



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:53 PM UTC

PDB ID : 7EY1 / pdb_00007ey1
Title : Bifunctional xylosidase/glucosidase LXYL with intermediate substrate xylose
Authors : Gong, W.M.; Yang, L.Y.
Deposited on : 2021-05-29
Resolution : 2.46 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

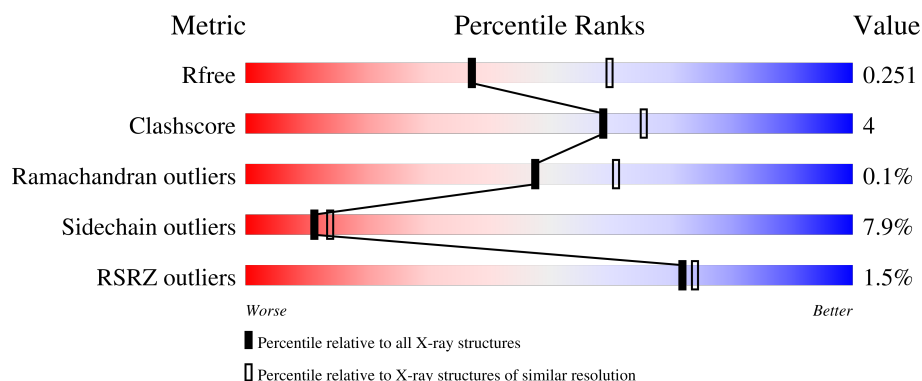
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



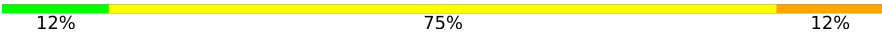
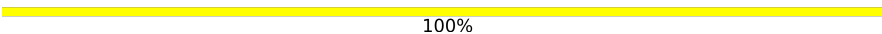
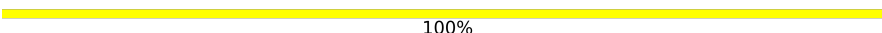
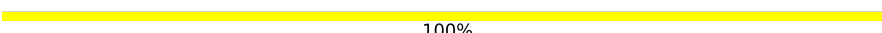
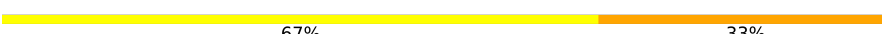
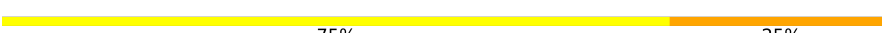
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	803	82% 10% 6%
1	B	803	83% 9% 6%
1	C	803	2% 81% 11% 6%
1	D	803	2% 80% 12% 6%
2	E	8	88% 12%

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Mol	Chain	Length	Quality of chain
2	G	8	
3	F	4	
4	I	3	
4	K	3	
4	M	3	
5	J	4	
6	L	8	
7	N	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	L	1	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 24651 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	756	Total	C	N	O	S	0	2	0
			5719	3621	957	1124	17			
1	B	756	Total	C	N	O	S	0	4	0
			5736	3633	958	1128	17			
1	C	756	Total	C	N	O	S	0	2	0
			5716	3621	955	1123	17			
1	D	756	Total	C	N	O	S	0	2	0
			5720	3624	956	1123	17			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			92	50	1	41			
2	G	8	Total	C	N	O	0	0	0
			92	50	1	41			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-3)-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
3	F	4	Total	C	N	O	0	0	0
			53	30	3	20			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 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
5	J	4	Total	C	N	O	0	0	0
			48	26	1	21			

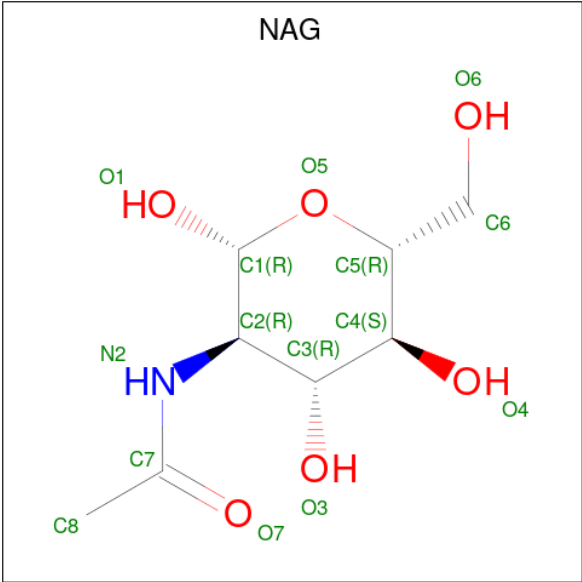
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(6-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	8	Total	C	N	O	0	0	0
			95	52	2	41			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	N	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



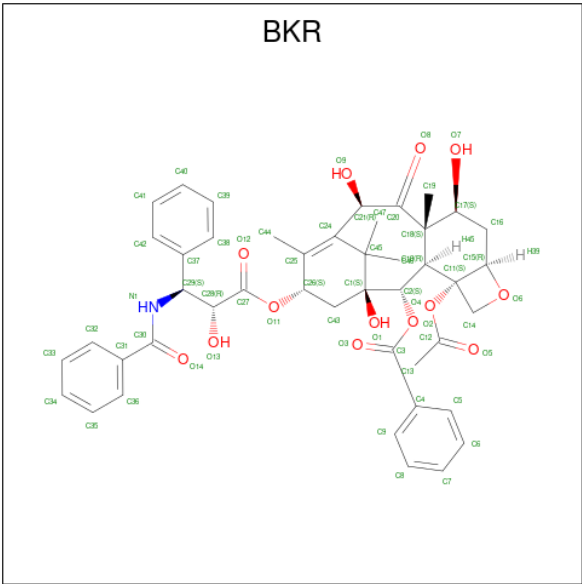
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			13	8	1	4		
8	A	1	Total	C	N	O	0	0
			15	8	1	6		
8	A	1	Total	C	N	O	0	0
			13	8	1	4		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			13	8	1	4		
8	B	1	Total	C	N	O	0	0
			15	8	1	6		
8	B	1	Total	C	N	O	0	0
			13	8	1	4		
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		
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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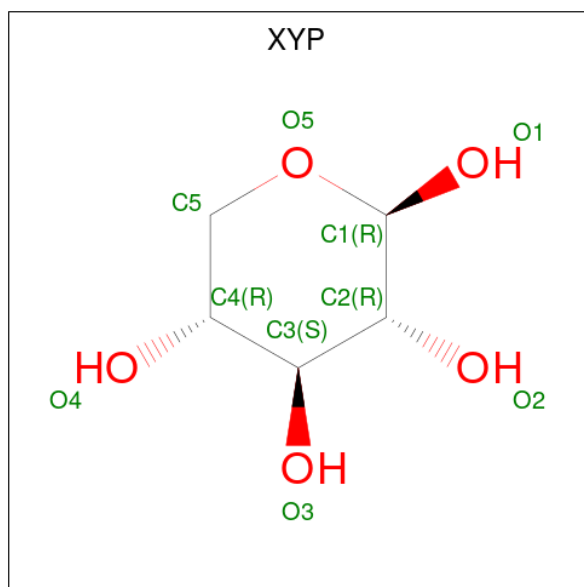
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			13	8	1	4		
8	C	1	Total	C	N	O	0	0
			15	8	1	6		
8	C	1	Total	C	N	O	0	0
			13	8	1	4		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			13	8	1	4		
8	D	1	Total	C	N	O	0	0
			15	8	1	6		
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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is Deacetyltaxol (CCD ID: BKR) (formula: C₄₅H₄₉NO₁₃) (labeled as "Ligand of Interest" by depositor).



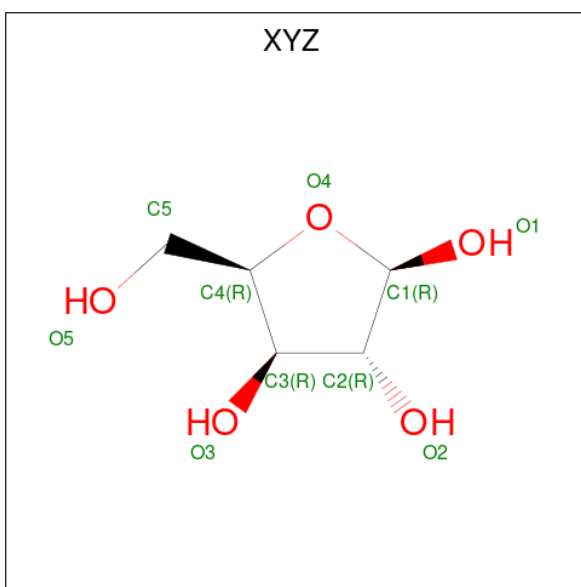
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			59	45	1	13		
9	B	1	Total	C	N	O	0	0
			59	45	1	13		

- Molecule 10 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



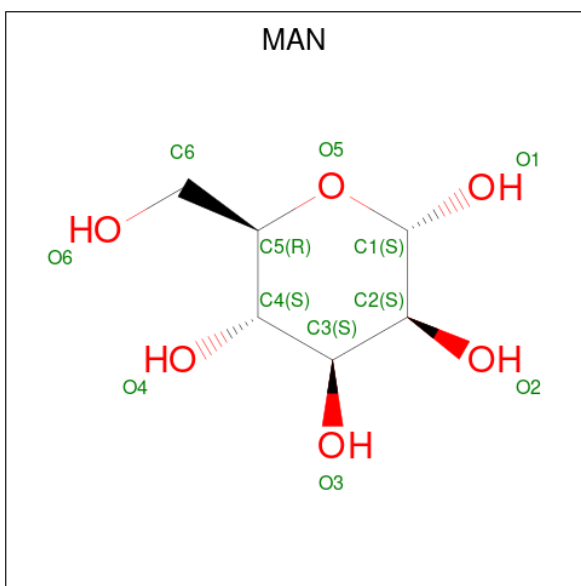
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			9	5	4		

- Molecule 11 is beta-D-xylofuranose (CCD ID: XYZ) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



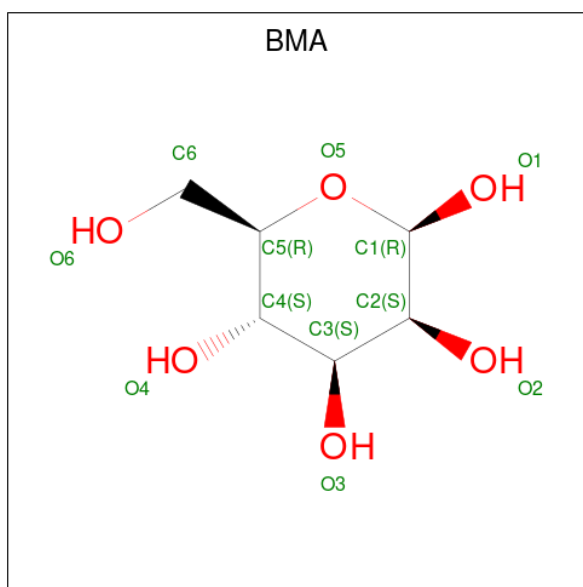
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 12 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 13 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



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

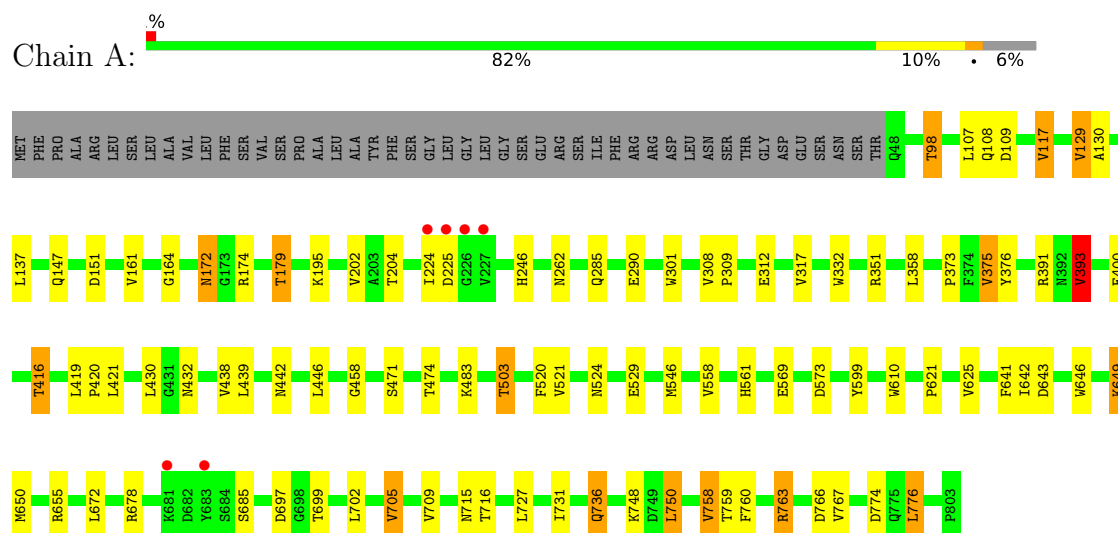
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	277	Total	O	0	0
			277	277		
14	B	242	Total	O	0	0
			242	242		
14	C	120	Total	O	0	0
			120	120		
14	D	96	Total	O	0	0
			96	96		

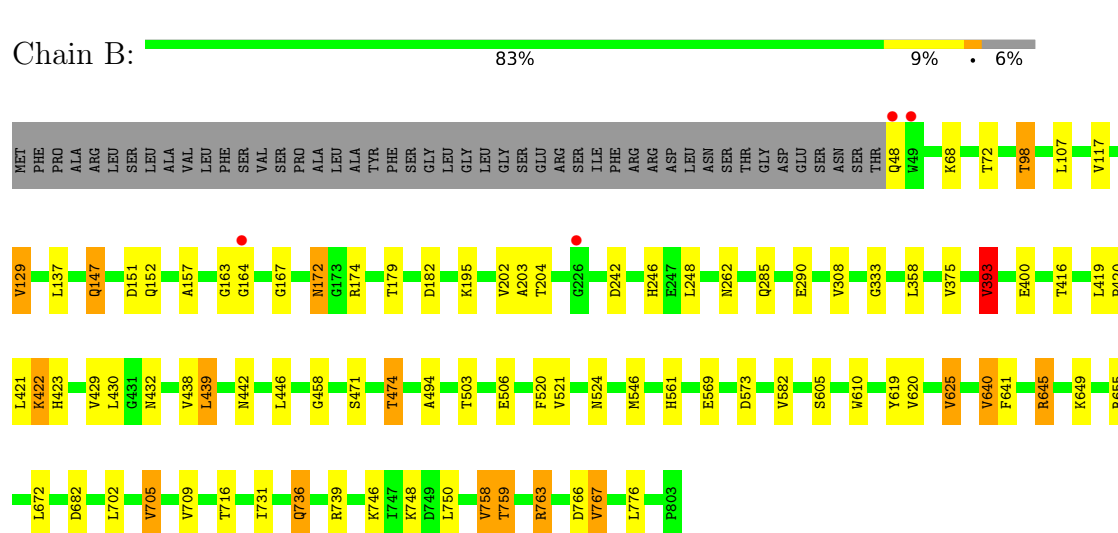
3 Residue-property plots [i](#)

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.

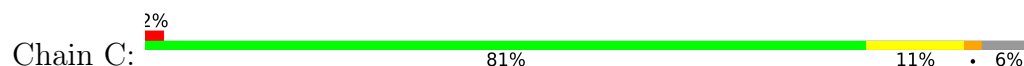
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

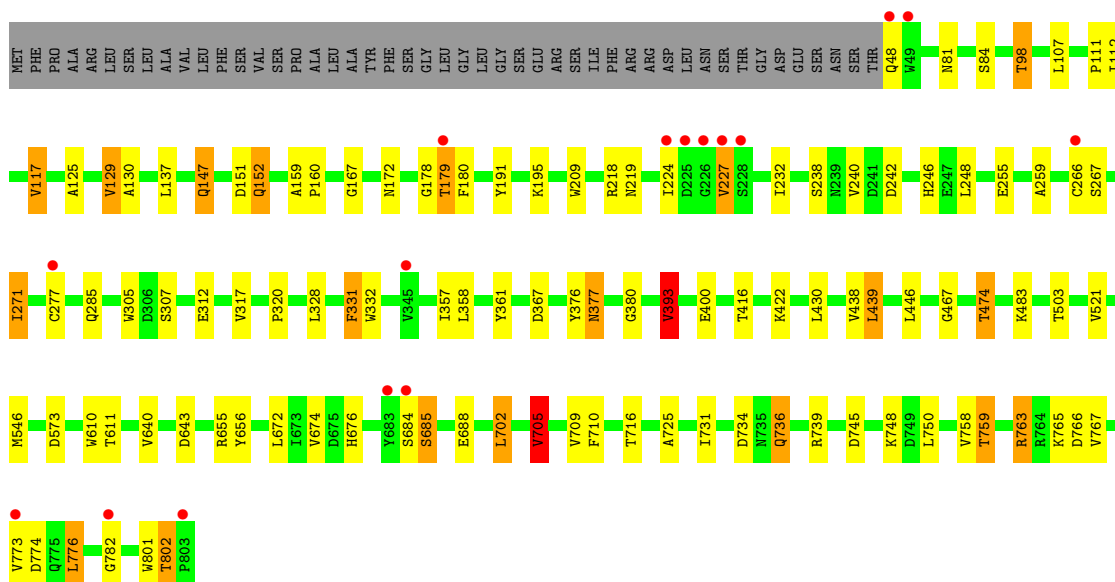


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

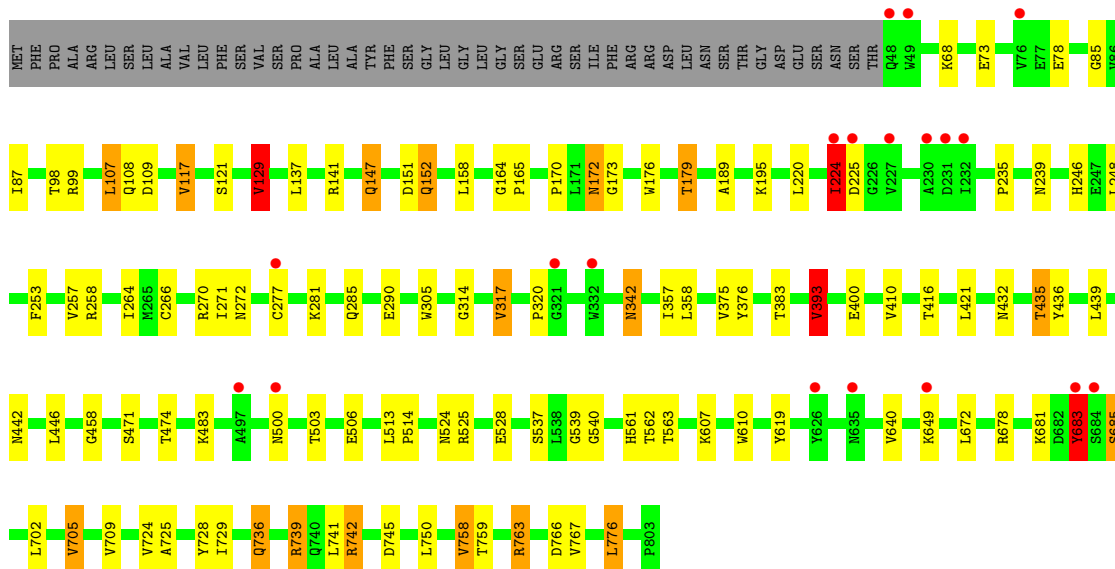
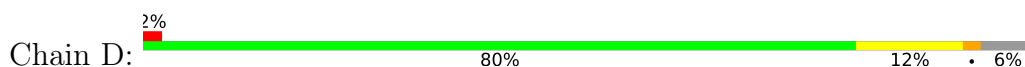


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

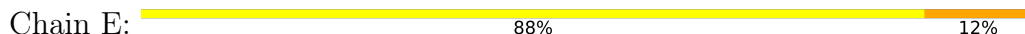




• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

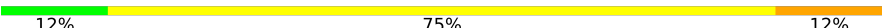


• Molecule 2: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



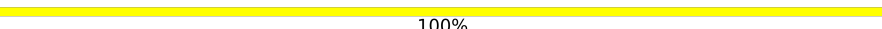
• Molecule 2: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  12% 75% 12%

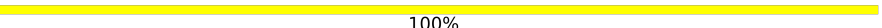


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

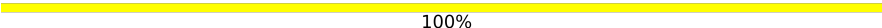


- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



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

Chain K:  100%



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

Chain M:  67% 33%



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

Chain J:  75% 25%



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(6-4)]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 L:  12% 75% 12%

MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7	MAN8
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- Molecule 7: α -D-mannopyranose-(1-2)- β -D-mannopyranose

Chain N:  100%

MAN1	MAN2
------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	228.51Å 88.17Å 218.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	218.50 – 2.46 218.50 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.7 (218.50-2.46) 98.7 (218.50-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.196 , 0.249 0.203 , 0.251	Depositor DCC
R_{free} test set	7844 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24651	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BKR, NAG, XYZ, XYP, BMA, MAN

