Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:16 AM JST

PDB ID	:	7EY2
Title	:	Bifunctional xylosidase/glucosidase LXYL D300N mutant with intermediate substrate xylose
Authors	:	Gong, W.M.; Yang, L.Y.
Deposited on	:	2021-05-29
Resolution	:	2.43 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:

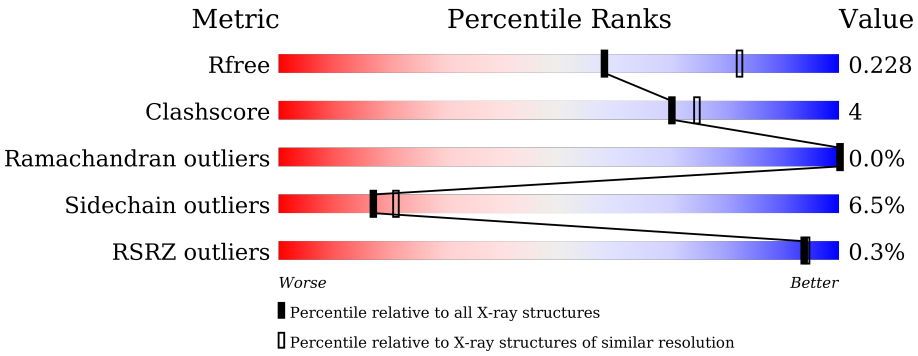
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	805	83% 9% • 6%
1	B	805	84% 9% • 6%
1	C	805	83% 9% • 6%
1	D	805	82% 10% • 6%
1	E	805	83% 10% • 6%
1	F	805	84% 9% • 6%

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Mol	Chain	Length	Quality of chain
2	G	3	100%
2	J	3	33% 67%
2	M	3	33% 67%
2	P	3	33% 67%
2	S	3	33% 67%
2	V	3	33% 67%
3	H	7	71% 29%
3	N	7	71% 29%
3	T	7	71% 29%
3	W	7	71% 29%
4	I	5	100%
4	R	5	100%
5	K	8	50% 50%
6	L	6	100%
6	O	6	100%
6	U	6	100%
6	X	6	100%
7	Q	6	83% 17%

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
11	XYL	C	907	-	X	-	-
5	MAN	K	6	-	-	X	-
5	MAN	K	8	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 37142 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 Beta-D-xylosidase/beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	1	0
			5724	3624	958	1125	17			
1	B	758	Total	C	N	O	S	0	1	0
			5736	3632	963	1124	17			
1	C	756	Total	C	N	O	S	0	1	0
			5712	3618	956	1121	17			
1	D	756	Total	C	N	O	S	0	1	0
			5712	3618	956	1121	17			
1	E	757	Total	C	N	O	S	0	1	0
			5726	3626	960	1123	17			
1	F	757	Total	C	N	O	S	0	1	0
			5726	3626	960	1123	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ASN	ASP	engineered mutation	UNP G8GLP2
A	804	HIS	-	expression tag	UNP G8GLP2
A	805	HIS	-	expression tag	UNP G8GLP2
B	300	ASN	ASP	engineered mutation	UNP G8GLP2
B	804	HIS	-	expression tag	UNP G8GLP2
B	805	HIS	-	expression tag	UNP G8GLP2
C	300	ASN	ASP	engineered mutation	UNP G8GLP2
C	804	HIS	-	expression tag	UNP G8GLP2
C	805	HIS	-	expression tag	UNP G8GLP2
D	300	ASN	ASP	engineered mutation	UNP G8GLP2
D	804	HIS	-	expression tag	UNP G8GLP2
D	805	HIS	-	expression tag	UNP G8GLP2
E	300	ASN	ASP	engineered mutation	UNP G8GLP2
E	804	HIS	-	expression tag	UNP G8GLP2
E	805	HIS	-	expression tag	UNP G8GLP2
F	300	ASN	ASP	engineered mutation	UNP G8GLP2
F	804	HIS	-	expression tag	UNP G8GLP2

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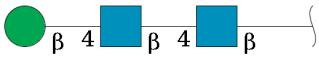
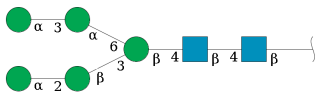
Chain	Residue	Modelled	Actual	Comment	Reference
F	805	HIS	-	expression tag	UNP G8GLP2

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



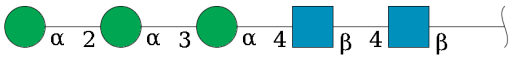
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	3	Total C N O 39 22 2 15	0	0	0
2	J	3	Total C N O 39 22 2 15	0	0	0
2	M	3	Total C N O 39 22 2 15	0	0	0
2	P	3	Total C N O 39 22 2 15	0	0	0
2	S	3	Total C N O 39 22 2 15	0	0	0
2	V	3	Total C N O 39 22 2 15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



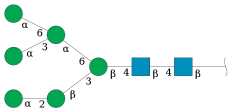
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	H	7	Total C N O 83 46 2 35	0	0	0
3	N	7	Total C N O 83 46 2 35	0	0	0
3	T	7	Total C N O 83 46 2 35	0	0	0
3	W	7	Total C N O 83 46 2 35	0	0	0

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



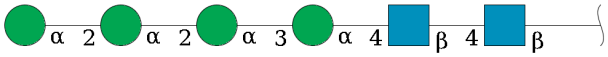
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



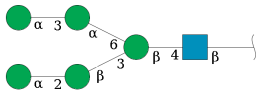
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



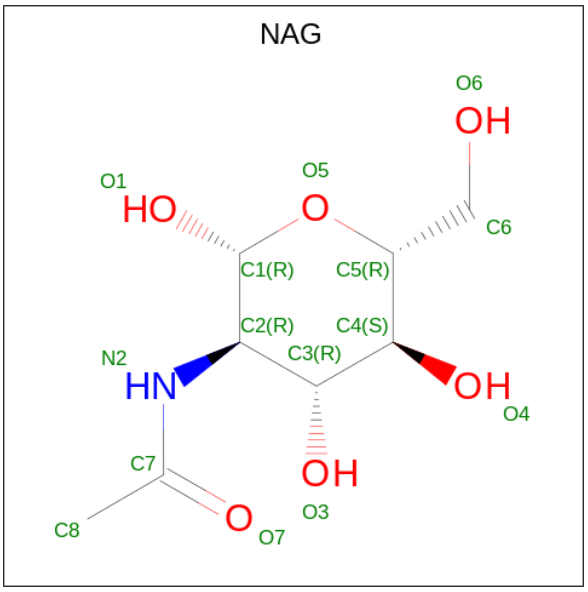
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	O	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	U	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	X	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Q	6	Total	C	N	O	0	0	0
			70	38	1	31			

- 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	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			13	8	1	4		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

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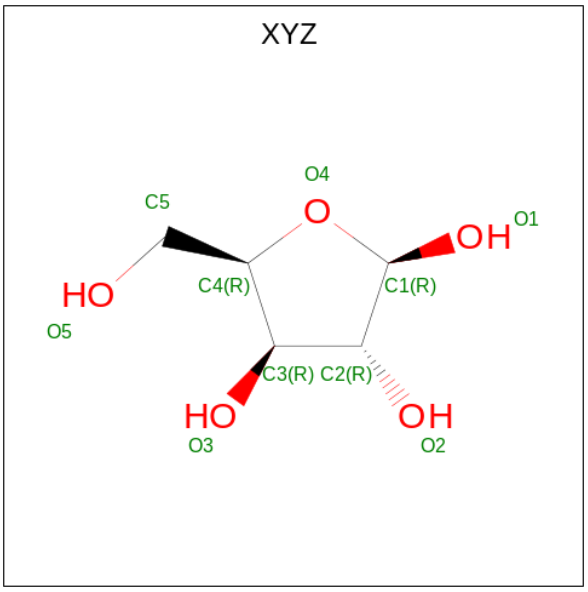
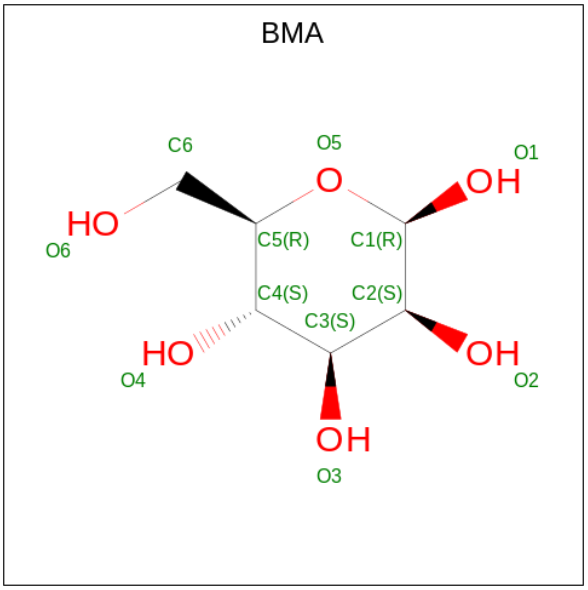
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			13	8	1	4		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			13	8	1	4		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			13	8	1	4		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is beta-D-xylofuranose (three-letter code: XYZ) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 10 5 5	0	0
9	B	1	Total C O 10 5 5	0	0

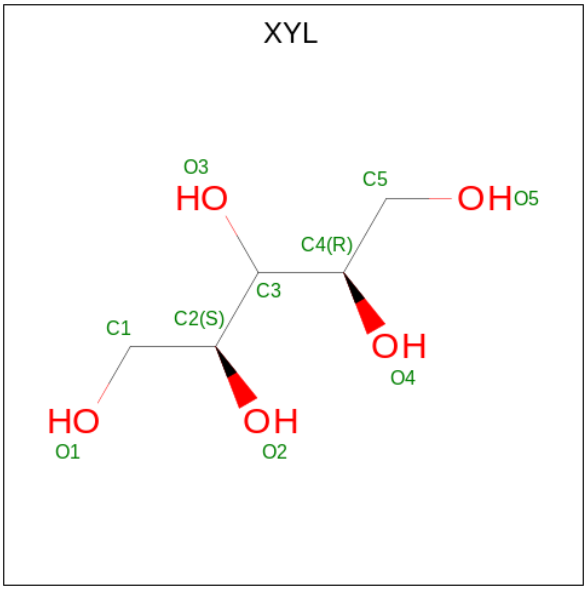
- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 11 6 5	0	0

- Molecule 11 is Xylitol (three-letter code: XYL) (formula: $C_5H_{12}O_5$) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 10 5 5	0	0
11	D	1	Total C O 10 5 5	0	0
11	E	1	Total C O 10 5 5	0	0

- Molecule 12 is water.

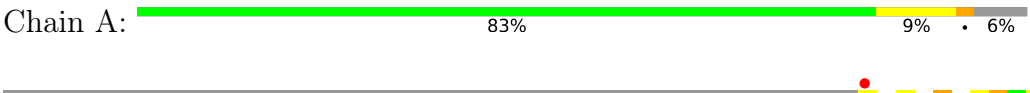
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	239	Total O 239 239	0	0
12	B	304	Total O 304 304	0	0
12	C	177	Total O 177 177	0	0
12	D	177	Total O 177 177	0	0
12	E	204	Total O 204 204	0	0
12	F	200	Total O 200 200	0	0

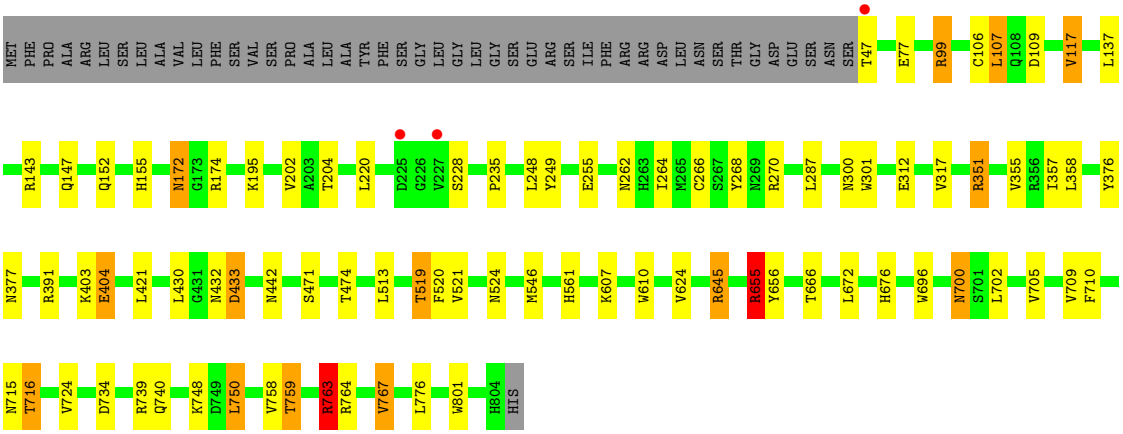
3 Residue-property plots (i)

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: Beta-D-xylosidase/beta-D-glucosidase

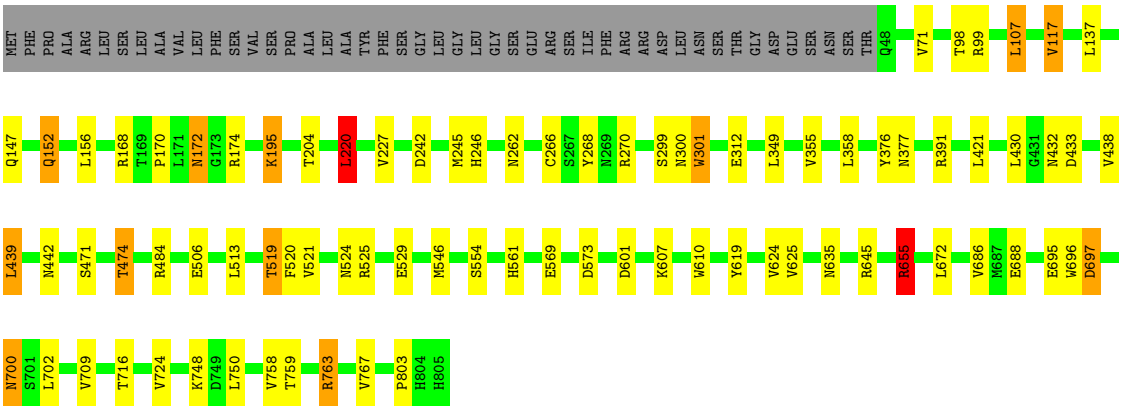
Chain A:





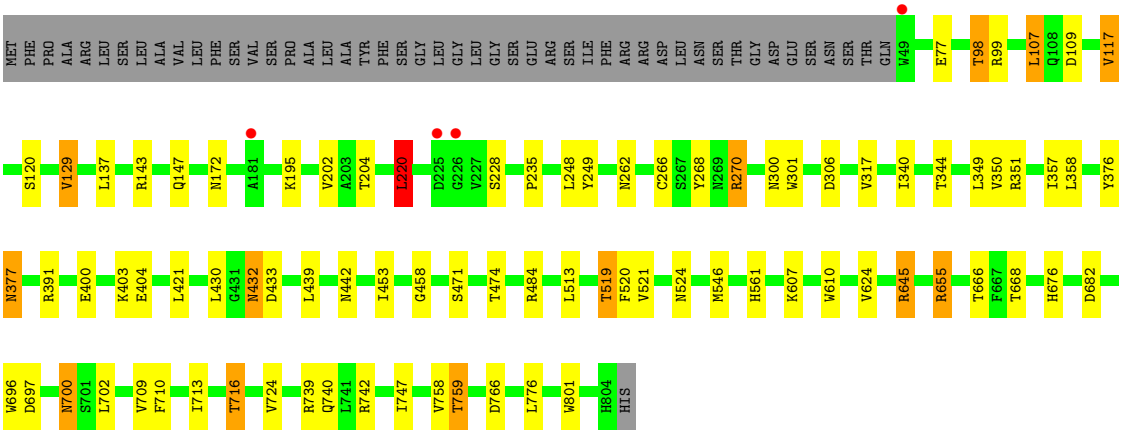
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain B:



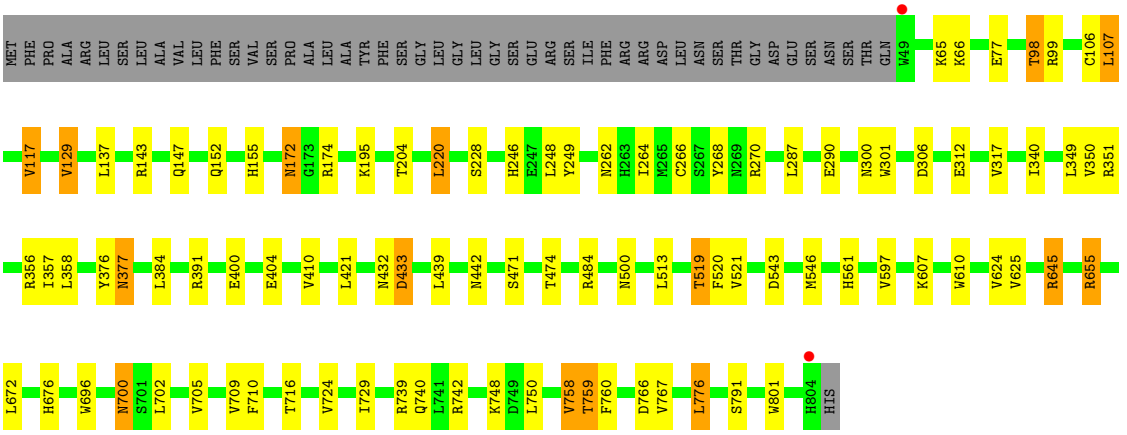
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain C:



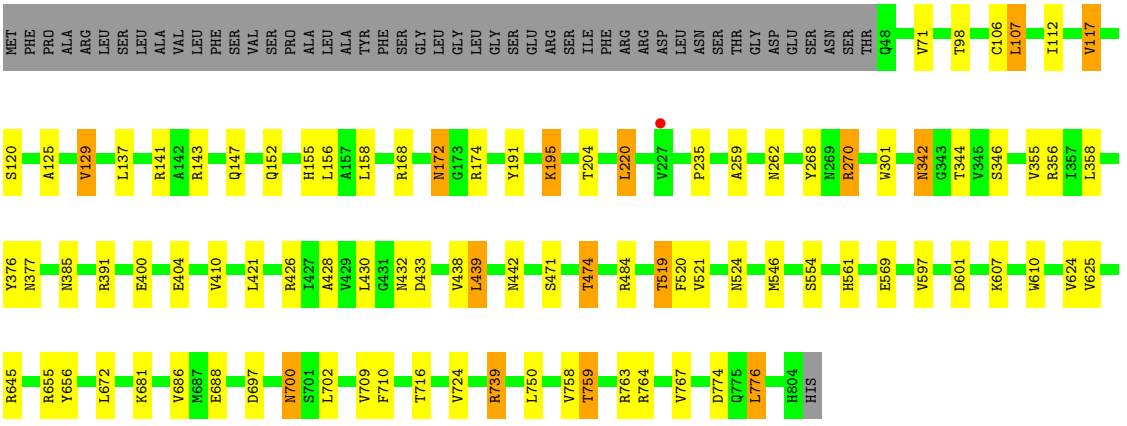
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain D:



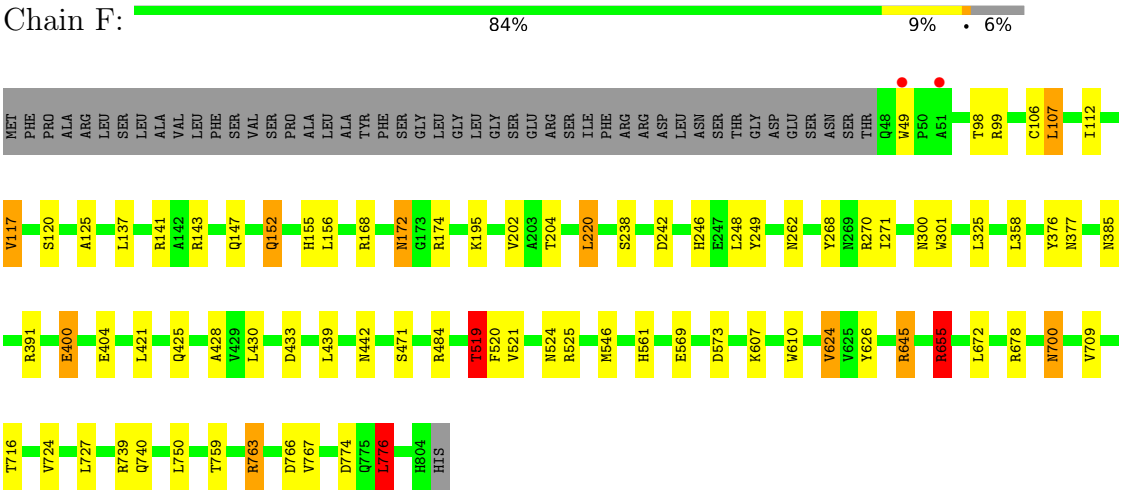
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain E:



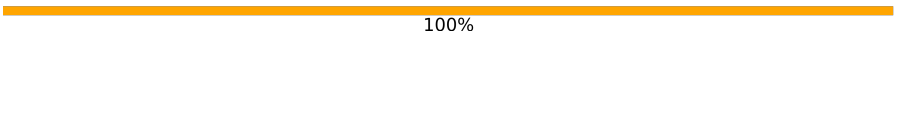
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain F:



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

Chain G:



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

Chain J:

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

Chain M:

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

Chain P:

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

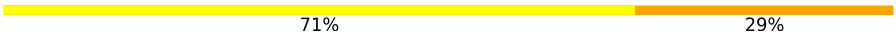
Chain S:

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

Chain V:

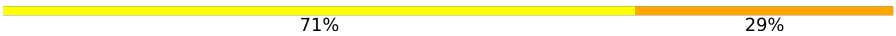
• Molecule 3: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



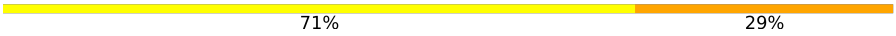
• Molecule 3: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



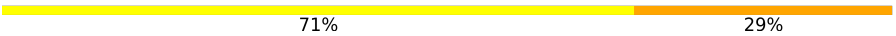
• Molecule 3: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



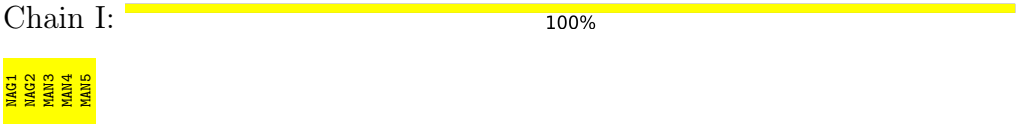
• Molecule 3: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



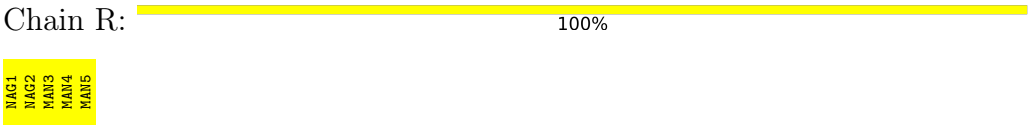
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain R:

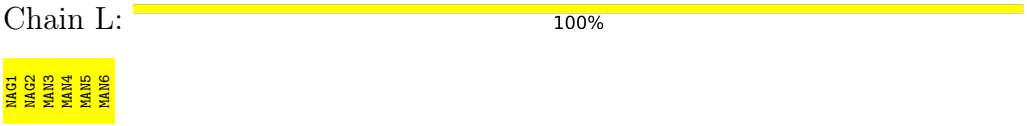


• Molecule 5: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

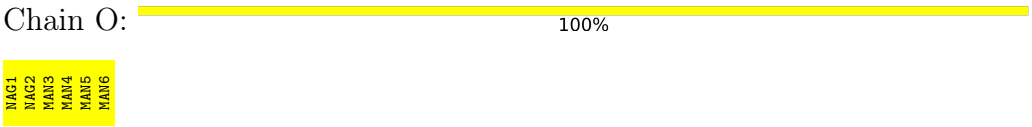
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



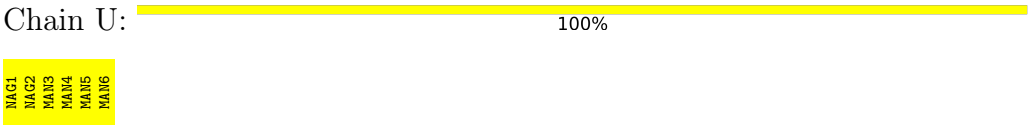
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



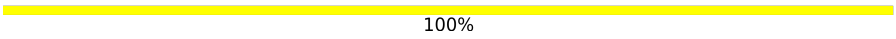
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



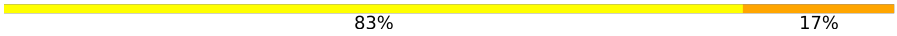
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 7: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	149.15Å 258.23Å 320.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	160.12 – 2.43 49.33 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (160.12-2.43) 98.9 (49.33-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.04 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.175 , 0.226 0.181 , 0.228	Depositor DCC
R_{free} test set	11385 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 4.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.456 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	37142	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: MAN, XYL, NAG, XYZ, BMA

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	0.83	1/5868 (0.0%)	0.93	15/8030 (0.2%)
1	B	0.86	3/5882 (0.1%)	0.94	19/8047 (0.2%)
1	C	0.84	2/5856 (0.0%)	0.92	16/8012 (0.2%)
1	D	0.86	1/5856 (0.0%)	0.93	21/8012 (0.3%)
1	E	0.87	1/5871 (0.0%)	0.95	18/8032 (0.2%)
1	F	0.89	2/5871 (0.0%)	0.95	17/8032 (0.2%)
All	All	0.86	10/35204 (0.0%)	0.94	106/48165 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	400	GLU	CG-CD	5.68	1.60	1.51
1	F	519	THR	CB-CG2	-5.33	1.34	1.52
1	F	400	GLU	CD-OE1	5.27	1.31	1.25
1	C	400	GLU	CD-OE1	5.21	1.31	1.25
1	B	695	GLU	CG-CD	5.19	1.59	1.51
1	A	404	GLU	CG-CD	5.12	1.59	1.51
1	B	301	TRP	CB-CG	5.11	1.59	1.50
1	E	400	GLU	CG-CD	5.08	1.59	1.51
1	B	635	ASN	CG-ND2	5.06	1.45	1.32
1	C	400	GLU	CG-CD	5.02	1.59	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	655	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	C	391	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	99	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	D	655	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	B	763	ARG	NE-CZ-NH1	9.20	124.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	270	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	F	484	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	E	391	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	A	391	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	655	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	C	391	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	A	391	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	D	107	LEU	CA-CB-CG	8.40	134.63	115.30
1	D	99	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	E	391	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	D	391	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	270	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	E	763	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	F	655	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	E	270	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	E	168	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	F	525	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	484	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	107	LEU	CA-CB-CG	7.72	133.05	115.30
1	F	270	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	351	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	66	LYS	CD-CE-NZ	7.60	129.19	111.70
1	D	270	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	356	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	F	270	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	655	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	C	270	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	764	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	C	655	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	391	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	F	484	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	109	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	391	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	D	391	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	107	LEU	CA-CB-CG	7.25	131.97	115.30
1	E	270	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	763	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	B	168	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	D	220	LEU	CA-CB-CG	6.89	131.16	115.30
1	F	763	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	763	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	B	484	ARG	NE-CZ-NH1	6.83	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	484	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	99	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	764	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	99	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	99	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	655	ARG	CG-CD-NE	-6.35	98.47	111.80
1	A	763	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	99	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	433	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	351	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	655	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	F	391	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	F	168	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	E	141	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	601	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	99	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	E	601	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	143	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	D	143	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	270	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	697	ASP	CB-CG-OD1	5.84	123.56	118.30
1	F	655	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	655	ARG	CG-CD-NE	-5.78	99.66	111.80
1	E	426	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	484	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	342	ASN	CB-CA-C	5.69	121.78	110.40
1	C	129	VAL	CB-CA-C	-5.67	100.62	111.40
1	D	655	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	739	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	655	ARG	CG-CD-NE	-5.62	99.99	111.80
1	A	433	ASP	CB-CG-OD1	5.58	123.32	118.30
1	F	655	ARG	CG-CD-NE	-5.57	100.10	111.80
1	D	270	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	764	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	776	LEU	CA-CB-CG	5.54	128.05	115.30
1	E	129	VAL	CB-CA-C	-5.53	100.89	111.40
1	B	525	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	220	LEU	CA-CB-CG	5.51	127.97	115.30
1	F	678	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	C	484	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	143	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	220	LEU	CA-CB-CG	5.42	127.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	543	ASP	CB-CG-OD1	5.39	123.15	118.30
1	F	776	LEU	CA-CB-CG	5.39	127.69	115.30
1	F	143	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	E	356	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	351	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	682	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	E	484	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	F	141	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	F	99	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	391	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	767	VAL	CB-CA-C	5.12	121.12	111.40
1	D	351	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	697	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	129	VAL	CB-CA-C	-5.08	101.75	111.40
1	B	245	MET	CG-SD-CE	5.07	108.31	100.20
1	D	433	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	E	141	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5724	0	5509	35	0
1	B	5736	0	5525	32	0
1	C	5712	0	5505	37	0
1	D	5712	0	5505	35	0
1	E	5726	0	5519	33	0
1	F	5726	0	5518	33	0
2	G	39	0	34	4	0
2	J	39	0	34	2	0
2	M	39	0	34	4	0
2	P	39	0	34	5	0
2	S	39	0	34	2	0
2	V	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	83	0	70	3	0
3	N	83	0	70	4	0
3	T	83	0	70	4	0
3	W	83	0	70	3	0
4	I	61	0	52	0	0
4	R	61	0	52	0	0
5	K	94	0	77	12	0
6	L	72	0	61	0	0
6	O	72	0	61	0	0
6	U	72	0	61	0	0
6	X	72	0	61	0	0
7	Q	70	0	60	3	0
8	A	55	0	50	0	0
8	B	42	0	38	2	0
8	C	55	0	50	0	0
8	D	68	0	61	3	0
8	E	42	0	39	2	0
8	F	42	0	38	0	0
9	A	10	0	7	1	0
9	B	10	0	7	1	0
10	A	11	0	10	0	0
11	C	10	0	12	2	0
11	D	10	0	12	0	0
11	E	10	0	12	1	0
12	A	239	0	0	3	0
12	B	304	0	0	3	0
12	C	177	0	0	3	0
12	D	177	0	0	2	0
12	E	204	0	0	5	0
12	F	200	0	0	3	0
All	All	37142	0	34386	253	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 4.

