



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:17 PM UTC

PDB ID : 3FUS / pdb_00003fus
Title : Improved Structure of the Unliganded Simian Immunodeficiency Virus gp120 Core
Authors : Chen, X.; Poon, B.; Wang, Q.; Ma, J.
Deposited on : 2009-01-14
Resolution : 4.00 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
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

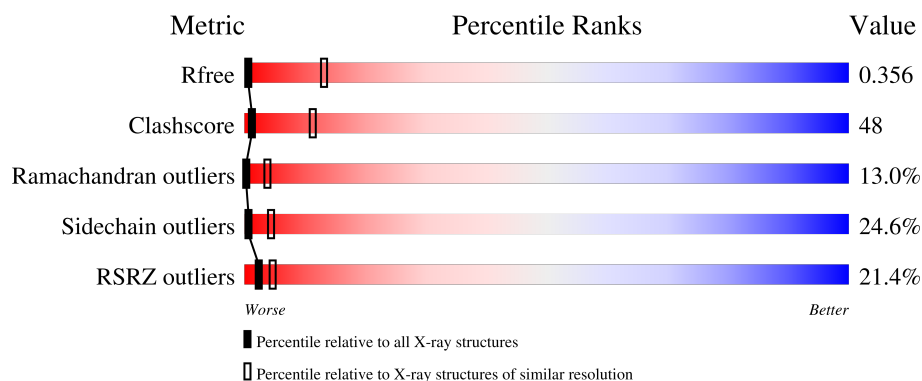
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.



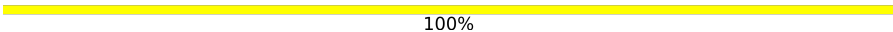
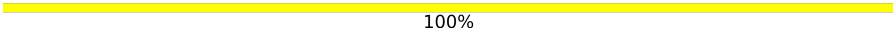
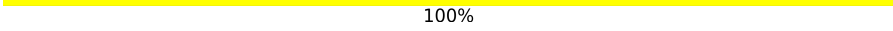
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	316	21% 26% 43% 24% • •
2	B	5	20% 20% 60%
3	C	6	33% 67%
3	K	6	33% 67%
4	D	3	100%

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Mol	Chain	Length	Quality of chain
5	E	4	 25% 75%
6	F	4	 100%
7	G	2	 100%
8	H	6	 83% 17%
9	I	7	 57% 43%
10	J	6	 67% 33%
11	L	4	 100%

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
12	NAG	A	1	X	-	-	-
2	NAG	B	1	X	-	-	-
4	NAG	D	1	X	-	-	-
7	NAG	G	1	X	-	-	-
8	NAG	H	1	X	-	-	-
9	NAG	I	1	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 3140 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.

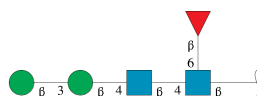
- Molecule 1 is a protein called EXTERIOR MEMBRANE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2470	1556	436	455	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

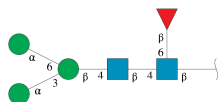
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	HIS	-	expression tag	UNP Q07374
A	65	MET	-	expression tag	UNP Q07374
A	110	GLY	-	linker	UNP Q07374
A	207	ALA	-	linker	UNP Q07374
A	208	GLY	-	linker	UNP Q07374
A	312	GLY	-	linker	UNP Q07374
A	313	ALA	-	linker	UNP Q07374
A	341	GLY	-	linker	UNP Q07374

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



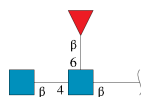
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	60	34	2	24	0	0	0

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



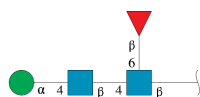
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	K	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



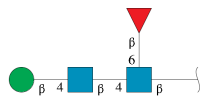
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



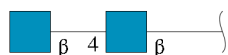
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



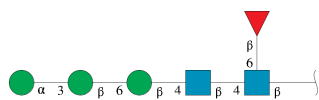
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



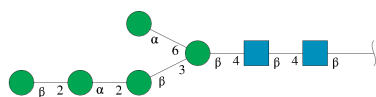
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



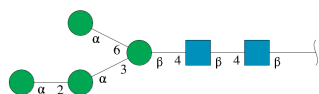
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



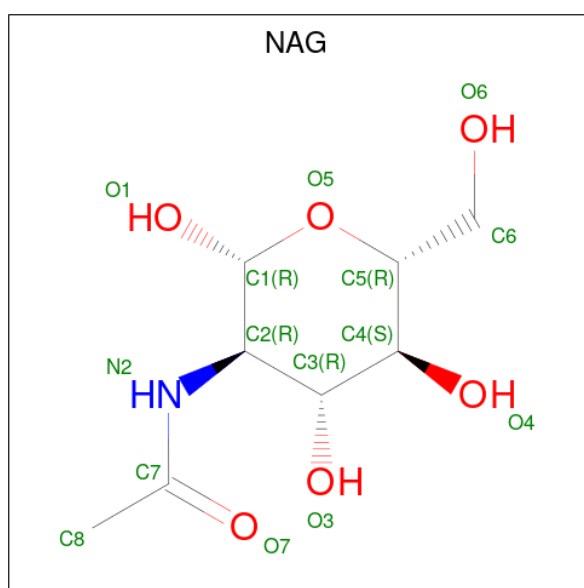
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

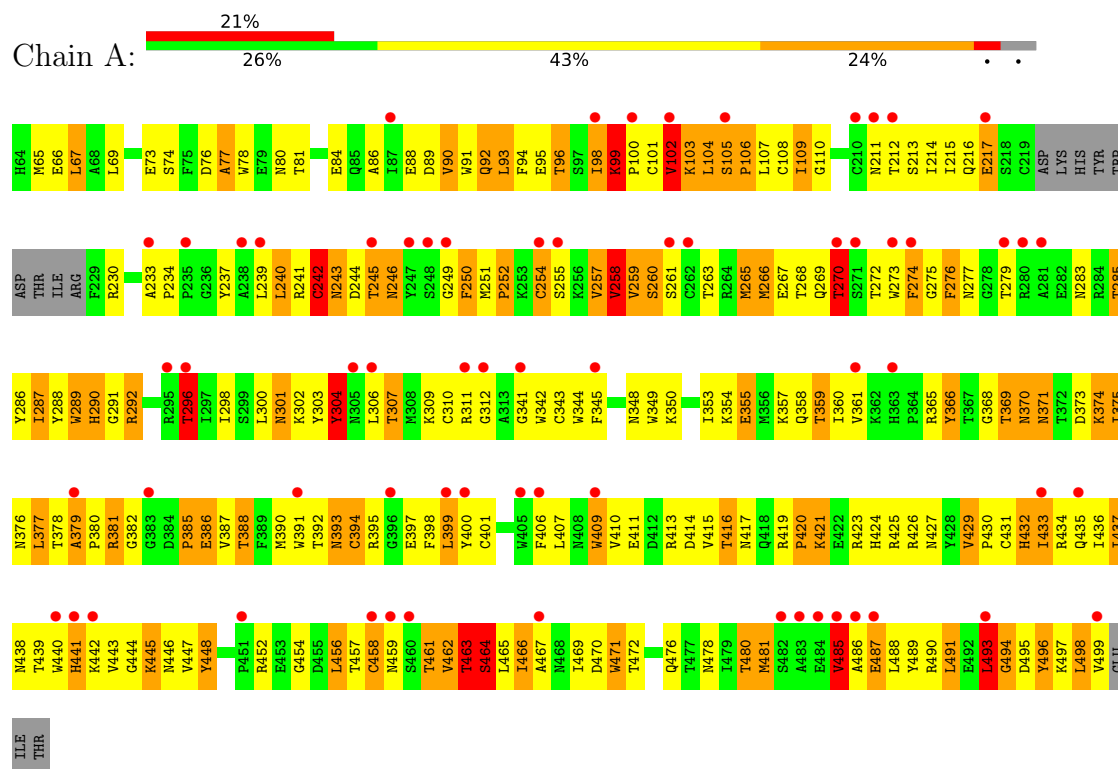


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	A	1	Total	C	N	O	0	0
			14	8	1	5		

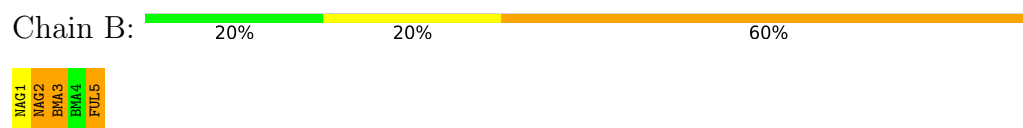
3 Residue-property plots

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

• Molecule 1: EXTERIOR MEMBRANE GLYCOPROTEIN GP120



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



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





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

Chain K:



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

Chain D:



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

Chain E:



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

Chain F:



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

Chain G:



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



- Molecule 9: beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  57% 43%

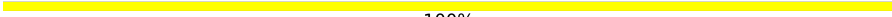
MAG1	MAG2	BMA3	BMA4	MAN5	BMA6	MAN7
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- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%

MAG1	MAG2	BMA3	MAN4	MAN5	MAN6
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- Molecule 11: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1	MAG2	BMA3	MAN4
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.05Å 108.05Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.58 – 4.00 25.58 – 4.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.58-4.00) 97.5 (25.58-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.346 , 0.354 0.347 , 0.356	Depositor DCC
R_{free} test set	279 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	174.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3140	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: BMA, FUL, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	2/2534 (0.1%)	1.16	24/3441 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	LEU	N-CA	5.02	1.52	1.45
1	A	102	VAL	C-N	5.01	1.40	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	TYR	N-CA-C	10.77	123.60	108.74
1	A	104	LEU	N-CA-C	9.06	123.82	109.50
1	A	106	PRO	N-CA-C	8.48	123.76	111.13
1	A	427	ASN	N-CA-C	7.96	121.57	109.23
1	A	409	TRP	N-CA-C	7.71	120.93	109.59
1	A	371	ASN	N-CA-C	7.65	118.36	108.34
1	A	250	PHE	N-CA-C	7.62	121.54	109.65
1	A	108	CYS	N-CA-C	7.24	117.53	108.19
1	A	103	LYS	N-CA-C	7.07	125.86	110.80
1	A	105	SER	CA-C-N	6.86	127.31	120.52
1	A	105	SER	C-N-CA	6.86	127.31	120.52
1	A	437	ILE	N-CA-C	6.66	116.21	106.55
1	A	258	VAL	N-CA-C	6.16	116.33	108.82
1	A	270	THR	N-CA-C	6.09	116.61	108.38
1	A	445	LYS	N-CA-C	5.89	118.23	108.99
1	A	377	LEU	N-CA-C	5.82	118.95	109.06
1	A	292	ARG	N-CA-C	-5.42	104.92	112.03
1	A	96	THR	N-CA-C	5.39	117.52	108.73
1	A	99	LYS	N-CA-C	5.34	121.62	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	VAL	N-CA-C	5.15	120.06	109.34
1	A	424	HIS	N-CA-C	5.15	117.56	108.24
1	A	289	TRP	N-CA-C	5.11	116.75	108.26
1	A	254	CYS	N-CA-C	5.09	116.68	110.41
1	A	296	THR	N-CA-C	5.01	114.76	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2470	0	2349	275	2
2	B	60	0	52	1	1
3	C	71	0	61	6	1
3	K	71	0	61	5	0
4	D	38	0	34	4	0
5	E	49	0	43	4	1
6	F	49	0	43	0	0
7	G	28	0	25	0	0
8	H	71	0	61	1	0
9	I	83	0	70	3	0
10	J	72	0	61	1	0
11	L	50	0	43	0	0
12	A	28	0	26	0	0
All	All	3140	0	2929	289	4

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 48.

