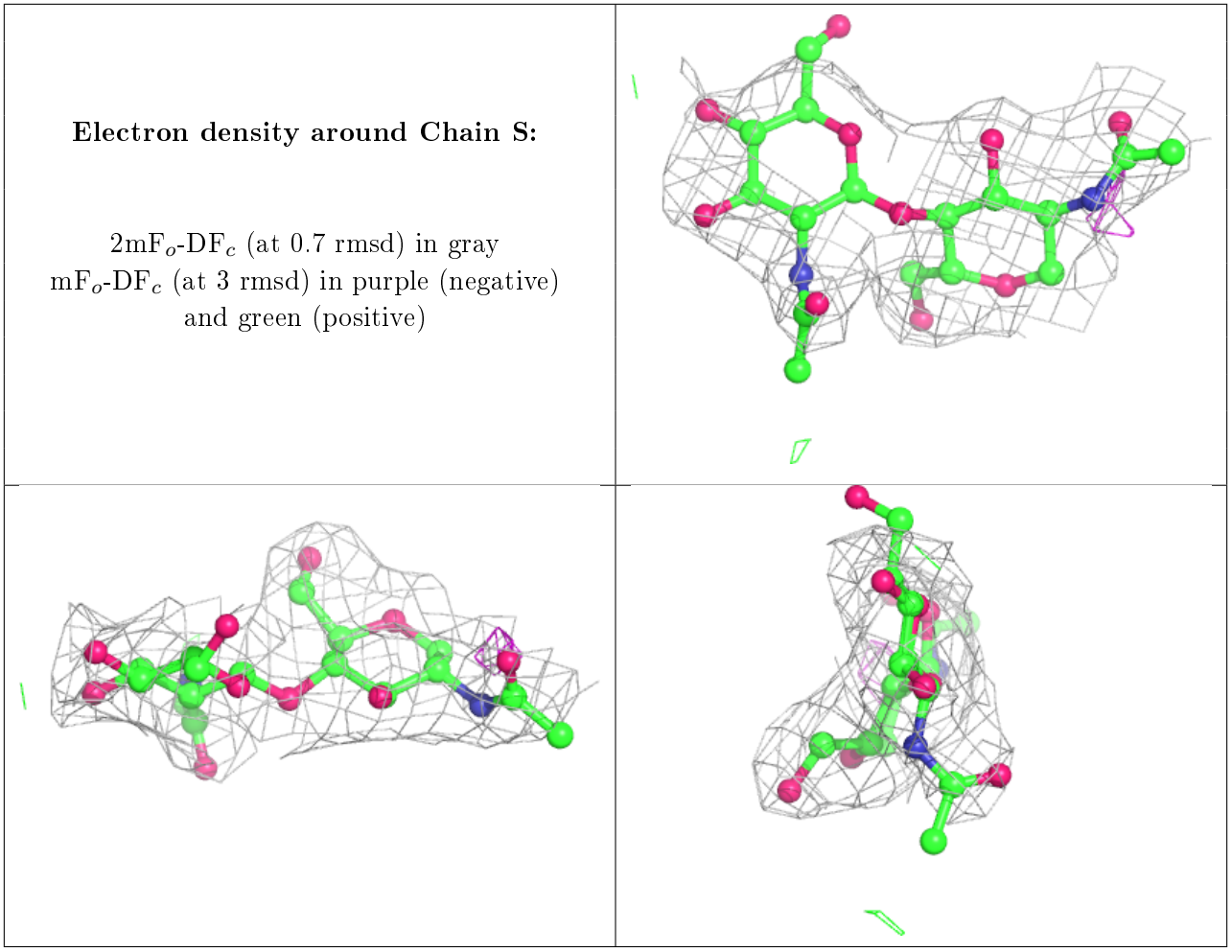






