



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 8GYX / pdb_00008gyx
Title : Bifunctional xylosidase/glucosidase LXYL with intermediate substrate xylose,
120 seconds
Authors : Yang, L.Y.
Deposited on : 2022-09-24
Resolution : 2.07 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

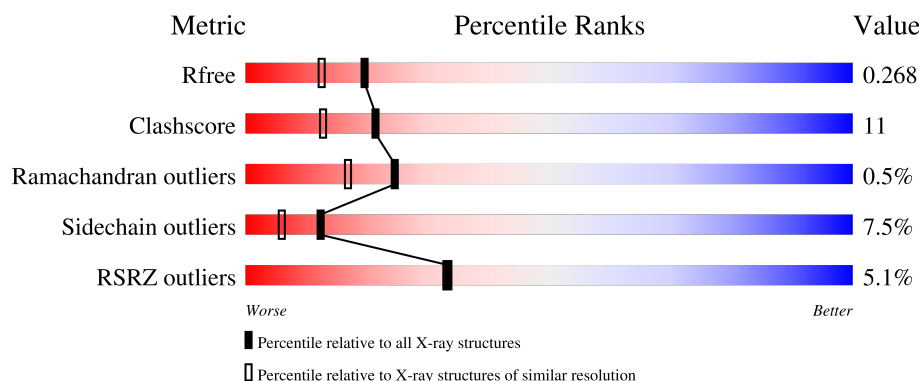
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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.



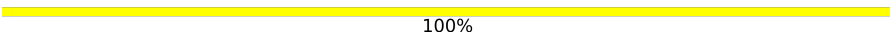
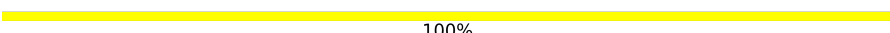
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	100% 78% 13% 6%
1	B	803	100% 79% 11% 6%
1	C	803	10% 73% 18% 6%
1	D	803	8% 71% 20% 6%
2	E	2	100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	A	901	-	-	X	-
10	MAN	A	903	-	-	X	-
10	MAN	A	904	-	-	X	-
10	MAN	B	904	-	-	X	-
10	MAN	B	906	-	-	X	-
10	MAN	B	910	-	-	X	-
10	MAN	C	903	-	-	X	-
10	MAN	C	904	-	-	X	-
11	NAG	C	901	-	-	X	-
12	BMA	D	901	-	-	X	-
2	NAG	H	2	-	-	X	-
2	NAG	P	1	-	-	X	-
4	MAN	G	1	-	-	X	-
4	BMA	G	2	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25439 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.

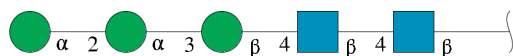
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	756	Total	C	N	O	S	0	3	0
			5738	3636	958	1127	17			
1	A	757	Total	C	N	O	S	0	1	0
			5721	3625	957	1122	17			
1	C	756	Total	C	N	O	S	0	2	0
			5717	3621	956	1123	17			
1	D	756	Total	C	N	O	S	0	2	0
			5720	3624	956	1123	17			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



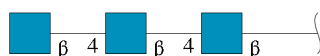
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-alpha-D-mannopyranos e.



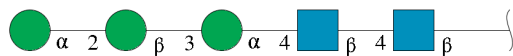
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			

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



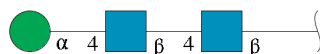
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			42	24	3	15			

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



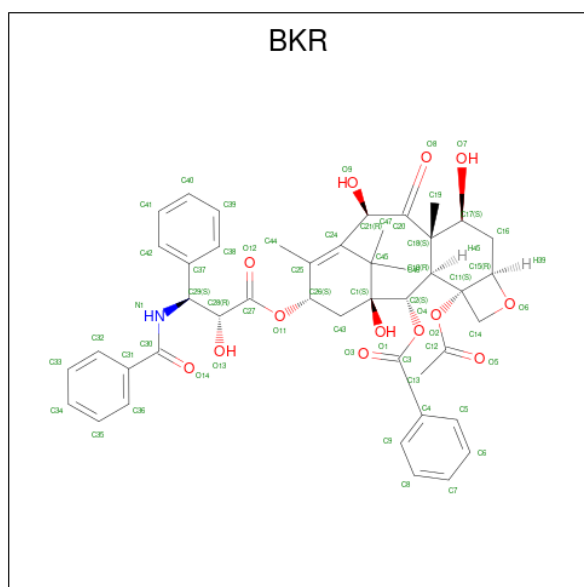
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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
7	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

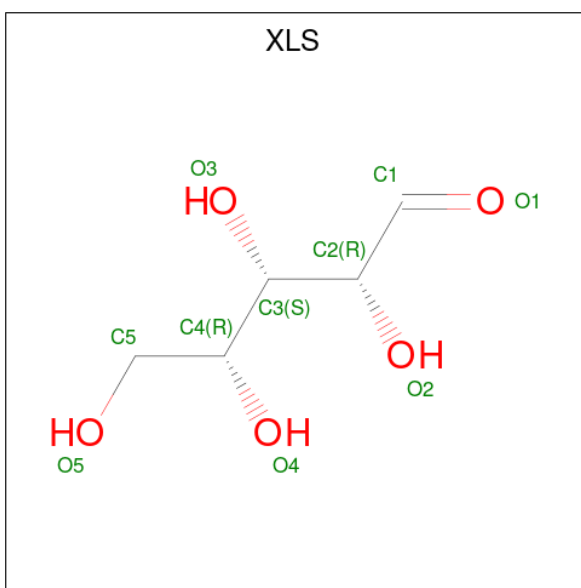
- Molecule 8 is Deacetyltaxol (CCD ID: BKR) (formula: C₄₅H₄₉NO₁₃) (labeled as "Ligand of Interest" by depositor).



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

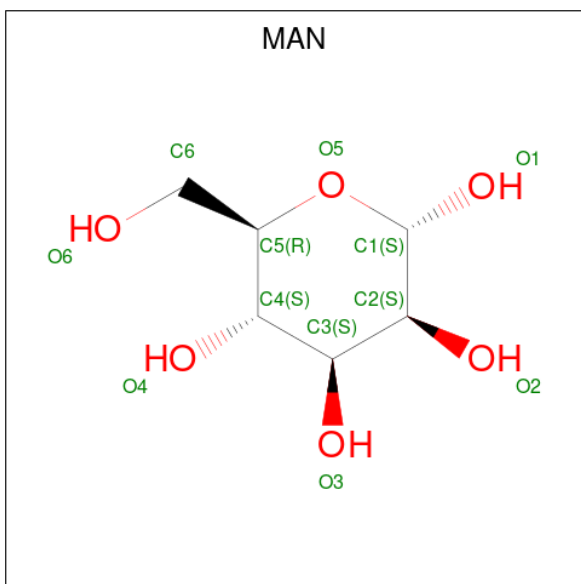
- Molecule 9 is D-xylose (CCD ID: XLS) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest")

by depositor).



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

- Molecule 10 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



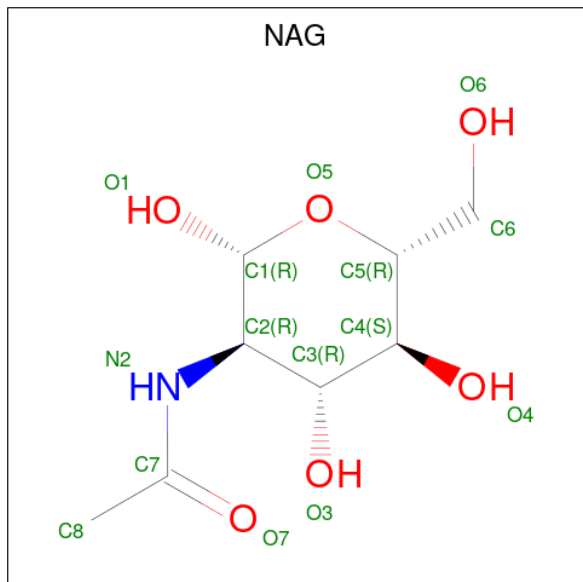
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			11	6	5		

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



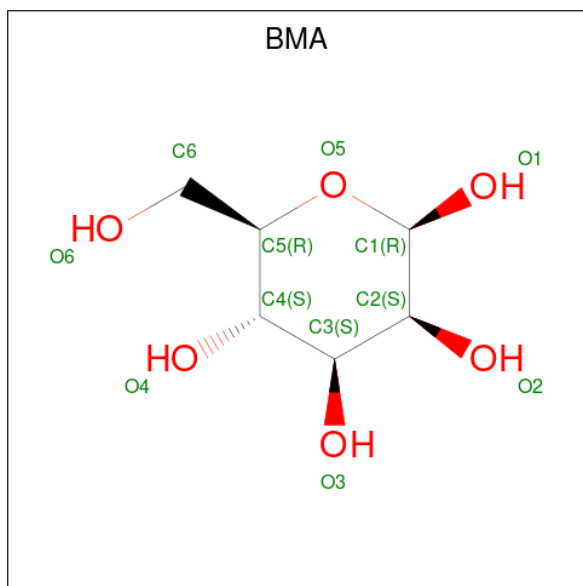
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			15	8	1	6		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			15	8	1	6		
11	B	1	Total	C	N	O	0	0
			14	8	1	5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

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

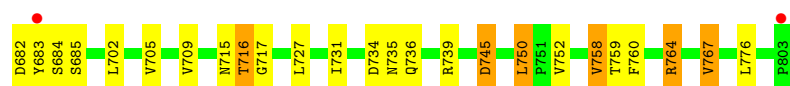
- Molecule 12 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



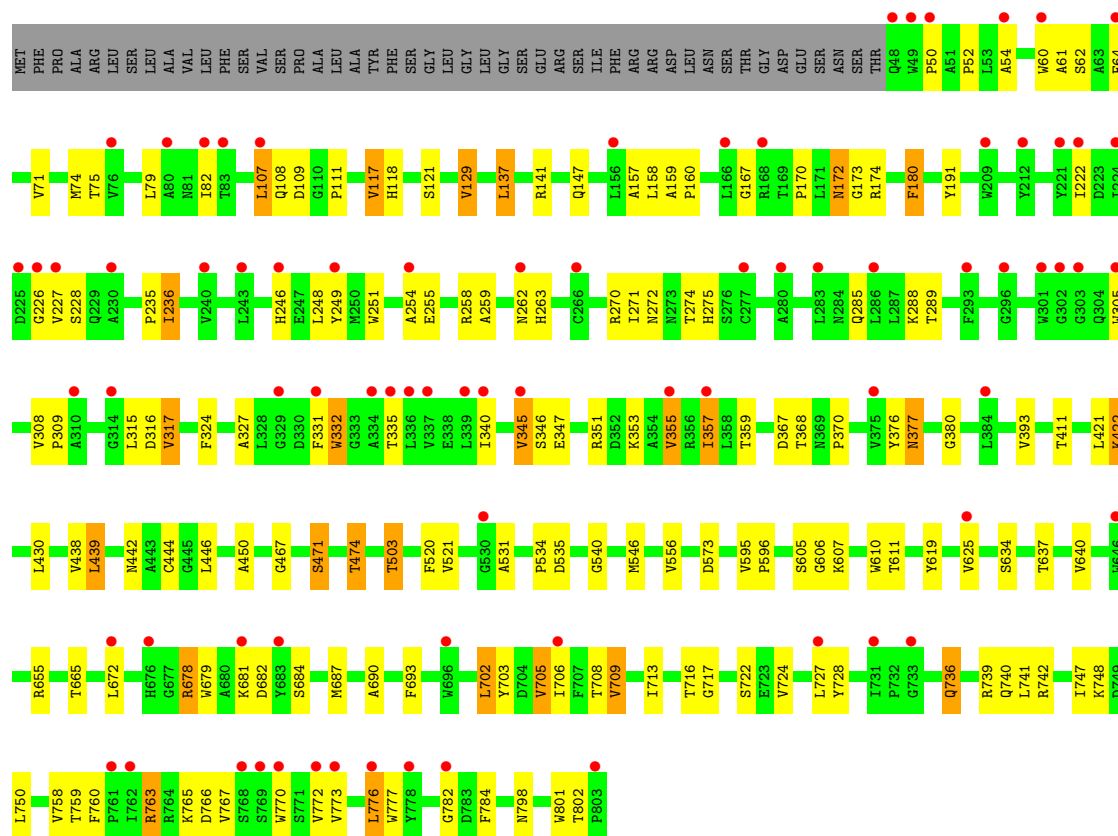
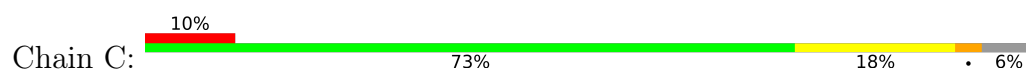
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	479	Total 479	O 479	0	0
13	A	436	Total 436	O 436	0	0
13	C	198	Total 198	O 198	0	0
13	D	181	Total 181	O 181	0	0

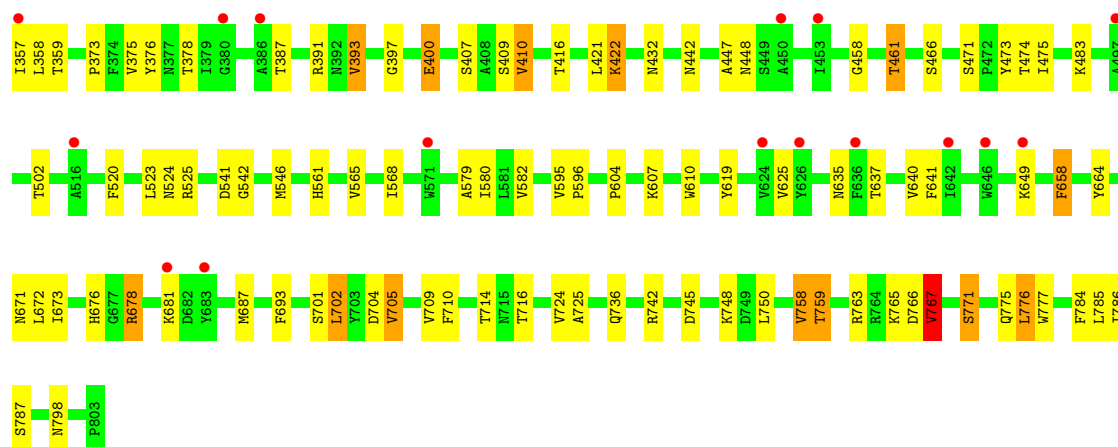


• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



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





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

Chain E: 100%



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

Chain H: 50% 50%



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

Chain L: 100%



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

Chain O: 100%



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

Chain P: 100%

NAG1
NAG2

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

Chain F:  20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 4: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose

Chain G:  50% 50%

MAN1
BMA2

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

Chain I:  100%

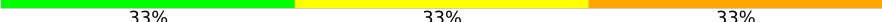
NAG1
NAG2
NAG3

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

Chain J:  60% 40%

NAG1
NAG2
AH23
BMA4
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 33% 33%

NAG1
NAG2
MAN3

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%

NAG1
NAG2
MAN3

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	228.43Å 89.23Å 218.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.97 – 2.07 35.97 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.97-2.07) 95.1 (35.97-2.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.219 , 0.259 0.231 , 0.268	Depositor DCC
R_{free} test set	12691 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25439	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: MAN, BMA, XLS, NAG, BKR, AH2

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	0.60	0/5865	1.04	10/8025 (0.1%)
1	B	0.62	0/5883	1.04	11/8049 (0.1%)
1	C	0.56	0/5864	1.02	4/8023 (0.0%)
1	D	0.58	0/5867	1.06	8/8027 (0.1%)
All	All	0.59	0/23479	1.04	33/32124 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	D	0	1
All	All	0	10

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	THR	CB-CA-C	8.94	123.67	110.26
1	A	48	GLN	N-CA-C	-7.96	103.57	113.20
1	B	218	ARG	N-CA-C	-7.51	103.17	111.36
1	A	675	ASP	CA-CB-CG	6.88	119.48	112.60
1	D	704	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	474	THR	CB-CA-C	6.62	121.67	109.70
1	A	129	VAL	N-CA-CB	6.17	119.83	110.58
1	B	375	VAL	CB-CA-C	6.12	117.23	110.62
1	D	129	VAL	N-CA-CB	6.12	118.12	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	VAL	N-CA-CB	-6.08	105.09	112.33
1	D	736	GLN	CB-CA-C	6.07	117.08	108.76
1	B	129	VAL	N-CA-CB	6.05	118.76	110.54
1	B	393	VAL	N-CA-CB	-5.82	104.80	112.36
1	C	367	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	370	PRO	N-CA-CB	5.76	106.42	103.19
1	B	342	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	129	VAL	CB-CA-C	-5.57	104.62	112.14
1	A	272	ASN	CB-CA-C	-5.57	103.67	111.80
1	C	180	PHE	CA-CB-CG	5.51	119.31	113.80
1	D	285	GLN	CB-CA-C	5.45	119.44	110.83
1	D	714	THR	CA-CB-OG1	-5.44	101.44	109.60
1	B	705	VAL	N-CA-CB	5.39	116.41	110.53
1	A	393	VAL	N-CA-CB	-5.36	104.47	112.67
1	D	658	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	81	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	479	GLU	CB-CA-C	-5.28	102.59	110.88
1	B	758	VAL	N-CA-CB	-5.26	104.10	111.25
1	A	503	THR	CB-CA-C	5.23	118.10	110.26
1	A	745	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	625	VAL	N-CA-CB	5.09	116.27	110.72
1	D	129	VAL	CB-CA-C	-5.04	105.44	112.04
1	D	767	VAL	N-CA-C	-5.04	108.37	113.20
1	B	655	ARG	N-CA-C	-5.02	105.72	111.14

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	391	ARG	Sidechain
1	A	678	ARG	Sidechain
1	A	764	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	218	ARG	Sidechain
1	B	270	ARG	Sidechain
1	B	391	ARG	Sidechain
1	B	484	ARG	Sidechain
1	B	655	ARG	Sidechain
1	D	678	ARG	Sidechain