All (289) 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:A:395:ARG:O	1:A:395:ARG:HG3	1.44	1.14
1:A:65:MET:HE1	1:A:240:LEU:HD21	1.26	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:HA	1:A:212:THR:HA	1.05	1.03
1:A:285:THR:HG23	1:A:302:LYS:HB2	1.40	1.03
1:A:489:TYR:O	1:A:493:LEU:HG	1.62	0.99
1:A:91:TRP:O	1:A:448:TYR:OH	1.80	0.98
1:A:290:HIS:HE1	1:A:292:ARG:HG2	1.31	0.96
1:A:437:ILE:O	1:A:445:LYS:HA	1.64	0.95
1:A:65:MET:CE	1:A:240:LEU:HD21	1.97	0.94
1:A:106:PRO:CA	1:A:212:THR:HA	1.98	0.93
1:A:237:TYR:OH	1:A:498:LEU:HB2	1.69	0.92
1:A:375:ILE:HG12	1:A:411:GLU:HB2	1.51	0.92
1:A:470:ASP:HB2	1:A:478:ASN:HB3	1.51	0.92
1:A:106:PRO:HA	1:A:212:THR:CA	1.99	0.91
1:A:306:LEU:O	1:A:462:VAL:HG21	1.71	0.90
1:A:80:ASN:HB3	1:A:84:GLU:HG2	1.53	0.90
1:A:244:ASP:O	1:A:245:THR:OG1	1.91	0.88
1:A:287:ILE:O	1:A:287:ILE:HG13	1.73	0.88
1:A:353:ILE:HG22	1:A:357:LYS:HE3	1.55	0.88
1:A:241:ARG:HG2	1:A:242:CYS:H	1.40	0.86
1:A:381:ARG:HH21	1:A:382:GLY:HA2	1.39	0.86
1:A:415:VAL:HG12	1:A:416:THR:H	1.41	0.86
1:A:380:PRO:HG2	1:A:385:PRO:HG3	1.57	0.85
1:A:65:MET:HE1	1:A:240:LEU:CD2	2.06	0.85
1:A:269:GLN:HE21	3:C:1:NAG:C8	1.89	0.85
1:A:269:GLN:HE21	3:C:1:NAG:H83	1.41	0.84
1:A:275:GLY:HA3	1:A:464:SER:HB2	1.60	0.84
1:A:496:TYR:HD1	1:A:496:TYR:C	1.85	0.84
1:A:395:ARG:O	1:A:395:ARG:CG	2.25	0.82
1:A:107:LEU:N	1:A:211:ASN:O	2.12	0.82
1:A:391:TRP:CZ2	1:A:393:ASN:HB2	2.15	0.82
1:A:258:VAL:HG12	1:A:259:VAL:H	1.46	0.81
1:A:306:LEU:O	1:A:462:VAL:CG2	2.28	0.80
1:A:105:SER:O	1:A:213:SER:N	2.14	0.80
1:A:269:GLN:HA	1:A:393:ASN:O	1.81	0.80
1:A:290:HIS:CE1	1:A:292:ARG:HG2	2.16	0.79
1:A:496:TYR:C	1:A:496:TYR:CD1	2.58	0.79
1:A:241:ARG:HG2	1:A:242:CYS:N	1.98	0.78
1:A:77:ALA:HA	1:A:80:ASN:HD22	1.48	0.78
1:A:266:MET:SD	1:A:398:PHE:HZ	2.07	0.77
1:A:80:ASN:CB	1:A:84:GLU:HG2	2.15	0.75
1:A:93:LEU:O	1:A:96:THR:HG22	1.88	0.74
9:I:5:MAN:H4	9:I:6:BMA:C1	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:CE2	1:A:349:TRP:CH2	2.75	0.73
4:D:1:NAG:H62	4:D:2:NAG:N2	2.03	0.73
1:A:289:TRP:NE1	1:A:291:GLY:HA2	2.04	0.73
1:A:94:PHE:CZ	1:A:265:MET:SD	2.82	0.73
1:A:435:GLN:O	1:A:447:VAL:HA	1.89	0.72
1:A:265:MET:HE1	1:A:485:VAL:HG13	1.70	0.72
1:A:381:ARG:NH2	1:A:382:GLY:HA2	2.04	0.72
1:A:273:TRP:CE3	1:A:481:MET:HG3	2.24	0.72
1:A:89:ASP:HA	1:A:92:GLN:HB3	1.72	0.72
1:A:486:ALA:O	1:A:490:ARG:HB2	1.90	0.72
1:A:283:ASN:HA	1:A:303:TYR:HB3	1.73	0.71
1:A:342:TRP:HA	1:A:429:VAL:O	1.90	0.71
1:A:354:LYS:O	1:A:358:GLN:N	2.23	0.71
1:A:435:GLN:OE1	1:A:435:GLN:N	2.24	0.71
1:A:437:ILE:HB	1:A:446:ASN:HB2	1.72	0.70
1:A:98:ILE:O	1:A:99:LYS:HG3	1.91	0.69
1:A:86:ALA:O	1:A:90:VAL:HB	1.92	0.69
1:A:290:HIS:HE1	1:A:292:ARG:CG	2.05	0.69
1:A:343:CYS:HB2	1:A:429:VAL:CG2	2.24	0.68
1:A:480:THR:O	1:A:481:MET:HB2	1.94	0.68
1:A:421:LYS:NZ	1:A:423:ARG:HH21	1.92	0.67
1:A:400:TYR:OH	1:A:437:ILE:HG23	1.95	0.66
1:A:415:VAL:HG12	1:A:416:THR:N	2.08	0.66
1:A:78:TRP:HH2	1:A:381:ARG:NH1	1.93	0.66
1:A:287:ILE:O	1:A:287:ILE:CG1	2.43	0.66
1:A:421:LYS:HZ2	1:A:423:ARG:HH21	1.41	0.66
1:A:290:HIS:ND1	1:A:290:HIS:C	2.54	0.65
1:A:240:LEU:O	1:A:497:LYS:HB2	1.97	0.65
1:A:273:TRP:HB2	1:A:390:MET:SD	2.37	0.65
1:A:241:ARG:HH11	1:A:494:GLY:HA3	1.61	0.64
1:A:269:GLN:NE2	3:C:1:NAG:H83	2.13	0.64
1:A:349:TRP:CZ2	1:A:353:ILE:HD11	2.33	0.64
1:A:289:TRP:HE1	1:A:291:GLY:HA2	1.63	0.63
1:A:487:GLU:HA	1:A:490:ARG:HB3	1.80	0.63
1:A:245:THR:HG22	1:A:246:ASN:H	1.62	0.63
1:A:241:ARG:NH1	1:A:494:GLY:HA3	2.13	0.63
1:A:268:THR:HG22	1:A:269:GLN:H	1.62	0.63
1:A:471:TRP:HA	1:A:476:GLN:O	1.98	0.63
1:A:275:GLY:CA	1:A:464:SER:HB2	2.29	0.63
1:A:343:CYS:HB2	1:A:429:VAL:HG21	1.80	0.62
3:K:1:NAG:H61	3:K:6:FUL:O2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:TRP:CE2	5:E:1:NAG:H81	2.34	0.62
1:A:289:TRP:HE1	1:A:296:THR:HG21	1.65	0.62
1:A:268:THR:HG22	1:A:269:GLN:N	2.14	0.62
1:A:302:LYS:HZ2	1:A:304:TYR:H	1.48	0.62
1:A:307:THR:O	1:A:345:PHE:HA	1.99	0.62
1:A:394:CYS:O	1:A:395:ARG:HB3	2.00	0.62
1:A:273:TRP:HD1	1:A:274:PHE:CZ	2.18	0.62
1:A:307:THR:OG1	9:I:2:NAG:H83	2.00	0.62
1:A:243:ASN:CG	1:A:244:ASP:H	2.08	0.61
1:A:273:TRP:CZ3	1:A:481:MET:HG3	2.35	0.61
1:A:406:PHE:O	1:A:409:TRP:NE1	2.33	0.61
1:A:266:MET:SD	1:A:398:PHE:CZ	2.91	0.61
1:A:439:THR:HB	1:A:442:LYS:O	2.01	0.60
1:A:355:GLU:O	1:A:359:THR:N	2.33	0.60
1:A:290:HIS:C	1:A:290:HIS:HD1	2.08	0.60
1:A:496:TYR:HD1	1:A:496:TYR:O	1.84	0.60
1:A:285:THR:OG1	1:A:302:LYS:HD3	2.01	0.60
1:A:244:ASP:C	1:A:245:THR:OG1	2.45	0.60
1:A:488:LEU:O	1:A:491:LEU:HB2	2.02	0.59
1:A:269:GLN:NE2	3:C:1:NAG:C8	2.63	0.59
1:A:381:ARG:NH2	1:A:382:GLY:CA	2.65	0.59
1:A:400:TYR:O	1:A:431:CYS:HB3	2.02	0.59
1:A:268:THR:HG22	1:A:269:GLN:HG2	1.85	0.58
1:A:391:TRP:CD1	1:A:392:THR:H	2.21	0.58
1:A:241:ARG:O	1:A:257:VAL:HG12	2.04	0.58
1:A:342:TRP:CD1	1:A:430:PRO:HA	2.39	0.57
1:A:306:LEU:C	1:A:462:VAL:HG21	2.30	0.57
1:A:234:PRO:HG3	1:A:263:THR:N	2.19	0.57
1:A:269:GLN:CA	1:A:393:ASN:O	2.50	0.57
1:A:241:ARG:CG	1:A:242:CYS:H	2.15	0.56
1:A:385:PRO:O	1:A:386:GLU:HB2	2.04	0.56
1:A:498:LEU:O	1:A:499:VAL:HB	2.05	0.56
1:A:302:LYS:NZ	1:A:304:TYR:H	2.04	0.56
1:A:401:CYS:HA	1:A:431:CYS:HA	1.87	0.56
1:A:486:ALA:HB1	1:A:490:ARG:HH21	1.70	0.56
1:A:365:ARG:O	1:A:366:TYR:C	2.49	0.56
1:A:303:TYR:O	1:A:304:TYR:O	2.24	0.55
1:A:237:TYR:CZ	1:A:498:LEU:HB2	2.41	0.55
1:A:437:ILE:HD12	1:A:446:ASN:HB2	1.87	0.55
1:A:417:ASN:HA	1:A:420:PRO:HG2	1.86	0.55
1:A:309:LYS:O	1:A:344:TRP:HD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TYR:O	1:A:300:LEU:HA	2.06	0.55
1:A:498:LEU:O	1:A:499:VAL:CB	2.54	0.55
1:A:270:THR:N	1:A:393:ASN:O	2.39	0.54
1:A:259:VAL:O	1:A:260:SER:HB2	2.07	0.54
1:A:265:MET:HE2	1:A:488:LEU:HD23	1.90	0.54
1:A:437:ILE:HB	1:A:446:ASN:CB	2.37	0.54
1:A:269:GLN:HE21	3:C:1:NAG:H82	1.69	0.54
1:A:421:LYS:HD2	1:A:423:ARG:HE	1.72	0.54
1:A:241:ARG:CG	1:A:242:CYS:N	2.71	0.53
1:A:102:VAL:HG22	1:A:103:LYS:N	2.23	0.53
1:A:237:TYR:OH	1:A:498:LEU:CB	2.51	0.53
1:A:380:PRO:HG2	1:A:385:PRO:CG	2.34	0.53
2:B:2:NAG:H61	2:B:3:BMA:H2	1.91	0.53
1:A:102:VAL:HG22	1:A:103:LYS:H	1.73	0.53
1:A:498:LEU:O	1:A:499:VAL:HG23	2.09	0.53
1:A:391:TRP:CG	1:A:392:THR:N	2.77	0.52
1:A:286:TYR:CD2	1:A:288:TYR:CE1	2.96	0.52
1:A:489:TYR:C	1:A:491:LEU:H	2.18	0.52
1:A:234:PRO:HG3	1:A:263:THR:H	1.73	0.52
1:A:306:LEU:HD23	1:A:462:VAL:HG11	1.91	0.52
1:A:215:ILE:HG22	1:A:216:GLN:N	2.25	0.52
1:A:273:TRP:CE3	1:A:481:MET:CG	2.93	0.52
1:A:415:VAL:CG1	1:A:416:THR:H	2.16	0.52
1:A:306:LEU:O	1:A:462:VAL:HG23	2.09	0.51
4:D:1:NAG:H62	4:D:2:NAG:C7	2.41	0.51
1:A:309:LYS:HG3	1:A:459:ASN:HA	1.92	0.51
1:A:357:LYS:O	1:A:361:VAL:HG23	2.11	0.51
1:A:354:LYS:O	1:A:358:GLN:HG3	2.11	0.51
3:K:1:NAG:C6	3:K:6:FUL:O2	2.59	0.51
1:A:80:ASN:CG	1:A:81:THR:H	2.18	0.50
1:A:77:ALA:HA	1:A:80:ASN:ND2	2.23	0.50
1:A:104:LEU:HB3	1:A:214:ILE:HG12	1.93	0.50
1:A:273:TRP:CZ3	1:A:481:MET:CG	2.95	0.50
1:A:437:ILE:CD1	1:A:446:ASN:HB2	2.40	0.50
1:A:269:GLN:HA	1:A:393:ASN:C	2.36	0.50
1:A:274:PHE:CE2	1:A:349:TRP:HH2	2.28	0.50
1:A:311:ARG:HB2	1:A:344:TRP:HE1	1.77	0.50
1:A:447:VAL:O	1:A:448:TYR:CG	2.64	0.50
1:A:109:ILE:O	1:A:499:VAL:HG22	2.11	0.50
1:A:273:TRP:CD1	1:A:274:PHE:CZ	2.99	0.50
1:A:357:LYS:HE2	1:A:411:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HE	1:A:452:ARG:HA	1.76	0.50
1:A:432:HIS:O	1:A:434:ARG:HG2	2.11	0.50
1:A:311:ARG:HG3	1:A:344:TRP:NE1	2.27	0.50
1:A:388:THR:HB	1:A:407:LEU:HD13	1.93	0.50
1:A:463:THR:HG22	1:A:464:SER:N	2.27	0.50
1:A:310:CYS:N	1:A:458:CYS:O	2.45	0.50
1:A:490:ARG:HG3	1:A:495:ASP:HA	1.92	0.50
1:A:381:ARG:HH21	1:A:382:GLY:CA	2.16	0.50
5:E:2:NAG:O3	5:E:3:MAN:H5	2.11	0.50
1:A:239:LEU:O	1:A:260:SER:HB3	2.12	0.49
1:A:78:TRP:HH2	1:A:381:ARG:HH11	1.60	0.49
1:A:243:ASN:OD1	1:A:244:ASP:N	2.39	0.49
1:A:391:TRP:CD1	1:A:392:THR:N	2.80	0.49
1:A:90:VAL:O	1:A:94:PHE:CD1	2.66	0.49
1:A:437:ILE:N	1:A:446:ASN:O	2.30	0.49
3:K:2:NAG:O3	3:K:3:BMA:H62	2.13	0.49
1:A:480:THR:O	1:A:481:MET:HE2	2.13	0.49
1:A:487:GLU:HA	1:A:490:ARG:CB	2.43	0.49
1:A:395:ARG:HG2	1:A:456:LEU:HD13	1.95	0.48
1:A:397:GLU:O	1:A:399:LEU:HG	2.12	0.48
1:A:376:ASN:OD1	1:A:410:VAL:HG12	2.13	0.48
4:D:1:NAG:H62	4:D:2:NAG:HN2	1.74	0.48
1:A:258:VAL:HG12	1:A:259:VAL:N	2.22	0.48
1:A:496:TYR:CD1	1:A:496:TYR:O	2.64	0.48
5:E:2:NAG:O6	5:E:3:MAN:H2	2.14	0.48
1:A:466:ILE:HD13	1:A:481:MET:SD	2.54	0.48
1:A:273:TRP:CZ2	1:A:481:MET:HG2	2.49	0.47
1:A:391:TRP:HZ2	1:A:393:ASN:OD1	1.98	0.47
1:A:234:PRO:HD3	1:A:263:THR:H	1.79	0.47
1:A:306:LEU:HD22	1:A:349:TRP:CZ3	2.50	0.47
1:A:78:TRP:CH2	1:A:381:ARG:NH1	2.80	0.47
1:A:243:ASN:OD1	3:K:1:NAG:O5	2.33	0.47
1:A:353:ILE:HD13	1:A:353:ILE:HA	1.82	0.47
4:D:2:NAG:HN2	4:D:3:FUL:C1	2.28	0.47
1:A:399:LEU:HA	1:A:433:ILE:HG23	1.97	0.47
1:A:77:ALA:O	1:A:80:ASN:HB2	2.15	0.46
1:A:360:ILE:HD11	1:A:469:ILE:CD1	2.45	0.46
1:A:242:CYS:O	1:A:243:ASN:HB2	2.15	0.46
1:A:251:MET:N	1:A:252:PRO:HD3	2.31	0.46
1:A:289:TRP:NE1	1:A:296:THR:HG21	2.30	0.46
1:A:277:ASN:HA	1:A:461:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PHE:HD2	1:A:407:LEU:HG	1.80	0.46
1:A:249:GLY:O	1:A:250:PHE:HD1	1.99	0.46
1:A:416:THR:O	1:A:420:PRO:HG2	2.15	0.46
1:A:73:GLU:HB2	1:A:292:ARG:NH1	2.31	0.46
1:A:311:ARG:HE	1:A:344:TRP:HZ2	1.62	0.45
1:A:349:TRP:CE2	1:A:406:PHE:CZ	3.05	0.45
1:A:395:ARG:CB	1:A:456:LEU:HD13	2.46	0.45
1:A:273:TRP:HD1	1:A:274:PHE:CE2	2.35	0.45
1:A:277:ASN:CG	1:A:461:THR:HG21	2.42	0.45
1:A:343:CYS:HB2	1:A:429:VAL:HG23	1.97	0.45
1:A:290:HIS:CE1	1:A:292:ARG:CG	2.90	0.45
1:A:440:TRP:CG	1:A:441:HIS:H	2.35	0.45
1:A:489:TYR:C	1:A:491:LEU:N	2.73	0.45
1:A:349:TRP:NE1	1:A:353:ILE:HG13	2.32	0.45
1:A:413:ARG:HG2	1:A:414:ASP:OD2	2.16	0.45
1:A:493:LEU:CD1	1:A:496:TYR:HA	2.47	0.45
1:A:419:ARG:N	1:A:420:PRO:CD	2.79	0.45
1:A:374:LYS:HE2	8:H:2:NAG:H81	1.99	0.44
1:A:463:THR:O	1:A:465:LEU:N	2.51	0.44
1:A:393:ASN:HD22	1:A:394:CYS:N	2.15	0.44
1:A:486:ALA:HB1	1:A:496:TYR:CD2	2.52	0.44
1:A:378:THR:HG22	1:A:379:ALA:N	2.32	0.44
1:A:469:ILE:HA	1:A:478:ASN:O	2.17	0.44
1:A:274:PHE:HE2	1:A:349:TRP:CH2	2.35	0.44
1:A:426:ARG:HH11	1:A:426:ARG:HB3	1.83	0.44
1:A:471:TRP:NE1	5:E:1:NAG:O7	2.50	0.44
3:C:3:BMA:O4	3:C:5:MAN:H2	2.18	0.44
1:A:434:ARG:HH11	1:A:438:ASN:ND2	2.15	0.44
1:A:485:VAL:O	1:A:488:LEU:HB3	2.18	0.44
1:A:105:SER:HB3	1:A:106:PRO:HD2	1.99	0.44
1:A:109:ILE:HB	1:A:499:VAL:HG22	2.00	0.44
1:A:244:ASP:HA	3:K:1:NAG:O6	2.18	0.44
1:A:273:TRP:HB3	1:A:274:PHE:CE2	2.53	0.44
1:A:285:THR:CG2	1:A:302:LYS:HB2	2.29	0.44
1:A:303:TYR:C	1:A:303:TYR:CD2	2.95	0.44
1:A:88:GLU:HA	1:A:91:TRP:CZ2	2.53	0.43
1:A:102:VAL:C	1:A:103:LYS:HG2	2.43	0.43
1:A:391:TRP:HE1	1:A:398:PHE:HA	1.82	0.43
1:A:98:ILE:O	1:A:99:LYS:CG	2.63	0.43
1:A:302:LYS:HG3	1:A:304:TYR:H	1.83	0.43
1:A:498:LEU:O	1:A:499:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:O	1:A:371:ASN:ND2	2.52	0.43
1:A:273:TRP:CE2	1:A:481:MET:HG2	2.53	0.43
1:A:80:ASN:HB3	1:A:84:GLU:CG	2.36	0.43
1:A:80:ASN:CG	1:A:81:THR:N	2.77	0.43
1:A:465:LEU:HD23	1:A:465:LEU:C	2.44	0.43
1:A:107:LEU:O	1:A:211:ASN:O	2.37	0.43
1:A:353:ILE:HG22	1:A:357:LYS:CE	2.38	0.43
1:A:462:VAL:O	1:A:463:THR:CB	2.66	0.43
1:A:105:SER:HB3	1:A:106:PRO:CD	2.49	0.42
1:A:342:TRP:CD1	1:A:429:VAL:O	2.72	0.42
1:A:349:TRP:NE1	1:A:353:ILE:CG1	2.82	0.42
1:A:493:LEU:HB2	1:A:494:GLY:H	1.50	0.42
10:J:4:MAN:O3	10:J:5:MAN:C1	2.67	0.42
1:A:275:GLY:N	1:A:464:SER:O	2.48	0.42
1:A:470:ASP:N	1:A:478:ASN:O	2.47	0.42
1:A:215:ILE:HG22	1:A:216:GLN:H	1.85	0.42
1:A:302:LYS:HG3	1:A:304:TYR:N	2.34	0.42
1:A:290:HIS:ND1	1:A:290:HIS:O	2.53	0.42
9:I:5:MAN:C4	9:I:6:BMA:C1	2.87	0.42
1:A:273:TRP:HB3	1:A:274:PHE:CD2	2.55	0.41
1:A:437:ILE:HG21	1:A:446:ASN:HD22	1.85	0.41
1:A:466:ILE:HG12	1:A:467:ALA:N	2.34	0.41
1:A:90:VAL:HG22	1:A:94:PHE:CE1	2.56	0.41
1:A:241:ARG:HD3	1:A:493:LEU:CB	2.49	0.41
1:A:105:SER:C	1:A:212:THR:OG1	2.63	0.41
1:A:273:TRP:CH2	1:A:481:MET:HG2	2.55	0.41
1:A:304:TYR:CE1	1:A:348:ASN:HB2	2.56	0.41
1:A:417:ASN:HA	1:A:420:PRO:CG	2.51	0.41
1:A:441:HIS:H	1:A:441:HIS:CD2	2.37	0.41
1:A:496:TYR:O	1:A:497:LYS:HG3	2.21	0.41
1:A:289:TRP:CD1	1:A:289:TRP:C	2.99	0.41
1:A:357:LYS:HA	1:A:360:ILE:HG22	2.03	0.41
1:A:439:THR:HB	1:A:444:GLY:H	1.86	0.41
1:A:309:LYS:HG2	1:A:458:CYS:O	2.22	0.40
1:A:369:THR:HG22	1:A:370:ASN:H	1.86	0.40
1:A:276:PHE:HB3	1:A:461:THR:HG23	2.03	0.40
1:A:98:ILE:O	1:A:99:LYS:CB	2.69	0.40
1:A:276:PHE:CD2	1:A:461:THR:O	2.74	0.40
1:A:301:ASN:HD22	1:A:463:THR:CG2	2.34	0.40
1:A:309:LYS:O	1:A:344:TRP:CD1	2.72	0.40
1:A:376:ASN:OD1	1:A:410:VAL:HA	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:436:ILE:CD1[4_455]	1.88	0.32
1:A:66:GLU:OE1	1:A:445:LYS:CB[4_455]	2.02	0.18
2:B:5:FUL:O3	2:B:5:FUL:O3[8_555]	2.14	0.06
3:C:4:MAN:O3	5:E:4:FUL:O3[6_555]	2.17	0.03

