Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 07:45 pm BST

PDB ID	:	5M8T
Title	:	Crystal structure of human tyrosinase related protein 1 (T391V-R374S-Y362F) in complex with tropolone
Authors	:	Lai, X.; Soler-Lopez, M.; Wichers, H.J.; Dijkstra, B.W.
Deposited on	:	2016-10-29
Resolution	:	2.35 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

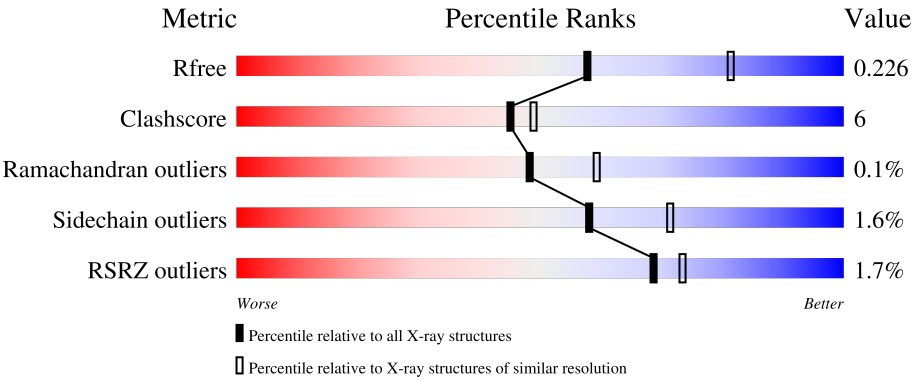
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	446	2% 89% 10%
1	B	446	2% 88% 12%
1	C	446	2% 85% 14%
1	D	446	% 87% 12%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	N	3	33% 67%
2	S	3	33% 67%
3	F	2	100%
3	J	2	100%
4	G	2	50% 50%
4	H	2	100%
4	K	2	50% 50%
4	M	2	50% 50%
4	P	2	50% 50%
4	Q	2	50% 50%
4	R	2	100%
4	U	2	100%
4	W	2	50% 50%
5	I	5	20% 60% 20%
6	L	3	67% 33%
6	O	3	100%
7	T	4	25% 50% 25%
7	V	4	50% 50%

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
10	0TR	A	513	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15515 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.

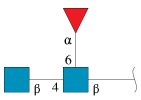
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	B	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	C	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			
1	D	446	Total	C	N	O	S	0	0	0
			3554	2231	629	671	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	PHE	TYR	engineered mutation	UNP P17643
A	374	SER	ARG	engineered mutation	UNP P17643
A	391	VAL	THR	engineered mutation	UNP P17643
B	362	PHE	TYR	engineered mutation	UNP P17643
B	374	SER	ARG	engineered mutation	UNP P17643
B	391	VAL	THR	engineered mutation	UNP P17643
C	362	PHE	TYR	engineered mutation	UNP P17643
C	374	SER	ARG	engineered mutation	UNP P17643
C	391	VAL	THR	engineered mutation	UNP P17643
D	362	PHE	TYR	engineered mutation	UNP P17643
D	374	SER	ARG	engineered mutation	UNP P17643
D	391	VAL	THR	engineered mutation	UNP P17643

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	3	Total C N O 38 22 2 14	0	0	0
2	N	3	Total C N O 38 22 2 14	0	0	0
2	S	3	Total C N O 38 22 2 14	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 24 14 1 9	0	0	0
3	J	2	Total C N O 24 14 1 9	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 28 16 2 10	0	0	0
4	H	2	Total C N O 28 16 2 10	0	0	0
4	K	2	Total C N O 28 16 2 10	0	0	0
4	M	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	Q	2	Total C N O 28 16 2 10	0	0	0
4	R	2	Total C N O 28 16 2 10	0	0	0

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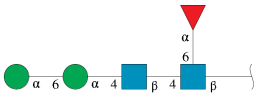
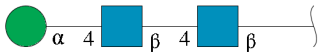
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	U	2	Total C N O 28 16 2 10	0	0	0
4	W	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



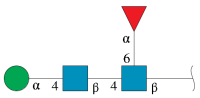
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	I	5	Total C N O 60 34 2 24	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	L	3	Total C N O 39 22 2 15	0	0	0
6	O	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	T	4	Total C N O 49 28 2 19	0	0	0

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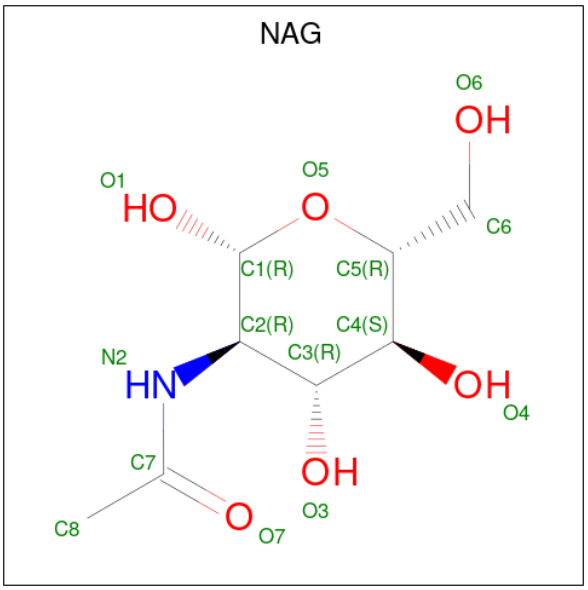
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	V	4	Total C N O 49 28 2 19	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

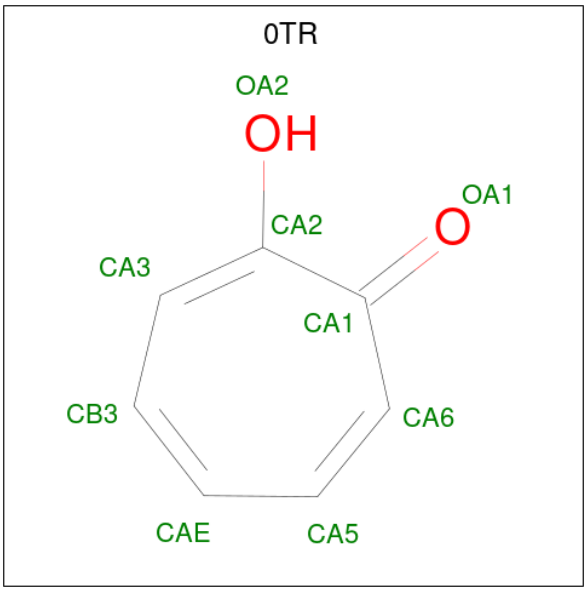


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Zn 2 2	0	0
9	B	2	Total Zn 2 2	0	0
9	C	2	Total Zn 2 2	0	0
9	D	2	Total Zn 2 2	0	0

- Molecule 10 is 2-HYDROXYCYCLOHEPTA-2,4,6-TRIEN-1-ONE (three-letter code: 0TR) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 9 7 2	0	0
10	B	1	Total C O 9 7 2	0	0
10	C	1	Total C O 9 7 2	0	0
10	D	1	Total C O 9 7 2	0	0

- Molecule 11 is water.

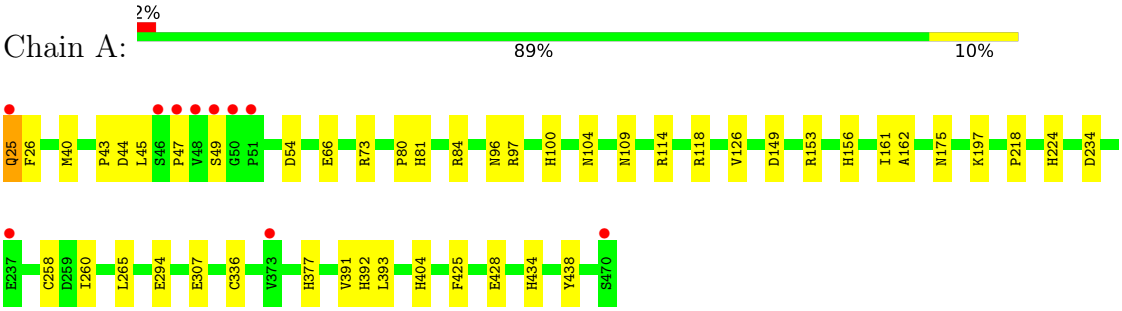
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	148	Total O 148 148	0	0
11	B	156	Total O 156 156	0	0
11	C	128	Total O 128 128	0	0
11	D	145	Total O 145 145	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

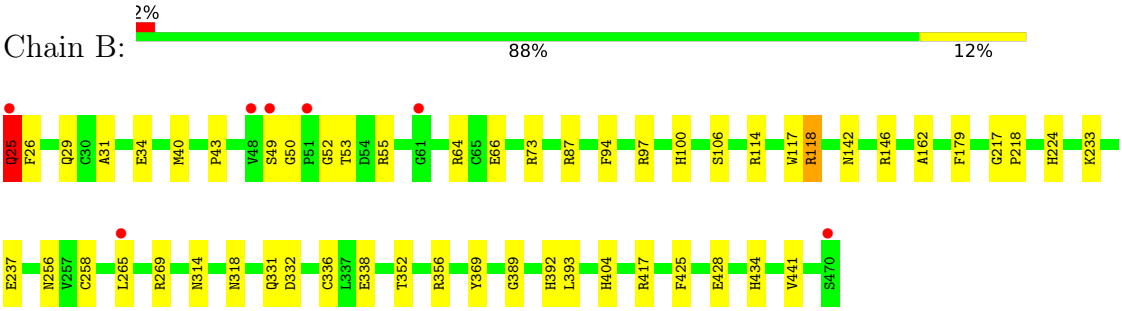
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain A:



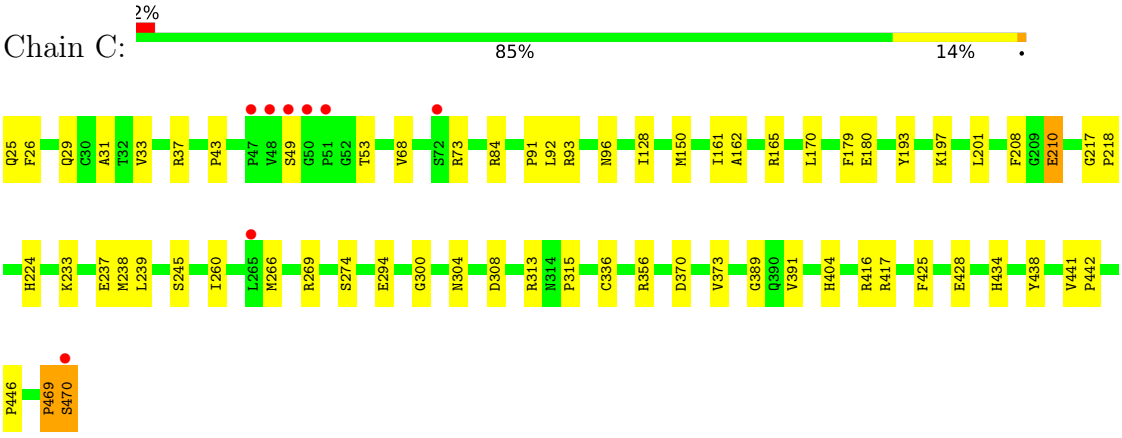
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain B:



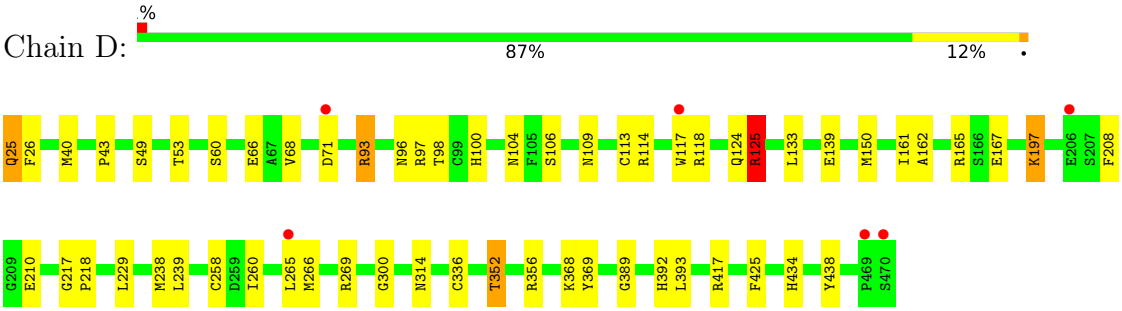
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain C:



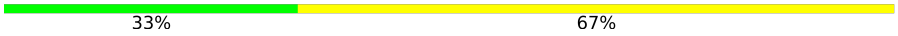
• Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

Chain D:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

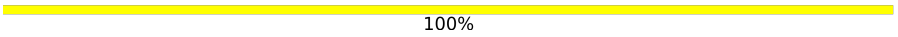
Chain N:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

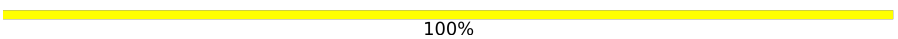
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

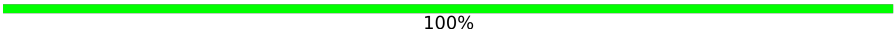


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain H:



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

Chain K:

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

Chain M:

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

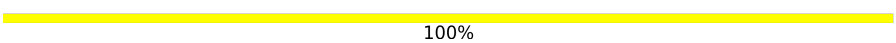
Chain P:

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

Chain Q:

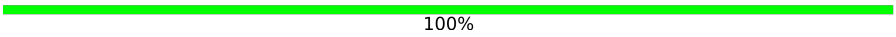
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



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

Chain U:

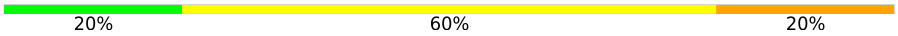


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

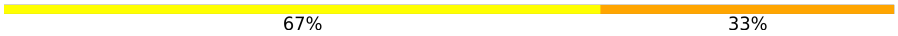
• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



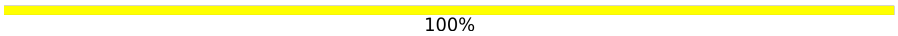
• Molecule 6: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



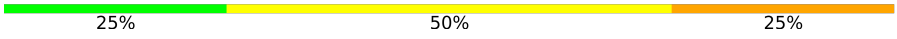
• Molecule 6: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.73Å 140.60Å 191.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.35 48.75 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.75-2.35) 92.8 (48.75-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.225 0.183 , 0.226	Depositor DCC
R_{free} test set	4972 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15515	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ZN, FUC, MAN, NAG, 0TR

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	0.50	0/3661	0.67	1/4990 (0.0%)
1	B	0.51	0/3661	0.67	2/4990 (0.0%)
1	C	0.48	0/3661	0.63	0/4990
1	D	0.53	2/3661 (0.1%)	0.75	9/4990 (0.2%)
All	All	0.51	2/14644 (0.0%)	0.68	12/19960 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	ARG	CB-CG	-6.12	1.36	1.52
1	D	125	ARG	CD-NE	-5.88	1.36	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	125	ARG	NE-CZ-NH2	-13.09	113.75	120.30
1	D	125	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	D	125	ARG	CG-CD-NE	-7.93	95.15	111.80
1	D	368	LYS	CD-CE-NZ	-6.55	96.62	111.70
1	D	125	ARG	CB-CG-CD	-6.44	94.86	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	25	GLN	C-N-CA	-5.93	106.88	121.70
1	B	25	GLN	CA-CB-CG	-5.61	101.06	113.40
1	A	25	GLN	C-N-CA	-5.41	108.17	121.70
1	D	93	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	125	ARG	CD-NE-CZ	5.31	131.04	123.60
1	D	93	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	118	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	469	PRO	Peptide
1	D	71	ASP	Sidechain