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	5721	0	5518	83	0
1	B	5738	0	5526	91	0
1	C	5717	0	5510	107	0
1	D	5720	0	5519	130	0
2	E	28	0	24	4	0
2	H	28	0	25	10	0
2	L	28	0	25	0	0
2	O	28	0	25	6	0
2	P	28	0	26	14	0
3	F	61	0	51	6	0
4	G	23	0	21	28	0
5	I	42	0	38	4	0
6	J	61	0	43	5	0
7	K	39	0	34	2	0
7	M	39	0	34	0	0
7	N	39	0	34	0	0
8	A	59	0	0	1	0
8	B	59	0	0	1	0
8	C	59	0	0	2	0
8	D	59	0	0	2	0
9	A	9	0	9	1	0
9	B	9	0	9	1	0
10	A	67	0	62	19	0
10	B	78	0	72	28	0
10	C	55	0	50	13	0
10	D	44	0	39	7	0
11	A	56	0	52	0	0
11	B	100	0	95	8	0
11	C	84	0	78	11	0
11	D	56	0	52	1	0
12	D	11	0	10	9	0
13	A	436	0	0	7	0
13	B	479	0	0	14	0
13	C	198	0	0	4	0
13	D	181	0	0	11	0
All	All	25439	0	22981	508	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 11.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:HD21	11:C:901:NAG:C1	1.31	1.40
10:B:904:MAN:O6	10:B:906:MAN:C1	1.70	1.38
1:D:272:ASN:HD21	2:P:1:NAG:C1	1.39	1.33
10:B:906:MAN:O2	10:B:907:MAN:C1	1.76	1.32
10:B:904:MAN:O3	10:B:905:MAN:C1	1.76	1.30
1:B:798:ASN:HD21	11:B:916:NAG:C1	1.53	1.21
1:C:272:ASN:ND2	11:C:901:NAG:C1	2.05	1.20
12:D:901:BMA:O6	10:D:902:MAN:C1	1.88	1.20
11:C:901:NAG:O4	11:C:902:NAG:C1	1.91	1.18
10:A:901:MAN:C1	6:J:3:AH2:O6	1.92	1.18
4:G:2:BMA:H5	2:H:2:NAG:O4	1.41	1.17
12:D:901:BMA:O3	10:D:904:MAN:C1	1.95	1.13
1:D:272:ASN:ND2	2:P:1:NAG:C1	2.12	1.10
12:D:901:BMA:C1	2:P:2:NAG:O4	1.98	1.10
10:A:901:MAN:O6	10:A:903:MAN:H2	1.51	1.10
2:O:1:NAG:C4	2:O:2:NAG:C1	2.30	1.10
10:A:901:MAN:O3	10:A:902:MAN:C1	2.04	1.05
10:C:903:MAN:O6	10:C:904:MAN:C1	2.07	1.02
10:A:901:MAN:O6	10:A:903:MAN:C2	2.14	0.95
10:C:903:MAN:O6	10:C:904:MAN:H2	1.67	0.94
1:C:346:SER:HB3	13:C:1051:HOH:O	1.67	0.94
10:B:910:MAN:H1	4:G:1:MAN:H61	1.49	0.93
10:B:903:MAN:C1	2:E:2:NAG:O4	2.16	0.93
12:D:901:BMA:O3	10:D:904:MAN:C2	2.17	0.93
1:D:272:ASN:HD21	2:P:1:NAG:C2	1.82	0.93
10:B:912:MAN:C1	4:G:1:MAN:H2	1.99	0.92
10:C:903:MAN:HO3	10:C:906:MAN:HO2	1.09	0.91
1:B:798:ASN:ND2	11:B:916:NAG:C1	2.33	0.91
10:C:903:MAN:O6	10:C:904:MAN:C2	2.20	0.90
4:G:2:BMA:C5	2:H:2:NAG:HO4	1.85	0.89
4:G:2:BMA:H5	2:H:2:NAG:HO4	1.35	0.89
10:A:901:MAN:O6	10:A:903:MAN:C1	2.22	0.88
10:B:910:MAN:O1	4:G:1:MAN:O5	1.93	0.87
5:I:2:NAG:HO4	5:I:3:NAG:C1	1.84	0.86
3:F:2:NAG:C4	3:F:3:BMA:C1	2.53	0.86
4:G:2:BMA:C5	2:H:2:NAG:O4	2.22	0.86
1:B:226:GLY:O	13:B:1001:HOH:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:904:MAN:HO6	10:B:906:MAN:C1	1.86	0.85
10:B:910:MAN:O1	4:G:1:MAN:H4	1.78	0.83
1:A:272:ASN:CG	6:J:1:NAG:C1	2.52	0.82
11:C:902:NAG:O4	10:C:903:MAN:C1	2.27	0.82
10:B:912:MAN:C1	4:G:1:MAN:C2	2.57	0.81
3:F:2:NAG:O4	3:F:3:BMA:C2	2.27	0.81
2:O:1:NAG:O4	2:O:2:NAG:C2	2.28	0.81
1:A:442:ASN:HD21	1:A:471:SER:H	1.28	0.81
1:D:565:VAL:HG23	13:D:1052:HOH:O	1.80	0.80
10:B:910:MAN:O1	4:G:1:MAN:C5	2.29	0.80
10:B:910:MAN:C1	4:G:1:MAN:H61	2.10	0.80
2:O:1:NAG:H4	2:O:2:NAG:C1	2.10	0.80
1:D:676:HIS:ND1	13:D:1001:HOH:O	2.15	0.79
4:G:2:BMA:O4	2:H:2:NAG:O4	1.98	0.79
4:G:2:BMA:O4	2:H:2:NAG:O3	1.99	0.79
10:B:910:MAN:O2	11:B:911:NAG:H1	1.81	0.79
1:C:52:PRO:HG3	1:C:289:THR:OG1	1.84	0.78
1:B:521:VAL:HG11	1:B:546:MET:HE3	1.66	0.78
1:A:421:LEU:HD11	1:A:520:PHE:HZ	1.49	0.78
1:B:272:ASN:CG	3:F:1:NAG:C1	2.54	0.77
1:D:373:PRO:O	1:D:391:ARG:NH2	2.17	0.77
1:C:377:ASN:C	1:C:377:ASN:HD22	1.93	0.77
10:A:907:MAN:O5	7:K:3:MAN:O3	2.02	0.77
1:B:272:ASN:ND2	3:F:1:NAG:C2	2.48	0.76
11:C:902:NAG:O4	10:C:903:MAN:C2	2.33	0.76
12:D:901:BMA:O3	10:D:904:MAN:H2	1.84	0.75
1:A:110:GLY:HA2	13:A:1171:HOH:O	1.85	0.75
1:B:474:THR:HG21	13:B:1376:HOH:O	1.87	0.75
1:D:109:ASP:OD2	1:D:466:SER:HB2	1.86	0.74
1:B:442:ASN:HD21	1:B:471:SER:H	1.34	0.74
1:B:731:ILE:O	1:B:736:GLN:HG2	1.86	0.74
1:A:521:VAL:HG11	1:A:546:MET:CE	2.17	0.74
11:C:902:NAG:O4	10:C:903:MAN:H2	1.86	0.74
1:D:246:HIS:HE1	1:D:290:GLU:OE2	1.71	0.74
2:P:1:NAG:O4	2:P:2:NAG:O7	2.06	0.74
10:B:910:MAN:O1	4:G:1:MAN:C4	2.34	0.74
10:B:904:MAN:C3	10:B:905:MAN:C1	2.65	0.73
10:A:901:MAN:C1	6:J:3:AH2:C6	2.67	0.73
1:D:272:ASN:CG	2:P:1:NAG:C1	2.62	0.73
1:D:78:GLU:OE2	1:D:99:ARG:NH1	2.21	0.73
4:G:2:BMA:O4	2:H:2:NAG:C4	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ALA:O	1:D:349:LEU:HD21	1.88	0.73
1:C:767:VAL:HG22	1:C:784:PHE:CE2	2.23	0.72
1:A:172:ASN:HD22	1:A:174:ARG:H	1.38	0.72
10:A:901:MAN:C3	10:A:902:MAN:C1	2.68	0.72
1:D:275:HIS:HB2	1:D:278:SER:OG	1.90	0.72
1:D:317:VAL:HG22	1:D:357:ILE:HD11	1.70	0.72
1:B:204:THR:H	1:B:262:ASN:HD22	1.38	0.71
1:D:109:ASP:OD1	1:D:158:LEU:HD12	1.90	0.71
1:D:759:THR:HG22	13:D:1011:HOH:O	1.90	0.71
1:B:273:ASN:HD21	1:B:633:GLN:HE22	1.37	0.71
1:D:776:LEU:C	1:D:776:LEU:HD23	2.15	0.71
1:D:236:ILE:CD1	1:D:625:VAL:HG11	2.22	0.70
1:A:649:LYS:NZ	13:A:1004:HOH:O	2.23	0.70
10:A:903:MAN:HO2	10:A:904:MAN:C1	2.04	0.70
1:D:98:THR:HB	2:O:2:NAG:O6	1.91	0.70
1:B:521:VAL:HG21	1:B:546:MET:CE	2.22	0.70
1:D:763:ARG:HD3	1:D:766:ASP:OD2	1.91	0.70
1:A:147:GLN:HG2	13:A:1291:HOH:O	1.91	0.70
4:G:2:BMA:C4	2:H:2:NAG:HO4	2.04	0.69
10:A:907:MAN:O1	10:A:908:MAN:C1	2.41	0.69
1:C:71:VAL:HG21	1:C:355:VAL:HG23	1.75	0.69
12:D:901:BMA:C6	10:D:902:MAN:C1	2.71	0.68
1:C:71:VAL:HA	1:C:74:MET:HE2	1.73	0.68
10:A:901:MAN:O3	10:A:902:MAN:C2	2.41	0.68
10:C:906:MAN:O2	10:C:907:MAN:C1	2.42	0.68
1:D:236:ILE:HD11	1:D:625:VAL:HG11	1.76	0.68
1:D:78:GLU:CD	1:D:99:ARG:HH12	2.02	0.68
1:A:425:GLN:NE2	13:A:1002:HOH:O	2.19	0.68
1:A:272:ASN:ND2	6:J:1:NAG:C2	2.57	0.67
1:D:122:GLN:OE1	1:D:461:THR:OG1	2.11	0.67
1:A:111:PRO:HD2	1:A:467:GLY:HA2	1.77	0.67
1:C:60:TRP:CD2	1:C:687:MET:HE2	2.30	0.67
1:C:272:ASN:CG	11:C:901:NAG:C1	2.67	0.67
10:A:901:MAN:HO6	10:A:903:MAN:H2	1.59	0.66
1:D:523:LEU:HD11	1:D:546:MET:SD	2.35	0.66
12:D:901:BMA:C1	2:P:2:NAG:C4	2.74	0.66
1:C:442:ASN:HD21	1:C:471:SER:H	1.42	0.65
1:C:713:ILE:HD11	1:C:747:ILE:HG13	1.79	0.65
1:A:246:HIS:HE1	1:A:290:GLU:OE2	1.79	0.65
1:D:272:ASN:HD21	2:P:1:NAG:H2	1.62	0.64
1:A:421:LEU:HD11	1:A:520:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:GLN:HA	1:C:736:GLN:HE21	1.63	0.64
4:G:2:BMA:O4	2:H:2:NAG:C3	2.45	0.64
1:B:521:VAL:CG1	1:B:546:MET:HE3	2.28	0.64
1:D:151:ASP:HB3	1:D:393:VAL:CG2	2.27	0.64
1:B:377:ASN:C	1:B:377:ASN:HD22	2.05	0.64
1:C:274:THR:HA	13:C:1005:HOH:O	1.97	0.63
1:A:474:THR:HG21	13:A:1353:HOH:O	1.98	0.63
1:B:438:VAL:HG23	1:B:439:LEU:HD13	1.81	0.63
1:A:377:ASN:C	1:A:377:ASN:HD22	2.05	0.63
1:B:701:SER:O	1:B:764:ARG:NH1	2.32	0.63
1:C:474:THR:HG21	13:C:1160:HOH:O	1.99	0.63
1:C:665:THR:OG1	1:C:717:GLY:HA3	1.99	0.62
10:B:910:MAN:O2	11:B:911:NAG:H5	1.98	0.62
10:C:904:MAN:H3	10:C:905:MAN:C1	2.28	0.62
1:C:421:LEU:HD11	1:C:520:PHE:HZ	1.63	0.62
1:C:702:LEU:HD22	1:C:765:LYS:HB2	1.82	0.62
10:B:903:MAN:C1	2:E:2:NAG:HO4	2.11	0.62
10:A:903:MAN:O2	10:A:904:MAN:C1	2.47	0.62
1:C:71:VAL:HG21	1:C:355:VAL:CG2	2.30	0.62
11:C:901:NAG:C4	11:C:902:NAG:C1	2.77	0.62
1:D:172:ASN:C	1:D:172:ASN:HD22	2.07	0.62
10:A:903:MAN:O2	10:A:904:MAN:H2	2.00	0.62
1:B:546:MET:HA	1:B:546:MET:HE2	1.81	0.61
1:A:204:THR:H	1:A:262:ASN:HD22	1.48	0.61
1:C:347:GLU:OE1	1:C:351:ARG:NH2	2.34	0.61
1:A:432:ASN:HB2	13:A:1335:HOH:O	2.00	0.60
1:D:134:ASP:OD1	1:D:136:THR:HB	2.01	0.60
10:B:906:MAN:C2	10:B:907:MAN:C1	2.77	0.60
1:C:605[A]:SER:OG	1:C:722:SER:HB2	2.01	0.60
1:C:272:ASN:HD21	11:C:901:NAG:C2	2.10	0.60
1:B:759:THR:HG23	13:B:1285:HOH:O	2.01	0.60
12:D:901:BMA:C3	10:D:904:MAN:C1	2.78	0.60
1:D:98:THR:HG21	2:O:1:NAG:O3	2.03	0.59
1:D:745:ASP:HB3	1:D:758:VAL:HG22	1.83	0.59
1:D:272:ASN:OD1	2:P:1:NAG:C1	2.50	0.59
1:C:377:ASN:HD21	1:C:380:GLY:H	1.49	0.59
1:A:715:ASN:HB2	1:A:750:LEU:HD13	1.84	0.58
10:C:904:MAN:C3	10:C:905:MAN:C1	2.81	0.58
1:C:763:ARG:NH1	1:C:766:ASP:OD1	2.35	0.58
1:D:502:THR:HA	13:D:1103:HOH:O	2.02	0.58
1:A:300:ASP:OD1	9:A:912:XLS:H3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASN:ND2	2:P:1:NAG:C2	2.59	0.58
10:A:907:MAN:C5	7:K:3:MAN:HO3	2.14	0.58
1:C:773:VAL:O	10:C:903:MAN:O4	2.13	0.58
1:D:421:LEU:HD11	1:D:520:PHE:HZ	1.69	0.58
1:D:776:LEU:HD23	1:D:776:LEU:O	2.02	0.58
1:A:152:GLN:HA	1:A:152:GLN:HE21	1.68	0.57
1:B:628:ASP:HA	11:B:911:NAG:H82	1.86	0.57
1:C:248:LEU:HD23	1:C:249:TYR:CE2	2.40	0.57
1:C:679:TRP:HB3	1:C:706:ILE:O	2.04	0.57
1:B:70:THR:HG22	1:B:74:MET:HE3	1.86	0.57
1:D:89:LEU:HB3	1:D:376:TYR:O	2.04	0.57
1:C:705:VAL:HA	1:C:763:ARG:HA	1.87	0.56
1:D:432:ASN:O	1:D:458:GLY:HA2	2.05	0.56
1:B:776:LEU:HD23	1:B:776:LEU:C	2.30	0.56
1:D:151:ASP:HB3	1:D:393:VAL:HG22	1.88	0.56
1:A:177:GLU:OE2	1:A:467:GLY:HA3	2.06	0.56
1:D:524:ASN:HA	1:D:561:HIS:O	2.06	0.56
1:C:438:VAL:HG23	1:C:439:LEU:HD13	1.88	0.55
1:D:76:VAL:HG23	13:D:1082:HOH:O	2.06	0.55
1:B:172:ASN:HD22	1:B:174:ARG:H	1.54	0.55
1:C:60:TRP:CE2	1:C:687:MET:HE2	2.41	0.55
1:D:152:GLN:HE21	1:D:152:GLN:HA	1.71	0.55
1:D:78:GLU:CD	1:D:99:ARG:NH1	2.65	0.55
1:B:432:ASN:HB2	13:B:1286:HOH:O	2.06	0.55
1:A:731:ILE:O	1:A:736:GLN:HG2	2.06	0.55
1:B:716:THR:HG22	1:B:716:THR:O	2.06	0.55
1:B:421:LEU:HD11	1:B:520:PHE:HZ	1.72	0.54
1:C:739:ARG:NH2	13:C:1004:HOH:O	2.40	0.54
1:C:258:ARG:HD2	1:C:703:TYR:CE2	2.42	0.54
8:A:911:BKR:C20	8:A:911:BKR:C47	2.86	0.54
1:B:89:LEU:HB3	1:B:376:TYR:O	2.08	0.54
1:B:702:LEU:HD13	1:B:765:LYS:HD2	1.88	0.54
1:C:693:PHE:HA	1:C:777:TRP:O	2.08	0.54
1:C:767:VAL:HG21	1:C:801:TRP:HZ3	1.73	0.54
1:D:51:ALA:HB2	1:D:284:ASN:HD21	1.72	0.54
8:B:901:BKR:C47	8:B:901:BKR:C20	2.86	0.54
1:B:626:TYR:CE1	4:G:1:MAN:H1	2.43	0.54
1:A:521:VAL:HG11	1:A:546:MET:HE3	1.87	0.54
1:D:776:LEU:C	1:D:776:LEU:CD2	2.81	0.54
1:B:108:GLN:HG3	1:B:109:ASP:O	2.08	0.53
1:A:122:GLN:HE21	1:A:587:GLY:HA2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLY:HA3	1:A:531:ALA:O	2.07	0.53
1:D:217:SER:HA	1:D:219:ASN:OD1	2.09	0.53
1:C:108:GLN:HG3	1:C:109:ASP:O	2.07	0.53
1:D:108:GLN:HG3	1:D:109:ASP:O	2.07	0.53
1:C:236:ILE:HD13	1:C:625:VAL:HG22	1.89	0.53
4:G:2:BMA:C4	2:H:2:NAG:O4	2.53	0.53
1:A:569:GLU:OE1	1:A:655:ARG:NH1	2.42	0.53
1:D:55:ASN:H	1:D:294:GLN:NE2	2.07	0.53
1:D:156:LEU:HD21	1:D:263:HIS:CD2	2.44	0.53
1:B:216:THR:HA	4:G:1:MAN:O6	2.09	0.53
1:B:515:ASP:N	13:B:1013:HOH:O	2.39	0.53
1:B:521:VAL:CB	1:B:546:MET:HE3	2.40	0.52
1:B:442:ASN:HD21	1:B:471:SER:N	2.05	0.52
1:D:607:LYS:HD2	1:D:724:VAL:HB	1.91	0.52
1:A:47:THR:C	1:A:49:TRP:H	2.15	0.52
1:A:258:ARG:NH2	1:A:685:SER:HB3	2.25	0.52
2:P:1:NAG:C4	2:P:2:NAG:C1	2.83	0.52
1:D:347:GLU:OE1	1:D:351:ARG:NH2	2.42	0.52
1:C:191:TYR:CD2	1:C:259:ALA:HB2	2.45	0.52
1:B:172:ASN:HD22	1:B:172:ASN:C	2.18	0.51
1:C:75:THR:O	1:C:79:LEU:HD12	2.10	0.51
1:C:728:TYR:CE1	1:C:741:LEU:HB2	2.45	0.51
10:B:912:MAN:H4	13:B:1392:HOH:O	2.09	0.51
1:C:255:GLU:OE2	1:C:763:ARG:NH2	2.43	0.51
1:D:641:PHE:CE2	1:D:649:LYS:HG3	2.45	0.51
5:I:2:NAG:C4	5:I:3:NAG:C1	2.84	0.51
1:C:305:TRP:O	1:C:331:PHE:CZ	2.62	0.51
1:C:377:ASN:C	1:C:377:ASN:ND2	2.64	0.51
1:D:49:TRP:CZ3	1:D:281:LYS:HB2	2.46	0.51
1:D:117:VAL:HG22	1:D:376:TYR:CD2	2.46	0.51
1:A:98:THR:CG2	5:I:1:NAG:O3	2.59	0.51
1:A:645:ARG:HG2	1:A:645:ARG:HH11	1.76	0.51
1:D:416:THR:O	1:D:416:THR:HG22	2.11	0.51
10:C:903:MAN:O3	10:C:906:MAN:O2	1.96	0.51
1:D:151:ASP:CB	1:D:393:VAL:HG22	2.40	0.51
1:D:205:VAL:HG22	1:D:263:HIS:HB2	1.92	0.51
1:B:203:ALA:HA	1:B:262:ASN:ND2	2.25	0.51
1:A:147:GLN:OE1	1:A:395:LYS:HG3	2.11	0.50
1:A:521:VAL:CG1	1:A:546:MET:CE	2.87	0.50
1:B:626:TYR:CE1	4:G:1:MAN:C1	2.94	0.50
10:D:904:MAN:O2	10:D:905:MAN:H3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:O	1:D:128:THR:N	2.41	0.50
1:D:798:ASN:HB3	13:D:1098:HOH:O	2.12	0.50
1:D:214:GLN:HG2	13:D:1161:HOH:O	2.11	0.50
1:D:253:PHE:O	1:D:257:VAL:HG23	2.11	0.50
1:D:108:GLN:NE2	1:D:378:THR:HG21	2.27	0.50
1:B:227:VAL:HG22	1:B:232:ILE:HD11	1.92	0.50
1:A:521:VAL:HB	1:A:546:MET:HE1	1.94	0.50
1:D:147:GLN:NE2	1:D:151:ASP:OD2	2.44	0.50
1:B:739:ARG:NH2	13:B:1027:HOH:O	2.44	0.49
1:A:525:ARG:HD2	1:A:525:ARG:C	2.37	0.49
1:C:191:TYR:CG	1:C:259:ALA:HB2	2.46	0.49
12:D:901:BMA:O5	2:P:2:NAG:O3	2.29	0.49
1:B:172:ASN:ND2	1:B:174:ARG:H	2.09	0.49
1:A:98:THR:HG21	5:I:1:NAG:O3	2.12	0.49
1:C:60:TRP:CE3	1:C:359:THR:HG21	2.47	0.49
10:B:910:MAN:O1	4:G:1:MAN:C6	2.61	0.49
1:B:246:HIS:HE1	1:B:290:GLU:OE2	1.96	0.49
1:D:129:VAL:HG13	1:D:141:ARG:HD2	1.94	0.49
1:A:503:THR:HG23	13:A:1208:HOH:O	2.11	0.49
1:C:235:PRO:O	1:C:236:ILE:C	2.55	0.49
1:D:107:LEU:N	1:D:107:LEU:HD23	2.28	0.49
2:O:1:NAG:O4	2:O:2:NAG:H2	2.09	0.49
10:B:910:MAN:C1	11:B:911:NAG:H5	2.42	0.49
1:A:524:ASN:HA	1:A:561:HIS:O	2.13	0.49
1:D:236:ILE:HD13	1:D:625:VAL:HG11	1.94	0.49
1:D:604:PRO:HD3	1:D:664:TYR:CE2	2.47	0.49
1:C:54:ALA:O	1:C:64:PHE:CE1	2.66	0.49
1:A:262:ASN:O	1:A:295:GLY:HA3	2.12	0.49
1:C:251:TRP:O	1:C:254:ALA:HB3	2.13	0.49
1:B:170:PRO:HG3	1:B:619:TYR:CD2	2.48	0.49
10:A:903:MAN:O2	10:A:904:MAN:C2	2.60	0.49
1:C:172:ASN:HD22	1:C:174:ARG:H	1.61	0.49
1:D:785:LEU:HD11	1:D:798:ASN:HB2	1.95	0.49
1:B:626:TYR:HE1	4:G:1:MAN:C1	2.26	0.48
1:A:484:ARG:NH1	1:A:599:TYR:HB3	2.28	0.48
1:B:521:VAL:HG21	1:B:546:MET:HE1	1.92	0.48
1:A:110:GLY:H	1:A:111:PRO:HD3	1.78	0.48
1:A:745:ASP:HB3	1:A:758:VAL:HG22	1.94	0.48
11:D:907:NAG:H83	13:D:1156:HOH:O	2.13	0.48
10:B:910:MAN:O1	4:G:1:MAN:H61	2.12	0.48
10:A:903:MAN:O2	10:A:904:MAN:O5	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASN:ND2	2:P:1:NAG:H2	2.27	0.48
1:B:524:ASN:HA	1:B:561:HIS:O	2.13	0.48
10:B:906:MAN:C1	10:B:907:MAN:O5	2.61	0.48
1:C:170:PRO:HG3	1:C:619:TYR:CD2	2.49	0.48
1:D:248:LEU:HD23	1:D:249:TYR:CZ	2.49	0.48
1:C:521:VAL:HG11	1:C:546:MET:HE2	1.95	0.48
1:B:59:SER:OG	1:B:686:VAL:O	2.29	0.48
1:C:324:PHE:CE2	8:C:912:BKR:C14	2.97	0.48
1:B:216:THR:HG23	4:G:1:MAN:O6	2.14	0.47
1:B:300:ASP:OD1	9:B:902:XLS:H3	2.14	0.47
1:A:107:LEU:HD23	1:A:107:LEU:N	2.29	0.47
1:A:521:VAL:HG11	1:A:546:MET:HE2	1.94	0.47
1:B:758:VAL:HG13	1:B:760:PHE:CZ	2.50	0.47
10:B:912:MAN:C1	4:G:1:MAN:O2	2.62	0.47
1:C:288:LYS:NZ	1:C:316:ASP:OD2	2.40	0.47
1:D:107:LEU:HD22	1:D:156:LEU:HB2	1.97	0.47
1:D:284:ASN:OD1	1:D:314:GLY:HA3	2.14	0.47
1:D:771:SER:O	1:D:775:GLN:N	2.44	0.47
1:A:272:ASN:ND2	6:J:1:NAG:O5	2.40	0.47
1:C:50:PRO:O	1:C:52:PRO:HD3	2.15	0.47
1:D:473:TYR:CE1	1:D:475:ILE:CD1	2.97	0.47
1:C:236:ILE:HD11	1:C:634:SER:HB2	1.96	0.47
1:D:541:ASP:O	1:D:542:GLY:C	2.57	0.47
1:B:265:MET:HA	1:B:298:VAL:O	2.15	0.47
1:D:397:GLY:O	1:D:400:GLU:HG2	2.15	0.47
1:A:655:ARG:HD3	1:A:656:TYR:CE2	2.50	0.47
1:D:759:THR:CG2	13:D:1011:HOH:O	2.57	0.47
1:B:774:ASP:OD1	3:F:5:MAN:H62	2.15	0.46
1:D:242:ASP:O	1:D:246:HIS:HD2	1.99	0.46
1:D:473:TYR:HE1	1:D:475:ILE:CD1	2.28	0.46
1:A:160:PRO:HG2	1:A:162:THR:CG2	2.46	0.46
1:C:60:TRP:HE3	1:C:359:THR:HG21	1.80	0.46
10:B:910:MAN:HO1	4:G:1:MAN:C1	2.22	0.46
1:A:203:ALA:HA	1:A:262:ASN:ND2	2.31	0.46
1:D:702:LEU:HD22	1:D:765:LYS:HB2	1.97	0.46
1:B:74:MET:HE1	1:B:358:LEU:HD21	1.97	0.46
1:C:702:LEU:HD13	1:C:765:LYS:HD2	1.97	0.46
1:D:635:ASN:HB3	1:D:637:THR:HG23	1.97	0.46
1:A:134:ASP:OD1	1:A:136:THR:HB	2.16	0.46
1:A:645:ARG:HG2	1:A:645:ARG:NH1	2.30	0.46
1:B:645:ARG:NH1	13:B:1031:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ASP:OD1	1:C:353:LYS:HA	2.15	0.46
1:C:521:VAL:HG11	1:C:546:MET:CE	2.46	0.46
1:C:595:VAL:N	1:C:596:PRO:CD	2.79	0.46
1:D:151:ASP:CB	1:D:393:VAL:CG2	2.93	0.46
1:D:309:PRO:O	1:D:310:ALA:C	2.59	0.46
1:D:767:VAL:HG22	1:D:784:PHE:CE2	2.51	0.46
1:C:763:ARG:HD3	1:C:766:ASP:OD2	2.16	0.45
1:B:150:HIS:CE1	13:B:1087:HOH:O	2.68	0.45
1:B:645:ARG:NH2	13:B:1036:HOH:O	2.48	0.45
1:A:129:VAL:O	1:A:130:ALA:C	2.59	0.45
1:C:782:GLY:O	1:C:802:THR:HG23	2.16	0.45
1:C:678:ARG:HB3	1:C:708:THR:HB	1.97	0.45
1:B:107:LEU:N	1:B:107:LEU:HD12	2.32	0.45
1:C:60:TRP:O	1:C:61:ALA:C	2.59	0.45
1:C:758:VAL:CG1	1:C:760:PHE:CZ	3.00	0.45
1:D:725:ALA:HB3	1:D:758:VAL:HG21	1.98	0.45
1:A:81:ASN:ND2	1:A:96:ALA:O	2.49	0.45
1:C:52:PRO:HG3	1:C:289:THR:HG1	1.81	0.45
1:D:248:LEU:HD23	1:D:249:TYR:CE2	2.51	0.45
1:D:705:VAL:HA	1:D:763:ARG:HA	1.99	0.45
10:A:903:MAN:HO2	10:A:904:MAN:C2	2.29	0.45
1:C:111:PRO:HD2	1:C:467:GLY:HA2	1.98	0.45
1:C:222:ILE:HD12	1:C:327:ALA:O	2.17	0.45
11:C:901:NAG:H61	11:C:902:NAG:H82	1.99	0.45
1:D:324:PHE:CE1	8:D:910:BKR:C14	3.00	0.45
1:B:167:GLY:HA2	13:B:1410:HOH:O	2.16	0.44
1:A:47:THR:C	1:A:49:TRP:N	2.73	0.44
1:A:176:TRP:CZ2	1:A:463:GLY:HA3	2.52	0.44
1:C:246:HIS:CE1	1:C:770:TRP:CZ2	3.05	0.44
1:C:315:LEU:HD23	1:C:332:TRP:CZ2	2.52	0.44
1:C:317:VAL:HG22	1:C:357:ILE:HD11	1.99	0.44
1:B:525:ARG:HD2	1:B:525:ARG:C	2.43	0.44
1:C:713:ILE:HD11	1:C:747:ILE:CG1	2.47	0.44
1:D:93:VAL:HA	1:D:105:PHE:O	2.17	0.44
1:D:170:PRO:HG3	1:D:619:TYR:CD2	2.52	0.44
10:B:907:MAN:H62	10:B:907:MAN:O3	2.18	0.44
1:A:592:ASN:N	1:A:592:ASN:OD1	2.50	0.44
1:D:56:GLY:O	1:D:687:MET:HE1	2.18	0.44
1:D:214:GLN:NE2	1:D:625:VAL:HG12	2.32	0.44
1:B:377:ASN:HD21	1:B:380:GLY:H	1.66	0.44
1:C:107:LEU:HD23	1:C:107:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:THR:O	1:C:690:ALA:HB3	2.17	0.44
1:D:172:ASN:HD21	1:D:174:ARG:HG2	1.83	0.44
1:B:98:THR:HG21	2:E:1:NAG:O3	2.18	0.44
1:B:285:GLN:O	1:B:289:THR:HB	2.18	0.44
1:A:442:ASN:ND2	1:A:471:SER:H	2.04	0.44
1:C:226:GLY:O	1:C:228:SER:N	2.51	0.44
1:C:727:LEU:HD23	1:C:727:LEU:C	2.43	0.44
1:B:377:ASN:C	1:B:377:ASN:ND2	2.73	0.43
1:A:176:TRP:CE2	1:A:463:GLY:HA3	2.53	0.43
1:A:521:VAL:CG1	1:A:546:MET:HE3	2.47	0.43
1:D:120:SER:HB3	1:D:148:GLU:OE1	2.17	0.43
1:D:724:VAL:HG23	13:D:1088:HOH:O	2.18	0.43
1:B:421:LEU:HD11	1:B:520:PHE:CZ	2.52	0.43
1:A:109:ASP:HA	1:A:158:LEU:HB2	2.00	0.43
1:A:668:THR:OG1	1:A:716:THR:HG21	2.18	0.43
1:C:709:VAL:HG13	1:C:760:PHE:HB2	2.00	0.43
1:C:776:LEU:C	1:C:776:LEU:HD23	2.43	0.43
1:A:274:THR:O	1:A:275:HIS:C	2.60	0.43
1:A:377:ASN:HD21	1:A:380:GLY:H	1.65	0.43
1:A:758:VAL:HG13	1:A:760:PHE:CZ	2.54	0.43
1:C:308:VAL:N	1:C:309:PRO:CD	2.82	0.43
1:D:579:ALA:C	1:D:580:ILE:HG13	2.43	0.43
1:B:235:PRO:HB2	1:B:270:ARG:HG3	1.99	0.43
1:B:242:ASP:O	1:B:246:HIS:HD2	2.02	0.43
1:B:758:VAL:CG1	1:B:760:PHE:CE2	3.01	0.43
1:A:414:LYS:O	1:A:579:ALA:HA	2.19	0.43
1:D:172:ASN:HD22	1:D:174:ARG:H	1.66	0.43
10:A:901:MAN:H3	10:A:902:MAN:C1	2.46	0.43
1:C:157:ALA:O	1:C:159:ALA:N	2.52	0.43
1:D:442:ASN:HD21	1:D:471:SER:H	1.66	0.43
10:B:904:MAN:C6	10:B:906:MAN:C1	2.86	0.43
1:C:107:LEU:HB3	1:C:158:LEU:HD21	2.01	0.43
1:D:222:ILE:HG13	1:D:327:ALA:O	2.19	0.43
1:B:798:ASN:HD21	11:B:916:NAG:C2	2.22	0.43
1:A:433:ASP:HB3	1:A:522:PHE:HB3	2.00	0.43
1:C:740:GLN:HB3	1:C:742:ARG:HH12	1.84	0.43
1:A:734:ASP:O	1:A:735:ASN:C	2.62	0.43
1:D:51:ALA:HB2	1:D:284:ASN:ND2	2.34	0.43
1:D:248:LEU:HD22	1:D:640:VAL:HA	2.01	0.43
1:C:118:HIS:O	1:C:376:TYR:CZ	2.72	0.43
1:D:473:TYR:CE1	1:D:475:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:C	1:A:377:ASN:ND2	2.75	0.43
1:A:243:LEU:HD23	1:A:243:LEU:C	2.43	0.42
1:C:235:PRO:HD3	1:C:305:TRP:CZ2	2.54	0.42
1:C:444:CYS:O	1:C:450:ALA:HB3	2.19	0.42
1:C:521:VAL:HB	1:C:546:MET:HE1	2.01	0.42
8:D:910:BKR:C47	8:D:910:BKR:C20	2.97	0.42
10:B:904:MAN:O3	10:B:905:MAN:C2	2.58	0.42
1:D:409:SER:O	1:D:410:VAL:C	2.59	0.42
1:B:776:LEU:HD23	1:B:776:LEU:O	2.19	0.42
1:C:137:LEU:HD12	1:C:137:LEU:HA	1.94	0.42
1:C:534:PRO:O	1:C:535:ASP:HB3	2.19	0.42
1:D:693:PHE:HA	1:D:777:TRP:O	2.19	0.42
1:A:717:GLY:O	1:A:752:VAL:HG13	2.19	0.42
1:C:248:LEU:HD22	1:C:640:VAL:HA	2.01	0.42
1:C:262:ASN:C	1:C:263:HIS:CD2	2.98	0.42
1:C:270:ARG:HG2	1:C:275:HIS:ND1	2.34	0.42
1:D:109:ASP:HB3	1:D:110:GLY:CA	2.49	0.42
1:B:693:PHE:HA	1:B:777:TRP:O	2.20	0.42
1:C:173:GLY:HA3	1:C:531:ALA:O	2.19	0.42
1:C:411:THR:HG23	1:C:606:GLY:O	2.20	0.42
1:B:474:THR:HB	13:B:1240:HOH:O	2.20	0.42
1:D:60:TRP:CD2	1:D:687:MET:HE2	2.55	0.42
1:D:108:GLN:HE22	1:D:378:THR:HG21	1.84	0.42
1:A:129:VAL:HG13	1:A:141:ARG:HD2	2.01	0.42
1:C:702:LEU:HD22	1:C:765:LYS:CB	2.48	0.42
1:D:257:VAL:O	1:D:687:MET:HB2	2.20	0.42
1:D:671:ASN:ND2	1:D:673:ILE:HD11	2.34	0.42
1:C:117:VAL:HG22	1:C:376:TYR:CD2	2.55	0.42
10:C:903:MAN:HO6	10:C:904:MAN:H2	1.76	0.42
1:B:683[B]:TYR:HE2	13:B:1260:HOH:O	2.01	0.42
1:D:64:PHE:CD1	1:D:64:PHE:C	2.98	0.42
1:D:258:ARG:HA	1:D:687:MET:O	2.20	0.42
1:D:595:VAL:N	1:D:596:PRO:CD	2.82	0.42
1:D:702:LEU:HD13	1:D:765:LYS:HD2	2.01	0.42
1:B:227:VAL:CG2	1:B:232:ILE:HD11	2.50	0.41
1:C:340:ILE:HA	1:C:345:VAL:O	2.20	0.41
1:D:710:PHE:CD1	1:D:759:THR:HB	2.55	0.41
1:B:767:VAL:HG22	1:B:784:PHE:CE2	2.55	0.41
1:B:784:PHE:CD1	1:B:784:PHE:N	2.87	0.41
1:C:351:ARG:HH11	1:C:351:ARG:HG2	1.85	0.41
1:D:172:ASN:ND2	1:D:174:ARG:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:625:VAL:HG13	1:D:625:VAL:O	2.21	0.41
1:D:742:ARG:HD2	1:D:766:ASP:HB3	2.01	0.41
1:C:758:VAL:HG12	1:C:760:PHE:CE2	2.55	0.41
1:D:787:SER:HB3	13:D:1098:HOH:O	2.20	0.41
1:B:419:LEU:HA	1:B:420:PRO:C	2.45	0.41
1:D:172:ASN:C	1:D:172:ASN:ND2	2.73	0.41
1:B:238:SER:O	1:B:271:ILE:HA	2.21	0.41
1:A:172:ASN:ND2	1:A:174:ARG:H	2.14	0.41
1:A:439:LEU:HB3	1:A:443:ALA:CB	2.51	0.41
1:C:573:ASP:CG	1:C:655:ARG:HH22	2.27	0.41
1:B:786:ILE:O	1:B:798:ASN:HA	2.21	0.41
1:D:546:MET:HE3	1:D:546:MET:HA	2.03	0.41
1:B:798:ASN:CG	11:B:916:NAG:C1	2.91	0.41
1:A:727:LEU:HD23	1:A:727:LEU:C	2.46	0.41
1:D:209:TRP:CG	1:D:210:ILE:HB	2.56	0.41
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.88	0.41
1:C:607:LYS:HE3	1:C:724:VAL:HB	2.02	0.41
1:D:447:ALA:O	1:D:448:ASN:C	2.64	0.41
1:B:446:LEU:HD12	1:B:446:LEU:HA	1.85	0.41
1:B:484:ARG:HA	1:B:484:ARG:HD2	1.86	0.41
1:B:767:VAL:HG22	1:B:784:PHE:CD2	2.56	0.41
1:B:773:VAL:HA	3:F:3:BMA:H5	2.03	0.41
1:A:237:SER:OG	1:A:239:ASN:OD1	2.34	0.41
1:A:767:VAL:O	1:A:767:VAL:HG13	2.21	0.41
1:C:272:ASN:OD1	11:C:901:NAG:C1	2.69	0.41
8:C:912:BKR:C20	8:C:912:BKR:C47	2.99	0.41
1:D:190:SER:O	1:D:194:VAL:HG23	2.21	0.41
1:B:129:VAL:HG13	1:B:141:ARG:HD2	2.03	0.41
1:B:626:TYR:HH	4:G:1:MAN:C1	2.25	0.41
1:A:438:VAL:HG23	1:A:439:LEU:HD13	2.03	0.41
1:A:524:ASN:OD1	1:A:524:ASN:C	2.64	0.41
1:D:171:LEU:O	1:D:172:ASN:C	2.61	0.41
1:D:281:LYS:HG2	2:P:1:NAG:O7	2.21	0.41
1:B:98:THR:CG2	2:E:1:NAG:O3	2.69	0.40
1:C:159:ALA:HB1	1:C:160:PRO:HA	2.03	0.40
1:D:308:VAL:N	1:D:309:PRO:CD	2.84	0.40
1:D:324:PHE:O	1:D:325:LEU:HB2	2.21	0.40
1:D:525:ARG:HD2	1:D:525:ARG:C	2.46	0.40
1:B:422:LYS:HB2	13:B:1010:HOH:O	2.21	0.40
1:C:521:VAL:HG23	1:C:556:VAL:HG13	2.03	0.40
1:A:112:ILE:HG22	1:A:125:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.96	0.40
1:A:152:GLN:HE21	1:A:152:GLN:CA	2.31	0.40
1:A:377:ASN:HD22	1:A:379:ILE:H	1.69	0.40
1:C:170:PRO:HG3	1:C:619:TYR:CG	2.56	0.40
1:C:442:ASN:HD21	1:C:471:SER:N	2.16	0.40
1:D:786:ILE:O	1:D:798:ASN:HA	2.21	0.40
1:B:159:ALA:HB1	1:B:160:PRO:HA	2.02	0.40
1:B:525:ARG:HD2	1:B:526:TYR:O	2.21	0.40
1:B:748:LYS:HA	1:B:748:LYS:HD2	1.91	0.40
1:A:546:MET:HE2	1:A:546:MET:HA	2.04	0.40
1:A:767:VAL:O	1:A:767:VAL:CG1	2.69	0.40
1:C:776:LEU:HD23	1:C:776:LEU:O	2.22	0.40
1:D:207:LYS:HA	1:D:208:HIS:HA	1.82	0.40
1:D:275:HIS:HB2	1:D:278:SER:HG	1.84	0.40
1:B:239:ASN:HD21	1:B:633:GLN:HE21	1.70	0.40
1:B:521:VAL:CG2	1:B:546:MET:CE	2.94	0.40
1:B:595:VAL:N	1:B:596:PRO:CD	2.84	0.40
1:C:129:VAL:HG11	1:C:141:ARG:HD3	2.04	0.40
1:C:740:GLN:HB3	1:C:742:ARG:NH1	2.35	0.40
1:D:421:LEU:HD11	1:D:520:PHE:CZ	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	720 (95%)	34 (4%)	2 (0%)	36	30
1	B	757/803 (94%)	719 (95%)	37 (5%)	1 (0%)	48	44
1	C	756/803 (94%)	693 (92%)	56 (7%)	7 (1%)	14	7
1	D	756/803 (94%)	685 (91%)	67 (9%)	4 (0%)	24	17
All	All	3025/3212 (94%)	2817 (93%)	194 (6%)	14 (0%)	24	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	VAL
1	A	110	GLY
1	C	236	ILE
1	C	332	TRP
1	C	422	LYS
1	D	422	LYS
1	D	91	SER
1	D	224	ILE
1	C	357	ILE
1	C	540	GLY
1	A	167	GLY
1	D	309	PRO
1	B	167	GLY
1	C	167	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/648 (94%)	563 (92%)	47 (8%)	12	5
1	B	612/648 (94%)	574 (94%)	38 (6%)	16	9
1	C	610/648 (94%)	564 (92%)	46 (8%)	12	6
1	D	611/648 (94%)	559 (92%)	52 (8%)	10	4
All	All	2443/2592 (94%)	2260 (92%)	183 (8%)	12	6