All (253) 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)
5:K:8:MAN:O6	5:K:8:MAN:C6	1.66	1.40
5:K:6:MAN:C5	5:K:8:MAN:O6	1.68	1.36
3:W:1:NAG:O4	3:W:1:NAG:C4	1.73	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1:NAG:C4	2:M:1:NAG:O4	1.73	1.36
5:K:1:NAG:O4	5:K:1:NAG:C4	1.77	1.33
2:G:1:NAG:O4	2:G:1:NAG:C4	1.76	1.33
2:P:1:NAG:O4	2:P:1:NAG:C4	1.77	1.31
2:J:1:NAG:C4	2:J:1:NAG:O4	1.78	1.31
2:V:1:NAG:O4	2:V:1:NAG:C4	1.79	1.30
3:H:1:NAG:C4	3:H:1:NAG:O4	1.78	1.29
3:T:1:NAG:C4	3:T:1:NAG:O4	1.78	1.29
2:S:1:NAG:O4	2:S:1:NAG:C4	1.80	1.28
3:N:1:NAG:O4	3:N:1:NAG:C4	1.82	1.26
8:D:902:NAG:C4	7:Q:1:NAG:O1	1.90	1.19
5:K:6:MAN:O5	5:K:8:MAN:O6	1.57	1.19
5:K:6:MAN:H5	5:K:8:MAN:O6	1.38	1.11
1:B:521:VAL:HG11	1:B:546:MET:CE	1.97	0.93
1:F:433:ASP:OD2	1:F:561:HIS:HD2	1.63	0.81
5:K:6:MAN:H5	5:K:8:MAN:C6	2.13	0.78
1:D:442:ASN:HD21	1:D:471:SER:H	1.32	0.77
1:A:442:ASN:HD21	1:A:471:SER:H	1.33	0.76
1:C:442:ASN:HD21	1:C:471:SER:H	1.32	0.75
1:C:433:ASP:OD2	1:C:561:HIS:HD2	1.70	0.74
3:W:1:NAG:C4	3:W:2:NAG:C1	2.65	0.74
1:B:433:ASP:OD2	1:B:561:HIS:HD2	1.68	0.74
1:E:739:ARG:HD3	12:E:1048:HOH:O	1.88	0.74
2:S:1:NAG:C4	2:S:2:NAG:C1	2.67	0.73
5:K:1:NAG:C4	5:K:2:NAG:C1	2.66	0.72
3:T:1:NAG:C4	3:T:2:NAG:C1	2.67	0.72
1:B:521:VAL:HG11	1:B:546:MET:HE2	1.72	0.72
1:D:521:VAL:HG11	1:D:546:MET:HE2	1.72	0.72
1:D:433:ASP:OD2	1:D:561:HIS:HD2	1.73	0.71
2:P:1:NAG:C4	2:P:2:NAG:C1	2.69	0.69
1:C:109:ASP:OD1	11:C:907:XYL:H12	1.90	0.69
2:J:1:NAG:C4	2:J:2:NAG:C1	2.69	0.69
2:V:1:NAG:C4	2:V:2:NAG:C1	2.71	0.68
3:H:1:NAG:C4	3:H:2:NAG:C1	2.71	0.68
2:M:1:NAG:C4	2:M:2:NAG:C1	2.70	0.68
1:E:442:ASN:HD21	1:E:471:SER:H	1.40	0.67
1:D:696:TRP:HA	1:D:700:ASN:HD21	1.59	0.67
1:E:433:ASP:OD2	1:E:561:HIS:HD2	1.77	0.67
2:G:1:NAG:C4	2:G:2:NAG:C1	2.72	0.67
1:C:432:ASN:HB2	12:C:1086:HOH:O	1.94	0.67
1:F:117:VAL:HG22	1:F:376:TYR:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1:NAG:C4	3:N:2:NAG:C1	2.74	0.66
1:F:521:VAL:HG11	1:F:546:MET:HE3	1.78	0.64
3:W:1:NAG:O4	3:W:1:NAG:C3	2.46	0.64
1:E:117:VAL:HG22	1:E:376:TYR:CD2	2.32	0.64
1:F:220:LEU:HD22	1:F:268:TYR:CZ	2.33	0.64
1:C:220:LEU:HD22	1:C:268:TYR:CZ	2.33	0.64
1:A:696:TRP:HA	1:A:700:ASN:HD21	1.62	0.64
1:B:117:VAL:HG22	1:B:376:TYR:CD2	2.33	0.64
5:K:6:MAN:H62	5:K:8:MAN:H3	1.78	0.64
1:B:432:ASN:HB2	12:B:1217:HOH:O	1.98	0.63
1:F:521:VAL:HG11	1:F:546:MET:CE	2.28	0.63
5:K:6:MAN:H5	5:K:8:MAN:C5	2.28	0.63
1:D:117:VAL:HG22	1:D:376:TYR:CD2	2.33	0.63
1:D:204:THR:H	1:D:262:ASN:HD22	1.46	0.63
1:E:521:VAL:HG11	1:E:546:MET:HE3	1.81	0.62
1:A:521:VAL:HG11	1:A:546:MET:HE2	1.82	0.62
1:A:300:ASN:ND2	9:A:907:XYZ:O1	2.33	0.61
8:D:902:NAG:C4	7:Q:1:NAG:C1	2.78	0.61
1:A:220:LEU:HD22	1:A:268:TYR:CZ	2.36	0.61
3:T:1:NAG:O4	3:T:1:NAG:C3	2.47	0.61
1:A:248:LEU:HD23	1:A:249:TYR:CE2	2.36	0.60
1:F:546:MET:CE	1:F:546:MET:HA	2.30	0.60
1:F:774:ASP:HB2	1:F:776:LEU:HD22	1.82	0.60
1:C:433:ASP:OD2	1:C:561:HIS:CD2	2.52	0.60
1:B:442:ASN:HD21	1:B:471:SER:H	1.46	0.60
1:D:220:LEU:HD22	1:D:268:TYR:CZ	2.37	0.60
1:B:607:LYS:HD2	1:B:724:VAL:HB	1.83	0.59
1:A:433:ASP:OD2	1:A:561:HIS:HD2	1.84	0.59
1:B:521:VAL:CG1	1:B:546:MET:CE	2.78	0.59
1:C:421:LEU:HD11	1:C:520:PHE:HZ	1.68	0.59
5:K:1:NAG:O4	5:K:1:NAG:C3	2.48	0.59
1:F:442:ASN:HD21	1:F:471:SER:H	1.48	0.59
1:A:317:VAL:HG22	1:A:357:ILE:HD11	1.84	0.58
1:C:759:THR:HG23	12:C:1122:HOH:O	2.02	0.58
1:D:248:LEU:HD23	1:D:249:TYR:CE2	2.38	0.58
12:F:1200:HOH:O	2:G:3:BMA:H5	2.03	0.58
1:A:521:VAL:HG11	1:A:546:MET:CE	2.35	0.57
1:D:645:ARG:HD3	12:D:1114:HOH:O	2.02	0.57
1:F:204:THR:H	1:F:262:ASN:HD22	1.52	0.57
1:A:204:THR:H	1:A:262:ASN:HD22	1.53	0.57
1:A:235:PRO:O	1:A:270:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:ASN:HA	1:E:561:HIS:O	2.05	0.56
1:B:521:VAL:HG11	1:B:546:MET:HE3	1.82	0.56
1:E:220:LEU:HD22	1:E:268:TYR:CZ	2.41	0.56
1:E:521:VAL:HG11	1:E:546:MET:CE	2.35	0.56
1:F:421:LEU:HD11	1:F:520:PHE:HZ	1.69	0.56
1:D:421:LEU:HD11	1:D:520:PHE:HZ	1.71	0.56
1:C:521:VAL:HG11	1:C:546:MET:HE3	1.88	0.55
1:B:421:LEU:HD11	1:B:520:PHE:HZ	1.72	0.55
5:K:1:NAG:O4	5:K:1:NAG:C5	2.53	0.55
1:A:220:LEU:HD22	1:A:268:TYR:CE1	2.41	0.55
1:A:666:THR:OG1	1:A:716:THR:HG22	2.07	0.55
1:D:710:PHE:CE1	1:D:759:THR:HB	2.42	0.55
1:E:774:ASP:HB2	1:E:776:LEU:HD22	1.88	0.54
1:D:172:ASN:HD22	1:D:174:ARG:H	1.54	0.54
1:D:521:VAL:HG11	1:D:546:MET:CE	2.35	0.54
1:C:117:VAL:HG22	1:C:376:TYR:CD2	2.42	0.54
1:D:246:HIS:HE1	1:D:290:GLU:OE2	1.90	0.54
1:B:524:ASN:HA	1:B:561:HIS:O	2.08	0.54
1:F:433:ASP:OD2	1:F:561:HIS:CD2	2.53	0.54
1:C:645:ARG:HH11	1:C:740:GLN:HE21	1.56	0.54
1:E:607:LYS:HD2	1:E:724:VAL:HB	1.89	0.54
1:F:573:ASP:OD1	1:F:655:ARG:NH2	2.41	0.54
1:D:98:THR:CG2	2:P:1:NAG:O3	2.55	0.54
1:A:99:ARG:NH2	12:A:1002:HOH:O	2.41	0.53
3:N:1:NAG:O4	3:N:1:NAG:C5	2.53	0.53
1:F:400:GLU:HB3	12:F:1185:HOH:O	2.07	0.53
1:E:428:ALA:HB3	1:E:519:THR:HB	1.90	0.53
1:E:474:THR:HG21	12:E:1113:HOH:O	2.09	0.53
1:D:645:ARG:NH1	1:D:740:GLN:HE21	2.07	0.52
1:A:172:ASN:HD22	1:A:174:ARG:H	1.56	0.52
1:C:666:THR:OG1	1:C:716:THR:HG22	2.10	0.52
1:C:676:HIS:CE1	1:C:801:TRP:CD1	2.98	0.52
1:D:500:ASN:ND2	12:D:1001:HOH:O	2.37	0.52
1:F:607:LYS:HD2	1:F:724:VAL:HB	1.91	0.52
1:A:106:CYS:H	1:A:155:HIS:CD2	2.27	0.52
1:D:317:VAL:HG22	1:D:357:ILE:HD11	1.91	0.52
1:E:546:MET:CE	1:E:546:MET:HA	2.39	0.52
1:F:172:ASN:HD22	1:F:174:ARG:H	1.57	0.52
1:B:107:LEU:HD22	1:B:156:LEU:HB2	1.93	0.51
1:B:573:ASP:OD1	1:B:655:ARG:NH2	2.43	0.51
1:A:759:THR:HG23	12:A:1121:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:HIS:HE1	1:A:801:TRP:CD1	2.28	0.51
1:C:607:LYS:HD2	1:C:724:VAL:HB	1.92	0.51
1:C:109:ASP:OD1	11:C:907:XYL:C1	2.58	0.51
1:C:696:TRP:HA	1:C:700:ASN:HD21	1.76	0.51
1:A:645:ARG:NH1	1:A:740:GLN:HE21	2.09	0.51
1:A:143:ARG:NE	12:A:1001:HOH:O	2.17	0.50
1:D:433:ASP:OD2	1:D:561:HIS:CD2	2.60	0.50
1:C:710:PHE:CE1	1:C:759:THR:HB	2.46	0.50
1:B:204:THR:H	1:B:262:ASN:HD22	1.58	0.50
1:C:645:ARG:NH1	1:C:740:GLN:HE21	2.09	0.50
3:H:1:NAG:O4	3:H:1:NAG:C3	2.56	0.50
1:E:204:THR:H	1:E:262:ASN:HD22	1.60	0.50
1:D:98:THR:HG21	2:P:1:NAG:O3	2.12	0.49
1:A:266:CYS:O	1:A:300:ASN:OD1	2.31	0.49
1:A:255:GLU:OE2	1:A:763:ARG:NH2	2.46	0.49
1:F:238:SER:O	1:F:271:ILE:HA	2.11	0.49
8:B:905:NAG:O7	8:B:905:NAG:C3	2.61	0.49
1:E:410:VAL:HG11	1:E:597:VAL:HG21	1.94	0.49
3:T:1:NAG:O4	3:T:1:NAG:C5	2.56	0.49
1:B:521:VAL:CG1	1:B:546:MET:HE3	2.42	0.48
1:C:204:THR:H	1:C:262:ASN:HD22	1.60	0.48
1:C:513:LEU:HG	1:C:519:THR:HG21	1.95	0.48
1:F:569:GLU:OE1	1:F:655:ARG:NH1	2.47	0.48
2:P:1:NAG:O4	2:P:1:NAG:C3	2.58	0.48
1:C:676:HIS:HE1	1:C:801:TRP:CD1	2.31	0.48
1:F:524:ASN:HA	1:F:561:HIS:O	2.13	0.48
1:C:235:PRO:O	1:C:270:ARG:HD3	2.14	0.48
1:E:191:TYR:CD1	1:E:259:ALA:HB2	2.49	0.48
1:F:220:LEU:HD22	1:F:268:TYR:CE1	2.48	0.48
1:E:172:ASN:HD22	1:E:174:ARG:H	1.61	0.47
1:F:106:CYS:H	1:F:155:HIS:CD2	2.32	0.47
12:F:1200:HOH:O	2:G:3:BMA:C5	2.62	0.47
1:B:513:LEU:HG	1:B:519:THR:HG21	1.96	0.47
1:B:561:HIS:HE1	12:B:1065:HOH:O	1.97	0.47
1:F:107:LEU:HD22	1:F:156:LEU:HB2	1.97	0.47
1:A:710:PHE:CE1	1:A:759:THR:HB	2.50	0.47
1:B:172:ASN:HD22	1:B:174:ARG:H	1.62	0.47
1:E:410:VAL:CG1	1:E:597:VAL:HG21	2.44	0.47
1:A:264:ILE:HD12	1:A:287:LEU:HD11	1.97	0.47
1:C:235:PRO:HD2	1:C:270:ARG:HD2	1.97	0.47
1:F:428:ALA:HB3	1:F:519:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG22	1:A:376:TYR:CD2	2.50	0.47
1:A:607:LYS:HD2	1:A:724:VAL:HB	1.97	0.47
1:B:300:ASN:ND2	9:B:906:XYZ:O2	2.48	0.47
1:C:248:LEU:HD23	1:C:249:TYR:CE2	2.50	0.47
1:D:513:LEU:HG	1:D:519:THR:HG21	1.96	0.47
1:B:152:GLN:HE21	1:B:152:GLN:HA	1.79	0.46
1:B:195:LYS:HE3	1:B:686:VAL:HG21	1.97	0.46
1:C:713:ILE:HD11	1:C:747:ILE:HG13	1.97	0.46
1:E:421:LEU:HD11	1:E:520:PHE:HZ	1.80	0.46
8:E:905:NAG:H83	12:E:1074:HOH:O	2.15	0.46
1:C:220:LEU:HD22	1:C:268:TYR:CE1	2.50	0.46
1:D:758:VAL:HG13	1:D:760:PHE:CE2	2.50	0.46
1:E:195:LYS:HE3	1:E:686:VAL:HG21	1.98	0.46
1:C:98:THR:CG2	2:M:1:NAG:O3	2.64	0.46
1:B:696:TRP:HA	1:B:700:ASN:HD21	1.80	0.46
1:D:248:LEU:HD23	1:D:249:TYR:CZ	2.51	0.46
1:C:266:CYS:O	1:C:300:ASN:OD1	2.34	0.45
1:E:106:CYS:H	1:E:155:HIS:CD2	2.35	0.45
1:F:242:ASP:O	1:F:246:HIS:HD2	1.99	0.45
3:N:1:NAG:O4	3:N:1:NAG:C3	2.59	0.45
1:B:474:THR:HG21	12:B:1198:HOH:O	2.15	0.45
1:C:524:ASN:HA	1:C:561:HIS:O	2.16	0.45
1:D:607:LYS:HD2	1:D:724:VAL:HB	1.98	0.45
1:E:561:HIS:HE1	12:E:1034:HOH:O	2.00	0.45
1:D:266:CYS:O	1:D:300:ASN:OD1	2.35	0.45
1:D:645:ARG:HH11	1:D:740:GLN:HE21	1.64	0.45
1:A:715:ASN:HB2	1:A:750:LEU:HD13	1.98	0.45
1:F:645:ARG:NH1	1:F:740:GLN:HE21	2.15	0.45
1:A:421:LEU:HD11	1:A:520:PHE:HZ	1.82	0.44
1:F:152:GLN:HE21	1:F:152:GLN:HA	1.82	0.44
1:C:340:ILE:HD11	1:C:350:VAL:HG21	1.99	0.44
1:E:438:VAL:HG23	1:E:439:LEU:HD13	1.98	0.44
1:C:742:ARG:HD2	1:C:766:ASP:HB3	2.00	0.44
1:F:521:VAL:HG21	1:F:546:MET:HE1	1.98	0.44
1:B:220:LEU:HD22	1:B:268:TYR:CZ	2.53	0.44
1:E:235:PRO:O	1:E:270:ARG:HD3	2.17	0.44
1:D:340:ILE:HD11	1:D:350:VAL:HG21	2.00	0.44
1:D:410:VAL:HG11	1:D:597:VAL:HG21	1.99	0.44
1:F:248:LEU:HD23	1:F:249:TYR:CE2	2.52	0.44
1:A:248:LEU:HD23	1:A:249:TYR:CZ	2.52	0.43
1:B:569:GLU:OE2	1:B:655:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:HIS:HE1	1:D:801:TRP:CD1	2.36	0.43
1:B:521:VAL:HG21	1:B:546:MET:HE1	2.01	0.43
1:E:774:ASP:CB	1:E:776:LEU:HD22	2.47	0.43
1:A:524:ASN:HA	1:A:561:HIS:O	2.19	0.43
1:B:266:CYS:SG	1:B:299:SER:HA	2.58	0.43
1:E:710:PHE:CE1	1:E:759:THR:HB	2.54	0.43
1:E:107:LEU:HD22	1:E:156:LEU:HB2	2.01	0.43
5:K:8:MAN:O6	5:K:8:MAN:C5	2.56	0.43
1:C:561:HIS:HE1	12:C:1037:HOH:O	2.02	0.43
1:B:438:VAL:HG23	1:B:439:LEU:HD13	2.01	0.42
1:C:317:VAL:HG22	1:C:357:ILE:HD11	2.01	0.42
1:E:655:ARG:HG2	1:E:656:TYR:CE2	2.54	0.42
1:F:546:MET:HA	1:F:546:MET:HE2	2.01	0.42
1:F:727:LEU:HD23	1:F:727:LEU:C	2.39	0.42
1:A:513:LEU:HG	1:A:519:THR:HG21	2.01	0.42
1:D:264:ILE:HD12	1:D:287:LEU:HD11	2.02	0.42
8:D:902:NAG:C5	7:Q:1:NAG:O1	2.64	0.42
1:E:569:GLU:OE1	1:E:655:ARG:NH1	2.53	0.42
1:F:546:MET:HE3	1:F:546:MET:HA	2.01	0.42
8:B:905:NAG:O7	8:B:905:NAG:H3	2.18	0.42
1:A:317:VAL:HG22	1:A:357:ILE:CD1	2.50	0.42
1:E:158:LEU:HD13	11:E:906:XYL:H52	2.02	0.42
1:F:624:VAL:HG22	1:F:626:TYR:CE2	2.55	0.42
1:F:112:ILE:HG22	1:F:125:ALA:HA	2.02	0.41
1:D:377:ASN:ND2	1:D:384:LEU:HD23	2.35	0.41
1:D:742:ARG:HD2	1:D:766:ASP:HB3	2.02	0.41
1:C:98:THR:HG21	2:M:1:NAG:O3	2.20	0.41
1:E:112:ILE:HG22	1:E:125:ALA:HA	2.02	0.41
1:F:763:ARG:HD3	1:F:766:ASP:OD2	2.20	0.41
1:D:710:PHE:CD1	1:D:759:THR:HB	2.55	0.41
8:E:905:NAG:C8	12:E:1074:HOH:O	2.68	0.41
1:C:668:THR:OG1	1:C:716:THR:HG21	2.21	0.41
1:D:106:CYS:H	1:D:155:HIS:CD2	2.38	0.41
1:D:729:ILE:HD12	1:D:742:ARG:HG3	2.02	0.41
1:A:433:ASP:OD2	1:A:561:HIS:CD2	2.70	0.40
1:A:655:ARG:HG2	1:A:656:TYR:CD2	2.57	0.40
1:E:697:ASP:OD1	1:E:697:ASP:C	2.59	0.40
1:E:71:VAL:HG21	1:E:355:VAL:HG23	2.03	0.40
1:A:351:ARG:O	1:A:355:VAL:HG23	2.21	0.40
1:B:71:VAL:HG21	1:B:355:VAL:HG23	2.04	0.40
1:B:697:ASP:H	1:B:700:ASN:HD21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ASN:O	1:C:458:GLY:HA2	2.22	0.40
1:B:242:ASP:O	1:B:246:HIS:HD2	2.04	0.40
1:B:170:PRO:HG3	1:B:619:TYR:CD2	2.57	0.40
1:C:377:ASN:C	1:C:377:ASN:HD22	2.24	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	757/805 (94%)	725 (96%)	32 (4%)	0	100	100
1	B	757/805 (94%)	722 (95%)	35 (5%)	0	100	100
1	C	755/805 (94%)	724 (96%)	31 (4%)	0	100	100
1	D	755/805 (94%)	718 (95%)	37 (5%)	0	100	100
1	E	756/805 (94%)	725 (96%)	30 (4%)	1 (0%)	51	64
1	F	756/805 (94%)	721 (95%)	34 (4%)	1 (0%)	51	64
All	All	4536/4830 (94%)	4335 (96%)	199 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	700	ASN
1	F	700	ASN

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	610/650 (94%)	570 (93%)	40 (7%)	16	20
1	B	612/650 (94%)	572 (94%)	40 (6%)	17	21
1	C	609/650 (94%)	570 (94%)	39 (6%)	17	22
1	D	609/650 (94%)	567 (93%)	42 (7%)	15	18
1	E	611/650 (94%)	569 (93%)	42 (7%)	15	18
1	F	611/650 (94%)	575 (94%)	36 (6%)	19	25
All	All	3662/3900 (94%)	3423 (94%)	239 (6%)	17	21

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	A	77	GLU
1	A	107	LEU
1	A	117	VAL
1	A	137	LEU
1	A	147	GLN
1	A	152	GLN
1	A	172	ASN
1	A	195	LYS
1	A	202	VAL
1	A	228	SER
1	A	301	TRP
1	A	312	GLU
1	A	351	ARG
1	A	358	LEU
1	A	377	ASN
1	A	403	LYS
1	A	404	GLU
1	A	430	LEU
1	A	432	ASN
1	A	474	THR
1	A	519	THR
1	A	610	TRP
1	A	624	VAL
1	A	645	ARG
1	A	655	ARG
1	A	672	LEU

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Mol	Chain	Res	Type
1	A	700	ASN
1	A	702	LEU
1	A	705	VAL
1	A	709	VAL
1	A	716	THR
1	A	734	ASP
1	A	748	LYS
1	A	750	LEU
1	A	758	VAL
1	A	759	THR
1	A	763	ARG
1	A	767	VAL
1	A	776	LEU
1	B	98	THR
1	B	107	LEU
1	B	117	VAL
1	B	137	LEU
1	B	147	GLN
1	B	152	GLN
1	B	172	ASN
1	B	195	LYS
1	B	220	LEU
1	B	227	VAL
1	B	301	TRP
1	B	312	GLU
1	B	349	LEU
1	B	358	LEU
1	B	377	ASN
1	B	430	LEU
1	B	439	LEU
1	B	474	THR
1	B	506	GLU
1	B	519	THR
1	B	529	GLU
1	B	554	SER
1	B	610	TRP
1	B	624	VAL
1	B	625	VAL
1	B	645	ARG
1	B	655	ARG
1	B	672	LEU
1	B	688	GLU

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Mol	Chain	Res	Type
1	B	700	ASN
1	B	702	LEU
1	B	709	VAL
1	B	716	THR
1	B	748	LYS
1	B	750	LEU
1	B	758	VAL
1	B	759	THR
1	B	763	ARG
1	B	767	VAL
1	B	803	PRO
1	C	77	GLU
1	C	98	THR
1	C	107	LEU
1	C	117	VAL
1	C	120	SER
1	C	129	VAL
1	C	137	LEU
1	C	147	GLN
1	C	172	ASN
1	C	195	LYS
1	C	202	VAL
1	C	220	LEU
1	C	228	SER
1	C	301	TRP
1	C	306	ASP
1	C	344	THR
1	C	349	LEU
1	C	358	LEU
1	C	377	ASN
1	C	403	LYS
1	C	404	GLU
1	C	430	LEU
1	C	432	ASN
1	C	439	LEU
1	C	453	ILE
1	C	474	THR
1	C	519	THR
1	C	610	TRP
1	C	624	VAL
1	C	645	ARG
1	C	655	ARG

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Mol	Chain	Res	Type
1	C	700	ASN
1	C	702	LEU
1	C	709	VAL
1	C	716	THR
1	C	739	ARG
1	C	758	VAL
1	C	759	THR
1	C	776	LEU
1	D	65	LYS
1	D	77	GLU
1	D	98	THR
1	D	107	LEU
1	D	117	VAL
1	D	129	VAL
1	D	137	LEU
1	D	147	GLN
1	D	152	GLN
1	D	172	ASN
1	D	195	LYS
1	D	228	SER
1	D	301	TRP
1	D	306	ASP
1	D	312	GLU
1	D	349	LEU
1	D	358	LEU
1	D	377	ASN
1	D	404	GLU
1	D	432	ASN
1	D	439	LEU
1	D	474	THR
1	D	519	THR
1	D	610	TRP
1	D	624	VAL
1	D	625	VAL
1	D	645	ARG
1	D	655	ARG
1	D	672	LEU
1	D	700	ASN
1	D	702	LEU
1	D	705	VAL
1	D	709	VAL
1	D	716	THR

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Mol	Chain	Res	Type
1	D	739	ARG
1	D	748	LYS
1	D	750	LEU
1	D	758	VAL
1	D	759	THR
1	D	767	VAL
1	D	776	LEU
1	D	791	SER
1	E	98	THR
1	E	107	LEU
1	E	117	VAL
1	E	120	SER
1	E	129	VAL
1	E	137	LEU
1	E	147	GLN
1	E	152	GLN
1	E	172	ASN
1	E	195	LYS
1	E	220	LEU
1	E	301	TRP
1	E	342	ASN
1	E	344	THR
1	E	346	SER
1	E	358	LEU
1	E	377	ASN
1	E	385	ASN
1	E	404	GLU
1	E	430	LEU
1	E	432	ASN
1	E	439	LEU
1	E	474	THR
1	E	519	THR
1	E	554	SER
1	E	610	TRP
1	E	624	VAL
1	E	625	VAL
1	E	645	ARG
1	E	672	LEU
1	E	681	LYS
1	E	688	GLU
1	E	700	ASN
1	E	702	LEU

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Mol	Chain	Res	Type
1	E	709	VAL
1	E	716	THR
1	E	739	ARG
1	E	750	LEU
1	E	758	VAL
1	E	759	THR
1	E	767	VAL
1	E	776	LEU
1	F	49	TRP
1	F	98	THR
1	F	107	LEU
1	F	117	VAL
1	F	120	SER
1	F	137	LEU
1	F	147	GLN
1	F	152	GLN
1	F	172	ASN
1	F	195	LYS
1	F	202	VAL
1	F	220	LEU
1	F	300	ASN
1	F	301	TRP
1	F	325	LEU
1	F	358	LEU
1	F	377	ASN
1	F	385	ASN
1	F	404	GLU
1	F	425	GLN
1	F	430	LEU
1	F	439	LEU
1	F	519	THR
1	F	610	TRP
1	F	624	VAL
1	F	645	ARG
1	F	655	ARG
1	F	672	LEU
1	F	700	ASN
1	F	709	VAL
1	F	716	THR
1	F	739	ARG
1	F	750	LEU
1	F	759	THR

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Mol	Chain	Res	Type
1	F	767	VAL
1	F	776	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	152	GLN
1	A	155	HIS
1	A	172	ASN
1	A	229	GLN
1	A	262	ASN
1	A	377	ASN
1	A	442	ASN
1	A	561	HIS
1	A	676	HIS
1	A	700	ASN
1	A	740	GLN
1	B	152	GLN
1	B	155	HIS
1	B	172	ASN
1	B	229	GLN
1	B	246	HIS
1	B	262	ASN
1	B	300	ASN
1	B	377	ASN
1	B	442	ASN
1	B	561	HIS
1	B	700	ASN
1	B	740	GLN
1	C	147	GLN
1	C	152	GLN
1	C	155	HIS
1	C	172	ASN
1	C	229	GLN
1	C	246	HIS
1	C	262	ASN
1	C	377	ASN
1	C	442	ASN
1	C	561	HIS
1	C	676	HIS
1	C	700	ASN

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Mol	Chain	Res	Type
1	C	740	GLN
1	D	147	GLN
1	D	152	GLN
1	D	155	HIS
1	D	172	ASN
1	D	229	GLN
1	D	246	HIS
1	D	262	ASN
1	D	377	ASN
1	D	442	ASN
1	D	561	HIS
1	D	676	HIS
1	D	700	ASN
1	D	740	GLN
1	E	152	GLN
1	E	155	HIS
1	E	172	ASN
1	E	229	GLN
1	E	246	HIS
1	E	262	ASN
1	E	275	HIS
1	E	377	ASN
1	E	425	GLN
1	E	442	ASN
1	E	561	HIS
1	E	700	ASN
1	E	740	GLN
1	F	152	GLN
1	F	155	HIS
1	F	172	ASN
1	F	229	GLN
1	F	246	HIS
1	F	262	ASN
1	F	275	HIS
1	F	300	ASN
1	F	377	ASN
1	F	442	ASN
1	F	561	HIS
1	F	700	ASN
1	F	740	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)

94 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	G	1	2,1	14,14,15	3.83	1 (7%)	17,19,21	1.42	2 (11%)
2	NAG	G	2	2	14,14,15	1.10	0	17,19,21	1.95	6 (35%)
2	BMA	G	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.40	4 (26%)
3	NAG	H	1	1,3	14,14,15	4.18	2 (14%)	17,19,21	1.92	5 (29%)
3	NAG	H	2	3	14,14,15	0.60	0	17,19,21	1.08	1 (5%)
3	BMA	H	3	3	11,11,12	0.67	0	15,15,17	2.18	4 (26%)
3	BMA	H	4	3	11,11,12	1.25	1 (9%)	15,15,17	3.18	7 (46%)
3	MAN	H	5	3	11,11,12	1.15	1 (9%)	15,15,17	1.39	3 (20%)
3	MAN	H	6	3	11,11,12	1.02	0	15,15,17	3.90	6 (40%)
3	MAN	H	7	3	11,11,12	0.62	0	15,15,17	1.73	5 (33%)
4	NAG	I	1	4,1	14,14,15	0.90	1 (7%)	17,19,21	1.59	4 (23%)
4	NAG	I	2	4	14,14,15	0.74	0	17,19,21	2.40	7 (41%)
4	MAN	I	3	4	11,11,12	1.40	1 (9%)	15,15,17	2.05	7 (46%)
4	MAN	I	4	4	11,11,12	1.31	2 (18%)	15,15,17	2.80	5 (33%)
4	MAN	I	5	4	11,11,12	0.68	0	15,15,17	2.62	7 (46%)
2	NAG	J	1	2,1	14,14,15	4.06	1 (7%)	17,19,21	1.61	4 (23%)
2	NAG	J	2	2	14,14,15	0.46	0	17,19,21	1.22	2 (11%)
2	BMA	J	3	2	11,11,12	0.92	0	15,15,17	1.57	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	K	1	5,1	14,14,15	3.97	1 (7%)	17,19,21	2.47	5 (29%)
5	NAG	K	2	5	14,14,15	0.68	0	17,19,21	1.22	2 (11%)
5	BMA	K	3	5	11,11,12	0.52	0	15,15,17	2.59	6 (40%)
5	BMA	K	4	5	11,11,12	1.39	2 (18%)	15,15,17	2.95	8 (53%)
5	MAN	K	5	5	11,11,12	1.26	2 (18%)	15,15,17	1.89	7 (46%)
5	MAN	K	6	5	11,11,12	1.92	1 (9%)	15,15,17	2.92	7 (46%)
5	MAN	K	7	5	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
5	MAN	K	8	5	11,11,12	2.23	2 (18%)	15,15,17	4.11	9 (60%)
6	NAG	L	1	1,6	14,14,15	0.49	0	17,19,21	1.39	1 (5%)
6	NAG	L	2	6	14,14,15	0.83	0	17,19,21	2.11	4 (23%)
6	MAN	L	3	6	11,11,12	1.38	1 (9%)	15,15,17	2.20	7 (46%)
6	MAN	L	4	6	11,11,12	0.97	0	15,15,17	2.46	6 (40%)
6	MAN	L	5	6	11,11,12	0.67	0	15,15,17	2.79	6 (40%)
6	MAN	L	6	6	11,11,12	0.73	0	15,15,17	1.89	3 (20%)
2	NAG	M	1	2,1	14,14,15	3.53	1 (7%)	17,19,21	1.43	2 (11%)
2	NAG	M	2	2	14,14,15	1.09	0	17,19,21	1.93	6 (35%)
2	BMA	M	3	2	11,11,12	1.40	1 (9%)	15,15,17	1.43	2 (13%)
3	NAG	N	1	1,3	14,14,15	4.56	2 (14%)	17,19,21	2.29	6 (35%)
3	NAG	N	2	3	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
3	BMA	N	3	3	11,11,12	0.90	0	15,15,17	2.64	4 (26%)
3	BMA	N	4	3	11,11,12	1.25	1 (9%)	15,15,17	3.07	9 (60%)
3	MAN	N	5	3	11,11,12	1.22	2 (18%)	15,15,17	1.57	4 (26%)
3	MAN	N	6	3	11,11,12	0.94	0	15,15,17	3.85	7 (46%)
3	MAN	N	7	3	11,11,12	0.67	0	15,15,17	1.46	2 (13%)
6	NAG	O	1	1,6	14,14,15	0.81	0	17,19,21	1.52	4 (23%)
6	NAG	O	2	6	14,14,15	0.93	1 (7%)	17,19,21	1.65	5 (29%)
6	MAN	O	3	6	11,11,12	1.26	0	15,15,17	2.42	7 (46%)
6	MAN	O	4	6	11,11,12	1.42	1 (9%)	15,15,17	2.72	5 (33%)
6	MAN	O	5	6	11,11,12	0.77	0	15,15,17	2.34	6 (40%)
6	MAN	O	6	6	11,11,12	0.83	0	15,15,17	1.71	4 (26%)
2	NAG	P	1	2,1	14,14,15	3.93	1 (7%)	17,19,21	1.49	3 (17%)
2	NAG	P	2	2	14,14,15	1.04	0	17,19,21	1.96	4 (23%)
2	BMA	P	3	2	11,11,12	1.19	1 (9%)	15,15,17	1.58	2 (13%)
7	NAG	Q	1	7	15,15,15	0.67	0	21,21,21	1.55	4 (19%)
7	BMA	Q	2	7	11,11,12	0.65	0	15,15,17	2.80	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	Q	3	7	11,11,12	1.32	2 (18%)	15,15,17	2.80	7 (46%)
7	MAN	Q	4	7	11,11,12	1.23	0	15,15,17	1.53	4 (26%)
7	MAN	Q	5	7	11,11,12	1.24	1 (9%)	15,15,17	3.99	7 (46%)
7	MAN	Q	6	7	11,11,12	0.49	0	15,15,17	1.27	3 (20%)
4	NAG	R	1	4,1	14,14,15	0.85	0	17,19,21	1.27	1 (5%)
4	NAG	R	2	4	14,14,15	0.79	0	17,19,21	1.72	6 (35%)
4	MAN	R	3	4	11,11,12	1.23	0	15,15,17	2.18	5 (33%)
4	MAN	R	4	4	11,11,12	1.28	1 (9%)	15,15,17	2.81	6 (40%)
4	MAN	R	5	4	11,11,12	1.43	2 (18%)	15,15,17	2.68	7 (46%)
2	NAG	S	1	2,1	14,14,15	4.25	1 (7%)	17,19,21	1.81	6 (35%)
2	NAG	S	2	2	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
2	BMA	S	3	2	11,11,12	1.08	0	15,15,17	1.62	4 (26%)
3	NAG	T	1	1,3	14,14,15	4.05	1 (7%)	17,19,21	2.39	4 (23%)
3	NAG	T	2	3	14,14,15	0.78	0	17,19,21	1.07	1 (5%)
3	BMA	T	3	3	11,11,12	0.70	0	15,15,17	2.55	5 (33%)
3	BMA	T	4	3	11,11,12	1.16	1 (9%)	15,15,17	2.66	7 (46%)
3	MAN	T	5	3	11,11,12	0.98	1 (9%)	15,15,17	2.49	7 (46%)
3	MAN	T	6	3	11,11,12	1.22	2 (18%)	15,15,17	3.98	7 (46%)
3	MAN	T	7	3	11,11,12	0.84	0	15,15,17	1.88	7 (46%)
6	NAG	U	1	1,6	14,14,15	0.61	0	17,19,21	1.25	3 (17%)
6	NAG	U	2	6	14,14,15	0.88	0	17,19,21	1.66	3 (17%)
6	MAN	U	3	6	11,11,12	1.47	2 (18%)	15,15,17	2.42	7 (46%)
6	MAN	U	4	6	11,11,12	1.10	1 (9%)	15,15,17	2.98	6 (40%)
6	MAN	U	5	6	11,11,12	0.67	0	15,15,17	2.81	6 (40%)
6	MAN	U	6	6	11,11,12	1.08	0	15,15,17	1.95	4 (26%)
2	NAG	V	1	2,1	14,14,15	4.24	1 (7%)	17,19,21	1.42	3 (17%)
2	NAG	V	2	2	14,14,15	0.58	0	17,19,21	1.44	1 (5%)
2	BMA	V	3	2	11,11,12	1.19	1 (9%)	15,15,17	1.68	2 (13%)
3	NAG	W	1	1,3	14,14,15	3.58	1 (7%)	17,19,21	2.28	5 (29%)
3	NAG	W	2	3	14,14,15	0.74	0	17,19,21	1.22	1 (5%)
3	BMA	W	3	3	11,11,12	0.57	0	15,15,17	2.55	5 (33%)
3	BMA	W	4	3	11,11,12	1.23	2 (18%)	15,15,17	2.72	7 (46%)
3	MAN	W	5	3	11,11,12	1.39	2 (18%)	15,15,17	2.95	8 (53%)
3	MAN	W	6	3	11,11,12	1.19	1 (9%)	15,15,17	4.06	5 (33%)
3	MAN	W	7	3	11,11,12	0.85	0	15,15,17	1.68	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	X	1	1,6	14,14,15	0.77	1 (7%)	17,19,21	1.57	3 (17%)
6	NAG	X	2	6	14,14,15	0.94	0	17,19,21	1.74	2 (11%)
6	MAN	X	3	6	11,11,12	1.57	2 (18%)	15,15,17	2.36	6 (40%)
6	MAN	X	4	6	11,11,12	1.11	1 (9%)	15,15,17	2.85	6 (40%)
6	MAN	X	5	6	11,11,12	0.57	0	15,15,17	1.95	4 (26%)
6	MAN	X	6	6	11,11,12	0.94	0	15,15,17	1.67	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	BMA	H	4	3	-	1/2/19/22	0/1/1/1
3	MAN	H	5	3	-	0/2/19/22	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
3	MAN	H	7	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	MAN	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	0/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1
5	BMA	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	1/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1
5	MAN	K	8	5	-	2/2/19/22	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	MAN	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
6	MAN	L	6	6	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	BMA	M	3	2	-	2/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	BMA	N	4	3	-	0/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1
3	MAN	N	6	3	-	2/2/19/22	0/1/1/1
3	MAN	N	7	3	-	0/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	MAN	O	3	6	-	1/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	0/1/1/1
6	MAN	O	5	6	-	2/2/19/22	0/1/1/1
6	MAN	O	6	6	-	2/2/19/22	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	BMA	P	3	2	-	1/2/19/22	0/1/1/1
7	NAG	Q	1	7	-	0/6/26/26	0/1/1/1
7	BMA	Q	2	7	-	0/2/19/22	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	MAN	R	3	4	-	1/2/19/22	0/1/1/1
4	MAN	R	4	4	-	1/2/19/22	0/1/1/1
4	MAN	R	5	4	-	1/2/19/22	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	BMA	S	3	2	-	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	BMA	T	4	3	-	0/2/19/22	0/1/1/1
3	MAN	T	5	3	-	0/2/19/22	0/1/1/1
3	MAN	T	6	3	-	2/2/19/22	0/1/1/1
3	MAN	T	7	3	-	0/2/19/22	0/1/1/1
6	NAG	U	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	MAN	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	0/1/1/1
6	MAN	U	5	6	-	0/2/19/22	0/1/1/1
6	MAN	U	6	6	-	0/2/19/22	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	BMA	V	3	2	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	BMA	W	4	3	-	0/2/19/22	0/1/1/1
3	MAN	W	5	3	-	1/2/19/22	0/1/1/1
3	MAN	W	6	3	-	2/2/19/22	0/1/1/1
3	MAN	W	7	3	-	0/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	MAN	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	MAN	X	5	6	-	0/2/19/22	0/1/1/1
6	MAN	X	6	6	-	2/2/19/22	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O4-C4	16.66	1.82	1.43
2	S	1	NAG	O4-C4	15.73	1.80	1.43
2	V	1	NAG	O4-C4	15.66	1.79	1.43
3	H	1	NAG	O4-C4	15.19	1.78	1.43
2	J	1	NAG	O4-C4	14.88	1.78	1.43
3	T	1	NAG	O4-C4	14.88	1.78	1.43
5	K	1	NAG	O4-C4	14.66	1.77	1.43
2	P	1	NAG	O4-C4	14.57	1.77	1.43
2	G	1	NAG	O4-C4	14.00	1.76	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	NAG	O4-C4	13.11	1.73	1.43
3	W	1	NAG	O4-C4	13.08	1.73	1.43
5	K	8	MAN	O6-C6	5.78	1.66	1.42
5	K	6	MAN	O5-C1	5.22	1.52	1.43
5	K	8	MAN	C2-C3	3.33	1.57	1.52
2	M	3	BMA	C2-C3	3.09	1.57	1.52
3	H	1	NAG	C2-N2	-3.01	1.41	1.46
4	R	5	MAN	C2-C3	2.78	1.56	1.52
3	W	6	MAN	O5-C1	2.75	1.48	1.43
6	O	4	MAN	C4-C5	2.69	1.58	1.53
3	W	5	MAN	O2-C2	2.61	1.48	1.43
3	W	4	BMA	C4-C5	2.58	1.58	1.53
3	H	5	MAN	C1-C2	2.58	1.58	1.52
2	P	3	BMA	C2-C3	2.58	1.56	1.52
6	X	3	MAN	C4-C5	2.52	1.58	1.53
3	N	1	NAG	C2-N2	-2.50	1.42	1.46
7	Q	5	MAN	C6-C5	2.48	1.60	1.51
2	G	3	BMA	C2-C3	2.46	1.56	1.52
6	U	3	MAN	C4-C5	2.46	1.58	1.53
5	K	4	BMA	C4-C5	2.45	1.58	1.53
3	W	5	MAN	C2-C3	2.45	1.56	1.52
6	O	2	NAG	O5-C1	-2.44	1.39	1.43
4	I	4	MAN	C4-C5	2.38	1.58	1.53
5	K	5	MAN	O2-C2	2.36	1.48	1.43
4	R	4	MAN	C4-C5	2.36	1.58	1.53
3	N	5	MAN	C1-C2	2.35	1.57	1.52
4	R	5	MAN	C1-C2	2.33	1.57	1.52
3	T	6	MAN	C4-C5	2.32	1.57	1.53
3	T	6	MAN	O5-C1	2.32	1.47	1.43
3	T	4	BMA	C4-C5	2.31	1.57	1.53
6	L	3	MAN	C4-C5	2.31	1.57	1.53
2	V	3	BMA	C4-C5	2.28	1.57	1.53
3	T	5	MAN	O2-C2	2.24	1.48	1.43
6	X	4	MAN	O5-C1	2.23	1.47	1.43
5	K	4	BMA	O5-C5	2.23	1.48	1.43
7	Q	3	BMA	O5-C5	2.21	1.47	1.43
6	X	3	MAN	C4-C3	2.19	1.57	1.52
5	K	5	MAN	C2-C3	2.18	1.55	1.52
7	Q	3	BMA	C4-C5	2.12	1.57	1.53
4	I	3	MAN	O5-C5	2.10	1.47	1.43
3	W	4	BMA	O5-C5	2.09	1.47	1.43
3	H	4	BMA	O5-C5	2.09	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	4	BMA	O2-C2	2.08	1.47	1.43
6	U	3	MAN	C4-C3	2.07	1.57	1.52
4	I	4	MAN	O5-C1	2.06	1.47	1.43
6	X	1	NAG	C2-N2	-2.06	1.42	1.46
3	N	5	MAN	C2-C3	2.05	1.55	1.52
4	I	1	NAG	C2-N2	-2.03	1.42	1.46
6	U	4	MAN	O5-C1	2.01	1.46	1.43