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	3554	0	3320	29	0
1	B	3554	0	3320	46	0
1	C	3554	0	3319	43	0
1	D	3554	0	3320	44	0
2	E	38	0	34	1	0
2	N	38	0	34	4	0
2	S	38	0	34	1	0
3	F	24	0	22	0	0
3	J	24	0	22	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	U	28	0	25	0	0
4	W	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	60	0	52	1	0
6	L	39	0	34	1	0
6	O	39	0	34	0	0
7	T	49	0	43	1	0
7	V	49	0	43	1	0
8	A	14	0	13	0	0
8	C	14	0	13	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
10	A	9	0	6	4	0
10	B	9	0	6	1	0
10	C	9	0	6	3	0
10	D	9	0	6	1	0
11	A	148	0	0	3	0
11	B	156	0	0	5	0
11	C	128	0	0	3	0
11	D	145	0	0	3	0
All	All	15515	0	13906	168	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 (168) 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)
10:A:513:0TR:OA2	11:A:601:HOH:O	1.58	1.14
1:B:142:ASN:OD1	1:B:146:ARG:NH2	1.96	0.97
1:D:150:MET:HE3	1:D:238:MET:HG2	1.50	0.93
1:A:25:GLN:HG3	1:A:26:PHE:H	1.41	0.84
1:D:25:GLN:HG3	1:D:26:PHE:H	1.45	0.82
1:D:117:TRP:CD2	1:D:125:ARG:NH2	2.51	0.79
1:C:25:GLN:HG3	1:C:26:PHE:H	1.45	0.79
1:D:106:SER:HB2	1:D:114:ARG:HG2	1.66	0.78
1:B:331:GLN:NE2	1:B:332:ASP:OD1	2.18	0.77
1:D:118:ARG:NH1	1:D:124:GLN:OE1	2.17	0.77
1:B:52:GLY:HA2	1:B:55:ARG:HH11	1.51	0.75
1:C:25:GLN:HG3	1:C:26:PHE:N	2.02	0.74
1:B:73:ARG:NH1	1:B:428:GLU:OE2	2.20	0.74
1:A:25:GLN:HG2	1:A:161:ILE:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ARG:NH1	1:D:314:ASN:OD1	2.23	0.69
1:A:25:GLN:HG3	1:A:26:PHE:N	2.08	0.68
1:B:269:ARG:NH1	1:B:314:ASN:OD1	2.24	0.67
1:C:218:PRO:HD2	1:C:434:HIS:HB3	1.76	0.66
1:B:40:MET:HE2	1:B:97:ARG:HD3	1.76	0.66
1:D:40:MET:HE2	1:D:97:ARG:HE	1.61	0.66
1:D:417:ARG:NH1	11:D:602:HOH:O	2.01	0.65
1:D:25:GLN:HG3	1:D:26:PHE:N	2.10	0.65
1:A:73:ARG:HB3	1:A:428:GLU:HG2	1.78	0.64
1:C:313:ARG:HG2	1:C:315:PRO:HD3	1.80	0.64
1:B:256:ASN:ND2	11:B:607:HOH:O	2.33	0.62
1:C:208:PHE:CZ	1:C:210:GLU:HB2	2.35	0.62
1:C:84:ARG:NH2	1:C:201:LEU:O	2.32	0.62
10:C:516:0TR:OA1	11:C:601:HOH:O	2.16	0.61
1:D:25:GLN:HE21	1:D:162:ALA:H	1.46	0.61
1:D:25:GLN:HG2	1:D:161:ILE:HA	1.82	0.61
1:D:352:THR:HG22	1:D:369:TYR:H	1.66	0.60
6:L:2:NAG:O3	6:L:3:MAN:H2	2.02	0.59
7:V:2:NAG:O3	7:V:3:MAN:H2	2.02	0.59
1:C:128:ILE:HG23	1:C:245:SER:HB3	1.85	0.59
1:B:73:ARG:HB3	1:B:428:GLU:HG2	1.83	0.59
1:D:389:GLY:C	10:D:518:0TR:HB3	2.24	0.59
1:C:25:GLN:HG2	1:C:161:ILE:HA	1.85	0.58
1:D:118:ARG:HD2	1:D:124:GLN:HB2	1.85	0.58
1:D:133:LEU:HD21	1:D:265:LEU:HD13	1.84	0.58
1:D:165:ARG:NH2	1:D:167:GLU:OE1	2.36	0.58
1:A:294:GLU:OE1	11:A:602:HOH:O	2.17	0.58
1:D:66:GLU:OE1	1:D:100:HIS:ND1	2.36	0.58
1:D:133:LEU:CD2	1:D:265:LEU:HD13	2.34	0.57
1:A:118:ARG:HD3	1:A:126:VAL:HG11	1.86	0.57
1:B:142:ASN:ND2	11:B:609:HOH:O	2.37	0.57
1:B:25:GLN:OE1	1:B:162:ALA:N	2.36	0.56
1:D:104:ASN:OD1	1:D:117:TRP:CH2	2.58	0.56
1:C:73:ARG:HB3	1:C:428:GLU:HG2	1.88	0.56
1:D:117:TRP:CE2	1:D:125:ARG:NH2	2.73	0.55
1:D:150:MET:HE3	1:D:238:MET:CG	2.32	0.55
1:C:33:VAL:HG13	1:C:37:ARG:HH12	1.72	0.55
1:A:40:MET:HE2	1:A:97:ARG:HD3	1.88	0.54
1:A:44:ASP:HB3	1:A:47:PRO:HD3	1.88	0.54
1:C:150:MET:HG2	1:C:238:MET:SD	2.48	0.54
1:C:96:ASN:HD22	2:N:1:NAG:H83	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:HA	1:A:114:ARG:HG3	1.91	0.53
1:B:73:ARG:HD2	1:B:428:GLU:HG2	1.90	0.53
1:B:389:GLY:C	10:B:517:0TR:HB3	2.28	0.53
1:C:233:LYS:O	1:C:237:GLU:HG2	2.08	0.53
1:A:25:GLN:HE21	1:A:162:ALA:H	1.55	0.52
1:A:224:HIS:CD2	1:A:404:HIS:CE1	2.96	0.52
1:D:113:CYS:HB3	1:D:117:TRP:HB2	1.91	0.52
1:B:392:HIS:CD2	1:B:393:LEU:HG	2.45	0.51
1:D:124:GLN:NE2	11:D:603:HOH:O	2.18	0.51
1:C:217:GLY:O	1:C:356:ARG:HD3	2.10	0.51
1:B:142:ASN:HD21	1:B:146:ARG:HH12	1.58	0.51
1:D:68:VAL:CG1	1:D:98:THR:HG23	2.41	0.51
1:A:149:ASP:OD2	1:A:153:ARG:NH1	2.43	0.50
1:B:34:GLU:CD	1:B:34:GLU:H	2.15	0.50
1:C:150:MET:HE3	1:C:238:MET:HG2	1.93	0.50
1:D:392:HIS:NE2	1:D:393:LEU:HG	2.26	0.50
1:B:218:PRO:HD2	1:B:434:HIS:HB3	1.93	0.50
1:C:49:SER:HB2	1:C:53:THR:OG1	2.13	0.49
1:C:416:ARG:HH21	1:C:417:ARG:HG2	1.76	0.49
1:B:25:GLN:HG3	1:B:26:PHE:H	1.78	0.49
1:D:217:GLY:O	1:D:356:ARG:HD3	2.13	0.49
1:B:224:HIS:CD2	1:B:404:HIS:CE1	3.01	0.49
1:C:165:ARG:HD3	1:C:300:GLY:O	2.13	0.49
1:B:106:SER:HB2	1:B:114:ARG:HG2	1.95	0.48
1:A:265:LEU:HD12	1:A:265:LEU:O	2.13	0.48
1:A:307:GLU:OE1	11:A:603:HOH:O	2.20	0.48
1:A:25:GLN:OE1	1:A:25:GLN:HA	2.14	0.48
2:N:1:NAG:O4	2:N:2:NAG:O7	2.31	0.48
1:B:52:GLY:HA2	1:B:55:ARG:NH1	2.23	0.47
1:D:25:GLN:HA	1:D:25:GLN:OE1	2.13	0.47
1:B:142:ASN:ND2	1:B:146:ARG:NH1	2.63	0.47
1:A:391:VAL:HA	10:A:513:0TR:CA3	2.44	0.47
1:B:318:ASN:OD1	4:M:1:NAG:H62	2.15	0.47
1:C:370:ASP:O	1:C:373:VAL:HG22	2.14	0.47
1:B:352:THR:HG22	1:B:369:TYR:H	1.80	0.46
1:D:139:GLU:H	1:D:139:GLU:CD	2.17	0.46
1:D:218:PRO:HD2	1:D:434:HIS:HB3	1.98	0.46
7:T:2:NAG:O3	7:T:3:MAN:H2	2.15	0.46
1:C:25:GLN:HA	1:C:25:GLN:OE1	2.15	0.46
1:A:80:PRO:HG2	1:A:81:HIS:CD2	2.50	0.46
1:B:338:GLU:OE2	1:B:417:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:HG22	1:C:170:LEU:HD22	1.96	0.46
1:C:29:GLN:NE2	11:C:613:HOH:O	2.49	0.45
1:A:156:HIS:NE2	1:A:234:ASP:OD2	2.48	0.45
1:D:208:PHE:CZ	1:D:210:GLU:HB2	2.50	0.45
1:A:392:HIS:CD2	1:A:393:LEU:HG	2.51	0.45
1:B:142:ASN:HD21	1:B:146:ARG:NH1	2.14	0.45
1:D:49:SER:HB2	1:D:53:THR:HG21	1.97	0.45
1:B:142:ASN:ND2	1:B:146:ARG:HH12	2.13	0.45
1:B:142:ASN:OD1	1:B:146:ARG:CZ	2.63	0.45
1:C:391:VAL:HA	10:C:516:0TR:HA3	1.98	0.45
1:A:391:VAL:HA	10:A:513:0TR:HA3	1.97	0.44
1:D:165:ARG:HD3	1:D:300:GLY:O	2.18	0.44
1:B:66:GLU:HG3	1:B:100:HIS:ND1	2.33	0.44
1:C:29:GLN:HG3	1:C:43:PRO:HB3	1.99	0.44
1:A:45:LEU:HB3	1:A:54:ASP:OD2	2.17	0.44
1:B:29:GLN:HG3	1:B:43:PRO:HB3	1.99	0.44
1:B:66:GLU:HA	1:B:97:ARG:NH2	2.32	0.44
1:A:66:GLU:HG3	1:A:100:HIS:HB2	1.99	0.44
1:B:49:SER:C	1:B:53:THR:HG21	2.38	0.44
1:B:31:ALA:HB1	1:B:179:PHE:CD2	2.52	0.44
1:B:142:ASN:CG	1:B:146:ARG:NH2	2.70	0.44
1:B:217:GLY:O	1:B:356:ARG:HD3	2.18	0.44
1:B:87:ARG:HG2	1:B:441:VAL:HG11	1.98	0.43
1:C:370:ASP:HB3	1:C:373:VAL:HG13	2.00	0.43
1:B:25:GLN:HG3	1:B:26:PHE:N	2.33	0.43
1:C:294:GLU:H	1:C:294:GLU:CD	2.21	0.43
1:D:40:MET:CE	1:D:97:ARG:HE	2.30	0.43
1:D:150:MET:CE	1:D:239:LEU:HD23	2.48	0.43
1:C:308:ASP:HB3	11:C:612:HOH:O	2.18	0.43
1:C:91:PRO:HG3	1:C:446:PRO:HG3	1.99	0.43
1:D:93:ARG:NH1	11:D:619:HOH:O	2.51	0.43
1:A:81:HIS:HB3	1:A:84:ARG:HG3	2.00	0.43
1:A:218:PRO:HD2	1:A:434:HIS:HB3	2.01	0.43
1:C:68:VAL:HG11	1:C:91:PRO:HD2	2.01	0.43
1:B:73:ARG:HD2	1:B:428:GLU:CG	2.49	0.43
1:A:43:PRO:HG2	1:A:109:ASN:HB3	2.01	0.42
1:C:33:VAL:CG1	1:C:37:ARG:HH12	2.31	0.42
1:D:265:LEU:O	1:D:266:MET:HB2	2.20	0.42
1:B:265:LEU:HD12	1:B:265:LEU:O	2.19	0.42
1:D:117:TRP:CE3	1:D:125:ARG:NH2	2.87	0.42
1:B:392:HIS:NE2	1:B:393:LEU:HG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HD3	1:C:274:SER:HB2	2.02	0.42
1:C:180:GLU:OE1	1:C:304:ASN:HB2	2.20	0.42
1:C:441:VAL:HA	1:C:442:PRO:HA	1.82	0.42
1:A:25:GLN:CG	1:A:26:PHE:N	2.81	0.41
1:C:93:ARG:HH21	2:N:3:FUC:C4	2.34	0.41
1:D:25:GLN:NE2	1:D:162:ALA:H	2.17	0.41
1:B:50:GLY:O	1:B:53:THR:HG23	2.20	0.41
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.82	0.41
1:C:389:GLY:C	10:C:516:0TR:HB3	2.40	0.41
1:C:469:PRO:O	1:C:470:SER:HB2	2.20	0.41
1:D:96:ASN:HD22	2:S:1:NAG:H83	1.86	0.41
1:B:94:PHE:O	5:I:5:FUC:H61	2.19	0.41
1:D:260:ILE:O	1:D:265:LEU:O	2.38	0.41
1:C:260:ILE:O	1:C:266:MET:HB2	2.21	0.41
1:D:43:PRO:HG2	1:D:109:ASN:HB3	2.03	0.41
1:D:352:THR:CG2	1:D:369:TYR:H	2.32	0.41
1:A:260:ILE:O	1:A:265:LEU:O	2.39	0.41
1:C:31:ALA:HB1	1:C:179:PHE:CD2	2.56	0.41
1:D:229:LEU:HA	1:D:229:LEU:HD12	1.90	0.41
1:B:25:GLN:HA	11:B:636:HOH:O	2.19	0.41
1:B:233:LYS:O	1:B:237:GLU:HG3	2.21	0.41
1:C:238:MET:HE2	1:C:239:LEU:HG	2.03	0.41
1:A:96:ASN:HD22	2:E:1:NAG:H83	1.86	0.41
1:B:117:TRP:O	1:B:118:ARG:HD3	2.21	0.41
1:D:197:LYS:HE2	1:D:197:LYS:HB2	1.94	0.41
1:B:331:GLN:HB3	11:B:673:HOH:O	2.20	0.40
1:A:377:HIS:HE1	10:A:513:0TR:OA1	2.03	0.40
1:B:256:ASN:ND2	11:B:625:HOH:O	2.55	0.40
1:C:25:GLN:HE21	1:C:162:ALA:H	1.69	0.40
1:C:224:HIS:CD2	1:C:404:HIS:CE1	3.09	0.40
1:C:93:ARG:O	2:N:3:FUC:H62	2.22	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	444/446 (100%)	426 (96%)	17 (4%)	1 (0%)	44	52
1	B	444/446 (100%)	425 (96%)	19 (4%)	0	100	100
1	C	444/446 (100%)	419 (94%)	25 (6%)	0	100	100
1	D	444/446 (100%)	427 (96%)	17 (4%)	0	100	100
All	All	1776/1784 (100%)	1697 (96%)	78 (4%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/395 (100%)	389 (98%)	6 (2%)	60	73
1	B	395/395 (100%)	390 (99%)	5 (1%)	65	77
1	C	395/395 (100%)	388 (98%)	7 (2%)	54	67
1	D	395/395 (100%)	387 (98%)	8 (2%)	50	63
All	All	1580/1580 (100%)	1554 (98%)	26 (2%)	58	71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	197	LYS
1	A	258	CYS
1	A	336	CYS
1	A	425	PHE
1	A	438	TYR
1	B	25	GLN

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Mol	Chain	Res	Type
1	B	64	ARG
1	B	258	CYS
1	B	336	CYS
1	B	425	PHE
1	C	193	TYR
1	C	197	LYS
1	C	210	GLU
1	C	336	CYS
1	C	425	PHE
1	C	438	TYR
1	C	470	SER
1	D	60	SER
1	D	125	ARG
1	D	197	LYS
1	D	258	CYS
1	D	336	CYS
1	D	352	THR
1	D	425	PHE
1	D	438	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	78	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

50 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	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	0.74	0
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.35	0
2	FUC	E	3	2	10,10,11	0.74	0	14,14,16	1.76	3 (21%)
3	NAG	F	1	1,3	14,14,15	2.04	3 (21%)	17,19,21	1.24	2 (11%)
3	FUC	F	2	3	10,10,11	2.16	4 (40%)	14,14,16	1.74	3 (21%)
4	NAG	G	1	1,4	14,14,15	0.27	0	17,19,21	0.71	1 (5%)
4	NAG	G	2	4	14,14,15	0.60	0	17,19,21	0.53	0
4	NAG	H	1	1,4	14,14,15	0.16	0	17,19,21	0.73	0
4	NAG	H	2	4	14,14,15	0.34	0	17,19,21	0.39	0
5	NAG	I	1	1,5	14,14,15	0.41	0	17,19,21	0.71	0
5	NAG	I	2	5	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
5	MAN	I	3	5	11,11,12	1.87	3 (27%)	15,15,17	2.01	4 (26%)
5	MAN	I	4	5	11,11,12	2.19	3 (27%)	15,15,17	1.98	6 (40%)
5	FUC	I	5	5	10,10,11	1.38	1 (10%)	14,14,16	1.69	4 (28%)
3	NAG	J	1	1,3	14,14,15	1.96	3 (21%)	17,19,21	1.20	2 (11%)
3	FUC	J	2	3	10,10,11	1.93	2 (20%)	14,14,16	1.73	3 (21%)
4	NAG	K	1	1,4	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
4	NAG	K	2	4	14,14,15	0.53	0	17,19,21	0.56	0
6	NAG	L	1	1,6	14,14,15	0.18	0	17,19,21	0.94	1 (5%)
6	NAG	L	2	6	14,14,15	0.40	0	17,19,21	0.59	0
6	MAN	L	3	6	11,11,12	2.15	5 (45%)	15,15,17	2.67	6 (40%)
4	NAG	M	1	1,4	14,14,15	1.26	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	M	2	4	14,14,15	0.43	0	17,19,21	0.47	0
2	NAG	N	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.85	1 (5%)
2	NAG	N	2	2	14,14,15	0.48	0	17,19,21	0.72	0
2	FUC	N	3	2	10,10,11	1.06	0	14,14,16	1.21	2 (14%)
6	NAG	O	1	1,6	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
6	NAG	O	2	6	14,14,15	0.56	0	17,19,21	1.85	1 (5%)
6	MAN	O	3	6	11,11,12	2.08	3 (27%)	15,15,17	1.65	5 (33%)
4	NAG	P	1	1,4	14,14,15	0.40	0	17,19,21	0.64	0
4	NAG	P	2	4	14,14,15	0.89	2 (14%)	17,19,21	0.58	0
4	NAG	Q	1	1,4	14,14,15	0.39	0	17,19,21	0.50	0
4	NAG	Q	2	4	14,14,15	0.42	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	R	1	1,4	14,14,15	0.28	0	17,19,21	0.91	1 (5%)
4	NAG	R	2	4	14,14,15	0.74	1 (7%)	17,19,21	0.57	0
2	NAG	S	1	1,2	14,14,15	0.36	0	17,19,21	0.63	0
2	NAG	S	2	2	14,14,15	0.46	0	17,19,21	0.37	0
2	FUC	S	3	2	10,10,11	0.93	1 (10%)	14,14,16	1.87	3 (21%)
7	NAG	T	1	1,7	14,14,15	0.46	0	17,19,21	0.71	0
7	NAG	T	2	7	14,14,15	0.37	0	17,19,21	0.68	0
7	MAN	T	3	7	11,11,12	2.29	4 (36%)	15,15,17	2.86	7 (46%)
7	FUC	T	4	7	10,10,11	2.08	3 (30%)	14,14,16	1.81	3 (21%)
4	NAG	U	1	1,4	14,14,15	0.49	0	17,19,21	0.65	0
4	NAG	U	2	4	14,14,15	0.40	0	17,19,21	0.40	0
7	NAG	V	1	1,7	14,14,15	0.73	1 (7%)	17,19,21	0.66	0
7	NAG	V	2	7	14,14,15	0.87	1 (7%)	17,19,21	2.41	1 (5%)
7	MAN	V	3	7	11,11,12	2.01	3 (27%)	15,15,17	2.17	4 (26%)
7	FUC	V	4	7	10,10,11	1.11	1 (10%)	14,14,16	1.15	1 (7%)
4	NAG	W	1	1,4	14,14,15	0.26	0	17,19,21	0.79	1 (5%)
4	NAG	W	2	4	14,14,15	0.25	0	17,19,21	0.62	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	MAN	I	3	5	-	2/2/19/22	1/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	FUC	I	5	5	-	-	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	J	2	3	-	-	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
6	MAN	L	3	6	-	1/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	FUC	N	3	2	-	-	0/1/1/1
6	NAG	O	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	3/6/23/26	0/1/1/1
6	MAN	O	3	6	-	1/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	4/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	1/6/23/26	0/1/1/1
2	FUC	S	3	2	-	-	0/1/1/1
7	NAG	T	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	1/6/23/26	0/1/1/1
7	MAN	T	3	7	-	2/2/19/22	0/1/1/1
7	FUC	T	4	7	-	-	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
7	NAG	V	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	V	2	7	-	4/6/23/26	0/1/1/1
7	MAN	V	3	7	-	2/2/19/22	1/1/1/1
7	FUC	V	4	7	-	-	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-6.18	1.33	1.43
3	J	1	NAG	O5-C1	-5.17	1.35	1.43
5	I	4	MAN	C4-C3	5.03	1.65	1.52
7	T	3	MAN	O5-C1	4.84	1.51	1.43
4	M	1	NAG	O5-C1	-4.65	1.36	1.43
7	V	3	MAN	C2-C3	-4.63	1.45	1.52
3	J	2	FUC	C1-C2	4.54	1.62	1.52
3	J	1	NAG	C1-C2	4.46	1.59	1.52
6	O	3	MAN	C2-C3	4.28	1.58	1.52
5	I	3	MAN	C4-C5	4.02	1.61	1.53
7	T	4	FUC	O5-C5	3.96	1.52	1.43
3	F	1	NAG	C1-C2	3.79	1.58	1.52
3	F	2	FUC	O5-C5	3.69	1.51	1.43
7	T	3	MAN	O5-C5	3.62	1.50	1.43
3	F	2	FUC	C1-C2	3.53	1.60	1.52
5	I	5	FUC	C6-C5	3.53	1.60	1.51
6	L	3	MAN	O5-C5	3.52	1.50	1.43
6	O	3	MAN	O5-C5	3.50	1.50	1.43
5	I	4	MAN	C4-C5	3.44	1.60	1.53
7	T	4	FUC	C2-C3	-3.31	1.47	1.52
7	T	4	FUC	C4-C5	3.30	1.60	1.52
5	I	3	MAN	C1-C2	3.30	1.59	1.52
3	F	2	FUC	C2-C3	3.21	1.57	1.52
7	V	2	NAG	O5-C1	3.00	1.48	1.43
6	L	3	MAN	O5-C1	2.93	1.48	1.43
6	L	3	MAN	C2-C3	-2.90	1.48	1.52
7	V	3	MAN	O5-C5	2.88	1.49	1.43
7	T	3	MAN	O3-C3	2.85	1.49	1.43
6	L	3	MAN	O3-C3	2.69	1.49	1.43
3	J	2	FUC	O5-C5	2.68	1.49	1.43
7	V	1	NAG	O5-C1	-2.64	1.39	1.43
7	T	3	MAN	C1-C2	2.56	1.58	1.52
5	I	4	MAN	C1-C2	2.56	1.58	1.52
4	P	2	NAG	O5-C1	2.55	1.47	1.43
6	O	3	MAN	C4-C3	2.54	1.58	1.52
5	I	3	MAN	C4-C3	2.48	1.58	1.52
6	L	3	MAN	C1-C2	2.47	1.57	1.52
4	R	2	NAG	C1-C2	2.47	1.56	1.52
3	F	2	FUC	C4-C5	2.37	1.58	1.52
3	J	1	NAG	C3-C2	2.28	1.57	1.52
7	V	3	MAN	O2-C2	-2.10	1.38	1.43
2	N	1	NAG	O5-C1	2.10	1.47	1.43
7	V	4	FUC	C2-C3	2.08	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C3-C2	2.08	1.56	1.52
6	O	1	NAG	C1-C2	2.06	1.55	1.52
4	P	2	NAG	C1-C2	2.03	1.55	1.52
2	S	3	FUC	O5-C5	2.01	1.47	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	2	NAG	C1-O5-C5	9.44	124.98	112.19
6	O	2	NAG	C1-O5-C5	6.72	121.29	112.19
7	V	3	MAN	O2-C2-C3	-5.99	98.13	110.14
6	L	3	MAN	C1-O5-C5	5.63	119.81	112.19
7	T	3	MAN	C1-O5-C5	5.18	119.22	112.19
5	I	4	MAN	C1-C2-C3	-4.94	103.59	109.67
6	L	3	MAN	O2-C2-C3	-4.72	100.68	110.14
7	T	3	MAN	O5-C5-C6	4.61	114.43	107.20
2	S	3	FUC	O5-C5-C4	4.59	117.75	109.52
7	T	4	FUC	O5-C5-C4	4.56	117.70	109.52
7	T	3	MAN	C3-C4-C5	-4.53	102.16	110.24
6	L	3	MAN	C1-C2-C3	4.39	115.06	109.67
7	T	3	MAN	O5-C1-C2	4.16	117.19	110.77
3	J	2	FUC	O2-C2-C1	4.06	117.47	109.15
5	I	3	MAN	O5-C5-C6	-3.93	101.05	107.20
5	I	5	FUC	O5-C5-C4	3.71	116.17	109.52
3	J	1	NAG	C4-C3-C2	3.68	116.41	111.02
3	F	1	NAG	C4-C3-C2	3.67	116.40	111.02
2	E	3	FUC	C1-O5-C5	3.66	121.08	112.78
6	O	3	MAN	C1-O5-C5	3.66	117.15	112.19
2	E	3	FUC	O5-C5-C4	3.62	116.02	109.52
5	I	3	MAN	C1-O5-C5	-3.49	107.47	112.19
4	R	1	NAG	C1-O5-C5	3.38	116.77	112.19
6	L	3	MAN	O5-C1-C2	3.36	115.95	110.77
2	S	3	FUC	C1-O5-C5	3.27	120.19	112.78
7	T	3	MAN	C1-C2-C3	3.21	113.61	109.67
3	F	2	FUC	O2-C2-C1	3.18	115.65	109.15
7	V	3	MAN	C2-C3-C4	-3.15	105.45	110.89
7	T	3	MAN	O3-C3-C4	3.14	117.61	110.35
6	L	1	NAG	C1-O5-C5	3.14	116.44	112.19
3	J	2	FUC	O5-C5-C4	3.08	115.04	109.52
3	F	2	FUC	C1-O5-C5	3.07	119.73	112.78
5	I	2	NAG	O4-C4-C5	-3.04	101.74	109.30
7	V	4	FUC	C1-C2-C3	3.00	113.35	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	FUC	O5-C1-C2	2.95	115.33	110.77
6	L	3	MAN	O5-C5-C6	2.93	111.79	107.20
3	F	2	FUC	O5-C5-C4	2.92	114.77	109.52
2	N	1	NAG	C1-O5-C5	2.89	116.10	112.19
3	J	2	FUC	C1-O5-C5	2.80	119.12	112.78
6	O	3	MAN	C1-C2-C3	-2.79	106.24	109.67
6	O	3	MAN	O2-C2-C1	2.77	114.81	109.15
4	M	1	NAG	C1-O5-C5	2.72	115.88	112.19
3	J	1	NAG	O5-C5-C4	-2.71	104.23	110.83
5	I	5	FUC	O5-C1-C2	2.69	114.93	110.77
4	Q	2	NAG	C1-O5-C5	2.69	115.84	112.19
7	T	4	FUC	C1-O5-C5	2.66	118.81	112.78
7	V	3	MAN	C1-O5-C5	2.66	115.80	112.19
3	F	1	NAG	O5-C5-C4	-2.66	104.36	110.83
7	T	3	MAN	O3-C3-C2	2.65	115.07	109.99
5	I	4	MAN	O2-C2-C1	2.65	114.56	109.15
5	I	4	MAN	O5-C1-C2	-2.64	106.69	110.77
5	I	3	MAN	C2-C3-C4	-2.62	106.37	110.89
2	S	3	FUC	O5-C1-C2	2.61	114.79	110.77
5	I	4	MAN	O4-C4-C3	2.56	116.26	110.35
7	V	3	MAN	C1-C2-C3	2.54	112.78	109.67
6	L	3	MAN	C2-C3-C4	-2.53	106.51	110.89
5	I	3	MAN	O5-C1-C2	-2.47	106.96	110.77
7	T	4	FUC	C3-C4-C5	2.46	113.60	109.77
4	W	1	NAG	C1-O5-C5	2.44	115.50	112.19
6	O	3	MAN	O5-C1-C2	-2.39	107.09	110.77
5	I	4	MAN	C1-O5-C5	-2.26	109.12	112.19
2	N	3	FUC	C1-O5-C5	2.25	117.87	112.78
5	I	5	FUC	C1-O5-C5	2.25	117.87	112.78
5	I	4	MAN	O3-C3-C4	2.18	115.38	110.35
2	N	3	FUC	O5-C5-C4	2.14	113.36	109.52
6	O	3	MAN	O3-C3-C2	2.08	113.98	109.99
5	I	5	FUC	C3-C4-C5	2.08	113.01	109.77
4	K	1	NAG	C1-O5-C5	2.06	114.98	112.19
4	G	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	V	3	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
5	I	3	MAN	O5-C5-C6-O6
7	T	3	MAN	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
7	V	3	MAN	C4-C5-C6-O6
5	I	3	MAN	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
7	V	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	V	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
7	T	3	MAN	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
6	O	3	MAN	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
6	L	3	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	3	MAN	C1-C2-C3-C4-C5-O5
7	V	3	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	3	MAN	1	0
6	L	2	NAG	1	0
2	S	1	NAG	1	0
2	N	1	NAG	2	0
7	V	2	NAG	1	0
5	I	5	FUC	1	0
2	E	1	NAG	1	0
2	N	3	FUC	2	0
7	T	3	MAN	1	0
4	M	1	NAG	1	0
7	T	2	NAG	1	0
2	N	2	NAG	1	0