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	LYS
1	B	98	THR
1	B	129	VAL
1	B	137	LEU
1	B	147	GLN
1	B	172	ASN

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	225	ASP
1	B	285	GLN
1	B	317	VAL
1	B	358	LEU
1	B	375	VAL
1	B	377	ASN
1	B	391	ARG
1	B	393	VAL
1	B	400	GLU
1	B	416	THR
1	B	430	LEU
1	B	439	LEU
1	B	446	LEU
1	B	474	THR
1	B	582	VAL
1	B	610	TRP
1	B	625	VAL
1	B	672	LEU
1	B	682	ASP
1	B	688	GLU
1	B	702	LEU
1	B	705	VAL
1	B	709	VAL
1	B	739	ARG
1	B	748	LYS
1	B	750	LEU
1	B	758	VAL
1	B	759	THR
1	B	767	VAL
1	B	776	LEU
1	B	784	PHE
1	A	48	GLN
1	A	66	LYS
1	A	77	GLU
1	A	98	THR
1	A	107	LEU
1	A	129	VAL
1	A	137	LEU
1	A	147	GLN
1	A	152	GLN
1	A	172	ASN

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Mol	Chain	Res	Type
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	391	ARG
1	A	393	VAL
1	A	400	GLU
1	A	430	LEU
1	A	439	LEU
1	A	446	LEU
1	A	474	THR
1	A	483	LYS
1	A	503	THR
1	A	554	SER
1	A	596	PRO
1	A	610	TRP
1	A	625	VAL
1	A	637	THR
1	A	655	ARG
1	A	672	LEU
1	A	682	ASP
1	A	683	TYR
1	A	684	SER
1	A	702	LEU
1	A	705	VAL
1	A	709	VAL
1	A	716	THR
1	A	739	ARG
1	A	750	LEU
1	A	758	VAL
1	A	759	THR
1	A	764	ARG
1	A	767	VAL
1	A	776	LEU
1	C	62	SER
1	C	82	ILE
1	C	107	LEU
1	C	117	VAL
1	C	121	SER

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Mol	Chain	Res	Type
1	C	129	VAL
1	C	137	LEU
1	C	147	GLN
1	C	172	ASN
1	C	180	PHE
1	C	271	ILE
1	C	285	GLN
1	C	317	VAL
1	C	335	THR
1	C	345	VAL
1	C	355	VAL
1	C	368	THR
1	C	377	ASN
1	C	393	VAL
1	C	422	LYS
1	C	430	LEU
1	C	439	LEU
1	C	446	LEU
1	C	471	SER
1	C	474	THR
1	C	503	THR
1	C	610	TRP
1	C	611	THR
1	C	637	THR
1	C	672	LEU
1	C	678	ARG
1	C	681	LYS
1	C	682	ASP
1	C	684	SER
1	C	702	LEU
1	C	705	VAL
1	C	709	VAL
1	C	716	THR
1	C	736	GLN
1	C	748	LYS
1	C	750	LEU
1	C	759	THR
1	C	763	ARG
1	C	772	VAL
1	C	776	LEU
1	C	798	ASN
1	D	72	THR

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Mol	Chain	Res	Type
1	D	82	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
1	D	227	VAL
1	D	243	LEU
1	D	271	ILE
1	D	285	GLN
1	D	299	SER
1	D	301	TRP
1	D	312	GLU
1	D	317	VAL
1	D	358	LEU
1	D	359	THR
1	D	375	VAL
1	D	387	THR
1	D	393	VAL
1	D	400	GLU
1	D	407	SER
1	D	410	VAL
1	D	422	LYS
1	D	461	THR
1	D	474	THR
1	D	483	LYS
1	D	568	ILE
1	D	582	VAL
1	D	610	TRP
1	D	658	PHE
1	D	672	LEU
1	D	678	ARG
1	D	681	LYS
1	D	701	SER
1	D	702	LEU
1	D	705	VAL

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Mol	Chain	Res	Type
1	D	709	VAL
1	D	716	THR
1	D	748	LYS
1	D	750	LEU
1	D	758	VAL
1	D	759	THR
1	D	767	VAL
1	D	771	SER
1	D	776	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	118	HIS
1	B	172	ASN
1	B	229	GLN
1	B	246	HIS
1	B	262	ASN
1	B	285	GLN
1	B	292	ASN
1	B	366	GLN
1	B	377	ASN
1	B	442	ASN
1	B	482	GLN
1	B	500	ASN
1	B	633	GLN
1	B	676	HIS
1	B	718	ASN
1	B	736	GLN
1	B	740	GLN
1	B	798	ASN
1	A	122	GLN
1	A	152	GLN
1	A	172	ASN
1	A	229	GLN
1	A	246	HIS
1	A	262	ASN
1	A	377	ASN
1	A	442	ASN
1	A	676	HIS
1	A	718	ASN

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Mol	Chain	Res	Type
1	A	740	GLN
1	C	48	GLN
1	C	118	HIS
1	C	152	GLN
1	C	172	ASN
1	C	246	HIS
1	C	262	ASN
1	C	263	HIS
1	C	272	ASN
1	C	377	ASN
1	C	442	ASN
1	C	482	GLN
1	C	622	ASN
1	C	676	HIS
1	C	736	GLN
1	C	740	GLN
1	D	48	GLN
1	D	147	GLN
1	D	150	HIS
1	D	172	ASN
1	D	229	GLN
1	D	246	HIS
1	D	272	ASN
1	D	275	HIS
1	D	294	GLN
1	D	377	ASN
1	D	423	HIS
1	D	442	ASN
1	D	622	ASN
1	D	671	ASN
1	D	676	HIS
1	D	740	GLN
1	D	798	ASN

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 ⓘ

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	3.23	4 (23%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.97	2 (11%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	1.22	1 (5%)
3	BMA	F	3	3	11,11,12	1.13	2 (18%)	15,15,17	1.29	2 (13%)
3	MAN	F	4	3	11,11,12	0.53	0	15,15,17	1.55	2 (13%)
3	MAN	F	5	3	11,11,12	0.65	0	15,15,17	1.49	2 (13%)
4	MAN	G	1	4	12,12,12	0.34	0	17,17,17	0.49	0
4	BMA	G	2	4	11,11,12	1.03	1 (9%)	15,15,17	1.78	4 (26%)
2	NAG	H	1	1,2	14,14,15	0.40	0	17,19,21	1.11	3 (17%)
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
5	NAG	I	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	I	2	5	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
5	NAG	I	3	5	14,14,15	0.34	0	17,19,21	1.78	3 (17%)
6	NAG	J	1	1,6	14,14,15	0.47	0	17,19,21	1.13	1 (5%)
6	NAG	J	2	6	14,14,15	0.43	0	17,19,21	1.16	3 (17%)
6	AH2	J	3	6	11,11,11	0.69	0	15,15,15	1.74	6 (40%)
6	BMA	J	4	6	11,11,12	0.47	0	15,15,17	1.29	2 (13%)
6	MAN	J	5	6	11,11,12	0.82	0	15,15,17	1.08	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.43	0	17,19,21	0.70	0
7	NAG	K	2	7	14,14,15	0.37	0	17,19,21	1.40	1 (5%)
7	MAN	K	3	7	11,11,12	0.86	1 (9%)	15,15,17	1.37	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.75	1 (7%)	17,19,21	2.51	4 (23%)
2	NAG	L	2	2	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
7	NAG	M	1	7,1	14,14,15	0.30	0	17,19,21	0.64	0
7	NAG	M	2	7	14,14,15	0.48	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	M	3	7	11,11,12	1.04	1 (9%)	15,15,17	1.35	2 (13%)
7	NAG	N	1	7,1	14,14,15	0.29	0	17,19,21	0.94	1 (5%)
7	NAG	N	2	7	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
7	MAN	N	3	7	11,11,12	0.95	0	15,15,17	1.19	3 (20%)
2	NAG	O	1	1,2	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
2	NAG	O	2	2	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
2	NAG	P	1	2	14,14,15	0.40	0	17,19,21	1.08	0
2	NAG	P	2	2	14,14,15	0.42	0	17,19,21	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
4	MAN	G	1	4	-	0/2/22/22	0/1/1/1
4	BMA	G	2	4	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	3	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	AH2	J	3	6	-	0/2/19/19	0/1/1/1
6	BMA	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	MAN	K	3	7	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	2.54	1.55	1.52
4	G	2	BMA	C2-C3	-2.42	1.48	1.52
7	K	3	MAN	O5-C5	2.33	1.48	1.43
3	F	3	BMA	C4-C5	-2.28	1.48	1.53
2	L	1	NAG	O4-C4	2.23	1.48	1.43
2	E	1	NAG	C1-C2	2.08	1.55	1.52
7	M	3	MAN	C4-C5	2.06	1.57	1.53
3	F	3	BMA	O5-C5	-2.02	1.39	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O4-C4-C5	9.93	133.79	109.32
2	L	1	NAG	O4-C4-C3	7.77	128.70	110.38
2	E	1	NAG	O5-C1-C2	-5.88	102.20	111.29
7	K	2	NAG	C2-N2-C7	5.29	129.98	122.90
3	F	4	MAN	C1-O5-C5	4.97	118.85	112.19
5	I	3	NAG	C1-C2-N2	4.80	117.99	110.43
4	G	2	BMA	C3-C4-C5	4.68	118.72	110.23
2	E	1	NAG	C1-O5-C5	4.47	118.17	112.19
2	L	1	NAG	C2-N2-C7	4.31	128.67	122.90
3	F	5	MAN	C1-O5-C5	3.99	117.53	112.19
5	I	1	NAG	O4-C4-C5	3.80	118.68	109.32
5	I	1	NAG	C1-O5-C5	3.69	117.13	112.19
2	E	1	NAG	C1-C2-N2	3.58	116.07	110.43
7	K	3	MAN	C1-O5-C5	3.46	116.82	112.19
6	J	4	BMA	C1-C2-C3	-3.34	104.78	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	L	1	NAG	O4-C4-C5	3.18	117.15	109.32
3	F	2	NAG	O5-C1-C2	-3.15	106.42	111.29
6	J	5	MAN	C1-O5-C5	3.15	116.40	112.19
7	M	3	MAN	C1-C2-C3	3.12	114.19	109.64
2	H	2	NAG	O3-C3-C2	-3.12	102.93	109.40
2	O	2	NAG	C4-C3-C2	3.08	115.53	111.02
3	F	5	MAN	O2-C2-C3	3.03	116.42	110.15
5	I	3	NAG	O5-C1-C2	-3.01	106.63	111.29
6	J	3	AH2	O2-C2-C3	2.96	116.27	110.15
4	G	2	BMA	O4-C4-C3	-2.89	103.57	110.38
7	K	3	MAN	C1-C2-C3	2.87	113.82	109.64
6	J	4	BMA	O2-C2-C3	2.82	115.99	110.15
3	F	3	BMA	C1-C2-C3	2.77	113.68	109.64
2	L	2	NAG	C4-C3-C2	2.77	115.07	111.02
2	H	2	NAG	C2-N2-C7	2.71	126.53	122.90
5	I	1	NAG	C1-C2-N2	2.70	114.69	110.43
2	O	2	NAG	C2-N2-C7	2.67	126.48	122.90
6	J	2	NAG	C4-C3-C2	-2.66	107.12	111.02
3	F	3	BMA	O5-C1-C2	2.66	117.13	110.79
5	I	3	NAG	C1-O5-C5	2.57	115.63	112.19
2	L	1	NAG	C1-O5-C5	2.47	115.49	112.19
2	E	2	NAG	C4-C3-C2	2.44	114.60	111.02
3	F	4	MAN	O2-C2-C3	2.44	115.21	110.15
6	J	2	NAG	O5-C1-C2	-2.43	107.54	111.29
2	L	2	NAG	O5-C1-C2	-2.39	107.59	111.29
4	G	2	BMA	C1-O5-C5	-2.38	109.00	112.19
2	H	1	NAG	C2-N2-C7	2.38	126.08	122.90
6	J	3	AH2	O5-C1-C2	2.36	116.41	110.79
6	J	3	AH2	C3-C4-C5	-2.36	105.96	110.23
7	N	3	MAN	C1-C2-C3	2.35	113.06	109.64
2	H	1	NAG	O4-C4-C3	-2.34	104.86	110.38
3	F	1	NAG	O5-C5-C4	-2.33	105.16	110.83
7	M	3	MAN	C3-C4-C5	2.33	114.46	110.23
6	J	1	NAG	C1-C2-N2	-2.30	106.81	110.43
6	J	3	AH2	C1-C2-C3	2.27	112.96	109.64
6	J	3	AH2	O3-C3-C2	2.21	114.56	110.05
7	N	3	MAN	C1-O5-C5	2.17	115.10	112.19
7	N	1	NAG	O3-C3-C2	2.15	113.86	109.40
5	I	2	NAG	C2-N2-C7	2.14	125.77	122.90
6	J	2	NAG	C1-C2-N2	2.12	113.77	110.43
3	F	1	NAG	C1-O5-C5	-2.09	109.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	2	NAG	C1-C2-N2	2.07	113.70	110.43
7	N	3	MAN	C3-C4-C5	2.07	113.98	110.23
4	G	2	BMA	O2-C2-C1	2.06	113.94	109.22
2	E	2	NAG	O5-C1-C2	-2.06	108.11	111.29
2	O	1	NAG	C2-N2-C7	2.05	125.65	122.90
6	J	3	AH2	C1-O5-C5	2.05	114.93	112.19
7	M	2	NAG	O3-C3-C2	-2.04	105.16	109.40
2	H	1	NAG	O5-C1-C2	2.01	114.40	111.29

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
5	I	3	NAG	C8-C7-N2-C2
5	I	3	NAG	O7-C7-N2-C2
4	G	2	BMA	C4-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
5	I	3	NAG	C4-C5-C6-O6
5	I	3	NAG	O5-C5-C6-O6
7	M	3	MAN	O5-C5-C6-O6
4	G	2	BMA	O5-C5-C6-O6
7	K	3	MAN	O5-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	N	3	MAN	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	N	3	MAN	C4-C5-C6-O6
7	M	3	MAN	C4-C5-C6-O6
2	P	1	NAG	C8-C7-N2-C2
2	P	2	NAG	C8-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
7	K	3	MAN	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6

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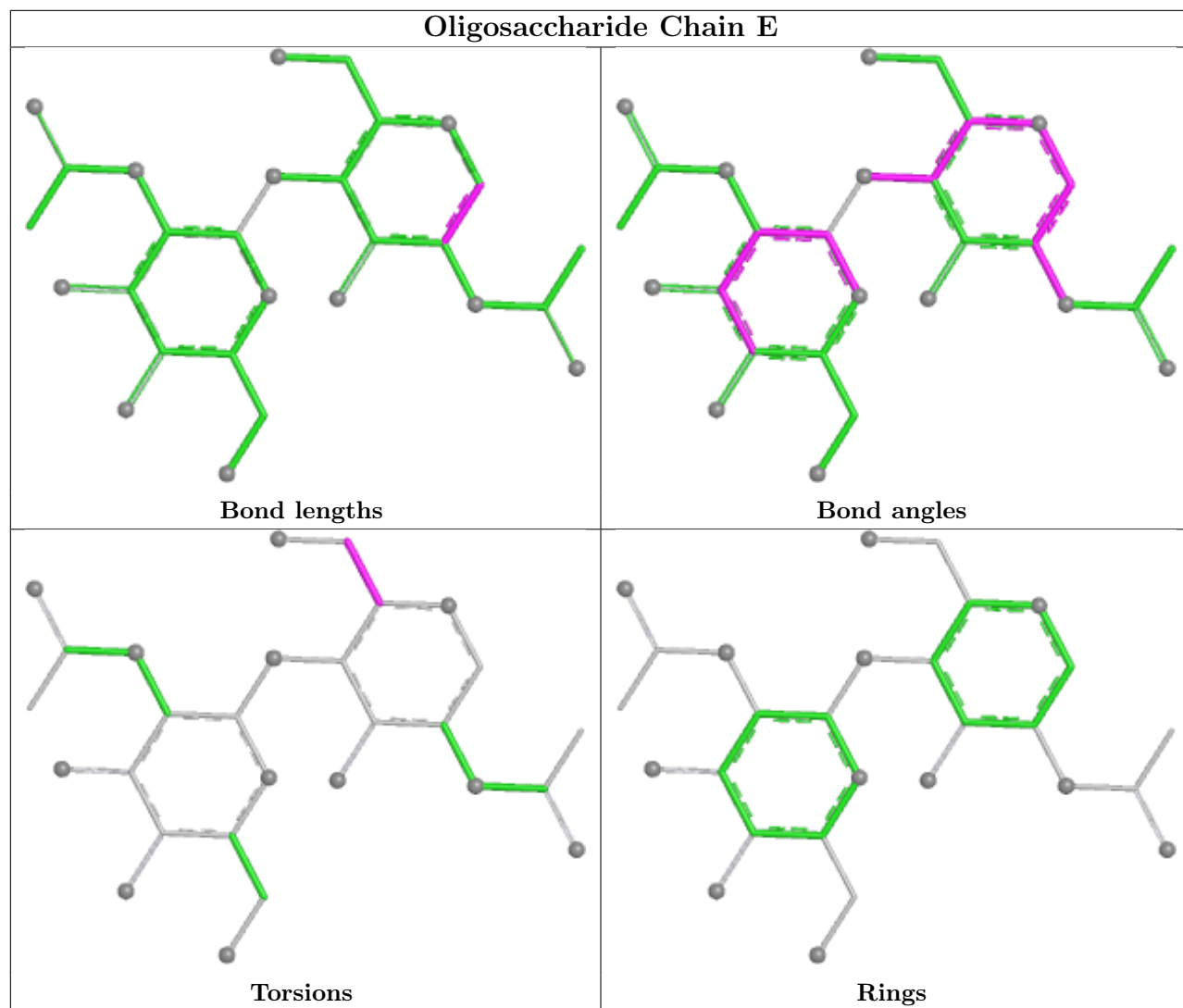
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C8-C7-N2-C2
6	J	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
2	P	2	NAG	C1-C2-N2-C7
2	L	1	NAG	O7-C7-N2-C2

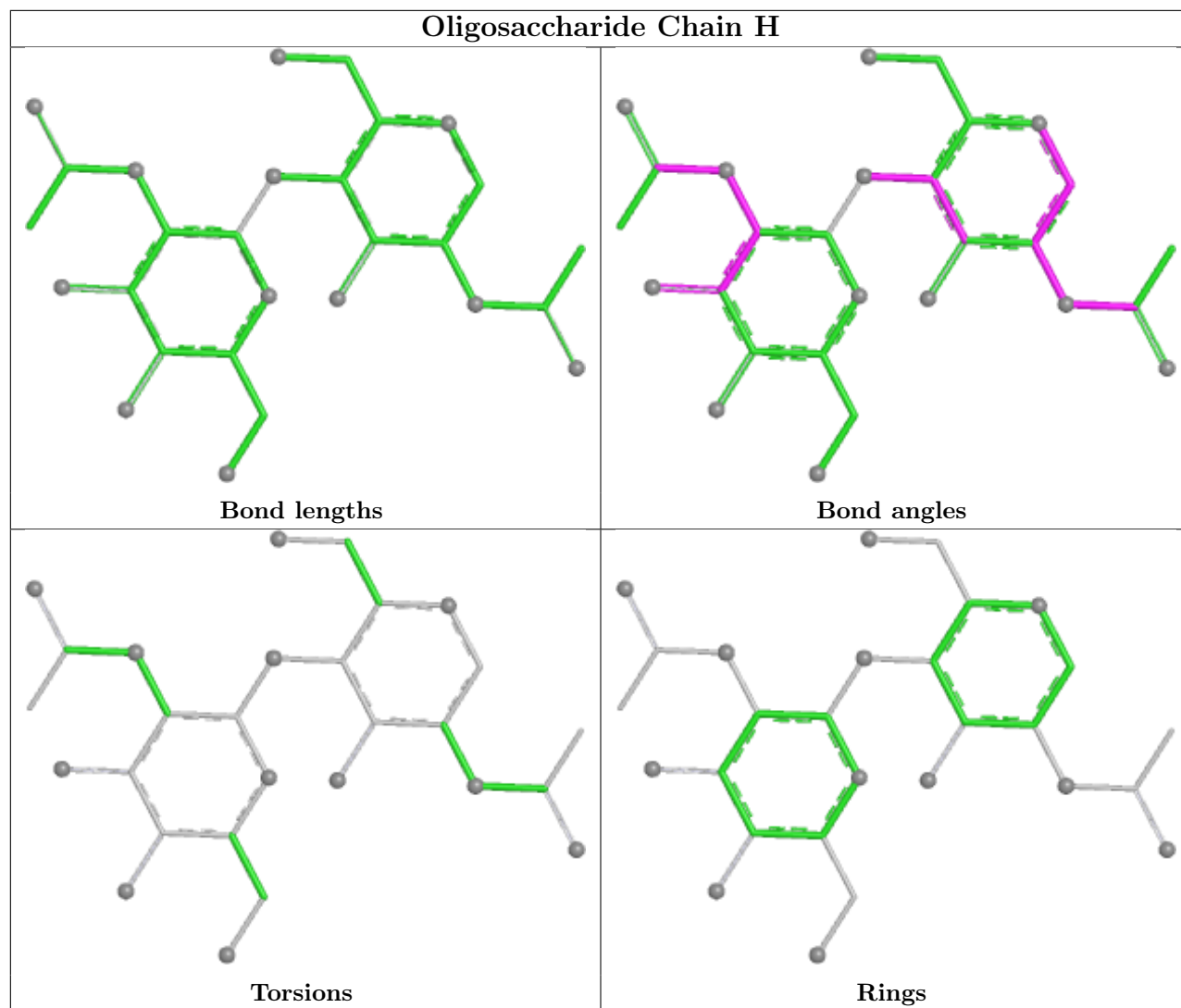
There are no ring outliers.