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	300/316 (95%)	204 (68%)	57 (19%)	39 (13%)	0 4

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	100	PRO
1	A	233	ALA
1	A	304	TYR
1	A	386	GLU
1	A	463	THR
1	A	481	MET
1	A	76	ASP
1	A	77	ALA
1	A	101	CYS
1	A	260	SER
1	A	265	MET
1	A	276	PHE
1	A	312	GLY
1	A	341	GLY
1	A	366	TYR
1	A	385	PRO

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Mol	Chain	Res	Type
1	A	454	GLY
1	A	493	LEU
1	A	217	GLU
1	A	242	CYS
1	A	243	ASN
1	A	246	ASN
1	A	252	PRO
1	A	485	VAL
1	A	261	SER
1	A	279	THR
1	A	368	GLY
1	A	379	ALA
1	A	464	SER
1	A	74	SER
1	A	98	ILE
1	A	102	VAL
1	A	109	ILE
1	A	255	SER
1	A	420	PRO
1	A	443	VAL
1	A	110	GLY
1	A	494	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/284 (96%)	205 (75%)	67 (25%)	1 4

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	69	LEU
1	A	90	VAL
1	A	92	GLN

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Mol	Chain	Res	Type
1	A	93	LEU
1	A	95	GLU
1	A	217	GLU
1	A	230	ARG
1	A	240	LEU
1	A	242	CYS
1	A	245	THR
1	A	254	CYS
1	A	257	VAL
1	A	258	VAL
1	A	259	VAL
1	A	266	MET
1	A	267	GLU
1	A	270	THR
1	A	272	THR
1	A	274	PHE
1	A	285	THR
1	A	287	ILE
1	A	290	HIS
1	A	296	THR
1	A	298	ILE
1	A	301	ASN
1	A	304	TYR
1	A	307	THR
1	A	350	LYS
1	A	355	GLU
1	A	359	THR
1	A	369	THR
1	A	370	ASN
1	A	373	ASP
1	A	374	LYS
1	A	375	ILE
1	A	377	LEU
1	A	381	ARG
1	A	387	VAL
1	A	388	THR
1	A	393	ASN
1	A	394	CYS
1	A	399	LEU
1	A	416	THR
1	A	421	LYS
1	A	425	ARG

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Mol	Chain	Res	Type
1	A	429	VAL
1	A	432	HIS
1	A	433	ILE
1	A	441	HIS
1	A	456	LEU
1	A	457	THR
1	A	458	CYS
1	A	461	THR
1	A	462	VAL
1	A	463	THR
1	A	464	SER
1	A	466	ILE
1	A	471	TRP
1	A	472	THR
1	A	480	THR
1	A	485	VAL
1	A	487	GLU
1	A	491	LEU
1	A	493	LEU
1	A	496	TYR
1	A	498	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	92	GLN
1	A	209	HIS
1	A	269	GLN
1	A	348	ASN
1	A	393	ASN
1	A	417	ASN
1	A	438	ASN
1	A	441	HIS
1	A	446	ASN
1	A	468	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 ⓘ

53 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	B	1	1,2	14,14,15	0.56	0	17,19,21	1.39	1 (5%)
2	NAG	B	2	2	14,14,15	0.74	0	17,19,21	1.24	2 (11%)
2	BMA	B	3	2	11,11,12	0.46	0	15,15,17	1.20	2 (13%)
2	BMA	B	4	2	11,11,12	0.68	0	15,15,17	0.78	0
2	FUL	B	5	2	10,10,11	0.47	0	14,14,16	0.98	1 (7%)
3	NAG	C	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	1.96	5 (29%)
3	NAG	C	2	3	14,14,15	0.77	0	17,19,21	1.43	2 (11%)
3	BMA	C	3	3	11,11,12	0.55	0	15,15,17	2.05	3 (20%)
3	MAN	C	4	3	11,11,12	0.49	0	15,15,17	1.57	2 (13%)
3	MAN	C	5	3	11,11,12	0.56	0	15,15,17	1.24	2 (13%)
3	FUL	C	6	3	10,10,11	0.54	0	14,14,16	1.59	2 (14%)
4	NAG	D	1	1,4	14,14,15	0.48	0	17,19,21	1.43	3 (17%)
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	1.45	4 (23%)
4	FUL	D	3	4	10,10,11	0.49	0	14,14,16	1.37	3 (21%)
5	NAG	E	1	1,5	14,14,15	0.53	0	17,19,21	1.78	3 (17%)
5	NAG	E	2	5	14,14,15	0.70	0	17,19,21	1.47	3 (17%)
5	MAN	E	3	5	11,11,12	0.47	0	15,15,17	1.38	2 (13%)
5	FUL	E	4	5	10,10,11	0.37	0	14,14,16	0.86	0
6	NAG	F	1	1,6	14,14,15	0.56	0	17,19,21	1.80	5 (29%)
6	NAG	F	2	6	14,14,15	0.43	0	17,19,21	1.40	3 (17%)
6	BMA	F	3	6	11,11,12	0.34	0	15,15,17	1.28	2 (13%)
6	FUL	F	4	6	10,10,11	0.54	0	14,14,16	1.36	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	1	1,7	14,14,15	0.31	0	17,19,21	1.27	2 (11%)
7	NAG	G	2	7	14,14,15	0.71	0	17,19,21	1.21	2 (11%)
8	NAG	H	1	1,8	14,14,15	0.35	0	17,19,21	1.78	3 (17%)
8	NAG	H	2	8	14,14,15	0.56	0	17,19,21	1.55	2 (11%)
8	BMA	H	3	8	11,11,12	0.57	0	15,15,17	1.38	2 (13%)
8	BMA	H	4	8	11,11,12	0.63	0	15,15,17	1.48	2 (13%)
8	MAN	H	5	8	11,11,12	0.53	0	15,15,17	1.42	2 (13%)
8	FUL	H	6	8	10,10,11	0.46	0	14,14,16	1.40	3 (21%)
9	NAG	I	1	1,9	14,14,15	0.52	0	17,19,21	1.20	2 (11%)
9	NAG	I	2	9	14,14,15	0.48	0	17,19,21	2.69	5 (29%)
9	BMA	I	3	9	11,11,12	0.62	0	15,15,17	2.44	4 (26%)
9	BMA	I	4	9	11,11,12	0.59	0	15,15,17	1.77	3 (20%)
9	MAN	I	5	9	11,11,12	0.68	0	15,15,17	1.52	2 (13%)
9	BMA	I	6	9	11,11,12	0.73	0	15,15,17	1.09	1 (6%)
9	MAN	I	7	9	11,11,12	0.58	0	15,15,17	1.94	5 (33%)
10	NAG	J	1	1,10	14,14,15	0.55	0	17,19,21	1.55	3 (17%)
10	NAG	J	2	10	14,14,15	0.74	1 (7%)	17,19,21	1.49	3 (17%)
10	BMA	J	3	10	11,11,12	0.71	0	15,15,17	1.46	2 (13%)
10	MAN	J	4	10	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
10	MAN	J	5	10	11,11,12	0.56	0	15,15,17	2.01	3 (20%)
10	MAN	J	6	10	11,11,12	0.53	0	15,15,17	1.21	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.47	0	17,19,21	1.27	2 (11%)
3	NAG	K	2	3	14,14,15	0.42	0	17,19,21	1.37	2 (11%)
3	BMA	K	3	3	11,11,12	0.63	0	15,15,17	1.77	3 (20%)
3	MAN	K	4	3	11,11,12	0.64	0	15,15,17	1.40	2 (13%)
3	MAN	K	5	3	11,11,12	0.59	0	15,15,17	1.83	3 (20%)
3	FUL	K	6	3	10,10,11	0.51	0	14,14,16	1.69	4 (28%)
11	NAG	L	1	11,1	14,14,15	0.56	0	17,19,21	1.47	3 (17%)
11	NAG	L	2	11	14,14,15	0.44	0	17,19,21	1.23	1 (5%)
11	BMA	L	3	11	11,11,12	0.46	0	15,15,17	1.11	1 (6%)
11	MAN	L	4	11	11,11,12	0.57	0	15,15,17	1.24	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	5/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	FUL	B	5	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	FUL	C	6	3	-	-	0/1/1/1
4	NAG	D	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	FUL	D	3	4	-	-	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	MAN	E	3	5	-	0/2/19/22	0/1/1/1
5	FUL	E	4	5	-	-	0/1/1/1
6	NAG	F	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	FUL	F	4	6	-	-	0/1/1/1
7	NAG	G	1	1,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
8	NAG	H	1	1,8	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	H	2	8	-	4/6/23/26	0/1/1/1
8	BMA	H	3	8	-	1/2/19/22	0/1/1/1
8	BMA	H	4	8	-	0/2/19/22	0/1/1/1
8	MAN	H	5	8	-	0/2/19/22	0/1/1/1
8	FUL	H	6	8	-	-	0/1/1/1
9	NAG	I	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	BMA	I	4	9	-	2/2/19/22	0/1/1/1
9	MAN	I	5	9	-	2/2/19/22	0/1/1/1
9	BMA	I	6	9	-	1/2/19/22	0/1/1/1
9	MAN	I	7	9	-	0/2/19/22	0/1/1/1
10	NAG	J	1	1,10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	2/2/19/22	0/1/1/1
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
10	MAN	J	5	10	-	0/2/19/22	0/1/1/1
10	MAN	J	6	10	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	MAN	K	5	3	-	0/2/19/22	0/1/1/1
3	FUL	K	6	3	-	-	0/1/1/1
11	NAG	L	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	L	2	11	-	2/6/23/26	0/1/1/1
11	BMA	L	3	11	-	2/2/19/22	0/1/1/1
11	MAN	L	4	11	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-2.12	1.40	1.43
10	J	2	NAG	C1-C2	2.10	1.55	1.52