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	0.97	2/5862 (0.0%)	1.04	13/8020 (0.2%)
1	B	1.00	4/5883 (0.1%)	1.05	15/8049 (0.2%)
1	C	0.90	2/5863 (0.0%)	1.05	14/8023 (0.2%)
1	D	0.94	0/5867	1.08	13/8027 (0.2%)
All	All	0.95	8/23475 (0.0%)	1.06	55/32119 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	643	ASP	C-O	-8.32	1.16	1.24
1	C	178	GLY	C-O	-6.54	1.15	1.23
1	B	163	GLY	C-O	-6.53	1.15	1.24
1	C	643	ASP	C-O	-6.04	1.18	1.24
1	B	640	VAL	C-O	-5.96	1.17	1.24
1	B	179	THR	C-O	-5.64	1.16	1.24
1	B	72	THR	CA-C	5.33	1.59	1.52
1	A	642	ILE	C-O	-5.16	1.18	1.24

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	ILE	N-CA-C	16.17	142.98	109.34
1	C	180	PHE	N-CA-CB	14.76	135.43	110.49
1	B	333	GLY	N-CA-C	-9.73	99.48	111.45
1	C	685	SER	N-CA-C	-9.02	93.53	108.32
1	C	179	THR	N-CA-C	8.71	129.35	110.80
1	D	224	ILE	CB-CA-C	-8.46	97.41	111.29
1	C	179	THR	CB-CA-C	-7.86	94.78	110.42
1	D	129	VAL	N-CA-CB	7.66	119.51	110.55
1	D	314	GLY	N-CA-C	7.51	123.83	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	VAL	N-CA-CB	-7.46	103.46	112.33
1	C	331	PHE	N-CA-C	7.44	120.45	111.82
1	D	271	ILE	O-C-N	7.28	130.09	123.03
1	A	179	THR	N-CA-C	7.21	126.15	110.80
1	D	179	THR	N-CA-C	7.11	125.95	110.80
1	B	705	VAL	N-CA-CB	7.11	118.28	110.53
1	C	227	VAL	N-CA-C	6.94	118.65	109.21
1	D	129	VAL	CB-CA-C	-6.89	103.16	111.97
1	C	180	PHE	N-CA-C	-6.61	96.72	110.80
1	B	164	GLY	C-N-CD	6.55	135.02	120.60
1	C	393	VAL	N-CA-CB	-6.50	103.91	112.36
1	D	705	VAL	CB-CA-C	6.49	118.95	110.91
1	C	332	TRP	N-CA-C	-6.46	100.19	109.29
1	D	435	THR	N-CA-C	6.44	116.78	108.34
1	B	767	VAL	CB-CA-C	6.41	121.80	111.29
1	A	393	VAL	N-CA-CB	-6.38	104.07	112.36
1	B	393	VAL	N-CA-CB	-6.09	104.44	112.36
1	A	129	VAL	N-CA-CB	6.08	121.78	110.77
1	A	224	ILE	N-CA-C	-6.00	99.83	108.53
1	C	81	ASN	N-CA-C	-5.98	104.46	110.97
1	C	129	VAL	CB-CA-C	-5.93	102.97	112.16
1	A	332	TRP	CA-C-N	-5.92	109.82	121.41
1	A	332	TRP	C-N-CA	-5.92	109.82	121.41
1	C	705	VAL	CB-CA-C	5.85	118.04	110.96
1	B	129	VAL	CB-CA-C	-5.78	103.20	112.16
1	B	179	THR	N-CA-C	5.72	122.99	110.80
1	A	129	VAL	CB-CA-C	-5.71	103.02	112.26
1	B	308	VAL	CA-C-N	-5.46	112.98	119.05
1	B	308	VAL	C-N-CA	-5.46	112.98	119.05
1	B	164	GLY	N-CA-C	-5.44	101.25	112.34
1	D	393	VAL	N-CA-CB	-5.39	104.42	112.67
1	D	147	GLN	N-CA-CB	5.33	118.06	110.16
1	C	332	TRP	CB-CA-C	-5.31	107.76	114.40
1	A	332	TRP	CB-CA-C	-5.30	101.42	111.97
1	B	129	VAL	N-CA-CB	5.29	119.70	110.65
1	A	503	THR	CB-CA-C	5.28	118.33	109.89
1	C	129	VAL	N-CA-CB	5.27	119.67	110.65
1	B	164	GLY	CA-C-N	-5.27	114.35	127.00
1	B	164	GLY	C-N-CA	-5.27	114.35	127.00
1	D	683	TYR	CA-CB-CG	5.24	123.33	113.90
1	B	625	VAL	N-CA-CB	5.24	116.43	110.72
1	A	705	VAL	N-CA-CB	5.14	116.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	758	VAL	CB-CA-C	5.14	118.49	110.83
1	A	393	VAL	N-CA-C	-5.10	108.16	113.10
1	D	685	SER	N-CA-C	5.07	117.69	110.24
1	A	225	ASP	CB-CA-C	-5.01	110.78	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5719	0	5511	38	0
1	B	5736	0	5528	44	0
1	C	5716	0	5507	48	0
1	D	5720	0	5519	58	0
2	E	92	0	78	2	0
2	G	92	0	78	3	0
3	F	53	0	46	0	0
4	I	39	0	34	0	0
4	K	39	0	34	0	0
4	M	39	0	34	1	0
5	J	48	0	42	2	0
6	L	95	0	78	9	0
7	N	22	0	17	0	0
8	A	97	0	89	6	0
8	B	97	0	89	8	0
8	C	83	0	75	5	0
8	D	70	0	64	1	0
9	A	59	0	0	4	0
9	B	59	0	0	1	0
10	A	9	0	0	1	0
11	B	10	0	7	0	0
12	B	11	0	10	0	0
13	C	11	0	10	0	0
14	A	277	0	0	2	0
14	B	242	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	120	0	0	1	0
14	D	96	0	0	2	0
All	All	24651	0	22850	206	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 (206) 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)
8:A:901:NAG:C4	8:A:902:NAG:O1	1.86	1.21
1:D:224:ILE:HD12	1:D:224:ILE:O	1.38	1.18
8:B:903:NAG:C4	2:G:1:NAG:O1	1.92	1.18
8:B:901:NAG:C4	8:B:902:NAG:O1	1.91	1.18
8:A:903:NAG:C4	2:E:1:NAG:O1	1.90	1.18
1:D:281:LYS:HG2	6:L:1:NAG:O7	1.45	1.15
1:D:224:ILE:HG23	1:D:225:ASP:H	1.24	1.01
1:D:224:ILE:HD12	1:D:224:ILE:C	1.89	0.97
1:D:281:LYS:CG	6:L:1:NAG:O7	2.17	0.92
8:C:901:NAG:C4	8:C:902:NAG:O1	2.23	0.86
1:D:281:LYS:HG3	6:L:1:NAG:H81	1.57	0.85
8:D:901:NAG:C4	8:D:902:NAG:O1	2.26	0.84
1:D:281:LYS:HG3	6:L:1:NAG:C8	2.08	0.83
1:C:130:ALA:CB	1:C:179:THR:O	2.27	0.81
1:C:736:GLN:HE21	1:C:736:GLN:HA	1.50	0.76
1:B:416[A]:THR:O	1:B:416[A]:THR:HG22	1.86	0.75
1:B:204:THR:H	1:B:262:ASN:HD22	1.35	0.74
1:C:227:VAL:HG13	1:C:232:ILE:HD11	1.70	0.73
1:D:745:ASP:HB3	1:D:758:VAL:HG22	1.70	0.72
1:D:281:LYS:HG2	6:L:1:NAG:C7	2.20	0.72
1:A:416:THR:HG21	14:A:1069:HOH:O	1.90	0.72
1:D:224:ILE:C	1:D:224:ILE:CD1	2.55	0.71
1:B:438:VAL:HG23	1:B:439:LEU:HD13	1.73	0.70
1:D:432:ASN:HD21	1:D:458:GLY:H	1.39	0.70
1:C:438:VAL:HG23	1:C:439:LEU:HD13	1.73	0.70
1:C:377:ASN:C	1:C:377:ASN:HD22	2.00	0.69
1:D:281:LYS:CG	6:L:1:NAG:C7	2.71	0.69
1:A:373:PRO:O	1:A:391:ARG:NH2	2.25	0.69
8:C:903:NAG:C4	5:J:1:NAG:O1	2.40	0.68
1:A:731:ILE:O	1:A:736:GLN:HG2	1.93	0.67
1:B:182:ASP:OD1	1:B:645:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:VAL:HG11	1:B:546:MET:HE3	1.77	0.67
1:A:421:LEU:HD11	1:A:520:PHE:HZ	1.59	0.66
1:B:759:THR:HG23	14:B:1005:HOH:O	1.95	0.66
1:B:422:LYS:O	1:B:423:HIS:CG	2.50	0.65
1:B:546:MET:HA	1:B:546:MET:HE2	1.79	0.64
1:B:649:LYS:HG3	14:B:1204:HOH:O	1.97	0.63
1:B:432:ASN:HD21	1:B:458:GLY:H	1.46	0.63
1:D:246:HIS:HE1	1:D:290:GLU:OE2	1.82	0.62
8:A:903:NAG:C4	2:E:1:NAG:C1	2.77	0.62
1:D:224:ILE:HG23	1:D:225:ASP:N	2.03	0.62
1:B:421:LEU:HD11	1:B:520:PHE:HZ	1.65	0.62
1:D:117:VAL:HG22	1:D:376:TYR:CD2	2.34	0.62
8:B:903:NAG:C4	2:G:1:NAG:C1	2.77	0.62
1:B:242:ASP:O	1:B:246:HIS:HD2	1.84	0.61
1:D:152:GLN:HE21	1:D:152:GLN:HA	1.66	0.61
1:B:474:THR:HG21	14:B:1193:HOH:O	2.01	0.59
1:C:130:ALA:HB1	1:C:179:THR:O	2.02	0.59
1:C:763:ARG:HD3	1:C:766:ASP:OD2	2.01	0.58
1:A:117:VAL:HG22	1:A:376:TYR:CD2	2.39	0.58
1:D:151:ASP:HB3	1:D:393:VAL:HG22	1.85	0.58
1:A:172:ASN:HD22	1:A:174:ARG:H	1.52	0.58
1:C:130:ALA:HB2	1:C:179:THR:O	2.04	0.58
1:D:763:ARG:HD3	1:D:766:ASP:OD2	2.04	0.58
1:A:432:ASN:HD21	1:A:458:GLY:H	1.50	0.58
1:B:416[A]:THR:O	1:B:416[A]:THR:CG2	2.50	0.58
1:D:683:TYR:HB2	14:D:1001:HOH:O	2.04	0.57
1:A:641:PHE:CE1	1:A:649:LYS:HG3	2.40	0.57
1:A:748:LYS:HE2	14:A:1172:HOH:O	2.03	0.57
1:A:650:MET:HA	1:A:650:MET:HE2	1.87	0.57
8:B:901:NAG:C4	8:B:902:NAG:C1	2.81	0.57
1:B:442:ASN:HD21	1:B:471:SER:H	1.52	0.57
1:A:521:VAL:HG11	1:A:546:MET:CE	2.35	0.56
9:A:908:BKR:C20	9:A:908:BKR:C46	2.84	0.56
1:C:702:LEU:HD22	1:C:765:LYS:HB2	1.86	0.56
1:D:253:PHE:O	1:D:257:VAL:HG23	2.06	0.56
1:B:246:HIS:HE1	1:B:290:GLU:OE2	1.88	0.56
1:C:320:PRO:HG3	1:C:328:LEU:HD12	1.87	0.55
1:D:224:ILE:CG2	1:D:225:ASP:H	2.08	0.55
1:D:172:ASN:HD22	1:D:172:ASN:C	2.15	0.55
1:C:117:VAL:HG22	1:C:376:TYR:CD2	2.42	0.55
1:C:731:ILE:O	1:C:736:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ASP:HB2	1:A:776:LEU:HD22	1.87	0.55
1:D:281:LYS:CG	6:L:1:NAG:C8	2.85	0.54
9:A:908:BKR:C19	9:A:908:BKR:C14	2.85	0.54
1:C:248:LEU:HD22	1:C:640:VAL:HA	1.89	0.54
1:A:130:ALA:CB	1:A:179:THR:O	2.57	0.53
1:B:763:ARG:HD3	1:B:766:ASP:OD2	2.09	0.53
1:A:521:VAL:HG11	1:A:546:MET:HE2	1.90	0.53
1:B:731:ILE:O	1:B:736:GLN:HG2	2.09	0.53
8:A:901:NAG:C4	8:A:902:NAG:C1	2.86	0.53
1:B:98:THR:HG21	8:B:901:NAG:O3	2.09	0.53
1:C:782:GLY:O	1:C:802:THR:HG23	2.08	0.53
1:D:524:ASN:HA	1:D:561:HIS:O	2.09	0.53
1:D:281:LYS:HG3	6:L:1:NAG:C7	2.38	0.53
1:D:435:THR:OG1	1:D:436:TYR:N	2.43	0.52
1:A:98:THR:CG2	8:A:901:NAG:O3	2.58	0.52
1:D:281:LYS:CG	6:L:1:NAG:H81	2.35	0.52
1:A:204:THR:H	1:A:262:ASN:HD22	1.58	0.52
9:A:908:BKR:C10	9:A:908:BKR:C24	2.88	0.51
1:B:98:THR:CG2	8:B:901:NAG:O3	2.58	0.51
1:A:151:ASP:HB3	1:A:393:VAL:HG22	1.91	0.51
1:B:172:ASN:HD22	1:B:174:ARG:H	1.58	0.51
1:B:157:ALA:HB2	1:B:202[B]:VAL:HG11	1.93	0.51
1:B:147:GLN:HG2	14:B:1124:HOH:O	2.12	0.50
1:C:152:GLN:HE21	1:C:152:GLN:HA	1.75	0.50
1:C:521:VAL:HG11	1:C:546:MET:CE	2.41	0.50
1:C:191:TYR:CD2	1:C:259:ALA:HB2	2.47	0.50
1:A:758:VAL:CG1	1:A:760:PHE:CE2	2.95	0.50
1:A:524:ASN:HA	1:A:561:HIS:O	2.12	0.49
9:B:908:BKR:C46	9:B:908:BKR:C20	2.90	0.49
1:C:774:ASP:HB2	1:C:776:LEU:HD22	1.94	0.49
1:A:246:HIS:HE1	1:A:290:GLU:OE2	1.95	0.49
1:C:745:ASP:HB3	1:C:758:VAL:HG22	1.94	0.49
1:D:729:ILE:HD12	1:D:742:ARG:HG2	1.94	0.49
1:A:438:VAL:HG23	1:A:439:LEU:HD13	1.94	0.49
1:C:242:ASP:O	1:C:246:HIS:HD2	1.96	0.49
1:C:705:VAL:HA	1:C:763:ARG:HA	1.95	0.48
1:D:725:ALA:HB3	1:D:758:VAL:HG21	1.94	0.48
1:B:203:ALA:HA	1:B:262:ASN:ND2	2.28	0.48
1:D:317:VAL:HG22	1:D:357:ILE:HD11	1.95	0.48
1:C:317:VAL:HG22	1:C:357:ILE:HD11	1.96	0.48
1:C:377:ASN:HD21	1:C:380:GLY:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:THR:O	1:C:416:THR:HG22	2.14	0.48
1:A:98:THR:HG21	8:A:901:NAG:O3	2.14	0.48
1:C:305:TRP:O	1:C:331:PHE:CZ	2.68	0.47
1:D:683:TYR:CB	14:D:1001:HOH:O	2.61	0.47
1:C:255:GLU:OE2	1:C:763:ARG:NH2	2.42	0.47
1:C:474:THR:HG21	14:C:1065:HOH:O	2.15	0.47
1:A:442:ASN:HD21	1:A:471:SER:H	1.61	0.47
1:B:641:PHE:CE2	1:B:649:LYS:HD3	2.49	0.46
1:D:736:GLN:HE21	1:D:736:GLN:HA	1.81	0.46
1:A:161:VAL:HG13	1:A:164:GLY:O	2.16	0.46
1:C:238:SER:O	1:C:271:ILE:HA	2.16	0.46
1:C:573:ASP:CG	1:C:655:ARG:HH22	2.23	0.46
1:D:224:ILE:O	1:D:224:ILE:CD1	2.32	0.45
1:C:147:GLN:NE2	1:C:151:ASP:OD2	2.49	0.45
1:C:725:ALA:HB3	1:C:758:VAL:HG21	1.99	0.45
1:B:569:GLU:OE1	1:B:655:ARG:NH1	2.49	0.45
1:D:728:TYR:HB3	1:D:739:ARG:HB2	1.98	0.45
1:C:112:ILE:HG22	1:C:125:ALA:HA	1.99	0.45
1:C:377:ASN:C	1:C:377:ASN:ND2	2.70	0.45
1:C:209:TRP:O	1:C:267:SER:N	2.49	0.45
8:C:903:NAG:C4	5:J:1:NAG:C1	2.95	0.45
1:A:421:LEU:HD12	1:A:599:TYR:CE1	2.52	0.44
1:C:702:LEU:HD22	1:C:765:LYS:CB	2.48	0.44
1:D:248:LEU:HD22	1:D:640:VAL:HA	1.99	0.44
1:A:774:ASP:CB	1:A:776:LEU:HD22	2.47	0.44
1:B:422:LYS:C	1:B:423:HIS:CG	2.94	0.44
1:B:521:VAL:HG21	1:B:546:MET:CE	2.48	0.44
1:D:179:THR:HG21	1:D:189:ALA:HB1	1.98	0.44
1:C:676:HIS:HE1	1:C:801:TRP:CD1	2.36	0.44
1:A:546:MET:HE1	1:A:558:VAL:HG22	2.00	0.44
1:B:641:PHE:CE2	1:B:649:LYS:CD	3.00	0.44
9:A:908:BKR:C19	10:A:909:XYP:O2	2.65	0.44
1:A:763:ARG:NH1	1:A:766:ASP:OD1	2.51	0.43
1:C:98:THR:HB	8:C:902:NAG:O6	2.19	0.43
1:D:342:ASN:C	1:D:342:ASN:OD1	2.60	0.43
1:C:361:TYR:CE2	1:C:367:ASP:HB3	2.54	0.43
1:D:78:GLU:OE2	1:D:99:ARG:NH1	2.47	0.43
1:B:442:ASN:HD21	1:B:471:SER:N	2.13	0.43
1:C:710:PHE:CE1	1:C:759:THR:HB	2.53	0.43
1:D:108:GLN:HG3	1:D:109:ASP:O	2.18	0.43
1:C:521:VAL:HG11	1:C:546:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASP:HB3	1:C:393:VAL:HG22	2.01	0.43
1:D:513:LEU:O	1:D:514:PRO:C	2.60	0.43
1:A:715:ASN:HB2	1:A:750:LEU:HD13	2.01	0.42
1:B:619:TYR:O	1:B:620:VAL:C	2.62	0.42
1:A:727:LEU:C	1:A:727:LEU:HD23	2.44	0.42
1:B:151:ASP:CB	1:B:393:VAL:HG22	2.48	0.42
1:D:258:ARG:NH1	1:D:685:SER:HB3	2.34	0.42
1:D:129:VAL:HG13	1:D:141:ARG:HD2	2.01	0.42
1:A:108:GLN:HG3	1:A:109:ASP:O	2.19	0.42
1:C:111:PRO:HD2	1:C:467:GLY:HA2	2.02	0.42
1:D:109:ASP:OD1	1:D:158:LEU:HD12	2.18	0.42
1:D:539:GLY:O	1:D:540:GLY:C	2.62	0.42
1:B:524:ASN:HA	1:B:561:HIS:O	2.20	0.42
1:C:736:GLN:HA	1:C:736:GLN:NE2	2.26	0.42
1:D:164:GLY:HA2	1:D:165:PRO:HA	1.92	0.42
1:B:248:LEU:HD22	1:B:640:VAL:HA	2.02	0.42
1:D:239:ASN:HA	1:D:272:ASN:ND2	2.35	0.42
1:B:429:VAL:O	1:B:494:ALA:HA	2.20	0.41
1:D:528:GLU:OE1	4:M:2:NAG:H5	2.20	0.41
1:D:776:LEU:C	1:D:776:LEU:HD23	2.45	0.41
1:B:48:GLN:N	14:B:1002:HOH:O	2.53	0.41
1:D:562:THR:OG1	1:D:563:THR:N	2.53	0.41
1:A:308:VAL:HB	1:A:309:PRO:HD3	2.02	0.41
1:A:697:ASP:OD1	1:A:699:THR:OG1	2.31	0.41
1:B:172:ASN:HD22	1:B:172:ASN:C	2.28	0.41
1:A:521:VAL:HB	1:A:546:MET:HE1	2.03	0.41
1:B:98:THR:HB	8:B:902:NAG:O6	2.19	0.41
1:B:521:VAL:CG1	1:B:546:MET:HE3	2.49	0.41
1:D:172:ASN:HD22	1:D:173:GLY:N	2.19	0.41
1:D:235:PRO:HD3	1:D:305:TRP:CZ2	2.55	0.41
1:D:442:ASN:HD21	1:D:471:SER:H	1.69	0.41
1:B:573:ASP:OD1	1:B:655:ARG:NH2	2.54	0.41
1:C:98:THR:CG2	8:C:901:NAG:O3	2.69	0.41
1:D:741:LEU:O	1:D:742:ARG:HD3	2.21	0.41
1:A:419:LEU:HA	1:A:420:PRO:C	2.46	0.40
1:A:621:PRO:HD3	1:A:646:TRP:CZ2	2.56	0.40
1:B:172:ASN:ND2	1:B:174:ARG:H	2.20	0.40
1:D:107:LEU:HB3	1:D:158:LEU:HD21	2.04	0.40
1:D:607:LYS:HD2	1:D:724:VAL:HB	2.02	0.40
1:B:419:LEU:HA	1:B:420:PRO:C	2.46	0.40
1:B:605[A]:SER:OG	1:B:746:LYS:CE	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:903:NAG:C5	2:G:1:NAG:O1	2.65	0.40
1:C:159:ALA:HB1	1:C:160:PRO:HA	2.03	0.40
1:C:655:ARG:HG2	1:C:656:TYR:CE2	2.56	0.40
1:D:85:GLY:HA3	1:D:320:PRO:O	2.21	0.40
1:D:176:TRP:CD1	1:D:563:THR:HB	2.57	0.40
1:A:569:GLU:OE1	1:A:655:ARG:NH1	2.55	0.40
1:B:151:ASP:HB3	1:B:393:VAL:HG22	2.03	0.40
1:C:218:ARG:O	1:C:219:ASN:C	2.64	0.40
1:C:776:LEU:HD23	1:C:776:LEU:O	2.21	0.40
1:A:573:ASP:CG	1:A:655:ARG:HH22	2.28	0.40
1:D:170:PRO:HG3	1:D:619:TYR:CD2	2.56	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	756/803 (94%)	722 (96%)	34 (4%)	0	100	100
1	B	758/803 (94%)	721 (95%)	36 (5%)	1 (0%)	48	61
1	C	756/803 (94%)	709 (94%)	46 (6%)	1 (0%)	48	61
1	D	756/803 (94%)	711 (94%)	45 (6%)	0	100	100
All	All	3026/3212 (94%)	2863 (95%)	161 (5%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	GLY
1	B	167	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/648 (94%)	567 (93%)	43 (7%)	14	18
1	B	613/648 (95%)	572 (93%)	41 (7%)	15	20
1	C	610/648 (94%)	558 (92%)	52 (8%)	10	11
1	D	611/648 (94%)	554 (91%)	57 (9%)	8	9
All	All	2444/2592 (94%)	2251 (92%)	193 (8%)	11	14