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	5	MAN	C1-O5-C5	12.57	129.22	112.19
3	N	6	MAN	C1-O5-C5	12.03	128.50	112.19
3	H	6	MAN	C1-O5-C5	11.91	128.32	112.19
3	W	6	MAN	C1-O5-C5	11.43	127.68	112.19
3	T	6	MAN	C1-O5-C5	10.91	126.98	112.19
5	K	8	MAN	C6-C5-C4	10.76	138.21	113.00
6	U	4	MAN	C1-O5-C5	8.64	123.90	112.19
4	I	4	MAN	C1-O5-C5	8.36	123.52	112.19
6	X	4	MAN	C1-O5-C5	8.20	123.30	112.19
4	R	4	MAN	C1-O5-C5	8.19	123.28	112.19
3	N	4	BMA	C1-C2-C3	-8.14	99.65	109.67
3	N	3	BMA	O3-C3-C2	7.99	125.29	109.99
7	Q	2	BMA	O3-C3-C2	7.88	125.08	109.99
6	O	4	MAN	C1-O5-C5	7.54	122.41	112.19
6	L	5	MAN	C1-O5-C5	7.49	122.34	112.19
6	U	5	MAN	C1-O5-C5	7.23	121.98	112.19
3	W	3	BMA	O3-C3-C2	7.20	123.79	109.99
7	Q	3	BMA	C1-C2-C3	-7.19	100.82	109.67
3	H	3	BMA	O3-C3-C2	6.92	123.25	109.99
5	K	6	MAN	C1-O5-C5	-6.91	102.83	112.19
3	H	4	BMA	C1-C2-C3	-6.90	101.18	109.67
3	H	4	BMA	O5-C5-C6	6.70	117.71	107.20
6	L	4	MAN	C1-O5-C5	6.52	121.02	112.19
5	K	8	MAN	C1-O5-C5	-6.07	103.97	112.19
6	O	5	MAN	C1-O5-C5	6.03	120.36	112.19
3	T	6	MAN	O5-C1-C2	5.94	119.95	110.77
6	L	6	MAN	C1-O5-C5	5.94	120.24	112.19
5	K	8	MAN	C3-C4-C5	-5.92	99.68	110.24
3	T	3	BMA	O3-C3-C2	5.91	121.31	109.99
3	T	6	MAN	C3-C4-C5	5.89	120.75	110.24
3	W	6	MAN	C3-C4-C5	5.87	120.72	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	3	BMA	O3-C3-C2	5.87	121.23	109.99
3	T	5	MAN	C1-O5-C5	5.76	120.00	112.19
4	I	5	MAN	C1-O5-C5	5.73	119.96	112.19
3	T	1	NAG	O4-C4-C3	-5.67	97.24	110.35
3	W	6	MAN	O5-C1-C2	5.64	119.47	110.77
3	W	1	NAG	O4-C4-C3	-5.53	97.55	110.35
5	K	1	NAG	O4-C4-C3	-5.47	97.70	110.35
3	T	1	NAG	C4-C3-C2	-5.32	103.22	111.02
6	O	3	MAN	C1-C2-C3	5.28	116.15	109.67
3	W	5	MAN	C1-C2-C3	-5.22	103.25	109.67
3	W	6	MAN	O4-C4-C3	-5.22	98.29	110.35
4	R	3	MAN	C1-C2-C3	5.18	116.04	109.67
3	W	4	BMA	C1-O5-C5	-5.16	105.20	112.19
3	W	1	NAG	C4-C3-C2	-5.13	103.51	111.02
3	T	3	BMA	O5-C5-C6	5.09	115.18	107.20
4	R	5	MAN	C1-O5-C5	5.07	119.06	112.19
3	W	5	MAN	C1-O5-C5	5.07	119.06	112.19
7	Q	5	MAN	C3-C4-C5	4.97	119.11	110.24
6	U	6	MAN	C1-O5-C5	4.93	118.87	112.19
2	V	3	BMA	C3-C4-C5	4.92	119.02	110.24
3	W	5	MAN	O3-C3-C4	4.88	121.62	110.35
4	I	3	MAN	C1-C2-C3	4.83	115.61	109.67
3	H	6	MAN	O5-C1-C2	4.81	118.19	110.77
6	U	5	MAN	O2-C2-C1	4.80	118.98	109.15
3	N	6	MAN	C3-C4-C5	4.78	118.77	110.24
6	X	5	MAN	C1-O5-C5	4.76	118.64	112.19
5	K	4	BMA	O4-C4-C3	-4.75	99.38	110.35
5	K	4	BMA	O5-C1-C2	-4.71	103.50	110.77
5	K	3	BMA	O5-C5-C6	4.69	114.56	107.20
6	X	6	MAN	O5-C5-C6	4.67	114.53	107.20
3	T	4	BMA	O5-C5-C6	4.67	114.52	107.20
6	U	4	MAN	O5-C5-C6	4.66	114.52	107.20
5	K	4	BMA	O5-C5-C6	4.65	114.49	107.20
5	K	4	BMA	C1-C2-C3	-4.64	103.96	109.67
6	X	1	NAG	O5-C1-C2	-4.63	103.98	111.29
3	T	4	BMA	O4-C4-C3	-4.63	99.65	110.35
3	H	6	MAN	C3-C4-C5	4.60	118.45	110.24
4	R	5	MAN	O5-C5-C6	4.59	114.41	107.20
3	H	1	NAG	C4-C3-C2	-4.57	104.32	111.02
3	N	1	NAG	C4-C3-C2	-4.53	104.37	111.02
6	U	3	MAN	O5-C5-C6	4.53	114.31	107.20
4	I	2	NAG	O7-C7-N2	4.51	130.24	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	5	MAN	O5-C1-C2	4.49	117.69	110.77
5	K	6	MAN	O5-C1-C2	4.47	117.67	110.77
6	L	2	NAG	O5-C5-C6	4.47	114.20	107.20
3	N	1	NAG	O4-C4-C5	-4.46	98.22	109.30
3	H	4	BMA	O5-C1-C2	-4.46	103.89	110.77
3	W	4	BMA	O4-C4-C3	-4.45	100.06	110.35
3	T	5	MAN	C1-C2-C3	-4.42	104.24	109.67
4	I	5	MAN	C3-C4-C5	4.41	118.11	110.24
3	T	6	MAN	O4-C4-C3	-4.41	100.15	110.35
3	N	4	BMA	O2-C2-C3	4.40	118.94	110.14
2	P	2	NAG	C1-C2-N2	-4.37	103.02	110.49
3	W	4	BMA	O5-C5-C6	4.37	114.05	107.20
6	X	2	NAG	O5-C5-C6	4.36	114.04	107.20
4	I	2	NAG	C2-N2-C7	4.34	129.08	122.90
5	K	1	NAG	C4-C3-C2	-4.34	104.66	111.02
3	N	3	BMA	O2-C2-C3	4.27	118.69	110.14
7	Q	2	BMA	C1-C2-C3	-4.24	104.45	109.67
6	U	2	NAG	O4-C4-C3	4.18	120.00	110.35
7	Q	3	BMA	O5-C5-C6	4.14	113.69	107.20
5	K	3	BMA	O3-C3-C4	-4.13	100.81	110.35
6	L	2	NAG	O4-C4-C3	4.12	119.88	110.35
3	T	4	BMA	C3-C4-C5	4.12	117.59	110.24
3	N	1	NAG	O4-C4-C3	-4.09	100.90	110.35
5	K	6	MAN	C6-C5-C4	4.09	122.57	113.00
3	N	6	MAN	O5-C1-C2	4.08	117.07	110.77
2	M	3	BMA	C1-C2-C3	4.05	114.64	109.67
6	X	3	MAN	O5-C5-C6	4.04	113.54	107.20
2	P	3	BMA	C1-C2-C3	4.04	114.63	109.67
4	I	2	NAG	C8-C7-N2	-4.01	109.31	116.10
6	U	3	MAN	C3-C4-C5	3.98	117.34	110.24
6	X	3	MAN	C1-C2-C3	3.97	114.55	109.67
6	L	5	MAN	O2-C2-C1	3.93	117.19	109.15
2	S	1	NAG	O5-C5-C6	3.93	113.36	107.20
3	H	1	NAG	O4-C4-C3	-3.92	101.28	110.35
4	R	3	MAN	C1-O5-C5	3.91	117.49	112.19
2	G	2	NAG	C1-C2-N2	-3.91	103.81	110.49
4	I	1	NAG	C1-O5-C5	3.88	117.45	112.19
6	O	3	MAN	O2-C2-C1	-3.87	101.24	109.15
5	K	1	NAG	O4-C4-C5	-3.86	99.70	109.30
6	X	3	MAN	C3-C4-C5	3.86	117.12	110.24
3	H	6	MAN	C2-C3-C4	3.83	117.52	110.89
4	I	5	MAN	C2-C3-C4	3.82	117.51	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	7	MAN	C1-O5-C5	3.82	117.37	112.19
6	O	3	MAN	C3-C4-C5	3.80	117.01	110.24
7	Q	5	MAN	O5-C1-C2	3.77	116.59	110.77
6	L	3	MAN	O5-C5-C6	3.77	113.11	107.20
3	W	5	MAN	O2-C2-C3	3.77	117.69	110.14
5	K	1	NAG	O5-C5-C4	-3.76	101.68	110.83
5	K	8	MAN	O4-C4-C5	3.73	118.56	109.30
6	L	4	MAN	O5-C1-C2	3.72	116.52	110.77
4	R	5	MAN	C2-C3-C4	3.71	117.32	110.89
6	O	3	MAN	C1-O5-C5	3.70	117.20	112.19
6	O	4	MAN	C1-C2-C3	-3.69	105.13	109.67
7	Q	1	NAG	C3-C2-N2	3.68	117.57	110.62
5	K	6	MAN	C1-C2-C3	3.67	114.17	109.67
6	X	2	NAG	O4-C4-C3	3.65	118.80	110.35
3	T	4	BMA	C1-C2-C3	-3.65	105.18	109.67
4	R	1	NAG	C2-N2-C7	3.63	128.07	122.90
2	V	2	NAG	C8-C7-N2	3.61	122.22	116.10
6	L	3	MAN	C1-C2-C3	3.60	114.09	109.67
3	N	4	BMA	O5-C5-C6	3.58	112.82	107.20
6	U	3	MAN	C1-C2-C3	3.58	114.06	109.67
3	W	4	BMA	C1-C2-C3	-3.56	105.29	109.67
4	R	4	MAN	O5-C1-C2	3.55	116.25	110.77
3	H	5	MAN	O2-C2-C1	3.54	116.39	109.15
7	Q	3	BMA	O2-C2-C3	3.53	117.22	110.14
3	N	4	BMA	O5-C1-C2	-3.52	105.34	110.77
2	J	3	BMA	C3-C4-C5	3.51	116.50	110.24
7	Q	5	MAN	O5-C5-C6	3.50	112.69	107.20
6	X	3	MAN	C2-C3-C4	3.50	116.95	110.89
6	O	5	MAN	O5-C1-C2	3.49	116.16	110.77
7	Q	5	MAN	C2-C3-C4	3.49	116.93	110.89
6	L	3	MAN	C3-C4-C5	3.47	116.43	110.24
6	X	4	MAN	O6-C6-C5	3.47	123.19	111.29
2	M	2	NAG	C4-C3-C2	3.47	116.10	111.02
3	N	3	BMA	C1-C2-C3	-3.46	105.41	109.67
4	R	2	NAG	C2-N2-C7	3.45	127.81	122.90
3	T	3	BMA	O3-C3-C4	-3.42	102.43	110.35
6	L	4	MAN	C3-C4-C5	3.40	116.31	110.24
3	H	7	MAN	O5-C5-C6	3.37	112.49	107.20
6	U	5	MAN	C3-C4-C5	3.37	116.26	110.24
6	L	1	NAG	O5-C1-C2	-3.34	106.01	111.29
2	G	2	NAG	C3-C4-C5	3.33	116.18	110.24
5	K	3	BMA	C1-O5-C5	3.29	116.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	6	MAN	C1-O5-C5	3.29	116.64	112.19
3	H	7	MAN	O5-C1-C2	-3.28	105.70	110.77
3	W	3	BMA	O5-C5-C6	3.27	112.33	107.20
6	X	4	MAN	O5-C5-C6	3.27	112.33	107.20
4	I	2	NAG	O3-C3-C2	-3.27	102.70	109.47
4	I	2	NAG	C1-C2-N2	3.27	116.07	110.49
6	X	4	MAN	O5-C1-C2	3.27	115.81	110.77
5	K	8	MAN	O3-C3-C4	3.26	117.89	110.35
3	H	4	BMA	O2-C2-C3	3.26	116.66	110.14
6	O	2	NAG	C1-C2-N2	3.25	116.04	110.49
5	K	8	MAN	O4-C4-C3	-3.25	102.84	110.35
3	T	1	NAG	O4-C4-C5	-3.24	101.25	109.30
2	G	1	NAG	C4-C3-C2	-3.24	106.27	111.02
5	K	4	BMA	C3-C4-C5	3.22	115.98	110.24
6	L	5	MAN	C3-C4-C5	3.20	115.95	110.24
6	U	6	MAN	O5-C1-C2	-3.19	105.85	110.77
3	N	6	MAN	C2-C3-C4	3.17	116.39	110.89
6	U	3	MAN	C2-C3-C4	3.17	116.38	110.89
7	Q	2	BMA	O2-C2-C3	3.17	116.49	110.14
6	O	4	MAN	O6-C6-C5	3.17	122.16	111.29
2	M	1	NAG	O4-C4-C5	3.15	117.12	109.30
6	U	4	MAN	O5-C1-C2	3.15	115.63	110.77
4	R	2	NAG	O7-C7-N2	3.15	127.74	121.95
5	K	1	NAG	C1-O5-C5	3.14	116.44	112.19
2	M	2	NAG	C2-N2-C7	3.13	127.35	122.90
6	U	6	MAN	O5-C5-C6	3.12	112.10	107.20
4	I	4	MAN	O5-C1-C2	3.11	115.58	110.77
3	T	4	BMA	O5-C1-C2	-3.11	105.97	110.77
2	J	1	NAG	O5-C1-C2	-3.11	106.38	111.29
2	P	3	BMA	C3-C4-C5	3.11	115.78	110.24
2	S	3	BMA	C1-C2-C3	3.10	113.48	109.67
3	H	4	BMA	O6-C6-C5	3.10	121.92	111.29
2	P	1	NAG	O4-C4-C3	-3.07	103.25	110.35
2	J	1	NAG	O5-C5-C4	-3.06	103.37	110.83
3	W	3	BMA	O3-C3-C4	-3.06	103.28	110.35
6	O	5	MAN	C3-C4-C5	3.06	115.69	110.24
7	Q	3	BMA	O5-C1-C2	-3.05	106.06	110.77
4	R	3	MAN	O2-C2-C1	-3.05	102.92	109.15
3	T	7	MAN	C1-C2-C3	3.04	113.40	109.67
3	H	3	BMA	C1-C2-C3	-3.03	105.94	109.67
6	O	4	MAN	C3-C4-C5	3.03	115.64	110.24
6	O	6	MAN	C3-C4-C5	3.02	115.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	1	NAG	O5-C5-C4	-3.02	103.48	110.83
6	X	4	MAN	C3-C4-C5	3.02	115.62	110.24
4	R	4	MAN	C1-C2-C3	-3.00	105.98	109.67
4	I	3	MAN	O5-C5-C6	3.00	111.90	107.20
7	Q	2	BMA	O4-C4-C3	-2.99	103.42	110.35
3	W	4	BMA	C3-C4-C5	2.99	115.57	110.24
2	J	3	BMA	C1-C2-C3	2.99	113.34	109.67
2	V	1	NAG	C4-C3-C2	-2.99	106.64	111.02
3	W	1	NAG	C8-C7-N2	-2.98	111.05	116.10
3	T	1	NAG	O5-C5-C4	-2.98	103.58	110.83
3	H	6	MAN	O3-C3-C2	-2.97	104.31	109.99
3	T	3	BMA	O4-C4-C3	-2.97	103.49	110.35
4	I	5	MAN	C6-C5-C4	-2.96	106.06	113.00
4	I	4	MAN	C3-C4-C5	2.95	115.50	110.24
5	K	3	BMA	O4-C4-C3	-2.94	103.54	110.35
3	T	5	MAN	O2-C2-C3	2.94	116.03	110.14
4	R	3	MAN	C3-C4-C5	2.92	115.46	110.24
2	M	2	NAG	O3-C3-C2	-2.92	103.42	109.47
3	T	4	BMA	C1-O5-C5	-2.92	108.24	112.19
4	I	5	MAN	C1-C2-C3	2.92	113.25	109.67
6	X	5	MAN	O2-C2-C1	2.91	115.11	109.15
2	P	2	NAG	C8-C7-N2	2.91	121.02	116.10
6	U	5	MAN	C6-C5-C4	-2.91	106.20	113.00
2	P	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	V	1	NAG	O5-C5-C4	-2.90	103.78	110.83
5	K	6	MAN	O3-C3-C4	-2.89	103.67	110.35
4	I	1	NAG	O5-C5-C6	2.88	111.72	107.20
3	T	7	MAN	C1-O5-C5	2.88	116.09	112.19
5	K	4	BMA	C1-O5-C5	-2.87	108.30	112.19
3	W	7	MAN	C1-C2-C3	2.86	113.19	109.67
4	I	3	MAN	C1-O5-C5	2.86	116.06	112.19
5	K	4	BMA	O6-C6-C5	2.85	121.08	111.29
6	L	2	NAG	C6-C5-C4	-2.85	106.33	113.00
7	Q	2	BMA	O3-C3-C4	-2.85	103.77	110.35
6	X	6	MAN	C1-C2-C3	2.83	113.14	109.67
2	M	2	NAG	O5-C5-C6	2.82	111.63	107.20
3	N	5	MAN	O2-C2-C1	2.82	114.92	109.15
3	H	7	MAN	O2-C2-C3	2.82	115.79	110.14
2	S	1	NAG	O5-C5-C4	-2.81	103.98	110.83
5	K	8	MAN	O2-C2-C3	2.81	115.78	110.14
3	W	5	MAN	C2-C3-C4	-2.81	106.03	110.89
2	J	2	NAG	O4-C4-C3	-2.81	103.86	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	4	BMA	O5-C1-C2	-2.79	106.46	110.77
5	K	5	MAN	C1-C2-C3	-2.79	106.23	109.67
6	U	1	NAG	O5-C5-C6	2.78	111.57	107.20
3	H	6	MAN	C1-C2-C3	2.78	113.08	109.67
6	L	5	MAN	C1-C2-C3	-2.78	106.25	109.67
5	K	7	MAN	C3-C4-C5	2.77	115.19	110.24
2	P	2	NAG	O7-C7-C8	-2.77	116.90	122.06
3	H	1	NAG	O5-C5-C4	-2.77	104.08	110.83
6	U	4	MAN	O6-C6-C5	2.77	120.79	111.29
6	X	5	MAN	C6-C5-C4	-2.77	106.53	113.00
6	O	6	MAN	C2-C3-C4	2.76	115.68	110.89
4	I	4	MAN	O6-C6-C5	2.76	120.76	111.29
6	O	2	NAG	O3-C3-C2	-2.76	103.76	109.47
4	R	4	MAN	O6-C6-C5	2.75	120.74	111.29
5	K	8	MAN	O2-C2-C1	-2.75	103.53	109.15
6	X	5	MAN	C3-C4-C5	2.74	115.12	110.24
5	K	5	MAN	O3-C3-C4	2.74	116.67	110.35
3	T	6	MAN	O6-C6-C5	2.73	120.67	111.29
5	K	2	NAG	C1-O5-C5	-2.73	108.50	112.19
4	I	3	MAN	O2-C2-C1	-2.72	103.58	109.15
6	O	6	MAN	C1-C2-C3	2.72	113.02	109.67
2	P	2	NAG	C4-C3-C2	2.71	114.99	111.02
6	L	5	MAN	C6-C5-C4	-2.71	106.67	113.00
3	T	3	BMA	C6-C5-C4	-2.70	106.68	113.00
3	W	3	BMA	O4-C4-C3	-2.69	104.12	110.35
4	I	2	NAG	O4-C4-C3	2.69	116.56	110.35
2	M	2	NAG	C1-C2-N2	-2.67	105.93	110.49
2	S	1	NAG	C4-C3-C2	-2.67	107.11	111.02
6	L	5	MAN	O5-C1-C2	2.66	114.88	110.77
5	K	7	MAN	O3-C3-C2	-2.65	104.92	109.99
5	K	5	MAN	O6-C6-C5	-2.64	102.22	111.29
3	N	6	MAN	O6-C6-C5	2.64	120.36	111.29
2	M	2	NAG	O7-C7-C8	-2.64	117.15	122.06
7	Q	3	BMA	C1-O5-C5	-2.64	108.62	112.19
4	I	1	NAG	C2-N2-C7	2.63	126.65	122.90
4	R	4	MAN	C3-C4-C5	2.62	114.92	110.24
2	S	1	NAG	C1-C2-N2	2.62	114.96	110.49
4	I	4	MAN	C1-C2-C3	-2.61	106.46	109.67
7	Q	3	BMA	O6-C6-C5	2.61	120.23	111.29
4	R	5	MAN	O2-C2-C1	2.60	114.48	109.15
2	J	2	NAG	C1-C2-N2	-2.59	106.06	110.49
3	N	1	NAG	O5-C5-C4	-2.59	104.53	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	3	BMA	O5-C5-C6	2.59	111.26	107.20
2	J	1	NAG	C4-C3-C2	-2.58	107.23	111.02
3	T	4	BMA	O6-C6-C5	2.58	120.14	111.29
6	L	4	MAN	O6-C6-C5	2.58	120.13	111.29
3	T	5	MAN	O5-C1-C2	2.57	114.75	110.77
6	O	5	MAN	C2-C3-C4	2.57	115.34	110.89
3	N	5	MAN	O3-C3-C2	2.56	114.89	109.99
3	H	4	BMA	C3-C4-C5	2.55	114.79	110.24
2	G	3	BMA	O3-C3-C2	2.55	114.88	109.99
6	L	3	MAN	C2-C3-C4	2.54	115.29	110.89
5	K	5	MAN	C1-O5-C5	2.54	115.63	112.19
2	P	1	NAG	C4-C3-C2	-2.54	107.30	111.02
6	O	5	MAN	C1-C2-C3	2.53	112.77	109.67
6	O	1	NAG	O5-C5-C6	2.52	111.15	107.20
2	G	2	NAG	C4-C3-C2	2.51	114.70	111.02
6	U	1	NAG	O5-C1-C2	-2.50	107.33	111.29
3	T	7	MAN	O2-C2-C3	-2.50	105.12	110.14
5	K	6	MAN	O2-C2-C1	2.50	114.27	109.15
6	X	4	MAN	O4-C4-C3	-2.50	104.56	110.35
3	N	1	NAG	C3-C4-C5	-2.50	105.78	110.24
2	S	2	NAG	O4-C4-C3	-2.50	104.57	110.35
3	N	4	BMA	O6-C6-C5	2.50	119.85	111.29
4	R	5	MAN	O2-C2-C3	2.49	115.12	110.14
6	O	2	NAG	C1-O5-C5	2.49	115.56	112.19
2	S	3	BMA	O5-C1-C2	2.48	114.60	110.77
3	N	4	BMA	C1-O5-C5	-2.48	108.83	112.19
3	T	5	MAN	O5-C5-C4	2.47	116.84	110.83
3	H	4	BMA	O3-C3-C4	2.46	116.04	110.35
2	G	2	NAG	C2-N2-C7	2.46	126.41	122.90
3	T	2	NAG	C1-O5-C5	-2.46	108.86	112.19
7	Q	6	MAN	C1-O5-C5	2.46	115.52	112.19
6	U	3	MAN	O4-C4-C3	-2.46	104.67	110.35
4	I	5	MAN	O5-C1-C2	2.45	114.56	110.77
2	S	1	NAG	O4-C4-C3	-2.45	104.68	110.35
6	O	1	NAG	O5-C1-C2	-2.45	107.42	111.29
7	Q	3	BMA	O3-C3-C4	2.44	116.00	110.35
3	H	3	BMA	O2-C2-C3	2.43	115.01	110.14
7	Q	1	NAG	C1-C2-N2	-2.43	107.91	110.73
6	L	4	MAN	O3-C3-C4	2.43	115.96	110.35
2	G	2	NAG	O7-C7-C8	-2.41	117.58	122.06
6	U	4	MAN	C3-C4-C5	2.41	114.53	110.24
4	I	2	NAG	C1-O5-C5	2.40	115.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	1	NAG	O5-C5-C6	2.40	110.97	107.20
6	U	3	MAN	O2-C2-C3	2.40	114.95	110.14
3	W	4	BMA	O6-C6-C5	2.39	119.50	111.29
3	H	7	MAN	C1-O5-C5	2.38	115.42	112.19
2	G	3	BMA	O4-C4-C3	-2.38	104.84	110.35
3	W	1	NAG	O5-C5-C6	2.36	110.91	107.20
3	T	7	MAN	C2-C3-C4	2.36	114.98	110.89
3	N	5	MAN	C1-O5-C5	2.35	115.37	112.19
3	T	6	MAN	C6-C5-C4	2.35	118.50	113.00
3	T	5	MAN	O2-C2-C1	2.34	113.94	109.15
4	R	3	MAN	O5-C5-C6	2.34	110.86	107.20
3	T	7	MAN	O3-C3-C2	-2.33	105.53	109.99
3	W	5	MAN	O4-C4-C5	-2.33	103.52	109.30
3	W	6	MAN	O6-C6-C5	2.33	119.28	111.29
6	L	3	MAN	O2-C2-C3	2.32	114.78	110.14
2	M	1	NAG	O7-C7-C8	-2.32	117.75	122.06
6	X	1	NAG	O3-C3-C2	2.31	114.24	109.47
3	N	6	MAN	O3-C3-C2	-2.30	105.58	109.99
3	T	6	MAN	O3-C3-C2	-2.30	105.58	109.99
7	Q	5	MAN	O6-C6-C5	2.30	119.17	111.29
3	T	7	MAN	O5-C5-C6	2.29	110.80	107.20
4	R	2	NAG	C8-C7-N2	-2.29	112.22	116.10
4	R	2	NAG	C1-C2-N2	2.29	114.40	110.49
3	N	5	MAN	O6-C6-C5	-2.29	103.45	111.29
6	U	5	MAN	O2-C2-C3	-2.28	105.57	110.14
5	K	5	MAN	O2-C2-C3	2.28	114.70	110.14
4	I	3	MAN	C3-C4-C5	2.27	114.30	110.24
3	W	5	MAN	O5-C1-C2	2.27	114.27	110.77
6	U	5	MAN	O5-C1-C2	2.27	114.27	110.77
3	N	4	BMA	C3-C4-C5	2.27	114.28	110.24
5	K	6	MAN	O5-C5-C4	2.26	116.33	110.83
2	V	3	BMA	O4-C4-C3	-2.26	105.13	110.35
6	L	6	MAN	O5-C1-C2	-2.26	107.29	110.77
6	O	4	MAN	O4-C4-C5	2.25	114.89	109.30
3	W	7	MAN	C2-C3-C4	2.25	114.79	110.89
6	O	3	MAN	O3-C3-C2	-2.24	105.71	109.99
3	N	1	NAG	C1-O5-C5	2.24	115.22	112.19
4	R	4	MAN	O4-C4-C5	2.24	114.85	109.30
7	Q	1	NAG	C1-C2-C3	-2.23	107.50	110.54
4	R	2	NAG	O4-C4-C3	2.23	115.50	110.35
3	N	4	BMA	C6-C5-C4	2.23	118.22	113.00
2	G	1	NAG	C1-O5-C5	2.23	115.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	5	MAN	O2-C2-C1	2.22	113.69	109.15
6	U	3	MAN	O5-C1-C2	2.21	114.19	110.77
2	G	3	BMA	C3-C4-C5	2.21	114.18	110.24
6	L	3	MAN	O3-C3-C2	-2.21	105.77	109.99
6	X	3	MAN	C1-O5-C5	2.21	115.18	112.19
6	O	2	NAG	O7-C7-N2	2.19	125.98	121.95
5	K	4	BMA	O2-C2-C1	2.19	113.63	109.15
5	K	2	NAG	C6-C5-C4	-2.19	107.89	113.00
2	G	2	NAG	O5-C5-C6	2.18	110.63	107.20
6	L	2	NAG	C2-N2-C7	2.17	126.00	122.90
7	Q	4	MAN	O2-C2-C1	2.17	113.60	109.15
6	U	4	MAN	O4-C4-C3	-2.17	105.33	110.35
5	K	3	BMA	O6-C6-C5	-2.17	103.85	111.29
7	Q	4	MAN	O3-C3-C2	2.17	114.14	109.99
3	W	7	MAN	C1-O5-C5	2.17	115.13	112.19
3	W	5	MAN	O2-C2-C1	2.16	113.57	109.15
2	J	3	BMA	O5-C5-C6	2.16	110.59	107.20
6	L	6	MAN	C6-C5-C4	-2.15	107.96	113.00
4	R	2	NAG	O3-C3-C2	-2.15	105.02	109.47
3	W	2	NAG	C1-O5-C5	-2.14	109.29	112.19
7	Q	6	MAN	O5-C5-C6	2.14	110.56	107.20
5	K	8	MAN	O5-C1-C2	-2.14	107.47	110.77
5	K	5	MAN	O4-C4-C5	-2.13	104.00	109.30
3	N	3	BMA	O4-C4-C3	-2.12	105.44	110.35
3	H	1	NAG	O5-C5-C6	2.11	110.51	107.20
6	O	5	MAN	O5-C5-C6	2.11	110.51	107.20
6	X	1	NAG	C1-C2-N2	-2.11	106.89	110.49
3	H	1	NAG	O3-C3-C2	2.11	113.83	109.47
7	Q	6	MAN	O5-C1-C2	-2.11	107.52	110.77
4	I	3	MAN	O6-C6-C5	2.10	118.50	111.29
6	U	2	NAG	C4-C3-C2	-2.10	107.94	111.02
7	Q	1	NAG	O1-C1-O5	-2.10	104.08	110.38
3	T	7	MAN	C3-C4-C5	2.10	113.98	110.24
2	M	3	BMA	O3-C3-C2	2.10	114.01	109.99
3	H	5	MAN	O6-C6-C5	-2.10	104.10	111.29
6	O	1	NAG	C3-C4-C5	-2.10	106.50	110.24
7	Q	4	MAN	O2-C2-C3	2.08	114.31	110.14
6	U	2	NAG	O3-C3-C2	-2.08	105.16	109.47
6	O	3	MAN	O6-C6-C5	2.08	118.43	111.29
7	Q	5	MAN	C1-C2-C3	2.08	112.22	109.67
3	H	2	NAG	C4-C3-C2	-2.08	107.97	111.02
2	S	1	NAG	O4-C4-C5	-2.08	104.14	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	2	NAG	O4-C4-C3	2.07	115.15	110.35
3	T	5	MAN	O3-C3-C4	2.07	115.13	110.35
7	Q	4	MAN	C2-C3-C4	-2.07	107.32	110.89
6	U	6	MAN	O4-C4-C3	2.06	115.12	110.35
2	G	3	BMA	C1-C2-C3	2.06	112.19	109.67
6	L	4	MAN	O5-C5-C6	2.05	110.42	107.20
2	J	1	NAG	O5-C5-C6	2.05	110.42	107.20
4	R	5	MAN	C1-C2-C3	2.05	112.19	109.67
3	W	3	BMA	O6-C6-C5	-2.05	104.27	111.29
3	N	2	NAG	C2-N2-C7	2.05	125.82	122.90
3	N	4	BMA	O3-C3-C4	2.04	115.07	110.35
6	L	3	MAN	O2-C2-C1	-2.04	104.97	109.15
4	I	1	NAG	C1-C2-N2	-2.04	107.00	110.49
2	S	3	BMA	C2-C3-C4	-2.03	107.38	110.89
6	X	3	MAN	O4-C4-C3	-2.03	105.67	110.35
4	I	5	MAN	O2-C2-C1	2.02	113.29	109.15
3	H	5	MAN	C2-C3-C4	-2.02	107.40	110.89
3	H	7	MAN	C2-C3-C4	2.02	114.39	110.89
6	O	1	NAG	C1-O5-C5	2.02	114.93	112.19
6	U	1	NAG	O3-C3-C4	2.01	115.00	110.35
3	N	6	MAN	O4-C4-C3	-2.01	105.70	110.35
3	N	7	MAN	O4-C4-C3	-2.01	105.71	110.35
4	I	3	MAN	O3-C3-C2	-2.01	106.15	109.99
3	H	3	BMA	O4-C4-C3	-2.01	105.71	110.35
6	O	3	MAN	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
6	X	6	MAN	O5-C5-C6-O6
2	S	3	BMA	C4-C5-C6-O6
5	K	8	MAN	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	N	6	MAN	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
6	O	6	MAN	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	U	3	MAN	O5-C5-C6-O6
6	L	3	MAN	O5-C5-C6-O6
6	X	3	MAN	O5-C5-C6-O6
7	Q	5	MAN	O5-C5-C6-O6
6	X	6	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
6	O	5	MAN	C4-C5-C6-O6
4	I	4	MAN	C4-C5-C6-O6
6	L	3	MAN	C4-C5-C6-O6
6	X	3	MAN	C4-C5-C6-O6
3	T	6	MAN	O5-C5-C6-O6
4	I	3	MAN	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
6	U	4	MAN	C4-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
3	W	6	MAN	O5-C5-C6-O6
6	O	6	MAN	O5-C5-C6-O6
6	U	3	MAN	C4-C5-C6-O6
6	O	3	MAN	O5-C5-C6-O6
4	R	3	MAN	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
4	R	5	MAN	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
7	Q	5	MAN	C4-C5-C6-O6
6	X	4	MAN	C4-C5-C6-O6
2	P	3	BMA	O5-C5-C6-O6
2	V	3	BMA	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
5	K	8	MAN	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
3	N	6	MAN	C4-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
2	M	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	H	4	BMA	C4-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
4	R	4	MAN	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
3	T	6	MAN	C4-C5-C6-O6
6	X	4	MAN	O5-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
3	W	6	MAN	C4-C5-C6-O6
4	I	3	MAN	C4-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
3	W	5	MAN	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6

There are no ring outliers.