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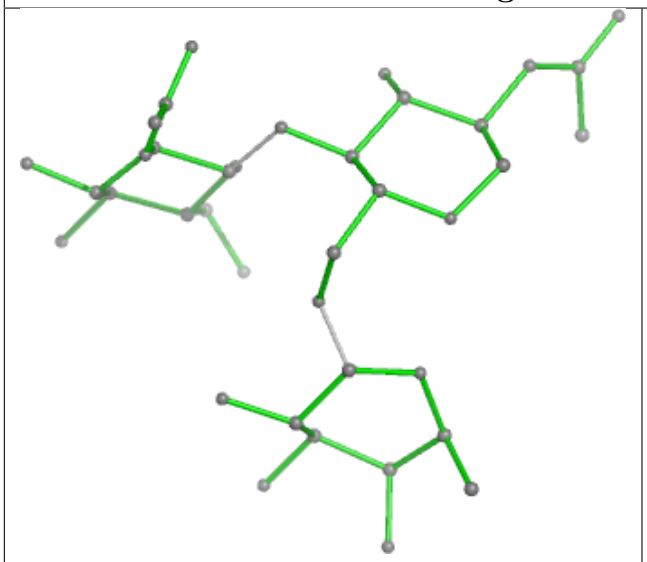
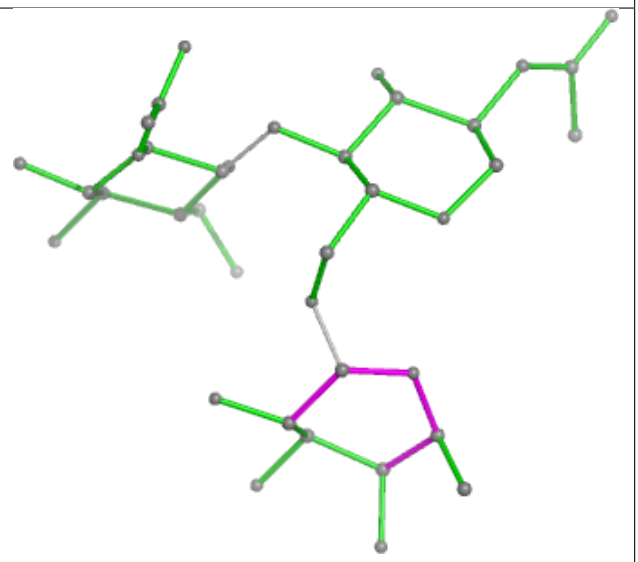
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	3	MAN	1	0