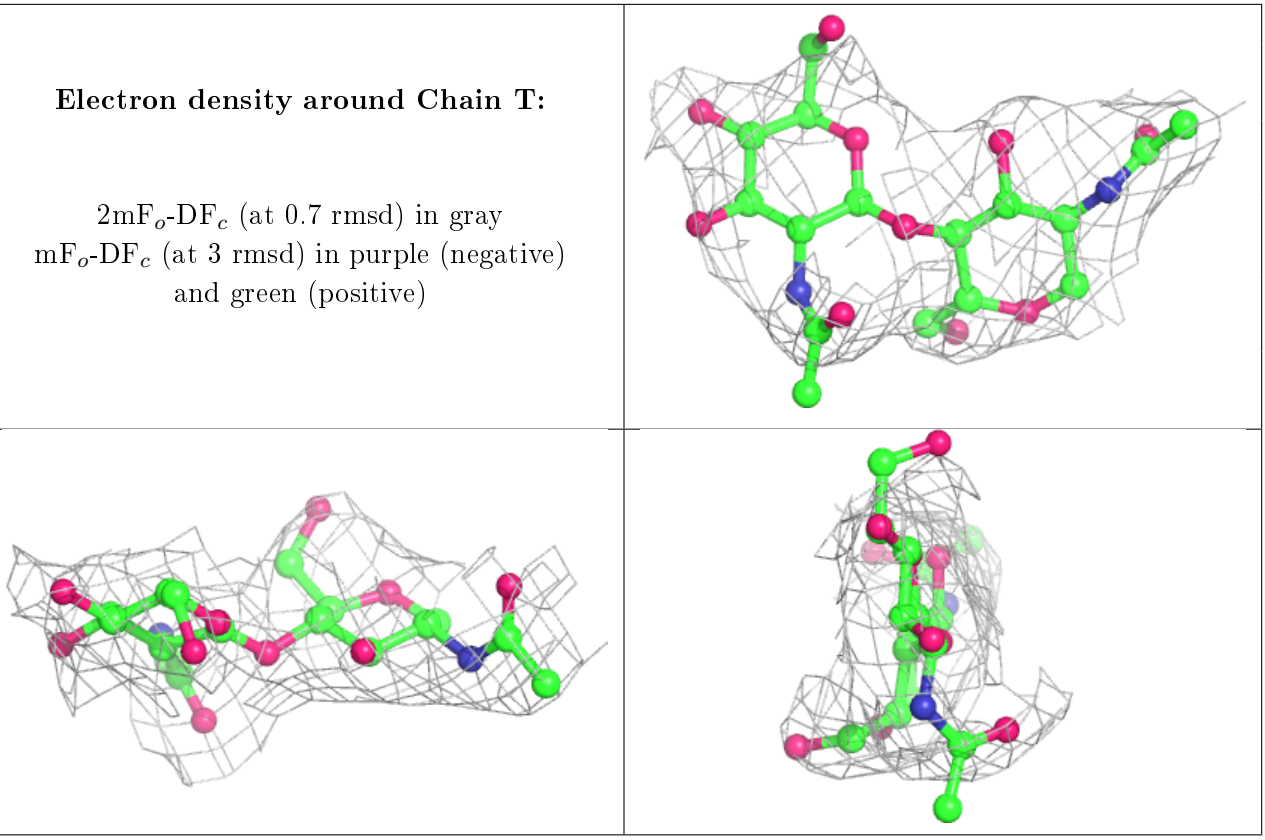
Electron density around Chain S:

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



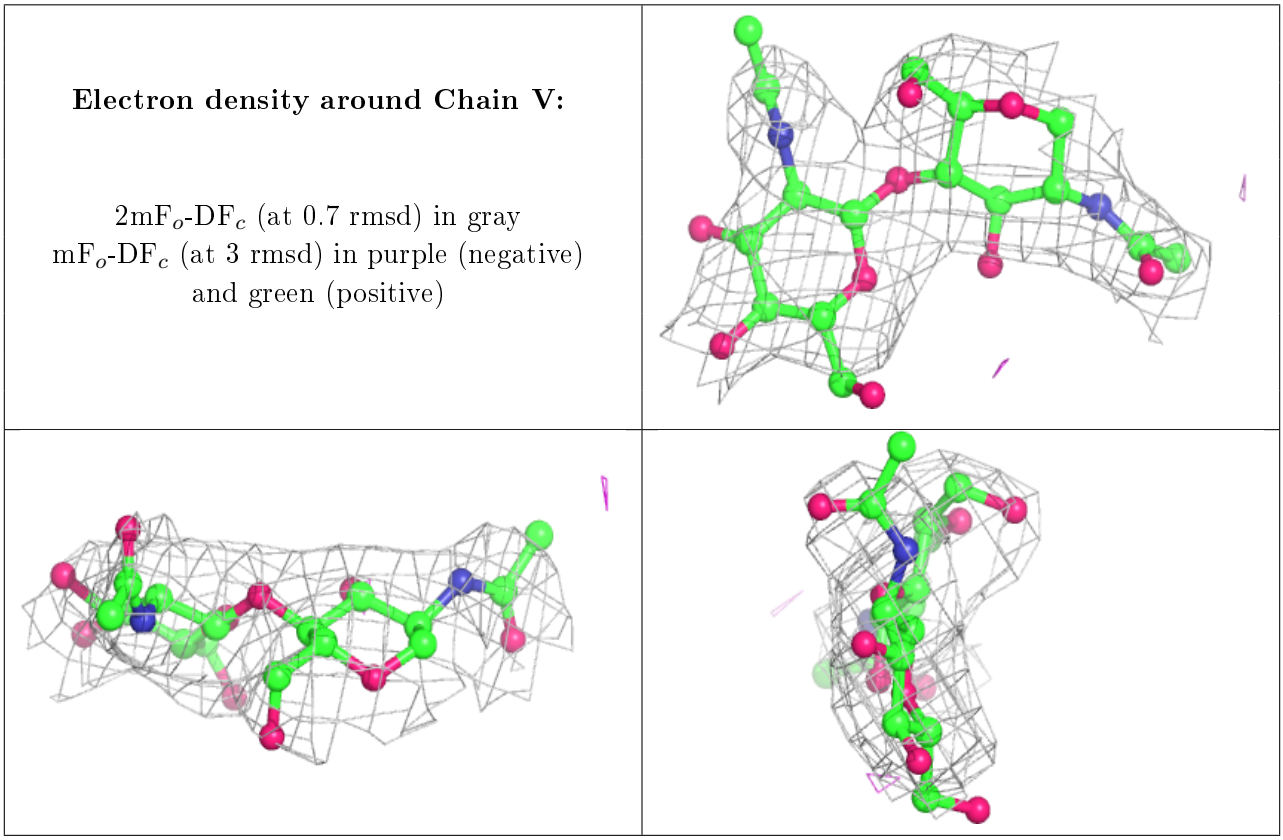
Electron density around Chain T:

$2mF_o$-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 V:

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



6.4 Ligands

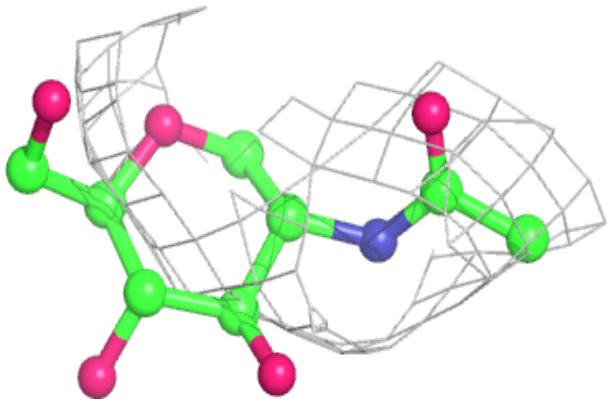
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