26 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	NAG	1	0
3	H	2	NAG	1	0
2	J	2	NAG	1	0
2	P	1	NAG	5	0
2	M	1	NAG	4	0
2	G	3	BMA	2	0
5	K	2	NAG	1	0
2	S	2	NAG	1	0
3	T	2	NAG	1	0
2	S	1	NAG	2	0
7	Q	1	NAG	3	0
5	K	6	MAN	6	0
3	H	1	NAG	3	0
2	G	2	NAG	1	0
2	J	1	NAG	2	0
2	M	2	NAG	1	0
3	W	2	NAG	1	0
2	G	1	NAG	2	0
5	K	1	NAG	4	0
3	T	1	NAG	4	0
2	P	2	NAG	1	0
2	V	1	NAG	2	0
3	W	1	NAG	3	0
5	K	8	MAN	8	0
3	N	1	NAG	4	0

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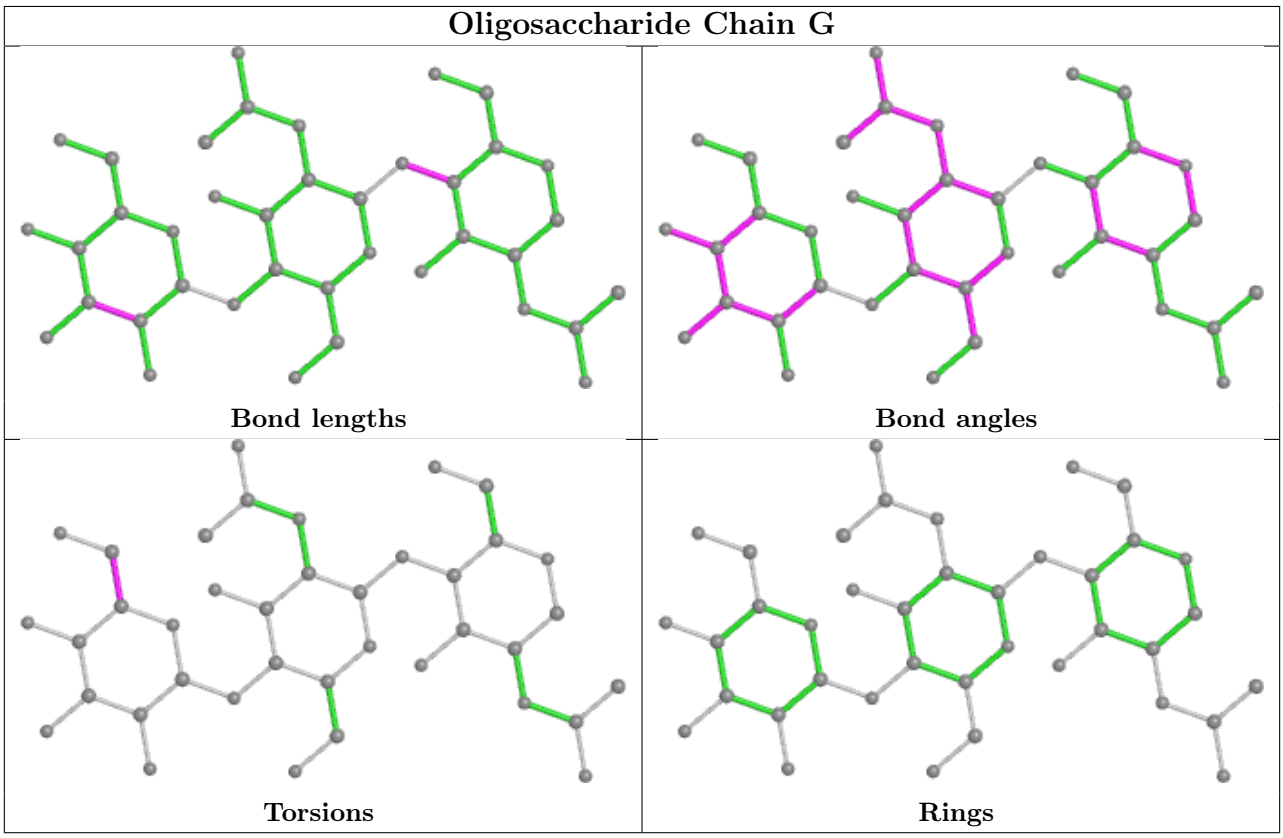
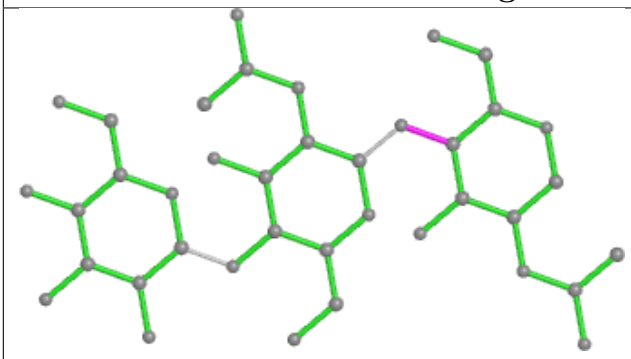
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	2	NAG	1	0

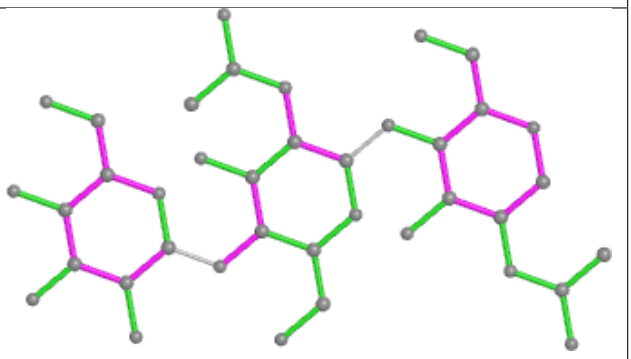
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