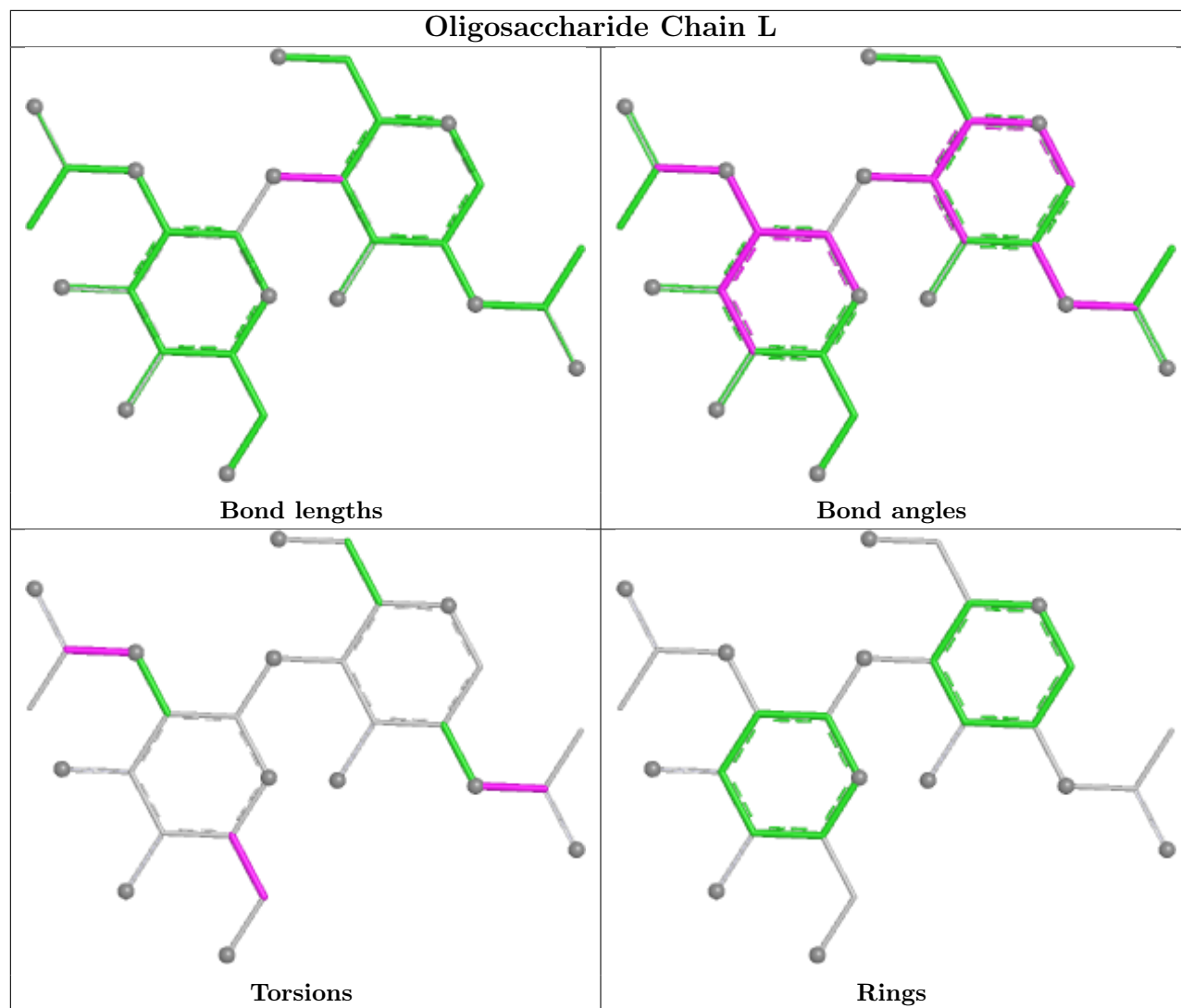
19 monomers are involved in 69 short contacts:

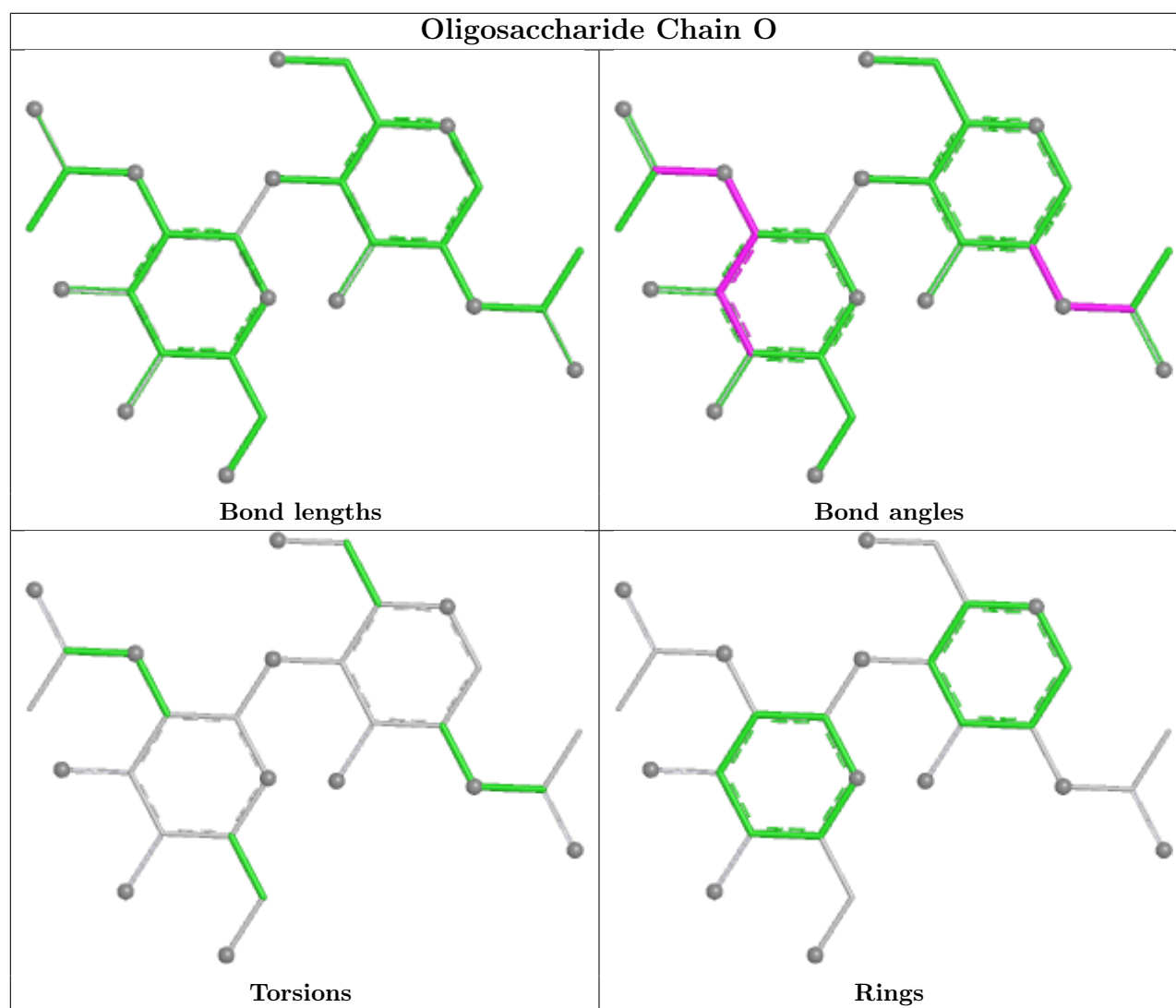
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	10	0
4	G	1	MAN	18	0
6	J	1	NAG	3	0
2	E	2	NAG	2	0
7	K	3	MAN	2	0
2	P	2	NAG	5	0
3	F	5	MAN	1	0
5	I	3	NAG	2	0
2	O	2	NAG	5	0
5	I	2	NAG	2	0
3	F	2	NAG	2	0
2	P	1	NAG	11	0
2	E	1	NAG	2	0
6	J	3	AH2	2	0
5	I	1	NAG	2	0
3	F	1	NAG	2	0
2	O	1	NAG	5	0
3	F	3	BMA	3	0
4	G	2	BMA	10	0

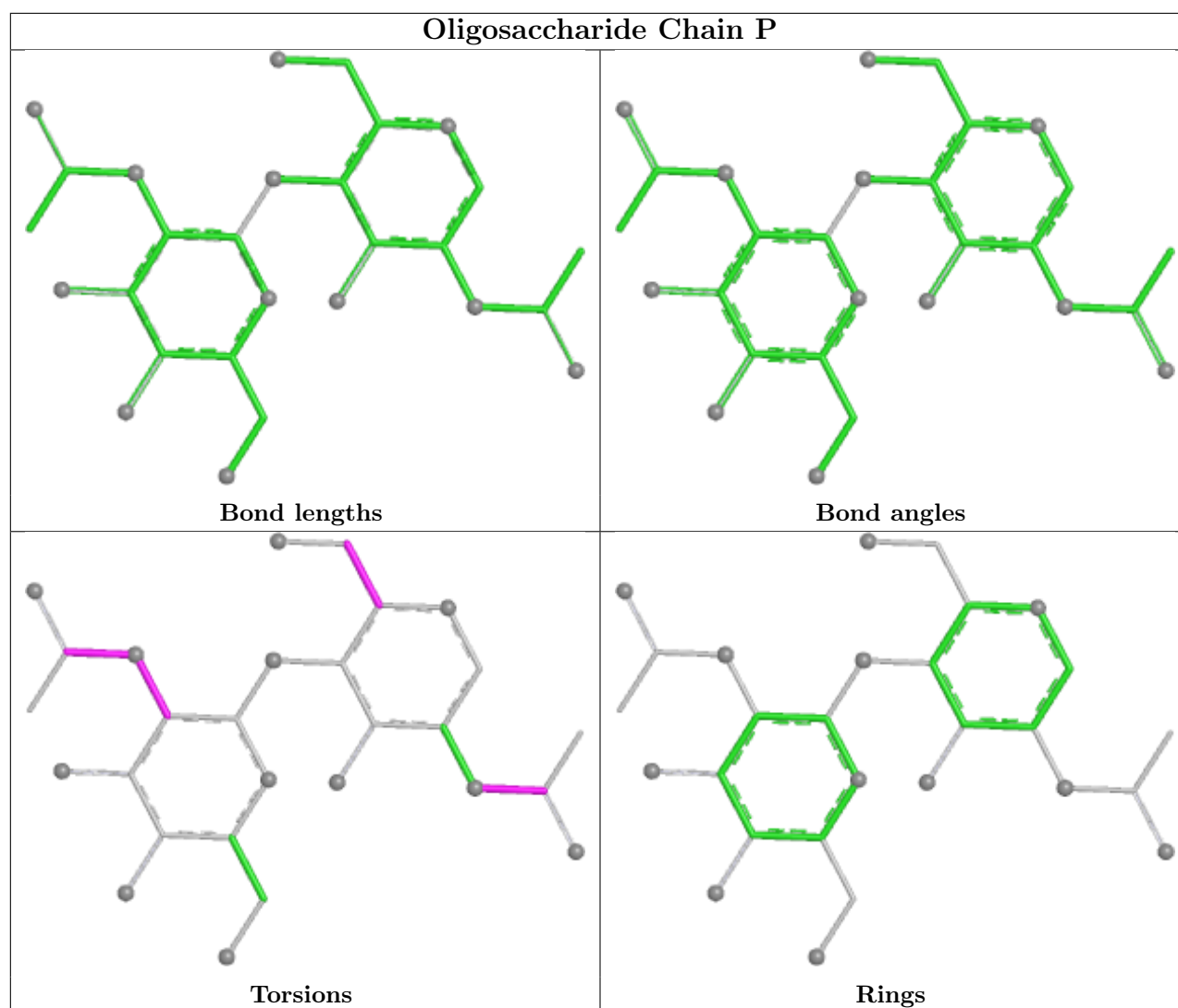
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

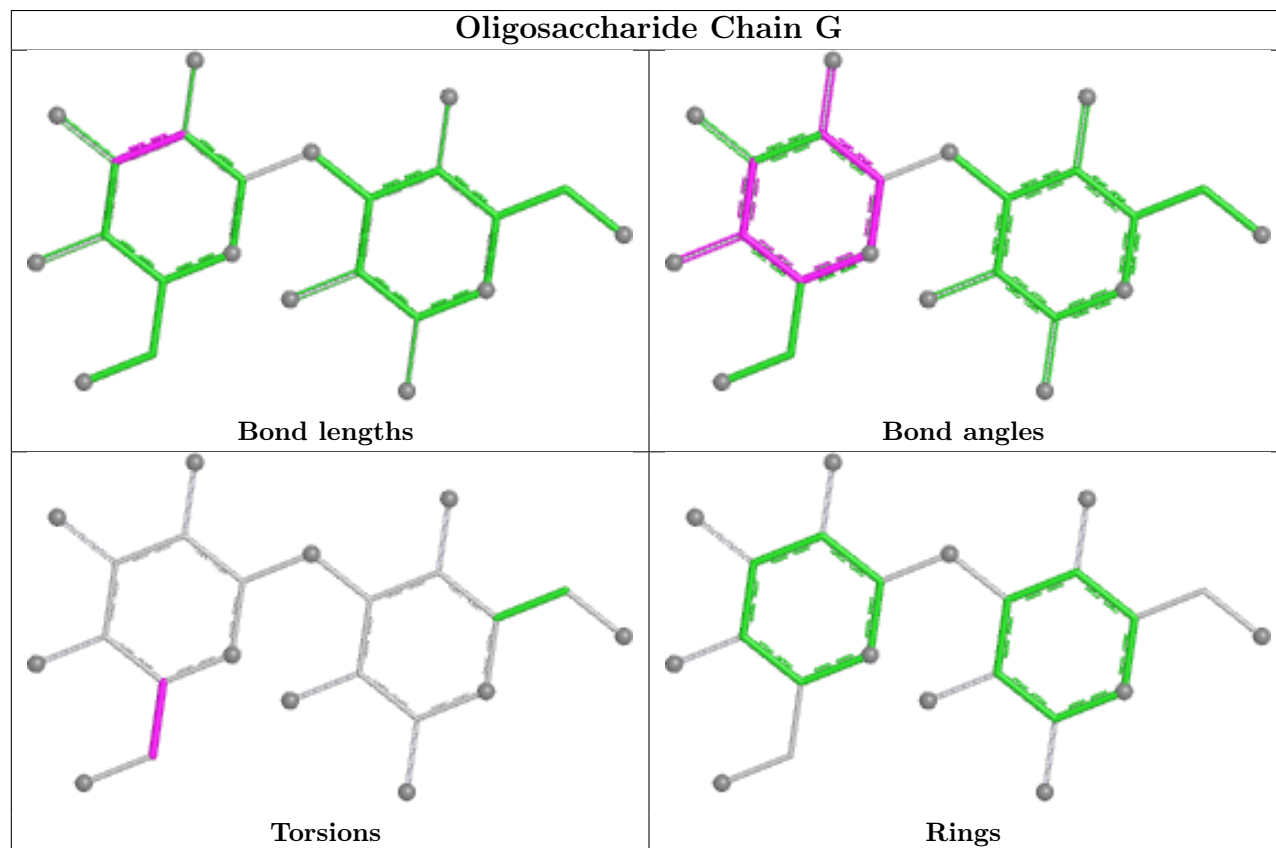
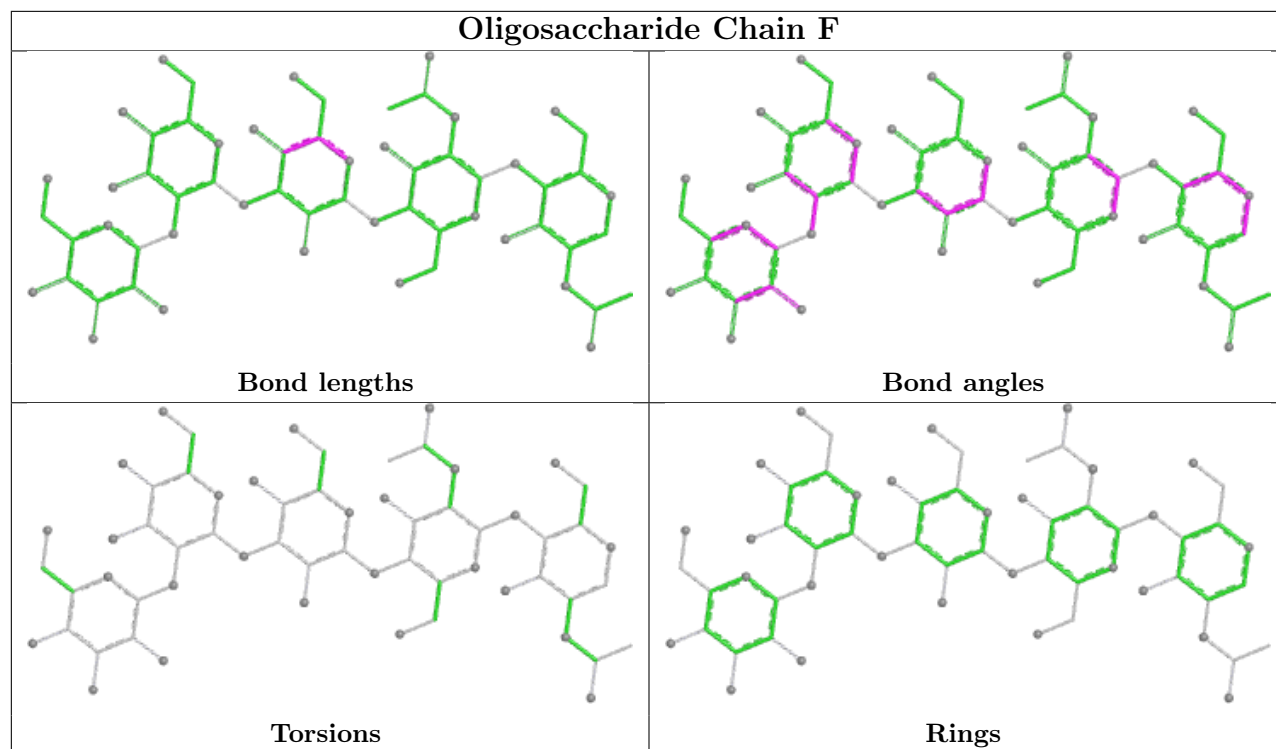


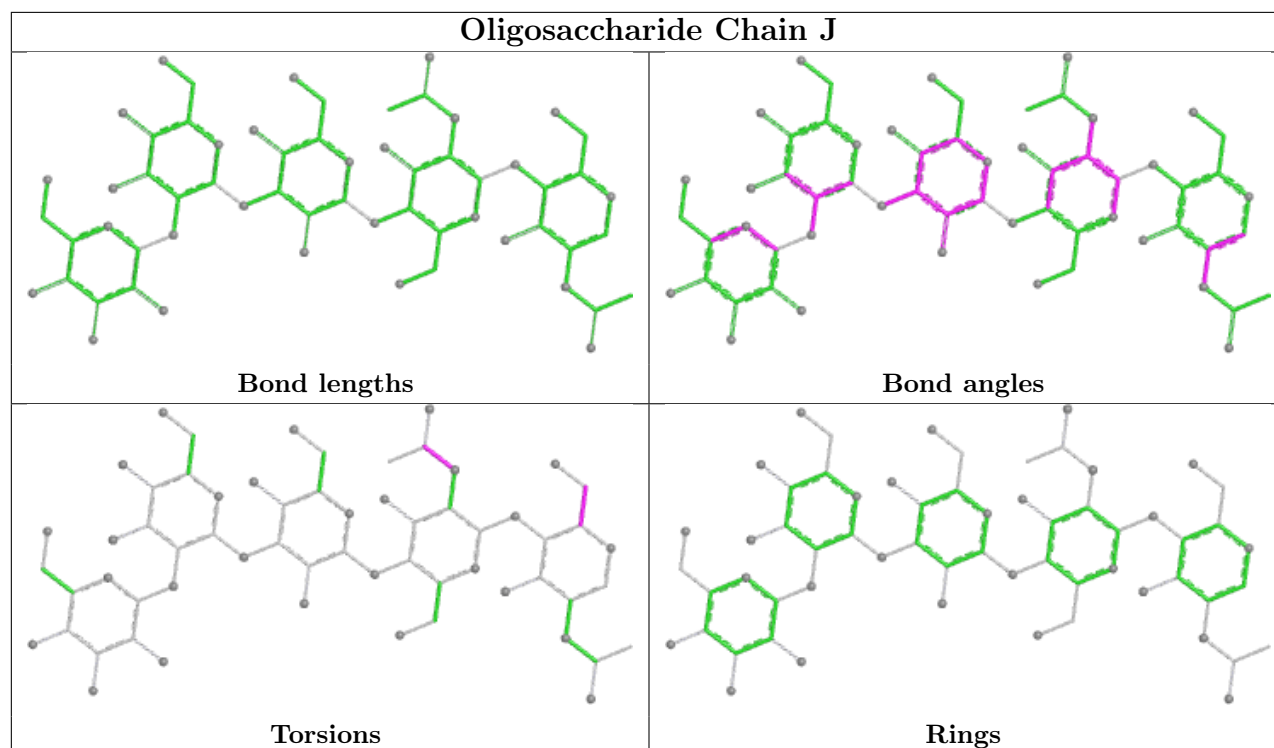
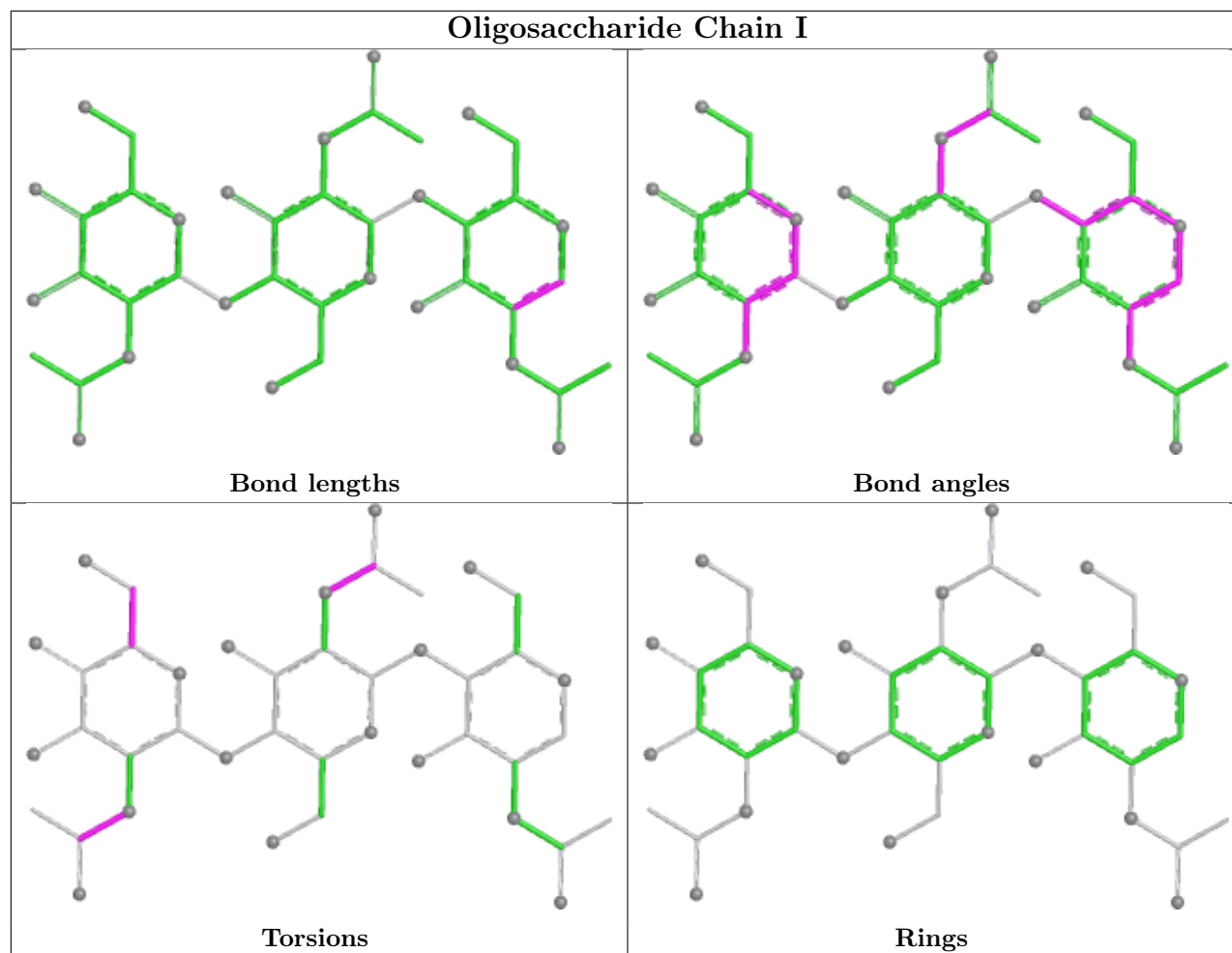