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	107	LEU
1	A	117	VAL
1	A	129	VAL
1	A	137	LEU
1	A	147	GLN
1	A	172	ASN
1	A	195	LYS
1	A	202[A]	VAL
1	A	202[B]	VAL
1	A	285	GLN
1	A	301	TRP
1	A	312	GLU
1	A	317	VAL
1	A	351	ARG
1	A	358	LEU
1	A	375	VAL
1	A	393	VAL
1	A	400	GLU
1	A	416	THR
1	A	430	LEU
1	A	446	LEU
1	A	474	THR
1	A	483	LYS

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Mol	Chain	Res	Type
1	A	503	THR
1	A	529	GLU
1	A	610	TRP
1	A	625	VAL
1	A	649	LYS
1	A	672	LEU
1	A	678	ARG
1	A	685	SER
1	A	702	LEU
1	A	705	VAL
1	A	709	VAL
1	A	716	THR
1	A	736	GLN
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	68	LYS
1	B	98	THR
1	B	107	LEU
1	B	117	VAL
1	B	129	VAL
1	B	137	LEU
1	B	147	GLN
1	B	152	GLN
1	B	172	ASN
1	B	195	LYS
1	B	285	GLN
1	B	358	LEU
1	B	375	VAL
1	B	393	VAL
1	B	400	GLU
1	B	422	LYS
1	B	430	LEU
1	B	439	LEU
1	B	446	LEU
1	B	474	THR
1	B	503	THR
1	B	506	GLU
1	B	582	VAL

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Mol	Chain	Res	Type
1	B	610	TRP
1	B	625	VAL
1	B	645	ARG
1	B	672	LEU
1	B	682	ASP
1	B	702	LEU
1	B	705	VAL
1	B	709	VAL
1	B	716	THR
1	B	736	GLN
1	B	739	ARG
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	776	LEU
1	C	48	GLN
1	C	84	SER
1	C	98	THR
1	C	107	LEU
1	C	117	VAL
1	C	129	VAL
1	C	137	LEU
1	C	147	GLN
1	C	152	GLN
1	C	172	ASN
1	C	195	LYS
1	C	224	ILE
1	C	240	VAL
1	C	266	CYS
1	C	271	ILE
1	C	277	CYS
1	C	285	GLN
1	C	307	SER
1	C	312	GLU
1	C	358	LEU
1	C	377	ASN
1	C	393	VAL
1	C	400	GLU
1	C	422	LYS

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Mol	Chain	Res	Type
1	C	430	LEU
1	C	439	LEU
1	C	446	LEU
1	C	474	THR
1	C	483	LYS
1	C	503	THR
1	C	610	TRP
1	C	611	THR
1	C	672	LEU
1	C	674	VAL
1	C	684	SER
1	C	685	SER
1	C	688	GLU
1	C	702	LEU
1	C	705	VAL
1	C	709	VAL
1	C	716	THR
1	C	734	ASP
1	C	736	GLN
1	C	739	ARG
1	C	748	LYS
1	C	750	LEU
1	C	759	THR
1	C	763	ARG
1	C	767	VAL
1	C	773	VAL
1	C	776	LEU
1	C	802	THR
1	D	68	LYS
1	D	73	GLU
1	D	87	ILE
1	D	98	THR
1	D	107	LEU
1	D	117	VAL
1	D	121	SER
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	220	LEU

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Mol	Chain	Res	Type
1	D	224	ILE
1	D	264	ILE
1	D	266	CYS
1	D	270	ARG
1	D	277	CYS
1	D	285	GLN
1	D	317	VAL
1	D	342	ASN
1	D	358	LEU
1	D	375	VAL
1	D	383	THR
1	D	393	VAL
1	D	400	GLU
1	D	410	VAL
1	D	416	THR
1	D	421	LEU
1	D	439	LEU
1	D	446	LEU
1	D	474	THR
1	D	483	LYS
1	D	500	ASN
1	D	503	THR
1	D	506	GLU
1	D	525	ARG
1	D	537	SER
1	D	610	TRP
1	D	649	LYS
1	D	672	LEU
1	D	678	ARG
1	D	681	LYS
1	D	683	TYR
1	D	702	LEU
1	D	705	VAL
1	D	709	VAL
1	D	736	GLN
1	D	739	ARG
1	D	742	ARG
1	D	750	LEU
1	D	758	VAL
1	D	759	THR
1	D	763	ARG
1	D	767	VAL

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Mol	Chain	Res	Type
1	D	776	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	172	ASN
1	A	208	HIS
1	A	246	HIS
1	A	262	ASN
1	A	285	GLN
1	A	377	ASN
1	A	432	ASN
1	A	442	ASN
1	A	455	ASN
1	A	676	HIS
1	A	736	GLN
1	B	147	GLN
1	B	152	GLN
1	B	172	ASN
1	B	229	GLN
1	B	246	HIS
1	B	262	ASN
1	B	377	ASN
1	B	432	ASN
1	B	442	ASN
1	B	735	ASN
1	B	736	GLN
1	B	740	GLN
1	C	147	GLN
1	C	152	GLN
1	C	172	ASN
1	C	229	GLN
1	C	239	ASN
1	C	246	HIS
1	C	285	GLN
1	C	377	ASN
1	C	442	ASN
1	C	676	HIS
1	C	736	GLN
1	D	48	GLN
1	D	147	GLN

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Mol	Chain	Res	Type
1	D	152	GLN
1	D	172	ASN
1	D	229	GLN
1	D	246	HIS
1	D	285	GLN
1	D	432	ASN
1	D	442	ASN
1	D	736	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

43 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2	15,15,15	0.52	0	21,21,21	1.12	2 (9%)
2	BMA	E	2	2	11,11,12	0.40	0	15,15,17	1.19	1 (6%)
2	MAN	E	3	2	11,11,12	0.82	0	15,15,17	2.23	3 (20%)
2	BMA	E	4	2	11,11,12	0.71	0	15,15,17	1.99	4 (26%)
2	MAN	E	5	2	11,11,12	0.61	0	15,15,17	1.53	3 (20%)
2	MAN	E	6	2	11,11,12	0.70	0	15,15,17	0.91	1 (6%)
2	MAN	E	7	2	11,11,12	0.64	0	15,15,17	2.34	2 (13%)
2	MAN	E	8	2	11,11,12	0.56	0	15,15,17	1.59	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.73	0	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.54	4 (23%)
3	MAN	F	3	3	11,11,12	1.79	2 (18%)	15,15,17	2.17	5 (33%)
3	NAG	F	4	3	14,14,15	2.67	4 (28%)	19,19,21	3.08	11 (57%)
2	NAG	G	1	2	15,15,15	0.50	0	21,21,21	1.56	4 (19%)
2	BMA	G	2	2	11,11,12	0.72	0	15,15,17	1.60	4 (26%)
2	MAN	G	3	2	11,11,12	0.27	0	15,15,17	0.61	0
2	BMA	G	4	2	11,11,12	0.76	0	15,15,17	2.32	6 (40%)
2	MAN	G	5	2	11,11,12	0.61	0	15,15,17	2.02	3 (20%)
2	MAN	G	6	2	11,11,12	0.45	0	15,15,17	1.31	2 (13%)
2	MAN	G	7	2	11,11,12	0.89	0	15,15,17	2.42	5 (33%)
2	MAN	G	8	2	11,11,12	0.94	0	15,15,17	2.00	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.58	0	17,19,21	1.23	1 (5%)
4	NAG	I	2	4	14,14,15	0.56	0	17,19,21	1.54	3 (17%)
4	MAN	I	3	4	11,11,12	0.94	0	15,15,17	2.24	6 (40%)
5	NAG	J	1	5	15,15,15	0.65	0	21,21,21	1.49	5 (23%)
5	BMA	J	2	5	11,11,12	1.09	1 (9%)	15,15,17	2.04	5 (33%)
5	MAN	J	3	5	11,11,12	0.49	0	15,15,17	2.19	6 (40%)
5	MAN	J	4	5	11,11,12	1.15	1 (9%)	15,15,17	1.14	0
4	NAG	K	1	4,1	14,14,15	0.53	0	17,19,21	1.17	2 (11%)
4	NAG	K	2	4	14,14,15	1.00	0	17,19,21	1.85	6 (35%)
4	MAN	K	3	4	11,11,12	1.50	2 (18%)	15,15,17	2.09	4 (26%)
6	NAG	L	1	6	14,14,15	1.25	3 (21%)	17,19,21	2.11	3 (17%)
6	NAG	L	2	6	14,14,15	0.46	0	17,19,21	1.24	3 (17%)
6	BMA	L	3	6	11,11,12	0.36	0	15,15,17	0.83	0
6	MAN	L	4	6	11,11,12	1.00	0	15,15,17	2.41	3 (20%)
6	MAN	L	5	6	11,11,12	0.87	0	15,15,17	1.73	3 (20%)
6	MAN	L	6	6	11,11,12	1.16	0	15,15,17	2.90	6 (40%)
6	MAN	L	7	6	11,11,12	0.60	0	15,15,17	1.62	3 (20%)
6	MAN	L	8	6	12,12,12	1.23	2 (16%)	17,17,17	1.74	4 (23%)
4	NAG	M	1	4,1	14,14,15	0.40	0	17,19,21	1.13	2 (11%)
4	NAG	M	2	4	14,14,15	0.55	0	17,19,21	1.73	4 (23%)
4	MAN	M	3	4	11,11,12	1.01	0	15,15,17	1.94	3 (20%)
7	BMA	N	1	7	11,11,12	1.07	1 (9%)	15,15,17	2.77	7 (46%)
7	MAN	N	2	7	11,11,12	1.37	2 (18%)	15,15,17	3.30	7 (46%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	L	6	6	-	2/2/19/22	0/1/1/1
6	MAN	L	7	6	-	0/2/19/22	0/1/1/1
6	MAN	L	8	6	-	1/2/22/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	MAN	M	3	4	-	2/2/19/22	0/1/1/1
7	BMA	N	1	7	-	2/2/19/22	0/1/1/1
7	MAN	N	2	7	-	1/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	NAG	C3-C2	7.18	1.59	1.53
3	F	4	NAG	C2-N2	4.05	1.52	1.45
3	F	4	NAG	C4-C3	3.84	1.60	1.52
3	F	3	MAN	C2-C3	3.73	1.58	1.52
7	N	1	BMA	O5-C1	-2.79	1.39	1.43
4	K	3	MAN	C2-C3	2.70	1.56	1.52
3	F	3	MAN	O3-C3	2.66	1.49	1.43
5	J	4	MAN	O5-C1	-2.66	1.39	1.43
5	J	2	BMA	O5-C5	-2.59	1.38	1.43
3	F	4	NAG	C1-C2	2.54	1.56	1.52
6	L	1	NAG	O4-C4	-2.42	1.37	1.43
7	N	2	MAN	O5-C5	2.35	1.48	1.43
6	L	8	MAN	O6-C6	2.30	1.52	1.42
6	L	1	NAG	O7-C7	-2.29	1.18	1.23
4	K	3	MAN	C4-C5	2.28	1.57	1.53
7	N	2	MAN	O4-C4	2.16	1.48	1.43
6	L	1	NAG	C2-N2	-2.05	1.42	1.46
6	L	8	MAN	C6-C5	2.00	1.58	1.51

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	6	MAN	C1-O5-C5	8.18	123.15	112.19
6	L	4	MAN	C1-O5-C5	7.96	122.85	112.19
2	E	7	MAN	C1-O5-C5	7.61	122.38	112.19
7	N	2	MAN	C1-O5-C5	6.59	121.02	112.19
3	F	4	NAG	O5-C1-C2	6.52	116.06	109.52
7	N	1	BMA	O2-C2-C3	6.40	123.41	110.15
2	E	3	MAN	C1-O5-C5	6.25	120.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	2	MAN	C2-C3-C4	6.23	121.82	110.86
3	F	4	NAG	C3-C2-N2	5.93	122.13	110.44
7	N	1	BMA	C1-O5-C5	5.68	119.80	112.19
6	L	1	NAG	C1-O5-C5	5.64	119.74	112.19
2	G	8	MAN	C1-O5-C5	5.17	119.11	112.19
2	E	4	BMA	C1-C2-C3	-5.09	102.23	109.64
4	K	3	MAN	C1-C2-C3	5.04	116.99	109.64
2	E	8	MAN	C1-O5-C5	5.04	118.94	112.19
4	M	3	MAN	C1-O5-C5	5.00	118.88	112.19
2	G	4	BMA	C1-O5-C5	-4.99	105.50	112.19
5	J	3	MAN	C1-O5-C5	4.98	118.86	112.19
2	G	5	MAN	C1-O5-C5	4.88	118.73	112.19
7	N	2	MAN	O4-C4-C3	4.80	121.69	110.38
7	N	2	MAN	O5-C5-C6	4.78	116.97	107.66
2	G	7	MAN	C1-O5-C5	4.77	118.58	112.19
2	G	7	MAN	C1-C2-C3	-4.75	102.73	109.64
3	F	3	MAN	O3-C3-C2	4.68	119.61	110.05
4	I	3	MAN	C1-C2-C3	4.68	116.46	109.64
6	L	5	MAN	C3-C4-C5	4.60	118.58	110.23
2	G	4	BMA	C1-C2-C3	-4.57	102.99	109.64
6	L	1	NAG	O4-C4-C3	4.40	120.76	110.38
3	F	4	NAG	C1-C2-N2	-4.36	105.67	110.73
2	G	1	NAG	C1-C2-C3	-4.31	104.66	110.54
2	G	7	MAN	O5-C5-C6	4.23	115.90	107.66
2	G	5	MAN	C1-C2-C3	4.14	115.68	109.64
3	F	4	NAG	O7-C7-C8	-4.03	114.87	122.05
4	K	2	NAG	O5-C5-C6	3.99	115.43	107.66
5	J	2	BMA	C1-O5-C5	3.98	117.52	112.19
3	F	4	NAG	O5-C5-C6	3.85	113.01	106.83
4	I	2	NAG	C2-N2-C7	3.80	128.00	122.90
6	L	1	NAG	C3-C4-C5	-3.72	103.48	110.23
7	N	2	MAN	O3-C3-C4	-3.72	101.61	110.38
6	L	8	MAN	O6-C6-C5	3.68	123.87	111.33
2	E	3	MAN	O5-C5-C6	-3.65	100.56	107.66
5	J	2	BMA	O5-C5-C6	-3.62	100.63	107.66
6	L	7	MAN	C1-C2-C3	3.61	114.90	109.64
3	F	3	MAN	C3-C4-C5	3.57	116.71	110.23
6	L	6	MAN	O5-C5-C6	-3.56	100.73	107.66
3	F	2	NAG	O3-C3-C2	-3.51	102.11	109.40
4	K	3	MAN	C3-C4-C5	3.46	116.51	110.23
4	I	3	MAN	C2-C3-C4	3.43	116.89	110.86
6	L	7	MAN	C1-O5-C5	3.42	116.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	NAG	C1-O5-C5	3.39	120.15	113.65
2	G	2	BMA	O3-C3-C4	-3.33	102.53	110.38
2	E	4	BMA	C3-C4-C5	3.33	116.26	110.23
2	G	5	MAN	C3-C4-C5	3.30	116.22	110.23
5	J	1	NAG	C3-C2-N2	3.29	116.67	110.62
5	J	2	BMA	O4-C4-C3	-3.27	102.68	110.38
3	F	1	NAG	C8-C7-N2	-3.23	110.76	116.12
5	J	3	MAN	C3-C4-C5	3.23	116.09	110.23
6	L	4	MAN	O5-C5-C6	3.20	113.90	107.66
3	F	2	NAG	C2-N2-C7	3.18	127.17	122.90
6	L	6	MAN	C2-C3-C4	3.13	116.37	110.86
2	E	5	MAN	C3-C4-C5	3.13	115.91	110.23
2	G	8	MAN	O2-C2-C1	3.12	116.37	109.22
4	I	3	MAN	O4-C4-C3	-3.12	103.03	110.38
2	G	4	BMA	O3-C3-C4	3.11	117.72	110.38
3	F	4	NAG	O5-C5-C4	-3.10	105.41	110.14
4	I	2	NAG	C1-O5-C5	3.10	116.34	112.19
5	J	1	NAG	C1-C2-N2	-3.10	107.14	110.73
3	F	3	MAN	O2-C2-C3	3.06	116.50	110.15
4	M	2	NAG	O3-C3-C2	-3.03	103.10	109.40
3	F	1	NAG	O5-C1-C2	-3.01	106.63	111.29
4	M	2	NAG	O4-C4-C3	3.00	117.44	110.38
4	M	3	MAN	C3-C4-C5	2.97	115.62	110.23
6	L	6	MAN	C6-C5-C4	2.96	120.29	113.02
6	L	6	MAN	O6-C6-C5	2.96	121.41	111.33
4	I	3	MAN	O2-C2-C1	-2.94	102.50	109.22
4	I	1	NAG	O5-C1-C2	-2.90	106.81	111.29
3	F	3	MAN	C1-C2-C3	2.81	113.73	109.64
6	L	6	MAN	C1-C2-C3	2.80	113.71	109.64
7	N	1	BMA	C6-C5-C4	-2.79	106.17	113.02
5	J	3	MAN	O5-C5-C6	2.76	113.04	107.66
2	G	7	MAN	C3-C4-C5	2.76	115.23	110.23
5	J	2	BMA	O3-C3-C4	2.74	116.85	110.38
4	K	2	NAG	C2-N2-C7	2.74	126.57	122.90
2	G	7	MAN	O6-C6-C5	2.73	120.64	111.33
4	I	3	MAN	C3-C4-C5	2.73	115.18	110.23
2	E	4	BMA	O2-C2-C3	2.73	115.80	110.15
5	J	1	NAG	O5-C1-C2	2.72	112.25	109.52
7	N	1	BMA	O5-C5-C4	2.69	117.38	110.83
6	L	8	MAN	C3-C4-C5	2.65	115.03	110.23
5	J	3	MAN	C1-C2-C3	2.63	113.47	109.64
4	K	3	MAN	C1-O5-C5	2.61	115.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	NAG	O7-C7-N2	2.61	126.59	121.98
6	L	8	MAN	O5-C5-C6	2.61	112.90	106.44
5	J	1	NAG	C1-C2-C3	-2.60	107.00	110.54
6	L	2	NAG	C1-C2-N2	2.58	114.49	110.43
6	L	5	MAN	O2-C2-C1	2.57	115.10	109.22
4	I	3	MAN	O5-C5-C6	2.56	112.65	107.66
2	G	2	BMA	C6-C5-C4	-2.56	106.74	113.02
2	E	5	MAN	C1-C2-C3	-2.48	106.03	109.64
4	M	3	MAN	O5-C5-C6	2.48	112.49	107.66
4	M	2	NAG	C3-C4-C5	-2.48	105.74	110.23
6	L	2	NAG	C8-C7-N2	2.46	120.20	116.12
3	F	4	NAG	C4-C3-C2	2.44	119.29	110.34
7	N	2	MAN	C6-C5-C4	-2.43	107.05	113.02
5	J	3	MAN	O2-C2-C3	2.42	115.17	110.15
2	E	1	NAG	C1-C2-N2	-2.42	107.93	110.73
6	L	7	MAN	O4-C4-C5	2.42	115.27	109.32
7	N	2	MAN	O3-C3-C2	-2.42	105.12	110.05
4	K	3	MAN	C2-C3-C4	2.41	115.10	110.86
4	K	2	NAG	O7-C7-N2	2.40	126.23	121.98
2	G	1	NAG	O7-C7-C8	-2.40	117.78	122.05
3	F	3	MAN	O5-C5-C6	2.40	112.33	107.66
2	E	1	NAG	C3-C2-N2	2.39	115.02	110.62
2	E	7	MAN	O3-C3-C2	-2.38	105.21	110.05
2	G	6	MAN	O3-C3-C4	-2.37	104.78	110.38
6	L	5	MAN	C2-C3-C4	2.37	115.03	110.86
2	G	2	BMA	C1-O5-C5	2.35	115.33	112.19
4	K	2	NAG	O4-C4-C3	2.35	115.90	110.38
3	F	2	NAG	C4-C3-C2	2.34	114.45	111.02
2	G	4	BMA	C3-C4-C5	2.33	114.45	110.23
2	G	4	BMA	C2-C3-C4	-2.31	106.80	110.86
7	N	1	BMA	O3-C3-C2	-2.30	105.37	110.05
4	K	1	NAG	O7-C7-N2	2.29	126.03	121.98
6	L	4	MAN	O6-C6-C5	2.29	119.12	111.33
2	G	1	NAG	C3-C2-N2	2.28	114.82	110.62
2	G	2	BMA	O3-C3-C2	2.27	114.68	110.05
6	L	8	MAN	O4-C4-C5	-2.26	103.75	109.32
4	K	2	NAG	C3-C4-C5	-2.26	106.14	110.23
5	J	2	BMA	C3-C4-C5	2.25	114.30	110.23
3	F	4	NAG	C2-N2-C7	2.23	128.33	123.11
7	N	1	BMA	C1-C2-C3	-2.23	106.40	109.64
2	E	4	BMA	O2-C2-C1	-2.22	104.14	109.22
2	E	5	MAN	O5-C1-C2	-2.22	105.50	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1	BMA	C2-C3-C4	2.22	114.76	110.86
4	I	2	NAG	O4-C4-C3	2.21	115.58	110.38
6	L	2	NAG	O7-C7-C8	-2.20	118.13	122.05
2	E	2	BMA	C3-C4-C5	2.19	114.21	110.23
2	E	3	MAN	O5-C1-C2	2.19	116.02	110.79
2	G	8	MAN	O5-C1-C2	2.19	116.01	110.79
2	G	4	BMA	C6-C5-C4	2.19	118.39	113.02
3	F	4	NAG	C4-C5-C6	2.17	116.51	112.50
2	G	1	NAG	O5-C1-C2	2.17	111.69	109.52
4	K	1	NAG	C2-N2-C7	2.15	125.78	122.90
4	M	1	NAG	O3-C3-C2	2.15	113.87	109.40
5	J	3	MAN	O4-C4-C5	-2.07	104.22	109.32
2	E	6	MAN	C1-O5-C5	2.05	114.93	112.19
3	F	2	NAG	O7-C7-N2	2.04	125.59	121.98
4	K	2	NAG	O7-C7-C8	-2.04	118.42	122.05
4	M	2	NAG	C1-C2-N2	2.03	113.64	110.43
4	M	1	NAG	O4-C4-C3	-2.03	105.60	110.38
2	G	6	MAN	C1-C2-C3	2.01	112.56	109.64
5	J	1	NAG	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	5	MAN	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	3	MAN	O5-C5-C6-O6
5	J	3	MAN	O5-C5-C6-O6
4	M	3	MAN	C4-C5-C6-O6
4	I	3	MAN	O5-C5-C6-O6
6	L	5	MAN	C4-C5-C6-O6
4	K	3	MAN	O5-C5-C6-O6
7	N	1	BMA	C4-C5-C6-O6
2	E	5	MAN	C4-C5-C6-O6
4	K	3	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	L	6	MAN	O5-C5-C6-O6
4	I	3	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
7	N	1	BMA	O5-C5-C6-O6
2	G	7	MAN	C4-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
5	J	2	BMA	O5-C5-C6-O6
3	F	3	MAN	O5-C5-C6-O6
2	E	4	BMA	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
5	J	2	BMA	C4-C5-C6-O6
2	E	7	MAN	C4-C5-C6-O6
5	J	3	MAN	C4-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6
7	N	2	MAN	O5-C5-C6-O6
2	E	7	MAN	O5-C5-C6-O6
3	F	4	NAG	O5-C5-C6-O6
2	E	2	BMA	C4-C5-C6-O6
2	G	7	MAN	O5-C5-C6-O6
3	F	4	NAG	C4-C5-C6-O6
6	L	8	MAN	O5-C5-C6-O6
6	L	6	MAN	C4-C5-C6-O6
2	E	4	BMA	O5-C5-C6-O6
2	G	4	BMA	C4-C5-C6-O6
2	E	2	BMA	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
2	E	8	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 17 short contacts:

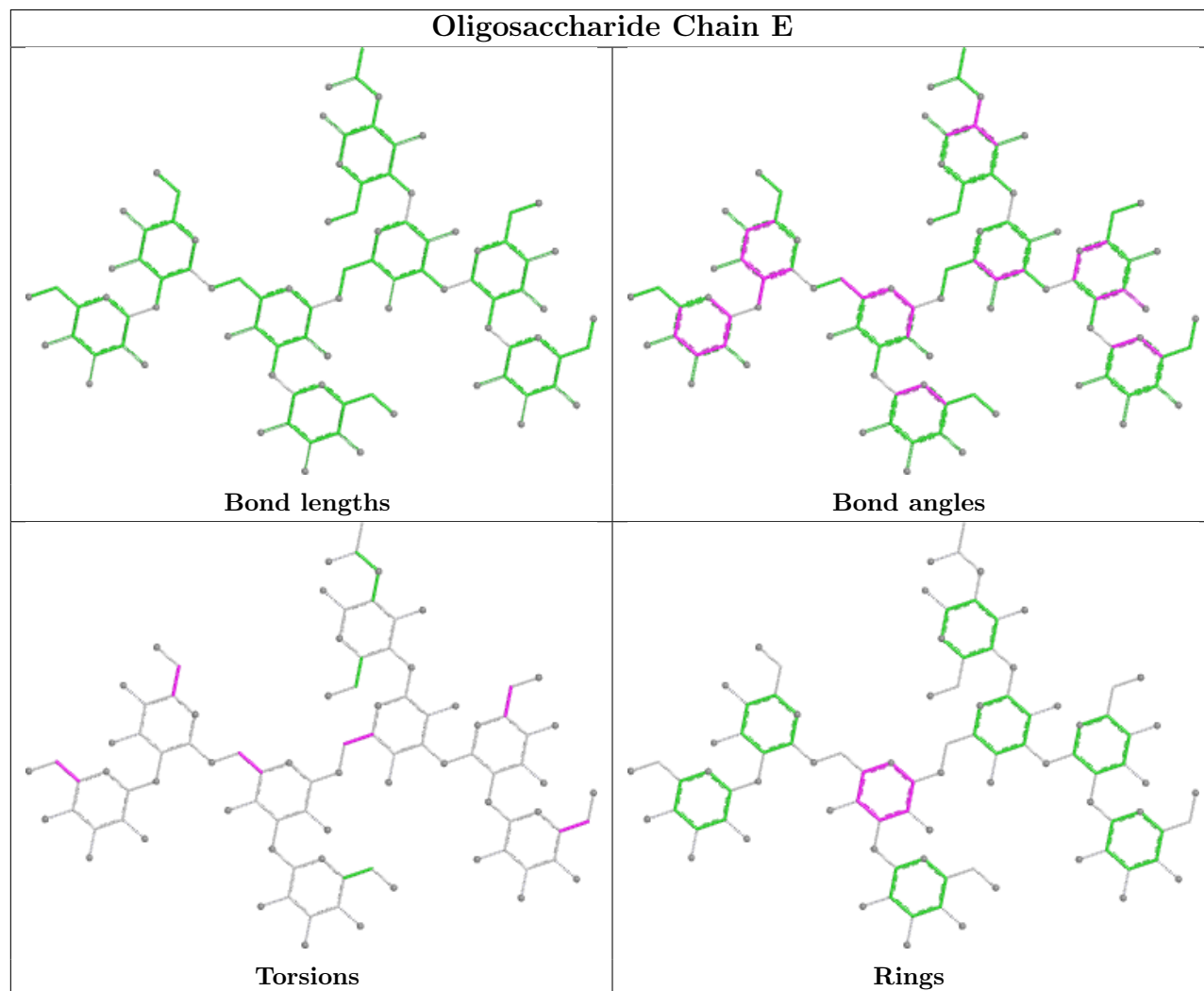
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	2	NAG	1	0
5	J	1	NAG	2	0
2	E	1	NAG	2	0
2	G	1	NAG	3	0

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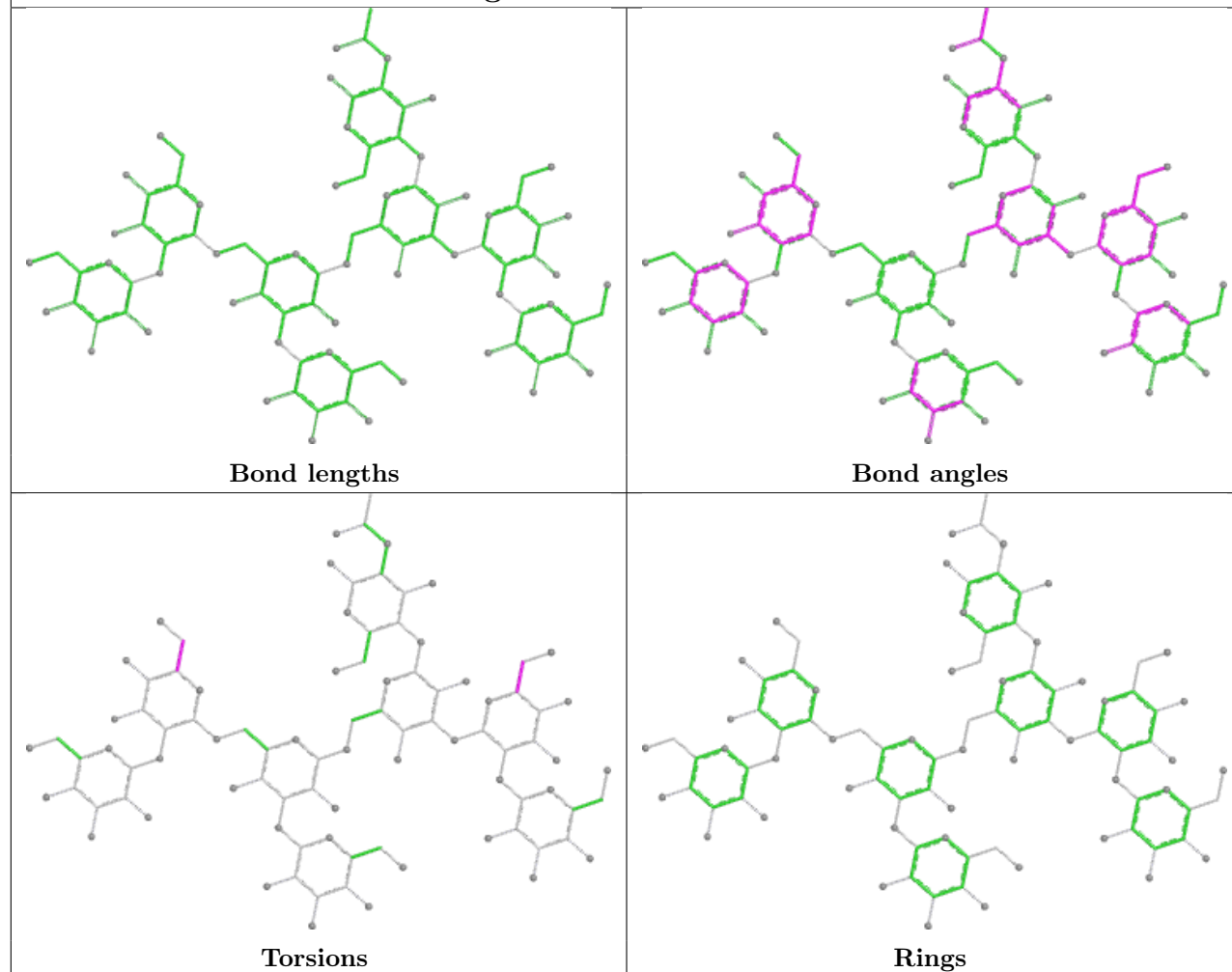
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1	NAG	9	0

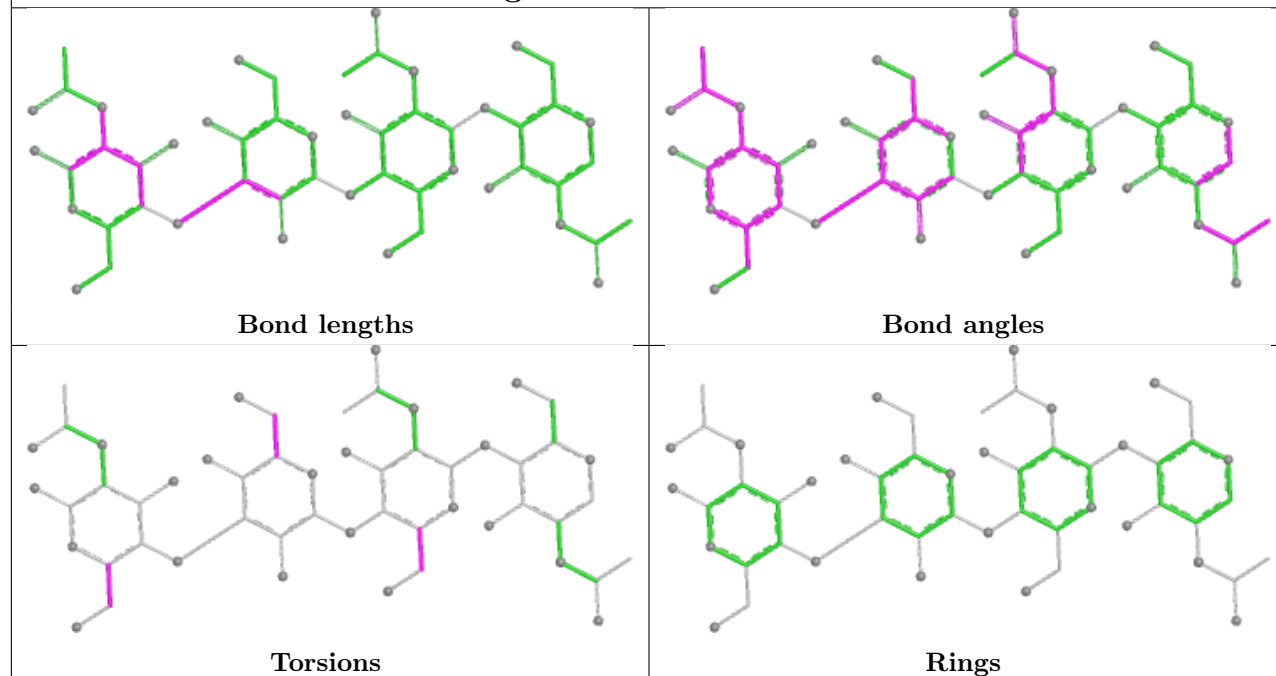
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

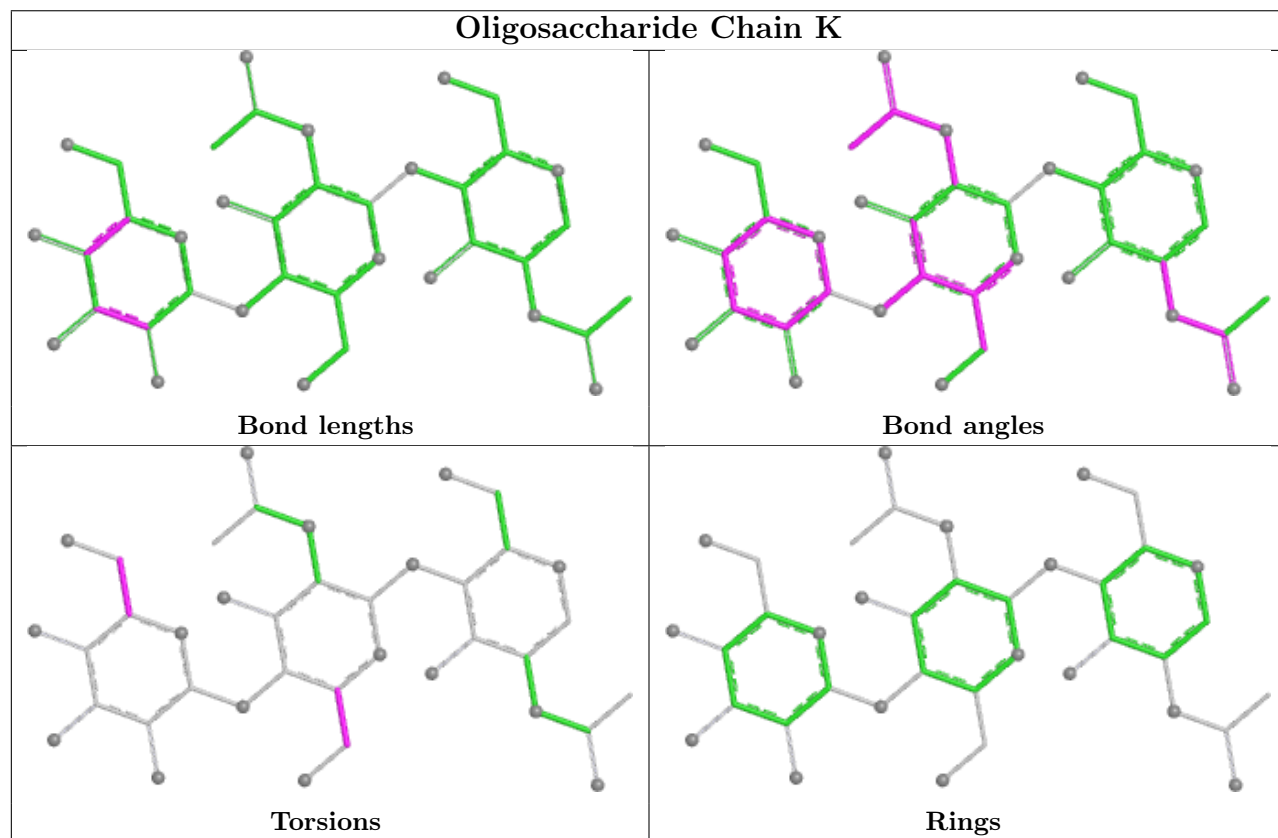
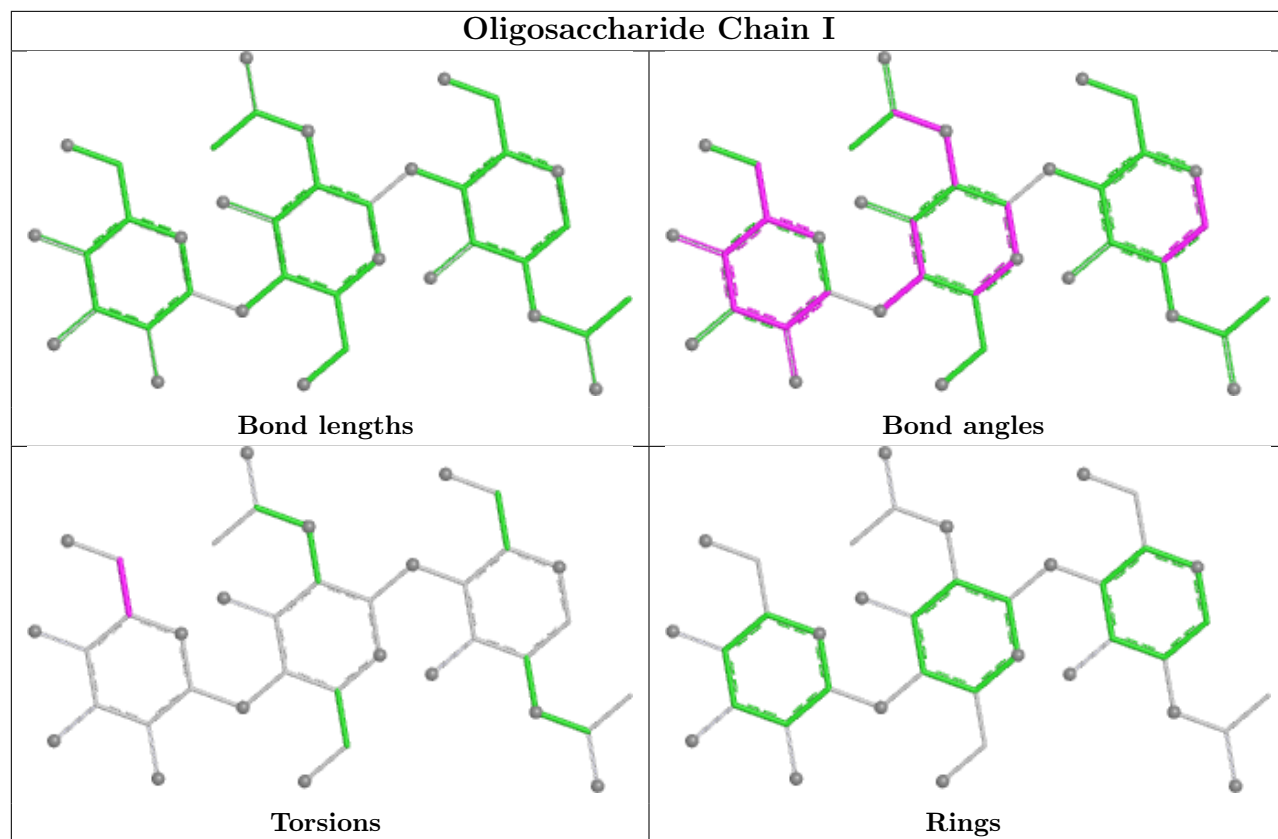