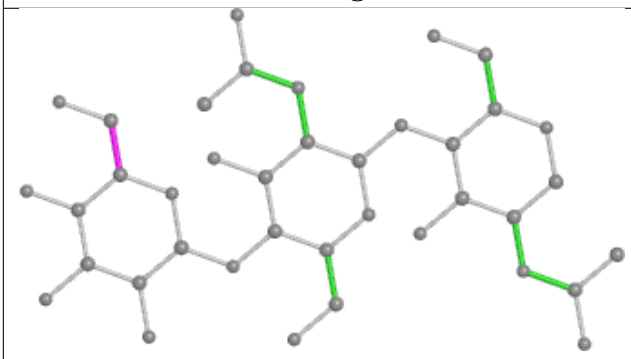
Oligosaccharide Chain J



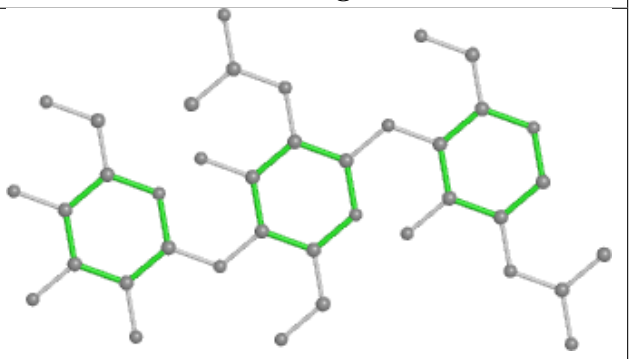
Bond lengths



Bond angles

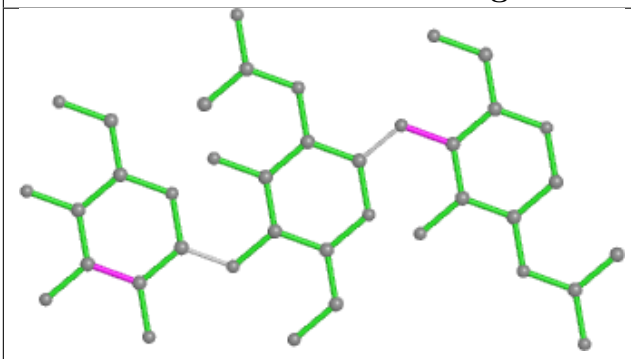


Torsions

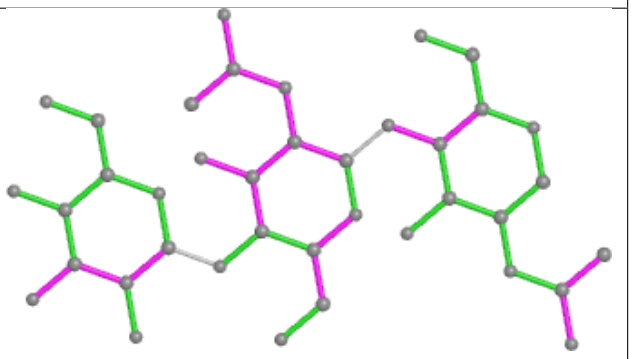


Rings

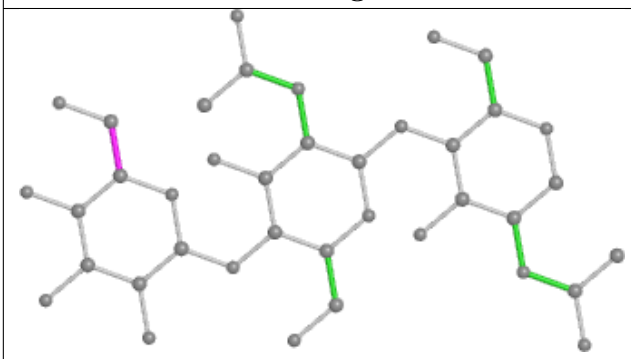
Oligosaccharide Chain M



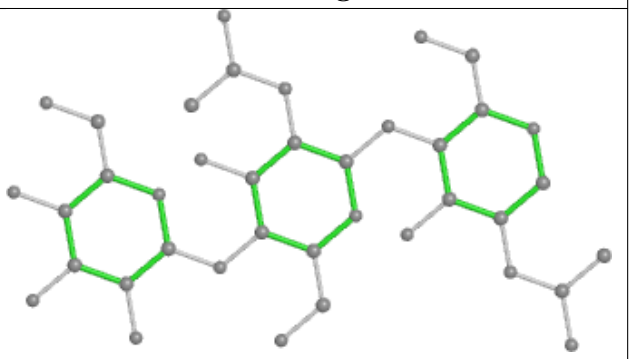
Bond lengths



Bond angles

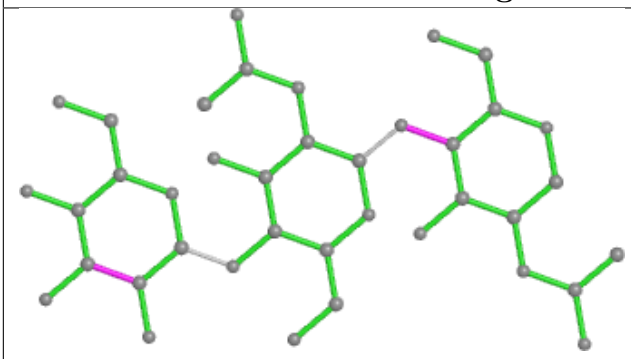


Torsions

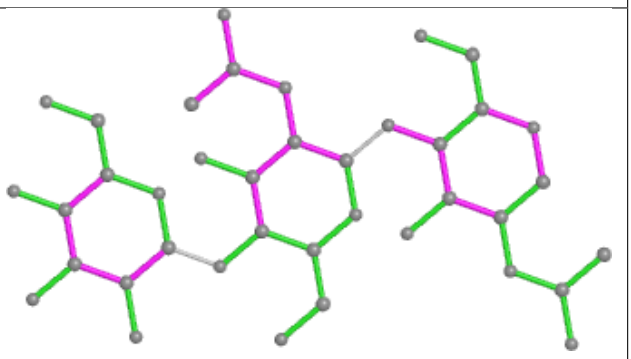


Rings

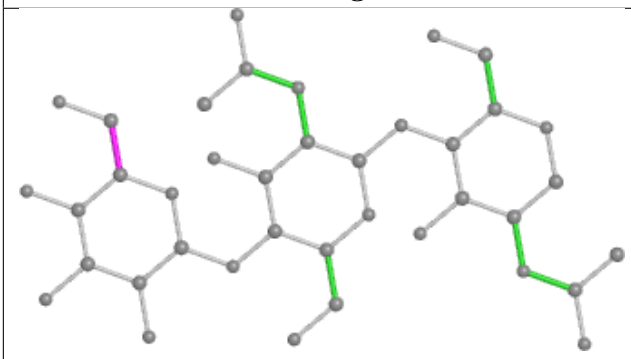
Oligosaccharide Chain P



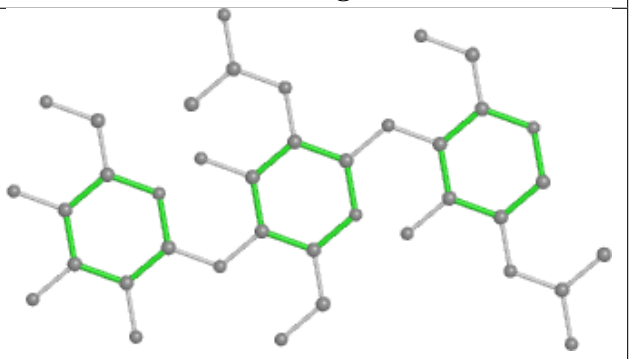
Bond lengths



Bond angles

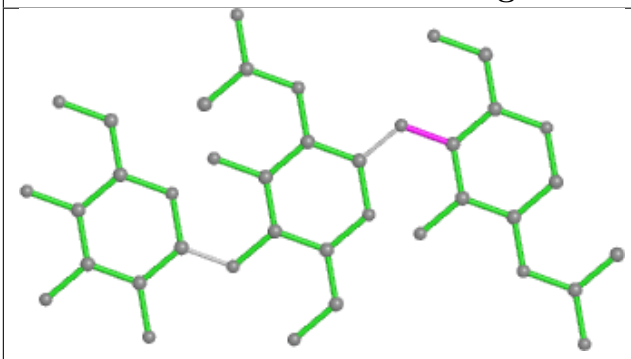


Torsions

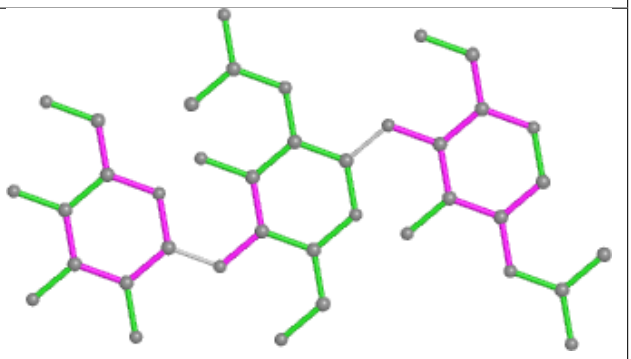


Rings

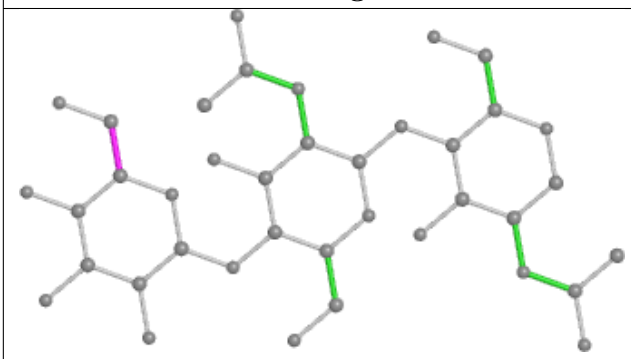
Oligosaccharide Chain S



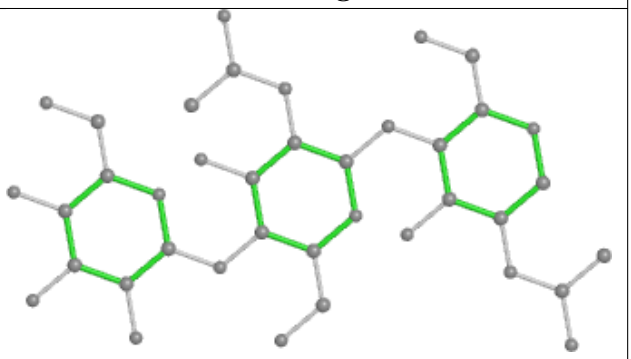
Bond lengths



Bond angles

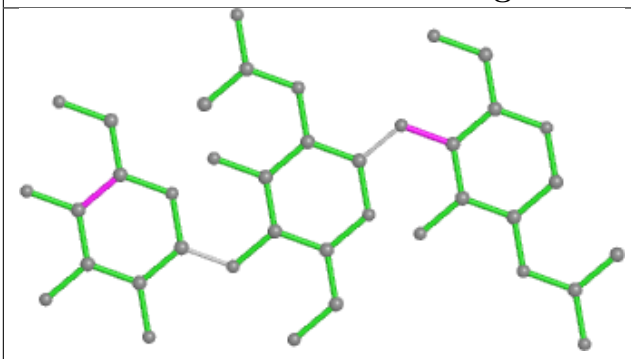


Torsions

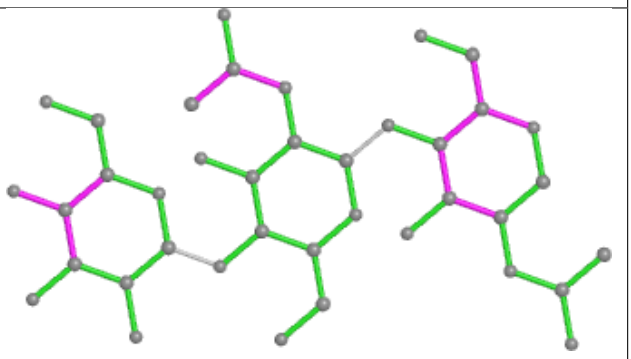


Rings

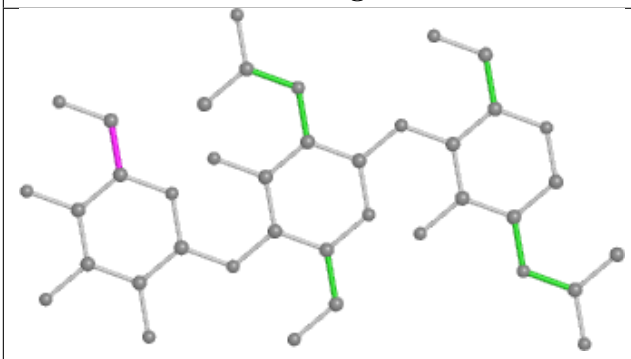
Oligosaccharide Chain V



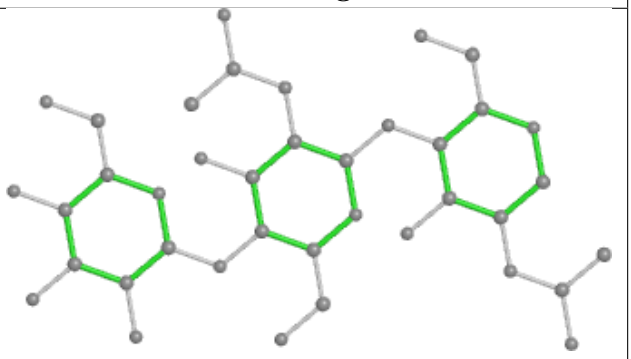
Bond lengths



Bond angles

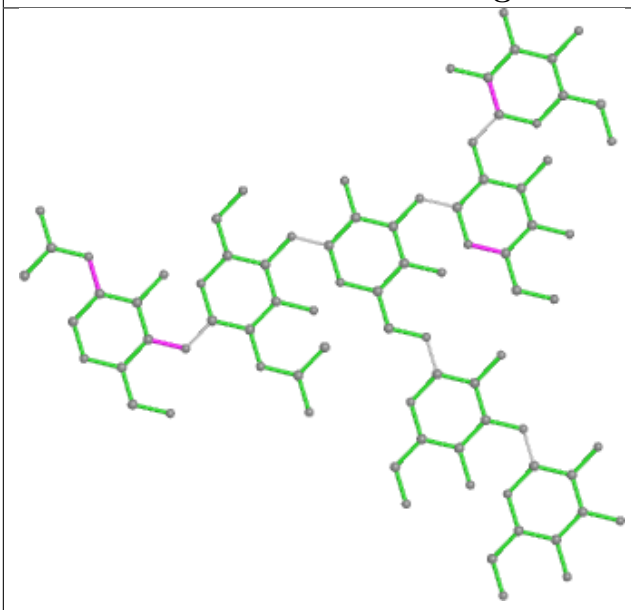


Torsions

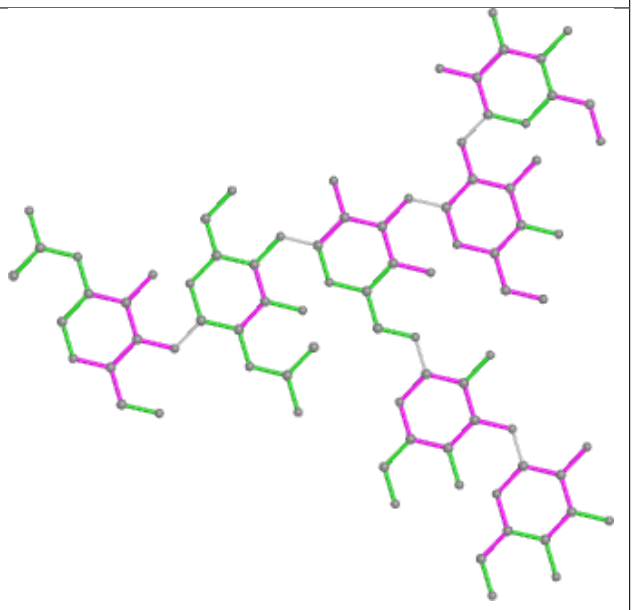


Rings

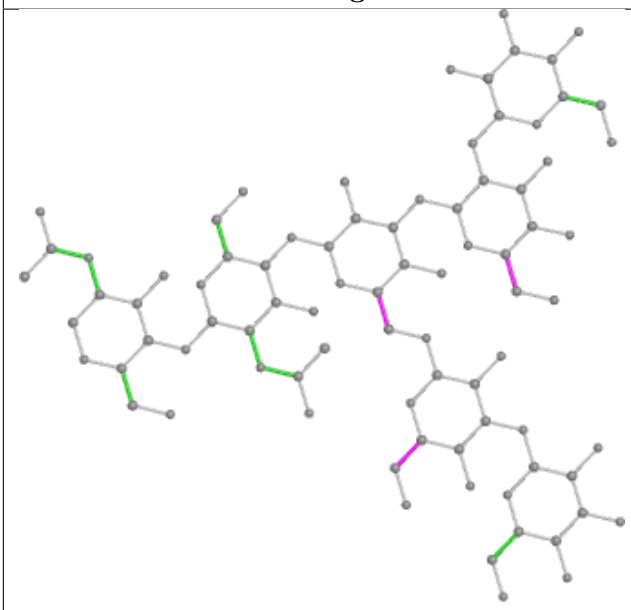
Oligosaccharide Chain H



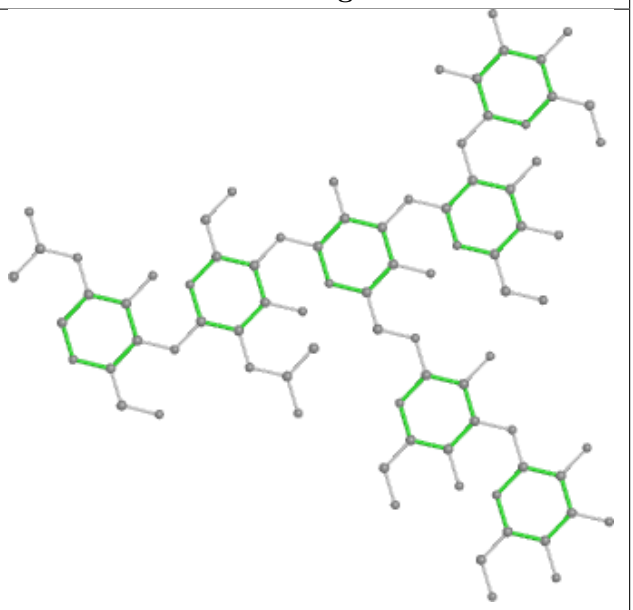
Bond lengths



Bond angles

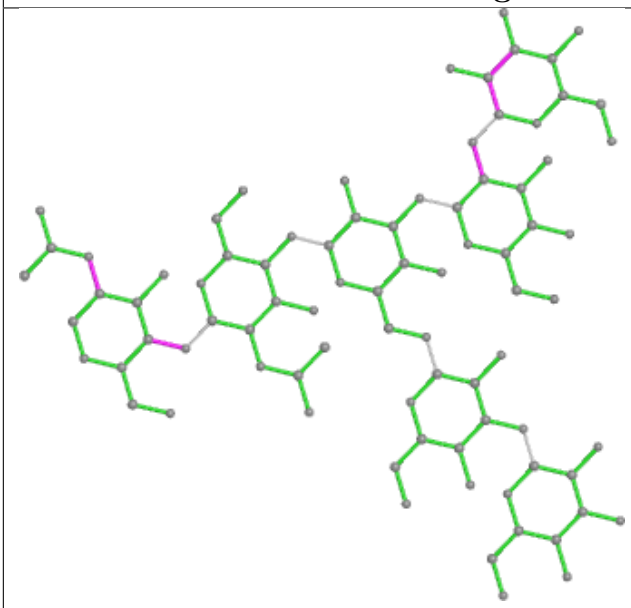


Torsions

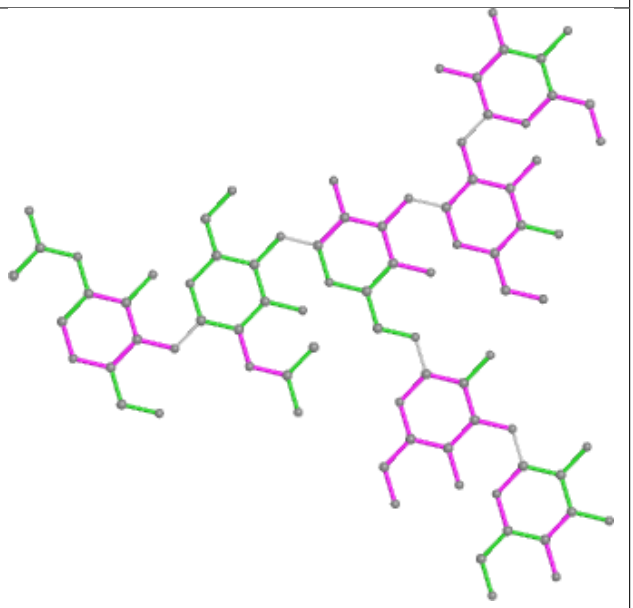


Rings

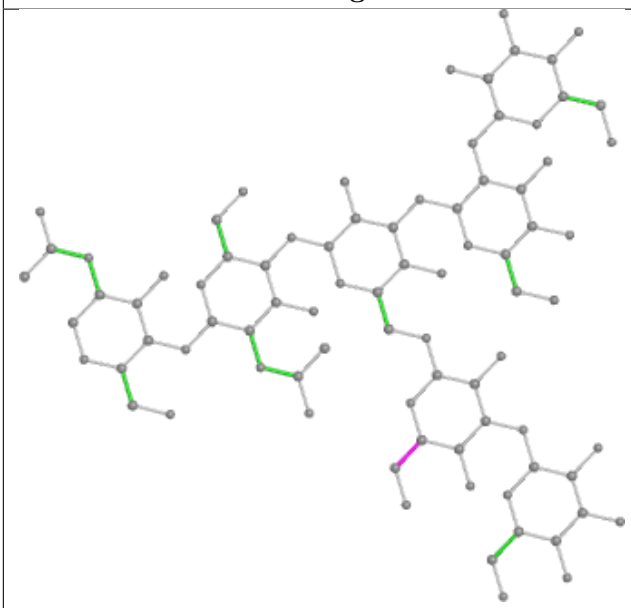
Oligosaccharide Chain N



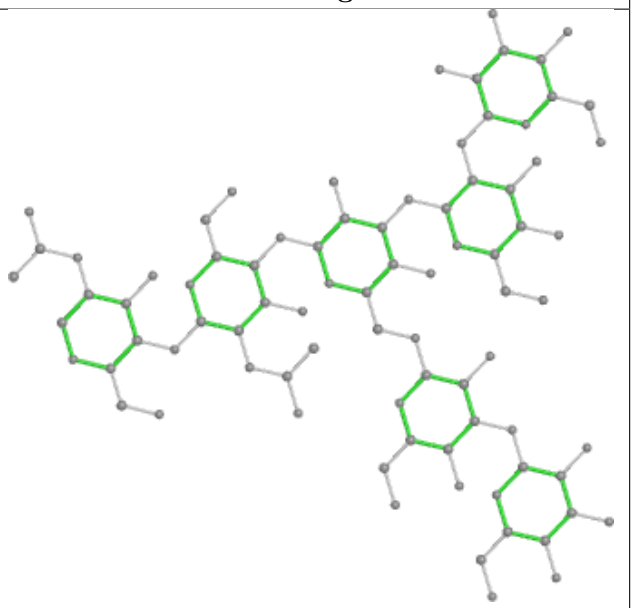
Bond lengths



Bond angles

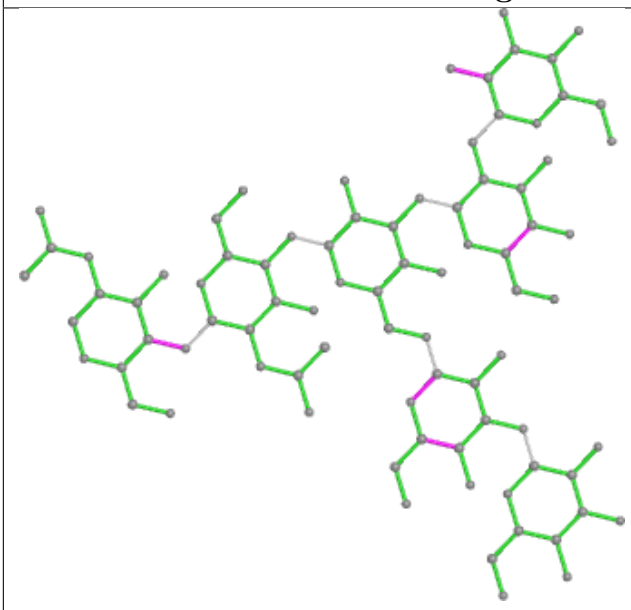


Torsions

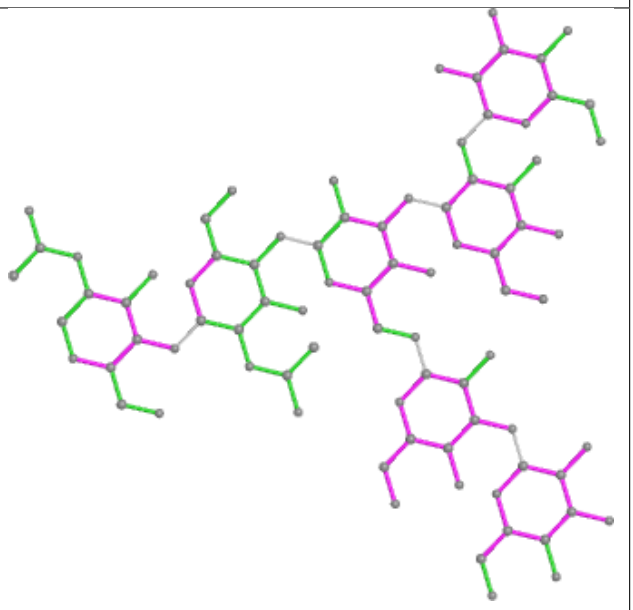


Rings

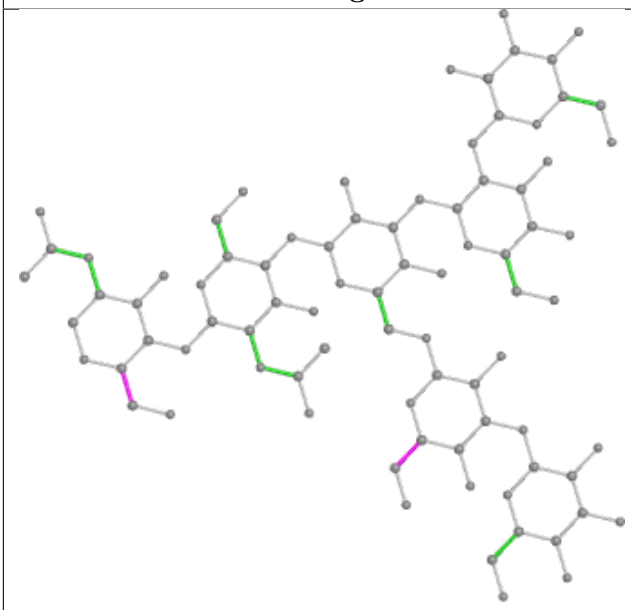
Oligosaccharide Chain T



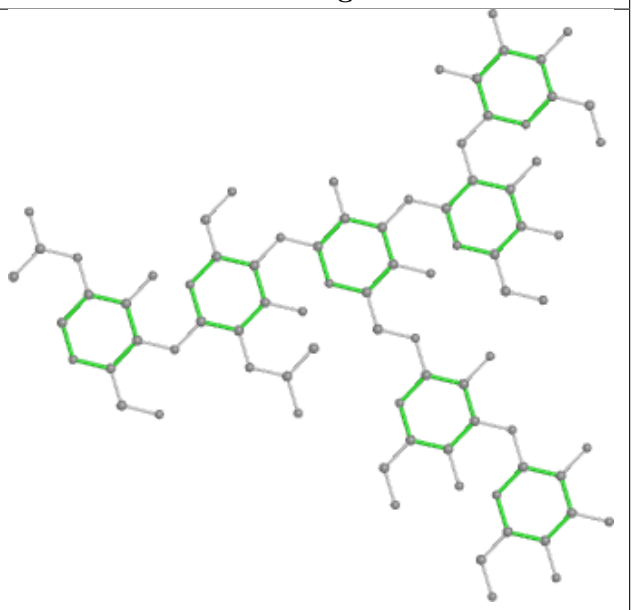
Bond lengths



Bond angles

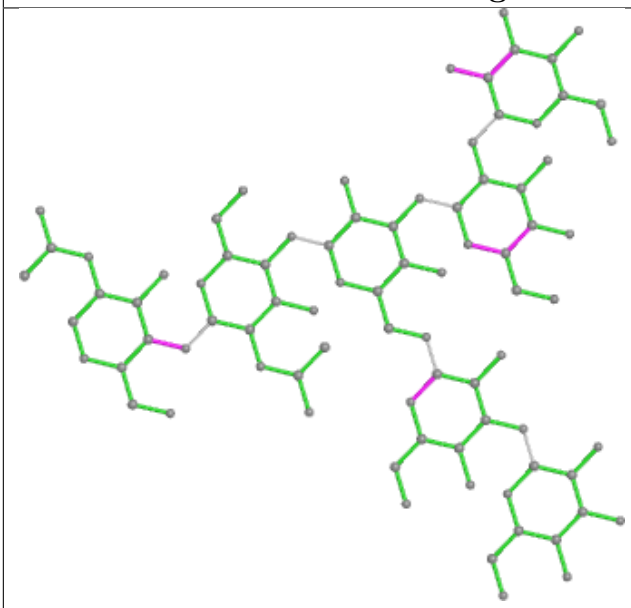


Torsions

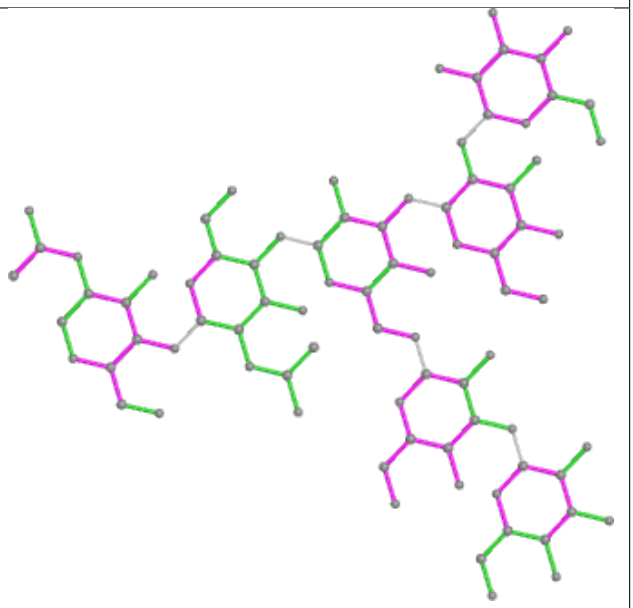


Rings

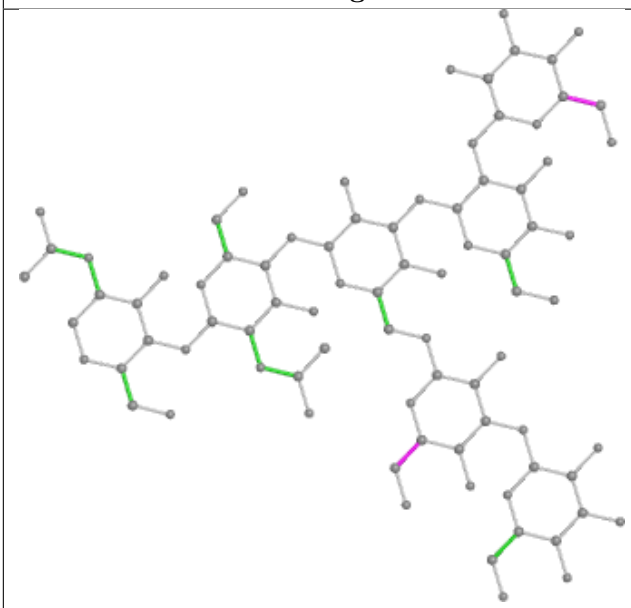
Oligosaccharide Chain W



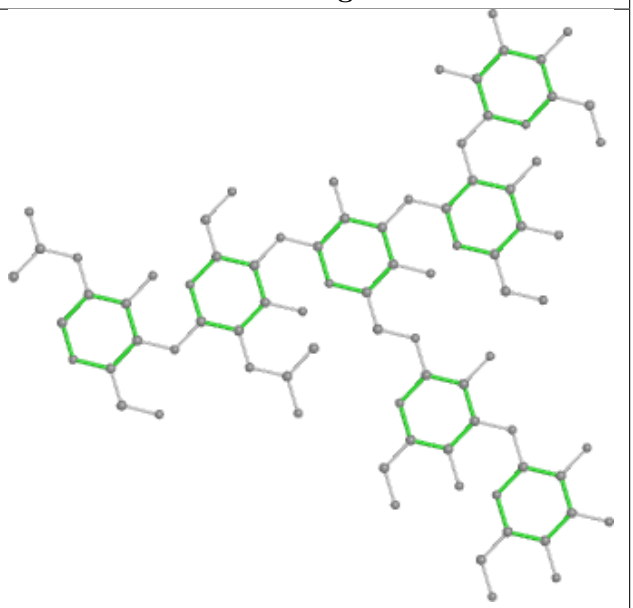
Bond lengths



Bond angles

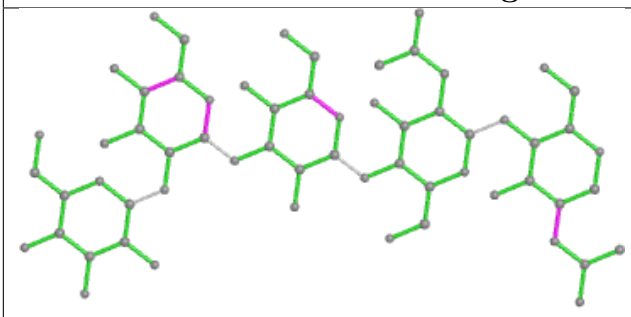


Torsions

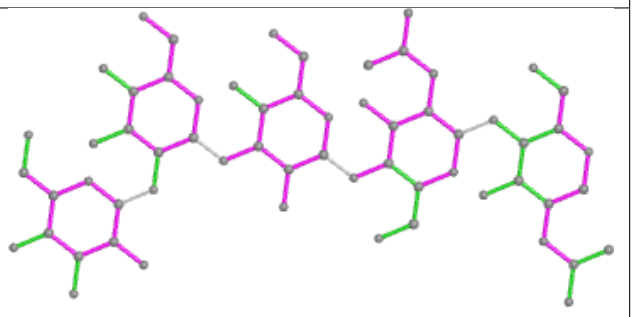


Rings

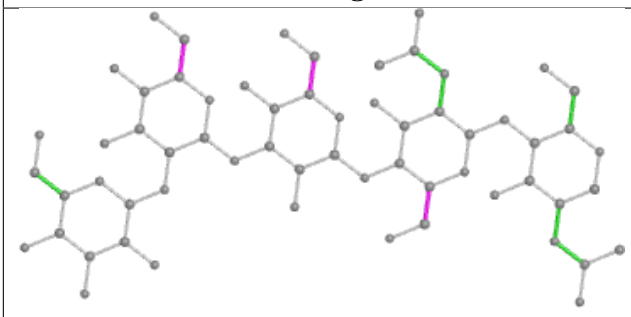
Oligosaccharide Chain I



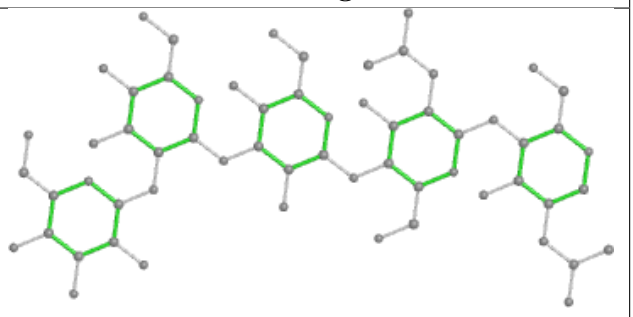
Bond lengths



Bond angles

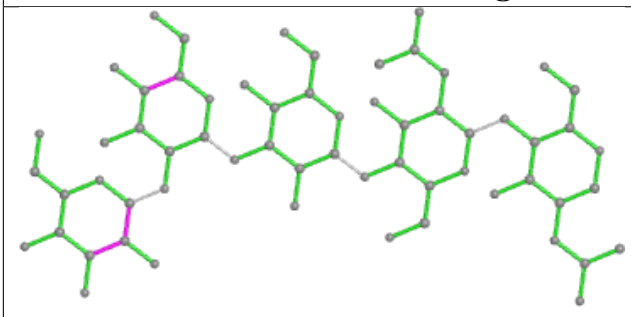


Torsions

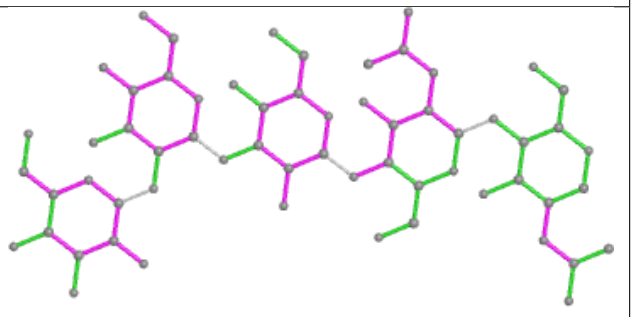


Rings

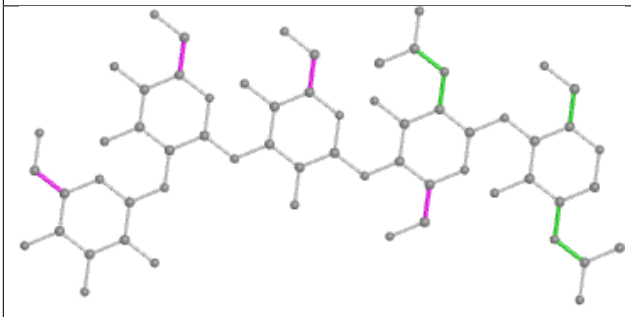
Oligosaccharide Chain R



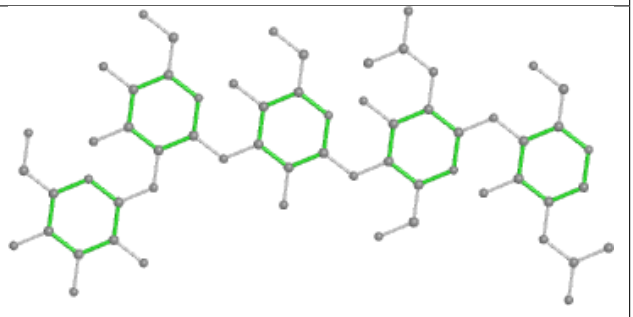
Bond lengths



Bond angles

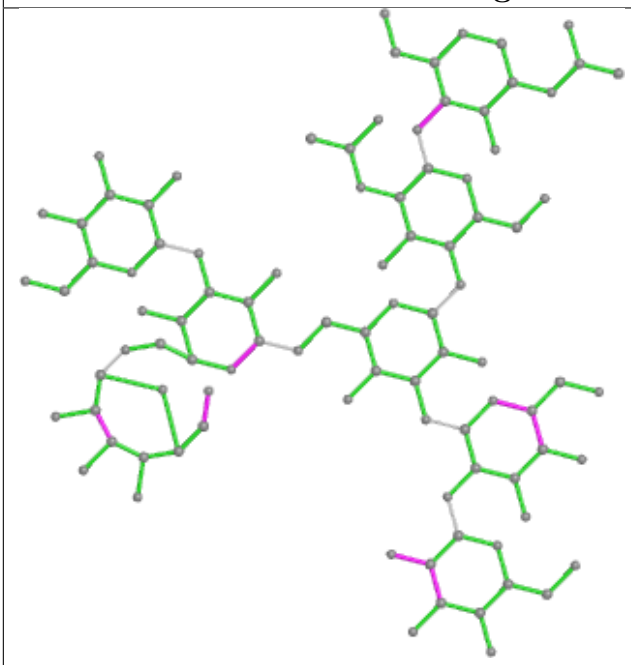


Torsions

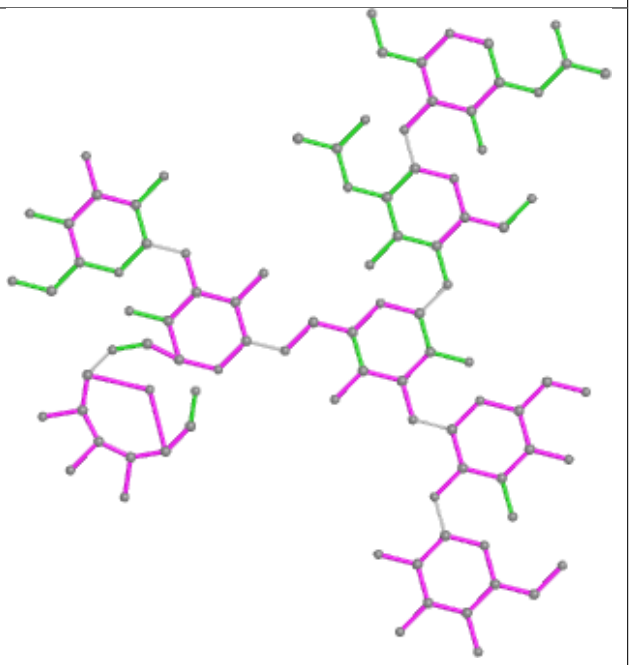


Rings

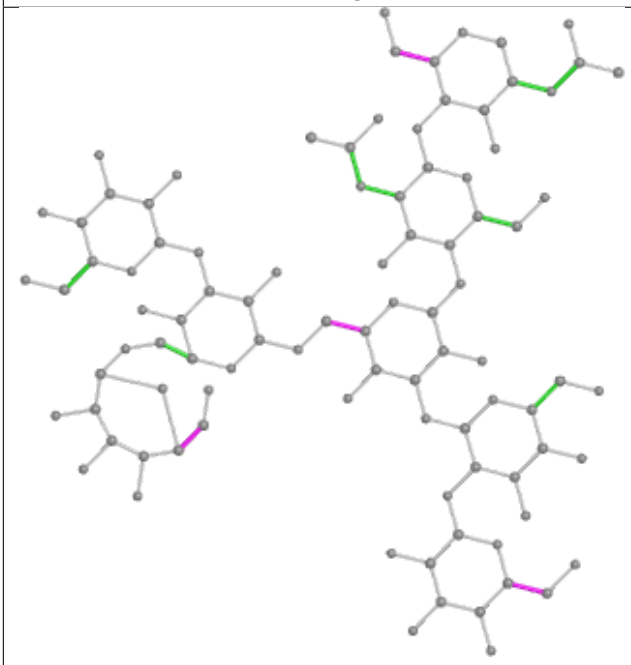
Oligosaccharide Chain K



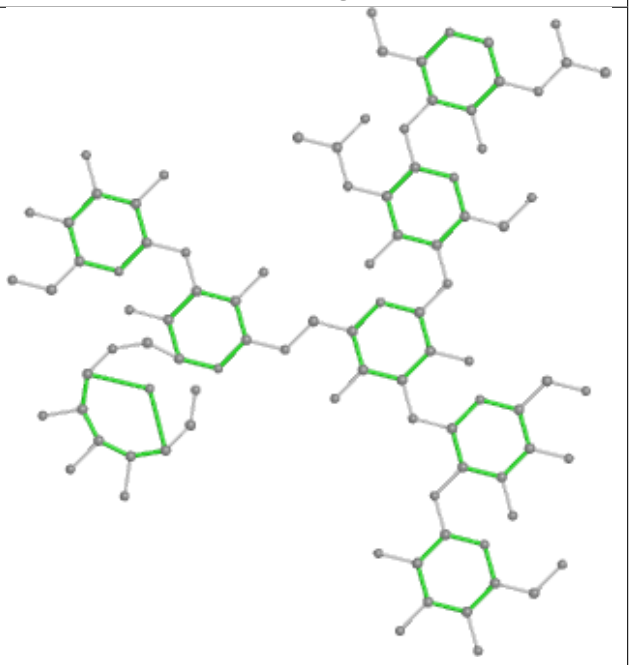
Bond lengths



Bond angles

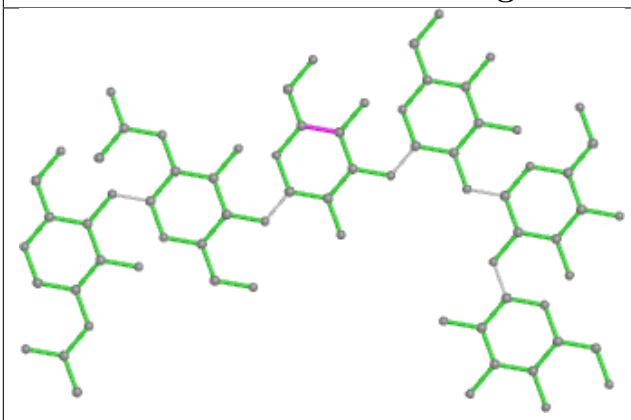


Torsions

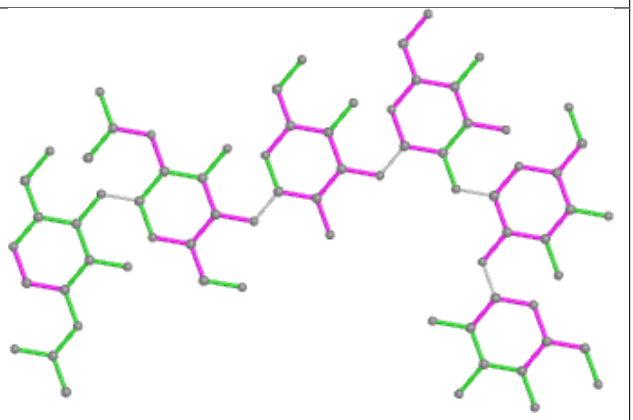


Rings

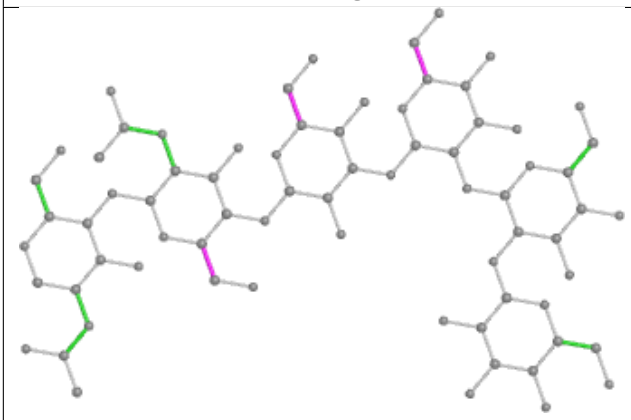
Oligosaccharide Chain L



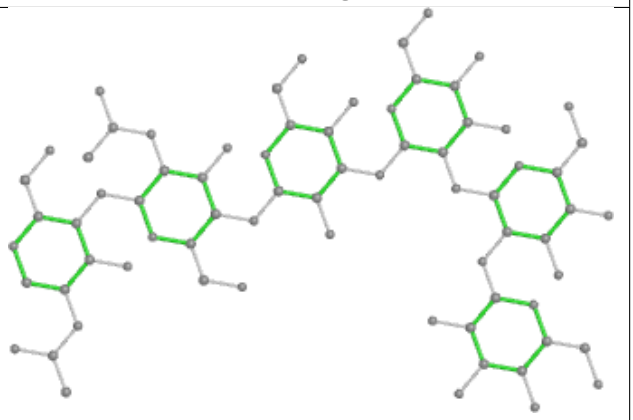
Bond lengths



Bond angles

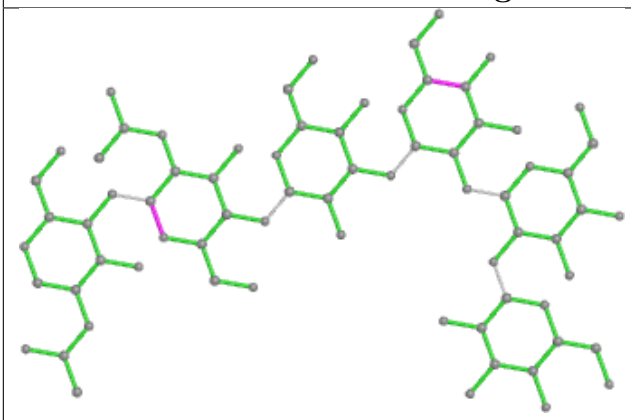


Torsions

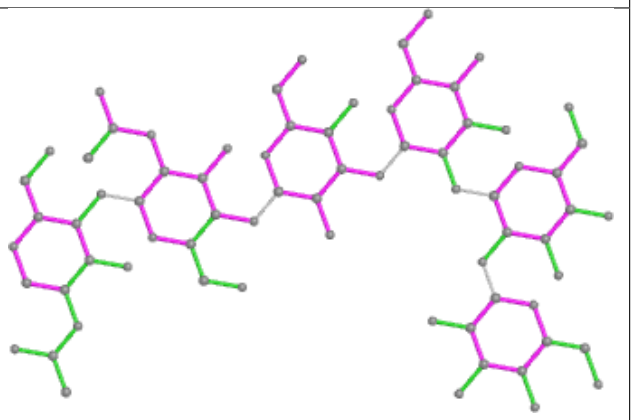


Rings

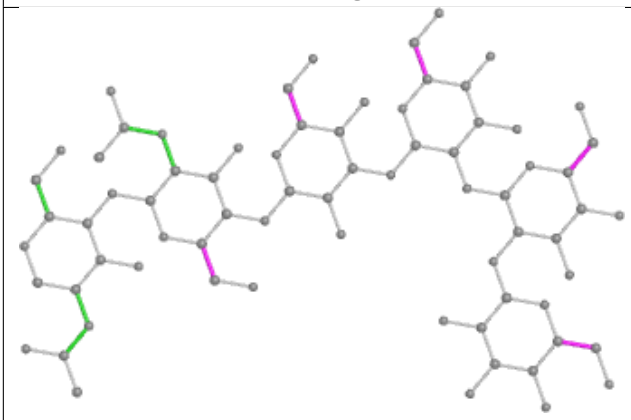
Oligosaccharide Chain O



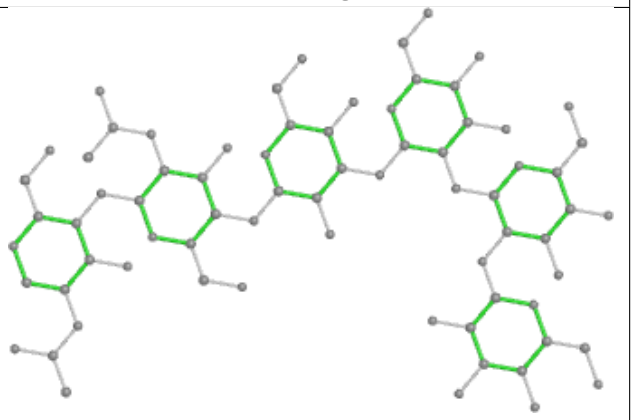
Bond lengths



Bond angles

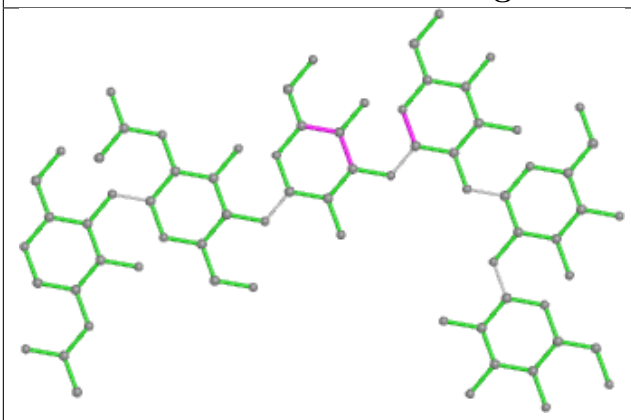


Torsions

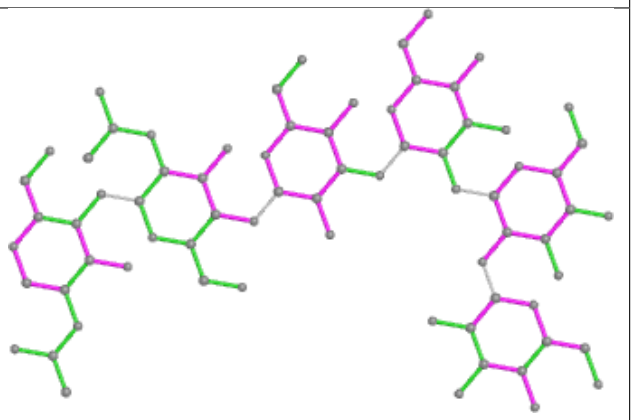


Rings

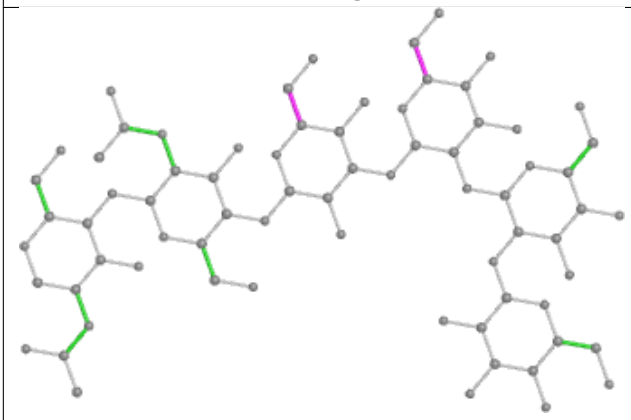
Oligosaccharide Chain U



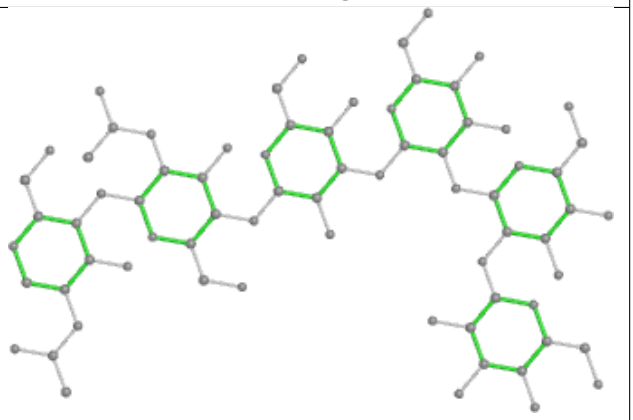
Bond lengths



Bond angles

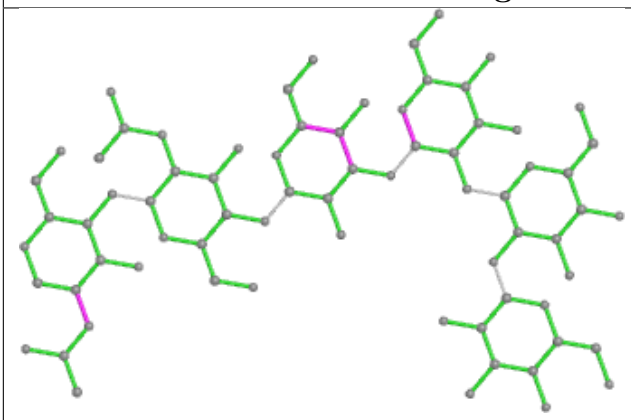


Torsions

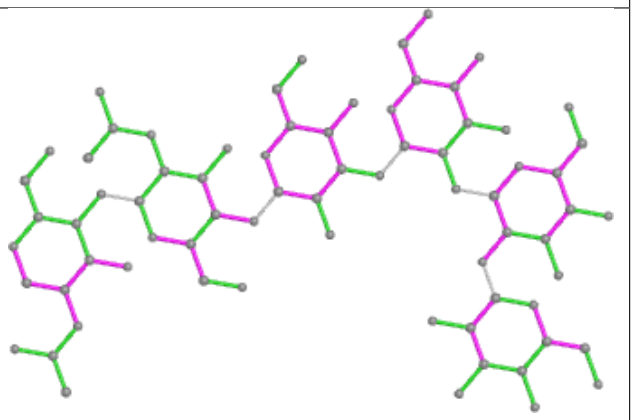


Rings

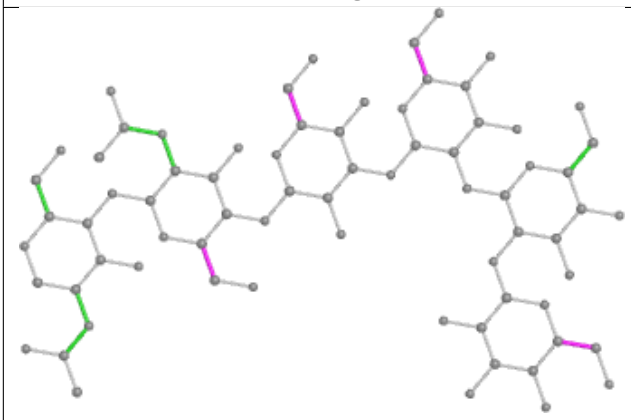
Oligosaccharide Chain X



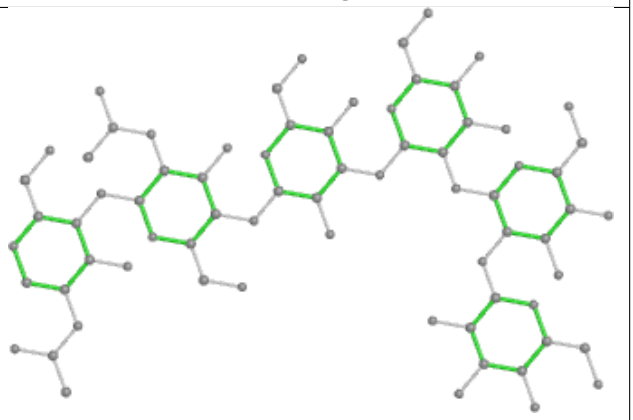
Bond lengths



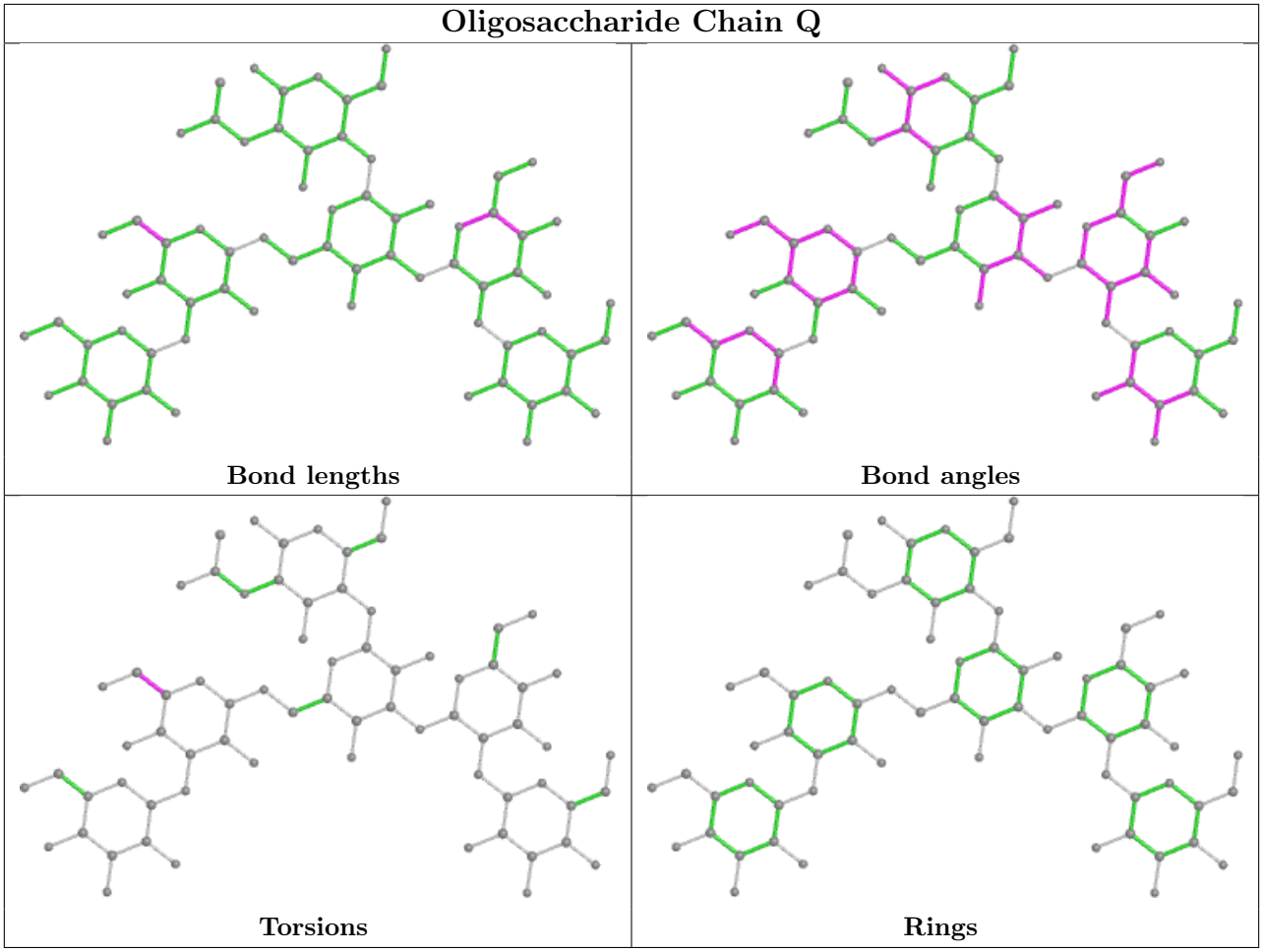
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	B	904	1	14,14,15	0.41	0	17,19,21	1.63	5 (29%)
8	NAG	B	905	1	14,14,15	1.67	2 (14%)	17,19,21	3.63	11 (64%)
8	NAG	D	905	1	14,14,15	1.94	4 (28%)	17,19,21	3.79	9 (52%)
11	XYL	D	907	-	9,9,9	1.09	1 (11%)	11,11,11	2.29	5 (45%)
8	NAG	A	903	1	14,14,15	0.88	1 (7%)	17,19,21	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	B	903	1	14,14,15	0.49	0	17,19,21	1.43	1 (5%)
9	XYZ	A	907	-	10,10,10	1.00	1 (10%)	13,14,14	2.90	6 (46%)
8	NAG	C	904	1	13,13,15	0.94	1 (7%)	16,17,21	2.21	3 (18%)
8	NAG	D	903	1	14,14,15	0.85	1 (7%)	17,19,21	1.31	4 (23%)
8	NAG	E	904	1	14,14,15	0.34	0	17,19,21	1.69	5 (29%)
8	NAG	E	905	1	14,14,15	0.81	0	17,19,21	3.73	9 (52%)
8	NAG	E	903	1	14,14,15	1.55	3 (21%)	17,19,21	2.73	5 (29%)
8	NAG	F	905	1	14,14,15	0.53	0	17,19,21	3.31	7 (41%)
10	BMA	A	908	-	11,11,12	1.15	2 (18%)	15,15,17	2.01	5 (33%)
11	XYL	E	906	-	9,9,9	1.24	1 (11%)	11,11,11	2.09	5 (45%)
8	NAG	C	906	1	14,14,15	0.45	0	17,19,21	1.50	2 (11%)
8	NAG	A	906	1	14,14,15	0.65	0	17,19,21	2.31	4 (23%)
8	NAG	F	903	1	14,14,15	1.09	2 (14%)	17,19,21	2.17	6 (35%)
8	NAG	D	904	1	13,13,15	1.27	1 (7%)	16,17,21	2.79	4 (25%)
11	XYL	C	907	-	9,9,9	1.22	1 (11%)	11,11,11	2.39	5 (45%)
8	NAG	A	905	1	14,14,15	0.77	1 (7%)	17,19,21	1.05	0
8	NAG	C	903	1	14,14,15	1.03	1 (7%)	17,19,21	2.07	4 (23%)
9	XYZ	B	906	-	10,10,10	1.23	1 (10%)	13,14,14	2.21	8 (61%)
8	NAG	C	905	1	14,14,15	0.75	1 (7%)	17,19,21	1.29	3 (17%)
8	NAG	F	904	1	14,14,15	0.47	0	17,19,21	1.48	3 (17%)
8	NAG	A	904	1	13,13,15	1.20	1 (7%)	16,17,21	3.07	5 (31%)
8	NAG	D	902	1	13,13,15	1.03	2 (15%)	14,17,21	1.80	3 (21%)
8	NAG	D	906	1	14,14,15	0.58	0	17,19,21	1.92	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
8	NAG	B	904	1	-	1/6/23/26	0/1/1/1
8	NAG	B	905	1	-	1/6/23/26	0/1/1/1
8	NAG	D	905	1	-	1/6/23/26	0/1/1/1
11	XYL	D	907	-	-	6/12/12/12	-
8	NAG	A	903	1	-	0/6/23/26	0/1/1/1
8	NAG	B	903	1	-	0/6/23/26	0/1/1/1
9	XYZ	A	907	-	-	2/2/18/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	904	1	-	0/6/19/26	0/1/1/1
8	NAG	D	903	1	-	0/6/23/26	0/1/1/1
8	NAG	E	904	1	-	0/6/23/26	0/1/1/1
8	NAG	E	905	1	-	2/6/23/26	0/1/1/1
8	NAG	E	903	1	-	0/6/23/26	0/1/1/1
8	NAG	F	905	1	-	3/6/23/26	0/1/1/1
10	BMA	A	908	-	-	2/2/19/22	0/1/1/1
11	XYL	E	906	-	-	2/12/12/12	-
8	NAG	C	906	1	-	0/6/23/26	0/1/1/1
8	NAG	A	906	1	-	2/6/23/26	0/1/1/1
8	NAG	F	903	1	-	3/6/23/26	0/1/1/1
8	NAG	D	904	1	-	1/6/19/26	0/1/1/1
11	XYL	C	907	-	-	8/12/12/12	-
8	NAG	A	905	1	-	0/6/23/26	0/1/1/1
8	NAG	C	903	1	-	2/6/23/26	0/1/1/1
9	XYZ	B	906	-	-	1/2/18/18	0/1/1/1
8	NAG	C	905	1	-	0/6/23/26	0/1/1/1
8	NAG	F	904	1	-	0/6/23/26	0/1/1/1
8	NAG	A	904	1	-	1/6/19/26	0/1/1/1
8	NAG	D	902	1	-	0/6/19/26	0/1/1/1
8	NAG	D	906	1	-	2/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	905	NAG	C1-C2	5.05	1.59	1.52
8	B	905	NAG	C1-C2	-4.46	1.45	1.52
8	E	903	NAG	C1-C2	4.05	1.58	1.52
8	D	904	NAG	C1-C2	3.82	1.55	1.51
8	B	905	NAG	C3-C2	3.75	1.60	1.52
8	A	904	NAG	C1-C2	3.17	1.54	1.51
8	D	905	NAG	O5-C1	-3.04	1.38	1.43
8	A	903	NAG	C1-C2	2.89	1.56	1.52
8	C	903	NAG	C1-C2	2.81	1.56	1.52
8	E	903	NAG	O5-C5	2.73	1.49	1.43
8	F	903	NAG	C1-C2	-2.72	1.48	1.52
11	C	907	XYL	C5-C4	2.68	1.59	1.52
8	D	905	NAG	O5-C5	2.60	1.48	1.43
8	D	903	NAG	C1-C2	2.55	1.56	1.52
9	B	906	XYZ	O4-C1	2.54	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	903	NAG	O5-C1	-2.53	1.39	1.43
8	D	902	NAG	C2-N2	-2.51	1.42	1.46
11	E	906	XYL	O2-C2	2.51	1.48	1.43
8	C	904	NAG	C1-C2	2.45	1.54	1.51
8	F	903	NAG	C3-C2	2.44	1.57	1.52
9	A	907	XYZ	C1-C2	2.43	1.55	1.52
11	D	907	XYL	C5-C4	2.42	1.58	1.52
8	D	905	NAG	C2-N2	-2.35	1.42	1.46
10	A	908	BMA	C2-C3	2.27	1.55	1.52
8	D	902	NAG	C3-C2	-2.18	1.50	1.52
10	A	908	BMA	C4-C5	2.17	1.57	1.53
8	A	905	NAG	C2-N2	-2.11	1.42	1.46
8	C	905	NAG	C2-N2	-2.08	1.42	1.46