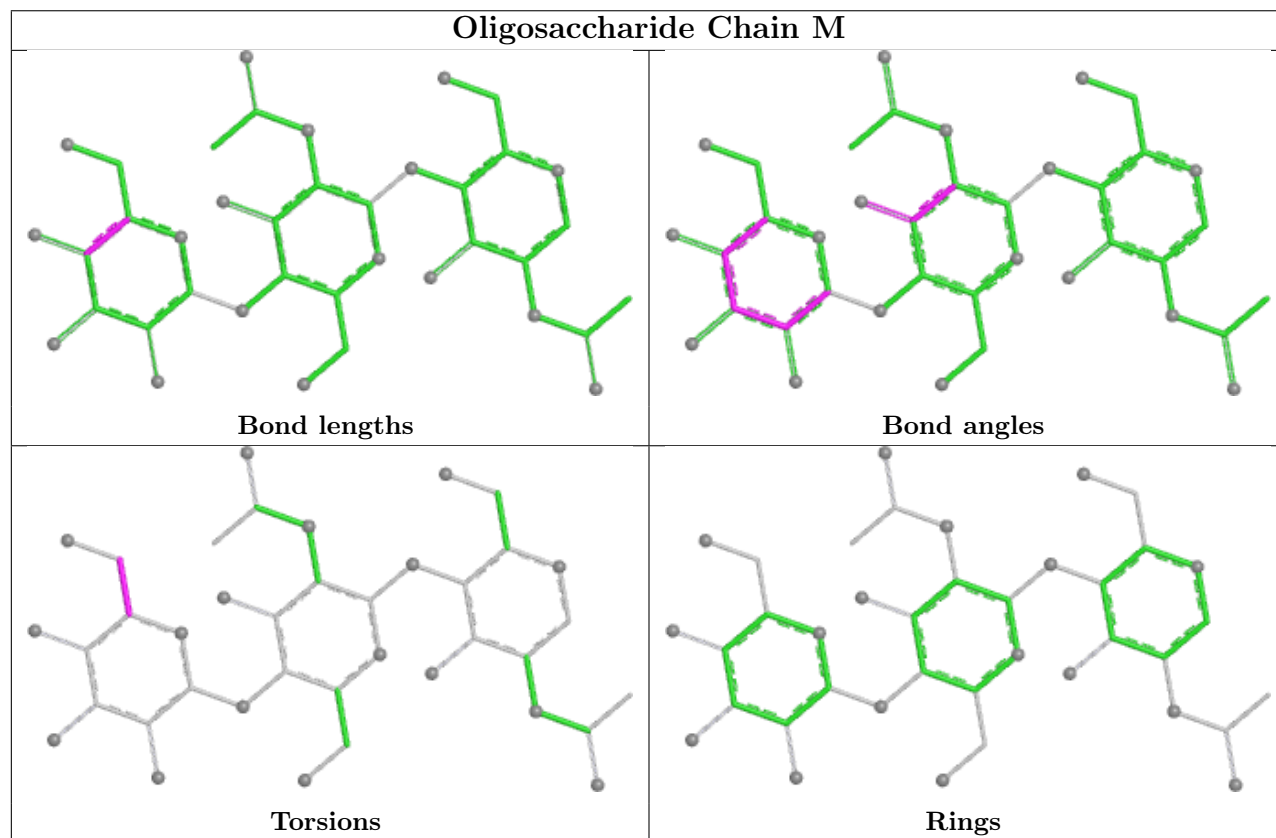
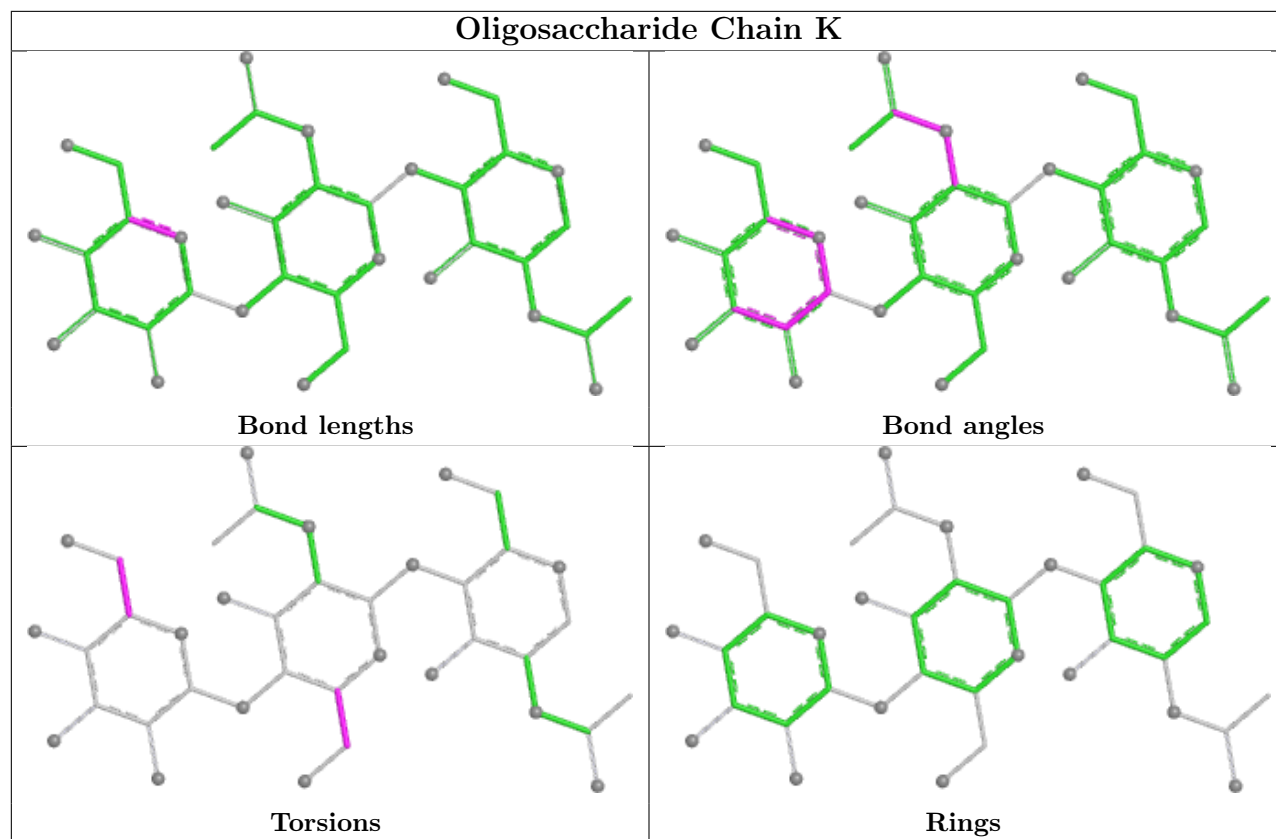


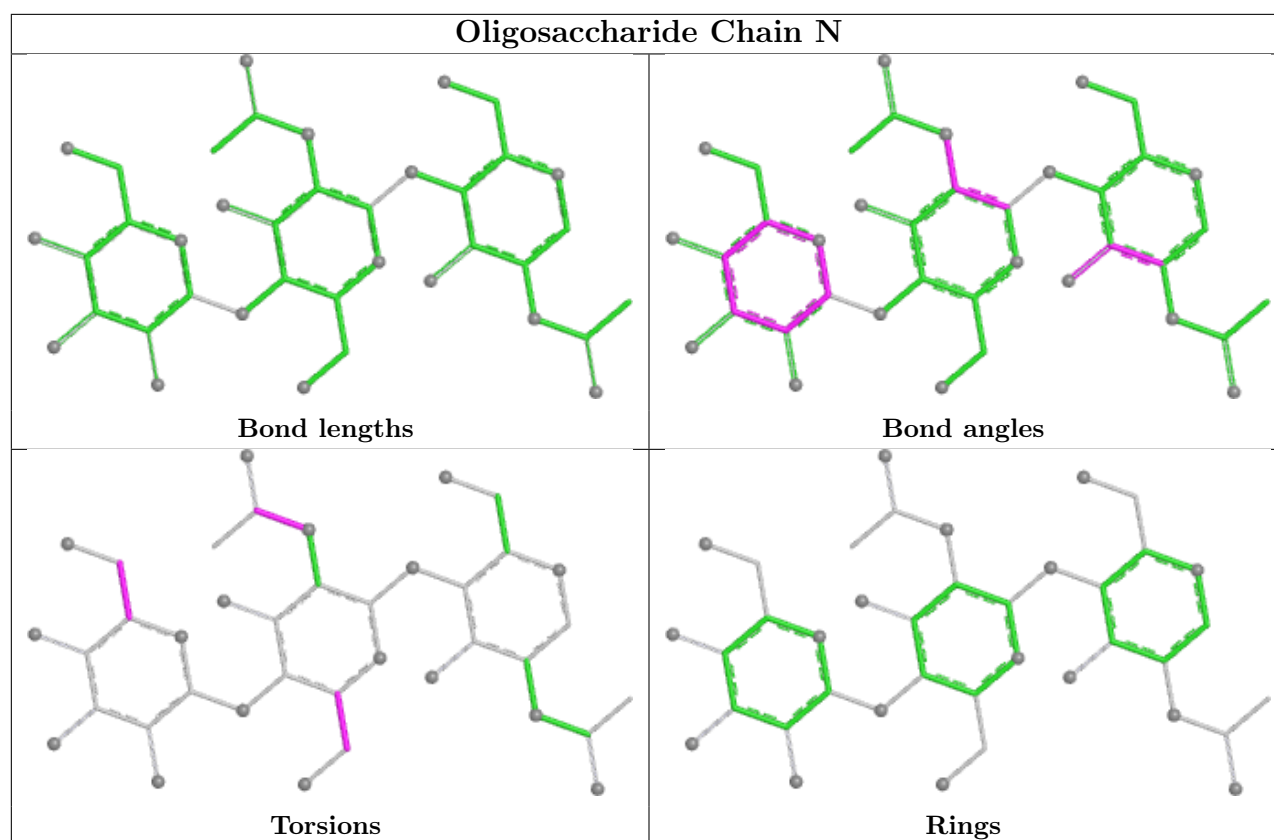












5.6 Ligand geometry [i](#)

50 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	$\# Z > 2$
11	NAG	D	909	1	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
11	NAG	C	901	-	14,14,15	0.41	0	17,19,21	1.06	0
8	BKR	A	911	-	65,65,65	0.69	0	101,101,101	0.95	7 (6%)
9	XLS	A	912	-	8,8,9	0.73	0	10,10,11	2.81	4 (40%)
10	MAN	D	904	-	11,11,12	0.61	0	15,15,17	1.47	3 (20%)
11	NAG	C	902	-	14,14,15	0.43	0	17,19,21	0.72	0
11	NAG	C	909	1	14,14,15	0.46	0	17,19,21	0.97	1 (5%)
10	MAN	C	904	-	11,11,12	0.92	0	15,15,17	2.01	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	A	907	-	12,12,12	0.70	0	17,17,17	1.35	3 (17%)
11	NAG	A	905	1	14,14,15	0.40	0	17,19,21	1.35	4 (23%)
11	NAG	D	907	1	14,14,15	0.39	0	17,19,21	1.66	2 (11%)
10	MAN	B	903	-	11,11,12	0.86	1 (9%)	15,15,17	0.99	1 (6%)
11	NAG	D	908	1	14,14,15	0.83	1 (7%)	17,19,21	2.04	2 (11%)
11	NAG	B	914	1	14,14,15	0.38	0	17,19,21	1.26	1 (5%)
10	MAN	B	912	-	11,11,12	1.26	1 (9%)	15,15,17	1.66	2 (13%)
11	NAG	B	911	-	15,15,15	0.21	0	21,21,21	0.42	0
8	BKR	B	901	-	65,65,65	0.69	0	101,101,101	0.95	7 (6%)
10	MAN	D	905	-	11,11,12	0.85	1 (9%)	15,15,17	0.90	1 (6%)
11	NAG	B	913	1	14,14,15	0.43	0	17,19,21	1.21	1 (5%)
11	NAG	A	906	1	14,14,15	0.47	0	17,19,21	1.15	1 (5%)
11	NAG	D	906	1	14,14,15	0.50	0	17,19,21	1.14	3 (17%)
11	NAG	C	908	1	14,14,15	0.50	0	17,19,21	0.88	0
11	NAG	A	910	1	14,14,15	0.44	0	17,19,21	1.46	3 (17%)
10	MAN	A	908	-	11,11,12	0.58	0	15,15,17	1.06	1 (6%)
10	MAN	D	902	-	11,11,12	1.11	1 (9%)	15,15,17	2.25	2 (13%)
10	MAN	B	904	-	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
11	NAG	A	909	1	14,14,15	0.39	0	17,19,21	0.95	2 (11%)
10	MAN	A	904	-	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
10	MAN	C	907	-	11,11,12	0.58	0	15,15,17	1.07	2 (13%)
10	MAN	D	903	-	11,11,12	0.52	0	15,15,17	1.73	3 (20%)
10	MAN	C	903	-	11,11,12	0.70	0	15,15,17	1.37	2 (13%)
8	BKR	D	910	-	65,65,65	0.52	0	101,101,101	0.90	5 (4%)
9	XLS	B	902	-	8,8,9	0.72	0	10,10,11	2.82	4 (40%)
10	MAN	A	901	-	11,11,12	0.45	0	15,15,17	1.39	2 (13%)
11	NAG	B	916	-	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	MAN	B	905	-	11,11,12	0.81	0	15,15,17	1.13	2 (13%)
10	MAN	A	903	-	11,11,12	0.77	0	15,15,17	1.19	1 (6%)
10	MAN	B	907	-	11,11,12	0.73	1 (9%)	15,15,17	1.02	2 (13%)
10	MAN	C	906	-	11,11,12	0.58	0	15,15,17	1.47	3 (20%)
11	NAG	C	910	1	14,14,15	0.48	0	17,19,21	0.81	0
10	MAN	C	905	-	11,11,12	0.43	0	15,15,17	1.09	1 (6%)
11	NAG	B	909	1	14,14,15	0.43	0	17,19,21	1.02	0
11	NAG	C	911	1	14,14,15	0.41	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	B	910	-	12,12,12	0.46	0	17,17,17	1.08	1 (5%)
10	MAN	A	902	-	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
11	NAG	B	915	-	15,15,15	0.17	0	21,21,21	0.60	0
12	BMA	D	901	-	11,11,12	0.79	0	15,15,17	0.93	1 (6%)
11	NAG	B	908	1	14,14,15	0.41	0	17,19,21	1.04	3 (17%)
10	MAN	B	906	-	11,11,12	0.92	1 (9%)	15,15,17	1.48	3 (20%)
8	BKR	C	912	-	65,65,65	0.55	0	101,101,101	0.85	3 (2%)

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
11	NAG	D	909	1	-	3/6/23/26	0/1/1/1
11	NAG	C	901	-	-	3/6/23/26	0/1/1/1
8	BKR	A	911	-	-	5/37/123/123	0/7/7/7
9	XLS	A	912	-	-	7/10/10/12	-
10	MAN	D	904	-	-	2/2/19/22	0/1/1/1
11	NAG	C	902	-	-	3/6/23/26	0/1/1/1
11	NAG	C	909	1	-	2/6/23/26	0/1/1/1
10	MAN	C	904	-	-	2/2/19/22	0/1/1/1
10	MAN	A	907	-	-	2/2/22/22	0/1/1/1
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1
11	NAG	D	907	1	-	4/6/23/26	0/1/1/1
10	MAN	B	903	-	-	2/2/19/22	0/1/1/1
11	NAG	D	908	1	-	4/6/23/26	0/1/1/1
11	NAG	B	914	1	-	2/6/23/26	0/1/1/1
10	MAN	B	912	-	-	0/2/19/22	1/1/1/1
11	NAG	B	911	-	-	4/6/26/26	0/1/1/1
8	BKR	B	901	-	-	5/37/123/123	0/7/7/7
10	MAN	D	905	-	-	2/2/19/22	0/1/1/1
11	NAG	B	913	1	-	0/6/23/26	0/1/1/1
11	NAG	A	906	1	-	0/6/23/26	0/1/1/1
11	NAG	D	906	1	-	2/6/23/26	0/1/1/1
11	NAG	C	908	1	-	0/6/23/26	0/1/1/1
11	NAG	A	910	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	A	908	-	-	0/2/19/22	0/1/1/1
10	MAN	D	902	-	-	2/2/19/22	0/1/1/1
10	MAN	B	904	-	-	2/2/19/22	0/1/1/1
11	NAG	A	909	1	-	0/6/23/26	0/1/1/1
10	MAN	A	904	-	-	2/2/19/22	0/1/1/1
10	MAN	C	907	-	-	1/2/19/22	0/1/1/1
10	MAN	D	903	-	-	2/2/19/22	0/1/1/1
10	MAN	C	903	-	-	0/2/19/22	1/1/1/1
8	BKR	D	910	-	-	8/37/123/123	0/7/7/7
9	XLS	B	902	-	-	7/10/10/12	-
10	MAN	A	901	-	-	0/2/19/22	0/1/1/1
11	NAG	B	916	-	-	0/6/23/26	0/1/1/1
10	MAN	B	905	-	-	0/2/19/22	0/1/1/1
10	MAN	A	903	-	-	0/2/19/22	0/1/1/1
10	MAN	B	907	-	-	2/2/19/22	0/1/1/1
10	MAN	C	906	-	-	1/2/19/22	0/1/1/1
11	NAG	C	910	1	-	0/6/23/26	0/1/1/1
10	MAN	C	905	-	-	0/2/19/22	0/1/1/1
11	NAG	B	909	1	-	2/6/23/26	0/1/1/1
11	NAG	C	911	1	-	4/6/23/26	0/1/1/1
10	MAN	B	910	-	-	2/2/22/22	0/1/1/1
10	MAN	A	902	-	-	0/2/19/22	0/1/1/1
11	NAG	B	915	-	-	0/6/26/26	0/1/1/1
12	BMA	D	901	-	-	0/2/19/22	0/1/1/1
11	NAG	B	908	1	-	2/6/23/26	0/1/1/1
10	MAN	B	906	-	-	2/2/19/22	0/1/1/1
8	BKR	C	912	-	-	7/37/123/123	0/7/7/7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	912	MAN	O5-C5	3.30	1.49	1.43
11	D	908	NAG	O5-C1	-2.57	1.39	1.43
10	D	902	MAN	O5-C5	2.53	1.48	1.43
10	B	903	MAN	O5-C5	2.43	1.48	1.43
10	B	906	MAN	C2-C3	-2.39	1.48	1.52
10	D	905	MAN	C2-C3	2.16	1.55	1.52
10	B	907	MAN	C2-C3	-2.07	1.49	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	902	MAN	C1-O5-C5	7.43	122.14	112.19
11	D	908	NAG	O5-C1-C2	-6.89	100.62	111.29
9	B	902	XLS	C1-C2-C3	5.98	119.44	112.11
9	A	912	XLS	C1-C2-C3	5.98	119.43	112.11
11	D	907	NAG	O5-C1-C2	-5.66	102.54	111.29
10	B	912	MAN	C1-O5-C5	5.30	119.28	112.19
9	B	902	XLS	O2-C2-C3	-5.01	101.48	109.77
9	A	912	XLS	O2-C2-C3	-4.99	101.51	109.77
10	D	903	MAN	C1-O5-C5	4.80	118.62	112.19
10	C	904	MAN	C3-C4-C5	4.46	118.33	110.23
11	A	910	NAG	O5-C1-C2	-4.42	104.46	111.29
10	C	904	MAN	C2-C3-C4	4.18	118.21	110.86
11	B	914	NAG	C1-C2-N2	3.96	116.68	110.43
11	B	913	NAG	C1-O5-C5	3.89	117.40	112.19
10	C	906	MAN	C3-C4-C5	3.76	117.05	110.23
10	B	910	MAN	O2-C2-C3	3.70	119.10	110.38
10	A	903	MAN	C1-O5-C5	3.50	116.88	112.19
10	B	906	MAN	C1-C2-C3	3.47	114.70	109.64
11	D	908	NAG	C1-O5-C5	-3.39	107.65	112.19
11	C	911	NAG	C2-N2-C7	3.28	127.30	122.90
11	D	906	NAG	C1-C2-N2	3.27	115.58	110.43
10	A	901	MAN	C1-O5-C5	3.26	116.56	112.19
11	D	907	NAG	C1-C2-N2	3.25	115.56	110.43
10	A	904	MAN	C1-O5-C5	3.25	116.54	112.19
8	A	911	BKR	C26-O11-C27	3.23	122.40	116.58
10	C	905	MAN	C1-C2-C3	3.23	114.34	109.64
11	D	909	NAG	C1-O5-C5	3.22	116.50	112.19
10	C	903	MAN	O2-C2-C3	3.22	116.82	110.15
8	B	901	BKR	C26-O11-C27	3.21	122.35	116.58
8	D	910	BKR	O9-C21-C24	-3.19	106.33	111.48
10	C	903	MAN	O3-C3-C2	3.14	116.45	110.05
10	A	902	MAN	C1-O5-C5	3.07	116.30	112.19
10	B	903	MAN	C1-O5-C5	3.07	116.30	112.19
11	C	909	NAG	O5-C1-C2	2.90	115.77	111.29
11	A	905	NAG	C1-C2-N2	2.89	114.99	110.43
10	D	904	MAN	C2-C3-C4	2.89	115.95	110.86
11	A	906	NAG	C2-N2-C7	2.88	126.75	122.90
10	D	904	MAN	C3-C4-C5	2.79	115.28	110.23
10	D	902	MAN	C3-C4-C5	2.74	115.20	110.23
10	D	903	MAN	O5-C1-C2	2.69	117.21	110.79
10	D	903	MAN	C1-C2-C3	2.65	113.50	109.64
11	A	909	NAG	C1-O5-C5	2.62	115.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	902	XLS	C4-C3-C2	2.61	116.50	112.48
9	A	912	XLS	C4-C3-C2	2.61	116.50	112.48
10	A	901	MAN	C1-C2-C3	2.60	113.43	109.64
8	D	910	BKR	C1-C2-C10	2.59	122.08	118.19
10	A	907	MAN	O1-C1-C2	-2.55	101.58	108.98
8	A	911	BKR	O7-C17-C18	2.55	116.82	110.53
10	B	905	MAN	C1-C2-C3	2.54	113.35	109.64
8	B	901	BKR	O7-C17-C18	2.53	116.78	110.53
10	D	904	MAN	C1-C2-C3	2.53	113.33	109.64
8	D	910	BKR	C1-C45-C24	-2.47	102.94	105.26
10	C	906	MAN	C2-C3-C4	2.43	115.13	110.86
11	A	905	NAG	C4-C3-C2	2.42	114.56	111.02
10	A	907	MAN	C3-C4-C5	-2.41	105.87	110.23
8	D	910	BKR	C45-C1-C2	2.40	114.57	111.93
11	A	905	NAG	O3-C3-C2	-2.37	104.47	109.40
10	C	907	MAN	C1-O5-C5	2.37	115.36	112.19
11	A	909	NAG	O5-C1-C2	2.36	114.95	111.29
11	A	910	NAG	C1-O5-C5	2.36	115.35	112.19
10	D	905	MAN	O2-C2-C3	2.36	115.04	110.15
10	A	907	MAN	O5-C5-C4	-2.34	105.48	109.70
11	C	911	NAG	C1-C2-N2	2.34	114.12	110.43
11	B	908	NAG	C1-O5-C5	2.32	115.30	112.19
10	B	912	MAN	O2-C2-C1	2.32	114.53	109.22
8	B	901	BKR	C2-O2-C3	2.29	121.99	117.80
8	B	901	BKR	C17-C18-C20	2.28	107.70	102.58
8	A	911	BKR	C2-O2-C3	2.28	121.96	117.80
8	A	911	BKR	C17-C18-C20	2.28	107.69	102.58
10	B	904	MAN	C2-C3-C4	2.26	114.84	110.86
12	D	901	BMA	C1-O5-C5	-2.24	109.18	112.19
8	A	911	BKR	C19-C18-C20	-2.24	100.78	106.56
8	B	901	BKR	C19-C18-C20	-2.23	100.80	106.56
10	A	902	MAN	O5-C1-C2	2.22	116.08	110.79
10	B	906	MAN	O2-C2-C3	-2.21	105.58	110.15
8	A	911	BKR	C18-C20-C21	-2.20	119.41	122.69
11	D	906	NAG	C1-O5-C5	2.20	115.13	112.19
10	B	904	MAN	C1-C2-C3	2.19	112.84	109.64
8	A	911	BKR	O1-C1-C2	-2.19	100.80	105.54
10	B	905	MAN	C1-O5-C5	2.19	115.11	112.19
11	A	910	NAG	C1-C2-N2	2.18	113.87	110.43
8	B	901	BKR	C18-C20-C21	-2.18	119.44	122.69
8	B	901	BKR	O1-C1-C2	-2.18	100.83	105.54
8	C	912	BKR	C18-C20-C21	-2.17	119.45	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	910	BKR	C10-C18-C17	2.17	110.67	106.55
8	C	912	BKR	C45-C1-C2	2.14	114.28	111.93
9	A	912	XLS	O3-C3-C4	-2.13	104.09	108.93
9	B	902	XLS	O3-C3-C4	-2.12	104.12	108.93
11	B	908	NAG	C1-C2-N2	2.09	113.73	110.43
10	B	906	MAN	O5-C5-C4	-2.09	105.75	110.83
10	C	904	MAN	O4-C4-C3	-2.07	105.50	110.38
11	B	916	NAG	C2-N2-C7	2.07	125.67	122.90
11	D	906	NAG	C2-N2-C7	2.07	125.67	122.90
10	B	907	MAN	C1-O5-C5	2.05	114.93	112.19
10	C	907	MAN	C1-C2-C3	2.04	112.62	109.64
10	A	908	MAN	C3-C4-C5	2.04	113.94	110.23
11	B	908	NAG	C2-N2-C7	2.04	125.64	122.90
11	A	905	NAG	O5-C1-C2	-2.04	108.13	111.29
10	C	906	MAN	O4-C4-C5	-2.04	104.31	109.32
10	B	907	MAN	C1-C2-C3	-2.03	106.69	109.64
8	C	912	BKR	C45-C24-C21	2.03	121.64	119.52