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

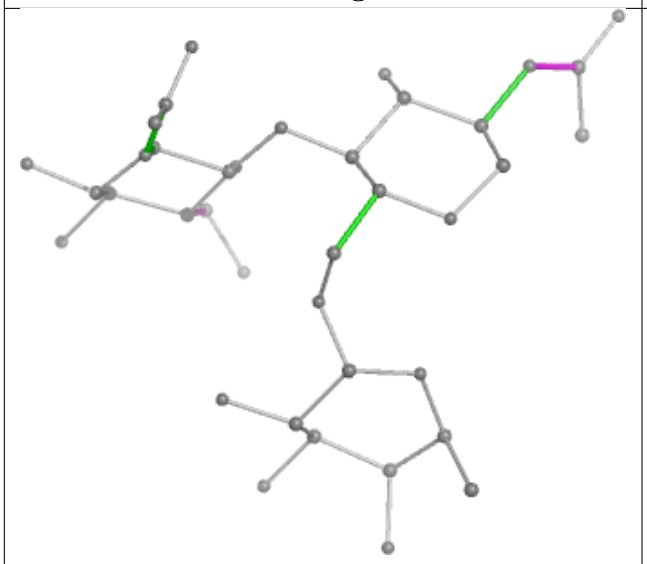
Oligosaccharide Chain E



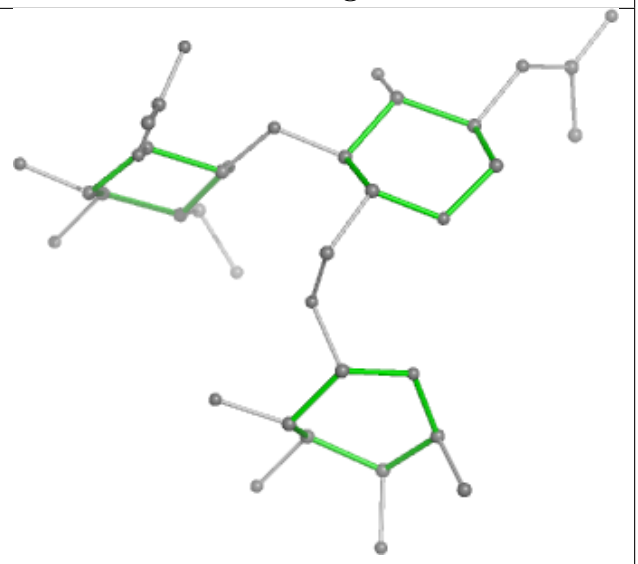
Bond lengths



Bond angles

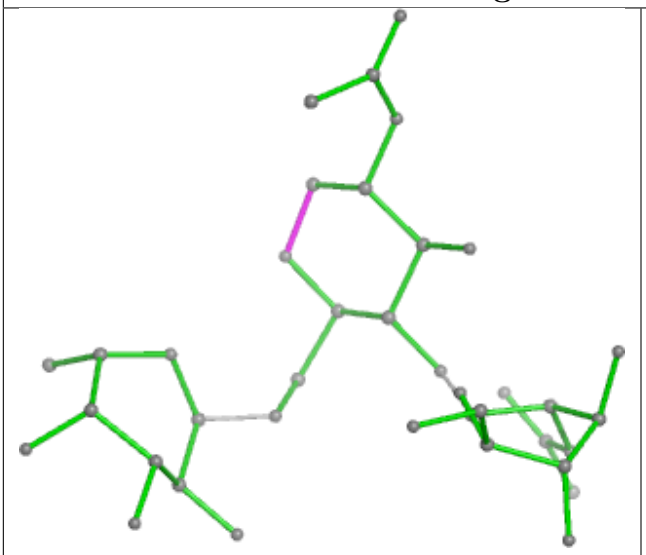


Torsions

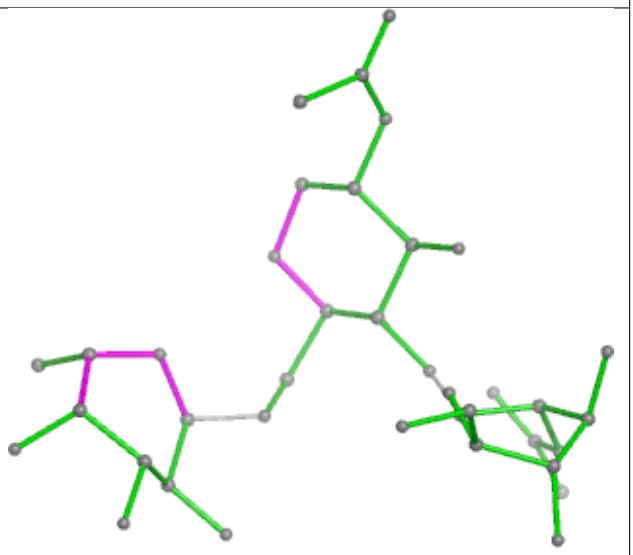


Rings

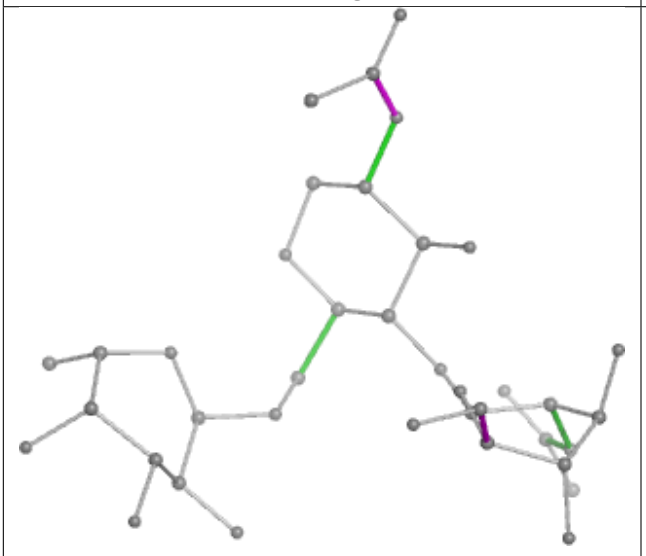
Oligosaccharide Chain N



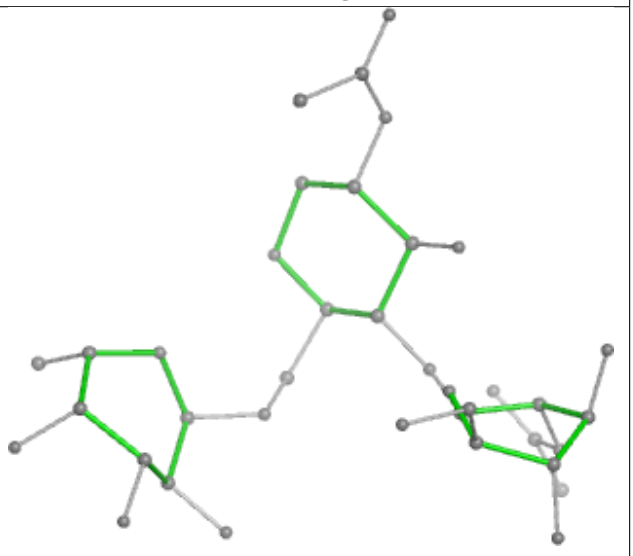
Bond lengths



Bond angles

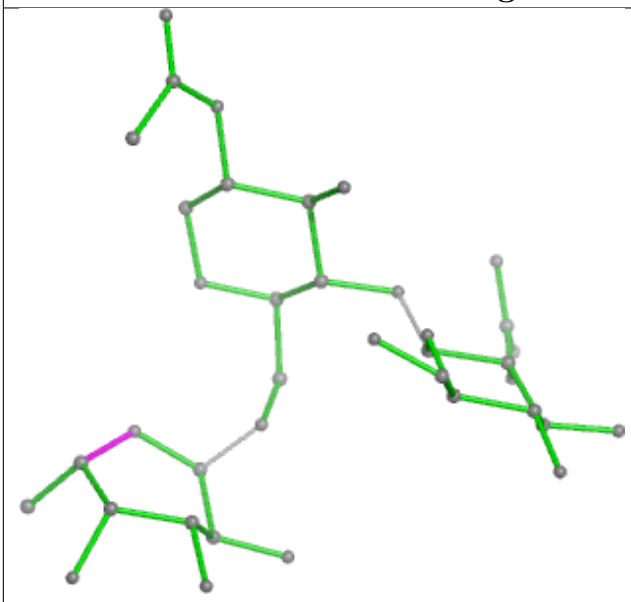


Torsions

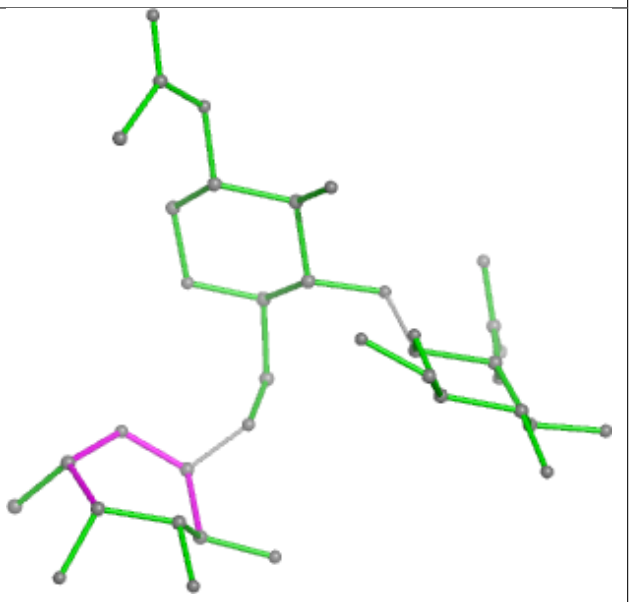


Rings

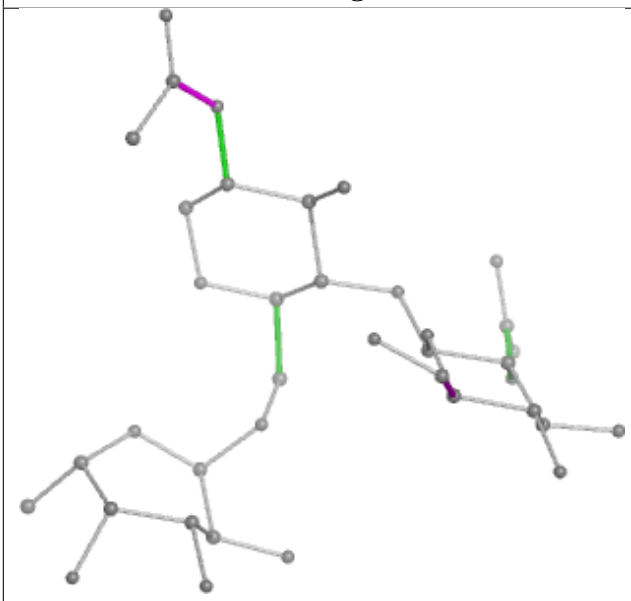
Oligosaccharide Chain S



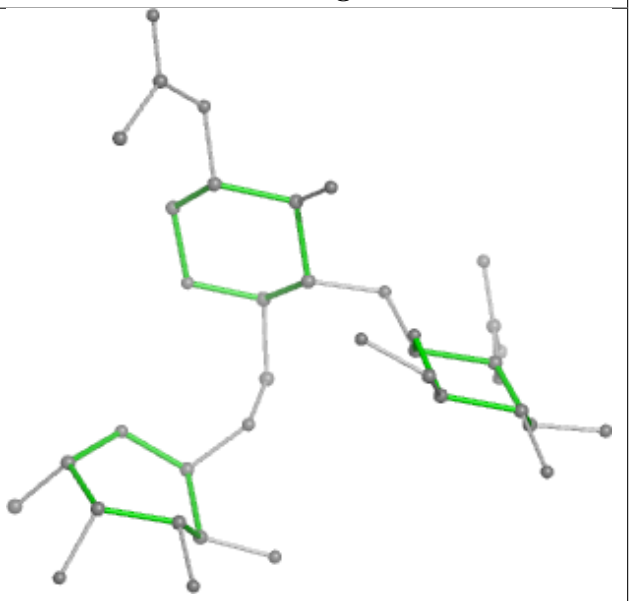
Bond lengths



Bond angles

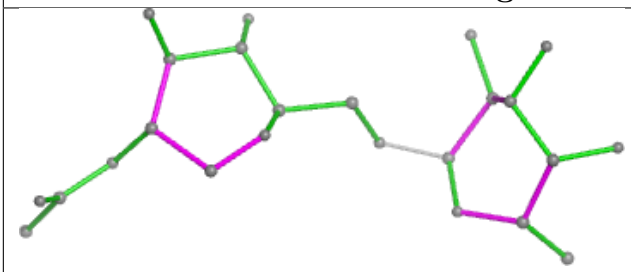


Torsions

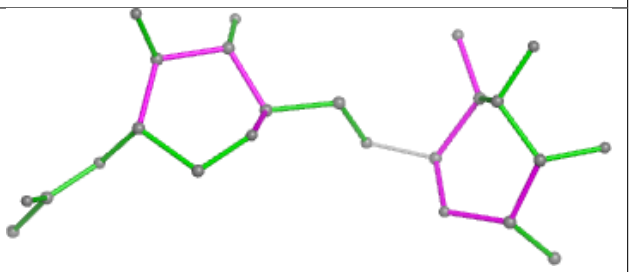


Rings

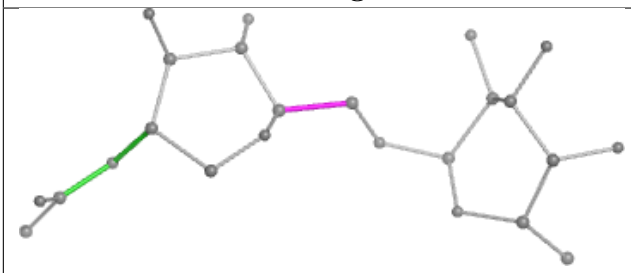
Oligosaccharide Chain F



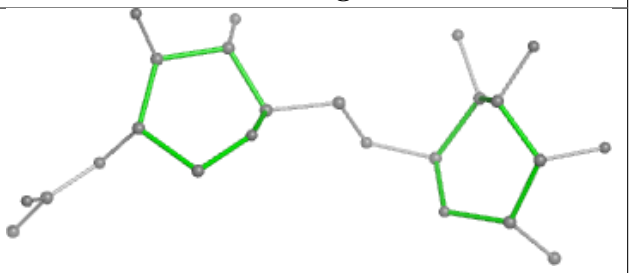
Bond lengths



Bond angles

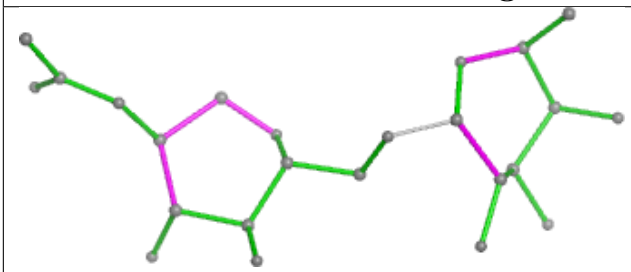


Torsions

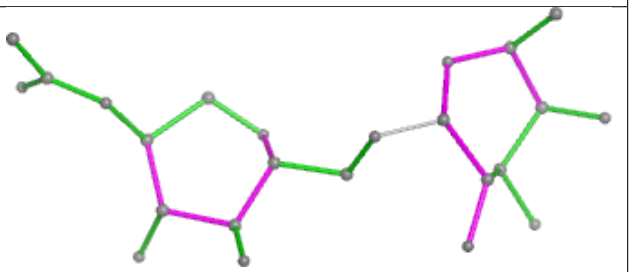


Rings

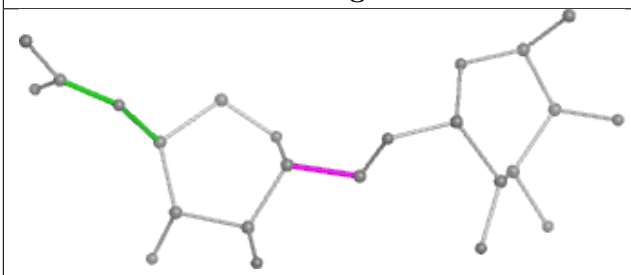
Oligosaccharide Chain J



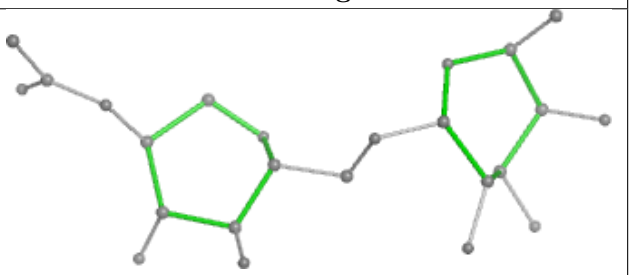
Bond lengths



Bond angles

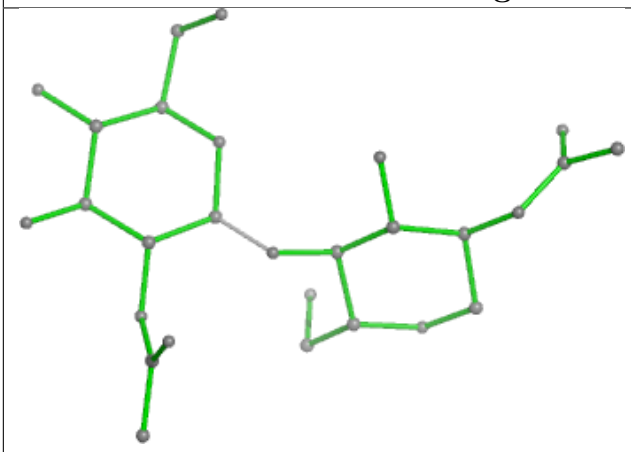


Torsions

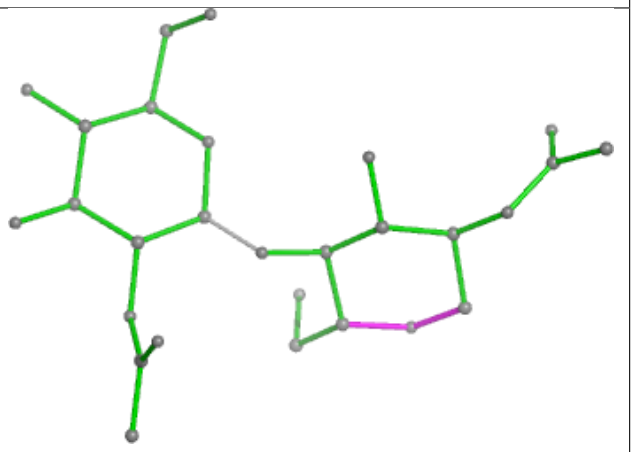


Rings

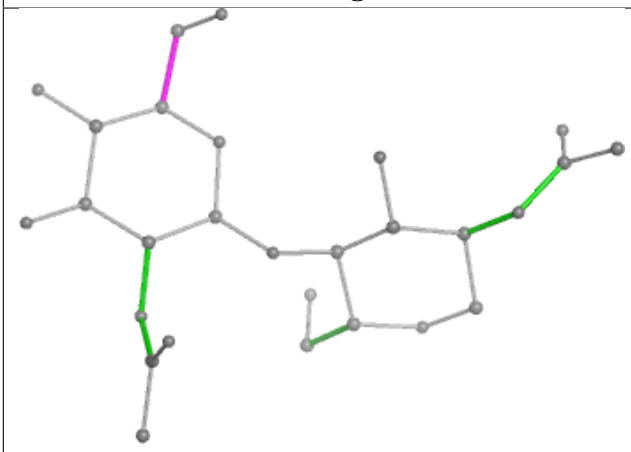
Oligosaccharide Chain G



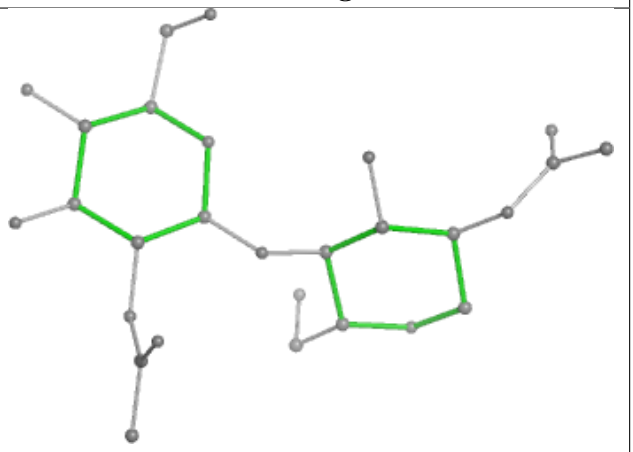
Bond lengths



Bond angles

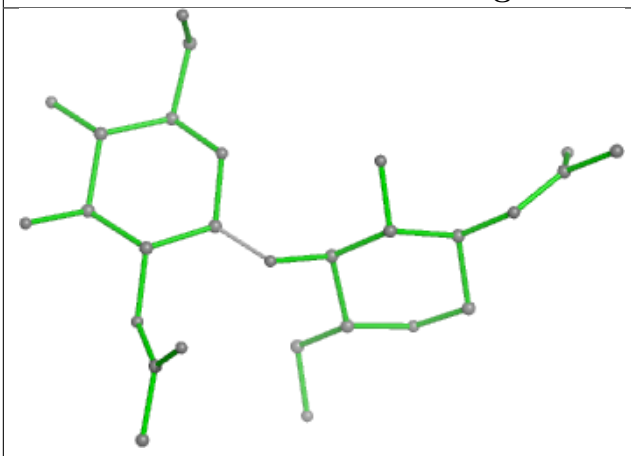


Torsions

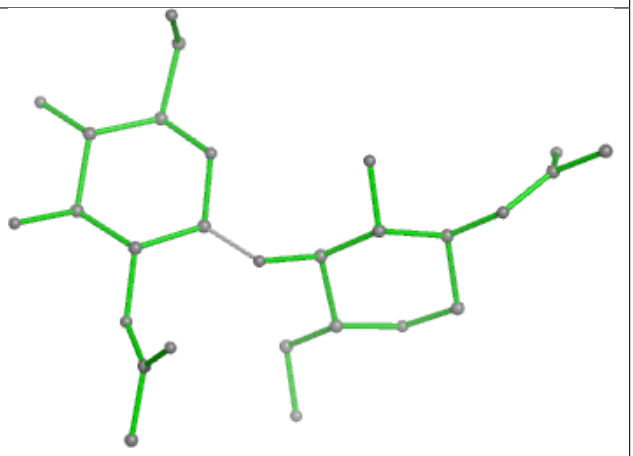


Rings

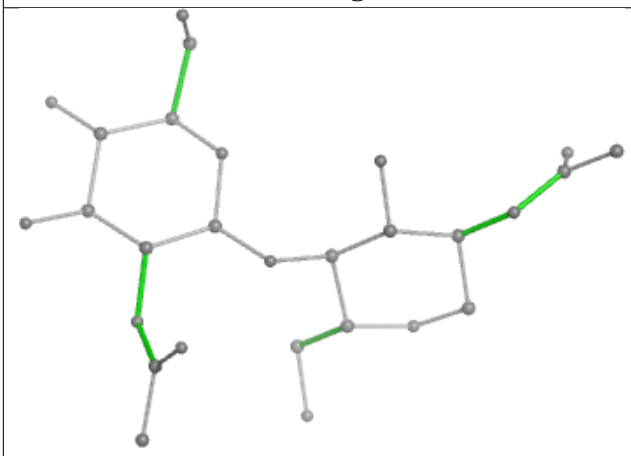
Oligosaccharide Chain H



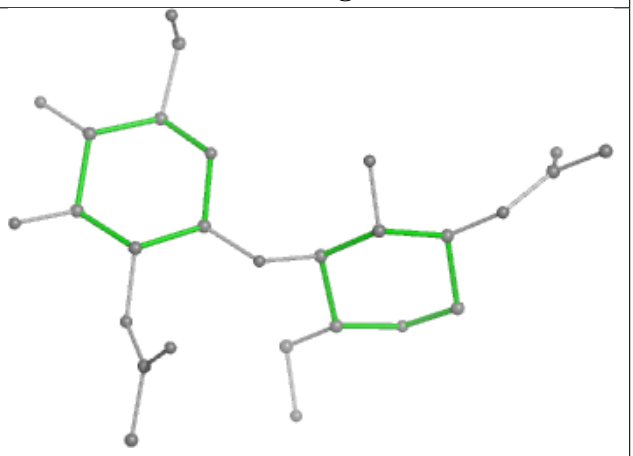
Bond lengths



Bond angles

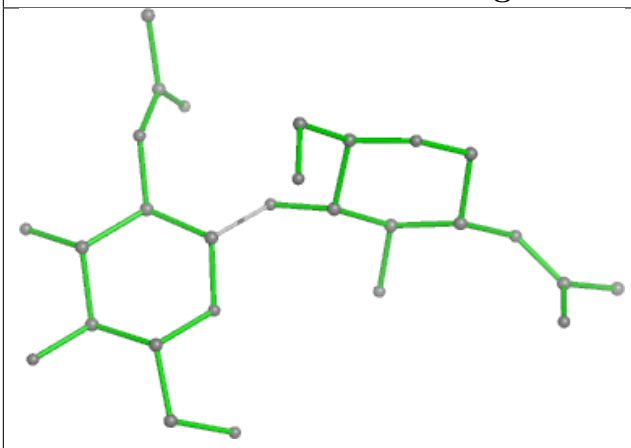


Torsions

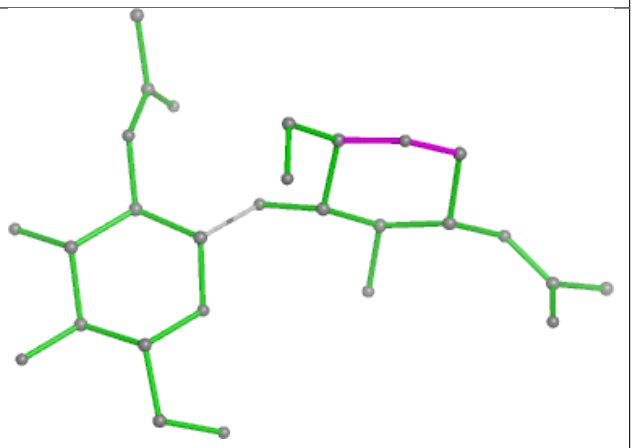


Rings

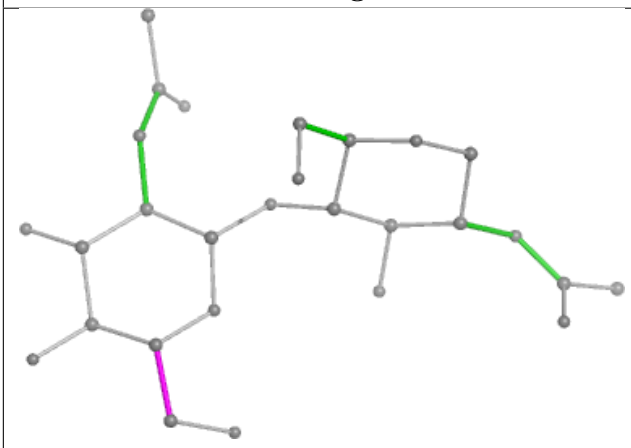
Oligosaccharide Chain K



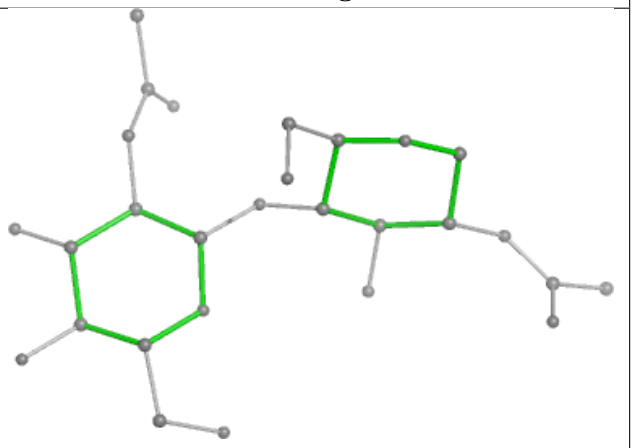
Bond lengths



Bond angles

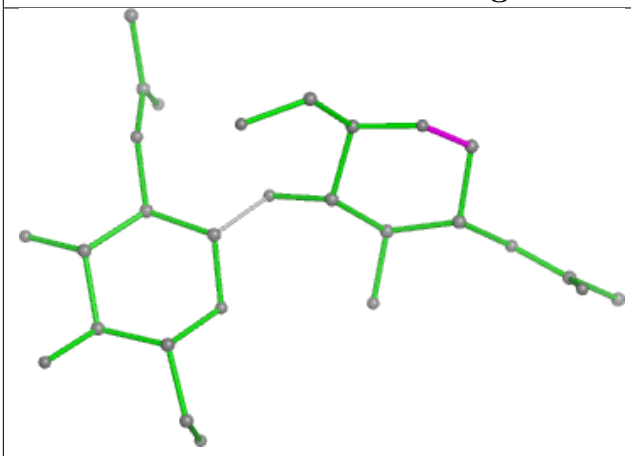


Torsions

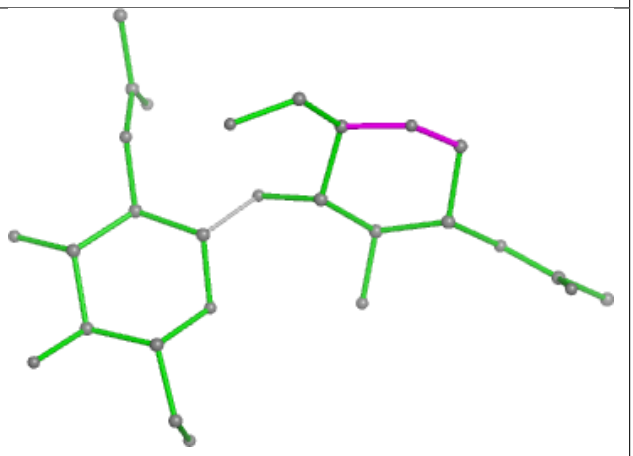


Rings

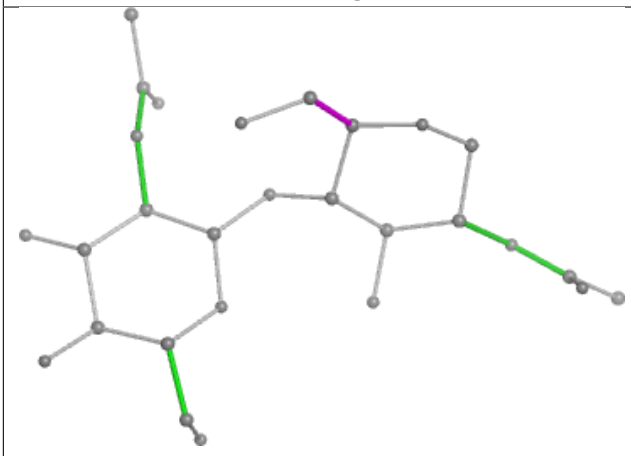
Oligosaccharide Chain M



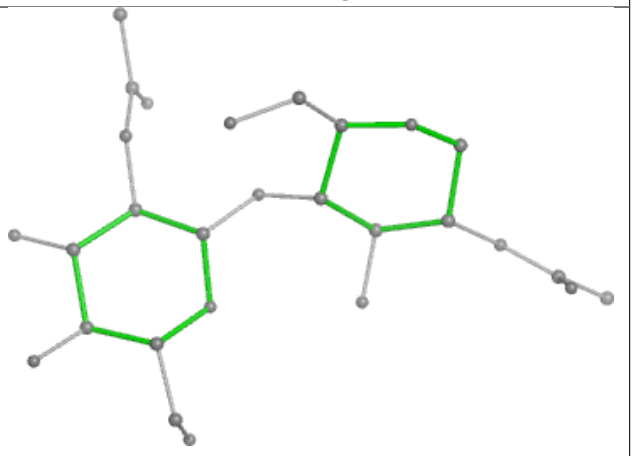
Bond lengths



Bond angles

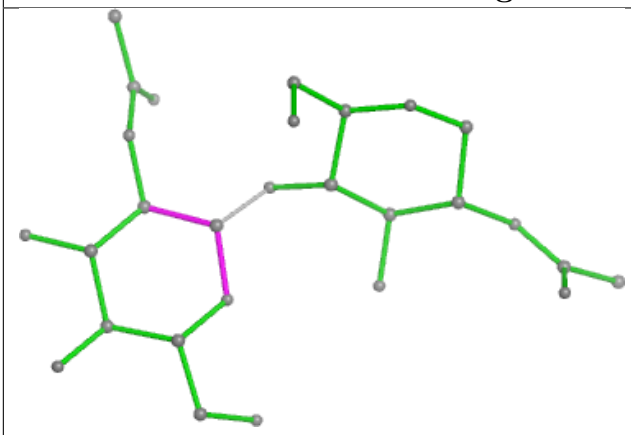


Torsions

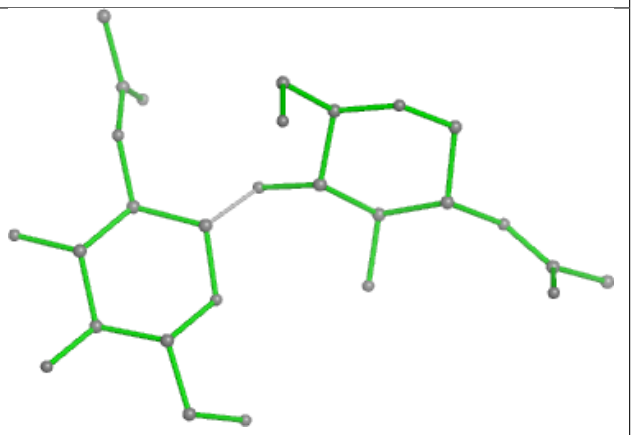


Rings

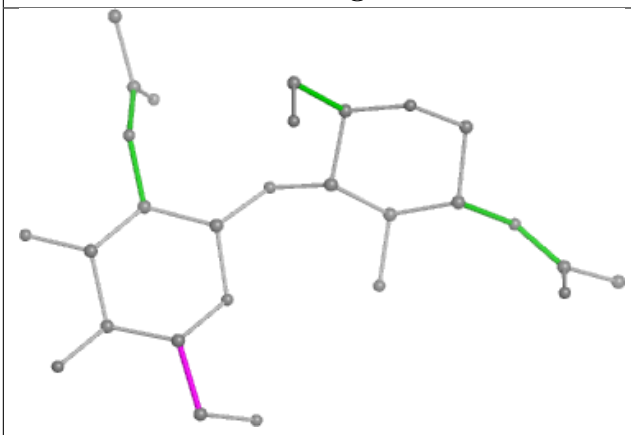
Oligosaccharide Chain P



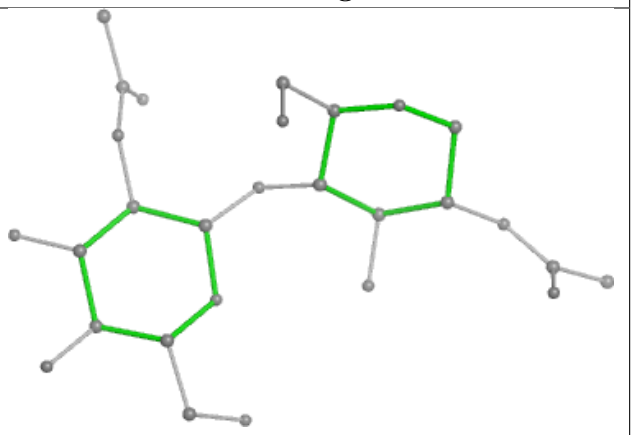
Bond lengths



Bond angles

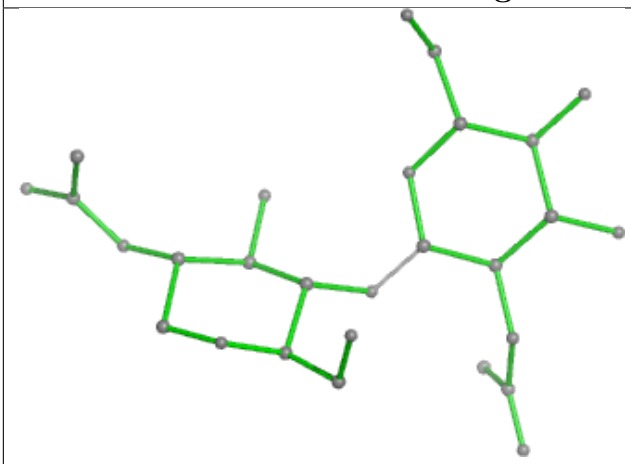


Torsions

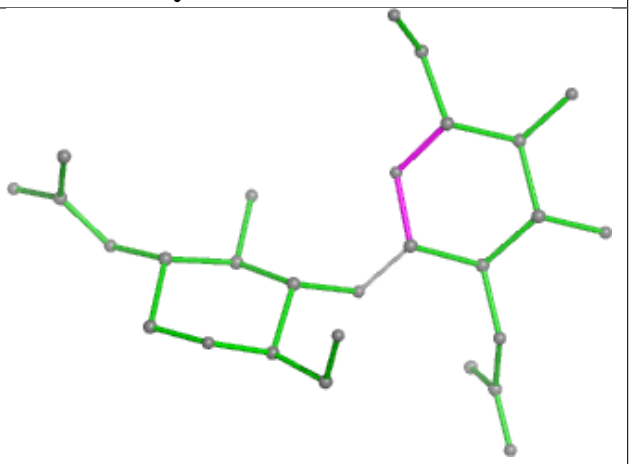


Rings

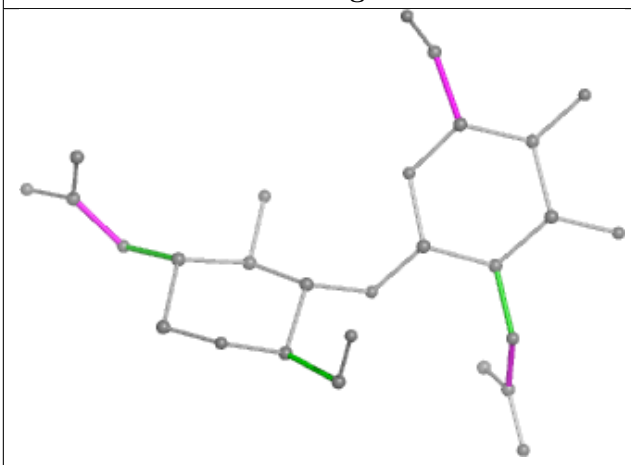
Oligosaccharide Chain Q



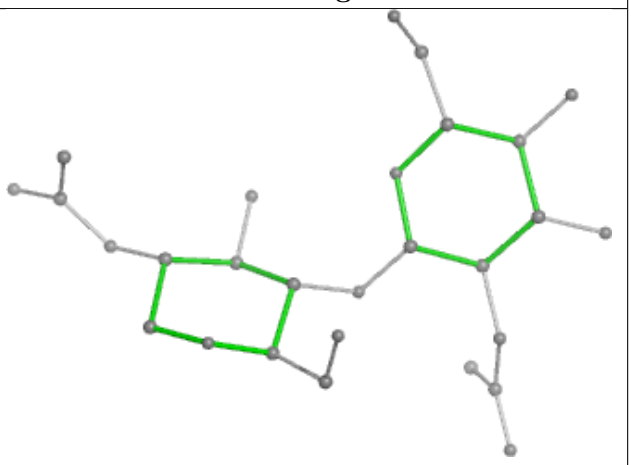
Bond lengths



Bond angles

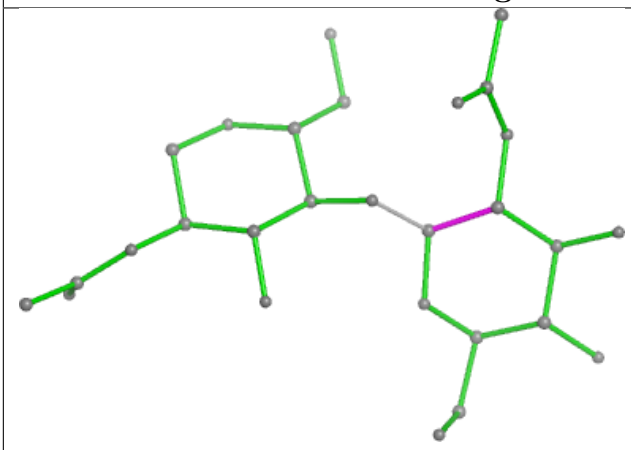


Torsions

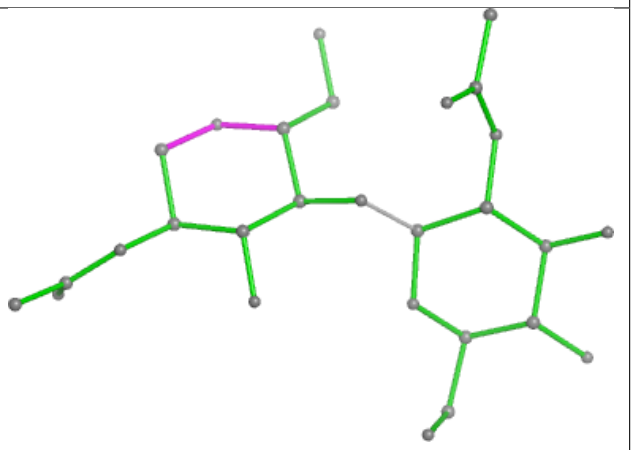


Rings

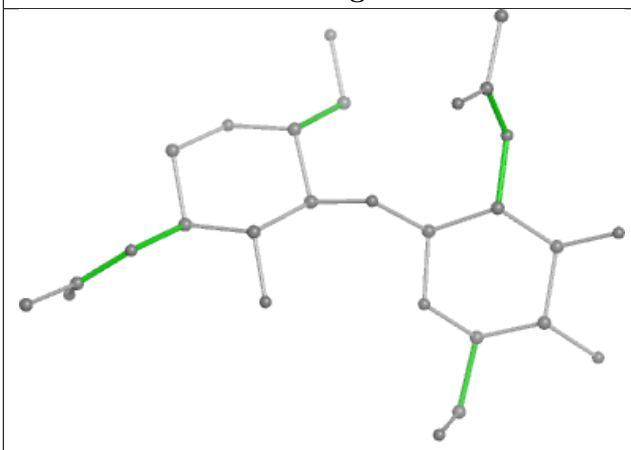
Oligosaccharide Chain R



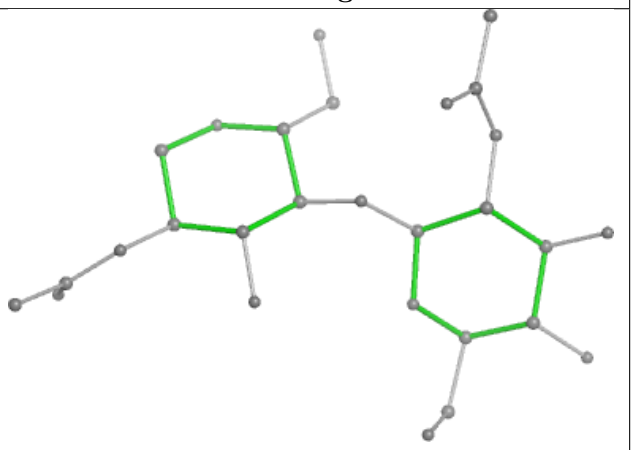
Bond lengths



Bond angles

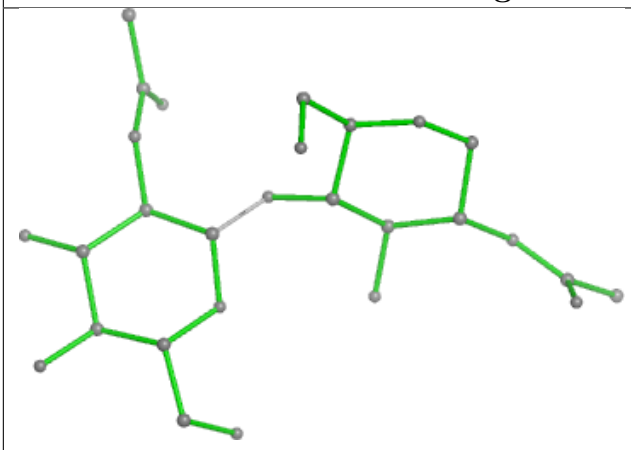


Torsions

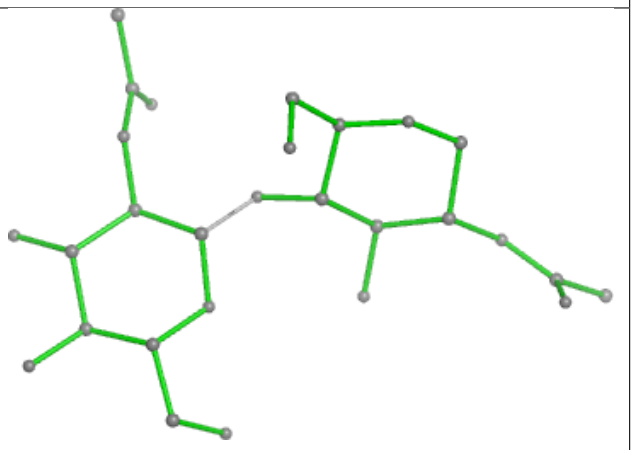


Rings

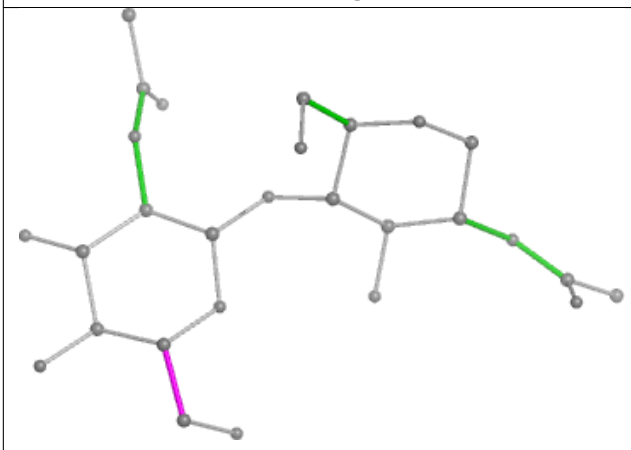
Oligosaccharide Chain U



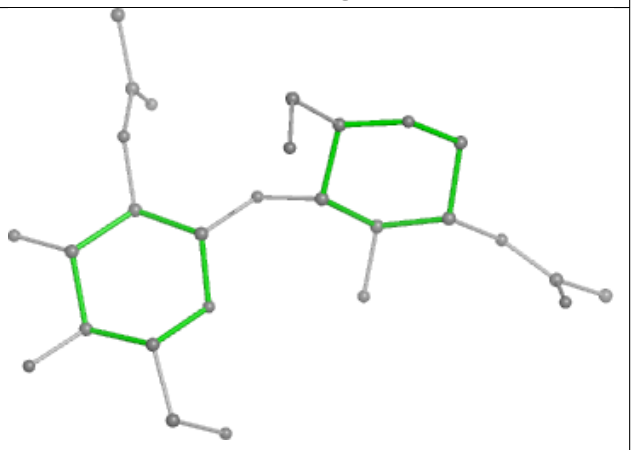
Bond lengths



Bond angles

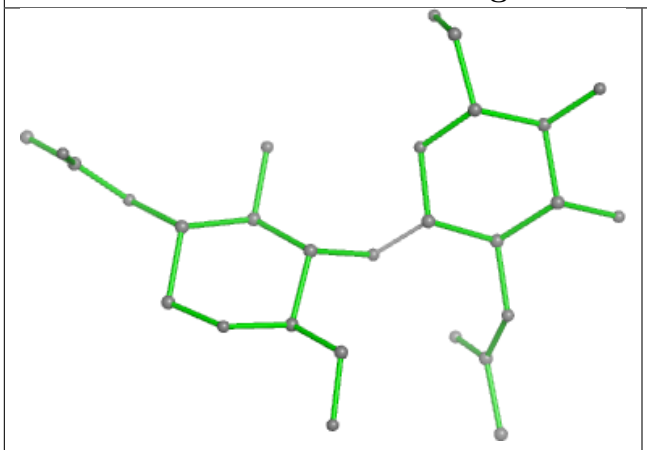


Torsions

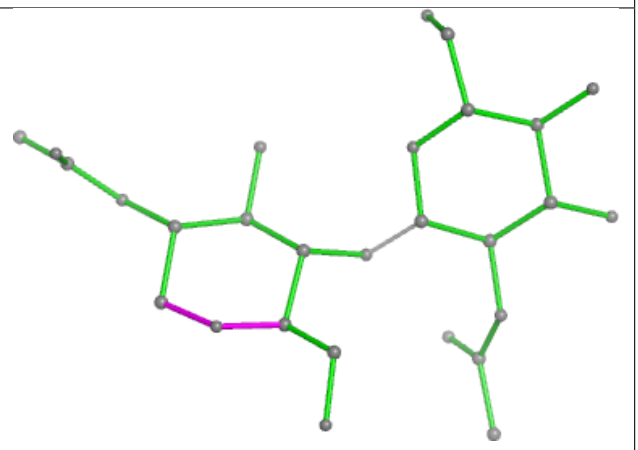