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	2	NAG	C4-C3-C2	-7.66	99.79	111.02
9	I	3	BMA	C1-O5-C5	6.31	120.64	112.19
3	C	3	BMA	C1-C2-C3	5.72	117.97	109.64
8	H	1	NAG	C1-O5-C5	5.24	119.21	112.19
10	J	1	NAG	C1-O5-C5	4.99	118.87	112.19
10	J	5	MAN	C1-O5-C5	4.75	118.55	112.19
5	E	1	NAG	C2-N2-C7	4.75	129.26	122.90
3	K	5	MAN	C1-O5-C5	4.71	118.50	112.19
8	H	2	NAG	C4-C3-C2	4.68	117.88	111.02
9	I	4	BMA	C1-C2-C3	-4.62	102.92	109.64
3	C	4	MAN	C1-O5-C5	4.54	118.26	112.19
10	J	5	MAN	C1-C2-C3	4.53	116.23	109.64
3	K	3	BMA	C1-O5-C5	4.41	118.10	112.19
3	K	2	NAG	C1-O5-C5	4.31	117.96	112.19
3	K	6	FUL	C3-C4-C5	4.28	116.33	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	7	MAN	C3-C4-C5	4.28	117.98	110.23
3	C	1	NAG	C3-C4-C5	4.27	117.98	110.23
9	I	3	BMA	C1-C2-C3	4.19	115.74	109.64
3	C	2	NAG	C4-C3-C2	4.11	117.04	111.02
10	J	6	MAN	C1-O5-C5	4.10	117.68	112.19
2	B	1	NAG	O5-C1-C2	-4.10	104.95	111.29
9	I	2	NAG	C1-O5-C5	4.06	117.63	112.19
6	F	1	NAG	C3-C4-C5	3.99	117.47	110.23
9	I	5	MAN	C1-O5-C5	3.92	117.43	112.19
9	I	7	MAN	C1-O5-C5	3.92	117.43	112.19
3	C	3	BMA	C1-O5-C5	3.88	117.39	112.19
9	I	2	NAG	O4-C4-C5	3.84	118.79	109.32
3	C	6	FUL	C3-C4-C5	3.77	115.55	109.81
7	G	1	NAG	O5-C1-C2	-3.72	105.54	111.29
5	E	3	MAN	C1-C2-C3	3.69	115.02	109.64
10	J	3	BMA	C1-C2-C3	3.67	114.99	109.64
8	H	5	MAN	C1-O5-C5	3.67	117.10	112.19
3	K	5	MAN	C3-C4-C5	3.64	116.84	110.23
5	E	2	NAG	C4-C3-C2	3.64	116.35	111.02
7	G	2	NAG	C4-C3-C2	3.63	116.34	111.02
11	L	4	MAN	C1-O5-C5	3.63	117.05	112.19
8	H	4	BMA	C1-O5-C5	3.59	116.99	112.19
9	I	2	NAG	C1-C2-N2	3.57	116.05	110.43
4	D	2	NAG	C2-N2-C7	3.56	127.67	122.90
6	F	1	NAG	O5-C1-C2	-3.50	105.88	111.29
11	L	1	NAG	C1-O5-C5	3.44	116.80	112.19
8	H	5	MAN	C1-C2-C3	3.40	114.60	109.64
3	C	6	FUL	C2-C3-C4	3.39	116.83	110.86
6	F	2	NAG	C1-C2-N2	3.33	115.68	110.43
10	J	5	MAN	O5-C1-C2	3.31	118.69	110.79
10	J	2	NAG	C2-N2-C7	3.31	127.33	122.90
9	I	3	BMA	C3-C4-C5	3.30	116.21	110.23
3	K	4	MAN	C1-C2-C3	3.23	114.35	109.64
8	H	4	BMA	O3-C3-C2	3.20	116.59	110.05
3	K	1	NAG	C1-O5-C5	3.18	116.45	112.19
5	E	1	NAG	O5-C5-C6	3.18	113.85	107.66
11	L	2	NAG	O5-C1-C2	-3.17	106.38	111.29
2	B	2	NAG	C4-C3-C2	3.15	115.63	111.02
8	H	3	BMA	O5-C5-C6	3.13	113.76	107.66
11	L	3	BMA	C1-O5-C5	3.09	116.33	112.19
3	C	1	NAG	C4-C3-C2	3.09	115.54	111.02
3	K	3	BMA	C1-C2-C3	3.08	114.14	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	NAG	C4-C3-C2	3.05	115.48	111.02
11	L	1	NAG	O5-C1-C2	-3.04	106.58	111.29
9	I	7	MAN	C2-C3-C4	3.00	116.14	110.86
6	F	4	FUL	C3-C4-C5	2.99	114.36	109.81
6	F	3	BMA	C3-C4-C5	2.99	115.65	110.23
3	C	5	MAN	C1-C2-C3	2.99	113.99	109.64
2	B	2	NAG	C1-O5-C5	2.98	116.18	112.19
3	K	4	MAN	C1-O5-C5	2.95	116.14	112.19
10	J	3	BMA	O5-C5-C6	2.94	113.39	107.66
3	C	1	NAG	C2-N2-C7	-2.88	119.04	122.90
6	F	2	NAG	C2-N2-C7	2.88	126.76	122.90
3	C	1	NAG	O5-C1-C2	-2.86	106.86	111.29
8	H	2	NAG	C3-C4-C5	2.82	115.35	110.23
8	H	6	FUL	C1-O5-C5	2.81	119.58	112.97
2	B	3	BMA	O5-C5-C6	2.79	113.09	107.66
9	I	1	NAG	O5-C1-C2	-2.77	107.01	111.29
9	I	2	NAG	O4-C4-C3	2.72	116.80	110.38
6	F	1	NAG	C1-O5-C5	2.72	115.84	112.19
8	H	1	NAG	C1-C2-N2	-2.69	106.20	110.43
8	H	6	FUL	O5-C5-C4	2.67	114.36	109.55
6	F	4	FUL	O5-C5-C4	2.67	114.35	109.55
3	K	5	MAN	O5-C5-C4	2.66	117.29	110.83
9	I	1	NAG	C1-O5-C5	2.65	115.73	112.19
3	C	5	MAN	C1-O5-C5	2.64	115.72	112.19
9	I	3	BMA	O3-C3-C2	2.62	115.39	110.05
9	I	6	BMA	C3-C4-C5	2.57	114.90	110.23
4	D	3	FUL	C1-C2-C3	2.51	113.31	109.64
10	J	1	NAG	O5-C1-C2	-2.51	107.41	111.29
3	K	3	BMA	O5-C5-C6	2.51	112.54	107.66
9	I	5	MAN	O4-C4-C5	2.47	115.41	109.32
5	E	2	NAG	C2-N2-C7	2.45	126.18	122.90
9	I	4	BMA	O2-C2-C3	2.44	115.22	110.15
4	D	2	NAG	C1-C2-N2	2.44	114.28	110.43
8	H	3	BMA	C1-C2-C3	2.42	113.17	109.64
3	C	2	NAG	C2-N2-C7	2.41	126.13	122.90
9	I	4	BMA	C1-O5-C5	2.40	115.40	112.19
5	E	3	MAN	C1-O5-C5	2.36	115.35	112.19
6	F	2	NAG	C1-O5-C5	2.36	115.35	112.19
2	B	3	BMA	C3-C4-C5	-2.33	106.00	110.23
2	B	5	FUL	O5-C5-C4	2.33	113.74	109.55
4	D	3	FUL	C3-C4-C5	2.29	113.30	109.81
3	C	4	MAN	C3-C4-C5	2.28	114.37	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	NAG	C4-C3-C2	-2.28	107.68	111.02
11	L	4	MAN	C1-C2-C3	2.26	112.94	109.64
9	I	7	MAN	C1-C2-C3	2.26	112.93	109.64
10	J	4	MAN	O2-C2-C3	2.22	114.75	110.15
11	L	1	NAG	C1-C2-N2	-2.21	106.95	110.43
7	G	2	NAG	O5-C5-C4	-2.20	105.47	110.83
4	D	1	NAG	C4-C3-C2	-2.18	107.82	111.02
10	J	2	NAG	C4-C3-C2	2.17	114.20	111.02
7	G	1	NAG	C1-C2-N2	-2.17	107.02	110.43
8	H	6	FUL	O5-C5-C6	2.15	112.07	107.40
9	I	7	MAN	O5-C5-C4	2.14	116.04	110.83
4	D	2	NAG	C3-C4-C5	2.13	114.09	110.23
4	D	1	NAG	O4-C4-C5	2.10	114.49	109.32
3	K	6	FUL	C1-C2-C3	-2.10	106.59	109.64
3	K	1	NAG	O4-C4-C5	2.09	114.46	109.32
10	J	1	NAG	C3-C4-C5	-2.08	106.46	110.23
4	D	1	NAG	O3-C3-C2	2.08	113.71	109.40
3	C	3	BMA	C2-C3-C4	2.07	114.50	110.86
3	K	6	FUL	O5-C5-C4	2.07	113.27	109.55
4	D	3	FUL	O5-C5-C6	2.06	111.87	107.40
10	J	2	NAG	O7-C7-C8	-2.06	118.39	122.05
6	F	3	BMA	C1-O5-C5	2.05	114.94	112.19
5	E	2	NAG	O5-C1-C2	-2.03	108.15	111.29
6	F	1	NAG	O5-C5-C4	2.03	115.77	110.83
8	H	1	NAG	O5-C1-C2	-2.03	108.15	111.29
3	C	1	NAG	O5-C5-C6	-2.03	103.72	107.66
3	K	6	FUL	O2-C2-C3	-2.02	105.96	110.15
4	D	2	NAG	O5-C5-C6	2.02	111.60	107.66
5	E	1	NAG	C8-C7-N2	-2.02	112.77	116.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
4	D	1	NAG	C1
7	G	1	NAG	C1
8	H	1	NAG	C1

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
6	F	2	NAG	C1-C2-N2-C7
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
7	G	2	NAG	C3-C2-N2-C7
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
8	H	2	NAG	C8-C7-N2-C2
8	H	2	NAG	O7-C7-N2-C2
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
11	L	2	NAG	C8-C7-N2-C2
11	L	2	NAG	O7-C7-N2-C2
6	F	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
11	L	1	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
11	L	3	BMA	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
9	I	5	MAN	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
11	L	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
9	I	2	NAG	C8-C7-N2-C2
2	B	4	BMA	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
11	L	3	BMA	O5-C5-C6-O6
9	I	5	MAN	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
9	I	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
3	C	5	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
8	H	1	NAG	C4-C5-C6-O6
8	H	1	NAG	O5-C5-C6-O6
11	L	4	MAN	C4-C5-C6-O6
2	B	4	BMA	C4-C5-C6-O6
9	I	4	BMA	O5-C5-C6-O6
8	H	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
11	L	4	MAN	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
10	J	4	MAN	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
9	I	3	BMA	O5-C5-C6-O6
3	K	1	NAG	C3-C2-N2-C7
9	I	6	BMA	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
9	I	1	NAG	C4-C5-C6-O6

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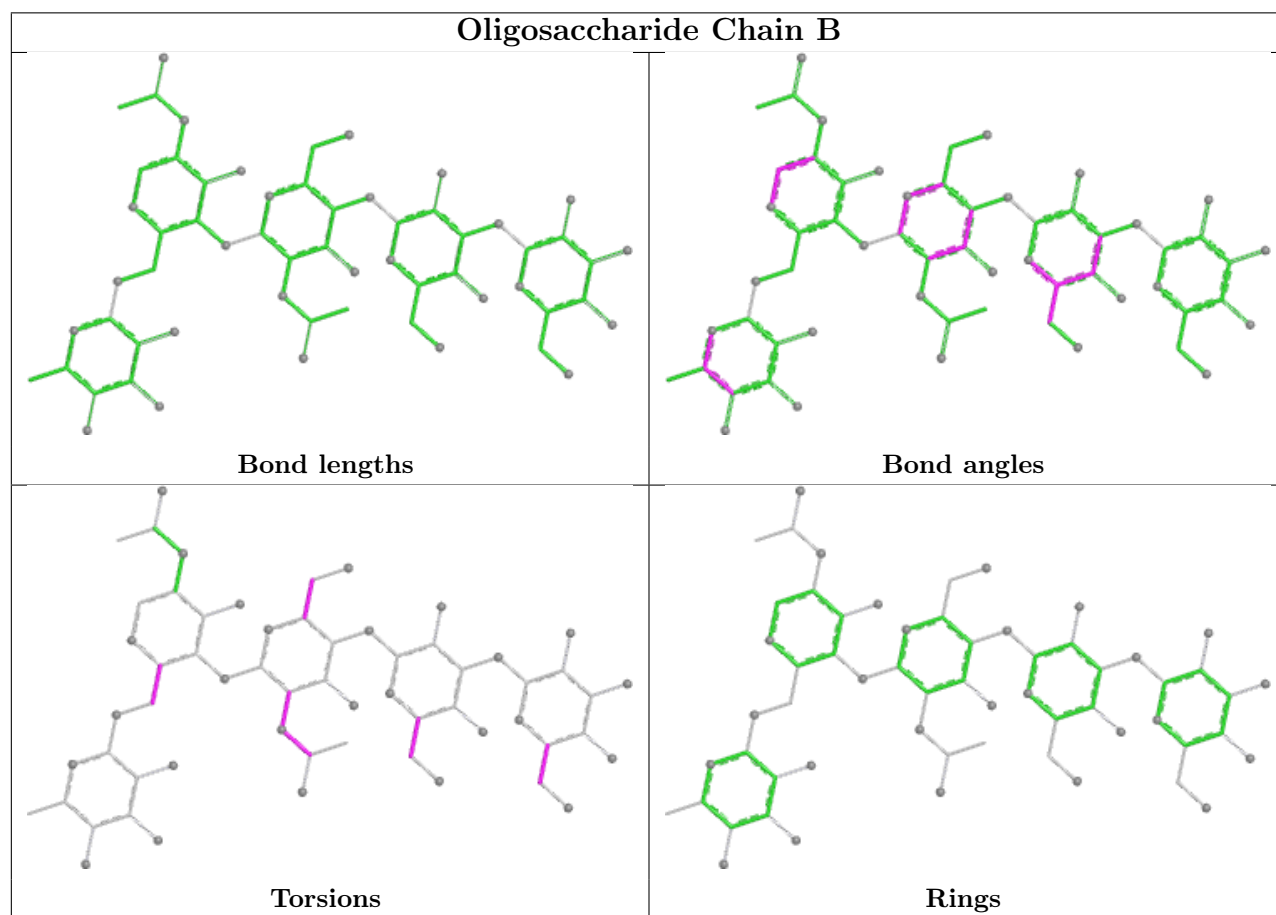
Mol	Chain	Res	Type	Atoms
10	J	3	BMA	C4-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
8	H	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
9	I	4	BMA	C4-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
3	C	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7
8	H	2	NAG	C1-C2-N2-C7
6	F	3	BMA	O5-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6

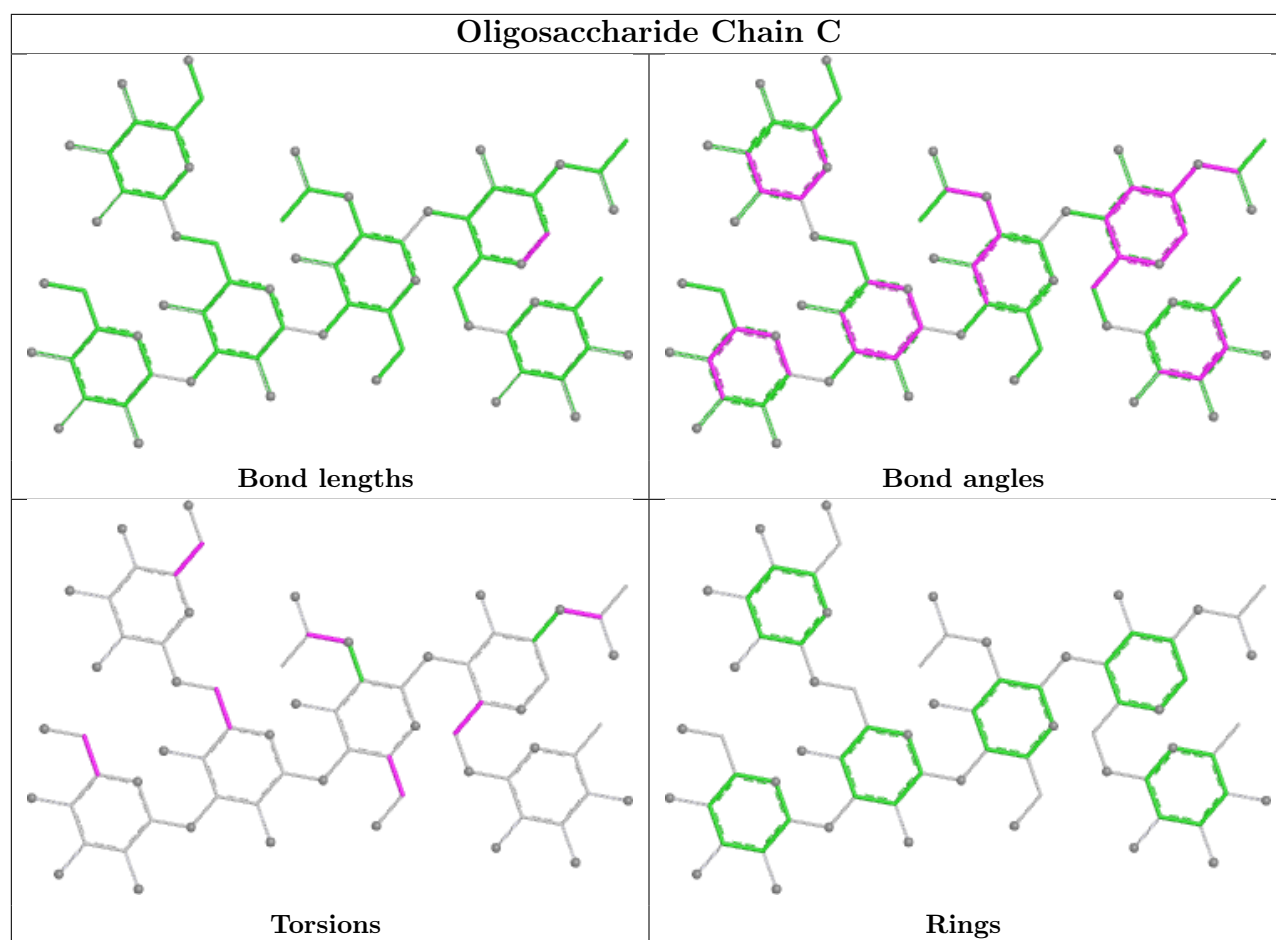
There are no ring outliers.