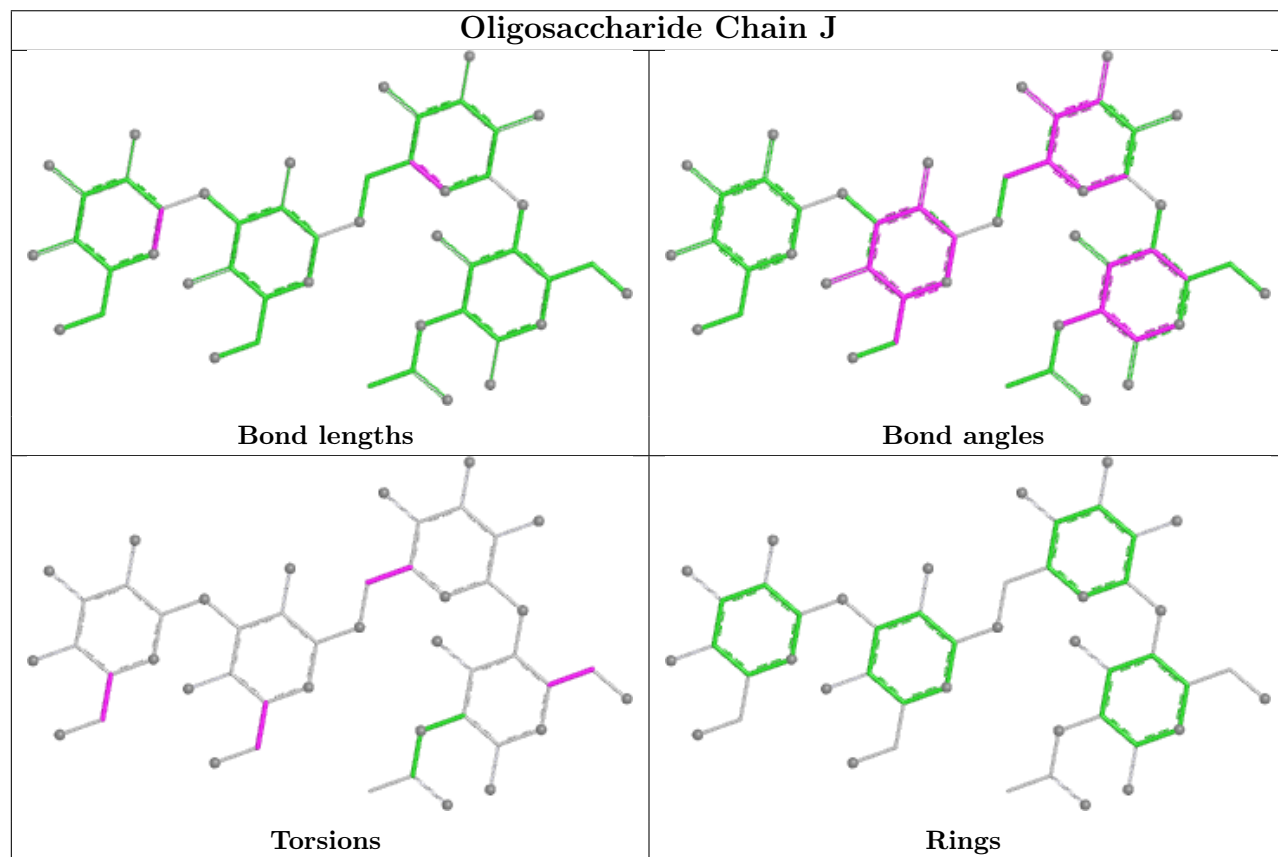
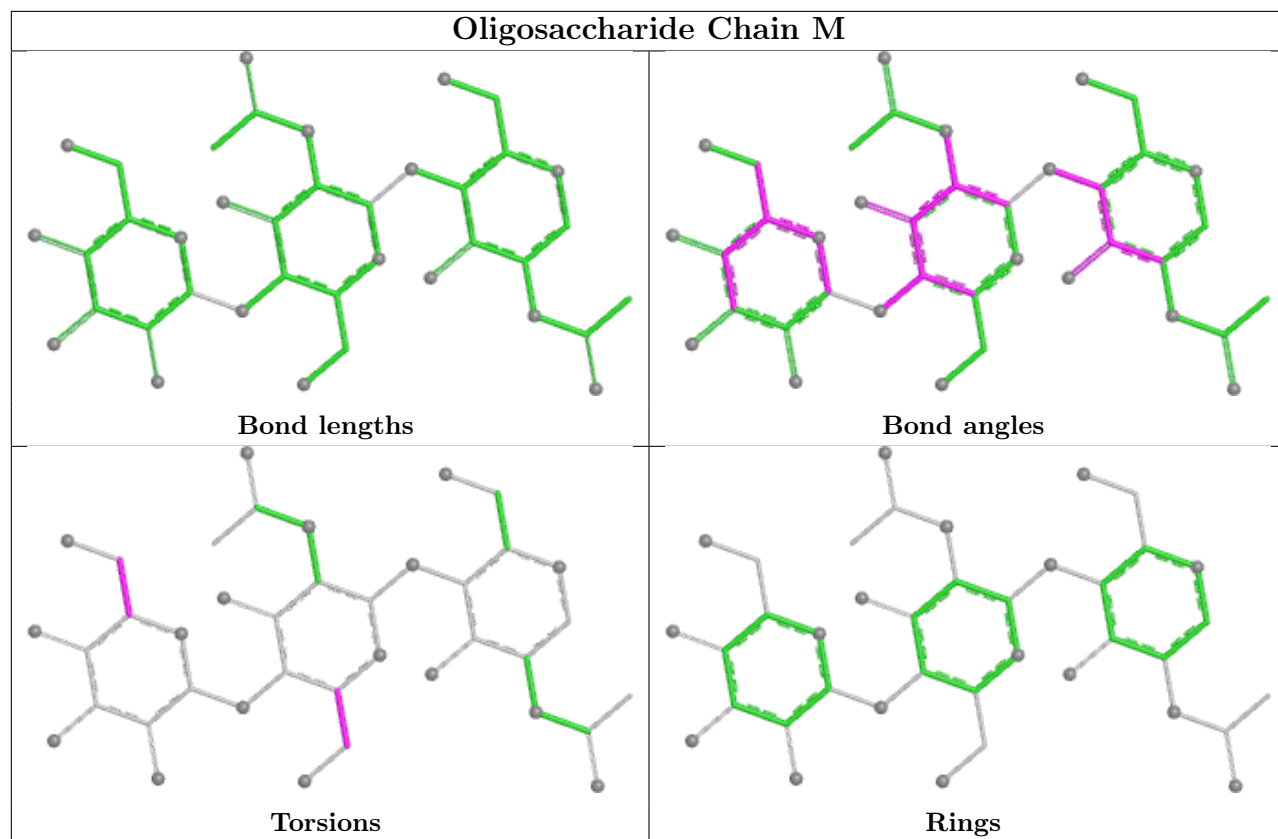
Oligosaccharide Chain G

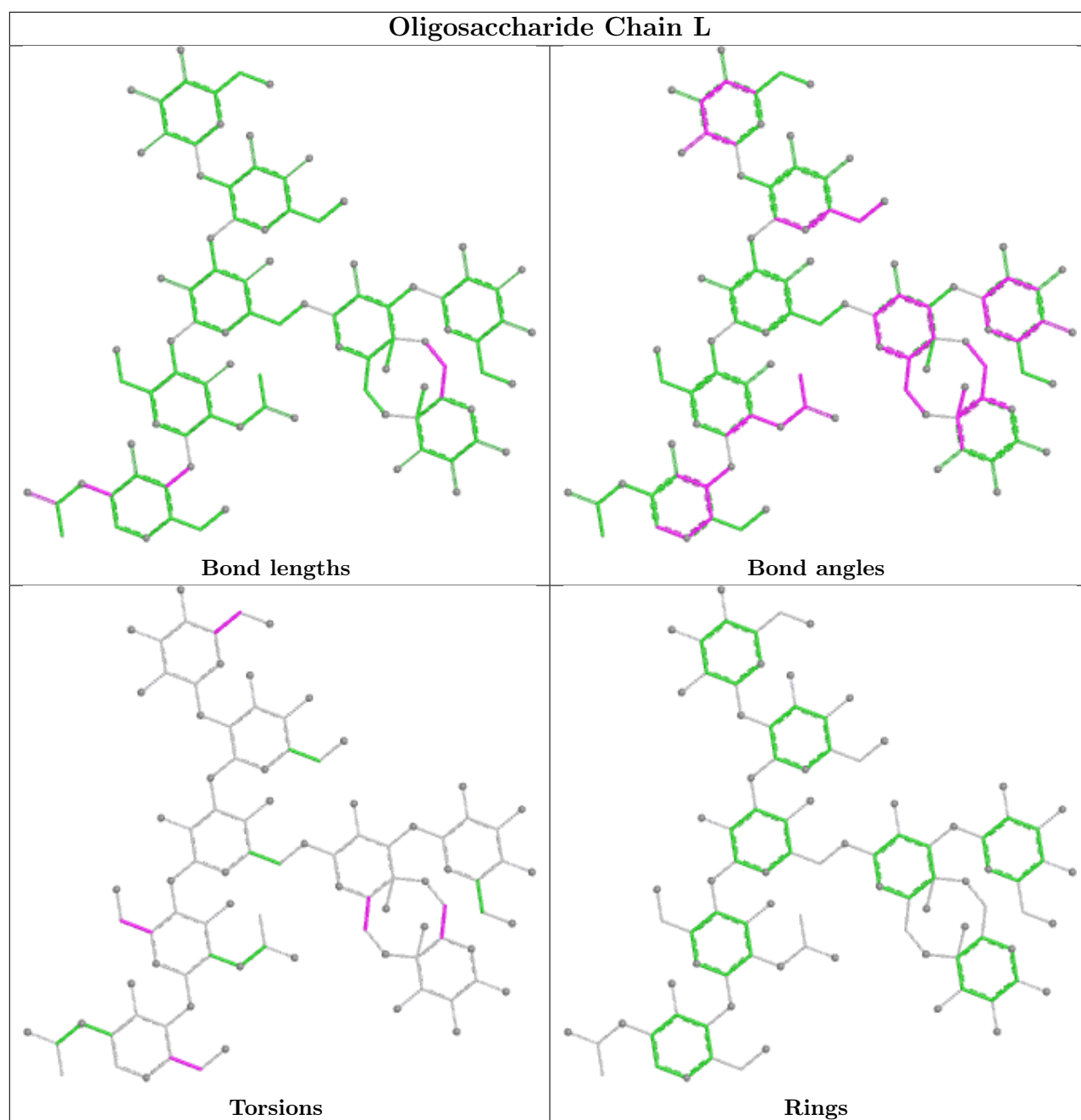


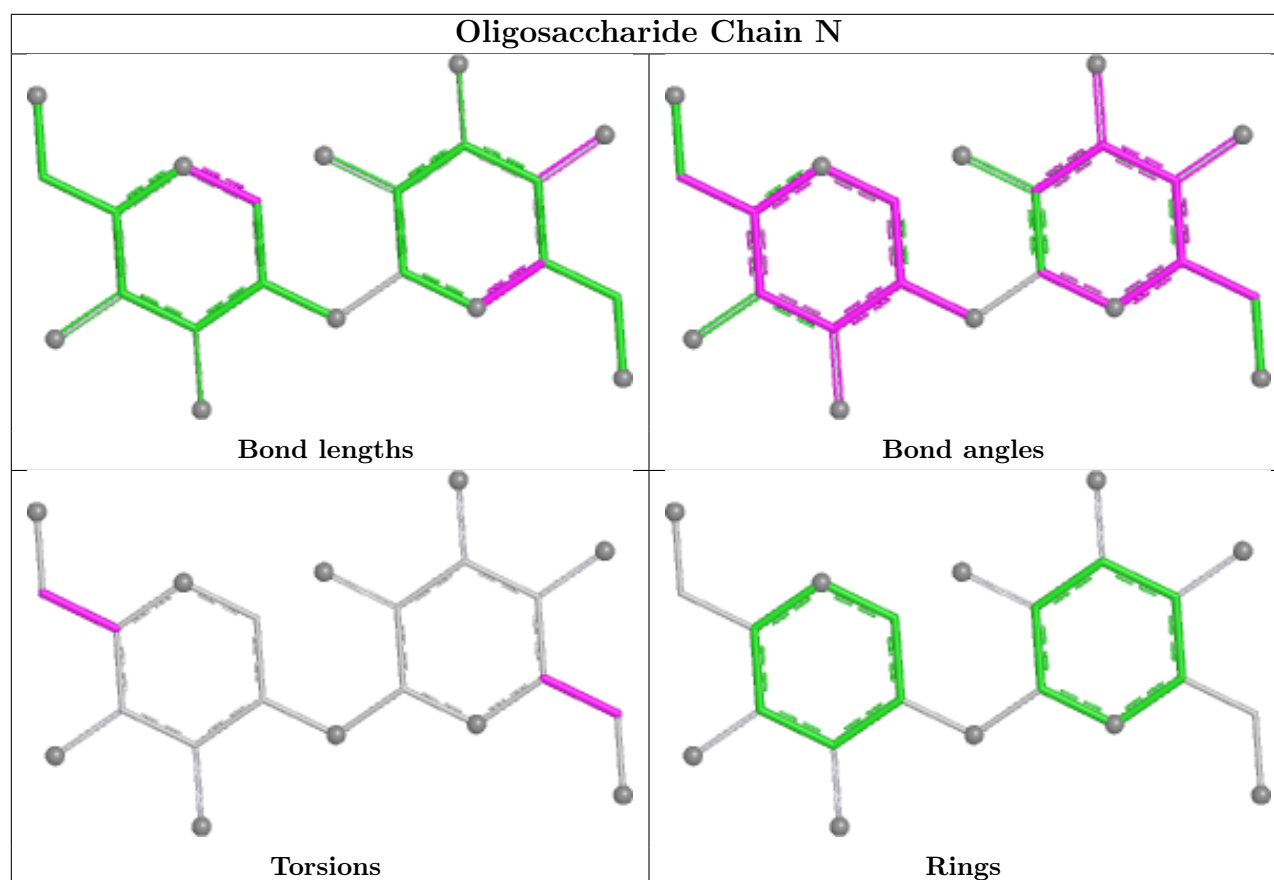
Oligosaccharide Chain F











5.6 Ligand geometry [i](#)

31 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	0.61	0	17,19,21	1.18	1 (5%)
8	NAG	A	904	1	14,14,15	0.72	1 (7%)	17,19,21	1.12	1 (5%)
8	NAG	D	904	1	14,14,15	0.42	0	17,19,21	1.56	5 (29%)
8	NAG	C	907	1	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
10	XYP	A	909	9	9,9,10	0.22	0	10,12,14	0.47	0
8	NAG	A	907	1	14,14,15	0.42	0	17,19,21	1.44	2 (11%)
9	BKR	A	908	10	65,65,65	1.47	9 (13%)	101,101,101	1.99	23 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	905	1	14,14,15	0.68	0	17,19,21	1.52	3 (17%)
8	NAG	B	901	1	13,13,15	1.64	2 (15%)	12,17,21	1.18	1 (8%)
8	NAG	B	907	1	14,14,15	0.53	0	17,19,21	1.42	2 (11%)
8	NAG	C	903	1	13,13,15	0.64	0	12,17,21	1.82	2 (16%)
9	BKR	B	908	11	65,65,65	1.61	6 (9%)	101,101,101	1.61	20 (19%)
8	NAG	B	903	1	13,13,15	0.59	0	12,17,21	2.03	4 (33%)
8	NAG	A	903	1	13,13,15	1.74	1 (7%)	12,17,21	1.83	2 (16%)
8	NAG	A	906	1	14,14,15	0.48	0	17,19,21	1.27	1 (5%)
8	NAG	D	901	1	13,13,15	1.33	1 (7%)	12,17,21	2.70	6 (50%)
11	XYZ	B	909	9	10,10,10	1.11	1 (10%)	13,14,14	2.08	5 (38%)
8	NAG	A	902	-	15,15,15	0.76	0	21,21,21	2.10	3 (14%)
8	NAG	B	902	-	15,15,15	0.88	1 (6%)	21,21,21	1.90	7 (33%)
8	NAG	C	906	1	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
12	MAN	B	910	1	11,11,12	0.80	0	15,15,17	2.17	6 (40%)
8	NAG	B	905	1	14,14,15	0.62	0	17,19,21	1.55	4 (23%)
8	NAG	A	901	1	13,13,15	0.93	1 (7%)	12,17,21	1.22	1 (8%)
13	BMA	C	904	-	11,11,12	0.72	0	15,15,17	1.81	2 (13%)
8	NAG	C	901	1	13,13,15	1.13	1 (7%)	12,17,21	2.53	7 (58%)
8	NAG	D	902	-	15,15,15	0.71	0	21,21,21	2.17	5 (23%)
8	NAG	D	903	1	14,14,15	1.23	1 (7%)	17,19,21	1.95	5 (29%)
8	NAG	C	902	-	15,15,15	0.98	0	21,21,21	1.53	4 (19%)
8	NAG	C	905	1	14,14,15	0.76	1 (7%)	17,19,21	1.47	2 (11%)
8	NAG	D	905	1	14,14,15	0.64	0	17,19,21	1.30	2 (11%)
8	NAG	B	906	1	14,14,15	0.39	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	904	1	-	0/6/23/26	0/1/1/1
8	NAG	A	904	1	-	0/6/23/26	0/1/1/1
8	NAG	D	904	1	-	2/6/23/26	0/1/1/1
8	NAG	C	907	1	-	0/6/23/26	0/1/1/1
10	XYP	A	909	9	-	-	0/1/1/1
8	NAG	A	907	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BKR	A	908	10	-	12/37/123/123	0/7/7/7
8	NAG	A	905	1	-	1/6/23/26	0/1/1/1
8	NAG	B	901	1	-	0/6/19/26	0/1/1/1
8	NAG	B	907	1	-	2/6/23/26	0/1/1/1
8	NAG	C	903	1	-	2/6/19/26	0/1/1/1
9	BKR	B	908	11	-	9/37/123/123	0/7/7/7
8	NAG	B	903	1	-	0/6/19/26	0/1/1/1
8	NAG	A	903	1	-	1/6/19/26	0/1/1/1
8	NAG	A	906	1	-	0/6/23/26	0/1/1/1
8	NAG	D	901	1	-	2/6/19/26	0/1/1/1
11	XYZ	B	909	9	-	2/2/18/18	0/1/1/1
8	NAG	A	902	-	-	0/6/26/26	0/1/1/1
8	NAG	B	902	-	-	0/6/26/26	0/1/1/1
8	NAG	C	906	1	-	2/6/23/26	0/1/1/1
12	MAN	B	910	1	-	2/2/19/22	0/1/1/1
8	NAG	B	905	1	-	1/6/23/26	0/1/1/1
8	NAG	A	901	1	-	0/6/19/26	0/1/1/1
13	BMA	C	904	-	-	1/2/19/22	0/1/1/1
8	NAG	C	901	1	-	1/6/19/26	0/1/1/1
8	NAG	D	902	-	-	0/6/26/26	0/1/1/1
8	NAG	D	903	1	-	3/6/23/26	0/1/1/1
8	NAG	C	902	-	-	0/6/26/26	0/1/1/1
8	NAG	C	905	1	-	3/6/23/26	0/1/1/1
8	NAG	D	905	1	-	2/6/23/26	0/1/1/1
8	NAG	B	906	1	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	908	BKR	O2-C3	6.23	1.47	1.34
9	B	908	BKR	O11-C27	6.09	1.48	1.34
8	A	903	NAG	O5-C1	-5.55	1.34	1.43
9	A	908	BKR	O11-C27	5.02	1.45	1.34
9	A	908	BKR	O2-C3	4.94	1.44	1.34
8	B	901	NAG	C3-C2	-4.78	1.48	1.52
9	B	908	BKR	O4-C12	4.14	1.44	1.35
9	A	908	BKR	O4-C12	3.53	1.43	1.35
8	D	903	NAG	O5-C1	-3.51	1.37	1.43
9	A	908	BKR	C37-C29	-3.40	1.47	1.52
8	D	901	NAG	C3-C2	3.28	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	901	NAG	C3-C2	3.15	1.55	1.52
9	A	908	BKR	O6-C15	-3.07	1.40	1.46
9	A	908	BKR	C11-C15	-2.77	1.49	1.55
9	B	908	BKR	O6-C15	-2.60	1.41	1.46
8	B	901	NAG	C2-N2	-2.39	1.42	1.46
8	A	901	NAG	C3-C2	-2.36	1.50	1.52
9	A	908	BKR	C21-C20	-2.32	1.47	1.53
8	A	904	NAG	C1-C2	2.24	1.55	1.52
11	B	909	XYZ	C1-C2	-2.19	1.50	1.52
9	A	908	BKR	O4-C11	-2.15	1.42	1.46
8	B	902	NAG	O4-C4	2.15	1.48	1.43
9	A	908	BKR	O6-C14	-2.12	1.40	1.45
9	B	908	BKR	C18-C10	2.12	1.61	1.57
8	C	905	NAG	C1-C2	2.11	1.55	1.52
9	B	908	BKR	C32-C31	2.00	1.42	1.39