Rings

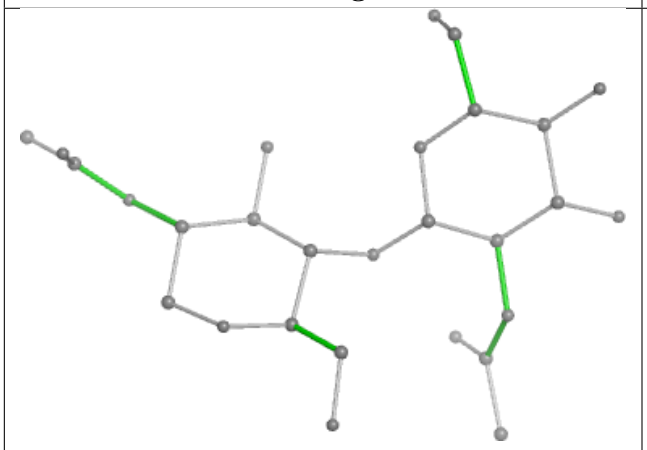
Oligosaccharide Chain W



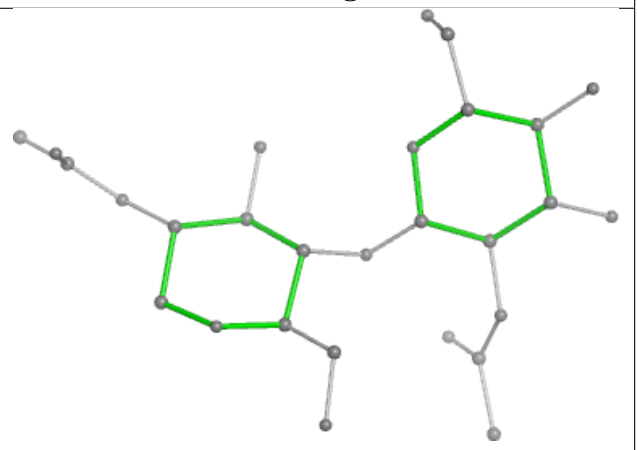
Bond lengths



Bond angles

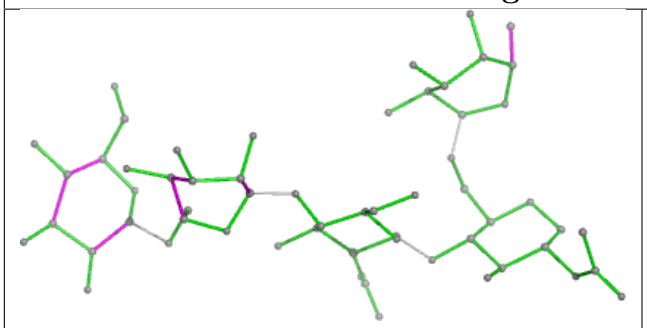


Torsions

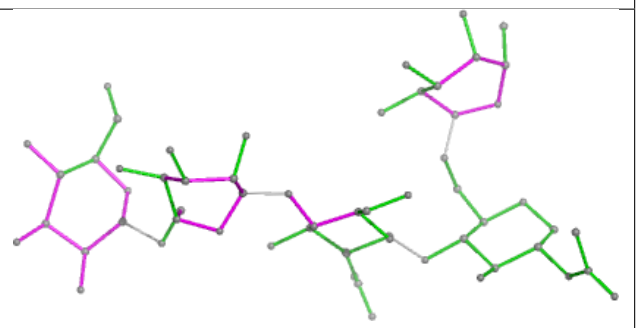


Rings

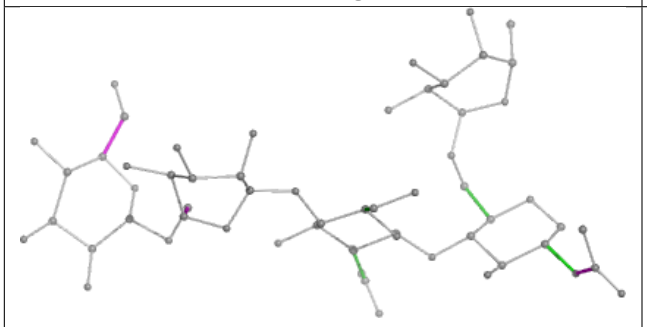
Oligosaccharide Chain I



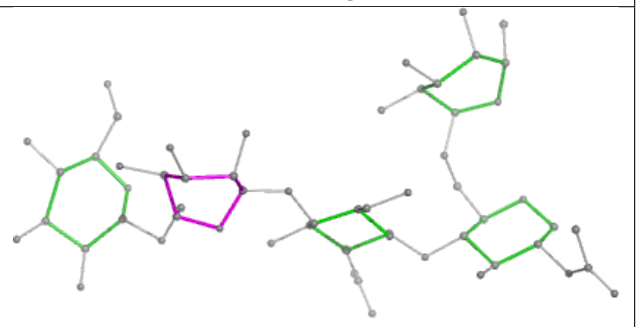
Bond lengths



Bond angles

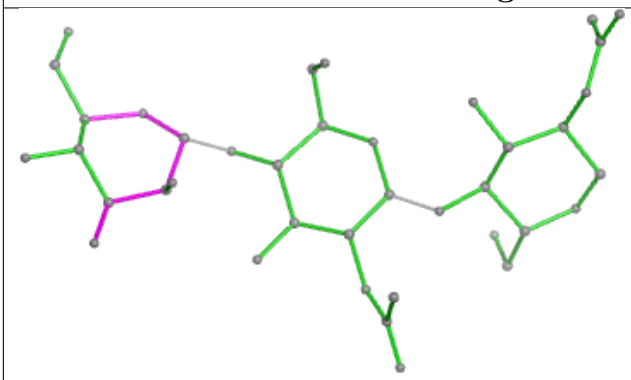


Torsions

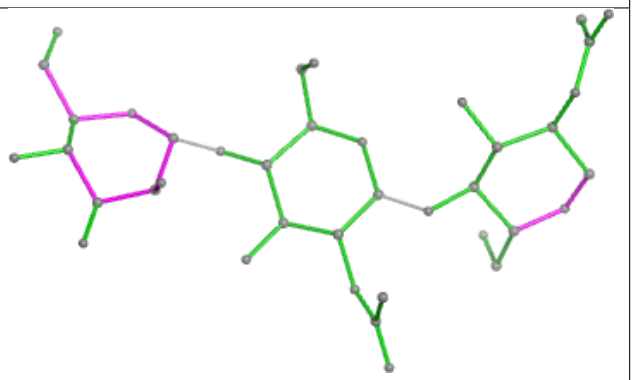


Rings

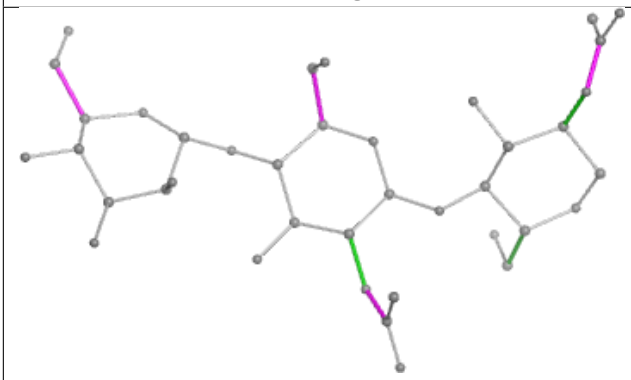
Oligosaccharide Chain L



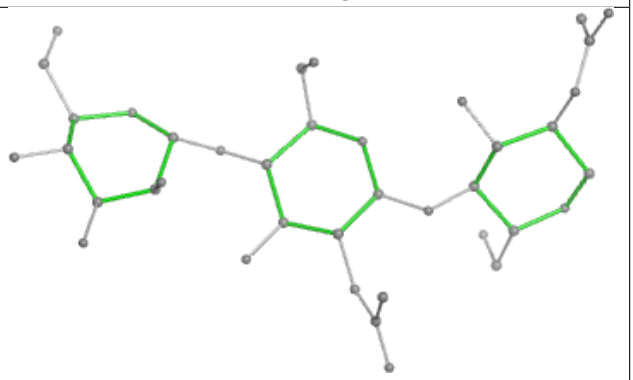
Bond lengths



Bond angles

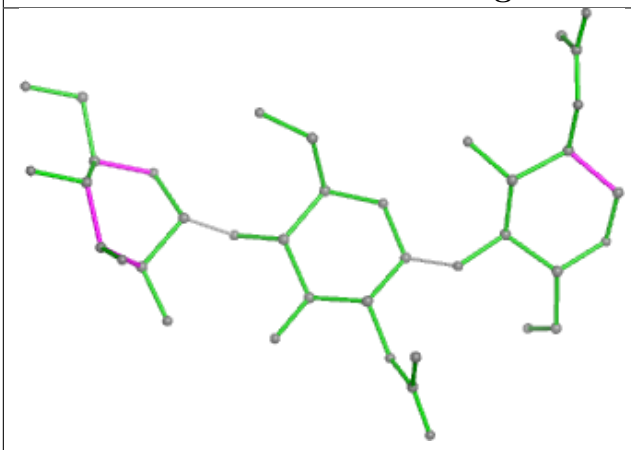


Torsions

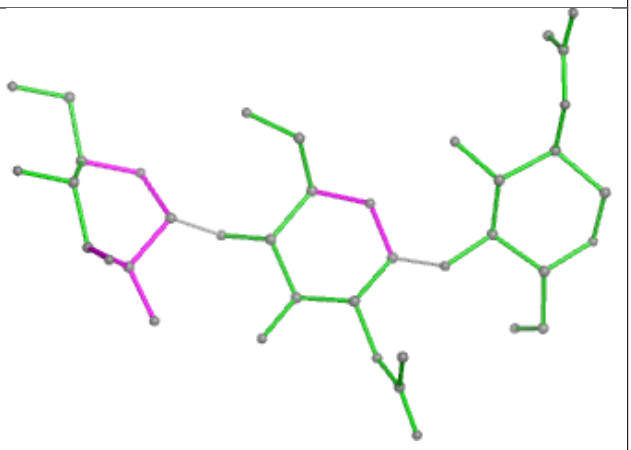


Rings

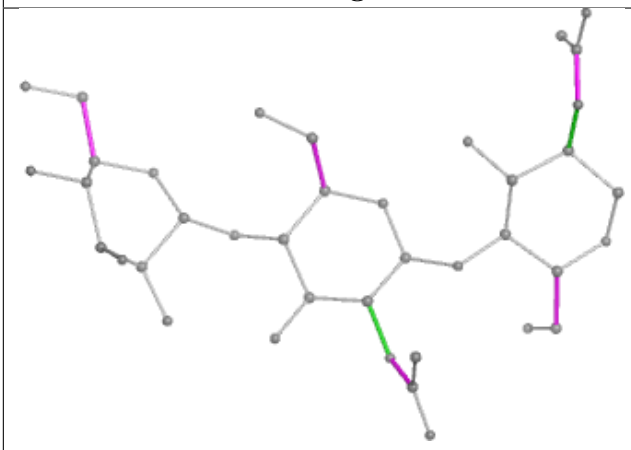
Oligosaccharide Chain O



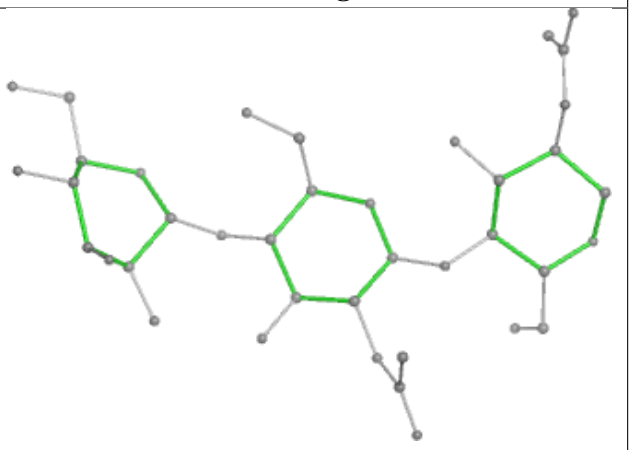
Bond lengths



Bond angles

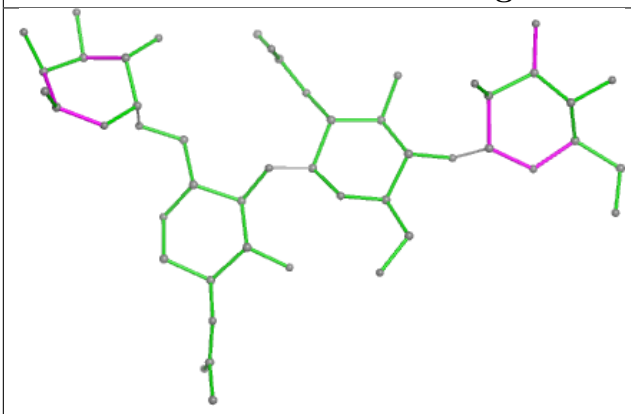


Torsions

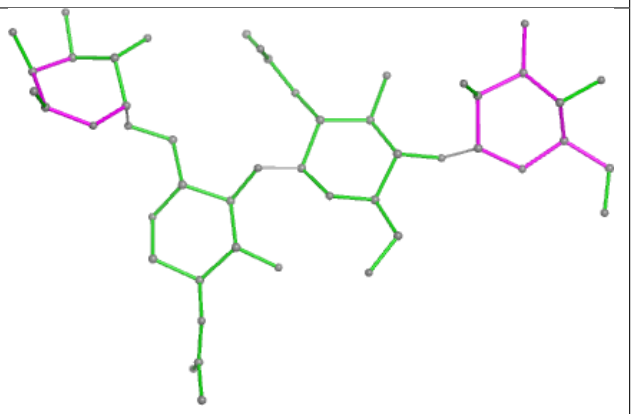


Rings

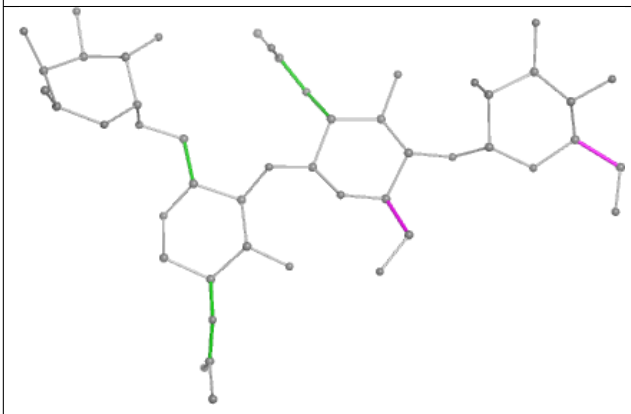
Oligosaccharide Chain T



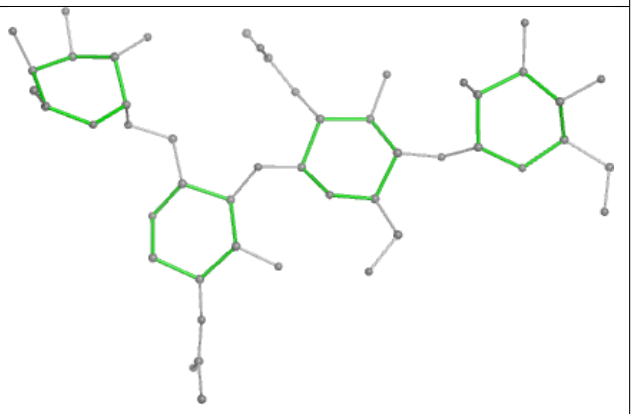
Bond lengths



Bond angles

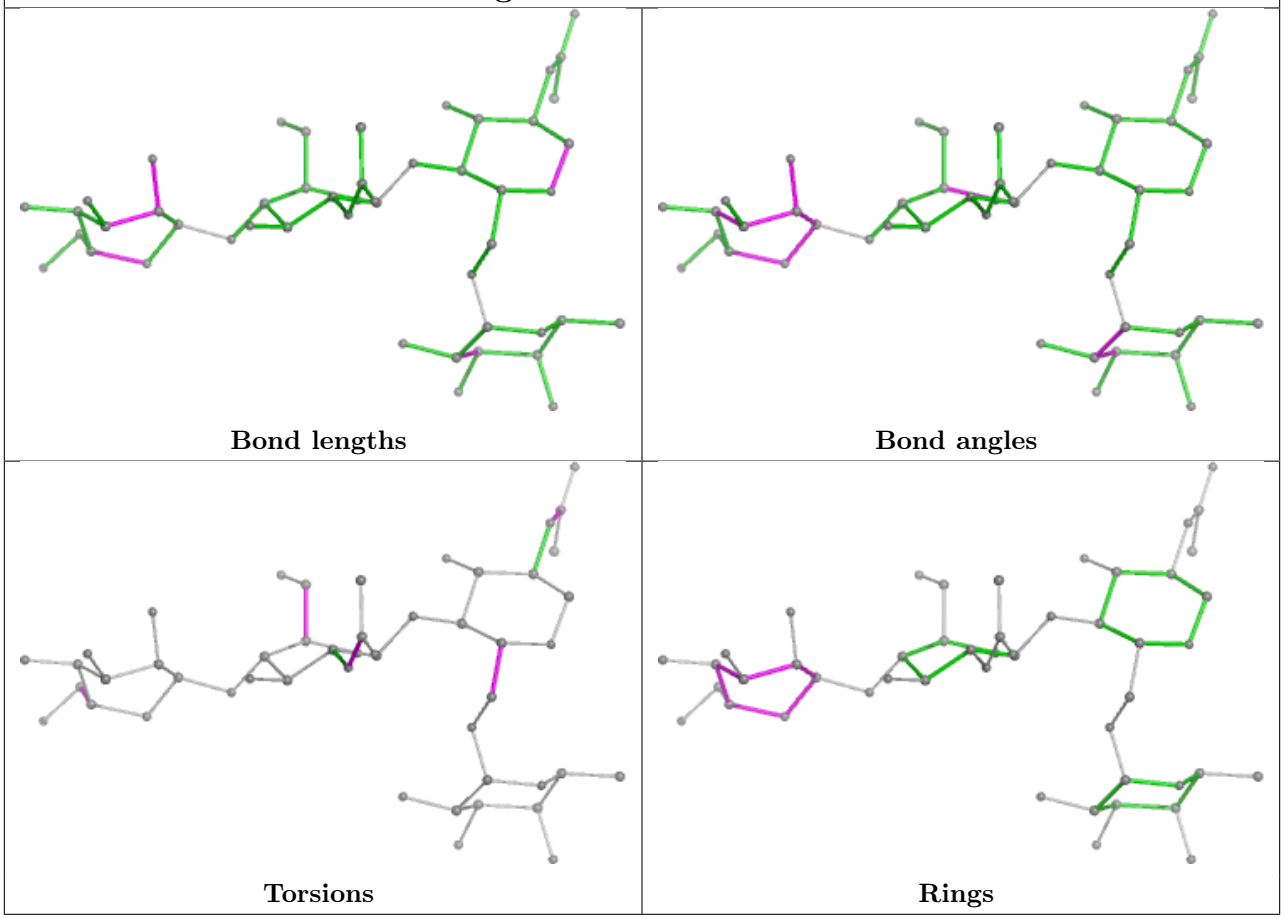


Torsions



Rings

Oligosaccharide Chain V



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
8	NAG	A	508	1	14,14,15	0.56	0	17,19,21	0.60	0
10	0TR	C	516	-	9,9,9	2.52	2 (22%)	11,11,11	3.00	2 (18%)
10	0TR	A	513	-	9,9,9	2.64	4 (44%)	11,11,11	2.91	3 (27%)
8	NAG	C	507	1	14,14,15	1.08	1 (7%)	17,19,21	0.76	1 (5%)
10	0TR	D	518	-	9,9,9	2.33	3 (33%)	11,11,11	2.30	2 (18%)
10	0TR	B	517	-	9,9,9	2.32	2 (22%)	11,11,11	2.85	2 (18%)

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
8	NAG	A	508	1	-	2/6/23/26	0/1/1/1
10	0TR	C	516	-	-	-	0/1/1/1
10	0TR	A	513	-	-	-	0/1/1/1
8	NAG	C	507	1	-	0/6/23/26	0/1/1/1
10	0TR	D	518	-	-	-	0/1/1/1
10	0TR	B	517	-	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	516	0TR	OA1-CA1	6.12	1.40	1.24
10	A	513	0TR	OA1-CA1	5.89	1.40	1.24
10	D	518	0TR	OA1-CA1	5.84	1.40	1.24
10	B	517	0TR	OA1-CA1	5.75	1.39	1.24
10	A	513	0TR	OA2-CA2	3.62	1.43	1.34
8	C	507	NAG	O5-C1	-3.41	1.38	1.43
10	C	516	0TR	OA2-CA2	2.99	1.41	1.34
10	B	517	0TR	OA2-CA2	2.73	1.41	1.34
10	A	513	0TR	CA3-CA2	2.54	1.40	1.37
10	D	518	0TR	OA2-CA2	2.46	1.40	1.34
10	D	518	0TR	CA6-CA1	-2.16	1.39	1.44
10	A	513	0TR	CA6-CA1	-2.01	1.40	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	516	0TR	CA6-CA1-CA2	8.82	130.79	122.76
10	A	513	0TR	CA6-CA1-CA2	8.63	130.61	122.76
10	B	517	0TR	CA6-CA1-CA2	8.23	130.25	122.76
10	D	518	0TR	CA6-CA1-CA2	6.56	128.73	122.76
10	C	516	0TR	OA1-CA1-CA6	-2.69	114.72	119.44
10	A	513	0TR	OA1-CA1-CA2	-2.31	112.26	116.14
10	B	517	0TR	OA1-CA1-CA6	-2.30	115.41	119.44
10	A	513	0TR	OA2-CA2-CA3	2.30	120.02	116.64
8	C	507	NAG	C4-C3-C2	2.11	114.12	111.02
10	D	518	0TR	OA2-CA2-CA3	-2.06	113.59	116.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	508	NAG	C8-C7-N2-C2
8	A	508	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	516	0TR	3	0
10	A	513	0TR	4	0
10	D	518	0TR	1	0
10	B	517	0TR	1	0

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	446/446 (100%)	-0.13	10 (2%)	62	67	27, 42, 59, 90	0
1	B	446/446 (100%)	-0.17	7 (1%)	70	75	28, 40, 56, 90	0