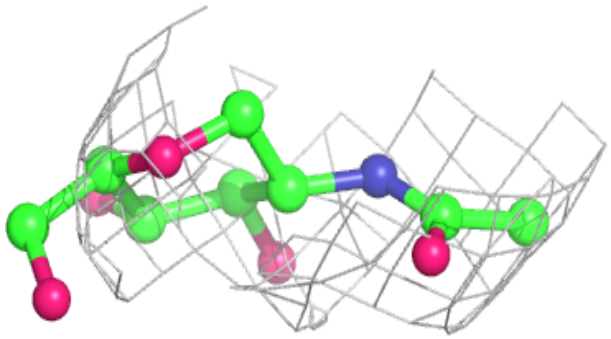
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	L	203	14/15	0.72	0.29	124,161,176,179	0
7	NAG	B	202	14/15	0.85	0.19	150,162,172,175	0
7	NAG	B	201	14/15	0.88	0.16	92,96,101,104	0
8	SIA	I	401	21/21	0.91	0.17	111,137,142,152	0
6	CA	I	402	1/1	0.93	0.06	104,104,104,104	0
6	CA	K	404	1/1	0.96	0.15	67,67,67,67	0
6	CA	A	404	1/1	0.97	0.18	72,72,72,72	0

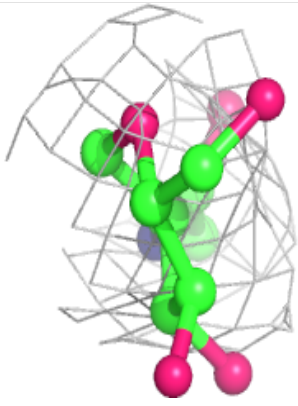
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG L 203:

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

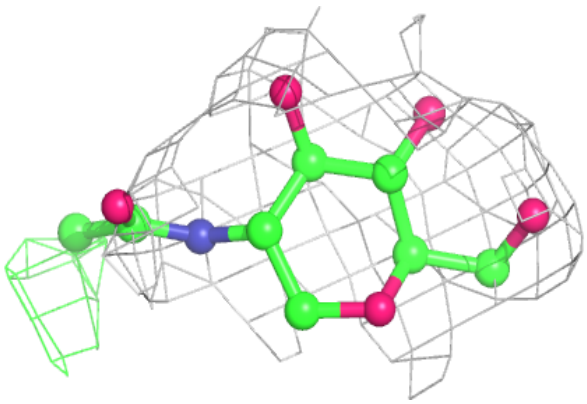


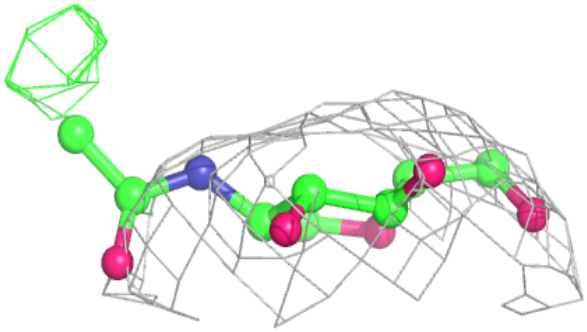


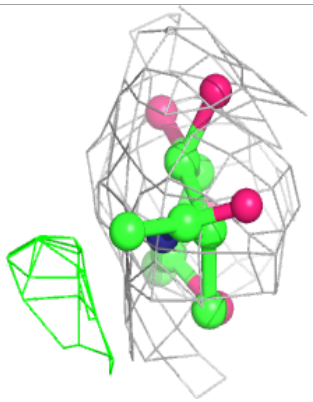


Electron density around NAG B 202:

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

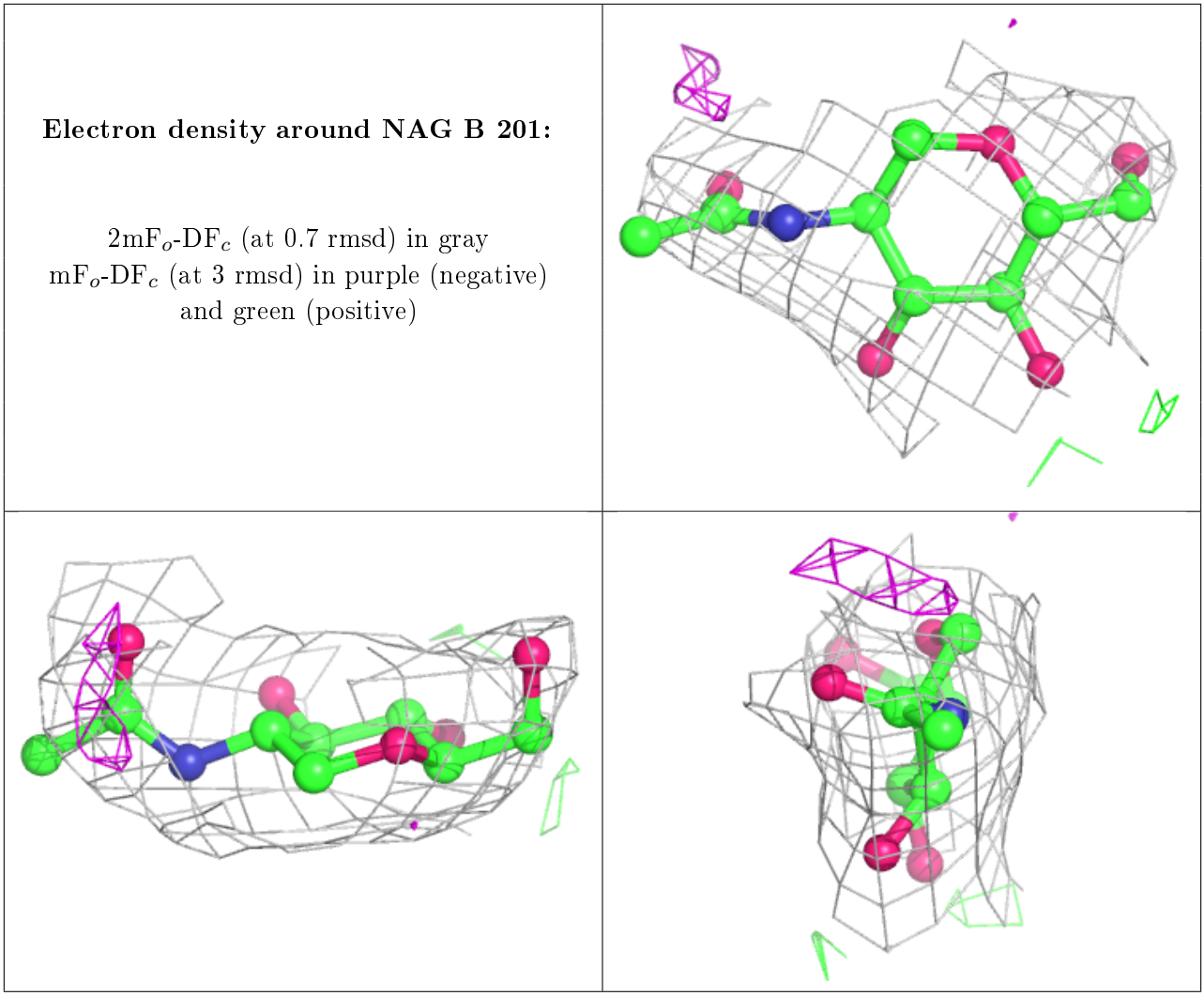






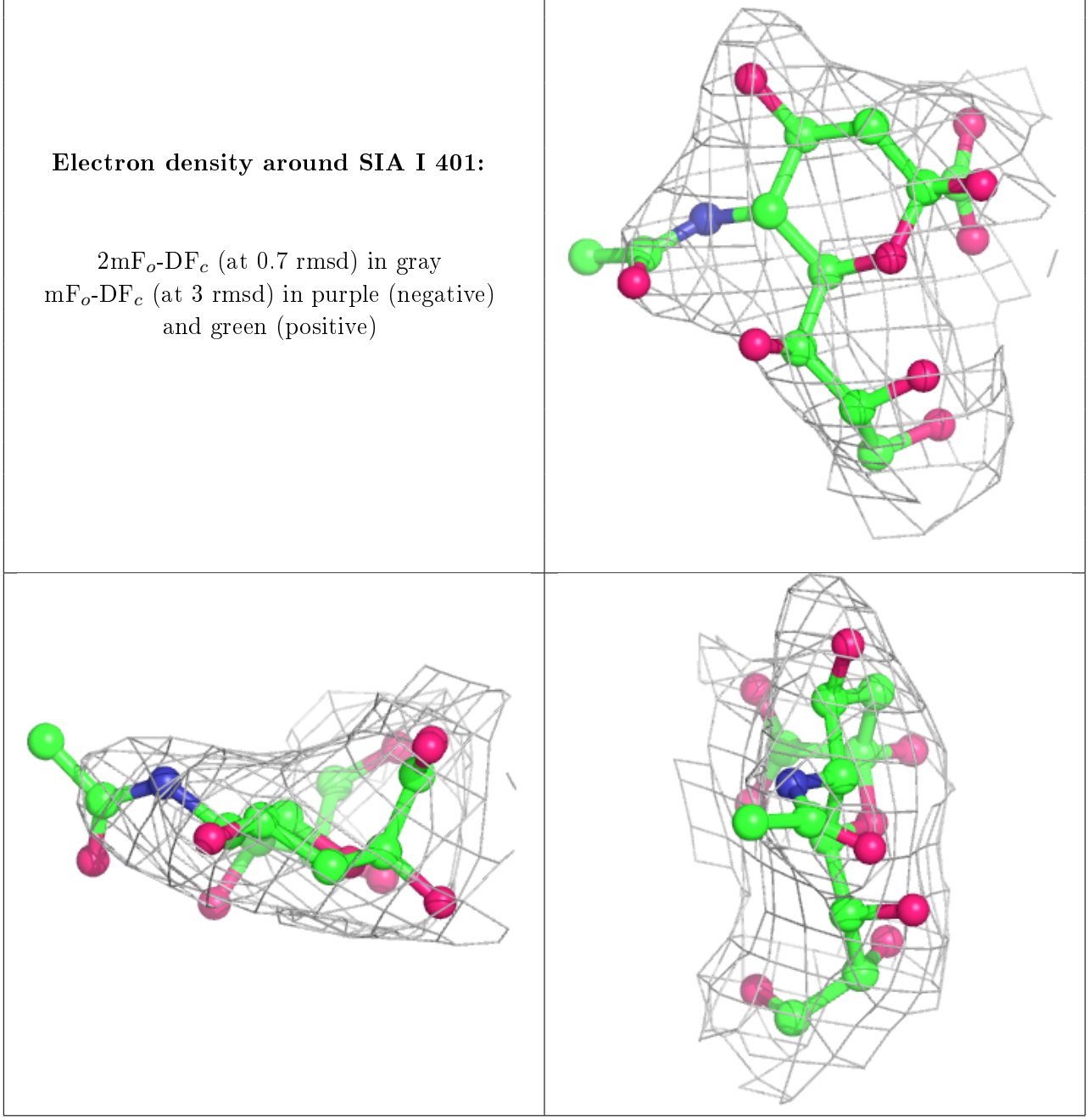
Electron density around NAG B 201:

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



Electron density around SIA I 401:

$2mF_o$-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.