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	908	BKR	C14-C11-C10	-8.06	107.85	120.32
9	A	908	BKR	O4-C12-C13	6.68	121.98	110.67
8	A	902	NAG	C1-C2-N2	-6.12	103.64	110.73
13	C	904	BMA	C1-O5-C5	5.78	119.94	112.19
8	D	902	NAG	C4-C3-C2	5.66	118.64	110.40
9	B	908	BKR	O11-C27-C28	5.37	119.64	111.13
8	D	901	NAG	C1-C2-N2	5.13	118.51	110.43
9	A	908	BKR	O11-C27-C28	5.08	119.19	111.13
8	D	903	NAG	C4-C3-C2	-4.89	103.86	111.02
8	B	903	NAG	O5-C5-C4	-4.70	101.17	110.26
11	B	909	XYZ	O2-C2-C1	-4.66	98.89	111.85
9	B	908	BKR	O2-C3-C4	4.65	119.38	111.90
8	D	902	NAG	C1-C2-N2	-4.65	105.34	110.73
8	A	903	NAG	C1-C2-N2	-4.58	103.22	110.43
9	A	908	BKR	C2-O2-C3	4.58	126.16	117.80
8	D	901	NAG	O3-C3-C2	4.44	119.28	109.88
9	A	908	BKR	O6-C14-C11	-4.41	87.12	91.94
8	C	905	NAG	C4-C3-C2	4.40	117.47	111.02
8	C	903	NAG	O5-C1-C2	4.40	118.09	111.29
8	D	902	NAG	O5-C1-C2	4.16	113.69	109.52
9	A	908	BKR	C45-C24-C21	4.11	123.82	119.52
9	A	908	BKR	C14-O6-C15	4.10	95.98	91.42
8	C	901	NAG	C2-N2-C7	3.94	128.18	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	903	NAG	C1-C2-N2	3.88	116.55	110.43
12	B	910	MAN	C6-C5-C4	3.88	122.54	113.02
8	A	902	NAG	O5-C1-C2	3.76	113.29	109.52
8	C	903	NAG	C1-C2-N2	-3.76	104.52	110.43
9	B	908	BKR	C14-C11-C10	-3.75	114.52	120.32
9	A	908	BKR	O4-C12-O5	-3.70	117.16	123.61
8	D	901	NAG	O5-C1-C2	-3.68	105.59	111.29
8	C	901	NAG	C1-C2-N2	3.63	116.16	110.43
8	C	901	NAG	O5-C1-C2	-3.62	105.69	111.29
8	C	901	NAG	O3-C3-C2	3.60	117.49	109.88
12	B	910	MAN	C1-C2-C3	3.58	114.86	109.64
9	B	908	BKR	C18-C10-C2	3.57	123.50	115.62
9	B	908	BKR	C31-C30-N1	3.53	123.58	117.04
9	B	908	BKR	C45-C1-C2	3.52	115.80	111.93
8	A	902	NAG	C3-C2-N2	3.51	117.08	110.62
9	B	908	BKR	C2-O2-C3	3.48	124.15	117.80
8	A	904	NAG	O5-C1-C2	-3.47	105.92	111.29
9	B	908	BKR	C44-C25-C24	-3.45	121.22	125.32
12	B	910	MAN	O5-C5-C4	-3.41	102.53	110.83
11	B	909	XYZ	C1-C2-C3	3.40	106.47	102.29
8	B	907	NAG	C8-C7-N2	3.31	121.61	116.12
9	A	908	BKR	O2-C3-C4	3.30	117.19	111.90
8	A	905	NAG	O5-C1-C2	-3.29	106.20	111.29
9	A	908	BKR	O4-C11-C10	3.29	114.33	109.24
9	A	908	BKR	C44-C25-C24	-3.27	121.43	125.32
8	B	902	NAG	C3-C4-C5	-3.26	104.32	110.23
8	A	906	NAG	C1-C2-N2	-3.25	105.31	110.43
8	C	906	NAG	C1-O5-C5	3.21	116.49	112.19
9	A	908	BKR	C18-C10-C2	3.16	122.61	115.62
9	A	908	BKR	O6-C15-C11	-3.16	87.13	90.58
8	D	902	NAG	C1-C2-C3	3.10	114.77	110.54
8	B	902	NAG	O7-C7-C8	-3.07	116.58	122.05
8	B	907	NAG	C1-C2-N2	-3.03	105.65	110.43
8	C	907	NAG	C1-C2-N2	-3.03	105.66	110.43
12	B	910	MAN	C3-C4-C5	-3.03	104.74	110.23
9	B	908	BKR	O6-C15-C16	-3.01	107.62	113.17
8	A	907	NAG	C8-C7-N2	2.94	121.00	116.12
8	B	902	NAG	O5-C1-C2	2.94	112.47	109.52
8	D	904	NAG	C4-C3-C2	2.91	115.29	111.02
8	B	905	NAG	C4-C3-C2	2.89	115.26	111.02
8	B	903	NAG	C4-C5-C6	2.87	117.81	112.50
8	B	906	NAG	C1-O5-C5	2.84	115.99	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	908	BKR	C14-C11-C15	2.84	88.30	85.38
8	D	904	NAG	C3-C4-C5	2.82	115.34	110.23
8	D	901	NAG	C2-N2-C7	2.80	126.65	122.90
8	B	904	NAG	O5-C1-C2	-2.77	107.00	111.29
8	A	901	NAG	O5-C1-C2	2.76	115.56	111.29
9	A	908	BKR	O11-C27-O12	-2.76	118.97	123.95
8	C	901	NAG	O7-C7-N2	2.75	126.83	121.98
11	B	909	XYZ	O3-C3-C2	2.73	120.57	111.82
8	B	902	NAG	C1-C2-N2	-2.69	107.61	110.73
9	B	908	BKR	C14-O6-C15	2.65	94.37	91.42
8	A	905	NAG	O3-C3-C2	2.64	114.89	109.40
8	B	903	NAG	C3-C4-C5	-2.63	106.74	111.19
8	D	904	NAG	O5-C1-C2	-2.62	107.23	111.29
9	A	908	BKR	O6-C15-C16	-2.60	108.37	113.17
8	B	902	NAG	O4-C4-C3	2.59	116.48	110.38
9	A	908	BKR	O13-C28-C29	-2.58	102.42	109.69
8	D	905	NAG	O5-C5-C6	2.55	112.62	107.66
9	B	908	BKR	O7-C17-C16	-2.55	103.94	109.12
8	C	902	NAG	C1-C2-N2	-2.53	107.80	110.73
9	B	908	BKR	O9-C21-C20	2.50	113.67	109.51
8	D	901	NAG	C3-C4-C5	-2.50	106.97	111.19
8	A	905	NAG	C1-O5-C5	2.48	115.51	112.19
8	C	902	NAG	C4-C3-C2	2.47	114.00	110.40
8	C	902	NAG	O5-C1-C2	2.45	111.98	109.52
8	D	902	NAG	O3-C3-C4	-2.44	104.63	110.38
12	B	910	MAN	O5-C1-C2	2.43	116.59	110.79
8	C	907	NAG	O5-C1-C2	-2.42	107.54	111.29
8	C	905	NAG	C3-C4-C5	2.39	114.56	110.23
8	B	902	NAG	O3-C3-C2	-2.38	104.85	109.58
12	B	910	MAN	O4-C4-C5	2.35	115.12	109.32
9	B	908	BKR	C45-C24-C21	2.35	121.98	119.52
9	B	908	BKR	O4-C12-O5	-2.32	119.56	123.61
8	D	904	NAG	O4-C4-C5	-2.32	103.61	109.32
8	B	905	NAG	C1-C2-N2	-2.32	106.78	110.43
9	B	908	BKR	C1-C43-C26	2.31	119.23	114.98
8	B	902	NAG	C1-C2-C3	-2.30	107.40	110.54
9	B	908	BKR	O4-C12-C13	2.29	114.56	110.67
8	D	904	NAG	O3-C3-C2	-2.29	104.64	109.40
8	C	901	NAG	C8-C7-N2	-2.28	112.34	116.12
9	B	908	BKR	O14-C30-N1	-2.26	118.17	122.47
8	D	901	NAG	O3-C3-C4	-2.25	104.26	109.86
11	B	909	XYZ	O1-C1-O4	2.24	113.97	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	904	BMA	O2-C2-C1	2.23	114.33	109.22
9	A	908	BKR	C46-C45-C1	-2.23	106.43	111.13
8	D	905	NAG	O5-C5-C4	-2.21	105.45	110.83
8	C	902	NAG	O4-C4-C5	2.20	114.74	109.32
9	A	908	BKR	C19-C18-C17	-2.19	105.40	109.61
8	C	901	NAG	C3-C4-C5	-2.19	107.48	111.19
8	A	907	NAG	O5-C5-C4	-2.19	105.49	110.83
8	A	903	NAG	O6-C6-C5	-2.19	106.15	111.77
9	A	908	BKR	C24-C21-C20	-2.18	111.54	114.05
8	D	903	NAG	C3-C4-C5	-2.15	106.34	110.23
9	B	908	BKR	C47-C45-C1	2.14	115.66	111.13
8	B	901	NAG	O3-C3-C2	-2.14	105.36	109.88
9	A	908	BKR	O2-C2-C10	2.13	112.03	108.17
8	B	905	NAG	O5-C5-C6	2.13	111.80	107.66
9	B	908	BKR	O9-C21-C24	-2.12	108.05	111.48
8	B	903	NAG	O6-C6-C5	-2.12	106.32	111.77
8	B	905	NAG	O3-C3-C4	-2.11	105.40	110.38
9	A	908	BKR	C45-C1-C2	2.10	114.23	111.93
11	B	909	XYZ	O4-C4-C5	2.06	113.56	109.22
9	B	908	BKR	O6-C14-C11	-2.05	89.70	91.94
9	A	908	BKR	C18-C20-C21	-2.03	119.66	122.69
8	D	903	NAG	O5-C1-C2	-2.02	108.16	111.29
8	D	903	NAG	O3-C3-C2	2.01	113.58	109.40

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	903	NAG	C4-C5-C6-O6
8	C	903	NAG	O5-C5-C6-O6
8	D	901	NAG	C4-C5-C6-O6
8	D	901	NAG	O5-C5-C6-O6
8	D	903	NAG	C1-C2-N2-C7
9	A	908	BKR	N1-C30-C31-C32
9	A	908	BKR	O14-C30-C31-C36
9	A	908	BKR	O14-C30-C31-C32
9	A	908	BKR	N1-C30-C31-C36
8	C	906	NAG	O5-C5-C6-O6
8	D	905	NAG	O5-C5-C6-O6
8	C	905	NAG	O5-C5-C6-O6
8	C	906	NAG	C4-C5-C6-O6
8	D	904	NAG	C4-C5-C6-O6

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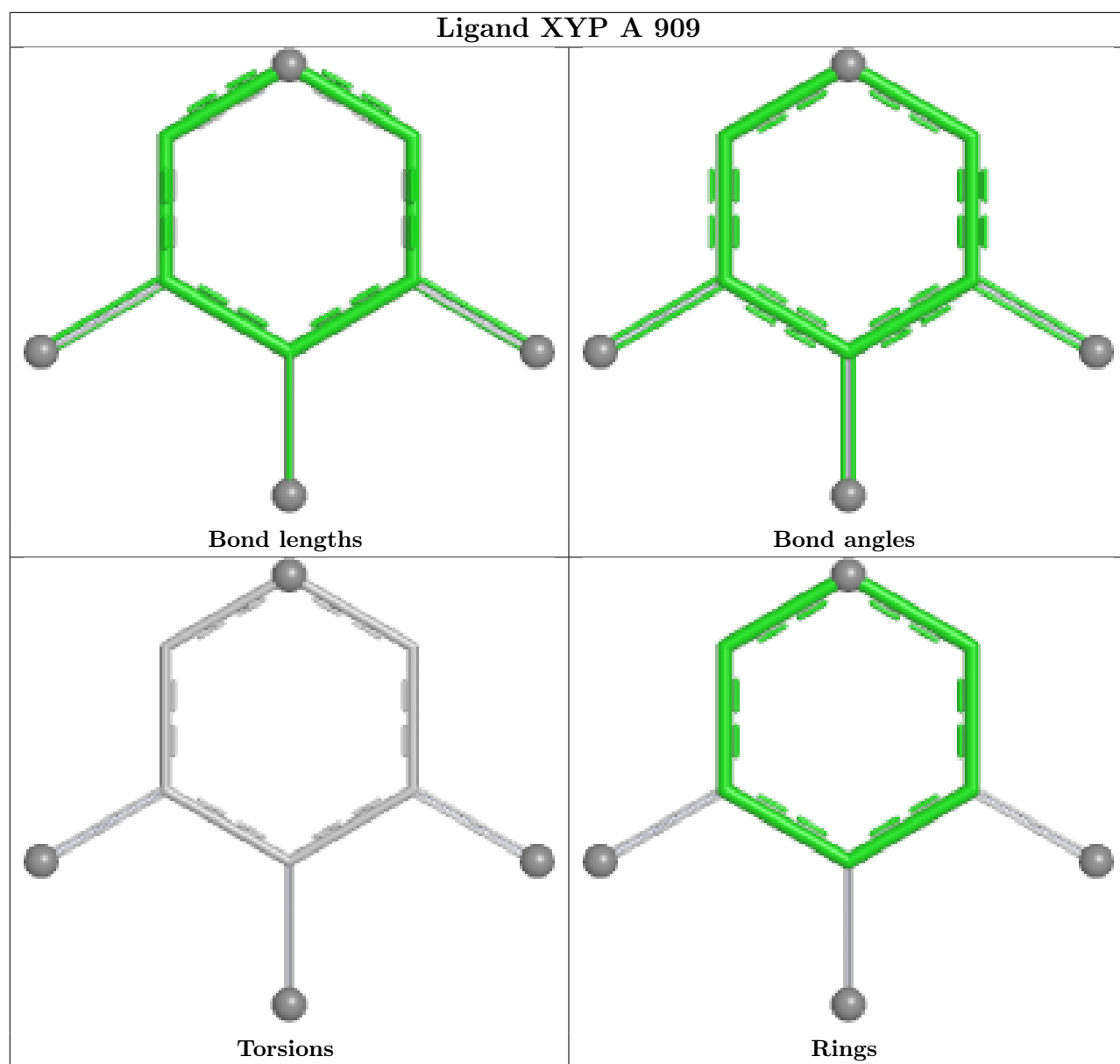
Mol	Chain	Res	Type	Atoms
11	B	909	XYZ	O4-C4-C5-O5
11	B	909	XYZ	C3-C4-C5-O5
8	D	905	NAG	C4-C5-C6-O6
8	D	904	NAG	O5-C5-C6-O6
8	A	907	NAG	C8-C7-N2-C2
8	A	907	NAG	O7-C7-N2-C2
8	B	907	NAG	C8-C7-N2-C2
8	B	907	NAG	O7-C7-N2-C2
8	C	905	NAG	C4-C5-C6-O6
8	A	905	NAG	O5-C5-C6-O6
8	D	903	NAG	O5-C5-C6-O6
9	B	908	BKR	N1-C30-C31-C32
9	B	908	BKR	O14-C30-C31-C32
8	D	903	NAG	C3-C2-N2-C7
9	B	908	BKR	O14-C30-C31-C36
9	B	908	BKR	N1-C30-C31-C36
12	B	910	MAN	C4-C5-C6-O6
9	A	908	BKR	C14-C11-O4-C12
12	B	910	MAN	O5-C5-C6-O6
13	C	904	BMA	C4-C5-C6-O6
9	A	908	BKR	C15-C11-O4-C12
9	A	908	BKR	O11-C27-C28-O13
8	B	905	NAG	C4-C5-C6-O6
9	B	908	BKR	C27-C28-C29-C37
8	C	905	NAG	C3-C2-N2-C7
9	A	908	BKR	C1-C2-O2-C3
8	A	903	NAG	C4-C5-C6-O6
8	C	901	NAG	C4-C5-C6-O6
9	A	908	BKR	C10-C2-O2-C3
8	A	907	NAG	C4-C5-C6-O6
9	A	908	BKR	O12-C27-C28-O13
9	A	908	BKR	O13-C28-C29-C37
9	B	908	BKR	O13-C28-C29-C37
9	B	908	BKR	O11-C27-C28-O13
9	A	908	BKR	O11-C27-C28-C29
9	B	908	BKR	O12-C27-C28-C29
9	B	908	BKR	O11-C27-C28-C29

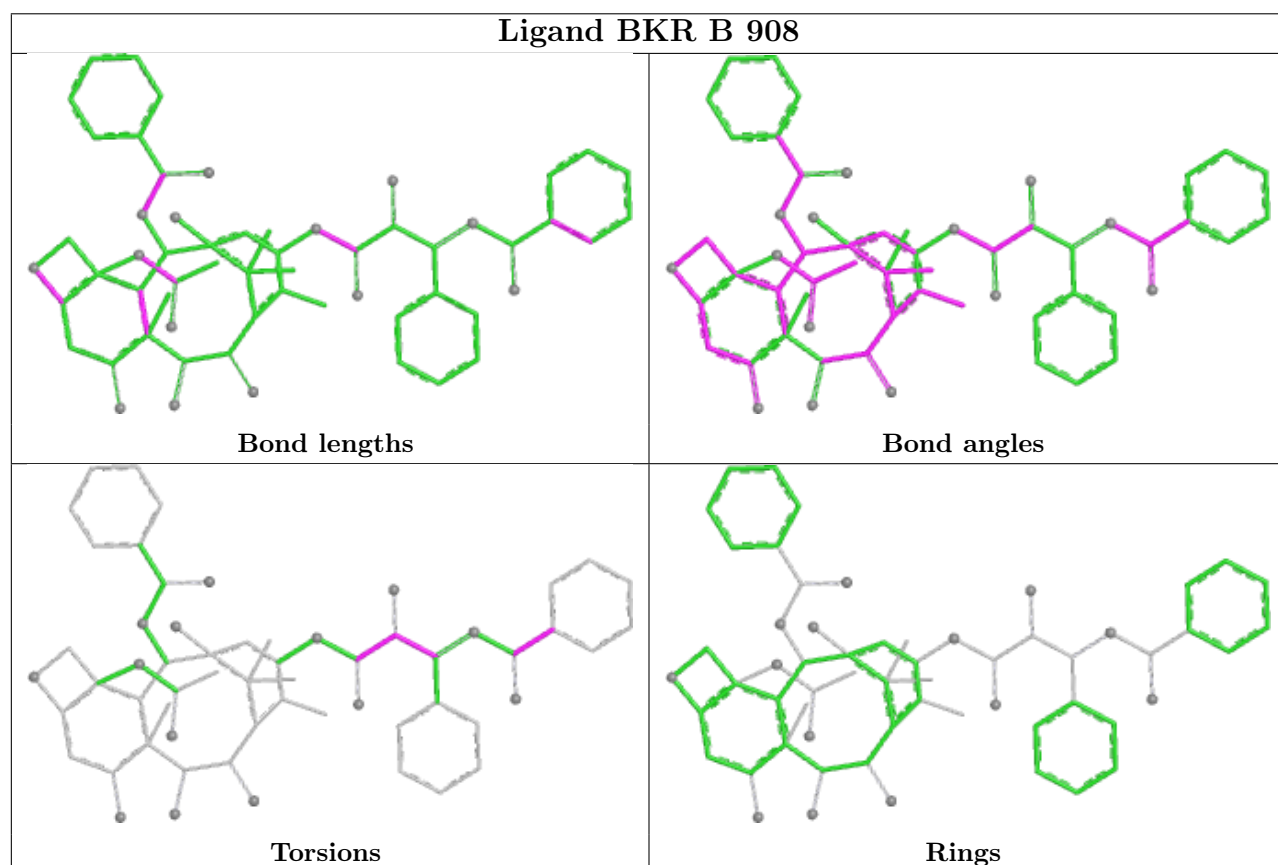
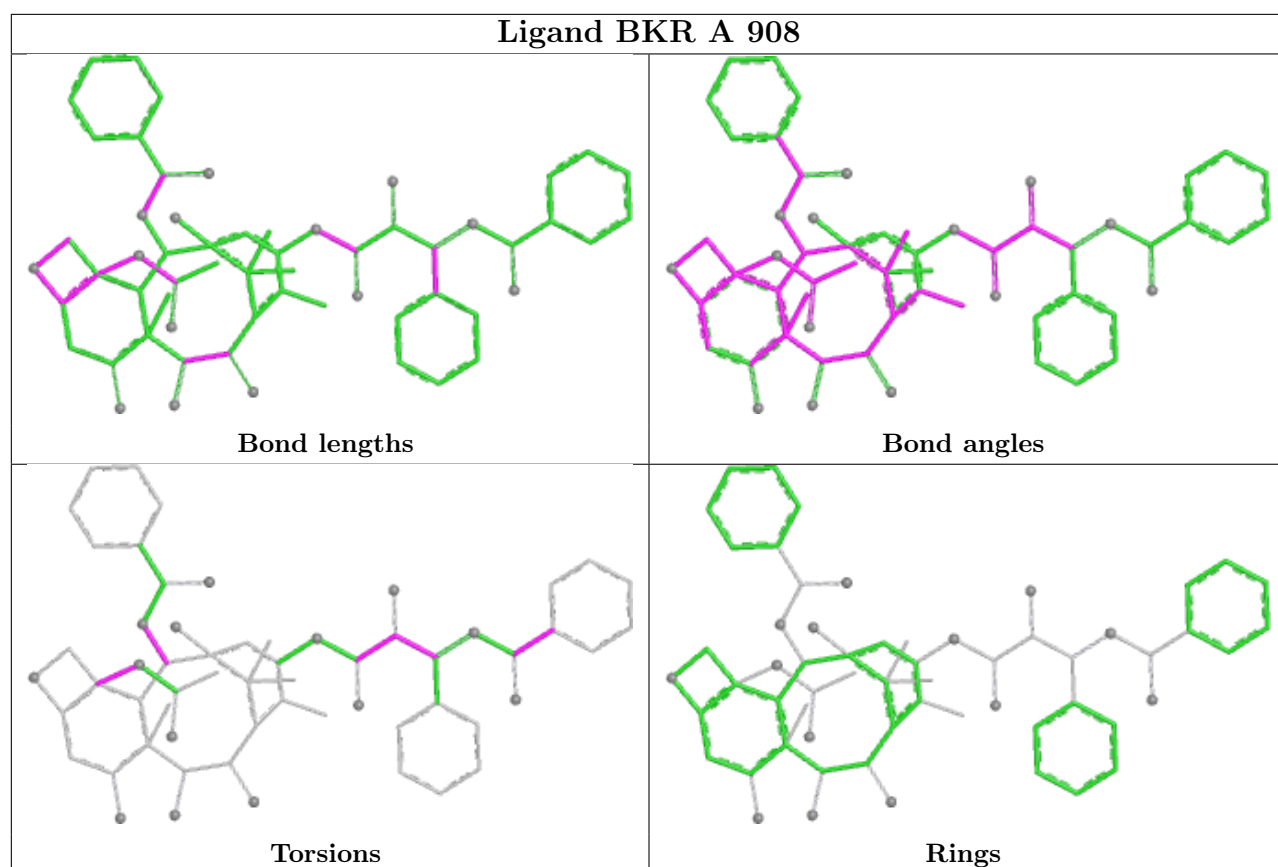
There are no ring outliers.