1	C	446/446 (100%)	-0.07	8 (1%)	67	72	29, 43, 61, 92	0
1	D	446/446 (100%)	-0.14	6 (1%)	74	79	27, 42, 59, 85	0
All	All	1784/1784 (100%)	-0.13	31 (1%)	69	73	27, 42, 59, 92	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	VAL	6.8
1	C	49	SER	5.1
1	A	48	VAL	4.4
1	D	117	TRP	4.0
1	A	49	SER	3.8
1	D	470	SER	3.7
1	C	47	PRO	3.3
1	B	48	VAL	3.3
1	A	470	SER	3.3
1	C	470	SER	3.3
1	C	50	GLY	3.1
1	B	61	GLY	3.0
1	B	470	SER	3.0
1	A	373	VAL	2.8
1	D	265	LEU	2.8
1	B	25	GLN	2.7
1	A	46	SER	2.7
1	A	47	PRO	2.7
1	B	51	PRO	2.3
1	D	469	PRO	2.3
1	C	51	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	25	GLN	2.3
1	C	265	LEU	2.3
1	A	237	GLU	2.2
1	A	51	PRO	2.2
1	B	265	LEU	2.1
1	A	50	GLY	2.1
1	C	72	SER	2.1
1	D	206	GLU	2.0
1	B	49	SER	2.0
1	D	71	ASP	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
2	NAG	N	2	14/15	0.56	0.19	72,88,91,94	0
6	MAN	O	3	11/12	0.58	0.20	55,69,73,75	0
3	NAG	F	1	14/15	0.60	0.16	67,72,78,81	0
5	MAN	I	3	11/12	0.65	0.17	64,71,78,78	0
3	NAG	J	1	14/15	0.66	0.16	48,66,73,80	0
4	NAG	Q	2	14/15	0.70	0.19	73,77,79,81	0
2	NAG	N	1	14/15	0.70	0.14	57,65,77,77	0
2	FUC	N	3	10/11	0.70	0.16	65,76,81,86	0
7	MAN	T	3	11/12	0.70	0.17	48,56,60,71	0
4	NAG	H	2	14/15	0.73	0.15	62,73,83,87	0
3	FUC	F	2	10/11	0.74	0.15	63,72,82,85	0
4	NAG	R	2	14/15	0.76	0.14	63,72,77,79	0
2	NAG	E	2	14/15	0.77	0.13	54,66,69,69	0
3	FUC	J	2	10/11	0.79	0.14	67,76,82,85	0
4	NAG	G	2	14/15	0.79	0.14	61,71,78,78	0
4	NAG	K	2	14/15	0.80	0.14	56,64,70,71	0
7	MAN	V	3	11/12	0.80	0.15	38,45,52,55	0
2	FUC	E	3	10/11	0.82	0.14	57,61,71,72	0

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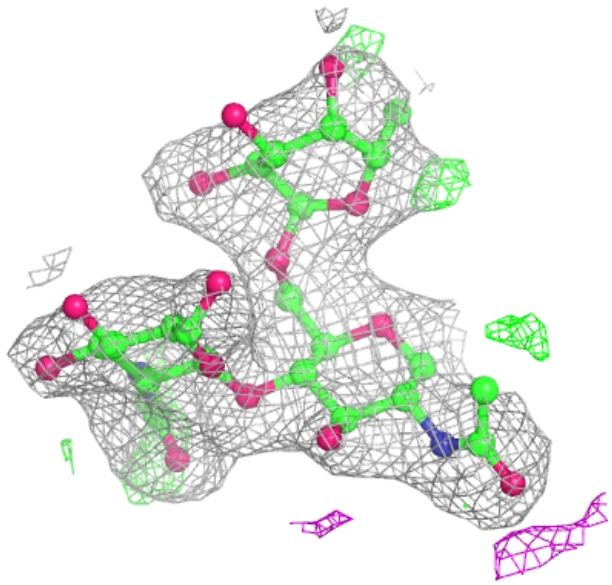
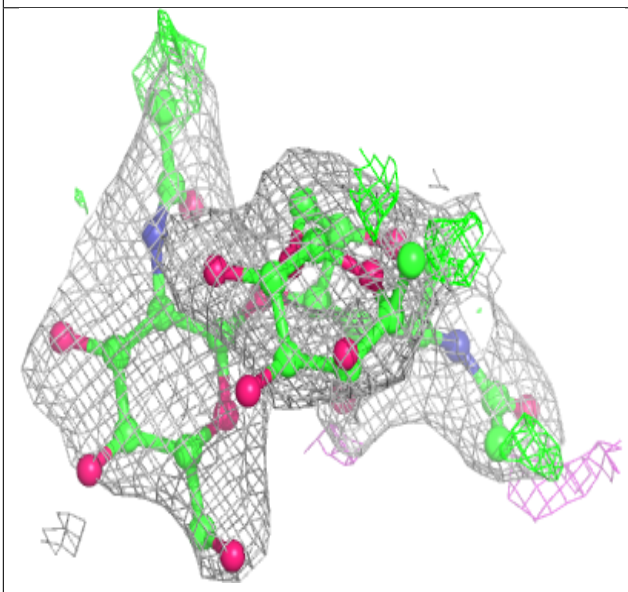
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	W	2	14/15	0.82	0.14	66,69,81,81	0
4	NAG	P	2	14/15	0.83	0.12	60,66,74,77	0
5	MAN	I	4	11/12	0.83	0.14	56,63,67,73	0
6	NAG	O	2	14/15	0.83	0.13	55,59,65,74	0
2	FUC	S	3	10/11	0.83	0.14	56,58,69,75	0
2	NAG	S	2	14/15	0.83	0.12	58,73,79,80	0
7	FUC	T	4	10/11	0.83	0.14	49,56,65,70	0
4	NAG	M	2	14/15	0.83	0.11	54,65,70,74	0
7	FUC	V	4	10/11	0.84	0.15	63,68,72,75	0
4	NAG	Q	1	14/15	0.86	0.12	57,65,71,77	0
5	FUC	I	5	10/11	0.86	0.11	39,46,49,53	0
6	MAN	L	3	11/12	0.86	0.12	45,49,55,61	0
4	NAG	H	1	14/15	0.87	0.10	44,57,64,66	0
6	NAG	O	1	14/15	0.87	0.10	50,55,56,57	0
4	NAG	M	1	14/15	0.88	0.10	47,54,61,63	0
2	NAG	E	1	14/15	0.88	0.11	46,52,61,62	0
4	NAG	U	2	14/15	0.88	0.11	49,55,58,59	0
6	NAG	L	2	14/15	0.90	0.11	41,49,54,55	0
2	NAG	S	1	14/15	0.90	0.10	56,59,67,69	0
4	NAG	W	1	14/15	0.90	0.09	44,52,63,65	0
5	NAG	I	2	14/15	0.91	0.10	47,54,66,67	0
7	NAG	V	2	14/15	0.91	0.12	44,49,55,55	0
7	NAG	T	2	14/15	0.92	0.09	47,50,57,58	0
4	NAG	R	1	14/15	0.92	0.09	47,56,63,63	0
4	NAG	P	1	14/15	0.93	0.08	45,48,52,60	0
4	NAG	U	1	14/15	0.94	0.08	37,42,48,51	0
5	NAG	I	1	14/15	0.94	0.07	33,44,46,50	0
4	NAG	K	1	14/15	0.94	0.08	44,49,54,57	0
7	NAG	T	1	14/15	0.94	0.08	34,43,49,52	0
4	NAG	G	1	14/15	0.94	0.09	40,47,53,60	0
7	NAG	V	1	14/15	0.95	0.08	43,48,53,59	0
6	NAG	L	1	14/15	0.95	0.07	39,44,49,49	0

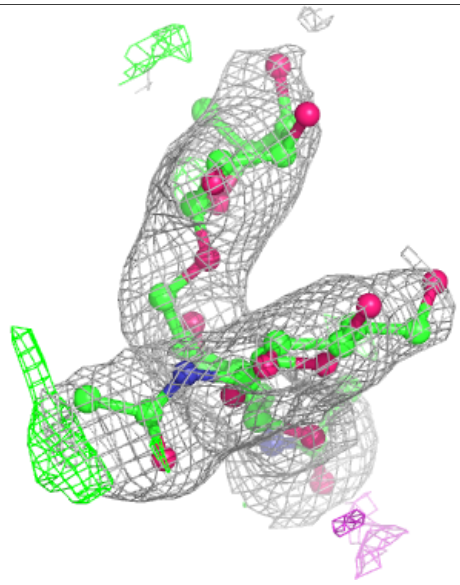
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

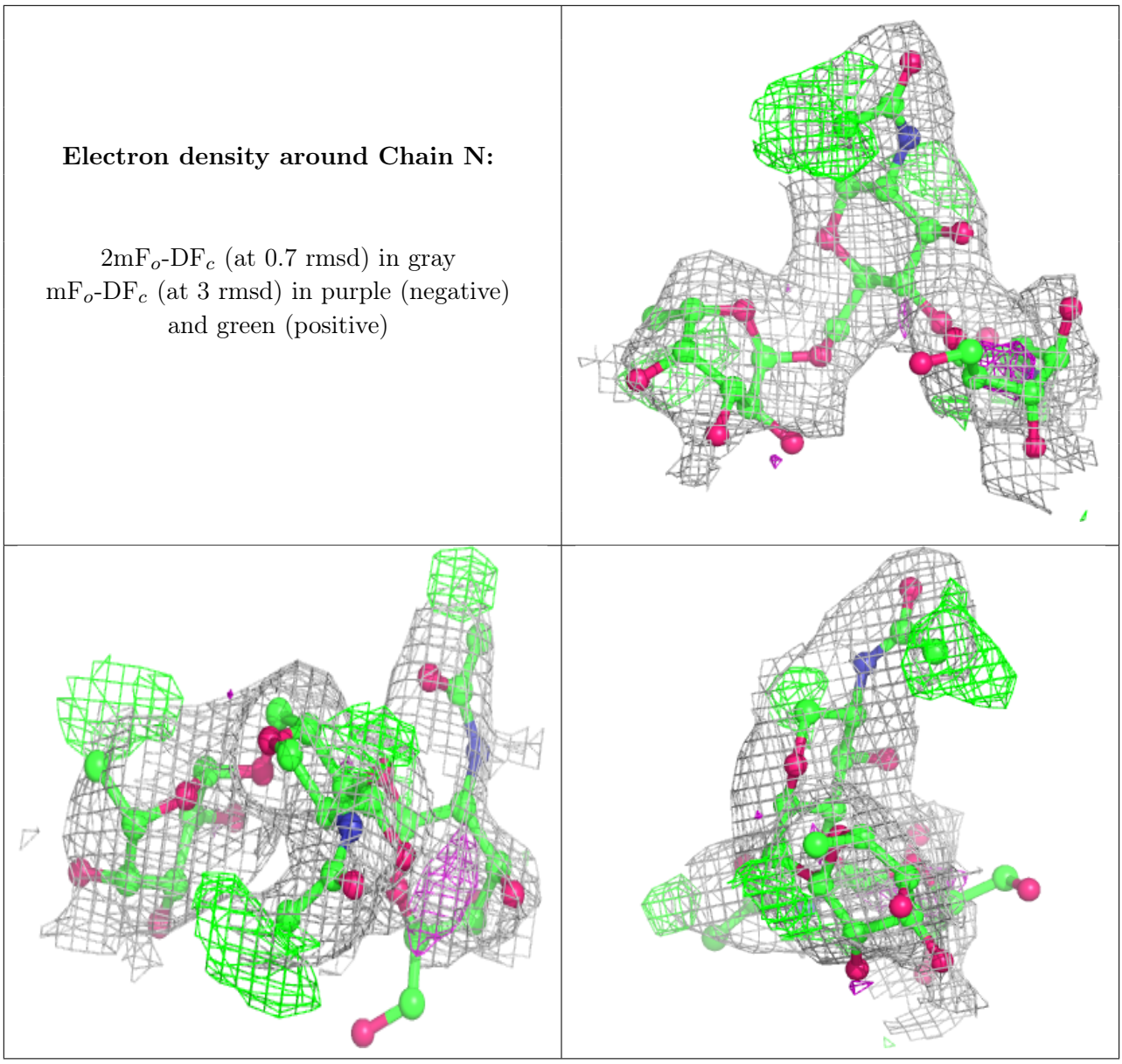






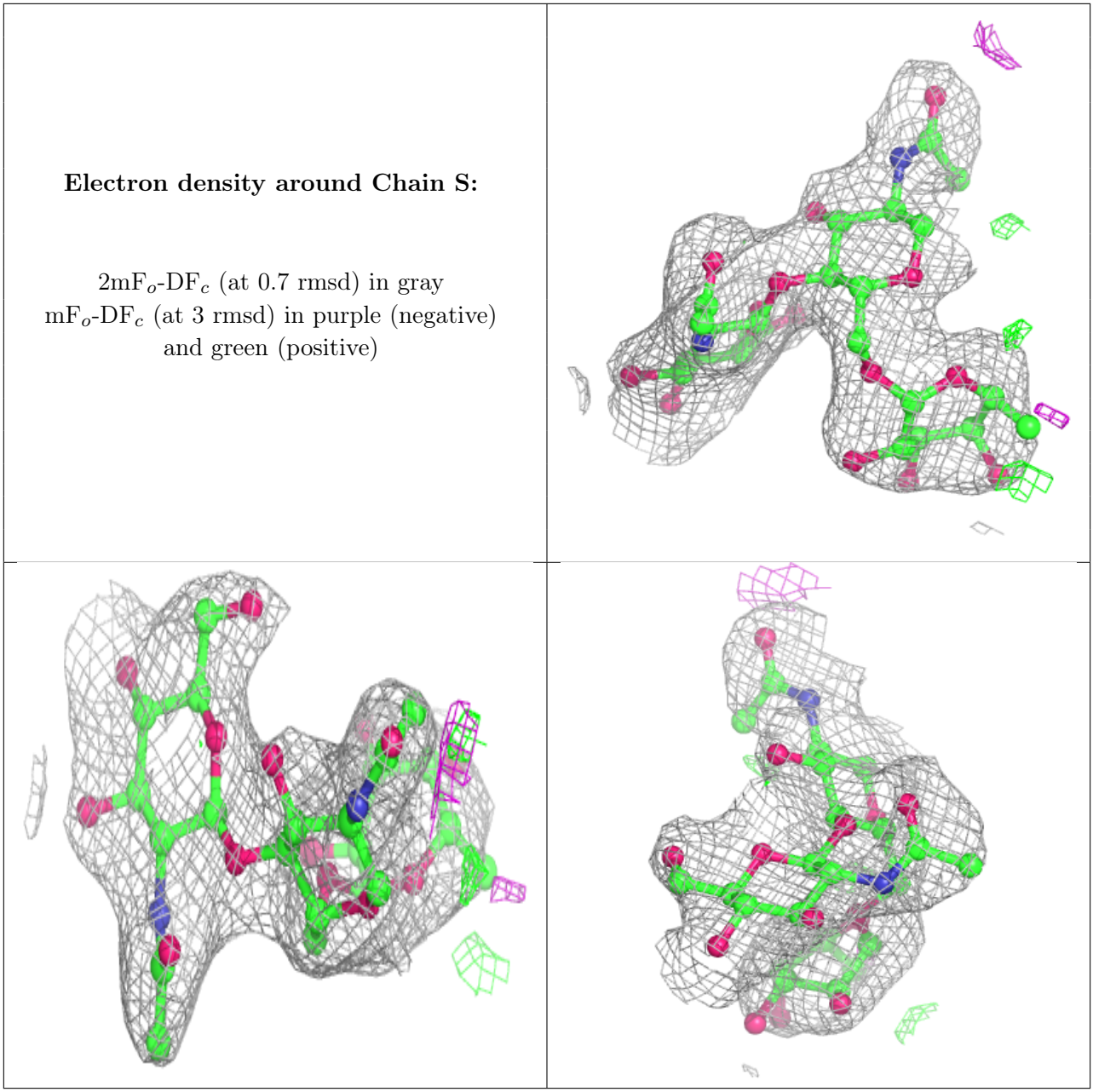
Electron density around Chain N:

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



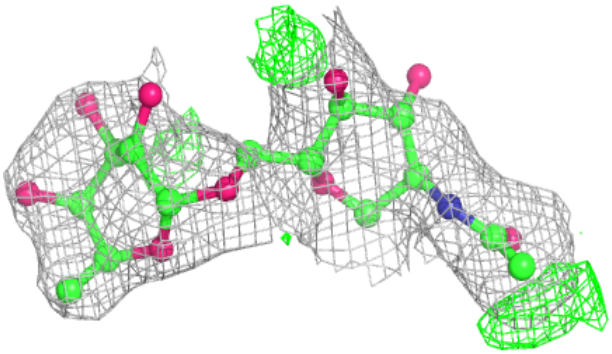
Electron density around Chain S:

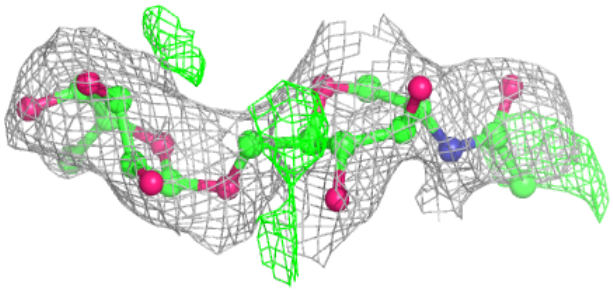
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

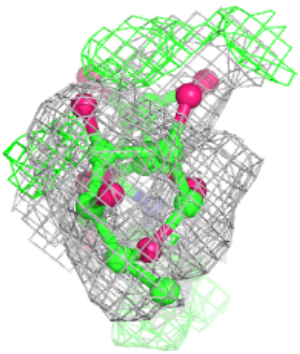


Electron density around Chain F:

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

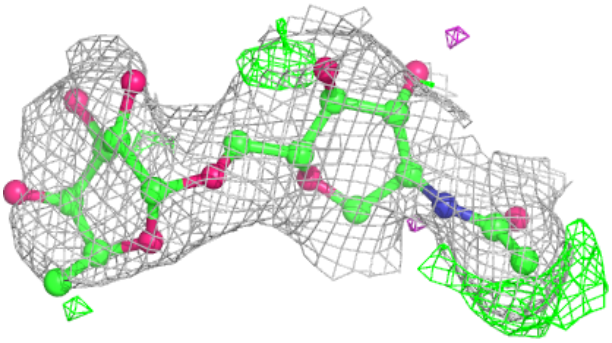


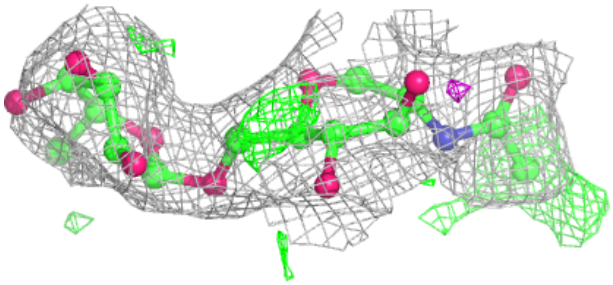


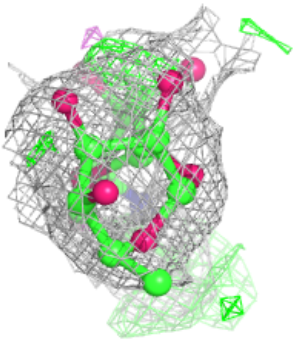


Electron density around Chain J:

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

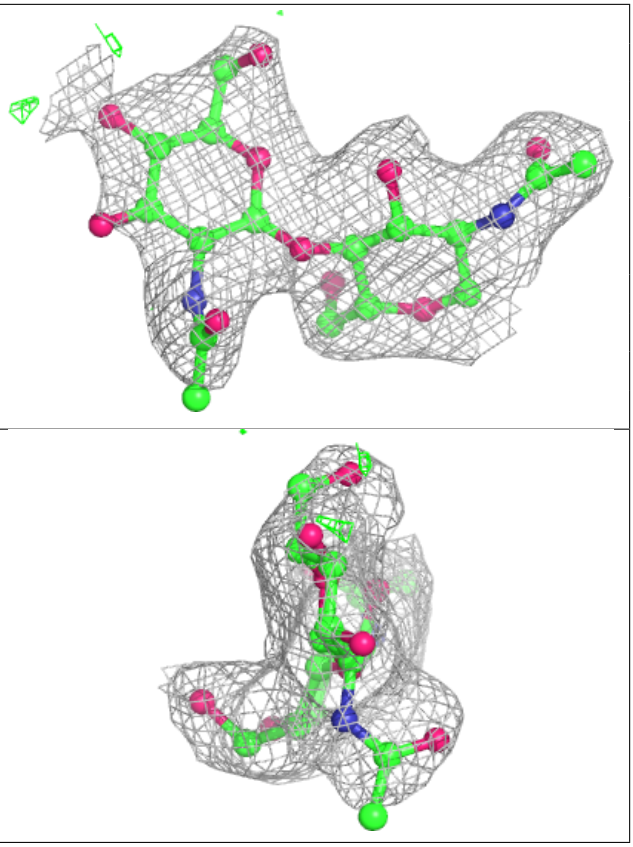


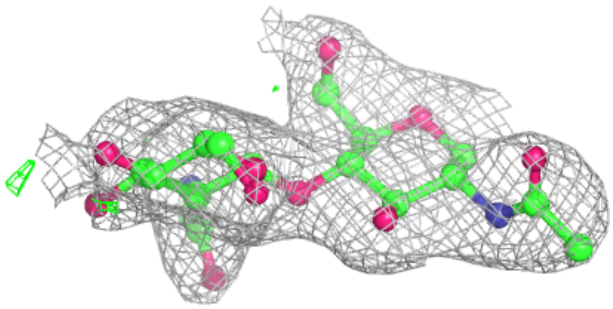




Electron density around Chain G:

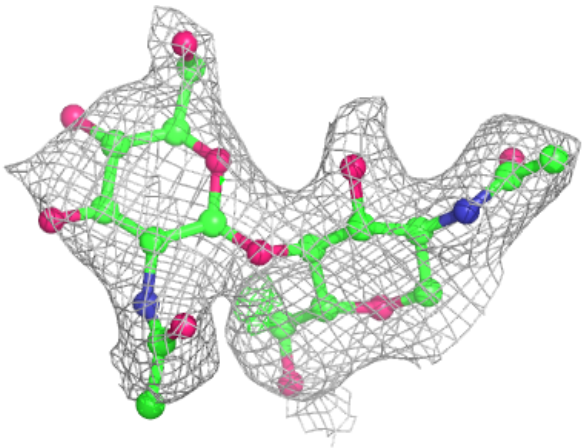
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

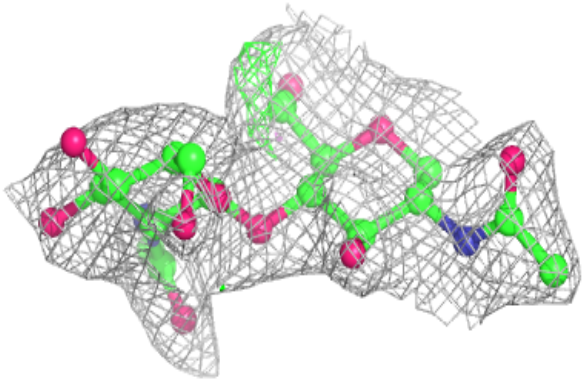


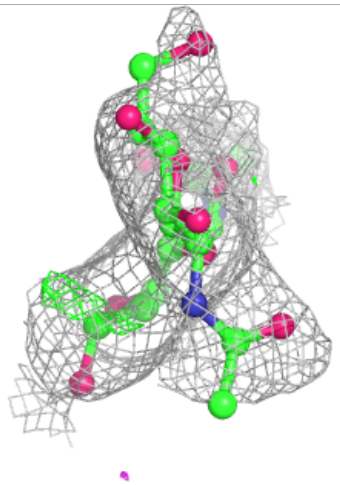


Electron density around Chain H:

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

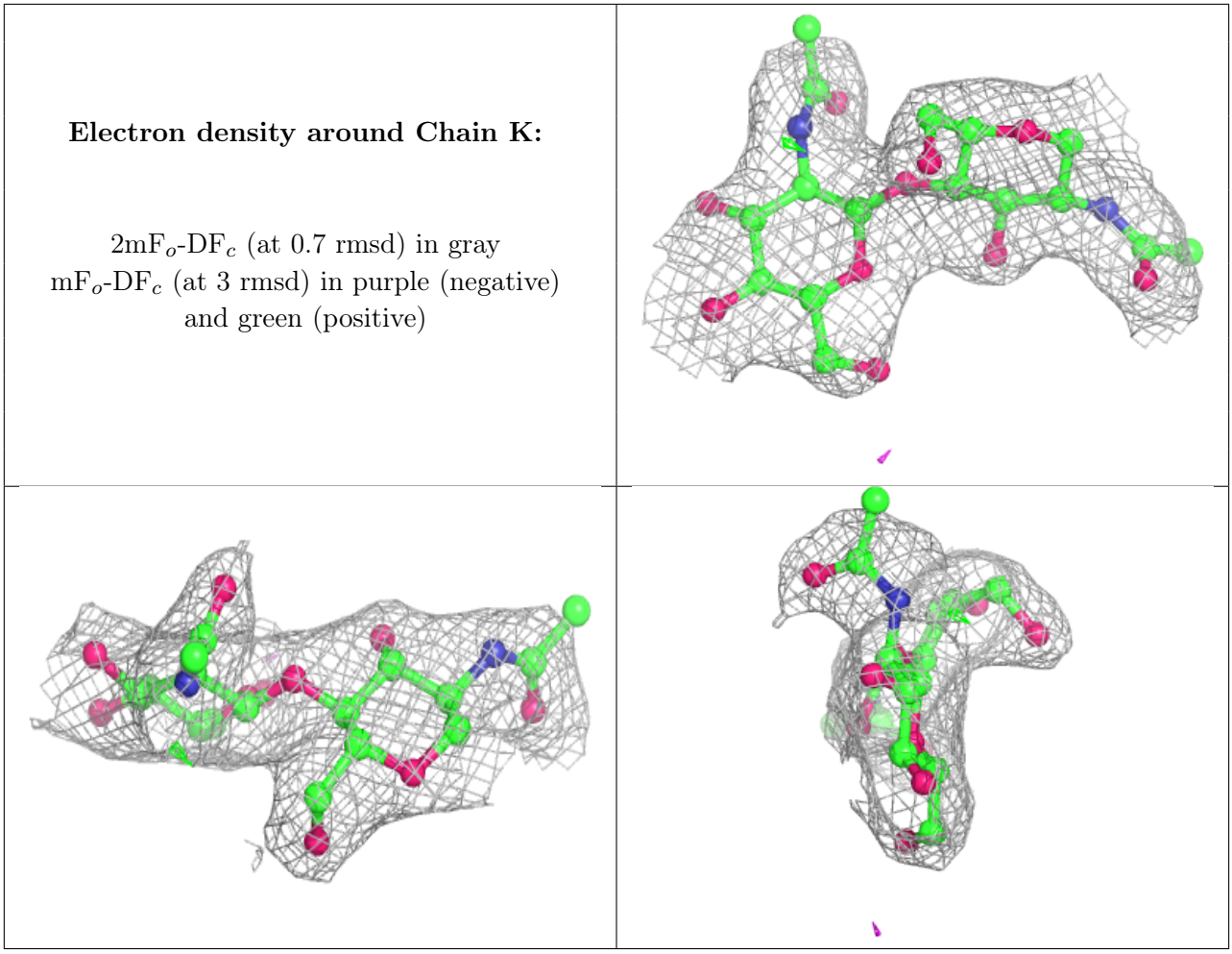






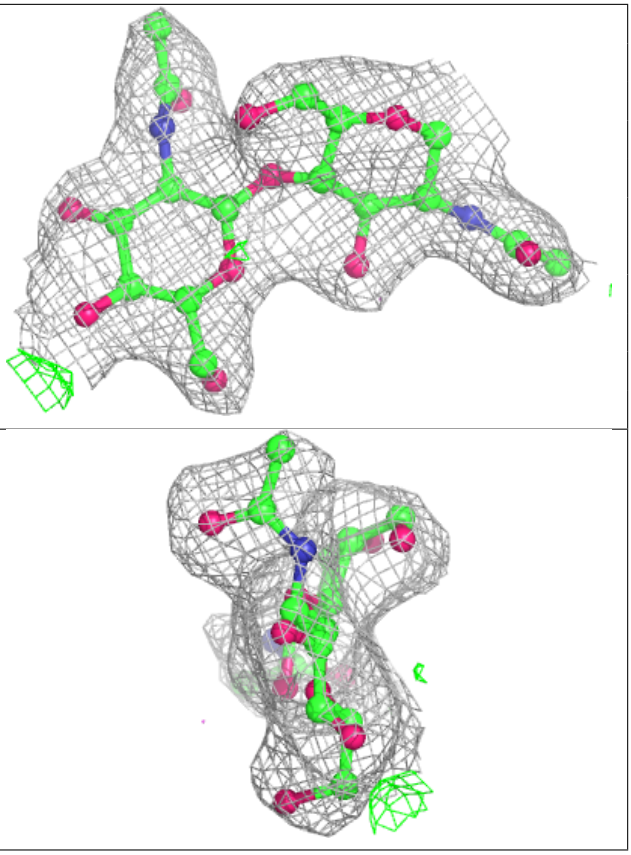
Electron density around Chain K:

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



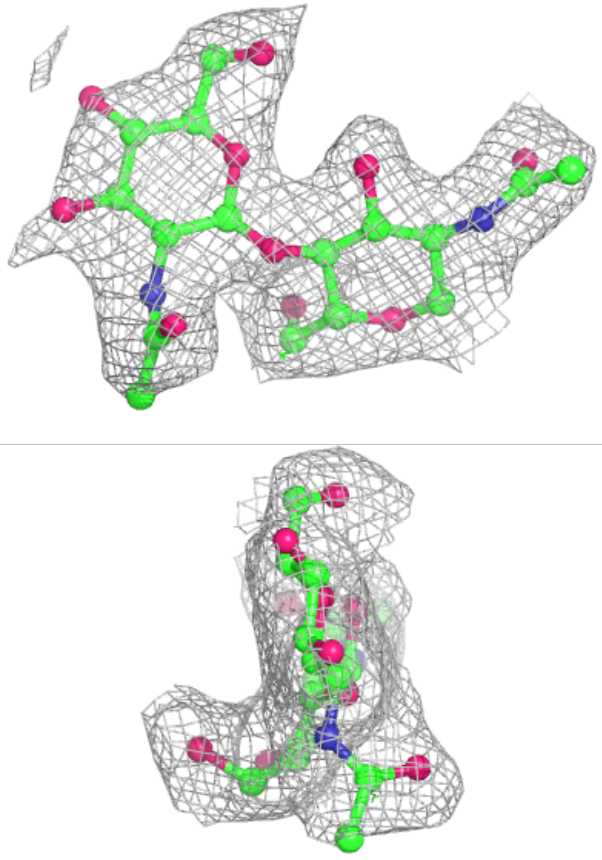
Electron density around Chain M:

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



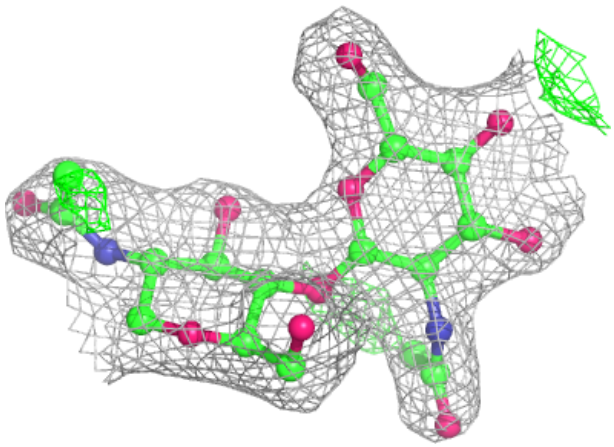
Electron density around Chain P:

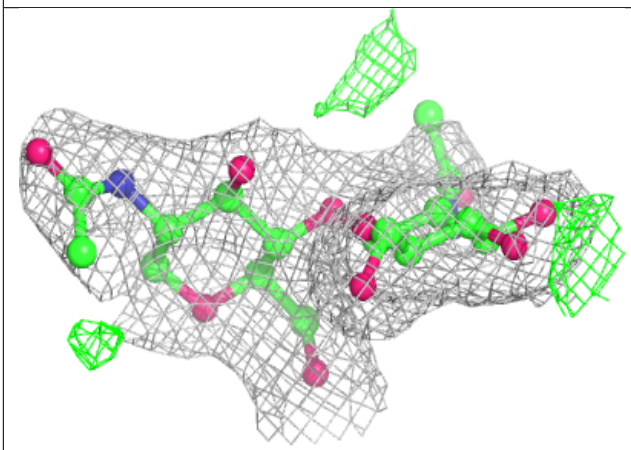
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

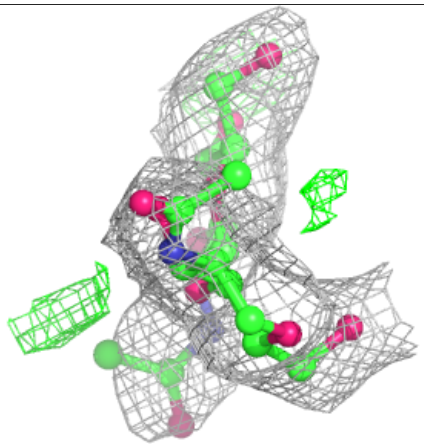


Electron density around Chain Q:

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

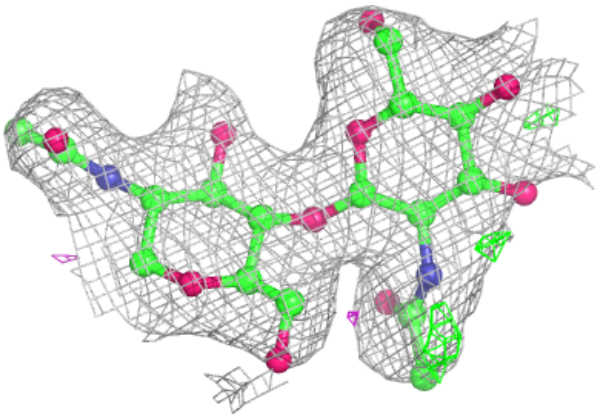


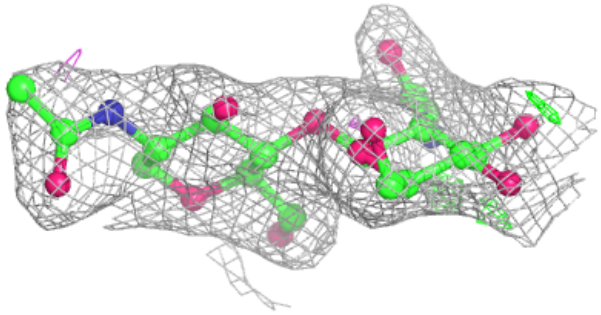


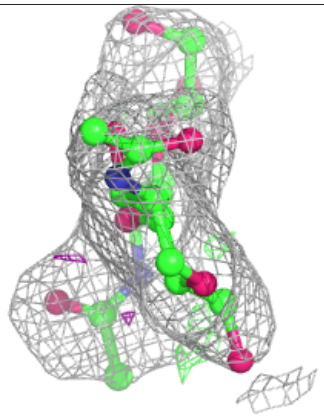


Electron density around Chain R:

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

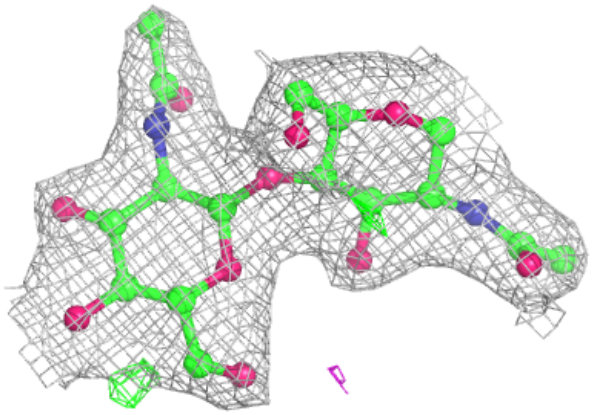


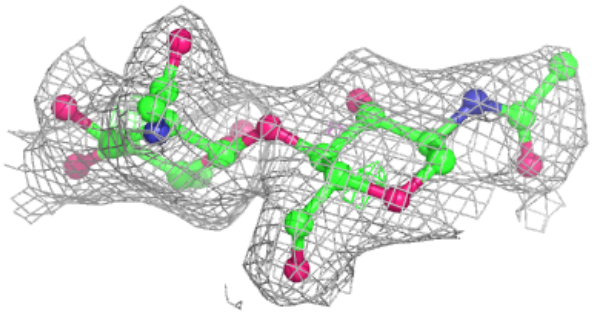


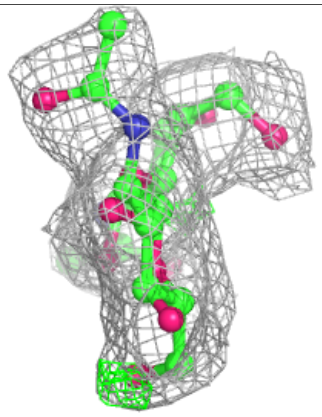


Electron density around Chain U:

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

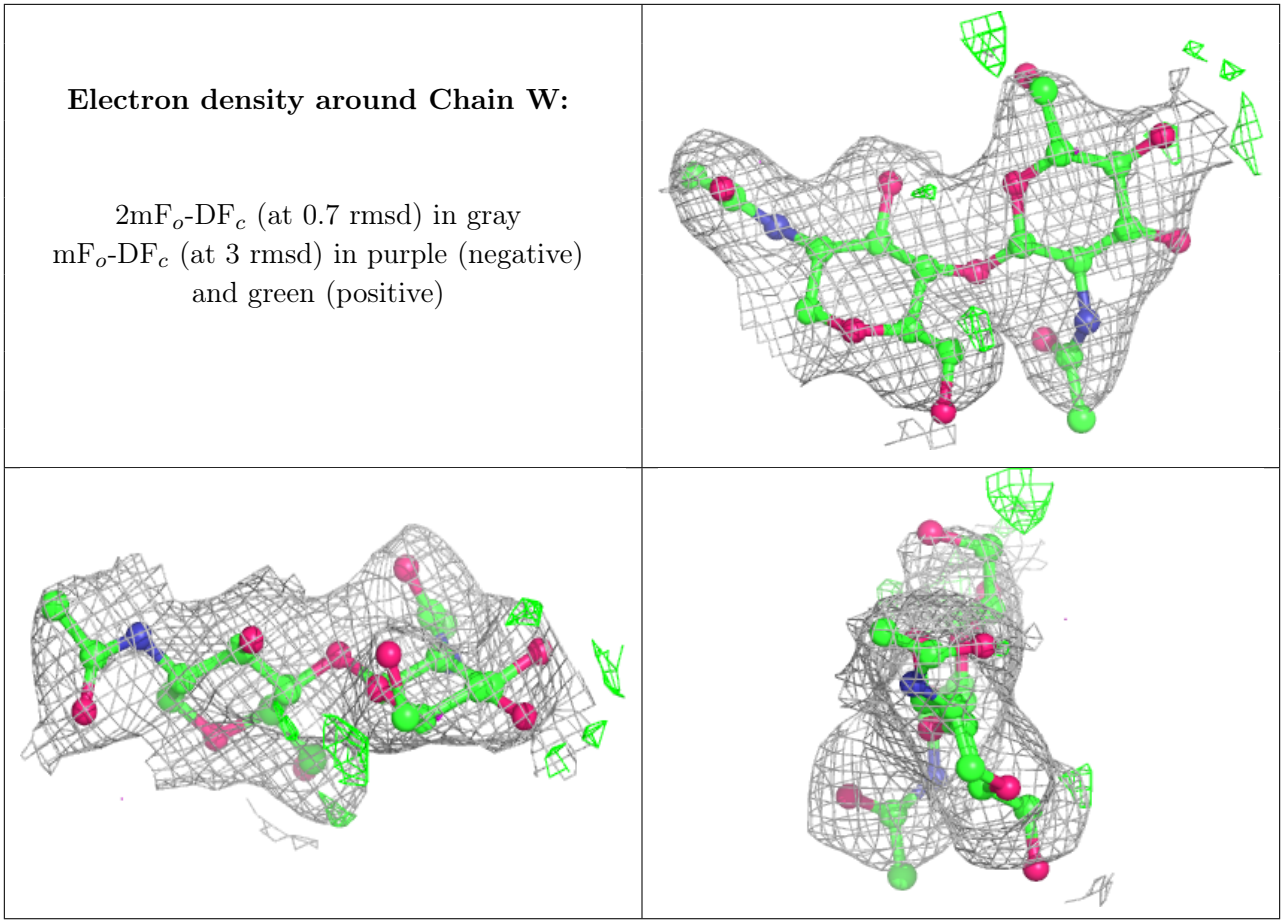






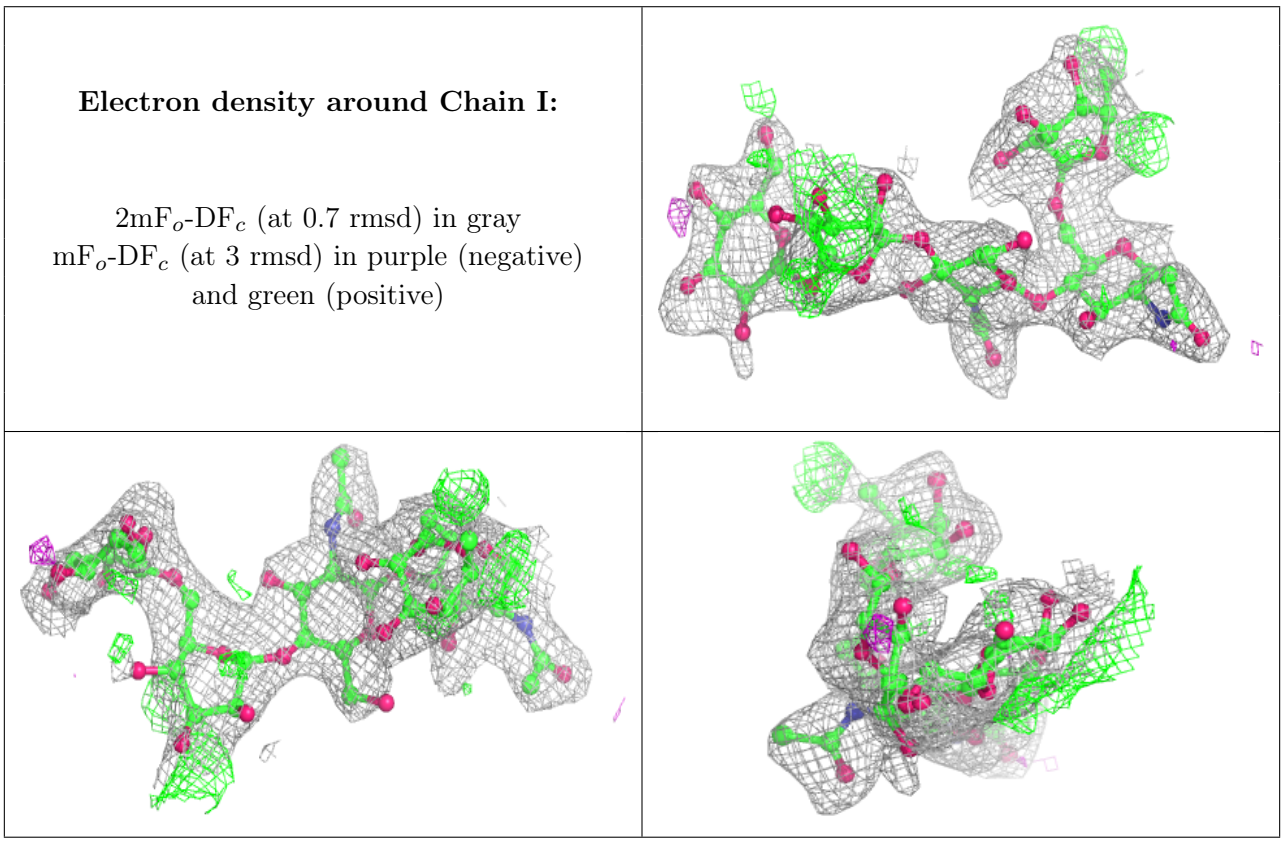
Electron density around Chain W:

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



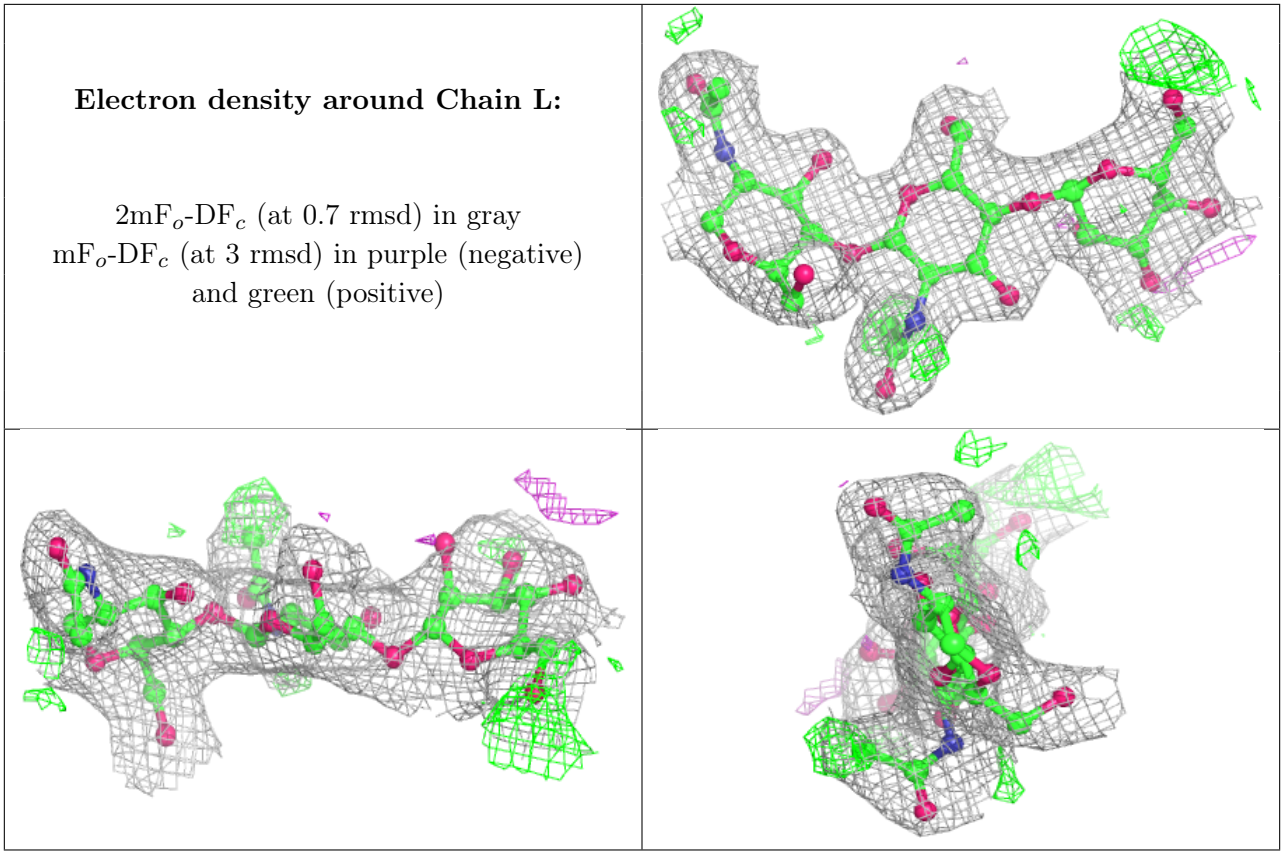
Electron density around Chain I:

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



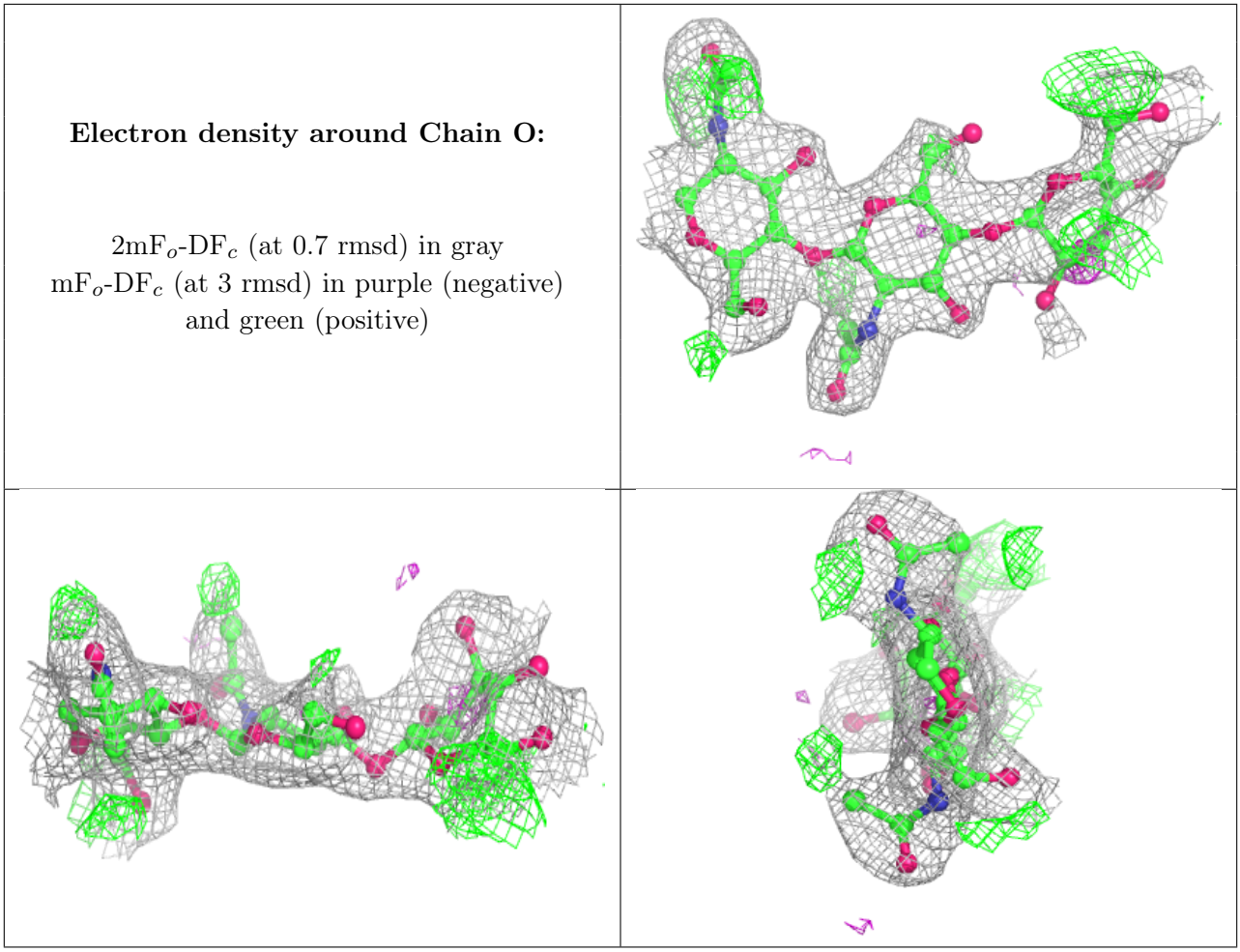
Electron density around Chain L:

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



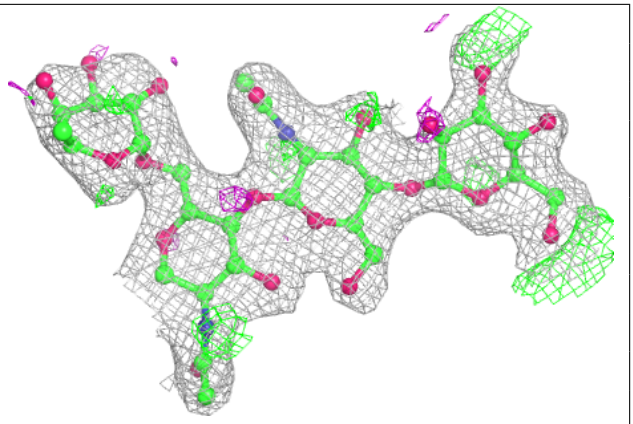
Electron density around Chain O:

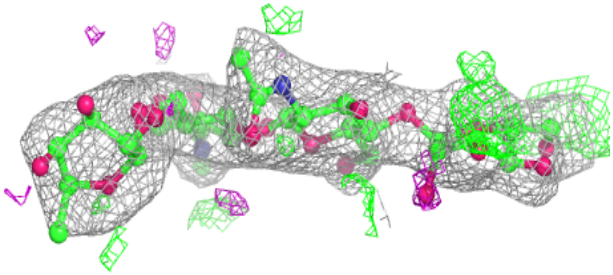
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

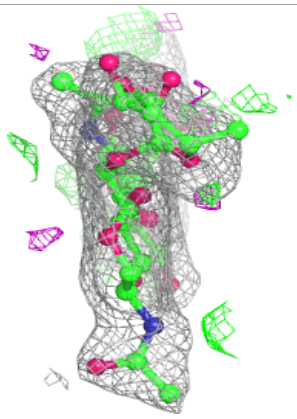


Electron density around Chain T:

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

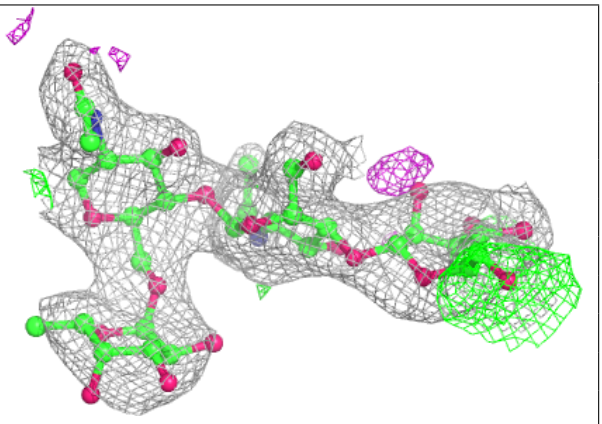


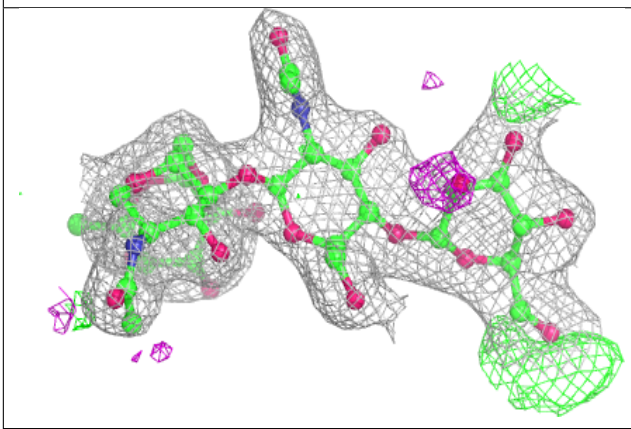


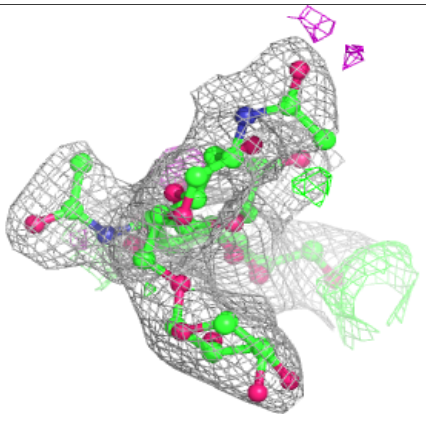


Electron density around Chain V:

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







6.4 Ligands (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
8	NAG	C	507	14/15	0.71	0.17	58,69,75,76	0
10	0TR	C	516	9/9	0.79	0.18	52,52,53,54	0
10	0TR	A	513	9/9	0.82	0.17	52,52,53,54	0
8	NAG	A	508	14/15	0.84	0.12	57,61,69,71	0
10	0TR	B	517	9/9	0.85	0.16	52,52,52,52	0
10	0TR	D	518	9/9	0.89	0.16	52,52,52,52	9
9	ZN	C	514	1/1	0.98	0.04	47,47,47,47	0
9	ZN	D	516	1/1	0.98	0.04	41,41,41,41	0
9	ZN	A	512	1/1	0.98	0.04	47,47,47,47	0
9	ZN	B	515	1/1	0.99	0.03	40,40,40,40	0
9	ZN	D	517	1/1	0.99	0.04	31,31,31,31	0
9	ZN	C	515	1/1	0.99	0.03	34,34,34,34	0
9	ZN	A	511	1/1	1.00	0.03	33,33,33,33	0
9	ZN	B	516	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.