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	905	NAG	O5-C1-C2	-11.29	93.46	111.29
8	E	905	NAG	C1-O5-C5	10.17	125.97	112.19
8	A	904	NAG	C3-C2-C1	10.14	118.83	109.50
8	D	904	NAG	C3-C2-C1	9.19	117.95	109.50
8	A	906	NAG	C1-O5-C5	7.79	122.74	112.19
8	B	905	NAG	C1-C2-N2	7.51	123.32	110.49
8	F	905	NAG	C2-N2-C7	7.38	133.42	122.90
8	F	905	NAG	C1-O5-C5	7.17	121.90	112.19
8	B	905	NAG	C1-O5-C5	7.08	121.78	112.19
8	E	903	NAG	O5-C5-C6	6.90	118.02	107.20
8	C	904	NAG	C3-C2-C1	6.78	115.73	109.50
8	E	903	NAG	O5-C1-C2	-6.74	100.65	111.29
8	D	905	NAG	O5-C5-C6	6.72	117.74	107.20
8	E	905	NAG	O5-C1-C2	-6.35	101.26	111.29
8	B	905	NAG	O5-C1-C2	-6.31	101.32	111.29
9	A	907	XYZ	O1-C1-O4	-6.12	103.30	111.13
9	A	907	XYZ	O4-C1-C2	5.96	111.80	104.46
8	D	906	NAG	C1-O5-C5	5.70	119.91	112.19
8	E	905	NAG	O5-C5-C6	-5.60	98.42	107.20
8	C	903	NAG	O5-C5-C6	5.47	115.79	107.20
8	F	903	NAG	C1-C2-N2	5.31	119.56	110.49
8	D	905	NAG	C1-O5-C5	4.49	118.28	112.19
8	F	905	NAG	O7-C7-N2	-4.42	113.83	121.95
8	F	905	NAG	C8-C7-N2	4.39	123.52	116.10
8	C	906	NAG	C1-O5-C5	4.37	118.11	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	904	NAG	C3-C4-C5	4.30	116.34	110.77
11	D	907	XYL	O4-C4-C5	4.30	119.23	109.14
10	A	908	BMA	C3-C4-C5	4.26	117.83	110.24
11	C	907	XYL	O4-C4-C5	4.20	119.01	109.14
8	A	904	NAG	C3-C2-N2	-4.20	104.20	110.57
8	F	905	NAG	O5-C1-C2	-4.07	104.86	111.29
8	F	903	NAG	O3-C3-C2	4.00	117.74	109.47
8	D	902	NAG	O5-C5-C4	-3.95	104.25	110.65
11	D	907	XYL	O5-C5-C4	3.92	119.62	111.07
8	F	905	NAG	C6-C5-C4	-3.84	104.01	113.00
8	C	904	NAG	C3-C4-C5	3.80	115.69	110.77
8	D	902	NAG	C4-C3-C2	-3.74	105.11	110.84
8	F	903	NAG	O5-C5-C6	3.70	113.00	107.20
8	A	904	NAG	C3-C4-C5	3.68	115.53	110.77
9	A	907	XYZ	C1-C2-C3	-3.64	97.75	102.30
8	B	905	NAG	C6-C5-C4	-3.62	104.53	113.00
11	C	907	XYL	O2-C2-C3	3.56	117.76	109.10
8	D	905	NAG	O3-C3-C2	3.56	116.83	109.47
8	E	904	NAG	C2-N2-C7	3.53	127.94	122.90
11	E	906	XYL	O4-C4-C3	3.34	117.21	109.10
8	E	905	NAG	C1-C2-N2	-3.32	104.81	110.49
8	B	905	NAG	C4-C3-C2	3.31	115.86	111.02
8	B	904	NAG	O5-C5-C6	3.27	112.32	107.20
8	E	905	NAG	C8-C7-N2	-3.23	110.63	116.10
9	B	906	XYZ	O3-C3-C2	-3.21	101.44	111.82
10	A	908	BMA	C1-O5-C5	3.16	116.47	112.19
11	C	907	XYL	O3-C3-C2	3.13	116.38	108.81
8	B	903	NAG	O5-C5-C6	3.11	112.07	107.20
8	D	906	NAG	C2-N2-C7	3.10	127.31	122.90
8	F	904	NAG	C1-O5-C5	3.10	116.39	112.19
8	B	905	NAG	C2-N2-C7	3.09	127.30	122.90
11	C	907	XYL	O5-C5-C4	3.06	117.75	111.07
8	E	904	NAG	C1-O5-C5	3.05	116.33	112.19
9	B	906	XYZ	O1-C1-O4	3.01	114.99	111.13
11	E	906	XYL	C1-C2-C3	-3.00	105.91	112.41
10	A	908	BMA	O3-C3-C2	3.00	115.74	109.99
10	A	908	BMA	O2-C2-C3	3.00	116.14	110.14
8	B	905	NAG	O7-C7-N2	2.98	127.44	121.95
9	A	907	XYZ	O2-C2-C1	2.98	120.05	111.82
8	C	903	NAG	C1-O5-C5	2.97	116.22	112.19
8	A	906	NAG	C3-C4-C5	2.92	115.45	110.24
9	B	906	XYZ	C1-C2-C3	2.91	105.94	102.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	906	XYL	C4-C3-C2	2.89	119.37	113.36
8	C	905	NAG	O5-C5-C6	2.88	111.71	107.20
8	D	903	NAG	O5-C5-C6	2.87	111.70	107.20
8	D	906	NAG	C3-C4-C5	2.85	115.33	110.24
8	E	905	NAG	O3-C3-C2	-2.85	103.56	109.47
8	B	905	NAG	O3-C3-C2	2.84	115.34	109.47
9	B	906	XYZ	C2-C3-C4	2.84	108.16	102.64
8	D	905	NAG	C2-N2-C7	2.83	126.93	122.90
8	F	904	NAG	O5-C5-C6	2.79	111.58	107.20
8	C	903	NAG	C4-C3-C2	-2.76	106.98	111.02
8	E	903	NAG	C3-C4-C5	-2.74	105.35	110.24
8	C	903	NAG	O5-C1-C2	2.72	115.59	111.29
9	A	907	XYZ	O5-C5-C4	-2.72	101.97	111.29
8	A	906	NAG	C2-N2-C7	2.67	126.70	122.90
8	B	905	NAG	O5-C5-C6	2.63	111.33	107.20
8	B	904	NAG	C2-N2-C7	2.62	126.64	122.90
11	E	906	XYL	O2-C2-C1	2.62	115.28	109.14
8	E	905	NAG	C6-C5-C4	2.61	119.11	113.00
8	D	905	NAG	C6-C5-C4	-2.60	106.90	113.00
8	E	905	NAG	O6-C6-C5	2.57	120.11	111.29
8	D	905	NAG	C3-C4-C5	-2.56	105.67	110.24
8	E	903	NAG	O3-C3-C2	2.52	114.67	109.47
9	B	906	XYZ	O2-C2-C1	2.51	118.75	111.82
8	B	904	NAG	C4-C3-C2	-2.48	107.39	111.02
11	E	906	XYL	O3-C3-C2	-2.47	102.85	108.81
8	D	905	NAG	C8-C7-N2	-2.43	111.99	116.10
9	B	906	XYZ	O5-C5-C4	-2.40	103.06	111.29
8	C	904	NAG	C3-C2-N2	-2.37	106.97	110.57
8	B	905	NAG	O6-C6-C5	2.36	119.40	111.29
8	D	902	NAG	C8-C7-N2	-2.36	112.10	116.10
8	F	905	NAG	O3-C3-C2	-2.35	104.61	109.47
11	D	907	XYL	O4-C4-C3	-2.35	103.40	109.10
8	E	905	NAG	C2-N2-C7	2.34	126.23	122.90
8	D	903	NAG	C4-C3-C2	-2.33	107.60	111.02
8	A	906	NAG	O5-C1-C2	2.31	114.94	111.29
8	F	903	NAG	C2-N2-C7	2.29	126.17	122.90
8	E	904	NAG	C4-C3-C2	-2.25	107.71	111.02
8	C	905	NAG	C8-C7-N2	-2.25	112.30	116.10
8	A	903	NAG	O5-C5-C6	2.24	110.71	107.20
9	B	906	XYZ	O4-C1-C2	2.22	107.19	104.46
8	C	906	NAG	C4-C3-C2	-2.22	107.77	111.02
11	D	907	XYL	O3-C3-C2	2.21	114.14	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	907	XYL	O1-C1-C2	2.20	115.86	111.07
8	A	904	NAG	O5-C5-C4	2.18	113.31	109.64
8	A	904	NAG	C6-C5-C4	-2.18	110.50	113.54
8	F	903	NAG	O3-C3-C4	-2.18	105.31	110.35
8	E	903	NAG	C1-O5-C5	2.18	115.15	112.19
8	D	905	NAG	C4-C3-C2	-2.18	107.83	111.02
8	D	903	NAG	O3-C3-C2	2.18	113.97	109.47
8	B	904	NAG	C3-C4-C5	-2.17	106.36	110.24
8	B	905	NAG	C8-C7-N2	-2.15	112.46	116.10
8	F	904	NAG	C2-N2-C7	2.14	125.94	122.90
9	A	907	XYZ	O3-C3-C2	-2.13	104.95	111.82
8	F	903	NAG	C4-C3-C2	2.10	114.10	111.02
8	D	904	NAG	O4-C4-C5	-2.10	105.55	110.01
10	A	908	BMA	O5-C5-C4	2.09	115.92	110.83
11	D	907	XYL	C5-C4-C3	2.08	116.92	112.41
8	E	904	NAG	O5-C5-C4	-2.08	105.78	110.83
8	E	904	NAG	O5-C1-C2	-2.05	108.05	111.29
8	B	904	NAG	O5-C5-C4	-2.05	105.84	110.83
8	D	903	NAG	O5-C5-C4	-2.02	105.92	110.83
8	C	905	NAG	C2-N2-C7	2.02	125.77	122.90
9	B	906	XYZ	O3-C3-C4	2.00	116.84	111.05
8	D	904	NAG	C3-C2-N2	-2.00	107.54	110.57

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	905	NAG	C3-C2-N2-C7
8	E	905	NAG	C3-C2-N2-C7
8	F	905	NAG	C3-C2-N2-C7
11	C	907	XYL	O1-C1-C2-C3
11	C	907	XYL	O1-C1-C2-O2
11	C	907	XYL	O2-C2-C3-O3
11	C	907	XYL	O4-C4-C5-O5
11	D	907	XYL	O2-C2-C3-C4
11	D	907	XYL	O2-C2-C3-O3
11	D	907	XYL	O4-C4-C5-O5
9	A	907	XYZ	C3-C4-C5-O5
8	C	903	NAG	O5-C5-C6-O6
10	A	908	BMA	O5-C5-C6-O6
11	C	907	XYL	C3-C4-C5-O5
11	D	907	XYL	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
9	A	907	XYZ	O4-C4-C5-O5
11	C	907	XYL	C1-C2-C3-O3
11	D	907	XYL	C1-C2-C3-O3
11	C	907	XYL	C1-C2-C3-C4
11	D	907	XYL	C1-C2-C3-C4
8	C	903	NAG	C4-C5-C6-O6
8	F	905	NAG	C8-C7-N2-C2
8	F	905	NAG	O7-C7-N2-C2
8	D	906	NAG	C4-C5-C6-O6
8	A	906	NAG	C4-C5-C6-O6
8	E	905	NAG	O5-C5-C6-O6
11	C	907	XYL	O2-C2-C3-C4
8	A	904	NAG	O5-C5-C6-O6
8	F	903	NAG	C4-C5-C6-O6
8	F	903	NAG	C1-C2-N2-C7
8	F	903	NAG	O5-C5-C6-O6
8	D	905	NAG	C4-C5-C6-O6
10	A	908	BMA	C4-C5-C6-O6
8	D	906	NAG	O5-C5-C6-O6
11	E	906	XYL	C2-C3-C4-C5
8	A	906	NAG	O5-C5-C6-O6
8	D	904	NAG	O5-C5-C6-O6
8	B	904	NAG	O5-C5-C6-O6
11	E	906	XYL	C2-C3-C4-O4
9	B	906	XYZ	O4-C4-C5-O5

There are no ring outliers.

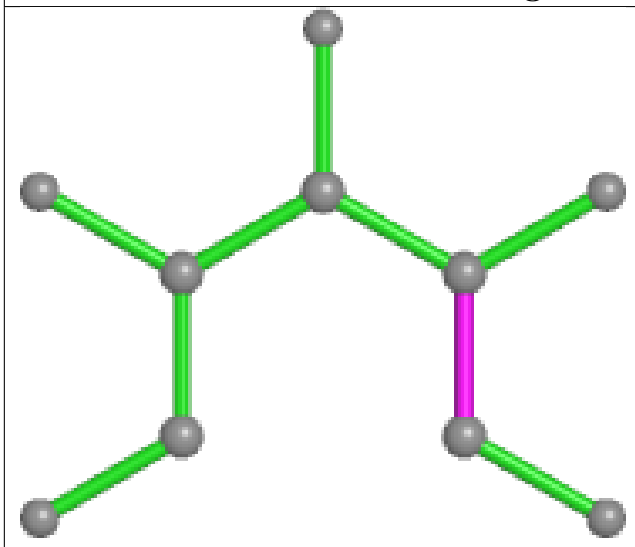
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	905	NAG	2	0
9	A	907	XYZ	1	0
8	E	905	NAG	2	0
11	E	906	XYL	1	0
11	C	907	XYL	2	0
9	B	906	XYZ	1	0
8	D	902	NAG	3	0

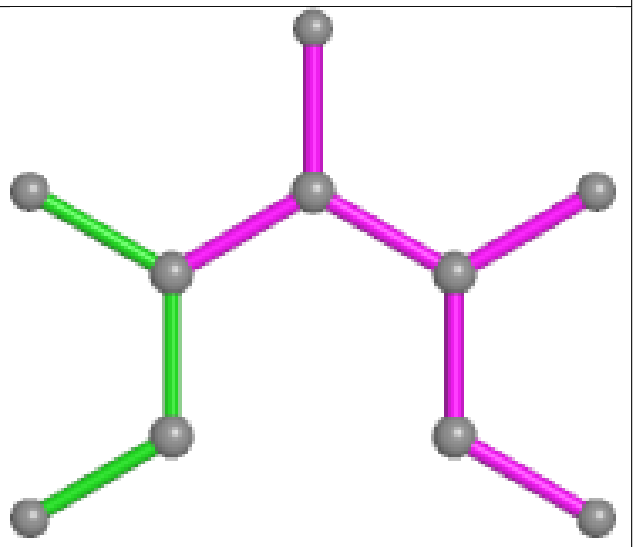
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

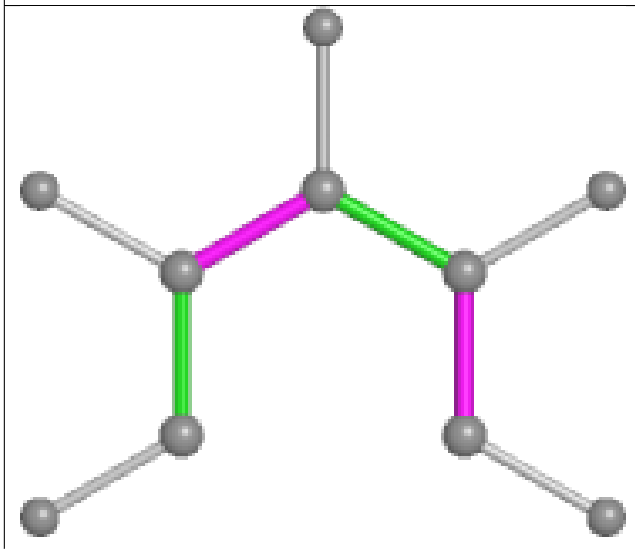
Ligand XYL D 907



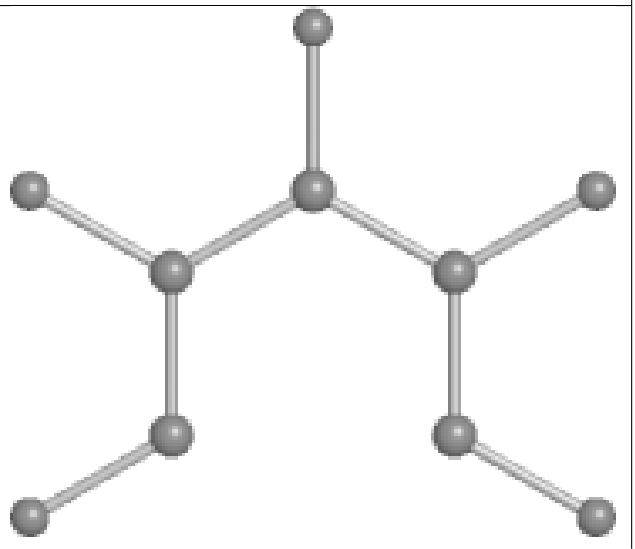
Bond lengths



Bond angles

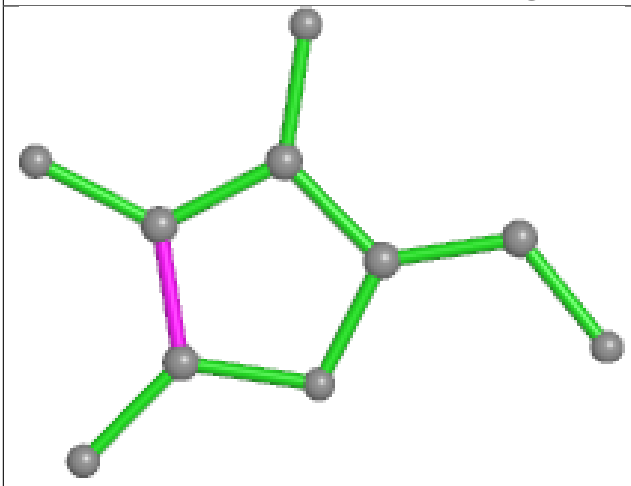


Torsions

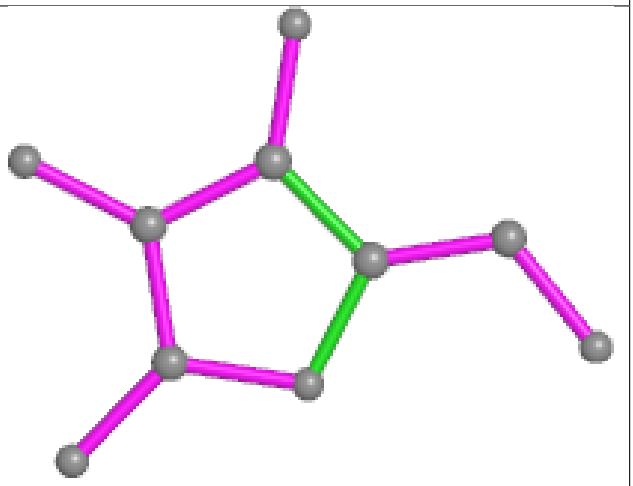


Rings

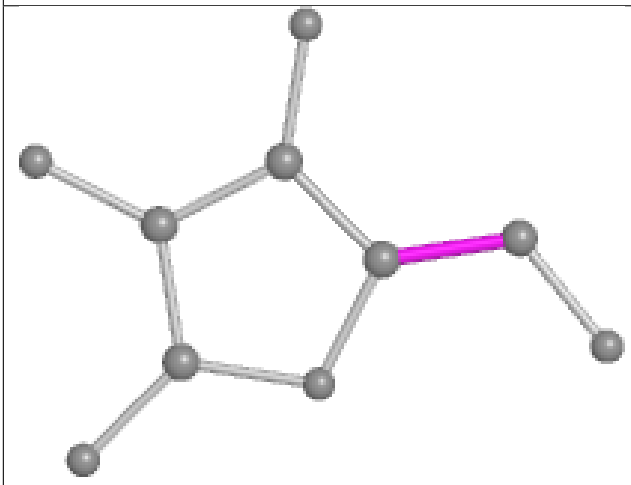
Ligand XYZ A 907



Bond lengths



Bond angles



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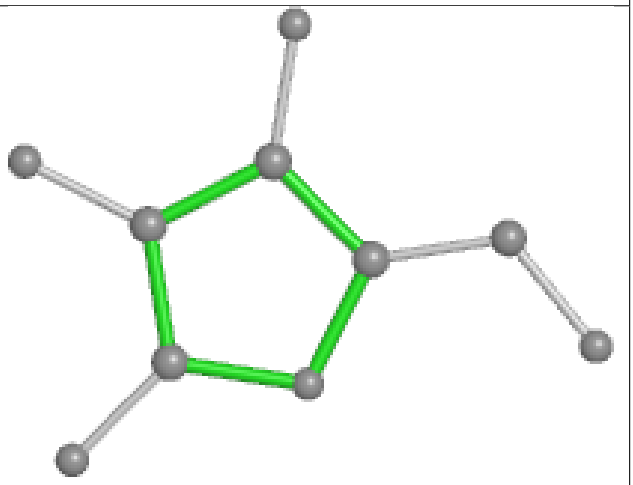
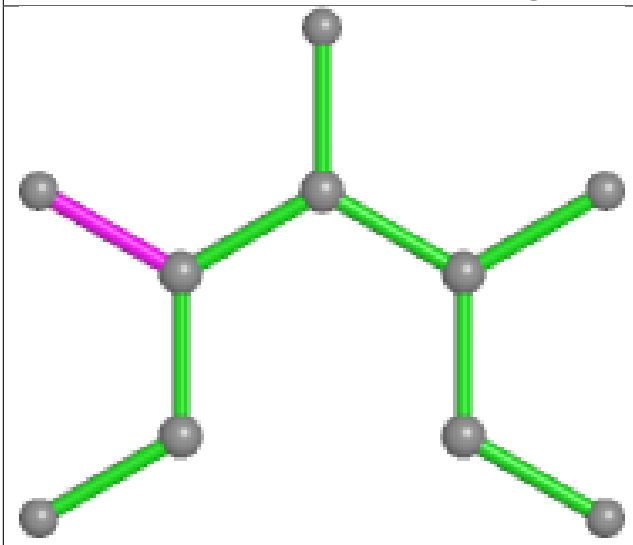
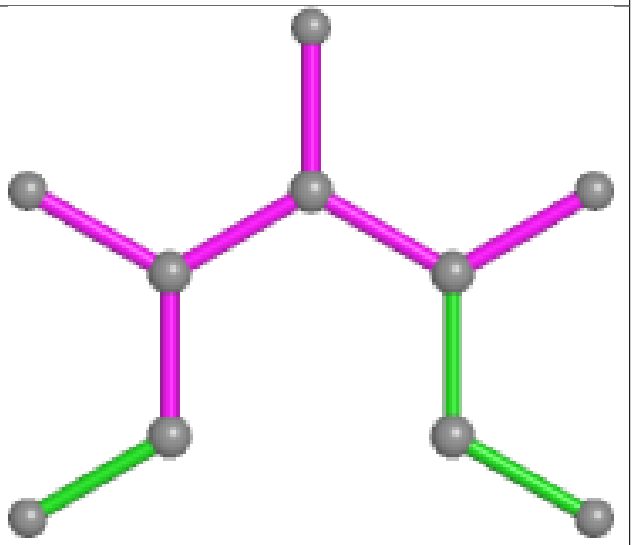