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	901	BKR	C37-C29-N1-C30
8	A	911	BKR	C37-C29-N1-C30
9	B	902	XLS	O4-C4-C5-O5
9	A	912	XLS	O4-C4-C5-O5
11	B	914	NAG	C8-C7-N2-C2
11	B	914	NAG	O7-C7-N2-C2
11	A	910	NAG	C8-C7-N2-C2
11	A	910	NAG	O7-C7-N2-C2
11	B	911	NAG	C8-C7-N2-C2
8	D	910	BKR	C31-C30-N1-C29
9	B	902	XLS	C3-C4-C5-O5
9	A	912	XLS	C3-C4-C5-O5
11	B	911	NAG	O7-C7-N2-C2
11	C	902	NAG	O7-C7-N2-C2
10	A	904	MAN	O5-C5-C6-O6
10	D	903	MAN	O5-C5-C6-O6
10	C	904	MAN	O5-C5-C6-O6
10	D	904	MAN	O5-C5-C6-O6
10	B	904	MAN	O5-C5-C6-O6
11	D	908	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	D	909	NAG	O5-C5-C6-O6
11	C	902	NAG	C8-C7-N2-C2
11	D	908	NAG	C8-C7-N2-C2
10	B	903	MAN	O5-C5-C6-O6
10	B	907	MAN	O5-C5-C6-O6
10	A	904	MAN	C4-C5-C6-O6
10	A	907	MAN	O5-C5-C6-O6
10	D	902	MAN	O5-C5-C6-O6
10	D	905	MAN	O5-C5-C6-O6
10	D	905	MAN	C4-C5-C6-O6
11	C	911	NAG	C4-C5-C6-O6
11	B	909	NAG	O5-C5-C6-O6
10	D	902	MAN	C4-C5-C6-O6
11	D	907	NAG	C4-C5-C6-O6
11	C	909	NAG	C8-C7-N2-C2
10	B	903	MAN	C4-C5-C6-O6
10	B	904	MAN	C4-C5-C6-O6
10	B	907	MAN	C4-C5-C6-O6
10	A	907	MAN	C4-C5-C6-O6
10	D	903	MAN	C4-C5-C6-O6
11	B	909	NAG	C4-C5-C6-O6
11	D	909	NAG	C4-C5-C6-O6
11	C	909	NAG	O7-C7-N2-C2
11	C	911	NAG	C8-C7-N2-C2
11	C	911	NAG	O7-C7-N2-C2
11	D	908	NAG	O7-C7-N2-C2
11	B	908	NAG	O5-C5-C6-O6
10	B	910	MAN	O5-C5-C6-O6
11	D	908	NAG	C4-C5-C6-O6
11	D	907	NAG	O5-C5-C6-O6
11	B	908	NAG	C4-C5-C6-O6
11	D	907	NAG	C8-C7-N2-C2
10	B	910	MAN	C4-C5-C6-O6
8	C	912	BKR	O12-C27-C28-O13
8	D	910	BKR	O12-C27-C28-O13
11	D	907	NAG	O7-C7-N2-C2
11	C	911	NAG	O5-C5-C6-O6
8	C	912	BKR	O11-C27-C28-O13
10	C	904	MAN	C4-C5-C6-O6
10	D	904	MAN	C4-C5-C6-O6
11	C	901	NAG	C8-C7-N2-C2
8	C	912	BKR	O11-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
10	C	907	MAN	O5-C5-C6-O6
10	C	906	MAN	O5-C5-C6-O6
8	D	910	BKR	O11-C27-C28-O13
11	C	901	NAG	O7-C7-N2-C2
8	D	910	BKR	O14-C30-N1-C29
11	D	906	NAG	C8-C7-N2-C2
11	B	911	NAG	C4-C5-C6-O6
9	B	902	XLS	C2-C3-C4-O4
9	A	912	XLS	C2-C3-C4-O4
10	B	906	MAN	O5-C5-C6-O6
9	B	902	XLS	O3-C3-C4-O4
9	A	912	XLS	O3-C3-C4-O4
11	C	902	NAG	C4-C5-C6-O6
9	B	902	XLS	C1-C2-C3-O3
9	A	912	XLS	C1-C2-C3-O3
11	D	906	NAG	O7-C7-N2-C2
8	C	912	BKR	O12-C27-C28-C29
8	C	912	BKR	O14-C30-N1-C29
8	C	912	BKR	C31-C30-N1-C29
8	D	910	BKR	C14-C11-O4-C12
9	B	902	XLS	O2-C2-C3-O3
9	A	912	XLS	O2-C2-C3-O3
11	D	909	NAG	C1-C2-N2-C7
8	B	901	BKR	O11-C27-C28-O13
8	A	911	BKR	O11-C27-C28-O13
8	D	910	BKR	O12-C27-C28-C29
8	D	910	BKR	O11-C27-C28-C29
9	B	902	XLS	C1-C2-C3-C4
9	A	912	XLS	C1-C2-C3-C4
11	B	911	NAG	O5-C5-C6-O6
11	C	901	NAG	C4-C5-C6-O6
8	D	910	BKR	C15-C11-O4-C12
10	B	906	MAN	C4-C5-C6-O6
8	B	901	BKR	O12-C27-C28-O13
8	A	911	BKR	O12-C27-C28-O13
8	B	901	BKR	C28-C29-N1-C30
8	A	911	BKR	C28-C29-N1-C30
8	B	901	BKR	O11-C27-C28-C29
8	A	911	BKR	O11-C27-C28-C29
8	C	912	BKR	C28-C27-O11-C26

All (2) ring outliers are listed below:

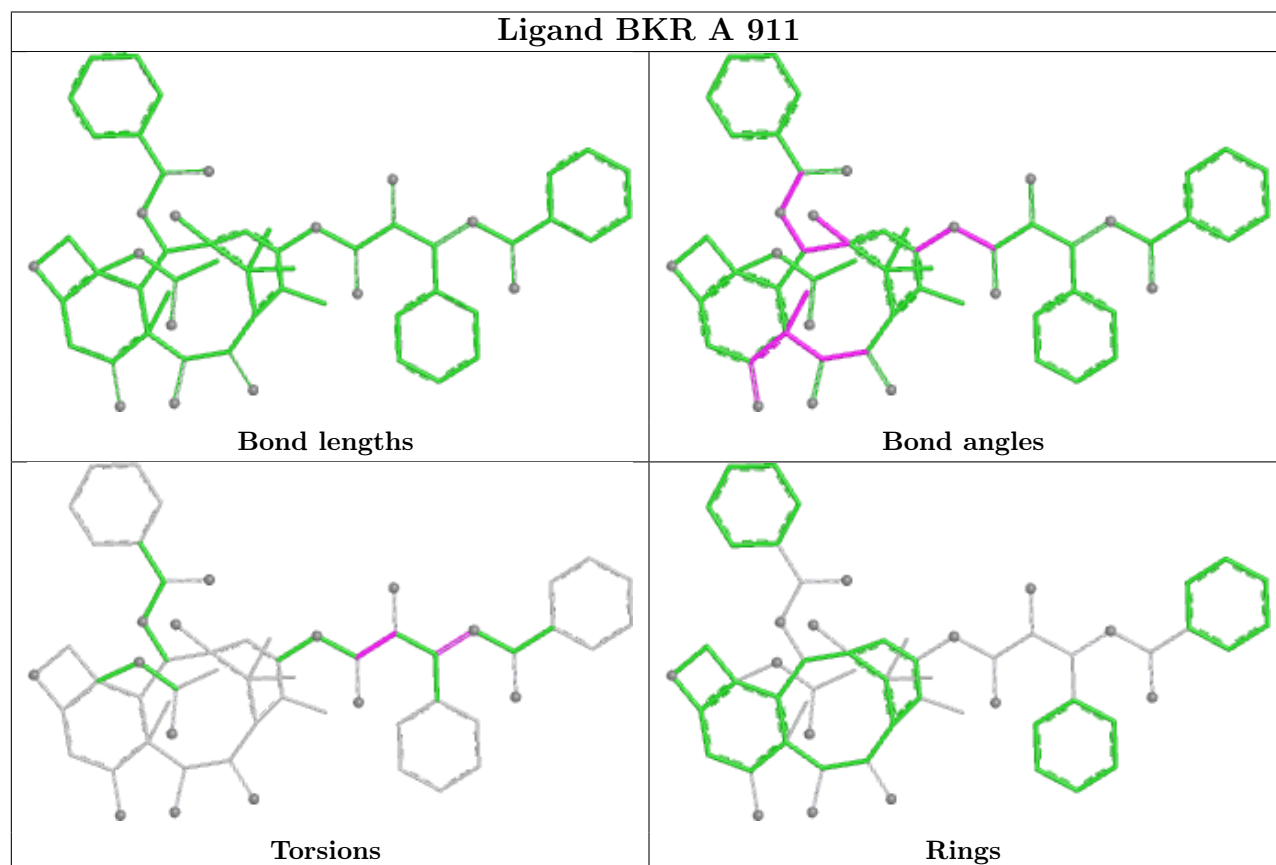
Mol	Chain	Res	Type	Atoms
10	B	912	MAN	C1-C2-C3-C4-C5-O5
10	C	903	MAN	C1-C2-C3-C4-C5-O5

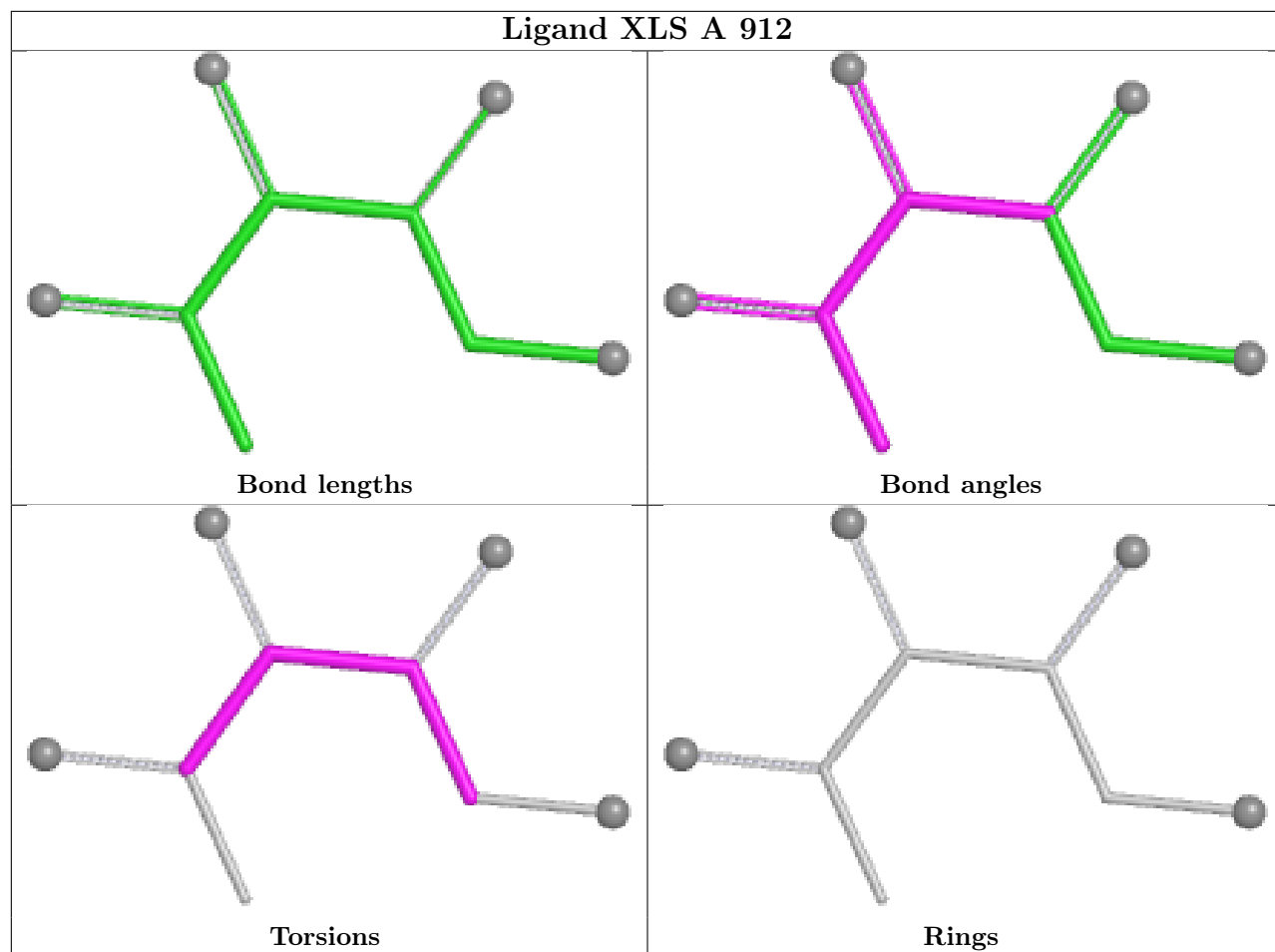
33 monomers are involved in 92 short contacts:

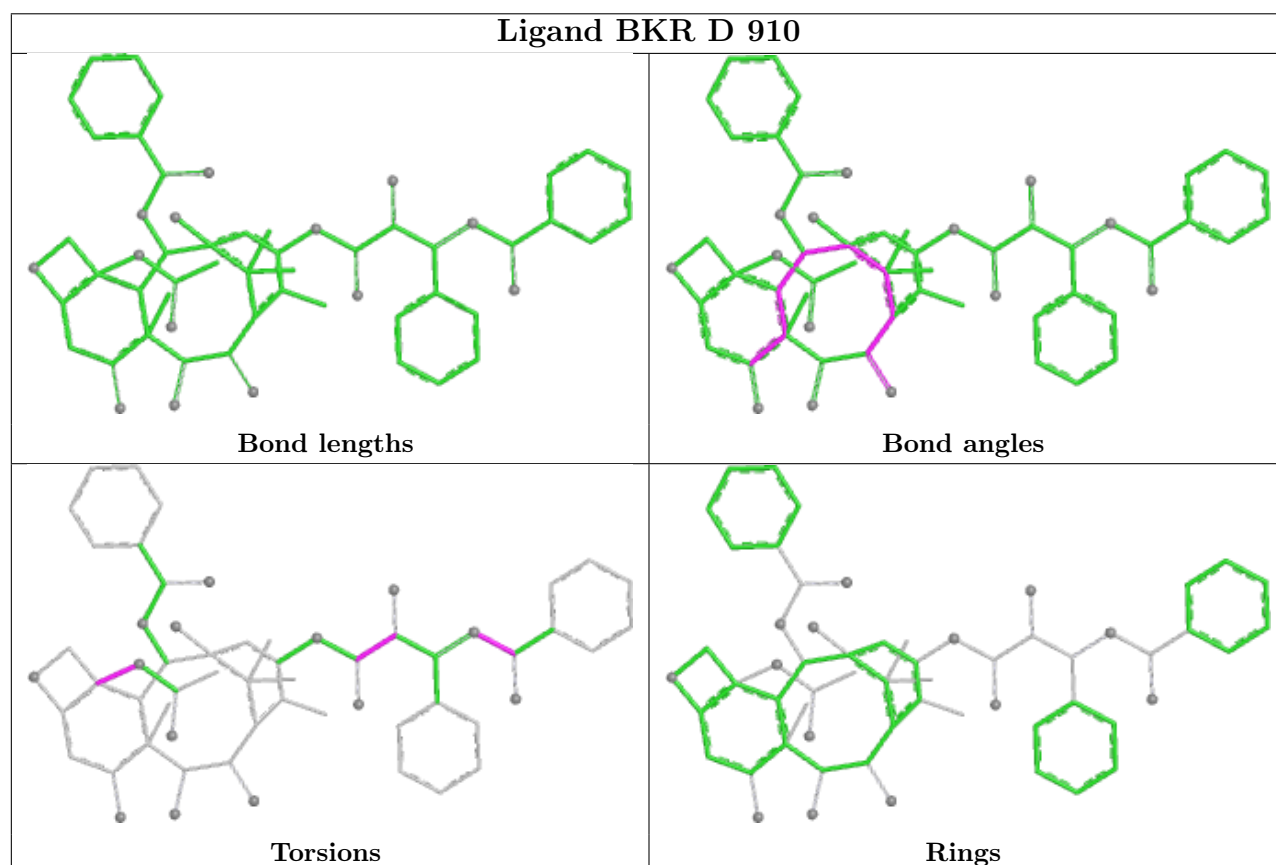
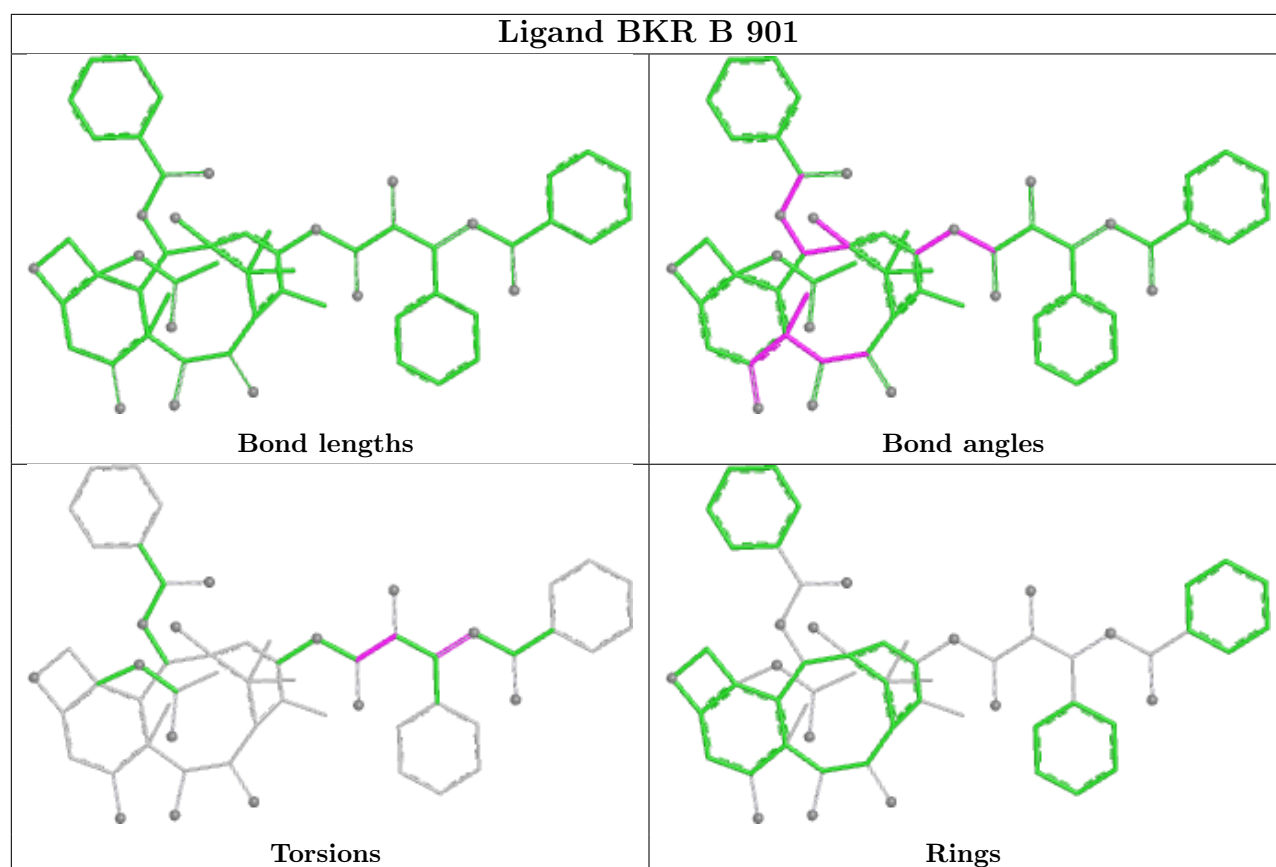
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	901	NAG	8	0
8	A	911	BKR	1	0
9	A	912	XLS	1	0
10	D	904	MAN	5	0
11	C	902	NAG	6	0
10	C	904	MAN	6	0
10	A	907	MAN	3	0
11	D	907	NAG	1	0
10	B	903	MAN	2	0
10	B	912	MAN	4	0
11	B	911	NAG	4	0
8	B	901	BKR	1	0
10	D	905	MAN	1	0
10	A	908	MAN	1	0
10	D	902	MAN	2	0
10	B	904	MAN	6	0
10	A	904	MAN	6	0
10	C	907	MAN	1	0
10	C	903	MAN	10	0
8	D	910	BKR	2	0
9	B	902	XLS	1	0
10	A	901	MAN	10	0
11	B	916	NAG	4	0
10	B	905	MAN	3	0
10	A	903	MAN	10	0
10	B	907	MAN	4	0
10	C	906	MAN	3	0
10	C	905	MAN	2	0
10	B	910	MAN	12	0
10	A	902	MAN	4	0
12	D	901	BMA	9	0
10	B	906	MAN	6	0
8	C	912	BKR	2	0

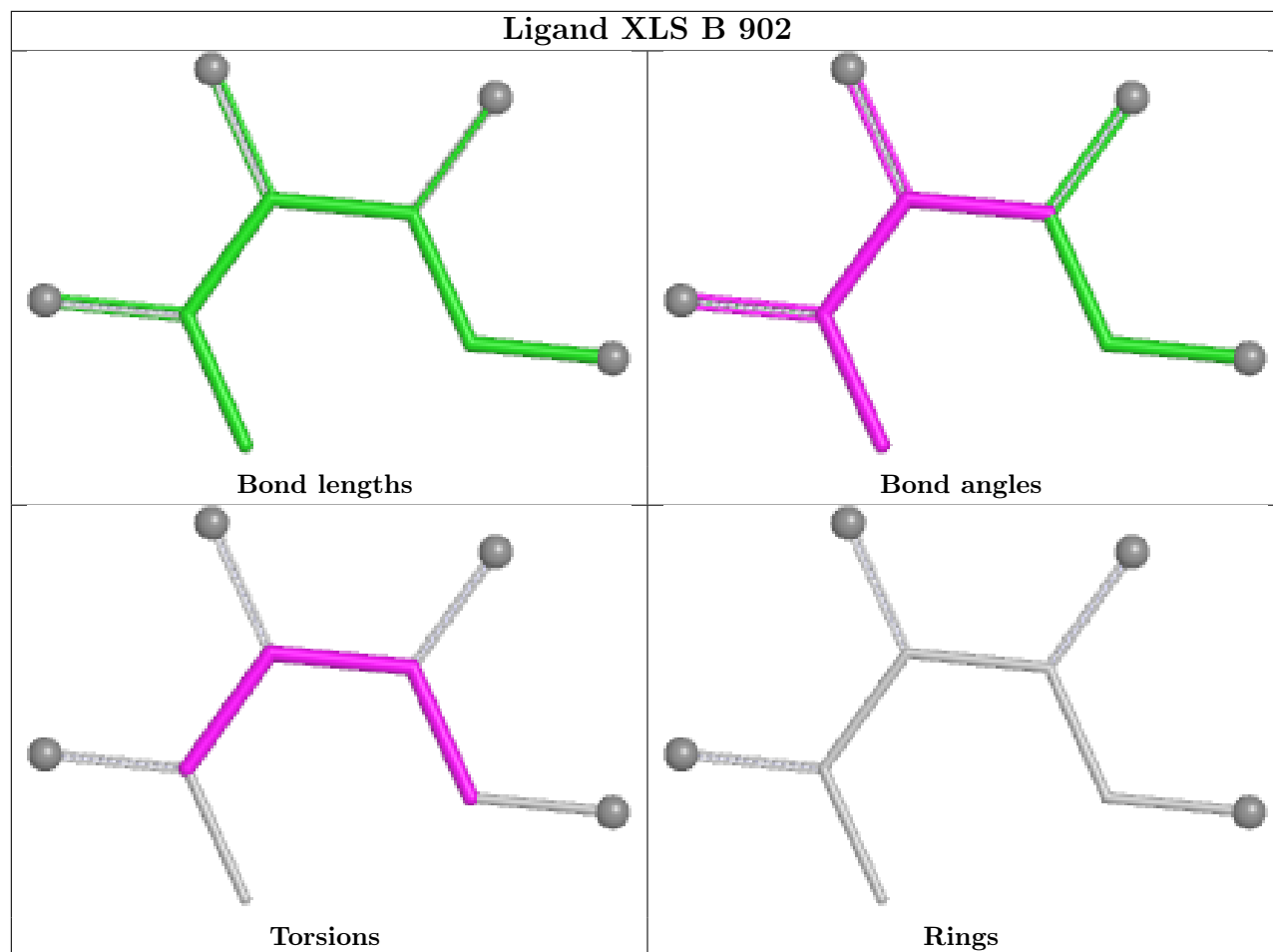
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