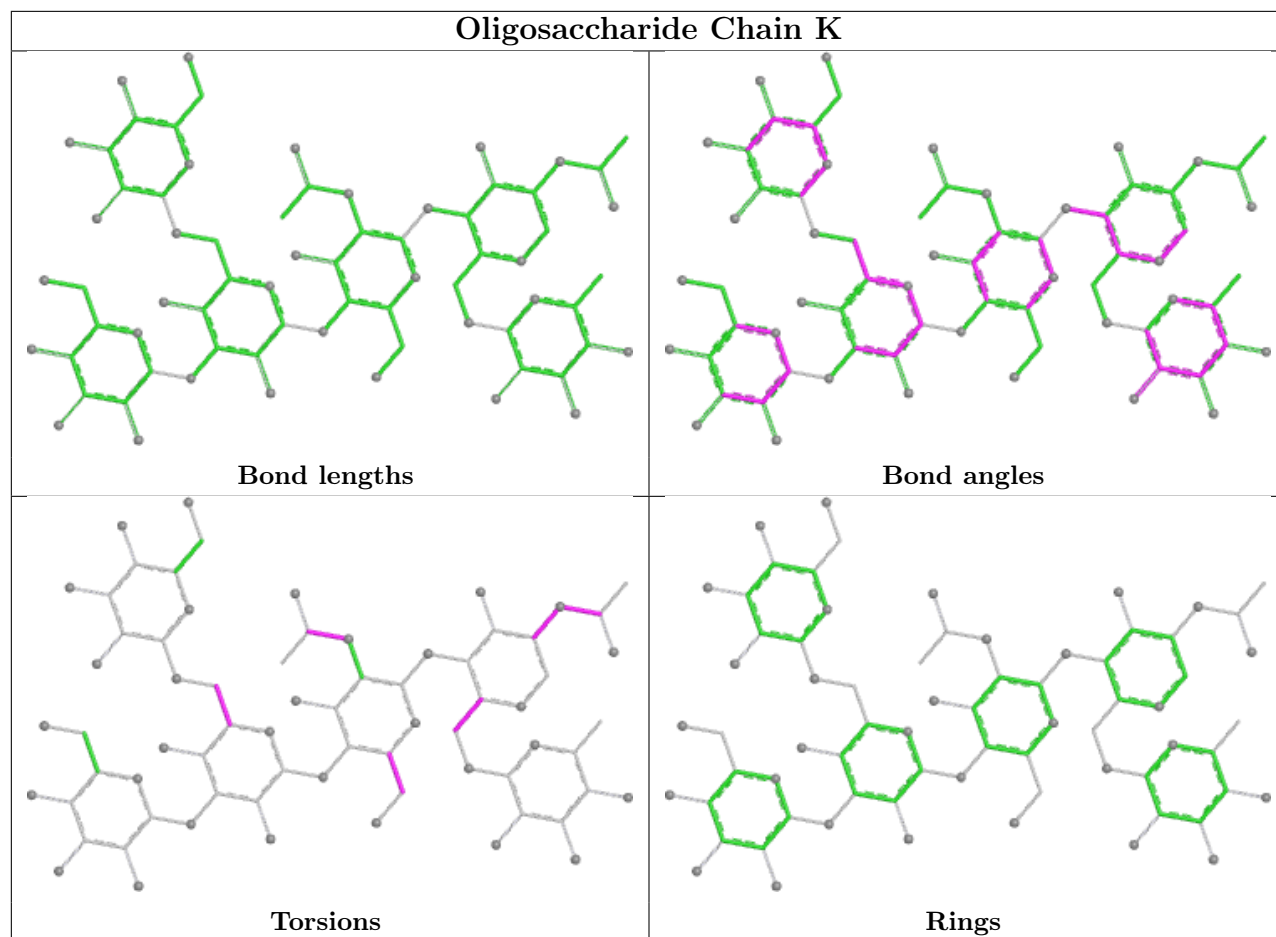
24 monomers are involved in 27 short contacts:

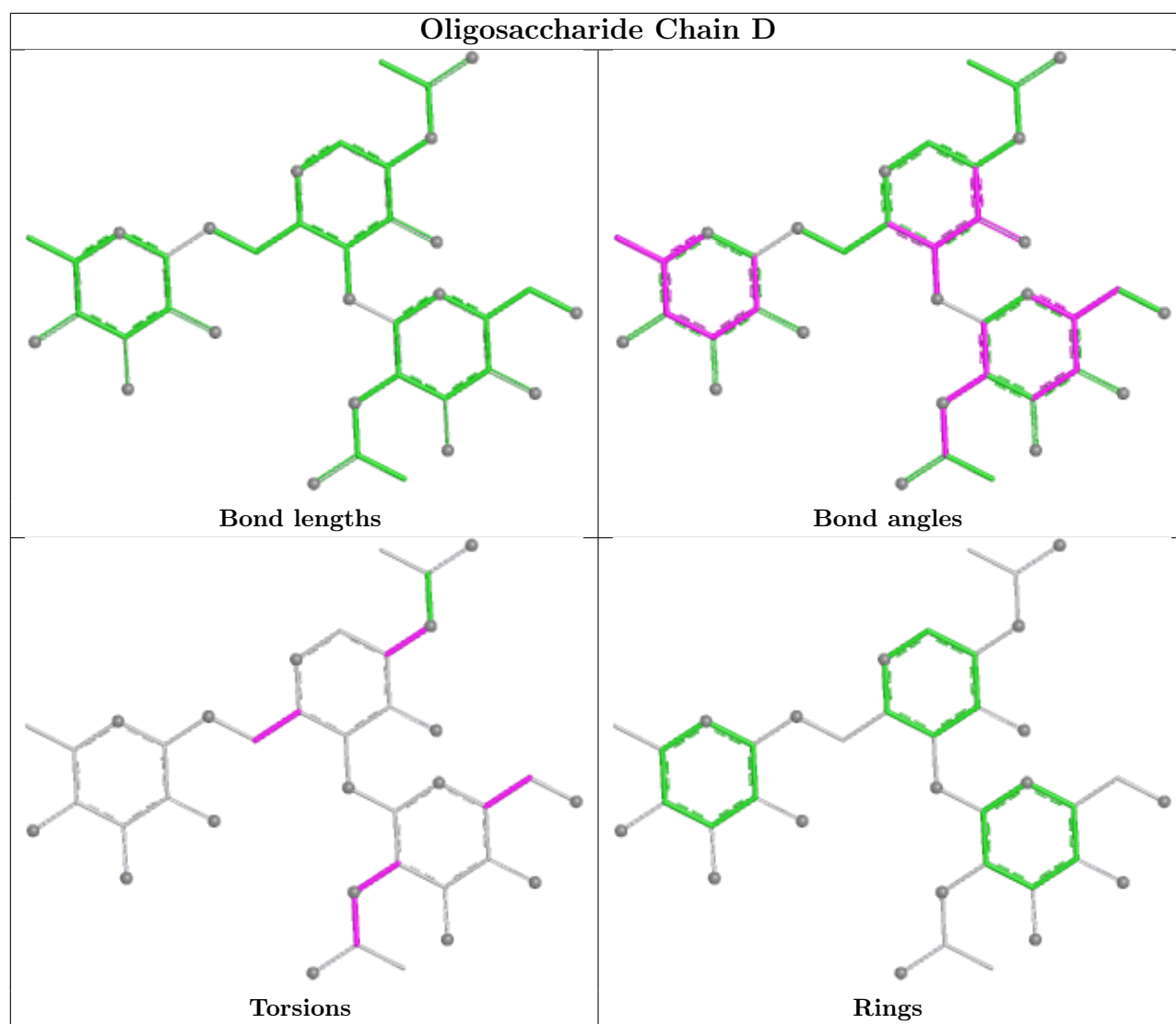
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
5	E	4	FUL	0	1
10	J	4	MAN	1	0
3	K	2	NAG	1	0
9	I	6	BMA	2	0
9	I	2	NAG	1	0
9	I	5	MAN	2	0
4	D	3	FUL	1	0
2	B	3	BMA	1	0
5	E	3	MAN	2	0
4	D	1	NAG	3	0
3	C	3	BMA	1	0
4	D	2	NAG	4	0
5	E	2	NAG	2	0
2	B	5	FUL	0	1
10	J	5	MAN	1	0
3	K	3	BMA	1	0
3	C	4	MAN	0	1
8	H	2	NAG	1	0
3	C	5	MAN	1	0
3	K	6	FUL	2	0
3	C	1	NAG	5	0
5	E	1	NAG	2	0
3	K	1	NAG	4	0

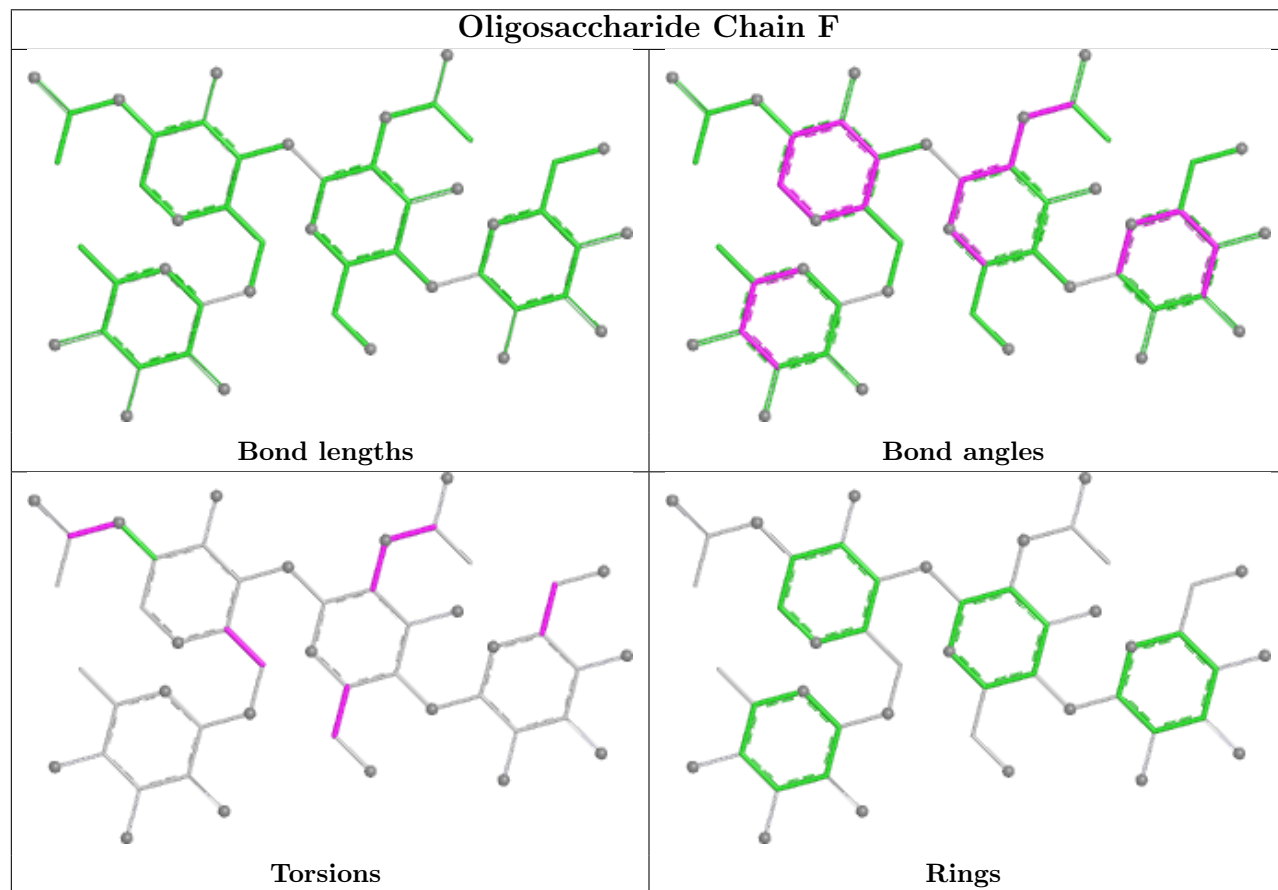
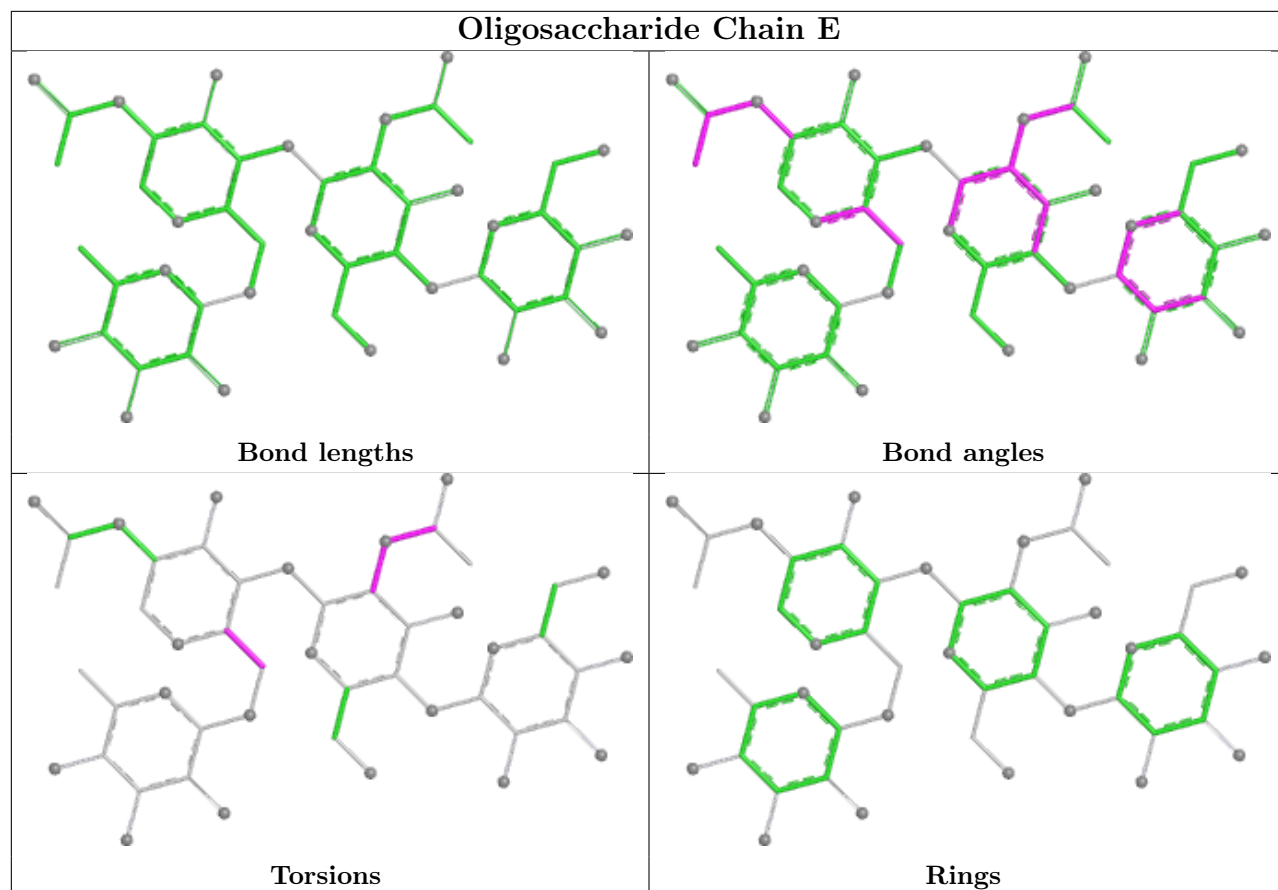
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