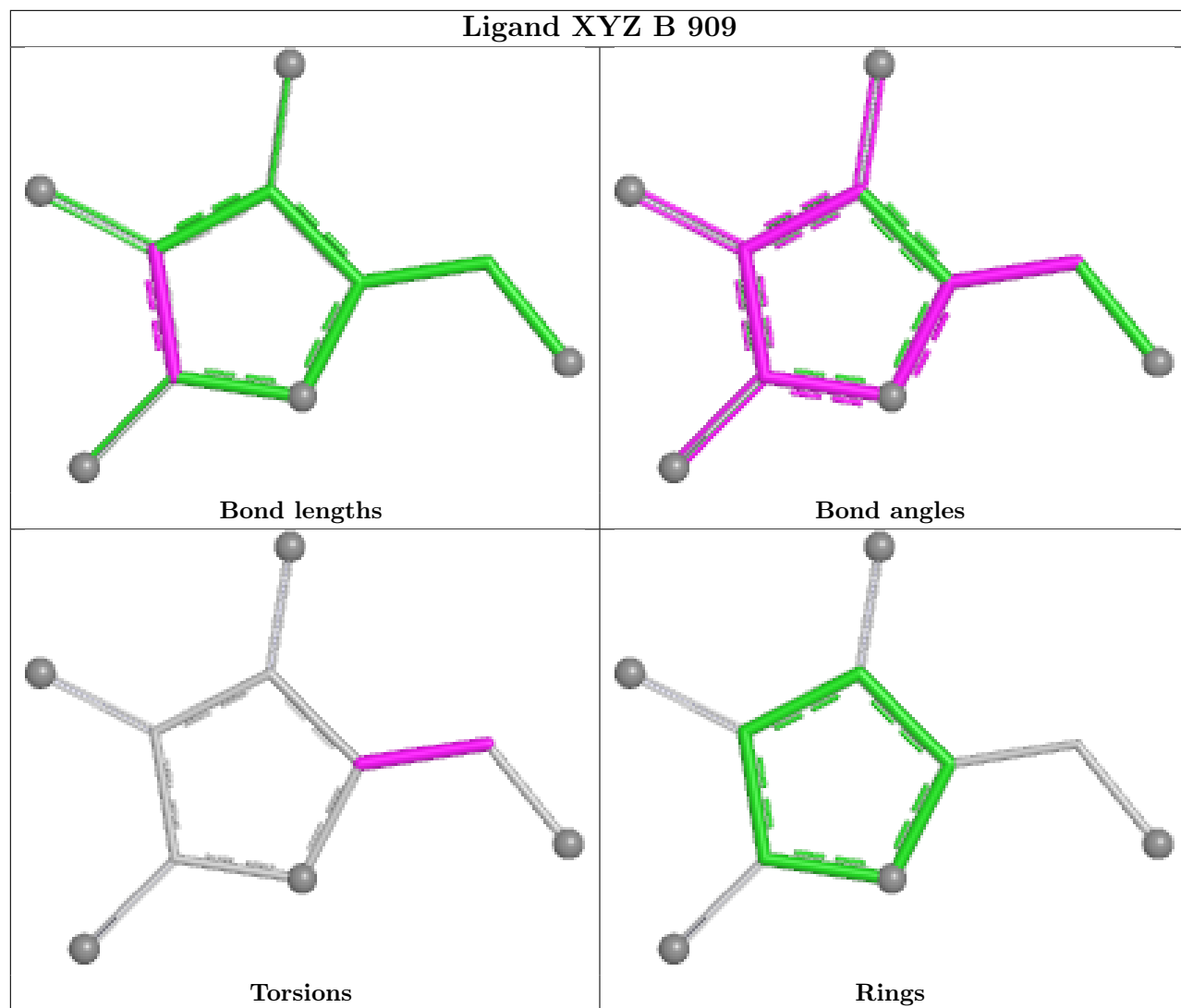
14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	909	XYP	1	0
9	A	908	BKR	4	0
8	B	901	NAG	4	0
8	C	903	NAG	2	0
9	B	908	BKR	1	0
8	B	903	NAG	3	0
8	A	903	NAG	2	0
8	D	901	NAG	1	0
8	A	902	NAG	2	0
8	B	902	NAG	3	0
8	A	901	NAG	4	0
8	C	901	NAG	2	0
8	D	902	NAG	1	0
8	C	902	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	756/803 (94%)	-0.49	6 (0%) 82 83	13, 24, 41, 97	2 (0%)
1	B	756/803 (94%)	-0.58	4 (0%) 87 88	12, 23, 36, 70	4 (0%)
1	C	756/803 (94%)	0.15	16 (2%) 63 65	19, 40, 62, 106	2 (0%)
1	D	756/803 (94%)	0.22	19 (2%) 58 61	17, 39, 59, 90	2 (0%)
All	All	3024/3212 (94%)	-0.18	45 (1%) 72 74	12, 31, 56, 106	10 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	683	TYR	6.0
1	D	224	ILE	5.6
1	A	227	VAL	5.5
1	C	227	VAL	5.4
1	C	228	SER	4.0
1	D	49	TRP	3.9
1	C	49	TRP	3.5
1	A	225	ASP	3.3
1	D	332	TRP	3.3
1	D	227	VAL	3.3
1	A	226	GLY	3.3
1	D	649	LYS	3.2
1	C	48	GLN	3.1
1	D	225	ASP	3.1
1	A	224	ILE	3.1
1	B	226	GLY	3.0
1	D	230	ALA	3.0
1	A	683	TYR	2.9
1	D	277	CYS	2.9
1	C	684	SER	2.8
1	D	684	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	224	ILE	2.8
1	D	48	GLN	2.7
1	C	179	THR	2.6
1	B	48	GLN	2.6
1	C	277	CYS	2.6
1	C	266	CYS	2.5
1	C	226	GLY	2.5
1	C	225	ASP	2.4
1	D	626	TYR	2.4
1	C	782	GLY	2.4
1	C	683	TYR	2.4
1	B	49	TRP	2.4
1	A	681	LYS	2.4
1	C	803	PRO	2.4
1	D	321	GLY	2.3
1	D	231	ASP	2.3
1	D	232	ILE	2.2
1	C	773	VAL	2.2
1	D	500	ASN	2.1
1	D	635	ASN	2.1
1	B	164	GLY	2.1
1	D	497	ALA	2.1
1	C	345	VAL	2.1
1	D	76	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	E	5	11/12	0.62	0.18	79,93,103,107	0
2	MAN	G	5	11/12	0.66	0.18	75,81,91,94	0
4	MAN	I	3	11/12	0.66	0.19	37,46,50,51	0
5	MAN	J	3	11/12	0.66	0.19	52,61,75,78	0

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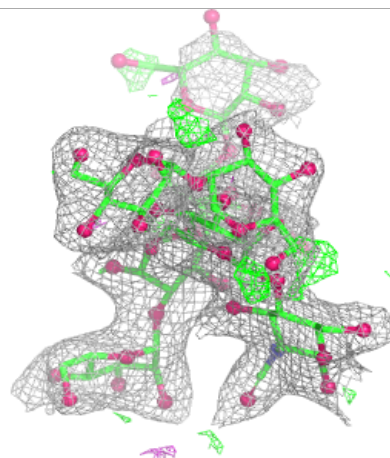
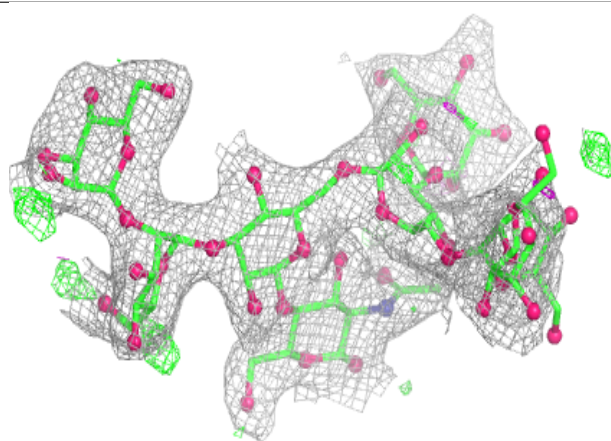
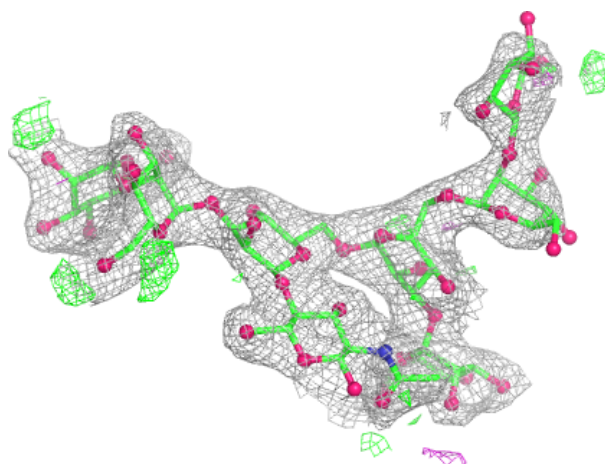
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	4	14/15	0.68	0.25	63,75,81,86	0
3	MAN	F	3	11/12	0.72	0.18	54,60,68,72	0
4	NAG	K	1	14/15	0.77	0.21	28,30,35,35	0
2	BMA	E	4	11/12	0.82	0.17	71,81,89,90	0
2	MAN	G	7	11/12	0.83	0.12	37,43,49,49	0
2	MAN	E	7	11/12	0.84	0.12	41,43,46,48	0
6	NAG	L	2	14/15	0.85	0.14	35,39,44,52	0
2	MAN	G	3	11/12	0.87	0.11	33,35,47,51	0
2	BMA	G	4	11/12	0.87	0.13	50,56,63,65	0
2	MAN	E	8	11/12	0.90	0.09	39,44,47,48	0
2	MAN	G	8	11/12	0.91	0.09	39,42,45,45	0
6	NAG	L	1	14/15	0.92	0.09	39,52,56,58	0
4	NAG	I	1	14/15	0.92	0.11	18,21,24,26	0
2	MAN	E	3	11/12	0.93	0.09	36,38,51,59	0
4	NAG	K	2	14/15	0.94	0.10	33,41,51,64	0
3	NAG	F	2	14/15	0.94	0.09	22,31,40,49	0
2	MAN	E	6	11/12	0.94	0.07	35,38,44,45	0
4	NAG	I	2	14/15	-	-	23,28,37,40	0
2	MAN	G	6	11/12	0.94	0.08	30,36,38,40	0
5	NAG	J	1	15/15	0.95	0.07	41,54,62,68	0
2	BMA	E	2	11/12	0.96	0.06	29,34,40,40	0
4	MAN	K	3	11/12	-	-	58,67,72,74	0
4	NAG	M	1	14/15	-	-	32,37,44,52	0
4	NAG	M	2	14/15	-	-	43,62,73,77	0
4	MAN	M	3	11/12	-	-	78,89,93,94	0
2	NAG	E	1	15/15	0.96	0.07	27,30,31,33	0
5	BMA	J	2	11/12	-	-	49,53,56,58	0
3	NAG	F	1	14/15	0.97	0.05	21,22,25,27	0
5	MAN	J	4	11/12	-	-	50,61,64,69	0
2	NAG	G	1	15/15	0.97	0.06	22,24,27,31	0
2	BMA	G	2	11/12	0.97	0.04	24,26,30,32	0
6	BMA	L	3	11/12	-	-	36,38,45,46	0
6	MAN	L	4	11/12	-	-	54,61,66,67	0
6	MAN	L	5	11/12	-	-	58,66,70,71	0
6	MAN	L	6	11/12	-	-	47,55,64,70	0
6	MAN	L	7	11/12	-	-	50,53,56,57	0
6	MAN	L	8	12/12	-	-	70,79,92,98	0
7	BMA	N	1	11/12	-	-	58,72,82,84	0
7	MAN	N	2	11/12	-	-	46,55,61,61	0

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

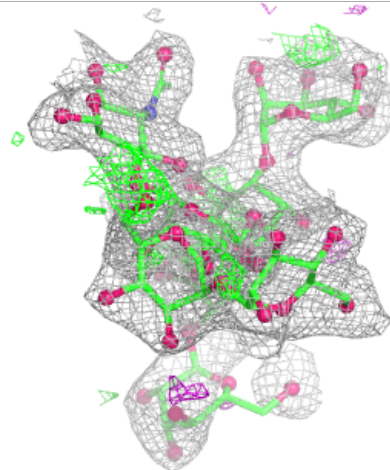
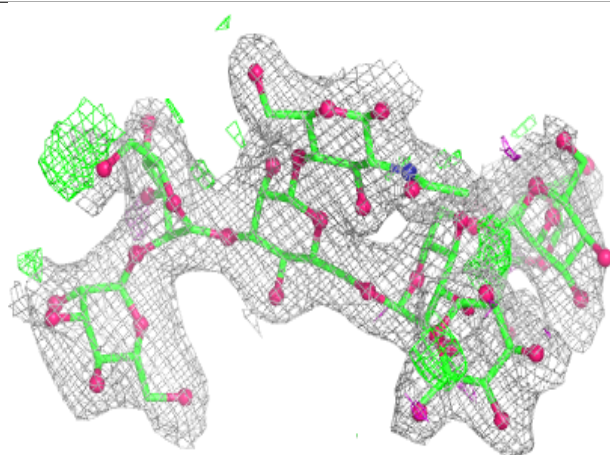
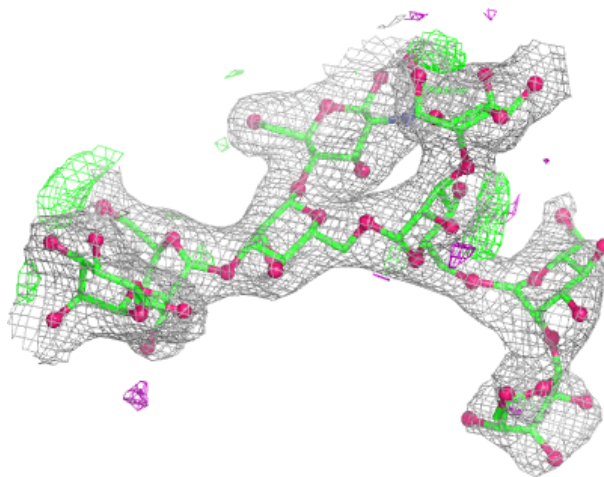
Electron density around Chain E:

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



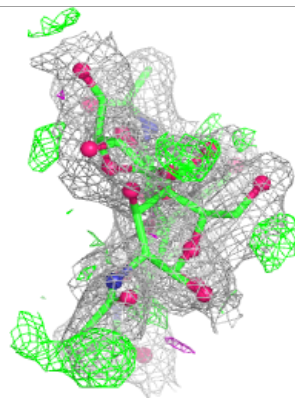
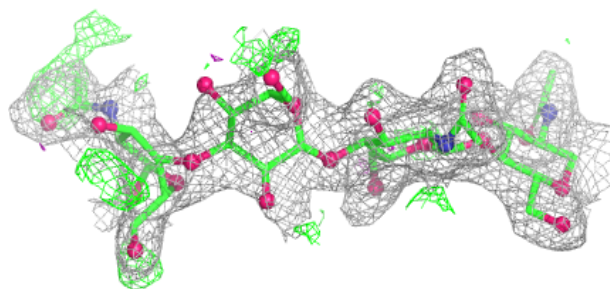
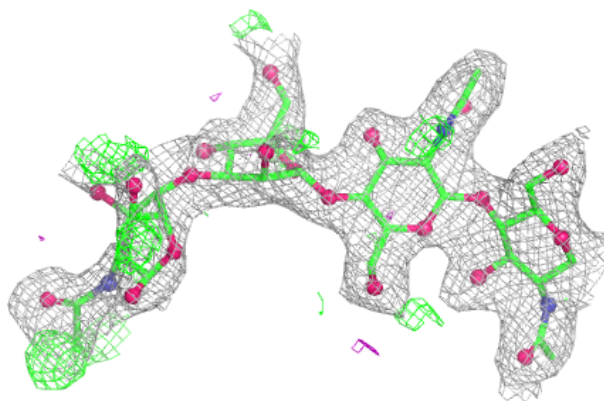
Electron density around Chain G:

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and green (positive)

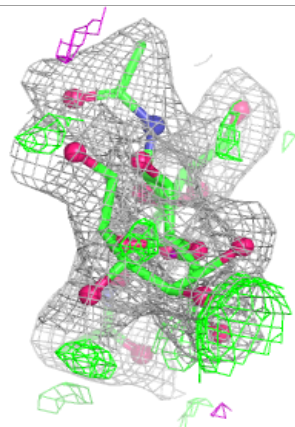
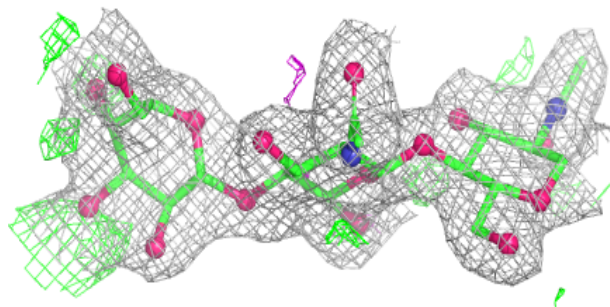
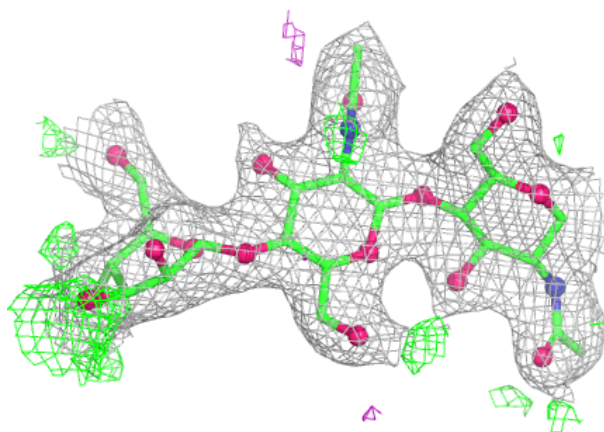


Electron density around Chain F:

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

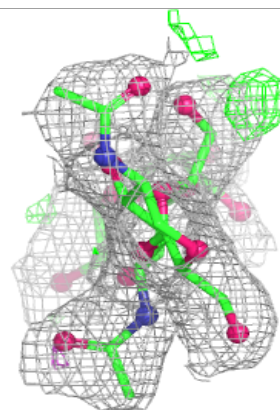
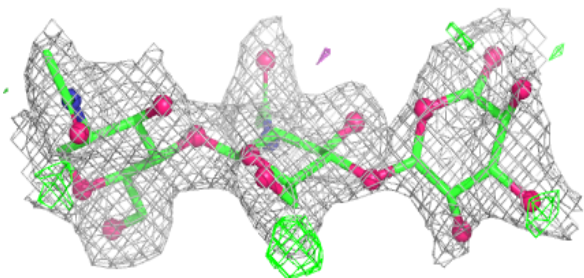
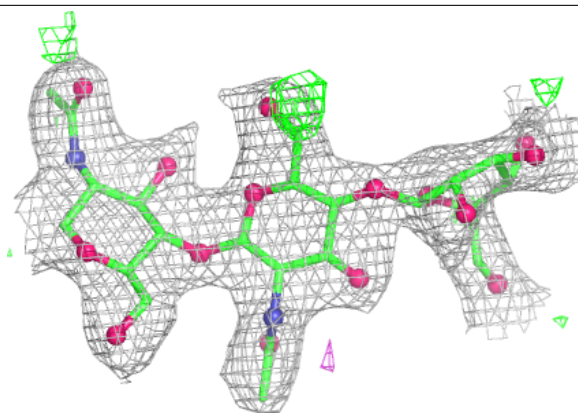
**Electron density around Chain I:**

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and green (positive)