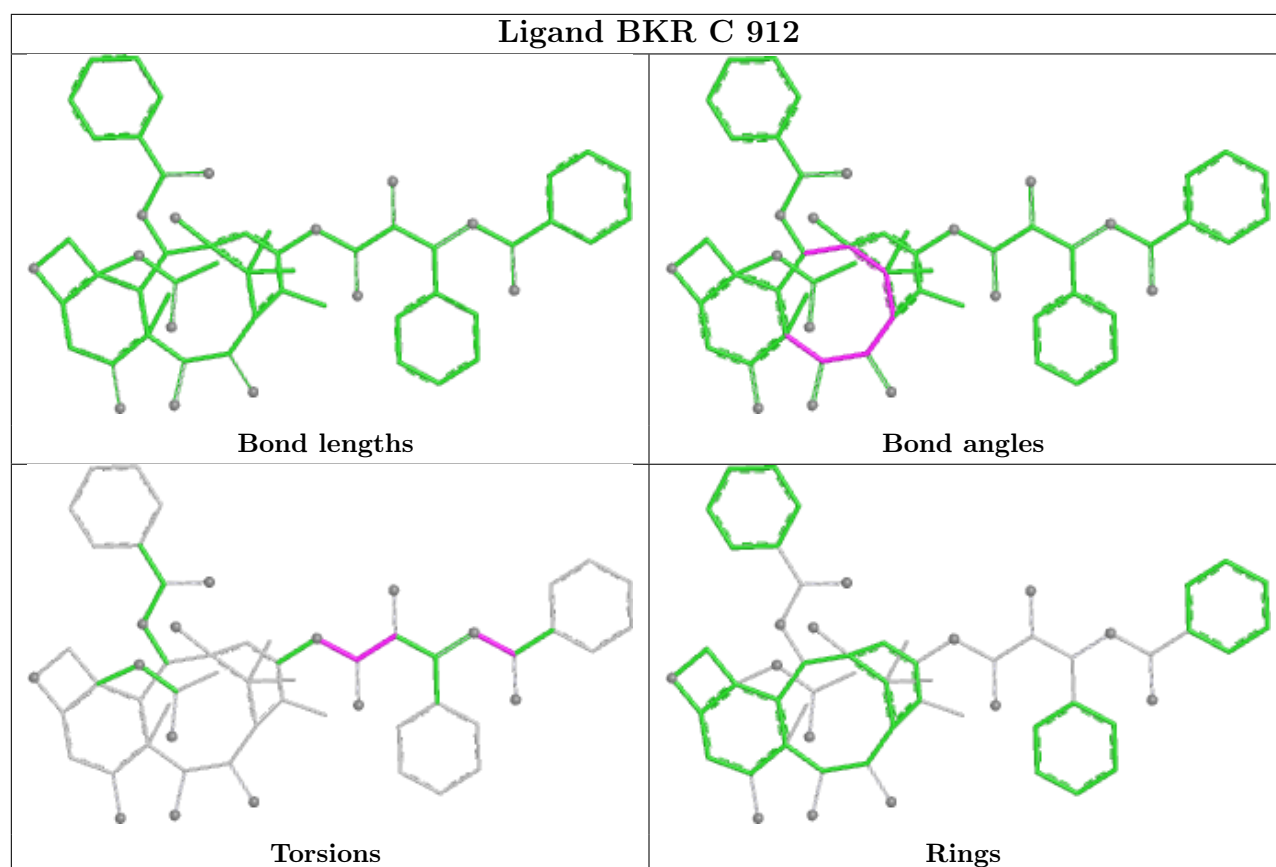
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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	757/803 (94%)	-0.15	10 (1%) 75 77	18, 31, 50, 101	1 (0%)
1	B	756/803 (94%)	-0.22	6 (0%) 82 84	14, 30, 42, 84	3 (0%)
1	C	756/803 (94%)	0.79	78 (10%) 12 12	24, 50, 73, 121	2 (0%)
1	D	756/803 (94%)	0.87	61 (8%) 18 18	22, 48, 69, 96	2 (0%)
All	All	3025/3212 (94%)	0.32	155 (5%) 33 33	14, 39, 67, 121	8 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	TYR	5.4
1	D	683	TYR	4.8
1	D	227	VAL	4.5
1	C	683	TYR	4.5
1	D	230	ALA	4.2
1	D	224	ILE	4.1
1	D	209	TRP	3.9
1	A	47	THR	3.8
1	C	773	VAL	3.8
1	B	683[A]	TYR	3.8
1	A	110	GLY	3.7
1	C	227	VAL	3.7
1	D	332	TRP	3.5
1	D	624	VAL	3.4
1	D	175	GLY	3.4
1	C	302	GLY	3.3
1	D	302	GLY	3.3
1	C	334	ALA	3.1
1	C	224	ILE	3.1
1	C	329	GLY	3.1
1	B	224	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	49	TRP	3.0
1	D	340	ILE	3.0
1	C	303	GLY	3.0
1	D	271	ILE	3.0
1	D	357	ILE	3.0
1	D	303	GLY	2.9
1	D	225	ASP	2.9
1	C	240	VAL	2.9
1	A	224	ILE	2.8
1	D	232	ILE	2.8
1	C	262	ASN	2.8
1	C	64	PHE	2.8
1	C	296	GLY	2.8
1	D	100	LEU	2.8
1	C	772	VAL	2.8
1	A	225	ASP	2.8
1	C	803	PRO	2.8
1	D	345	VAL	2.8
1	C	222	ILE	2.8
1	D	308	VAL	2.7
1	D	226	GLY	2.7
1	C	778	TYR	2.7
1	C	345	VAL	2.7
1	A	571	TRP	2.7
1	C	314	GLY	2.7
1	C	76	VAL	2.7
1	D	642	ILE	2.7
1	D	48	GLN	2.6
1	C	336	LEU	2.6
1	D	301	TRP	2.6
1	C	731	ILE	2.6
1	D	222	ILE	2.6
1	C	226	GLY	2.6
1	C	681	LYS	2.6
1	C	280	ALA	2.6
1	D	516	ALA	2.6
1	C	761	PRO	2.6
1	C	646	TRP	2.6
1	C	762	ILE	2.5
1	C	283	LEU	2.5
1	D	328	LEU	2.5
1	C	305	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	340	ILE	2.5
1	D	240	VAL	2.5
1	C	48	GLN	2.5
1	C	156	LEU	2.5
1	D	166	LEU	2.5
1	D	649	LYS	2.5
1	B	225	ASP	2.4
1	A	226	GLY	2.4
1	A	48	GLN	2.4
1	C	60	TRP	2.4
1	C	337	VAL	2.4
1	D	49	TRP	2.4
1	D	283	LEU	2.4
1	C	782	GLY	2.4
1	D	82	ILE	2.4
1	C	80	ALA	2.4
1	C	357	ILE	2.4
1	D	337	VAL	2.4
1	C	209	TRP	2.4
1	C	696	TRP	2.4
1	C	286	LEU	2.3
1	D	248	LEU	2.3
1	C	246	HIS	2.3
1	C	277	CYS	2.3
1	D	646	TRP	2.3
1	C	221	TYR	2.3
1	D	636	PHE	2.3
1	D	238	SER	2.3
1	C	706	ILE	2.3
1	A	227	VAL	2.3
1	D	450	ALA	2.3
1	C	339	LEU	2.3
1	C	727	LEU	2.3
1	C	769	SER	2.3
1	B	48	GLN	2.3
1	C	50	PRO	2.3
1	C	249	TYR	2.3
1	C	293	PHE	2.2
1	D	331	PHE	2.2
1	C	168	ARG	2.2
1	D	681	LYS	2.2
1	D	314	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	64	PHE	2.2
1	C	375	VAL	2.2
1	C	530	GLY	2.2
1	C	254	ALA	2.2
1	C	310	ALA	2.2
1	D	51	ALA	2.2
1	C	384	LEU	2.2
1	C	212	TYR	2.2
1	C	770	TRP	2.2
1	D	344	THR	2.2
1	D	173	GLY	2.2
1	D	380	GLY	2.2
1	C	54	ALA	2.2
1	D	626	TYR	2.2
1	D	571	TRP	2.2
1	D	111	PRO	2.1
1	D	453	ILE	2.1
1	C	733	GLY	2.1
1	C	776	LEU	2.1
1	C	768	SER	2.1
1	C	83	THR	2.1
1	C	331	PHE	2.1
1	D	236	ILE	2.1
1	B	227	VAL	2.1
1	C	625	VAL	2.1
1	C	676	HIS	2.1
1	D	228	SER	2.1
1	D	101	GLY	2.1
1	C	301	TRP	2.1
1	C	355	VAL	2.1
1	D	212	TYR	2.1
1	C	230	ALA	2.1
1	C	107	LEU	2.0
1	C	166	LEU	2.0
1	C	225	ASP	2.0
1	D	282	GLY	2.0
1	D	321	GLY	2.0
1	C	82	ILE	2.0
1	D	251	TRP	2.0
1	D	386	ALA	2.0
1	D	497	ALA	2.0
1	C	243	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	672	LEU	2.0
1	D	306	ASP	2.0
1	C	266	CYS	2.0
1	D	90	CYS	2.0
1	D	266	CYS	2.0
1	A	803	PRO	2.0
1	C	335	THR	2.0
1	B	226	GLY	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.

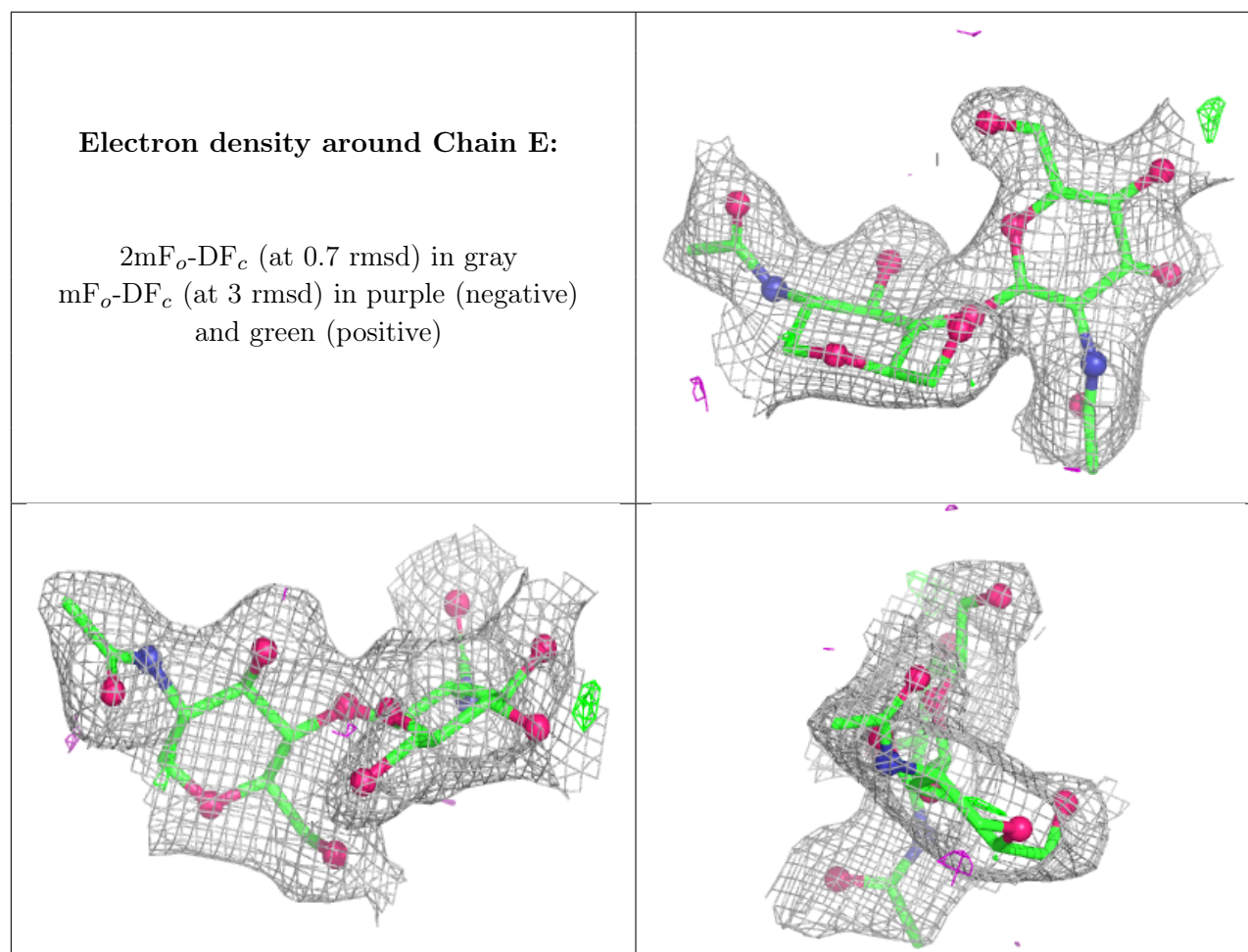
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	G	1	12/12	0.37	0.28	20,20,20,20	0
7	MAN	N	3	11/12	0.62	0.16	80,85,92,94	0
2	NAG	O	2	14/15	0.66	0.16	69,91,100,108	0
5	NAG	I	3	14/15	0.67	0.14	60,73,81,86	0
2	NAG	L	2	14/15	0.69	0.14	70,80,85,91	0
2	NAG	O	1	14/15	0.76	0.22	20,20,20,20	0
4	BMA	G	2	11/12	0.76	0.17	37,49,56,57	0
7	MAN	M	3	11/12	0.78	0.14	50,63,69,78	0
7	NAG	N	2	14/15	0.80	0.15	41,65,82,83	0
2	NAG	P	1	14/15	0.84	0.17	55,70,80,82	0
6	BMA	J	4	11/12	0.85	0.11	50,60,64,65	0
3	MAN	F	4	11/12	0.87	0.10	44,45,54,55	0
7	MAN	K	3	11/12	0.89	0.10	37,43,48,55	0
2	NAG	E	2	14/15	0.90	0.09	42,52,55,60	0
3	MAN	F	5	11/12	0.90	0.09	43,50,53,54	0
2	NAG	L	1	14/15	0.90	0.12	51,68,73,76	0
6	MAN	J	5	11/12	0.90	0.09	45,53,63,64	0
2	NAG	P	2	14/15	0.92	0.09	42,46,50,50	0
7	NAG	M	2	14/15	0.93	0.08	33,37,45,56	0
7	NAG	N	1	14/15	0.93	0.09	34,39,47,58	0

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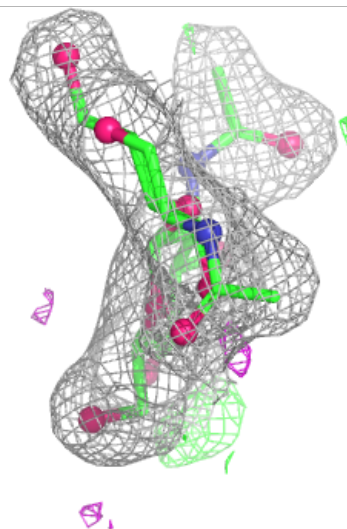
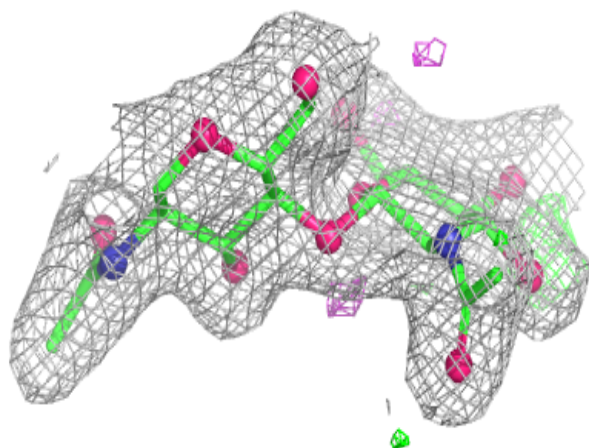
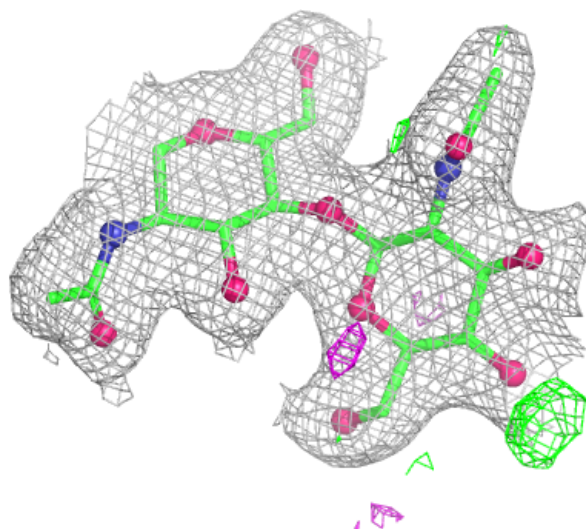
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AH2	J	3	11/11	0.94	0.07	35,45,48,50	0
5	NAG	I	2	14/15	0.94	0.07	38,44,48,49	0
2	NAG	H	2	14/15	0.94	0.07	27,31,38,39	0
6	NAG	J	2	14/15	0.95	0.07	37,40,48,49	0
7	NAG	K	2	14/15	0.95	0.06	23,29,32,35	0
6	NAG	J	1	14/15	0.96	0.06	27,30,36,42	0
3	NAG	F	1	14/15	0.96	0.06	24,28,31,34	0
3	NAG	F	2	14/15	0.96	0.06	25,29,34,38	0
7	NAG	M	1	14/15	0.97	0.06	33,37,38,39	0
3	BMA	F	3	11/12	0.97	0.05	24,27,30,31	0
2	NAG	H	1	14/15	0.97	0.06	25,28,33,34	0
7	NAG	K	1	14/15	0.97	0.06	25,29,32,32	0
5	NAG	I	1	14/15	0.97	0.06	24,28,30,38	0
2	NAG	E	1	14/15	0.97	0.07	30,35,39,46	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.



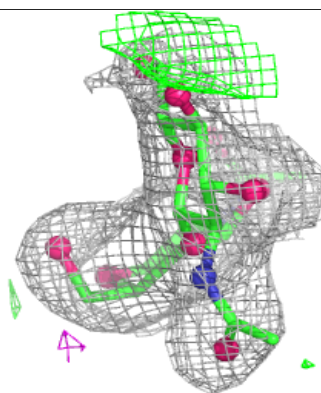
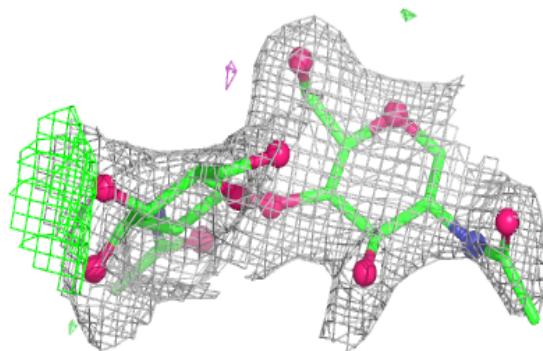
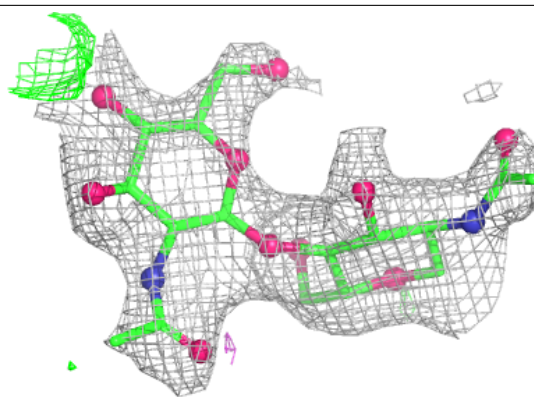
Electron density around Chain H:

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



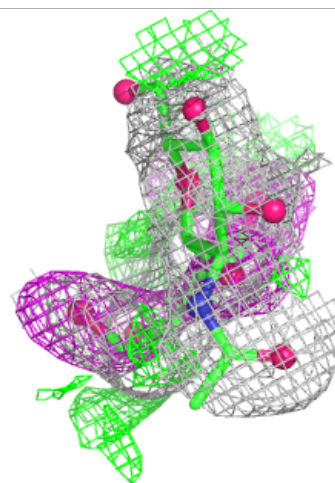
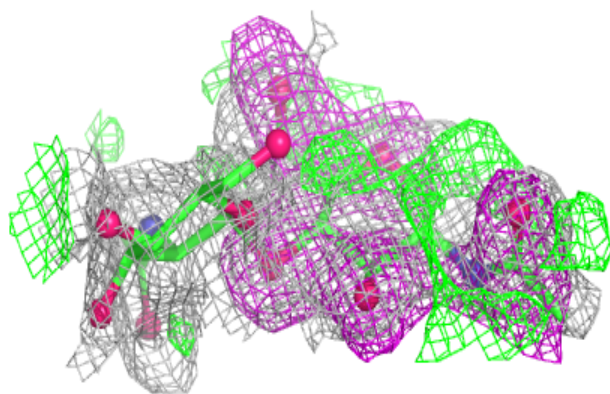
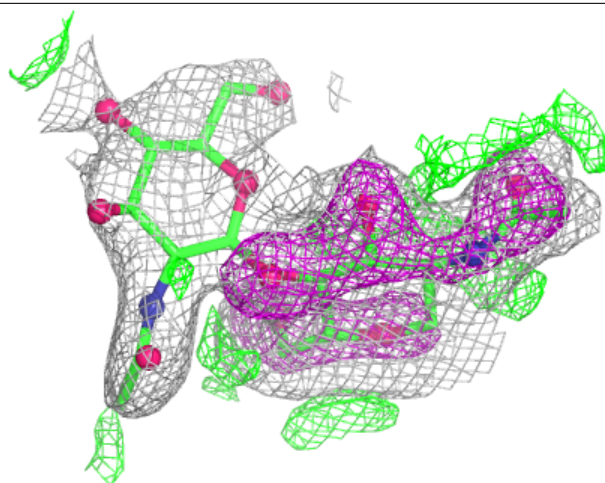
Electron density around Chain L:

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



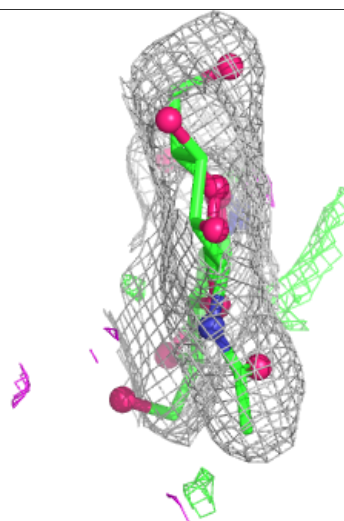
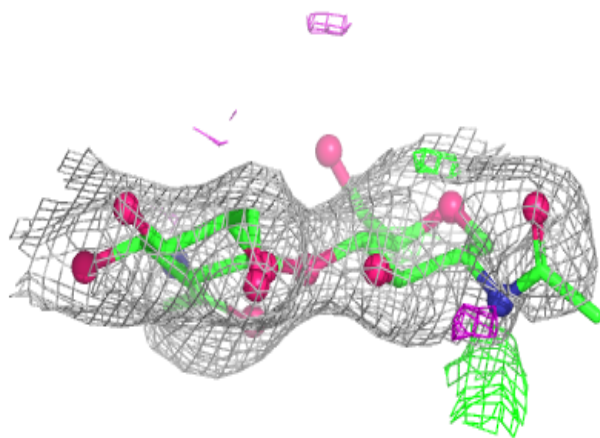
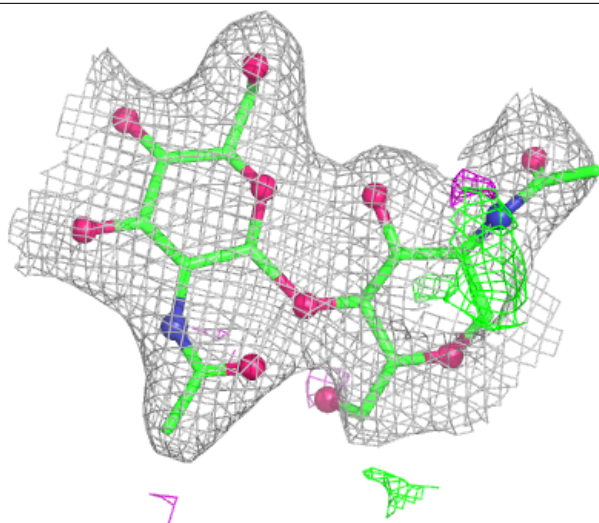
Electron density around Chain O:

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



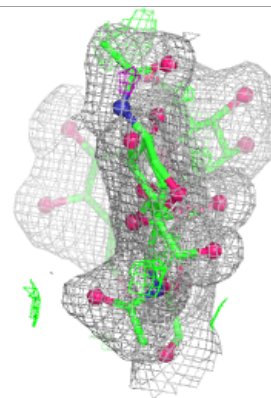
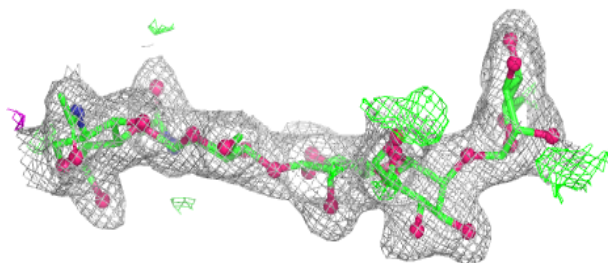
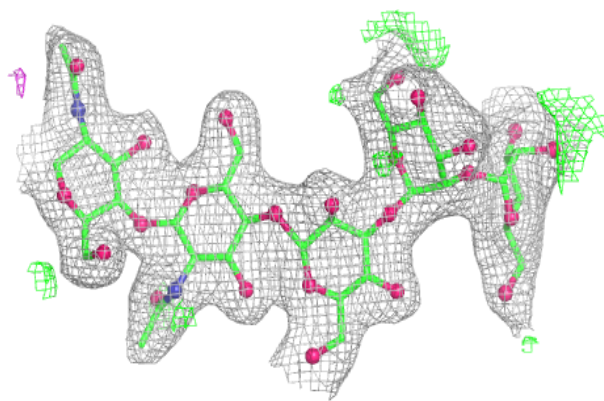
Electron density around Chain P:

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

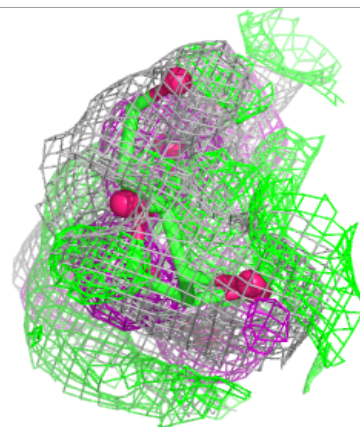
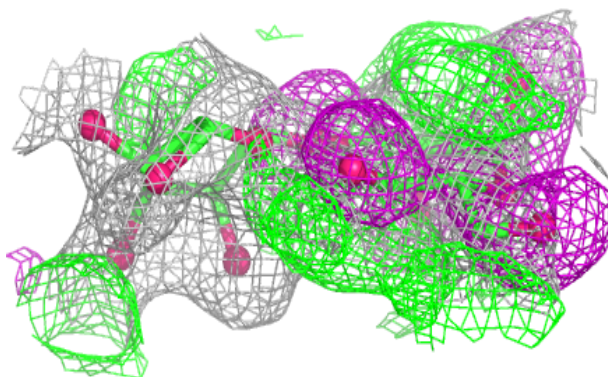
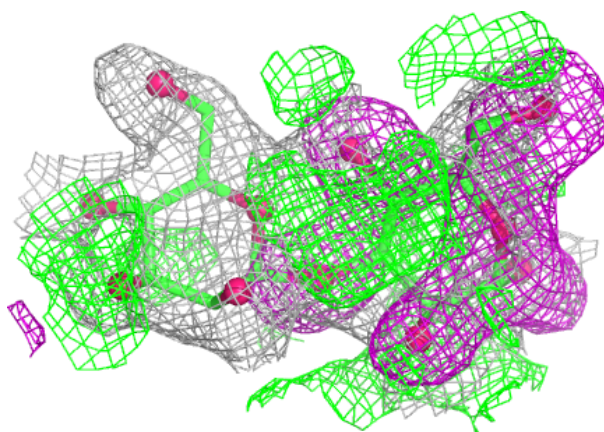


Electron density around Chain F:

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

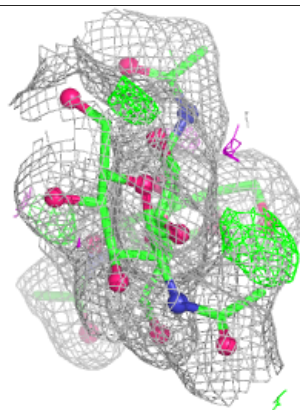
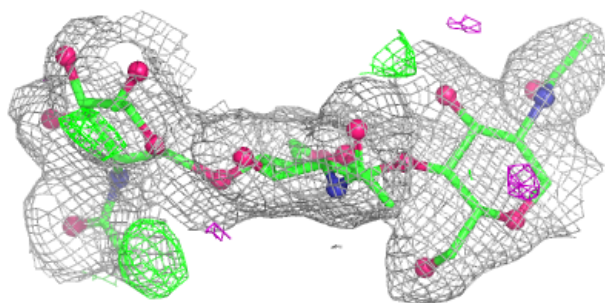
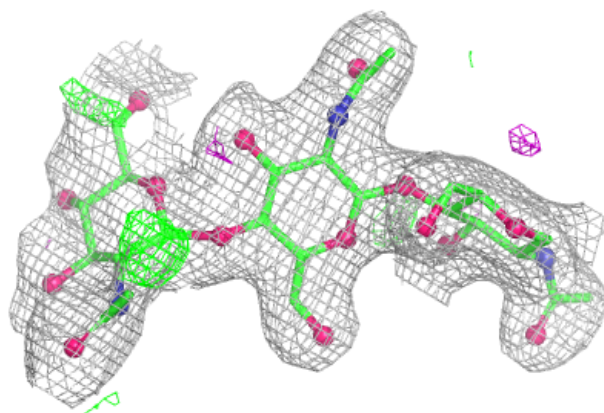
**Electron density around Chain G:**

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

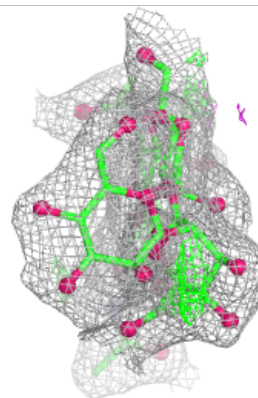
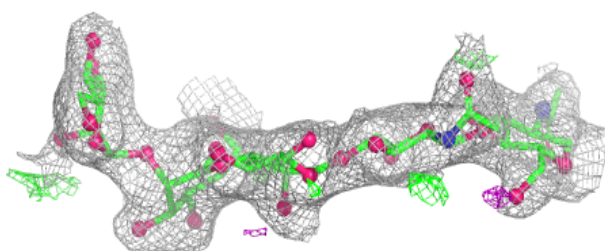
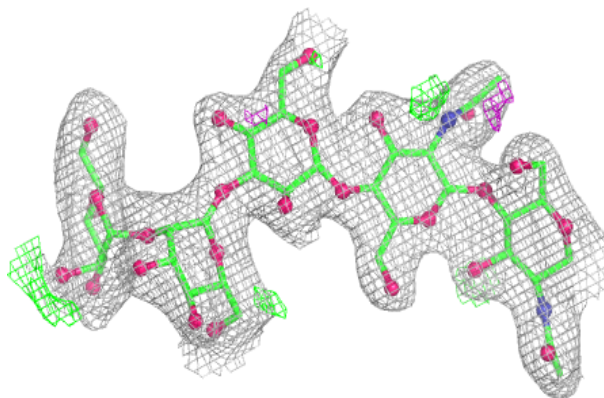


Electron density around Chain I:

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

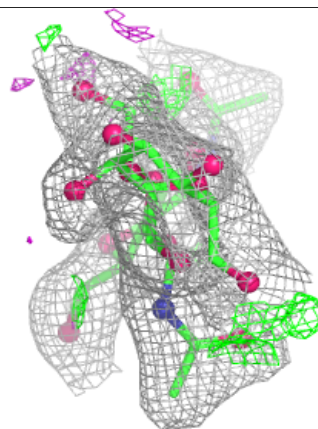
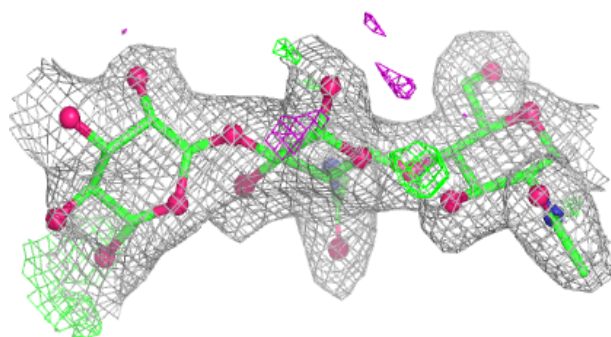
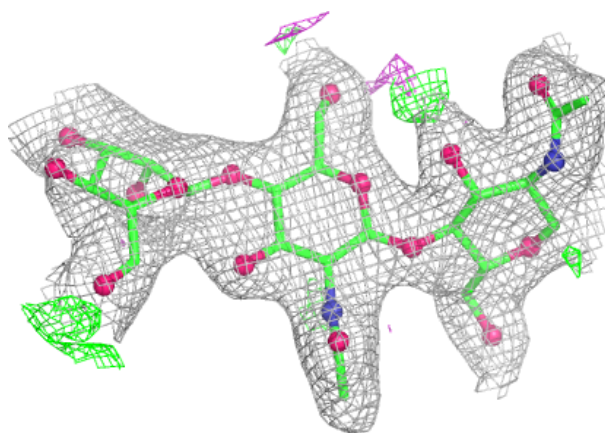
**Electron density around Chain J:**

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

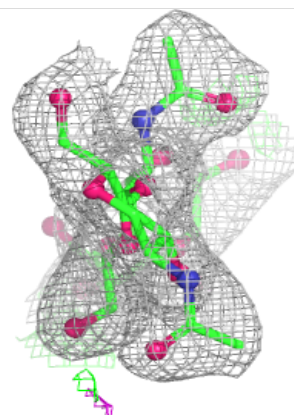
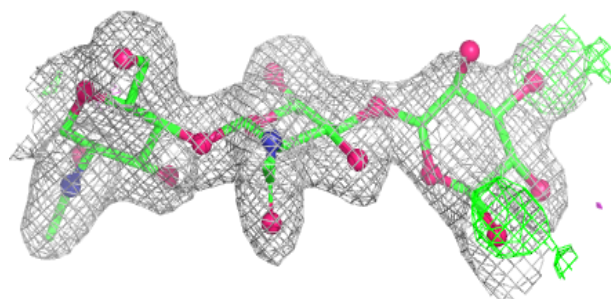
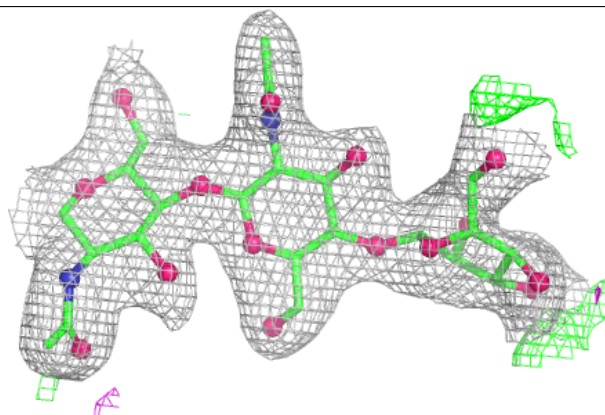


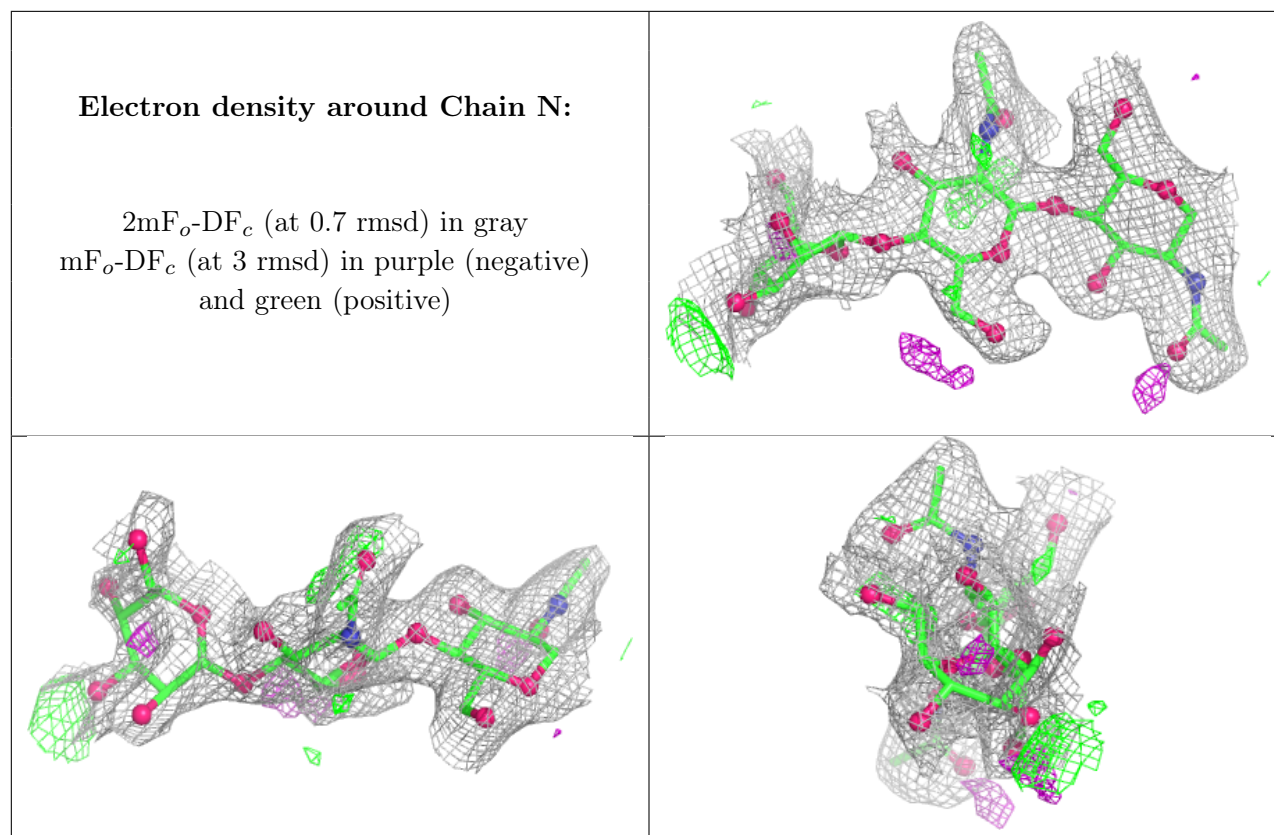
Electron density around Chain K:

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

**Electron density around Chain M:**

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





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
11	NAG	B	915	15/15	0.44	0.17	20,20,20,20	0
11	NAG	D	909	14/15	0.61	0.14	68,90,97,104	0
11	NAG	C	911	14/15	0.62	0.15	92,113,120,134	0
10	MAN	B	912	11/12	0.65	0.19	52,57,65,66	0
11	NAG	B	916	14/15	0.65	0.15	20,20,20,20	0
11	NAG	B	914	14/15	0.66	0.15	67,74,84,94	0
11	NAG	B	911	15/15	0.68	0.15	20,20,20,20	0
10	MAN	B	907	11/12	0.70	0.14	79,88,93,95	0
10	MAN	A	904	11/12	0.73	0.14	83,97,107,110	0
10	MAN	C	904	11/12	0.73	0.17	70,80,85,90	0
10	MAN	C	906	11/12	0.73	0.15	68,84,94,102	0
11	NAG	C	908	14/15	0.75	0.15	88,94,99,100	0
10	MAN	D	902	11/12	0.76	0.13	55,60,71,74	0
8	BKR	D	910	59/59	0.76	0.20	82,112,136,139	0

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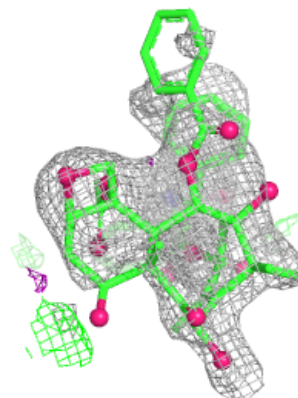
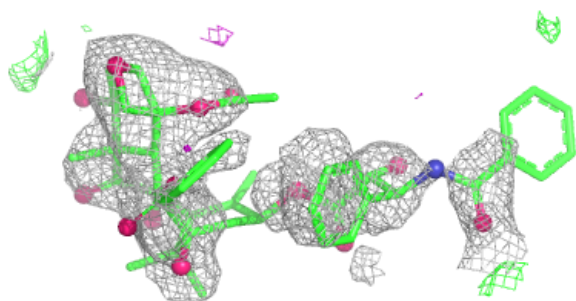
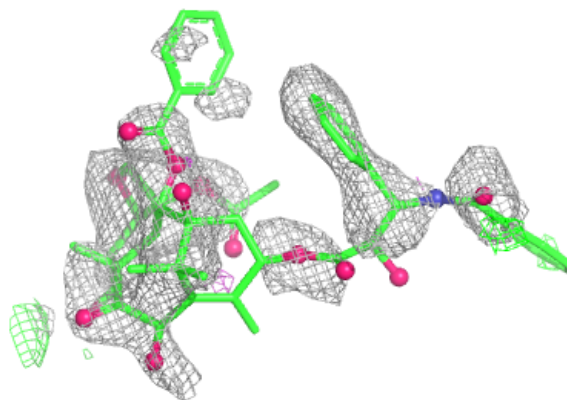
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	A	910	14/15	0.77	0.16	74,85,97,103	0
10	MAN	B	910	12/12	0.79	0.14	33,43,54,57	0
11	NAG	D	907	14/15	0.79	0.11	65,74,85,89	0
9	XLS	A	912	9/10	0.79	0.21	32,44,63,67	0
10	MAN	D	904	11/12	0.80	0.13	65,73,84,90	0
8	BKR	C	912	59/59	0.80	0.19	72,104,123,126	0
8	BKR	A	911	59/59	0.82	0.15	36,47,54,56	0
11	NAG	D	906	14/15	0.82	0.12	65,73,85,90	0
10	MAN	D	905	11/12	0.83	0.13	65,79,89,98	0
10	MAN	C	907	11/12	0.84	0.10	55,61,72,83	0
9	XLS	B	902	9/10	0.85	0.17	32,44,63,67	0
11	NAG	C	909	14/15	0.85	0.10	61,80,89,91	0
10	MAN	B	903	11/12	0.86	0.11	56,72,79,82	0
10	MAN	A	907	12/12	0.87	0.15	51,58,67,79	0
10	MAN	B	906	11/12	0.87	0.10	53,59,65,68	0
11	NAG	D	908	14/15	0.87	0.10	54,62,67,71	0
11	NAG	C	902	14/15	0.87	0.14	52,67,74,82	0
8	BKR	B	901	59/59	0.88	0.12	36,47,54,56	0
10	MAN	C	905	11/12	0.88	0.09	56,60,74,80	0
11	NAG	A	906	14/15	0.88	0.09	39,44,46,48	0
10	MAN	A	903	11/12	0.88	0.09	62,70,85,91	0
10	MAN	A	901	11/12	0.89	0.09	44,47,50,56	0
11	NAG	C	901	14/15	0.89	0.13	54,58,65,73	0
11	NAG	A	905	14/15	0.90	0.08	46,50,55,61	0
10	MAN	C	903	11/12	0.90	0.08	52,54,58,59	0
10	MAN	B	904	11/12	0.90	0.08	37,43,48,52	0
10	MAN	D	903	11/12	0.90	0.10	55,56,59,67	0
11	NAG	B	913	14/15	0.91	0.09	37,44,47,47	0
11	NAG	B	909	14/15	0.91	0.10	39,44,53,55	0
11	NAG	C	910	14/15	0.91	0.08	41,44,47,48	0
10	MAN	A	908	11/12	0.91	0.08	47,61,65,69	0
11	NAG	B	908	14/15	0.92	0.08	39,45,52,60	0
10	MAN	A	902	11/12	0.92	0.09	45,47,52,53	0
12	BMA	D	901	11/12	0.93	0.07	36,40,45,46	0
10	MAN	B	905	11/12	0.94	0.08	30,35,42,45	0
11	NAG	A	909	14/15	0.94	0.07	35,39,44,47	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.

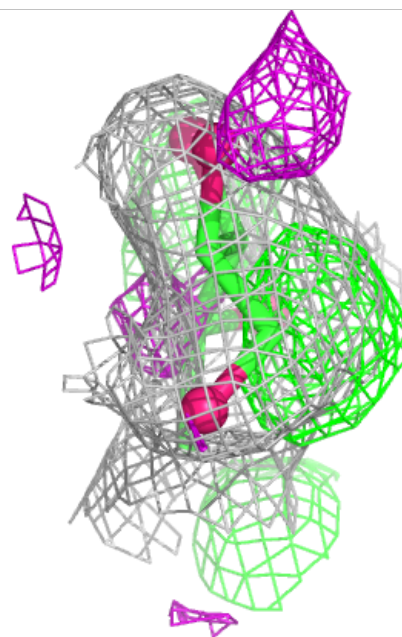
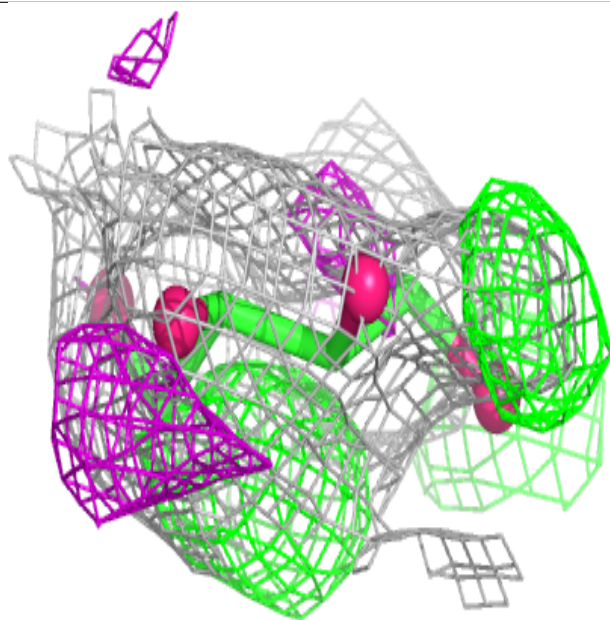
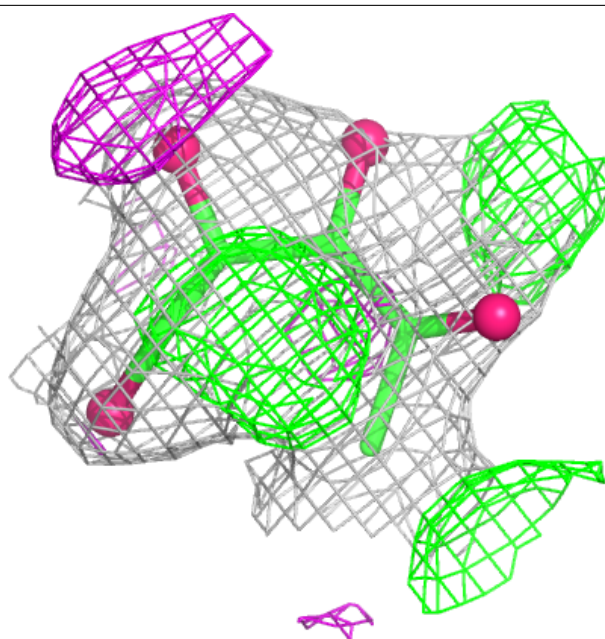
Electron density around BKR D 910:

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



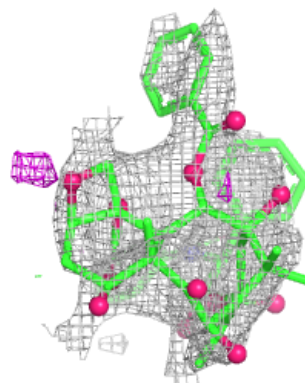
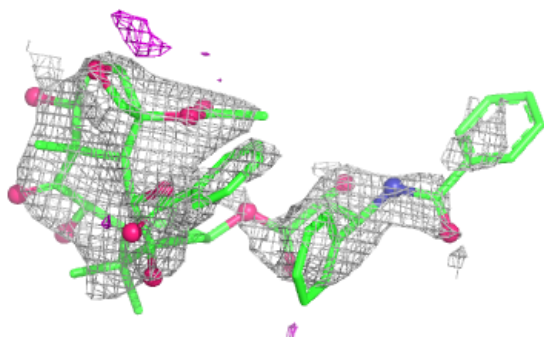
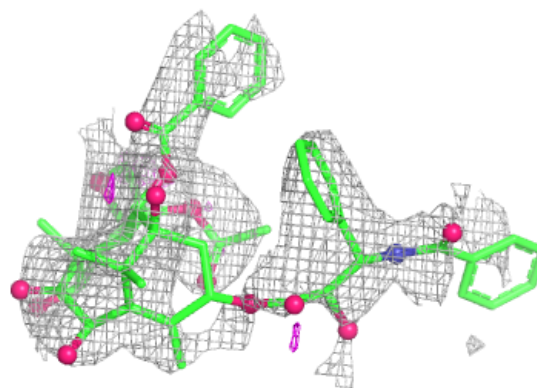
Electron density around XLS A 912:

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

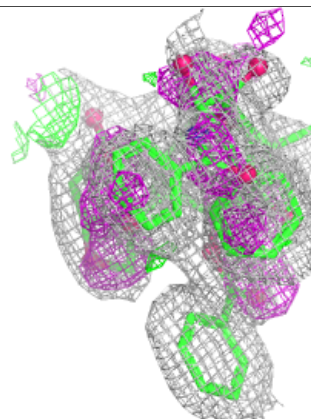
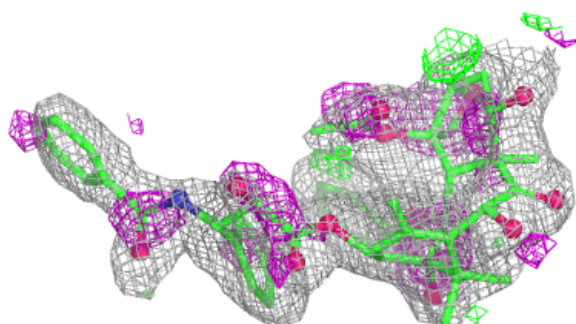
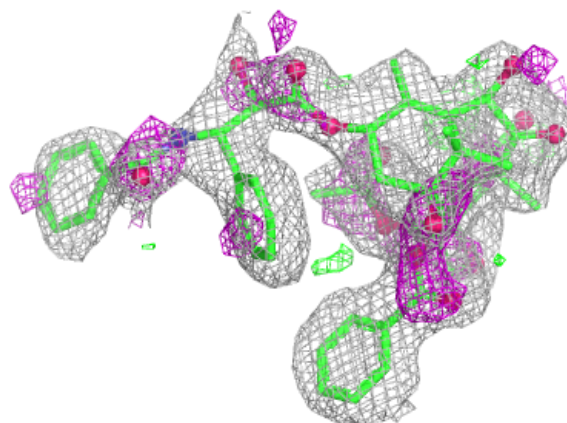


Electron density around BKR C 912:

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

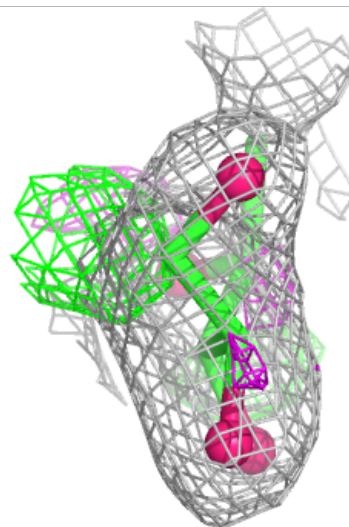
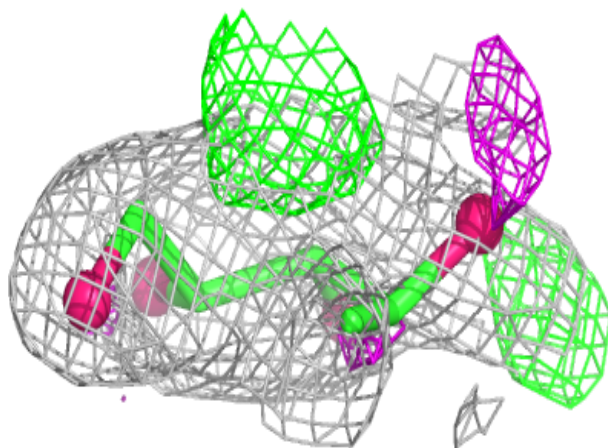
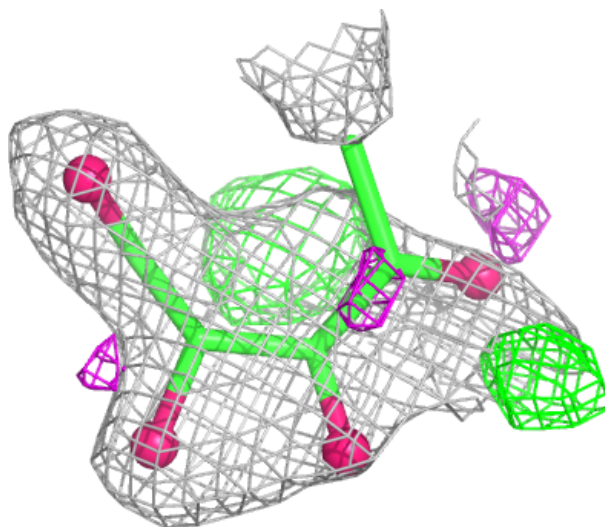
**Electron density around BKR A 911:**

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



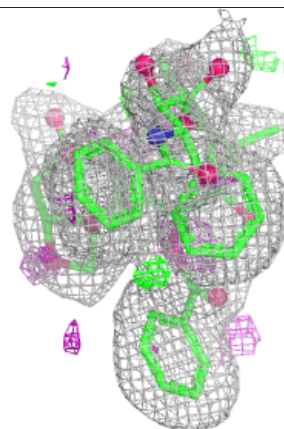
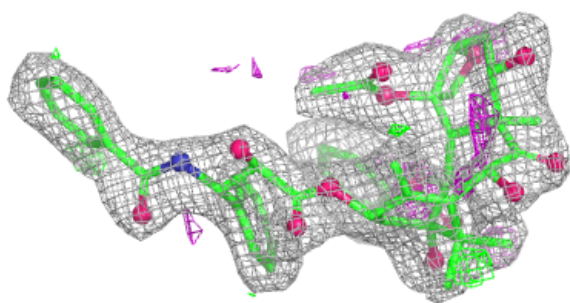
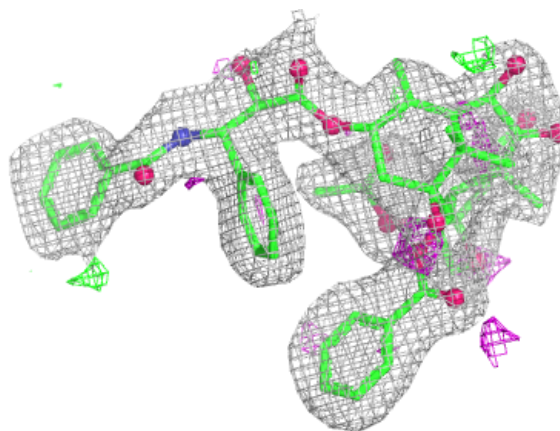
Electron density around XLS B 902:

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



Electron density around BKR B 901:

$2mF_o - DF_c$ (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.