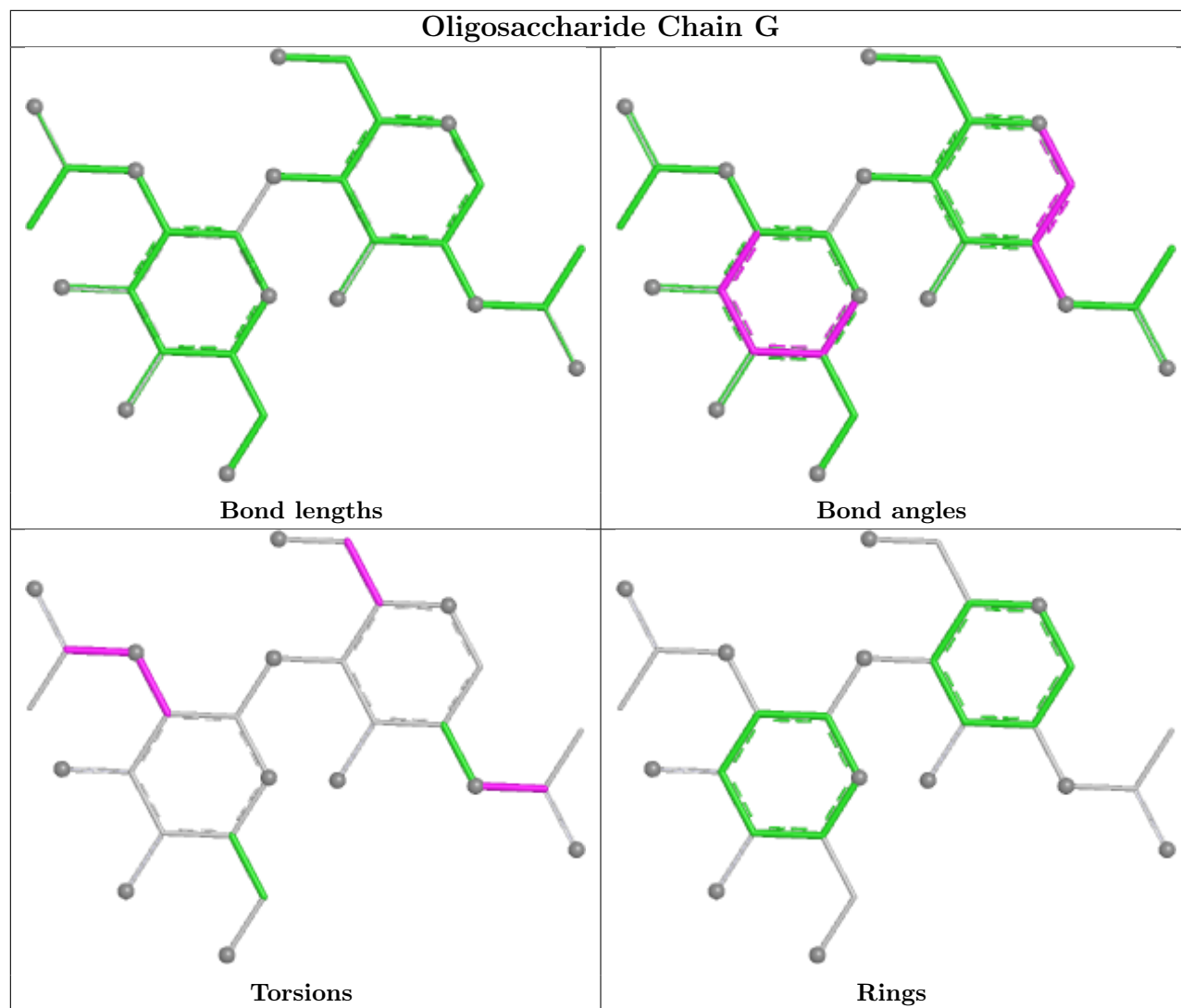


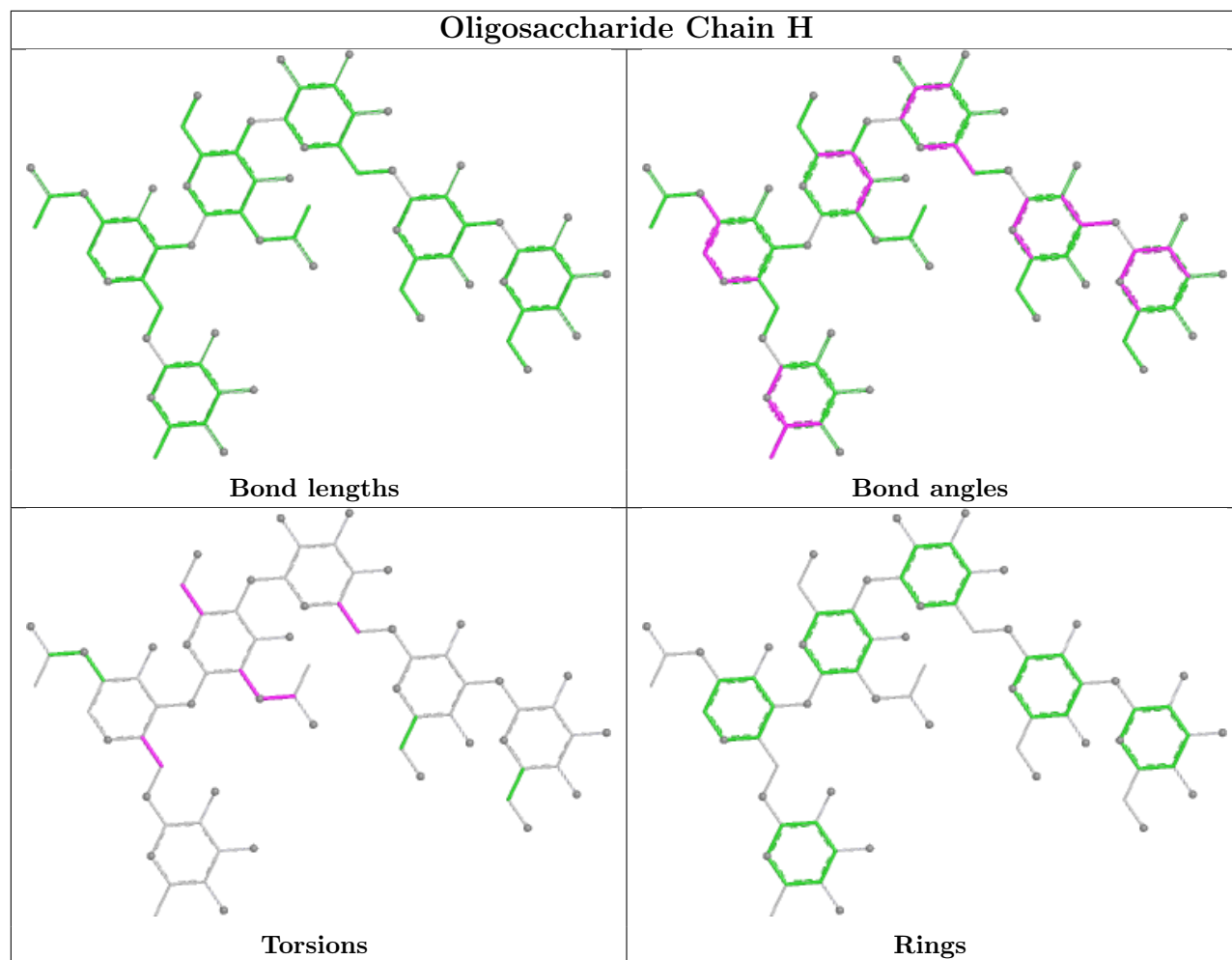


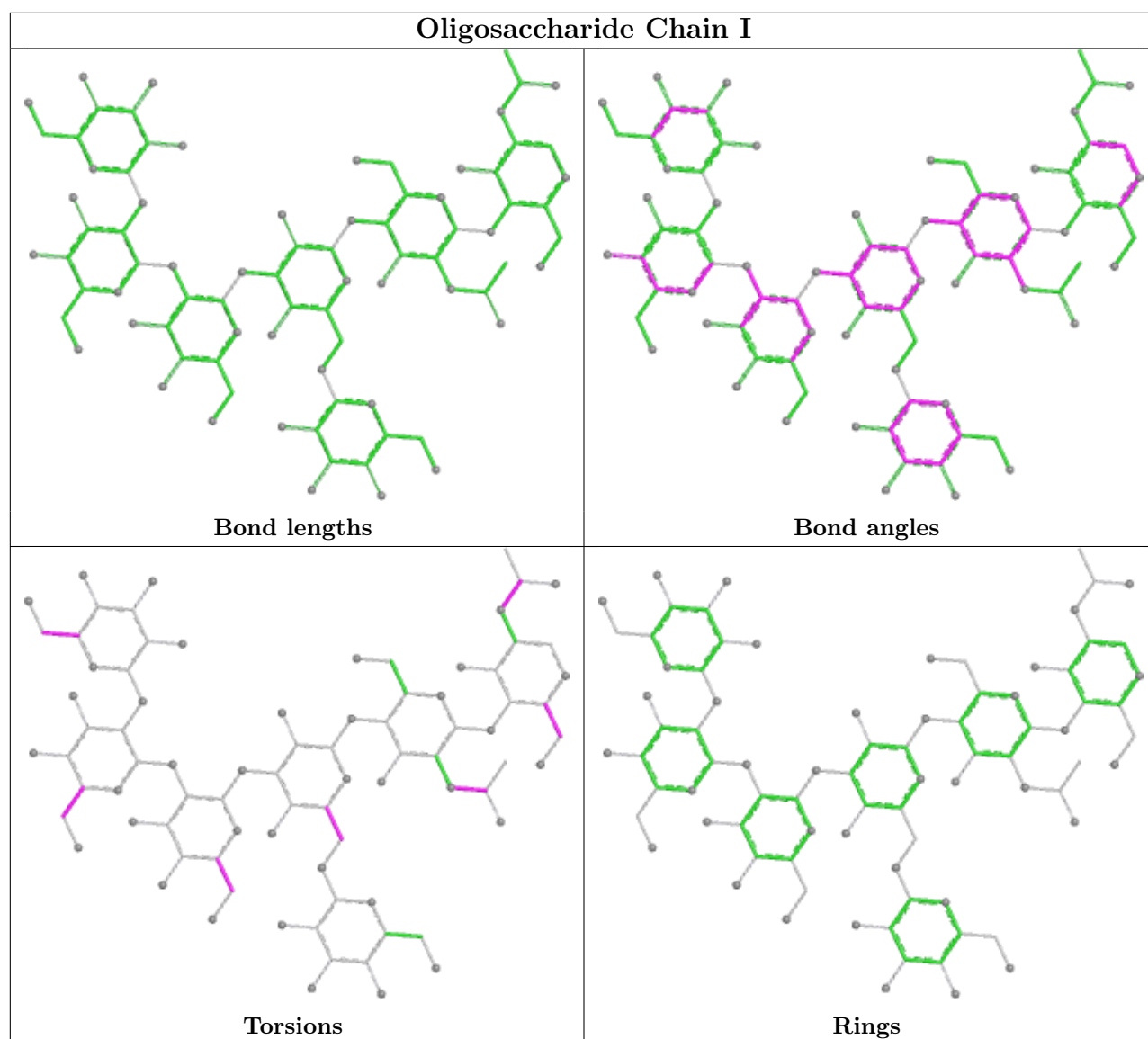


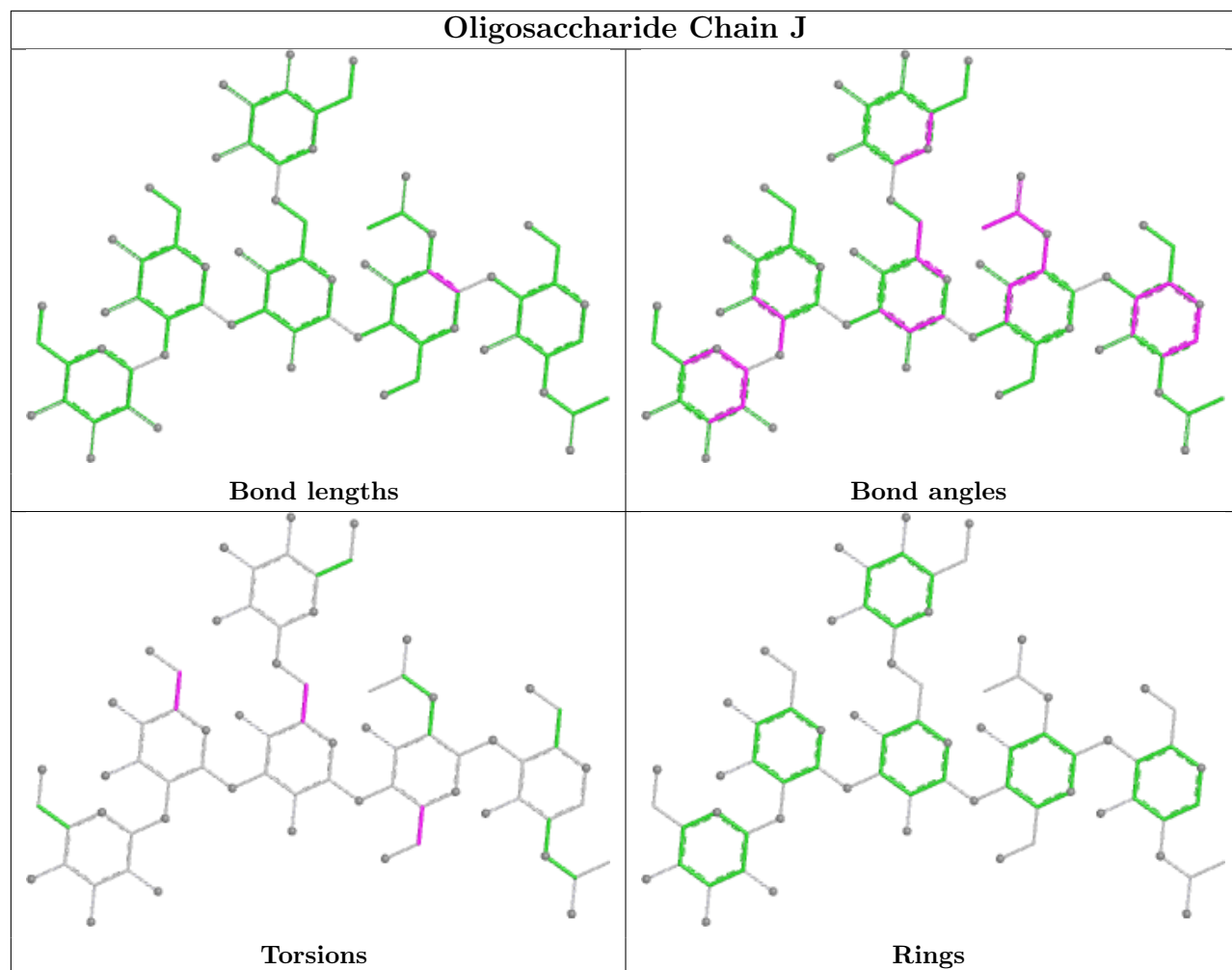


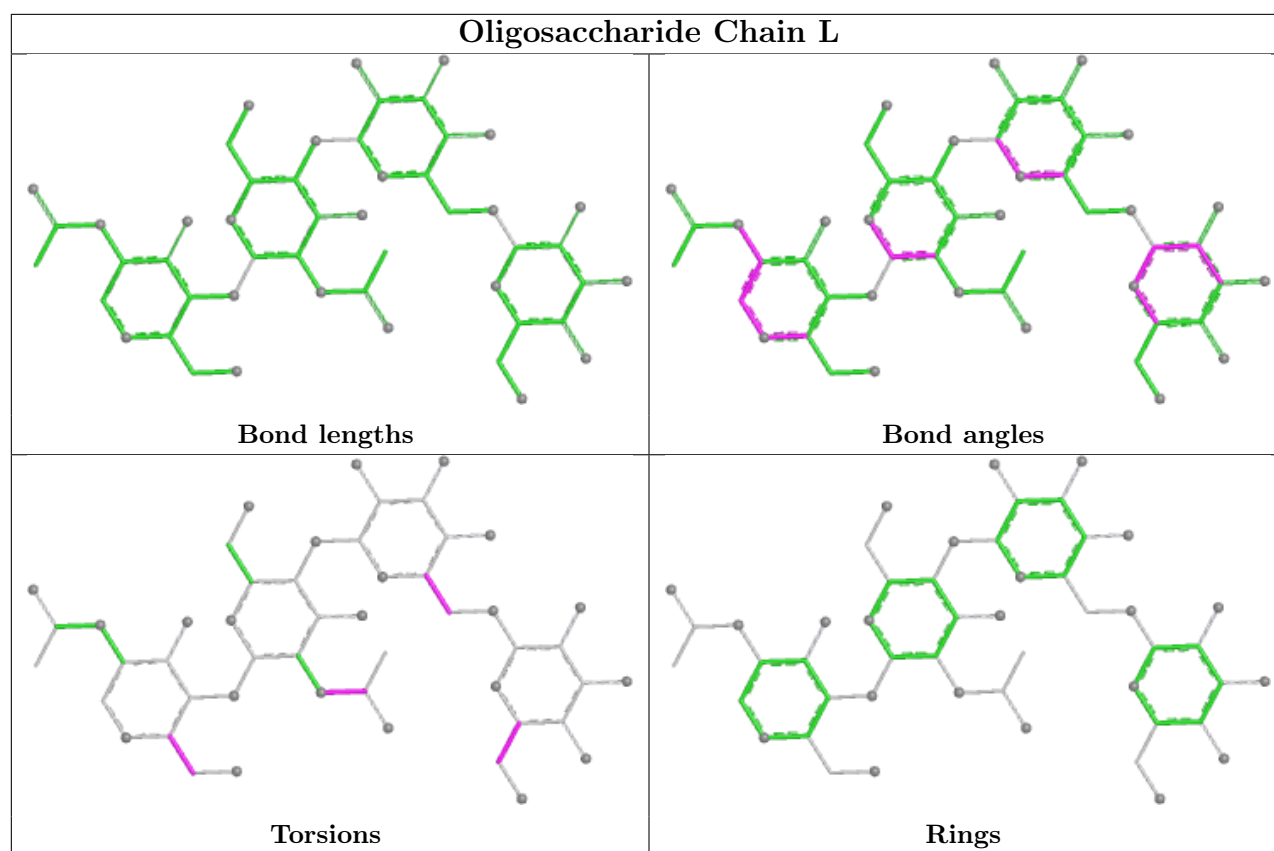












5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
12	NAG	A	1	1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
12	NAG	A	2	1	14,14,15	0.55	0	17,19,21	1.18	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	1	1	1/1/5/7	2/6/23/26	0/1/1/1
12	NAG	A	2	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	2	NAG	O5-C1-C2	-3.43	105.98	111.29
12	A	1	NAG	C4-C3-C2	2.30	114.38	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1	NAG	C8-C7-N2-C2
12	A	1	NAG	O7-C7-N2-C2
12	A	2	NAG	C8-C7-N2-C2
12	A	2	NAG	O7-C7-N2-C2
12	A	2	NAG	O5-C5-C6-O6
12	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	304/316 (96%)	1.21	65 (21%) 2 5	104, 124, 167, 245	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	ALA	6.4
1	A	484	GLU	6.3
1	A	255	SER	6.2
1	A	383	GLY	5.6
1	A	459	ASN	5.5
1	A	467	ALA	5.1
1	A	391	TRP	5.1
1	A	245	THR	4.9
1	A	400	TYR	4.3
1	A	238	ALA	4.0
1	A	306	LEU	3.9
1	A	261	SER	3.8
1	A	105	SER	3.6
1	A	279	THR	3.5
1	A	311	ARG	3.5
1	A	248	SER	3.4
1	A	442	LYS	3.4
1	A	460	SER	3.2
1	A	239	LEU	3.2
1	A	270	THR	3.1
1	A	482	SER	3.1
1	A	98	ILE	3.1
1	A	102	VAL	3.0
1	A	280	ARG	2.9
1	A	363	HIS	2.9
1	A	274	PHE	2.9
1	A	440	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	210	CYS	2.9
1	A	486	ALA	2.8
1	A	435	GLN	2.8
1	A	296	THR	2.8
1	A	345	PHE	2.8
1	A	485	VAL	2.7
1	A	262	CYS	2.7
1	A	433	ILE	2.7
1	A	406	PHE	2.6
1	A	312	GLY	2.6
1	A	396	GLY	2.6
1	A	211	ASN	2.5
1	A	100	PRO	2.5
1	A	409	TRP	2.5
1	A	295	ARG	2.5
1	A	271	SER	2.4
1	A	499	VAL	2.4
1	A	361	VAL	2.3
1	A	441	HIS	2.3
1	A	254	CYS	2.3
1	A	247	TYR	2.3
1	A	273	TRP	2.2
1	A	212	THR	2.2
1	A	379	ALA	2.2
1	A	458	CYS	2.2
1	A	87	ILE	2.2
1	A	405	TRP	2.2
1	A	235	PRO	2.2
1	A	233	ALA	2.1
1	A	399	LEU	2.1
1	A	281	ALA	2.1
1	A	451	PRO	2.1
1	A	305	ASN	2.1
1	A	341	GLY	2.1
1	A	487	GLU	2.1
1	A	217	GLU	2.0
1	A	493	LEU	2.0
1	A	249	GLY	2.0

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

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

6.3 Carbohydrates

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

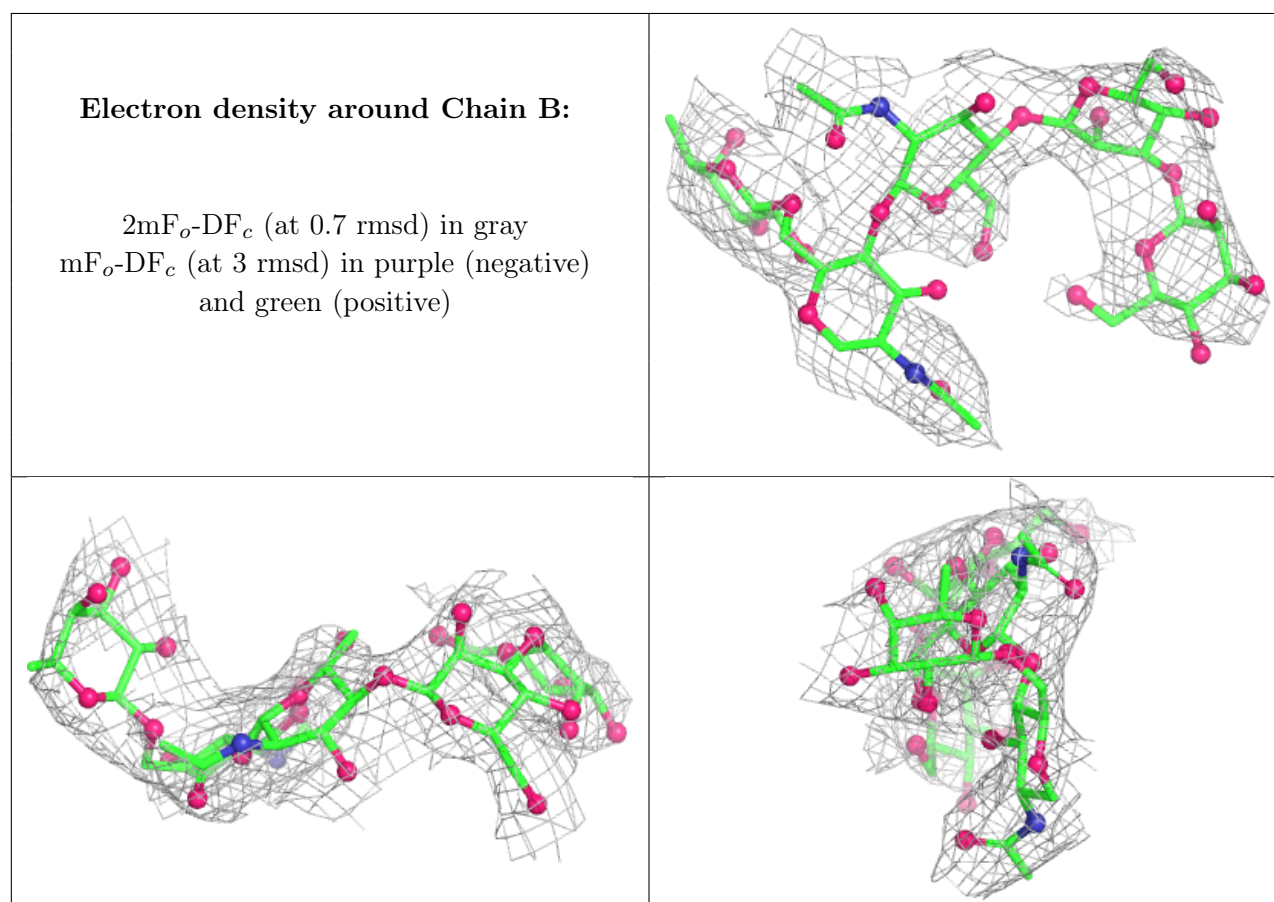
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.26	0.17	123,128,132,134	0
11	MAN	L	4	11/12	0.41	0.17	168,173,176,181	0
11	BMA	L	3	11/12	0.51	0.14	155,158,165,166	0
10	NAG	J	2	14/15	0.52	0.16	162,163,173,174	0