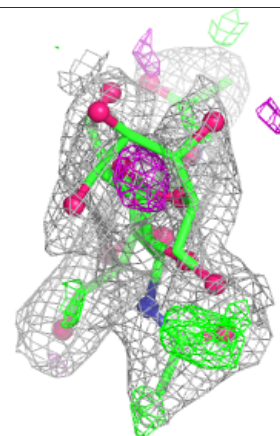
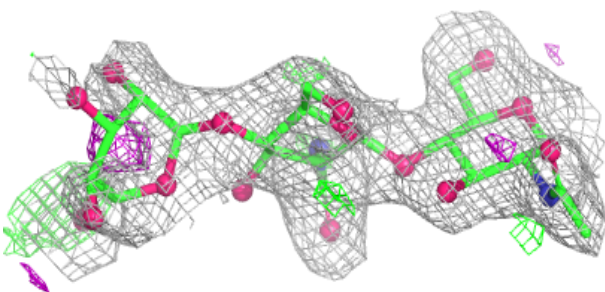
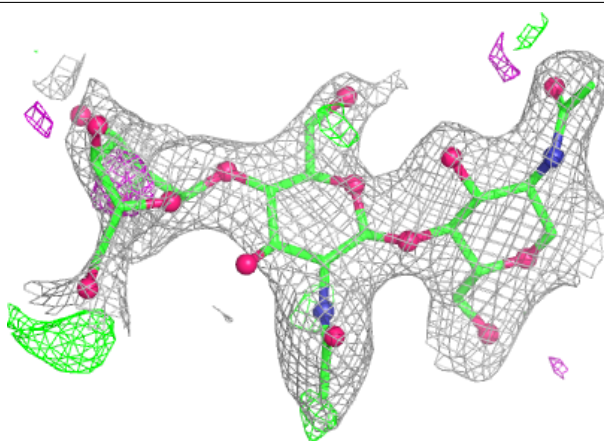


Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

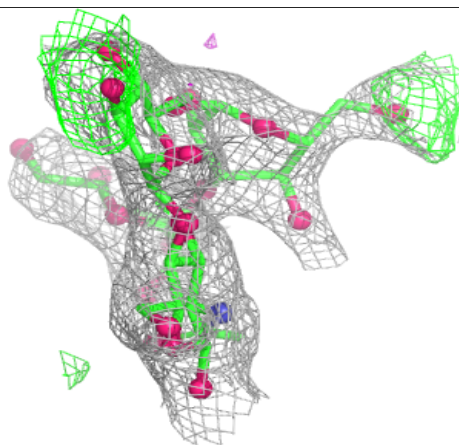
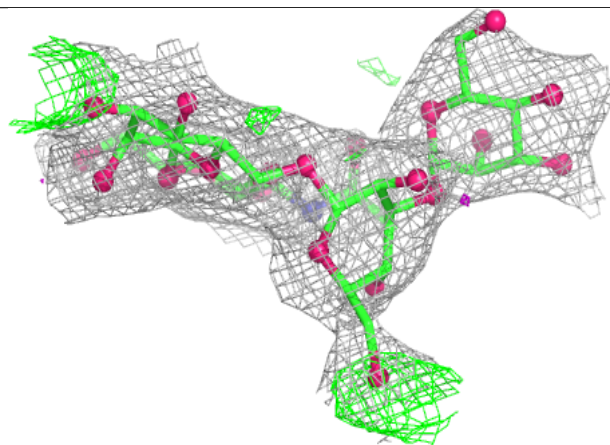
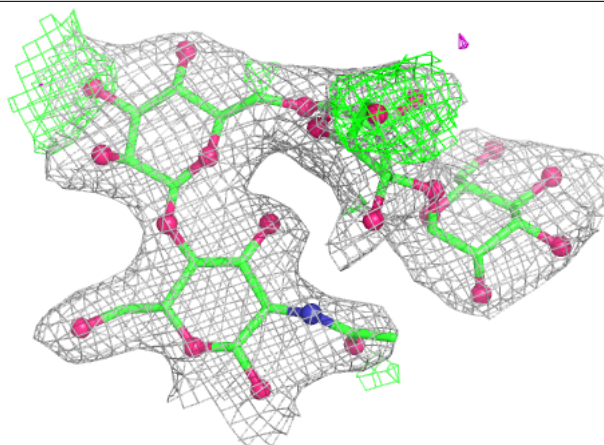
**Electron density around Chain M:**

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



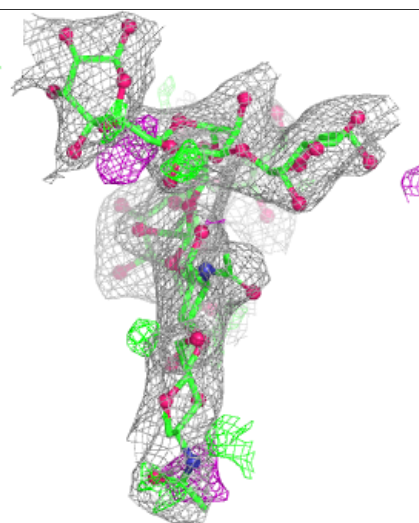
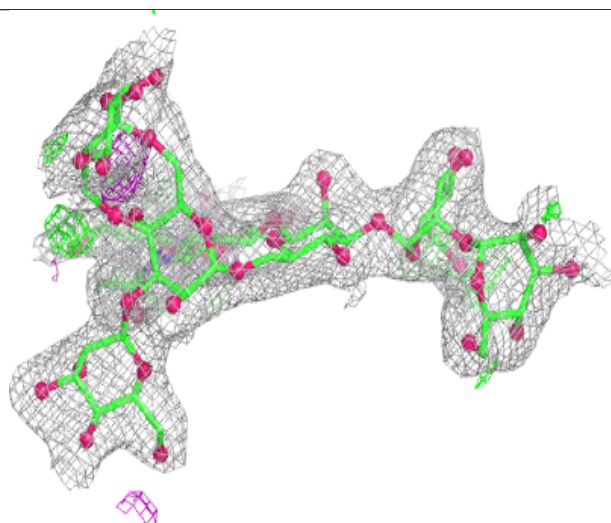
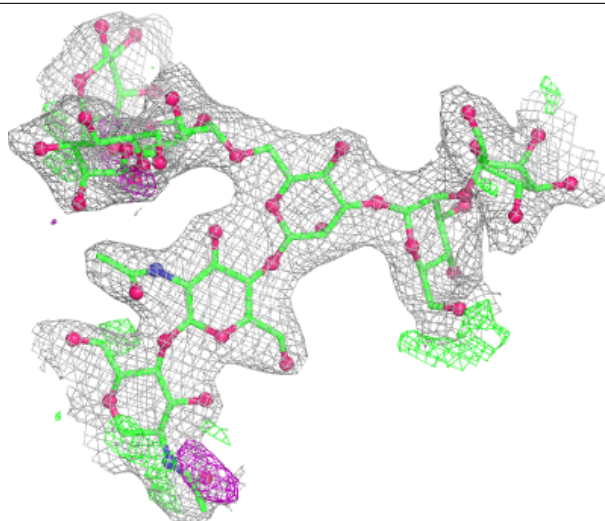
Electron density around Chain J:

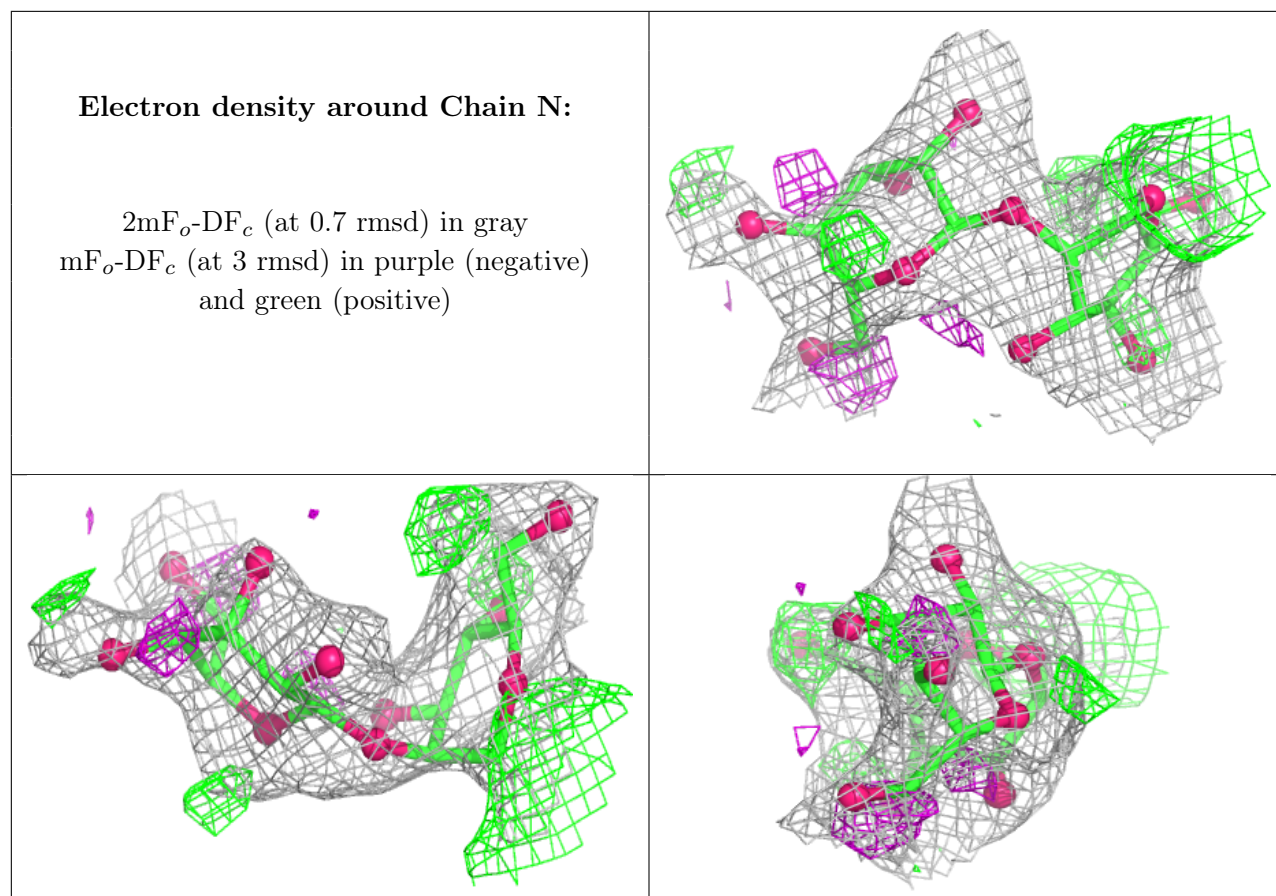
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	BMA	C	904	11/12	0.66	0.17	46,55,67,69	0
8	NAG	D	902	15/15	0.72	0.18	60,71,75,76	0
8	NAG	A	907	14/15	0.73	0.19	59,65,68,78	0
10	XYP	A	909	9/10	0.73	0.26	38,52,58,59	0
12	MAN	B	910	11/12	0.73	0.15	53,59,66,66	0
8	NAG	B	907	14/15	0.73	0.19	66,73,75,75	0
9	BKR	A	908	59/59	0.77	0.22	59,79,94,96	0
8	NAG	C	905	14/15	0.77	0.17	76,90,95,96	0
8	NAG	C	902	15/15	0.80	0.15	51,60,65,66	0
11	XYZ	B	909	10/10	0.81	0.23	20,20,20,20	0
8	NAG	D	904	14/15	0.83	0.14	57,68,70,72	0
8	NAG	D	903	14/15	0.83	0.14	68,71,79,83	0
9	BKR	B	908	59/59	0.86	0.15	44,56,61,64	0

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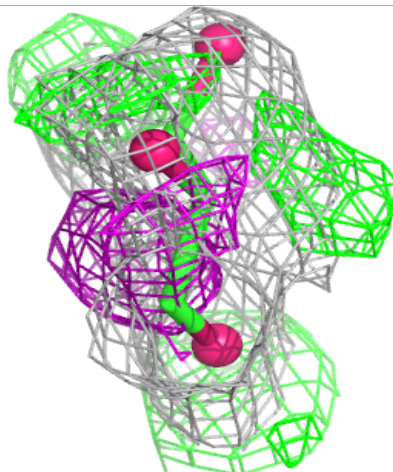
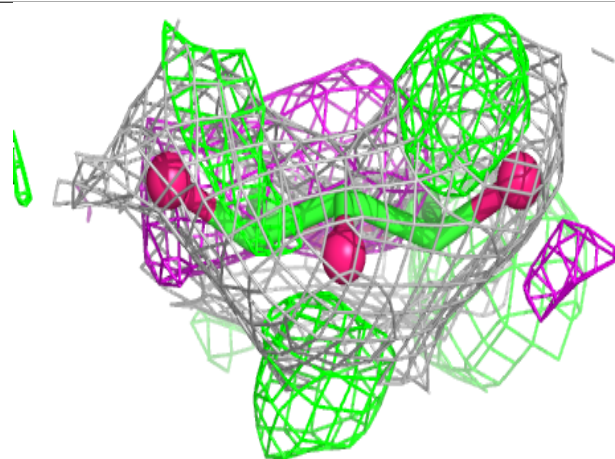
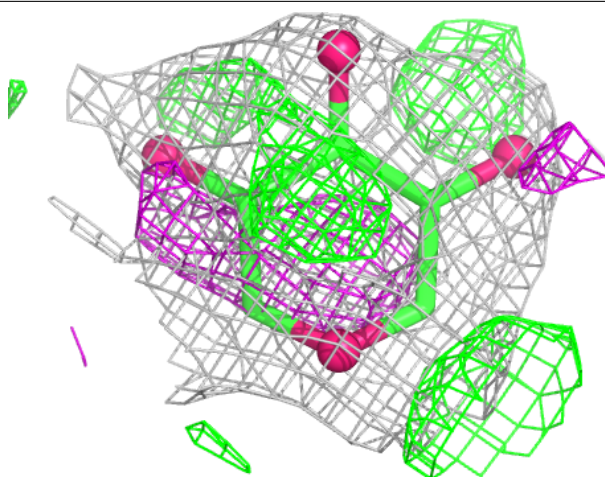
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	C	901	13/15	0.87	0.12	49,60,64,65	0
8	NAG	C	906	14/15	0.87	0.11	57,64,68,68	0
8	NAG	D	901	13/15	0.87	0.13	49,55,61,62	0
8	NAG	D	905	14/15	0.90	0.11	40,51,59,59	0
8	NAG	C	907	14/15	0.91	0.10	38,40,42,45	0
8	NAG	C	903	13/15	0.91	0.12	48,51,65,68	0
8	NAG	B	905	14/15	0.91	0.09	36,39,45,46	0
8	NAG	A	904	14/15	0.91	0.08	37,43,46,46	0
8	NAG	B	902	15/15	0.92	0.09	33,36,39,43	0
8	NAG	A	902	15/15	0.92	0.09	27,30,33,38	0
8	NAG	A	906	14/15	0.93	0.08	31,34,37,38	0
8	NAG	B	904	14/15	0.93	0.08	30,32,34,37	0
8	NAG	A	905	14/15	0.93	0.08	35,39,43,50	0
8	NAG	A	903	13/15	0.95	0.07	23,25,30,35	0
8	NAG	B	906	14/15	0.95	0.07	29,34,35,35	0
8	NAG	B	903	13/15	0.96	0.07	22,23,27,30	0
8	NAG	B	901	13/15	0.96	0.07	19,21,26,26	0
8	NAG	A	901	13/15	0.97	0.06	17,20,21,21	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.

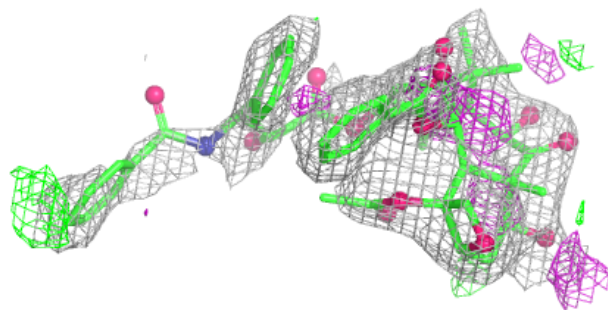
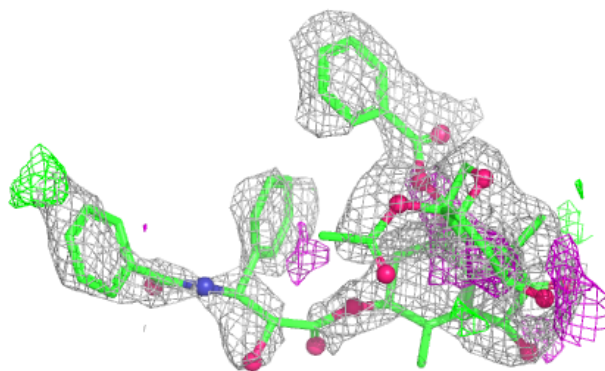
Electron density around XYP A 909:

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



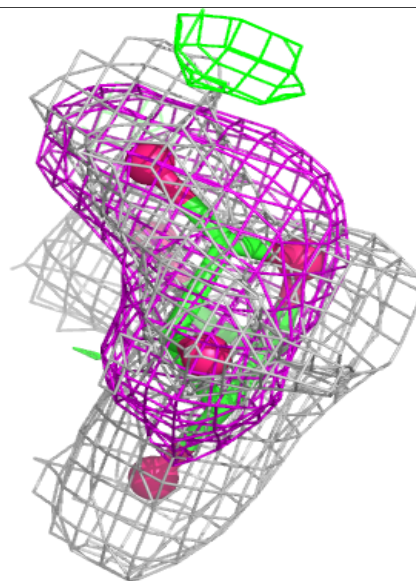
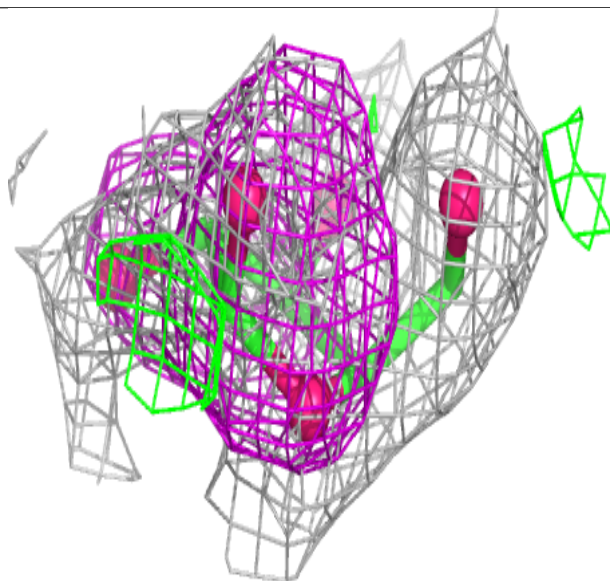
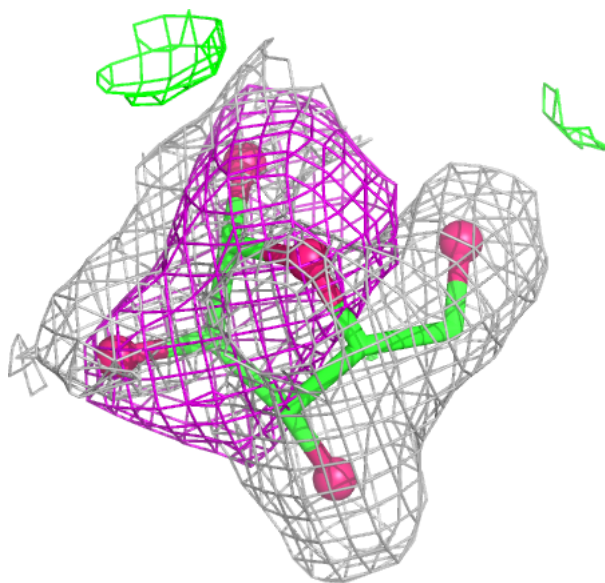
Electron density around BKR A 908:

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



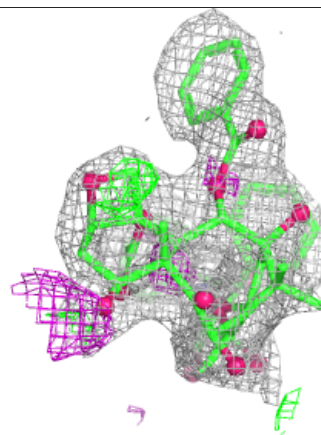
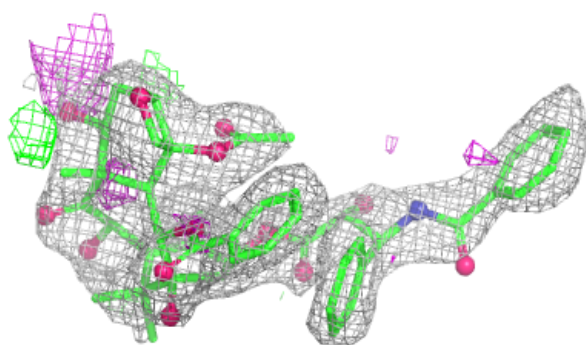
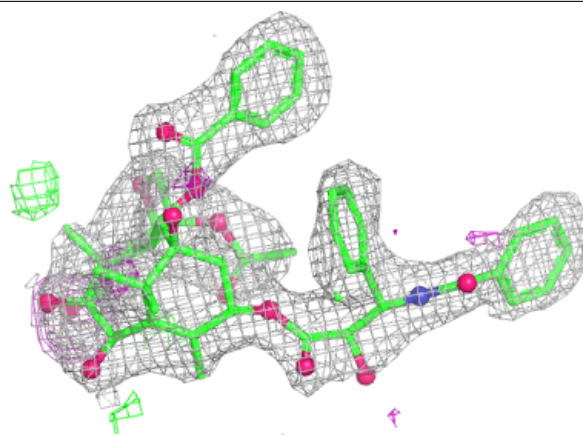
Electron density around XYZ B 909:

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



Electron density around BKR B 908:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.