Rings

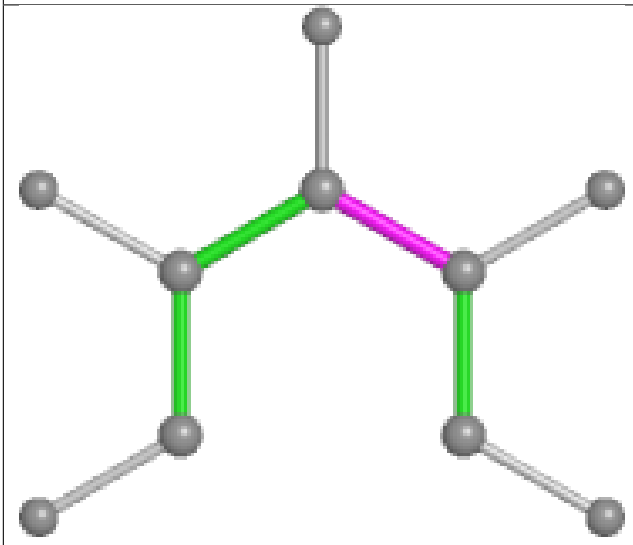
Ligand XYL E 906



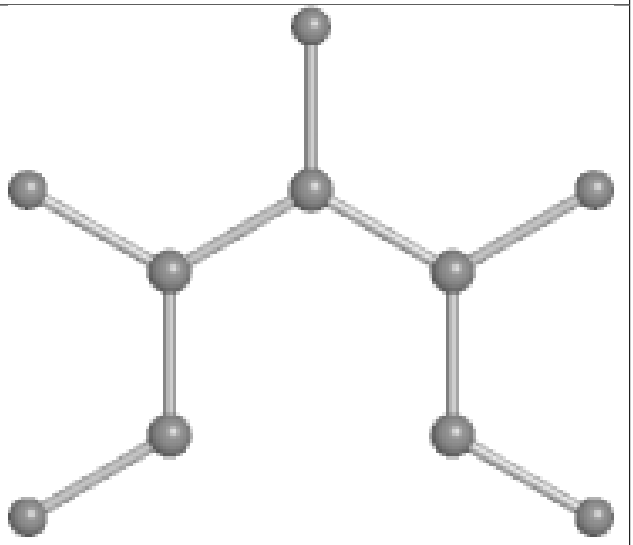
Bond lengths



Bond angles

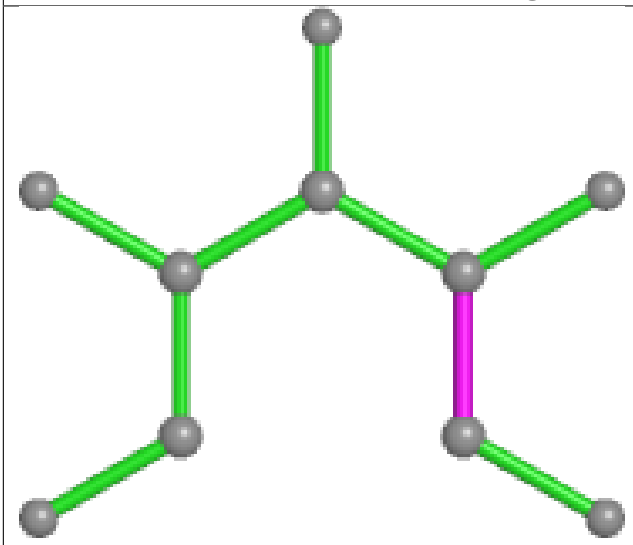


Torsions

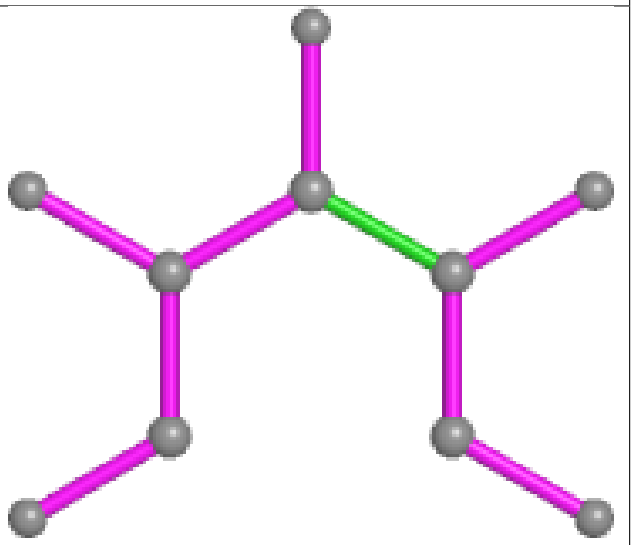


Rings

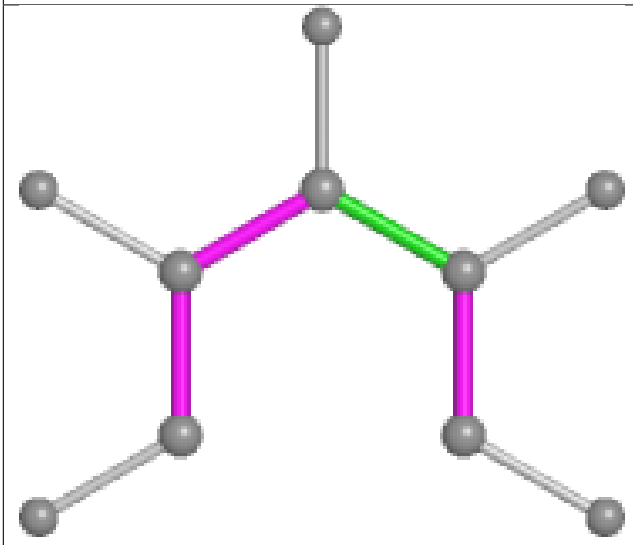
Ligand XYL C 907



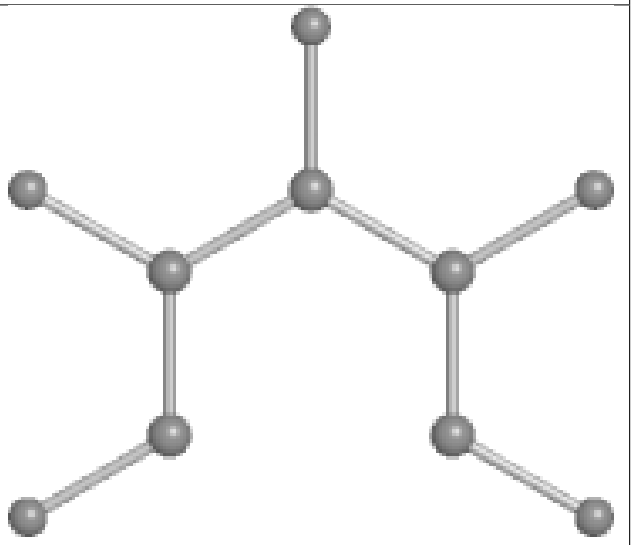
Bond lengths



Bond angles

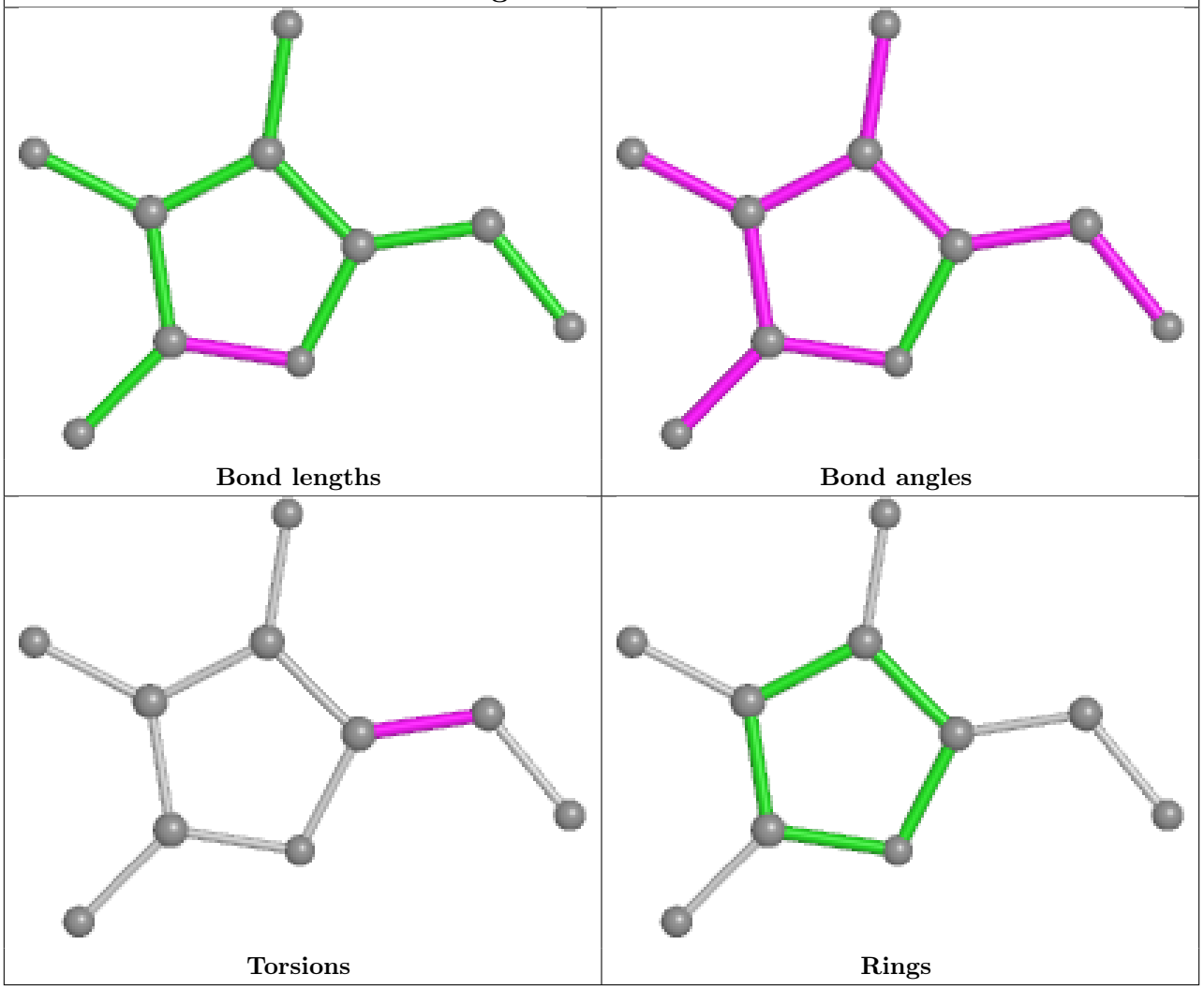


Torsions



Rings

Ligand XYZ B 906



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	758/805 (94%)	-0.28	3 (0%) 92 92	18, 29, 47, 98	0
1	B	758/805 (94%)	-0.32	0 100 100	18, 27, 44, 90	0
1	C	756/805 (93%)	-0.22	4 (0%) 91 91	19, 29, 46, 92	0
1	D	756/805 (93%)	-0.26	2 (0%) 94 94	18, 29, 46, 102	0
1	E	757/805 (94%)	-0.28	1 (0%) 95 96	18, 27, 44, 85	0
1	F	757/805 (94%)	-0.27	2 (0%) 94 94	18, 27, 44, 88	0
All	All	4542/4830 (94%)	-0.27	12 (0%) 94 94	18, 28, 45, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	3.9
1	A	225	ASP	3.8
1	C	226	GLY	2.9
1	C	181	ALA	2.7
1	C	49	TRP	2.5
1	F	51	ALA	2.1
1	D	804	HIS	2.1
1	D	49	TRP	2.1
1	F	49	TRP	2.1
1	E	227	VAL	2.1
1	C	225	ASP	2.0
1	A	47	THR	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	O	4	11/12	0.65	0.17	50,59,66,66	0
2	BMA	P	3	11/12	0.73	0.19	61,68,76,78	0
2	BMA	M	3	11/12	0.73	0.19	58,70,77,78	0
4	MAN	I	4	11/12	0.74	0.19	52,60,67,70	0
2	BMA	G	3	11/12	0.74	0.16	62,75,79,80	0
4	MAN	R	5	11/12	0.76	0.20	60,69,85,89	0
3	MAN	W	5	11/12	0.77	0.18	52,54,64,64	0
3	MAN	T	5	11/12	0.77	0.17	55,58,68,75	0
2	BMA	J	3	11/12	0.78	0.17	56,69,76,85	0
6	MAN	O	5	11/12	0.78	0.24	77,85,91,100	0
5	MAN	K	5	11/12	0.79	0.20	50,59,71,72	0
3	MAN	N	6	11/12	0.81	0.16	40,46,49,51	0
6	MAN	O	6	11/12	0.81	0.24	80,93,100,103	0
2	BMA	V	3	11/12	0.82	0.16	62,74,82,85	0
6	MAN	L	3	11/12	0.83	0.13	32,50,57,59	0
5	MAN	K	8	11/12	0.83	0.22	57,77,86,86	0
6	MAN	U	3	11/12	0.83	0.15	33,48,56,59	0
4	MAN	R	3	11/12	0.84	0.14	51,55,60,63	0
4	MAN	I	3	11/12	0.84	0.20	51,56,59,59	0
3	BMA	N	3	11/12	0.84	0.15	37,39,44,46	0
6	MAN	X	4	11/12	0.84	0.14	41,42,52,52	0
3	MAN	H	6	11/12	0.86	0.12	37,46,50,51	0
2	NAG	P	2	14/15	0.86	0.18	44,50,59,70	0
6	MAN	X	3	11/12	0.86	0.13	40,47,56,56	0
3	MAN	N	5	11/12	0.86	0.14	47,53,59,60	0
7	MAN	Q	5	11/12	0.86	0.18	36,44,51,54	0
3	BMA	H	4	11/12	0.87	0.12	44,48,53,53	0
4	MAN	R	4	11/12	0.87	0.15	51,56,61,61	0
6	MAN	L	6	11/12	0.87	0.27	59,66,72,74	0
3	BMA	T	4	11/12	0.87	0.13	43,45,50,50	0
2	BMA	S	3	11/12	0.87	0.15	61,68,76,76	0
3	BMA	W	4	11/12	0.88	0.14	42,47,53,53	0
5	MAN	K	6	11/12	0.88	0.17	41,50,79,88	0
3	MAN	H	7	11/12	0.88	0.18	47,52,54,59	0
3	MAN	W	6	11/12	0.88	0.13	39,42,44,45	0
6	MAN	U	6	11/12	0.88	0.33	49,60,64,65	0
6	MAN	L	4	11/12	0.88	0.14	40,42,49,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	L	5	11/12	0.88	0.20	62,68,82,86	0
3	BMA	N	4	11/12	0.88	0.11	47,52,57,59	0
2	NAG	G	2	14/15	0.89	0.17	43,52,66,76	0
6	MAN	O	3	11/12	0.89	0.17	46,52,56,56	0
3	MAN	T	6	11/12	0.89	0.14	40,42,45,46	0
3	MAN	N	7	11/12	0.89	0.15	44,46,49,50	0
6	MAN	X	6	11/12	0.89	0.27	57,66,72,72	0
7	MAN	Q	4	11/12	0.89	0.13	45,48,58,60	0
2	NAG	J	2	14/15	0.89	0.15	37,43,50,57	0
7	BMA	Q	2	11/12	0.90	0.16	40,41,44,47	0
4	MAN	I	5	11/12	0.90	0.12	72,82,90,91	0
3	MAN	T	7	11/12	0.90	0.14	41,46,52,53	0
6	MAN	U	5	11/12	0.91	0.15	59,63,71,75	0
2	NAG	P	1	14/15	0.91	0.16	28,33,35,40	0
2	NAG	V	2	14/15	0.91	0.14	36,41,48,55	0
3	NAG	N	2	14/15	0.91	0.20	34,39,42,44	0
3	MAN	W	7	11/12	0.91	0.17	38,43,45,47	0
3	MAN	H	5	11/12	0.91	0.12	45,52,58,59	0
5	BMA	K	4	11/12	0.91	0.14	41,45,49,52	0
6	MAN	U	4	11/12	0.91	0.11	40,43,48,58	0
2	NAG	J	1	14/15	0.92	0.13	27,34,36,37	0
6	MAN	X	5	11/12	0.92	0.19	57,62,66,71	0
3	BMA	H	3	11/12	0.93	0.14	37,37,44,48	0
6	NAG	L	1	14/15	0.93	0.13	20,21,25,26	0
3	NAG	N	1	14/15	0.93	0.13	27,28,34,36	0
5	NAG	K	1	14/15	0.93	0.17	25,27,31,36	0
7	NAG	Q	1	15/15	0.93	0.12	35,37,41,42	0
2	NAG	G	1	14/15	0.93	0.13	29,32,35,42	0
3	NAG	H	1	14/15	0.93	0.16	25,27,33,36	0
3	NAG	H	2	14/15	0.93	0.17	35,37,40,41	0
2	NAG	M	1	14/15	0.94	0.14	28,33,37,38	0
5	MAN	K	7	11/12	0.94	0.14	41,45,48,49	0
7	BMA	Q	3	11/12	0.94	0.12	46,50,54,56	0
3	NAG	W	1	14/15	0.94	0.13	23,26,30,34	0
2	NAG	M	2	14/15	0.94	0.15	41,45,57,68	0
7	MAN	Q	6	11/12	0.94	0.13	45,49,51,51	0
6	NAG	O	1	14/15	0.95	0.12	23,27,30,32	0
6	NAG	X	2	14/15	0.95	0.11	28,32,38,39	0
6	NAG	O	2	14/15	0.95	0.14	28,34,44,45	0
2	NAG	V	1	14/15	0.95	0.14	31,34,37,38	0
2	NAG	S	2	14/15	0.95	0.12	36,40,46,54	0
6	NAG	L	2	14/15	0.95	0.13	27,30,36,40	0

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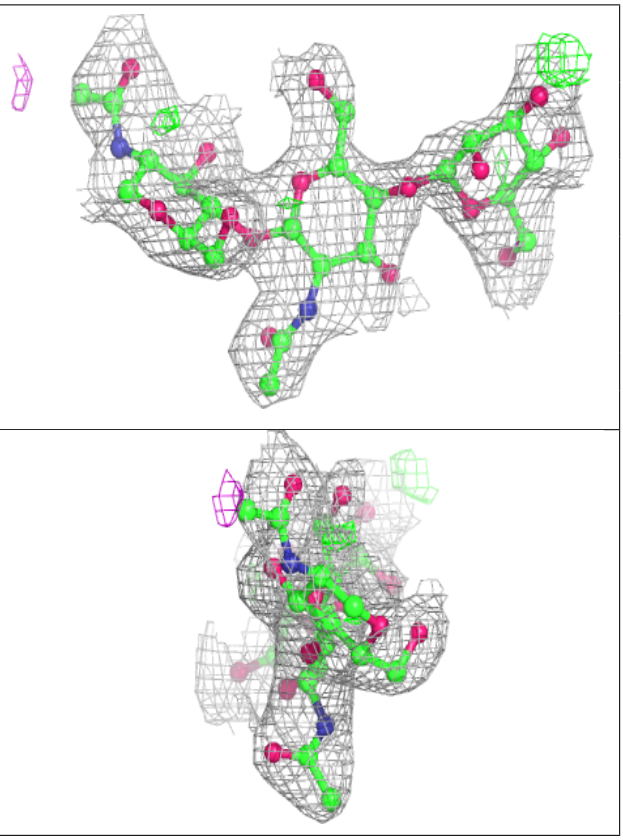
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	T	2	14/15	0.95	0.13	22,25,29,31	0
6	NAG	U	1	14/15	0.95	0.09	20,23,27,27	0
6	NAG	U	2	14/15	0.95	0.12	25,30,34,37	0
4	NAG	R	2	14/15	0.95	0.15	27,32,40,48	0
2	NAG	S	1	14/15	0.95	0.13	28,36,38,40	0
4	NAG	I	2	14/15	0.95	0.15	27,34,47,48	0
6	NAG	X	1	14/15	0.96	0.09	20,23,28,32	0
3	BMA	W	3	11/12	0.96	0.13	30,33,36,37	0
5	BMA	K	3	11/12	0.96	0.14	29,32,39,46	0
3	NAG	T	1	14/15	0.96	0.13	25,26,31,36	0
3	NAG	W	2	14/15	0.96	0.13	24,27,30,32	0
4	NAG	R	1	14/15	0.96	0.12	23,25,29,30	0
3	BMA	T	3	11/12	0.97	0.11	28,31,36,37	0
4	NAG	I	1	14/15	0.97	0.12	22,26,30,31	0
5	NAG	K	2	14/15	0.97	0.12	24,26,30,33	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.

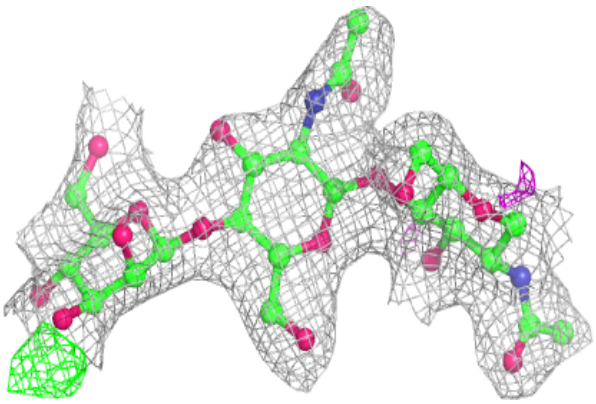
Electron density around Chain G:

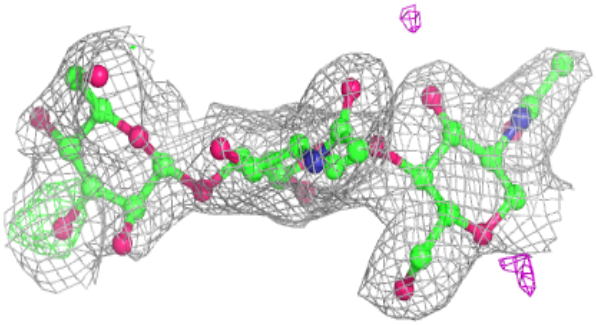
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

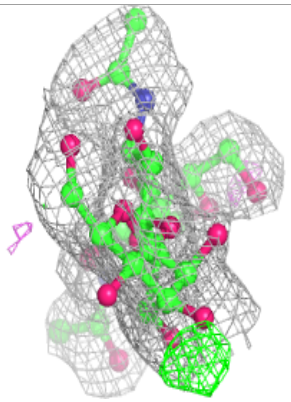


Electron density around Chain J:

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

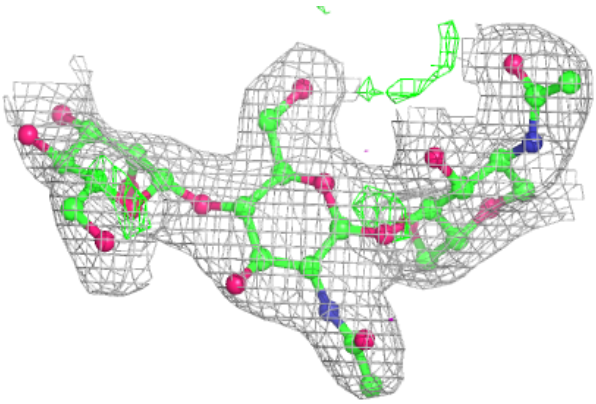


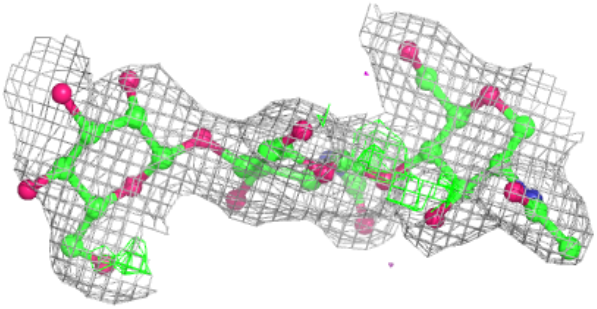


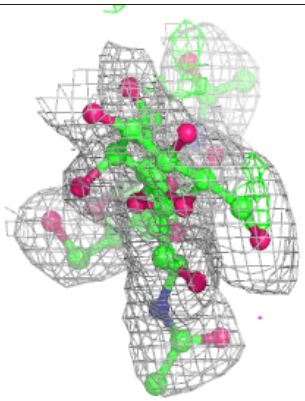


Electron density around Chain M:

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

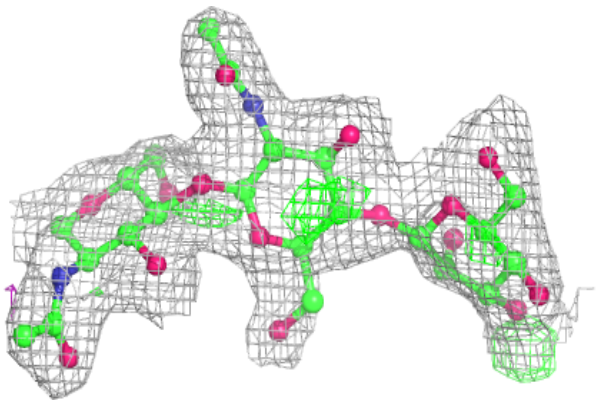


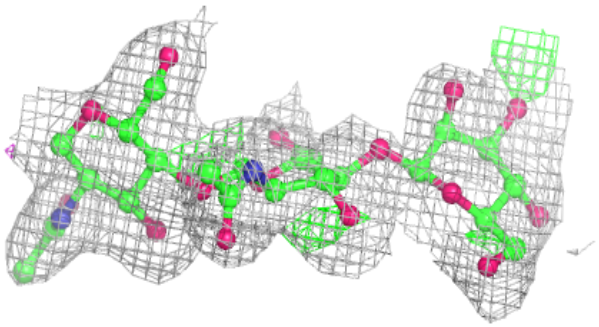


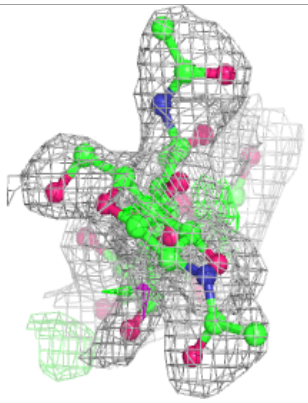


Electron density around Chain P:

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

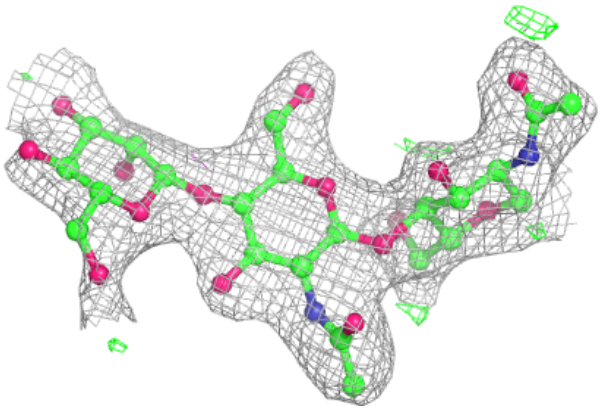


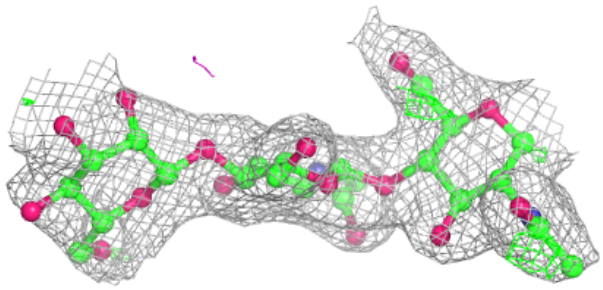


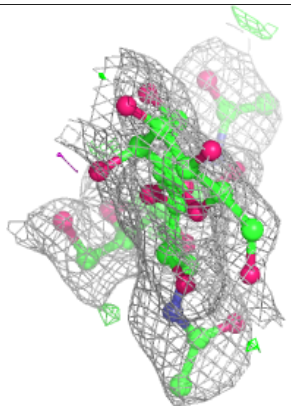


Electron density around Chain S:

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

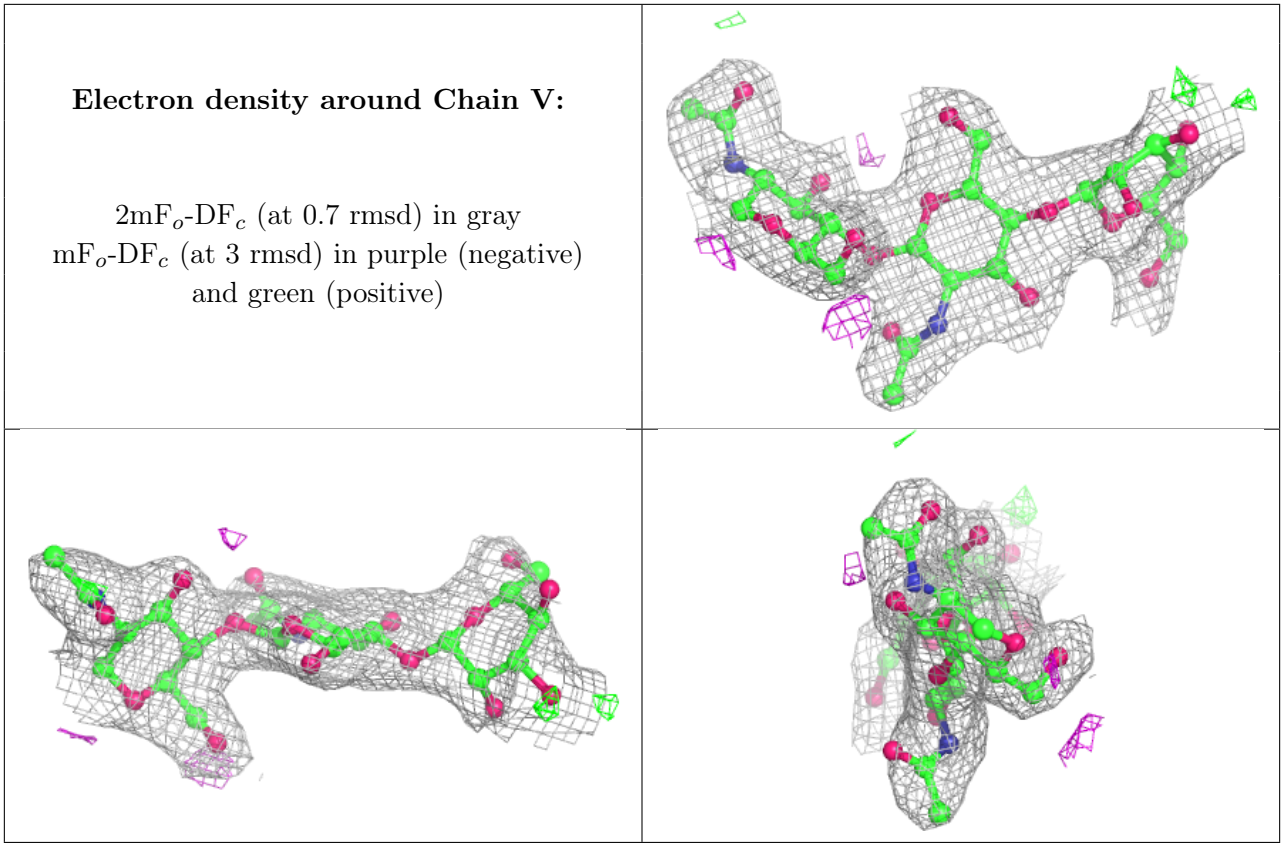






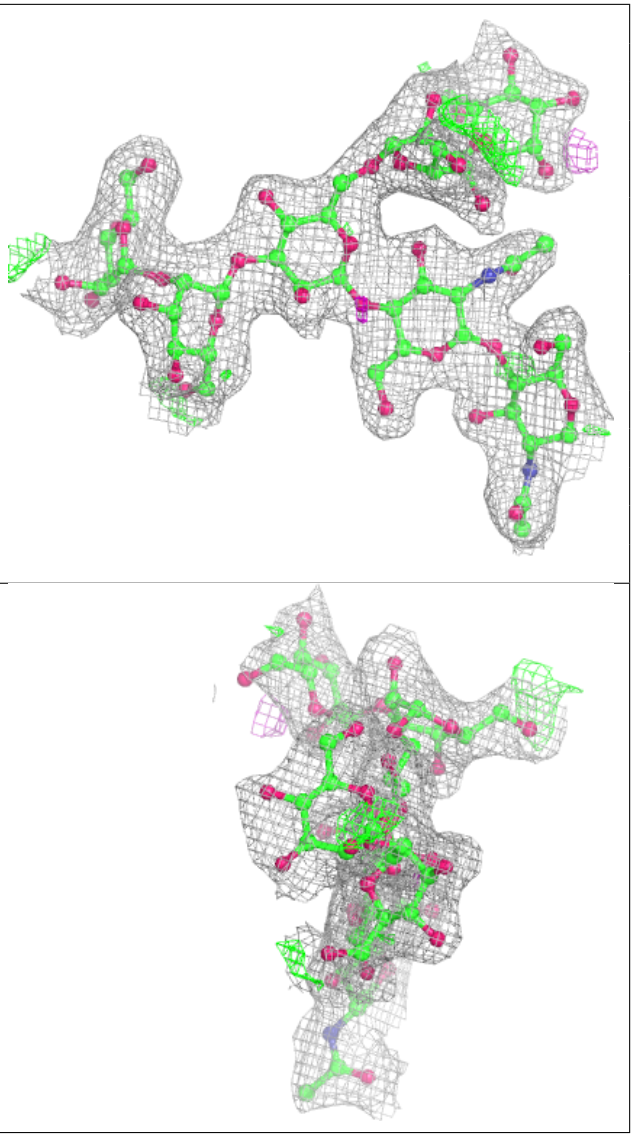
Electron density around Chain V:

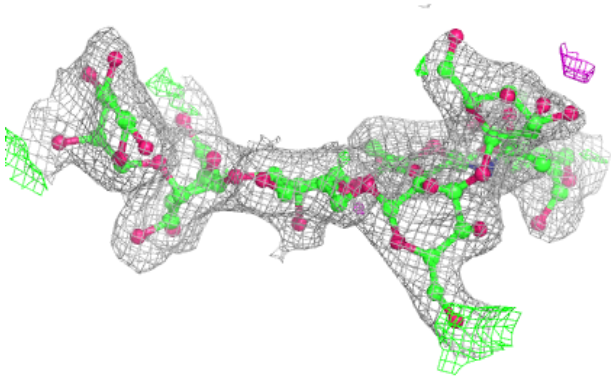
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain H:

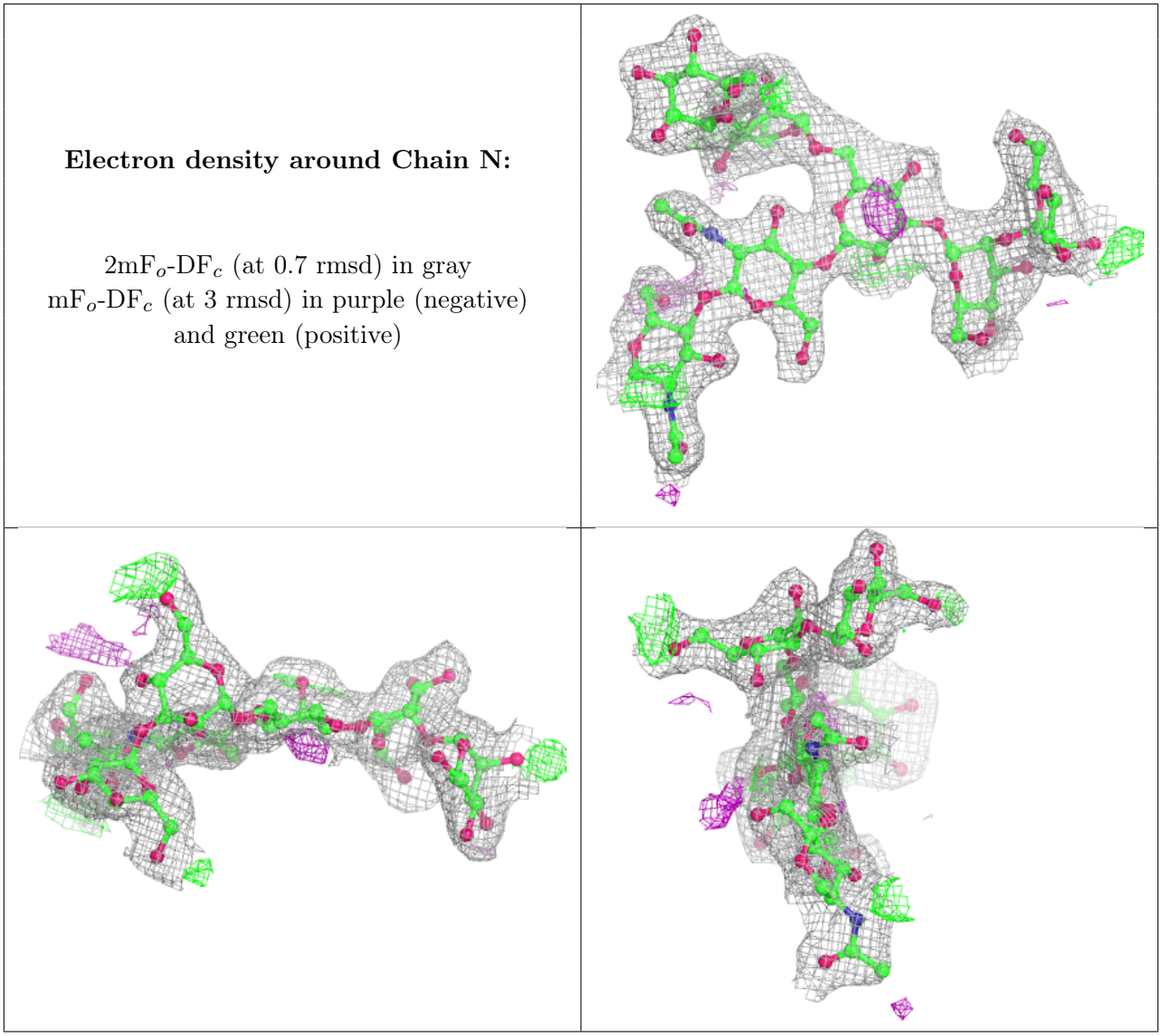
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





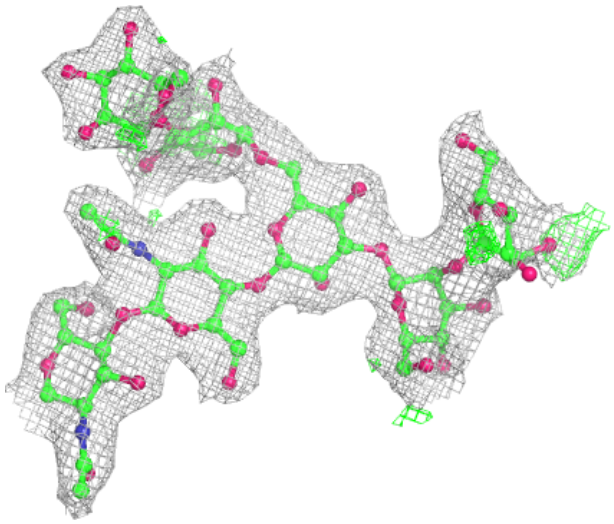
Electron density around Chain N:

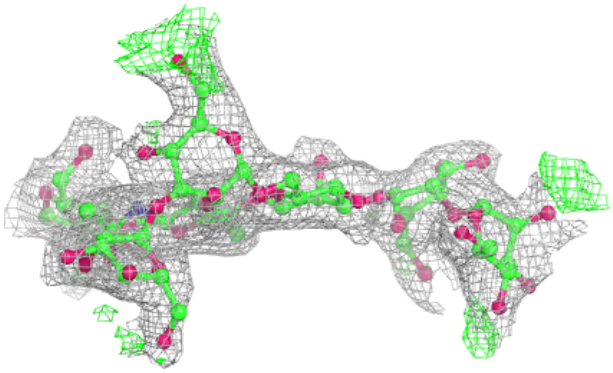
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

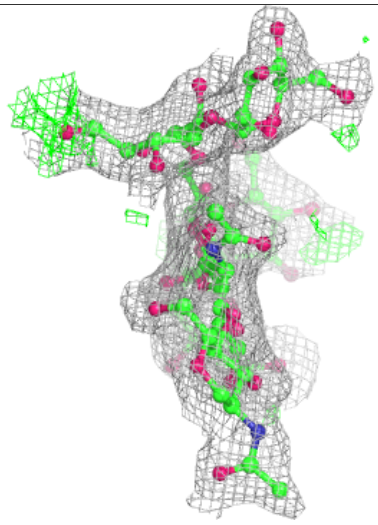


Electron density around Chain T:

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

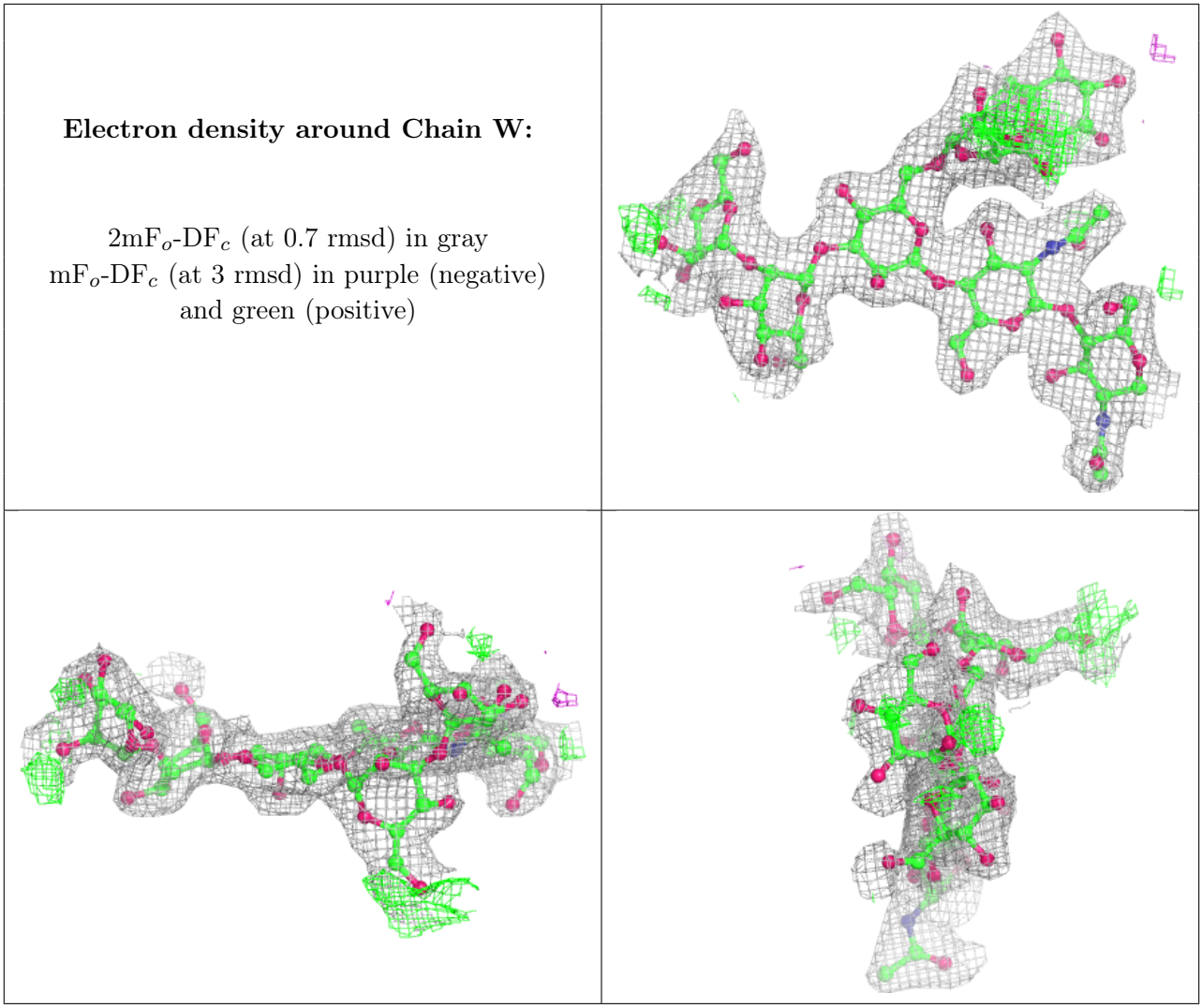






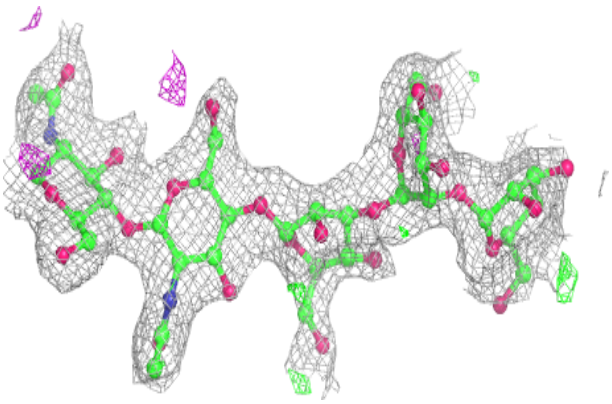
Electron density around Chain W:

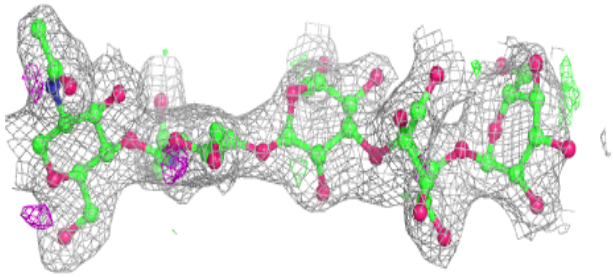
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

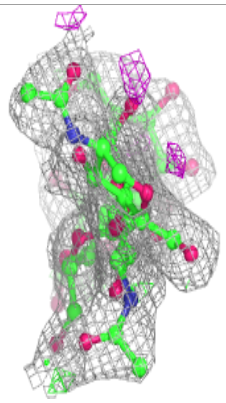


Electron density around Chain I:

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

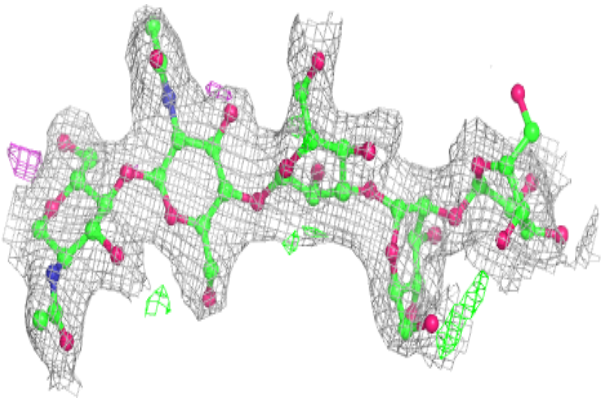


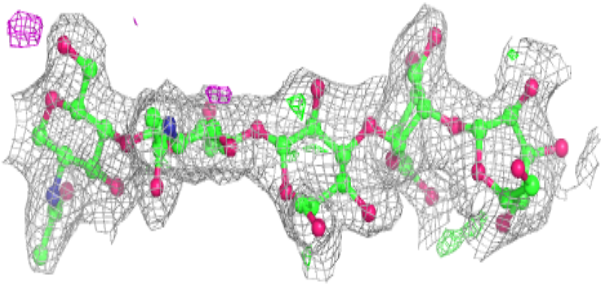


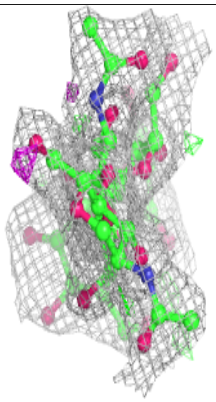


Electron density around Chain R:

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

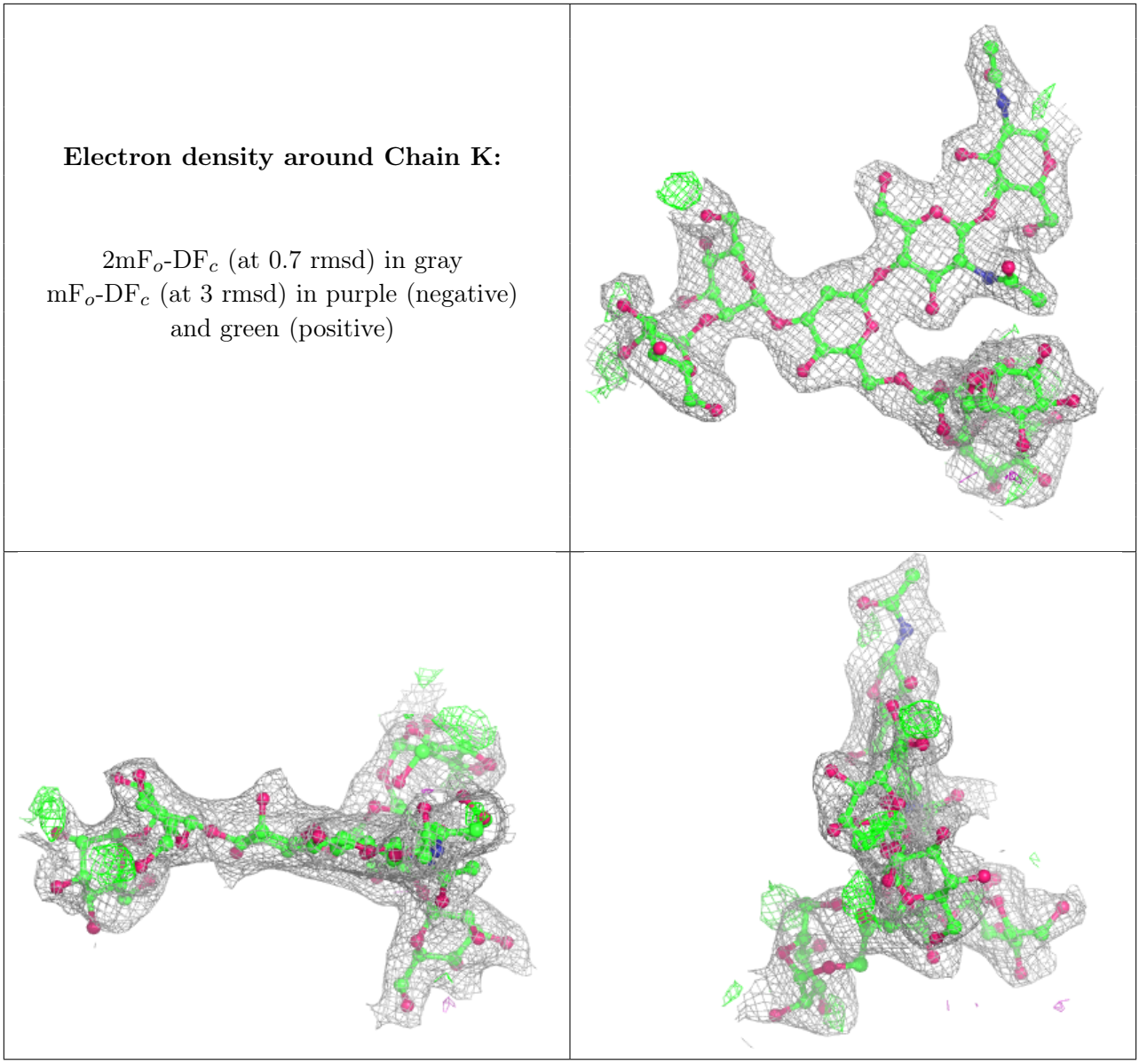






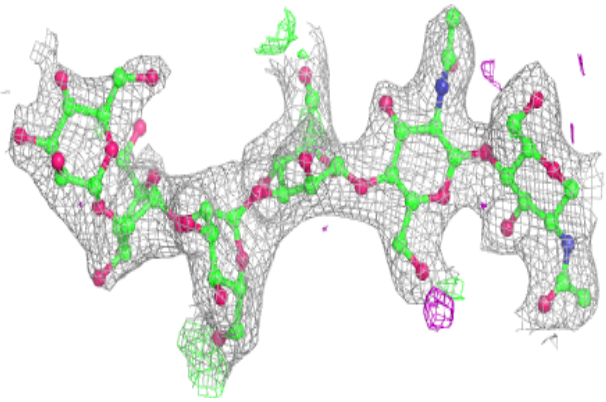
Electron density around Chain K:

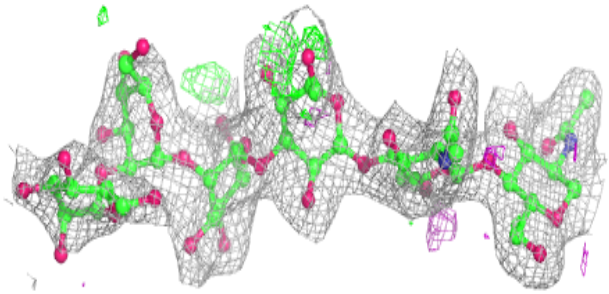
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

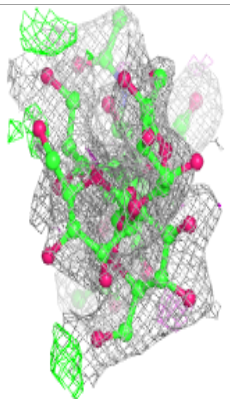


Electron density around Chain L:

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

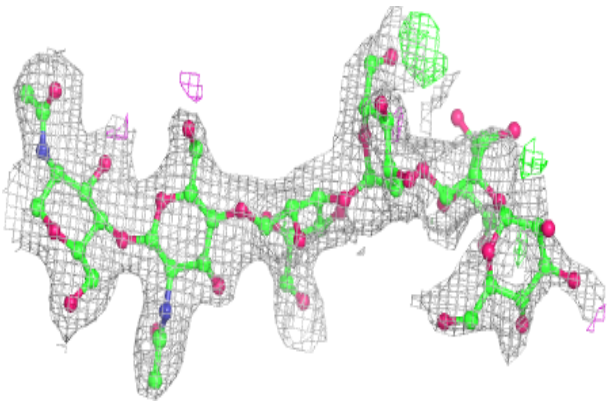


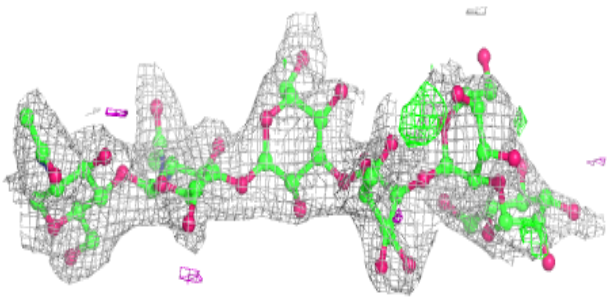


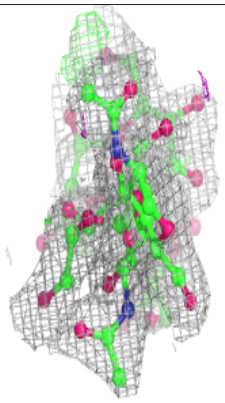


Electron density around Chain O:

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

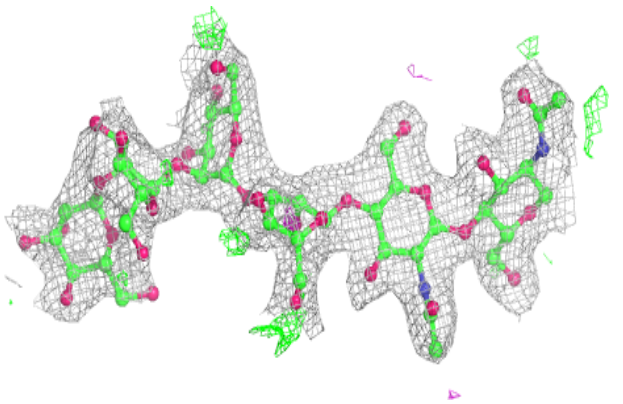


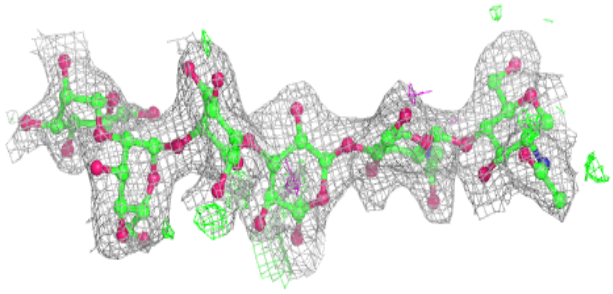


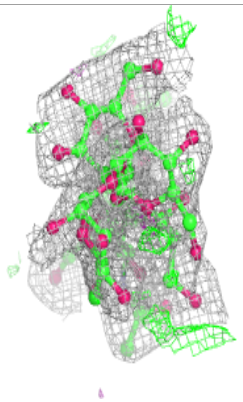


Electron density around Chain U:

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

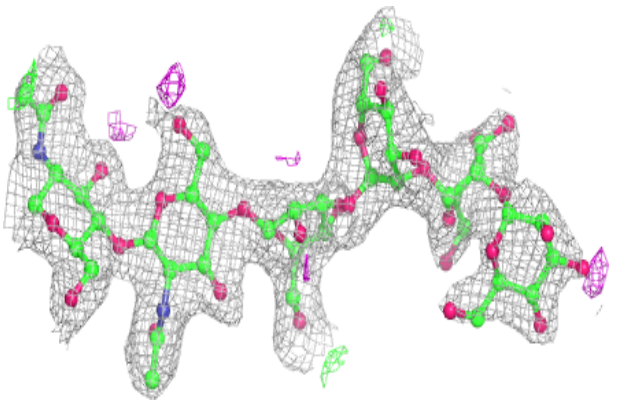


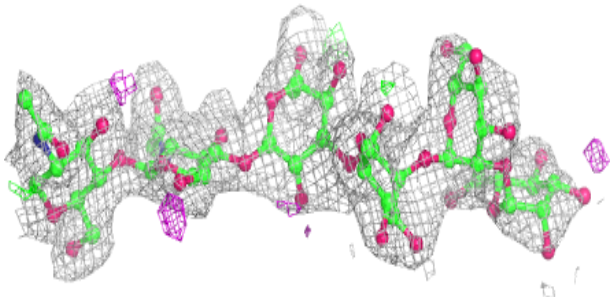


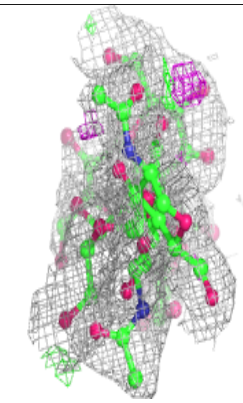


Electron density around Chain X:

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

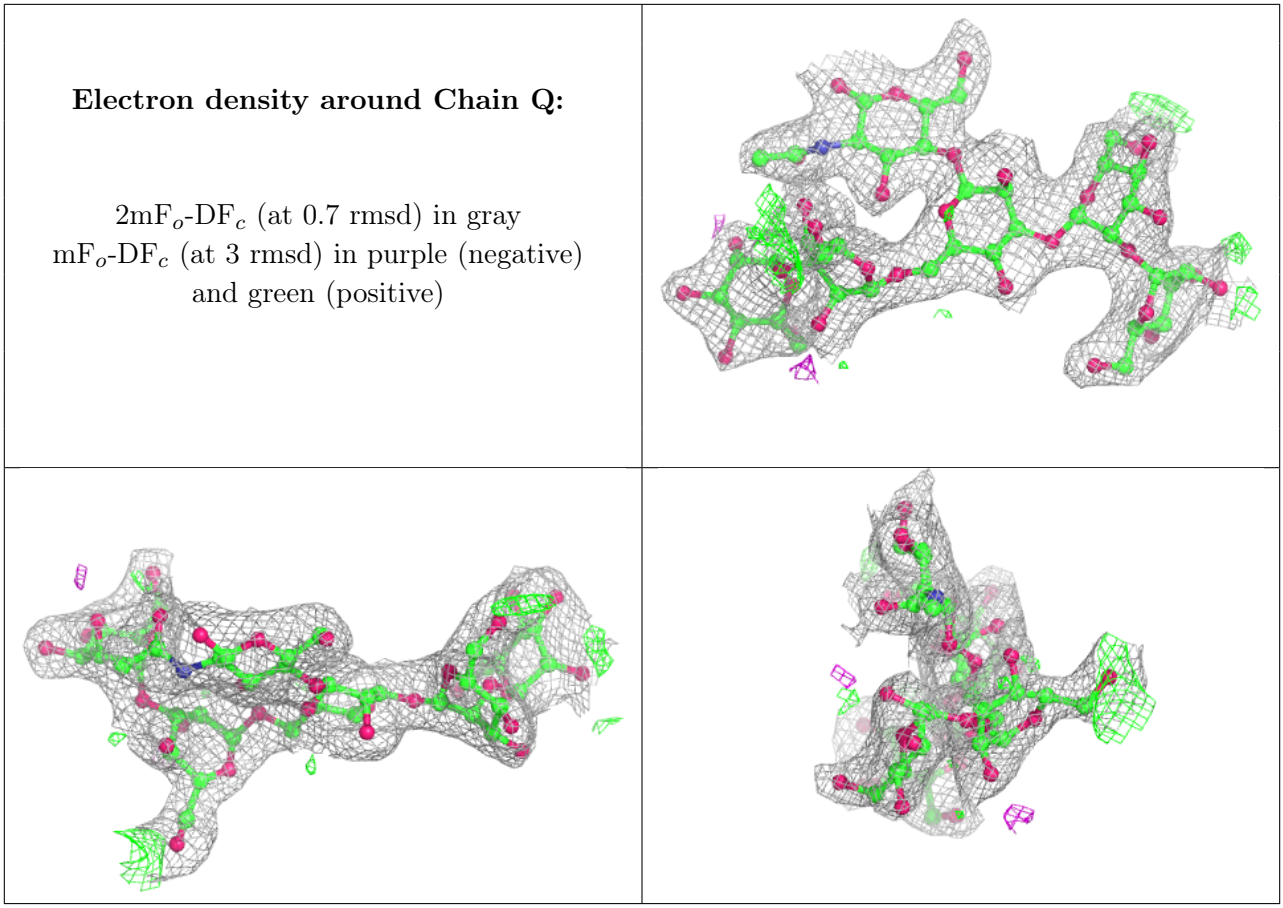






Electron density around Chain Q:

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



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
10	BMA	A	908	11/12	0.80	0.14	79,88,92,95	0
9	XYZ	A	907	10/10	0.81	0.18	37,47,54,54	0
8	NAG	D	903	14/15	0.81	0.23	55,63,67,68	0
11	XYL	C	907	10/10	0.81	0.22	37,45,50,67	0
9	XYZ	B	906	10/10	0.83	0.21	40,53,58,65	0
8	NAG	D	906	14/15	0.83	0.27	69,78,84,84	0
8	NAG	A	906	14/15	0.83	0.34	70,75,80,84	0
11	XYL	E	906	10/10	0.83	0.19	32,43,49,53	0
8	NAG	D	904	13/15	0.84	0.20	51,56,63,63	0
11	XYL	D	907	10/10	0.85	0.18	39,42,48,63	0
8	NAG	C	906	14/15	0.86	0.26	36,42,45,46	14
8	NAG	B	903	14/15	0.87	0.18	52,56,66,66	0
8	NAG	C	904	13/15	0.89	0.17	54,55,61,61	0

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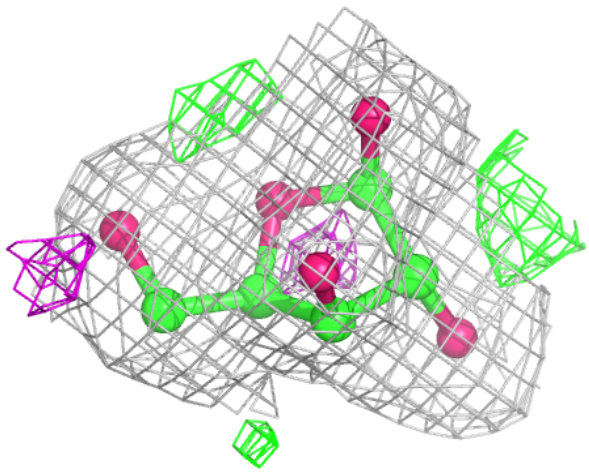
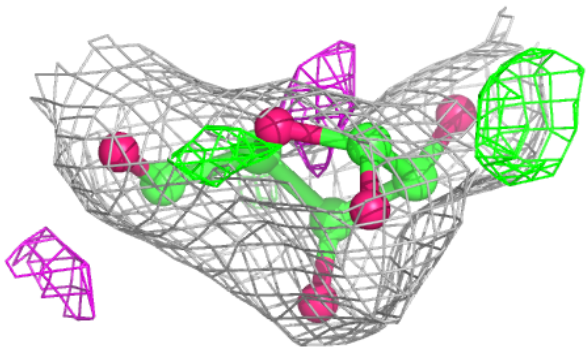
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	F	905	14/15	0.89	0.19	35,44,53,53	0
8	NAG	A	903	14/15	0.91	0.17	54,62,74,74	0
8	NAG	A	904	13/15	0.91	0.16	45,51,56,57	0
8	NAG	B	904	14/15	0.92	0.12	30,35,38,39	0
8	NAG	F	903	14/15	0.93	0.14	54,59,65,70	0
8	NAG	B	905	14/15	0.93	0.13	40,45,49,50	0
8	NAG	E	904	14/15	0.93	0.12	30,34,38,41	0
8	NAG	E	905	14/15	0.93	0.16	37,46,51,52	0
8	NAG	E	903	14/15	0.94	0.13	48,56,65,66	0
8	NAG	D	902	13/15	0.94	0.12	24,27,35,35	0
8	NAG	A	905	14/15	0.94	0.12	23,28,30,31	0
8	NAG	C	905	14/15	0.94	0.11	24,29,33,34	0
8	NAG	F	904	14/15	0.94	0.16	28,32,36,39	0
8	NAG	C	903	14/15	0.94	0.17	55,63,75,77	0
8	NAG	D	905	14/15	0.96	0.13	22,28,32,35	0

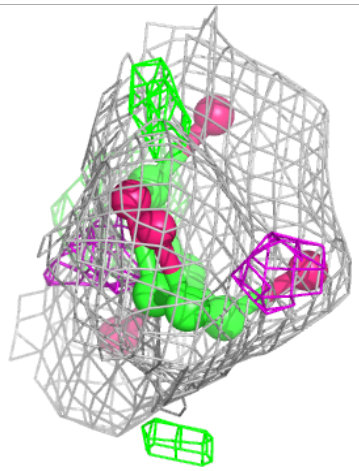
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XYZ A 907:

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

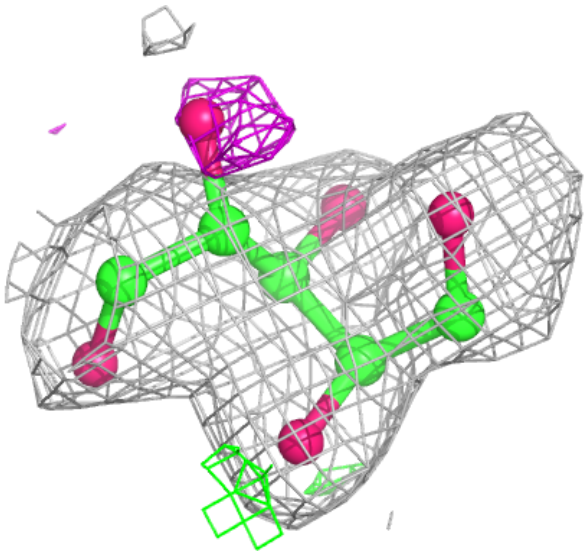


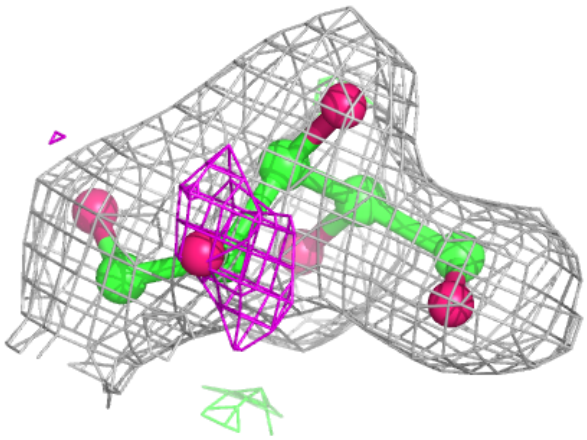


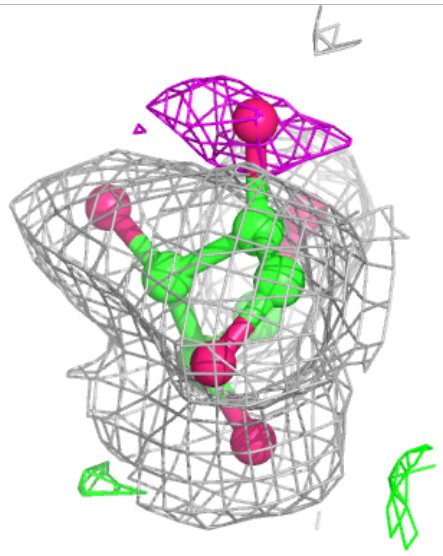


Electron density around XYL C 907:

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

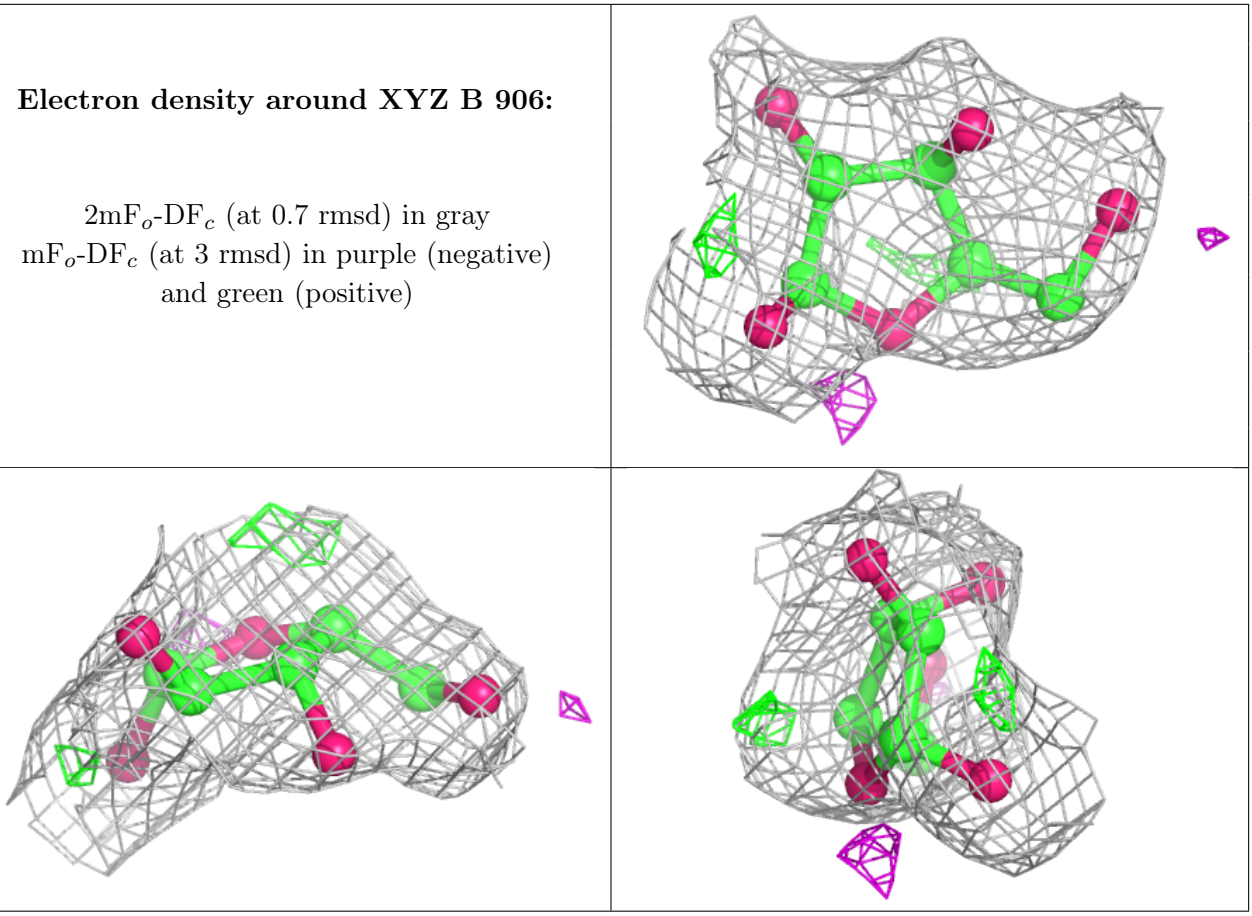






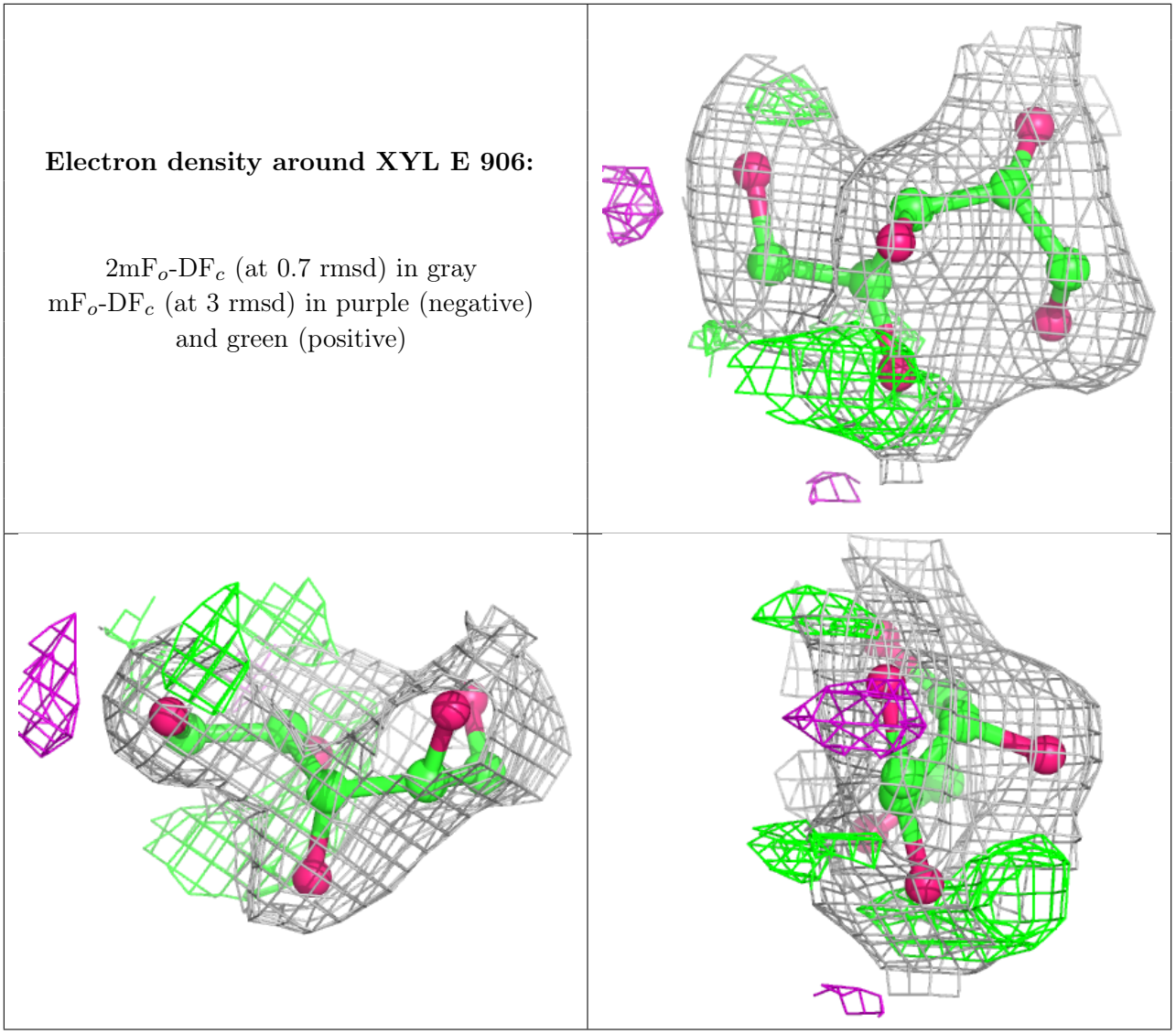
Electron density around XYZ B 906:

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



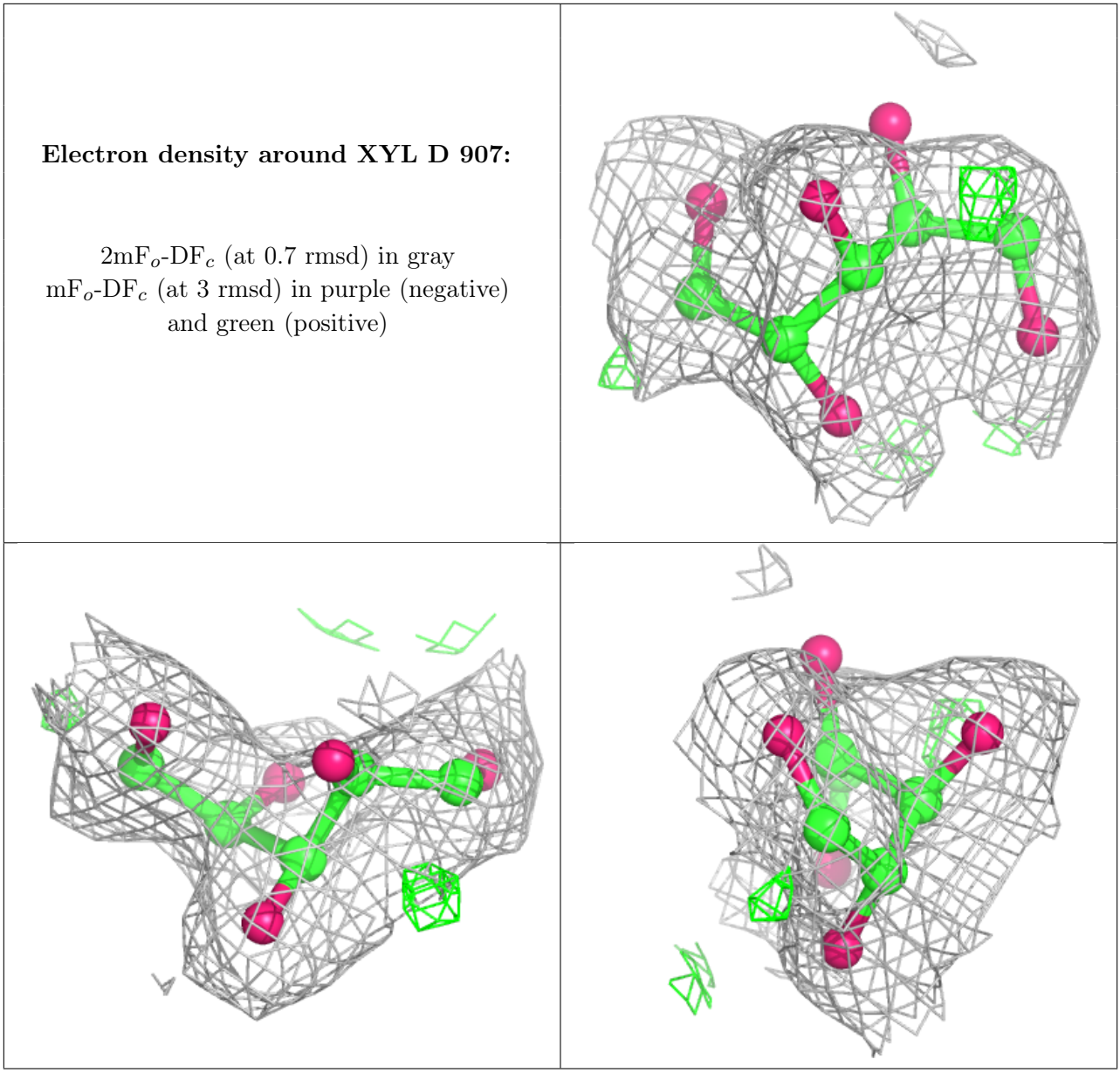
Electron density around XYL E 906:

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



Electron density around XYL D 907:

$2mF_o$-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.