2	BMA	B	3	11/12	0.53	0.16	139,141,145,146	0
8	BMA	H	3	11/12	0.56	0.15	163,169,172,174	0
9	BMA	I	4	11/12	0.57	0.20	138,142,148,148	0
8	NAG	H	2	14/15	0.59	0.16	144,148,152,152	0
3	MAN	K	5	11/12	0.60	0.12	125,129,131,132	0
3	NAG	C	2	14/15	0.61	0.30	118,121,125,126	0
6	FUL	F	4	10/11	0.61	0.15	125,128,131,132	0
10	BMA	J	3	11/12	0.63	0.13	175,178,185,189	0
8	MAN	H	5	11/12	0.64	0.12	185,191,200,202	0
10	MAN	J	5	11/12	0.64	0.14	209,217,221,225	0
4	NAG	D	2	14/15	0.67	0.13	128,131,136,136	0
5	MAN	E	3	11/12	0.67	0.15	159,163,171,171	0
3	BMA	C	3	11/12	0.69	0.14	129,133,136,137	0
6	NAG	F	2	14/15	0.69	0.09	127,133,137,138	0
3	FUL	C	6	10/11	0.71	0.10	116,118,120,122	0
7	NAG	G	1	14/15	0.72	0.19	179,187,196,201	0
8	BMA	H	4	11/12	0.73	0.10	185,189,199,199	0
4	NAG	D	1	14/15	0.73	0.12	117,121,122,122	0
9	NAG	I	2	14/15	0.74	0.15	120,124,129,130	0
10	MAN	J	6	11/12	0.74	0.12	157,163,165,166	0
6	BMA	F	3	11/12	0.75	0.08	147,150,156,156	0
9	MAN	I	5	11/12	0.75	0.13	141,142,144,147	0
8	NAG	H	1	14/15	0.76	0.18	133,135,139,141	0
2	BMA	B	4	11/12	0.76	0.12	137,140,143,147	0
7	NAG	G	2	14/15	0.78	0.13	186,194,202,204	0
9	BMA	I	3	11/12	0.78	0.15	125,129,132,132	0
10	NAG	J	1	14/15	0.78	0.20	150,153,156,157	0
9	NAG	I	1	14/15	0.79	0.41	119,124,129,130	0
3	MAN	K	4	11/12	0.79	0.09	126,128,132,133	0
3	BMA	K	3	11/12	0.80	0.11	118,119,121,122	0
11	NAG	L	2	14/15	0.81	0.13	140,143,147,148	0
5	NAG	E	1	14/15	0.81	0.12	133,140,146,148	0
3	NAG	K	2	14/15	0.81	0.13	113,116,117,118	0

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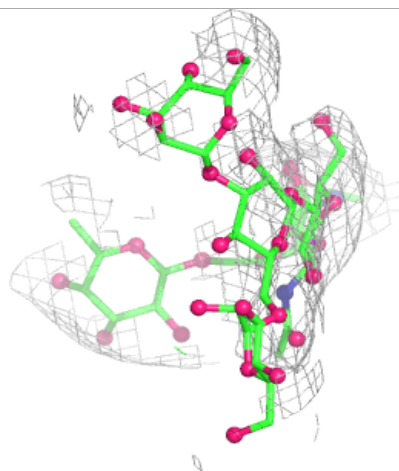
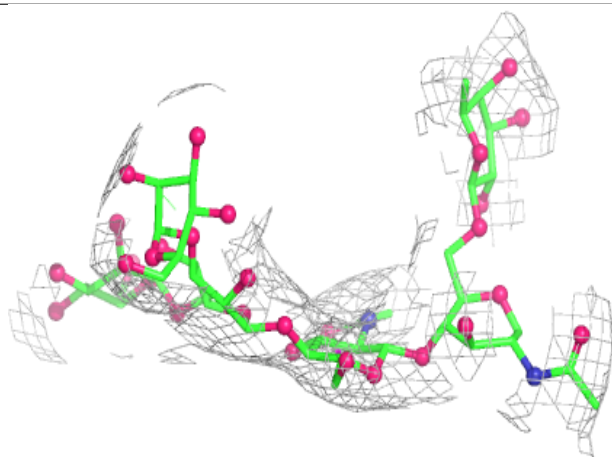
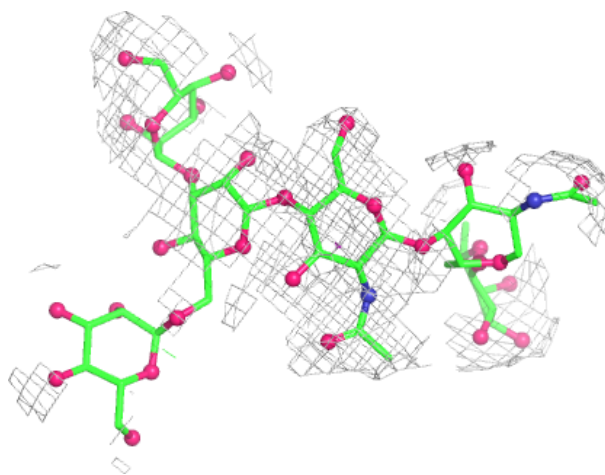
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MAN	J	4	11/12	0.82	0.10	194,198,206,209	0
3	MAN	C	5	11/12	0.82	0.18	134,136,141,142	0
11	NAG	L	1	14/15	0.84	0.10	124,127,132,133	0
5	NAG	E	2	14/15	0.85	0.11	153,157,165,167	0
3	FUL	K	6	10/11	0.85	0.15	120,123,126,127	0
3	MAN	C	4	11/12	0.85	0.10	142,145,149,149	0
4	FUL	D	3	10/11	0.86	0.10	118,122,124,126	0
2	NAG	B	1	14/15	0.86	0.12	116,119,122,122	0
8	FUL	H	6	10/11	0.86	0.10	131,133,135,135	0
2	FUL	B	5	10/11	0.88	0.12	118,120,123,123	0
6	NAG	F	1	14/15	0.88	0.20	120,123,126,127	0
5	FUL	E	4	10/11	0.89	0.11	141,147,153,154	0
3	NAG	C	1	14/15	0.90	0.09	111,114,116,117	0
9	BMA	I	6	11/12	0.90	0.14	151,152,157,160	0
3	NAG	K	1	14/15	0.91	0.15	113,114,117,118	0
9	MAN	I	7	11/12	0.92	0.11	120,124,127,128	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.



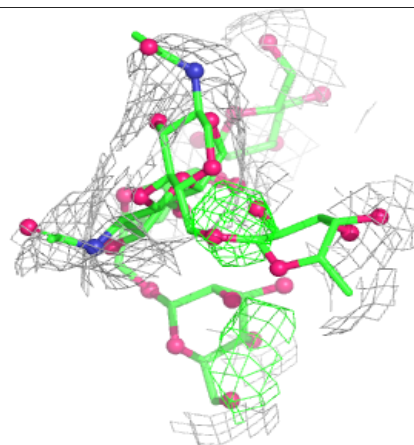
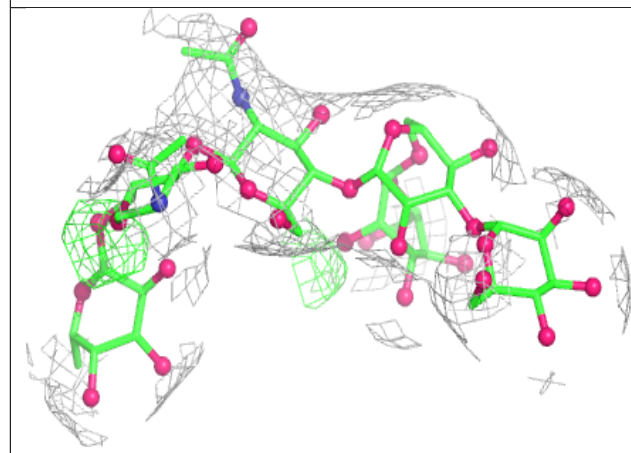
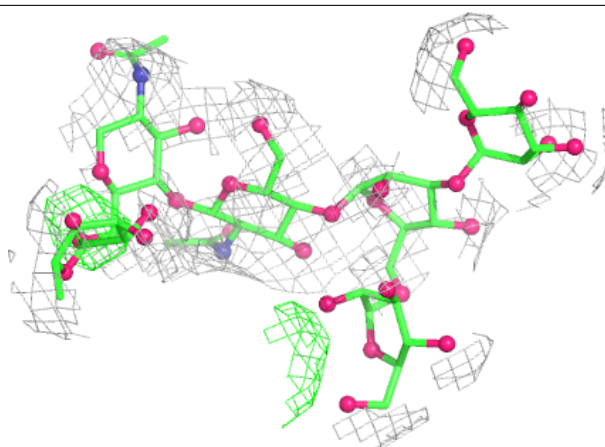
Electron density around Chain C:

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



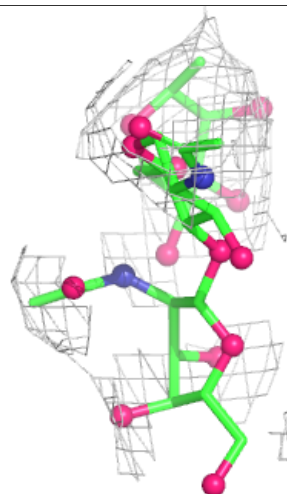
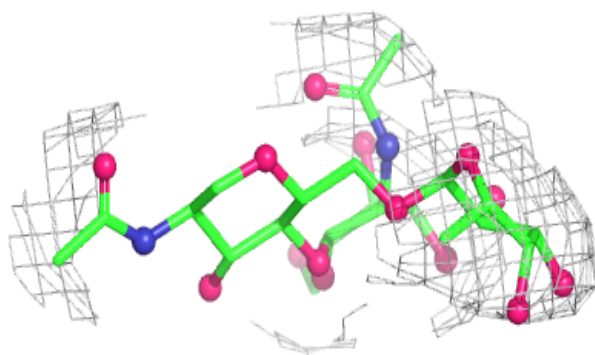
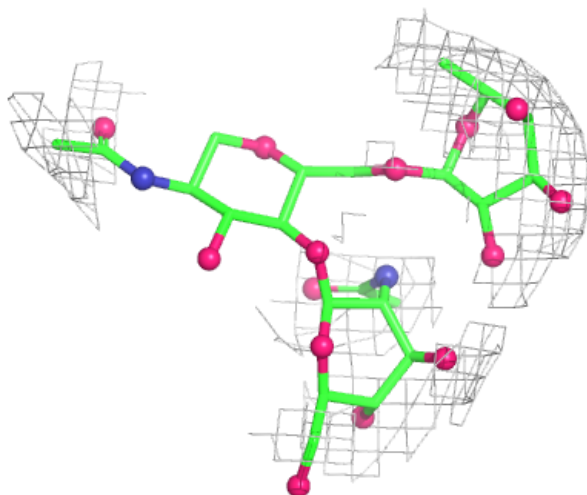
Electron density around Chain K:

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



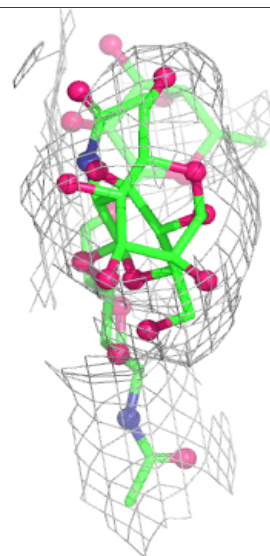
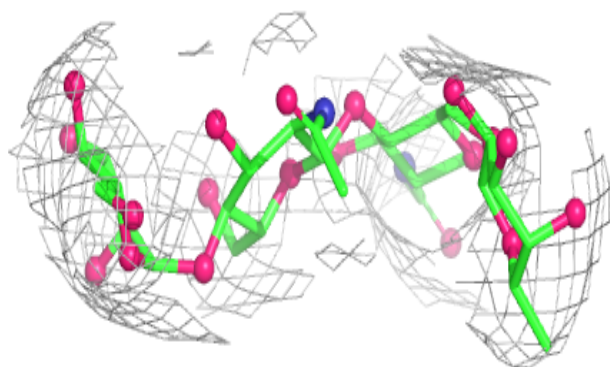
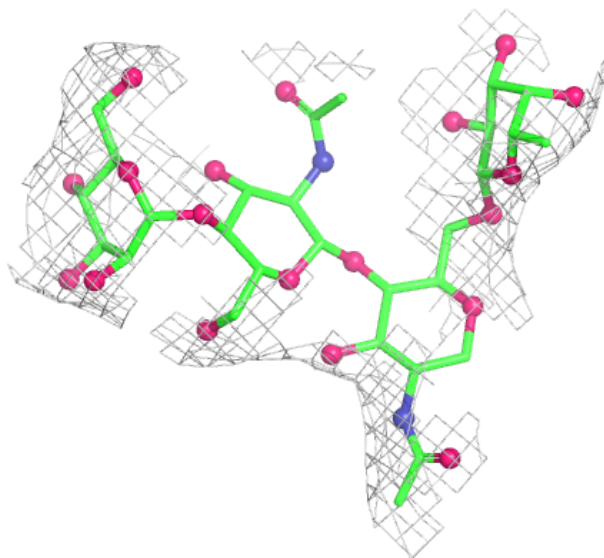
Electron density around Chain D:

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



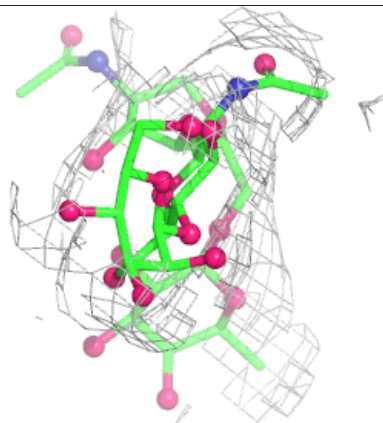
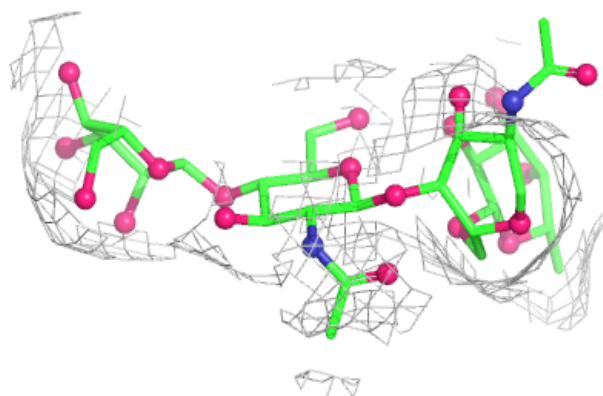
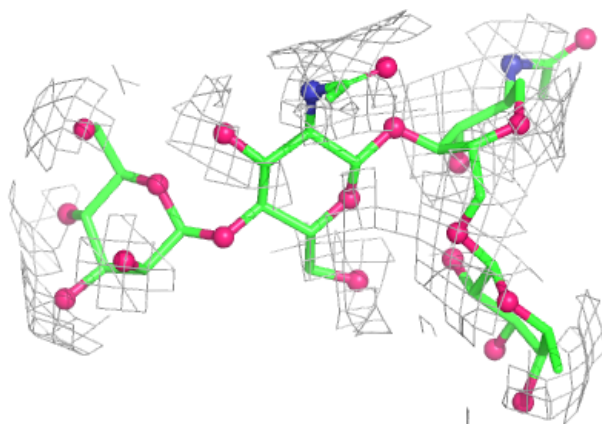
Electron density around Chain E:

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

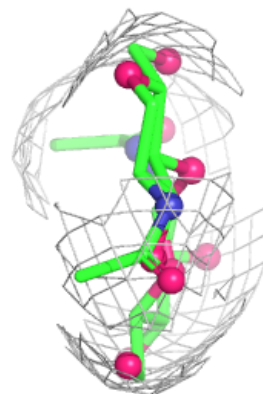
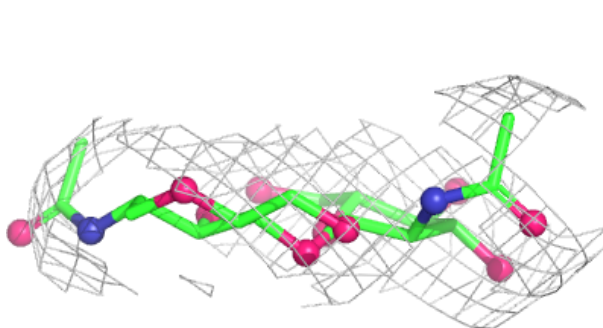
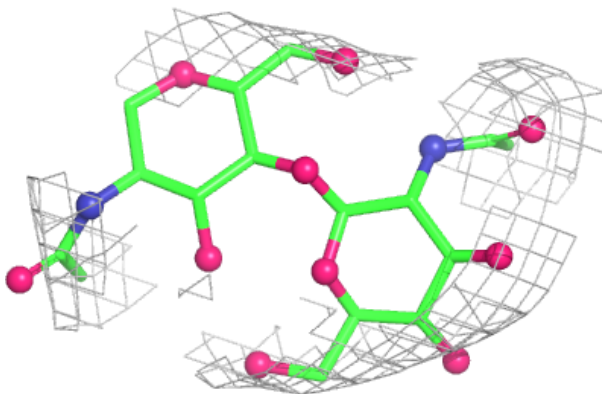


Electron density around Chain F:

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

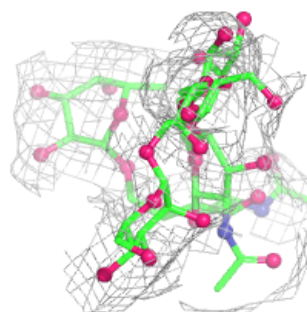
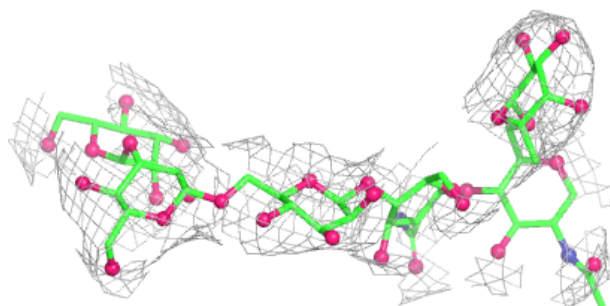
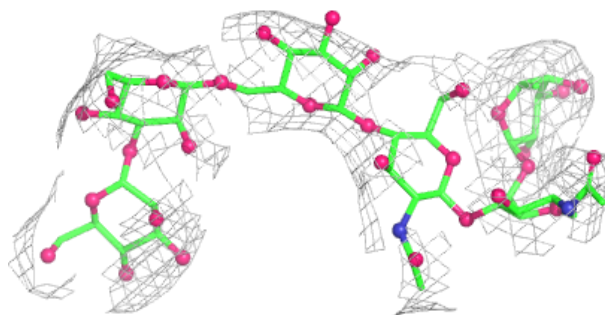
**Electron density around Chain G:**

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

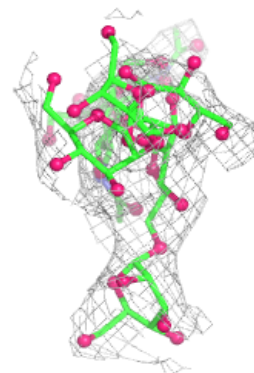
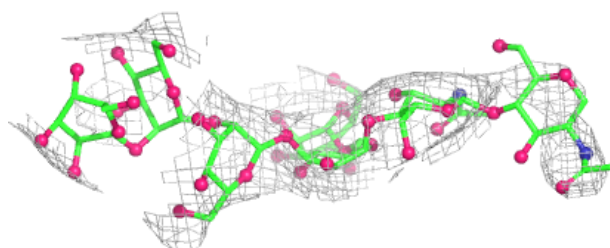
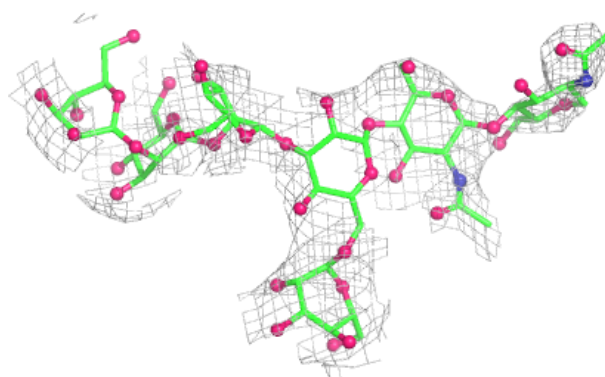


Electron density around Chain H:

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

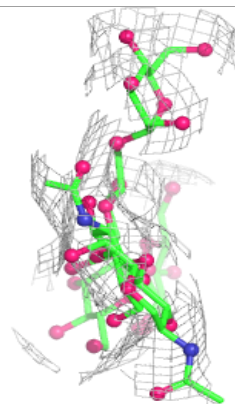
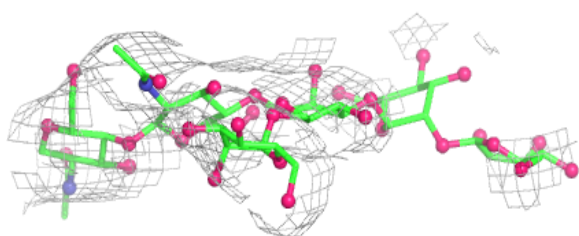
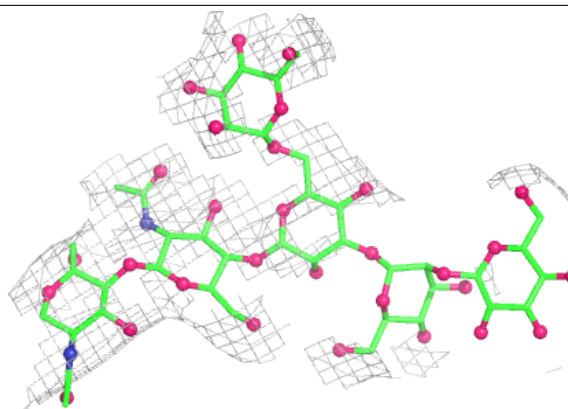
**Electron density around Chain I:**

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

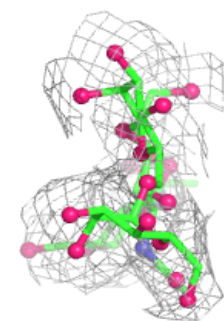
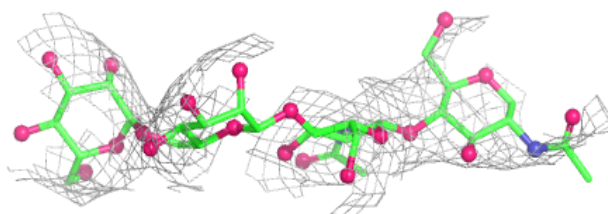
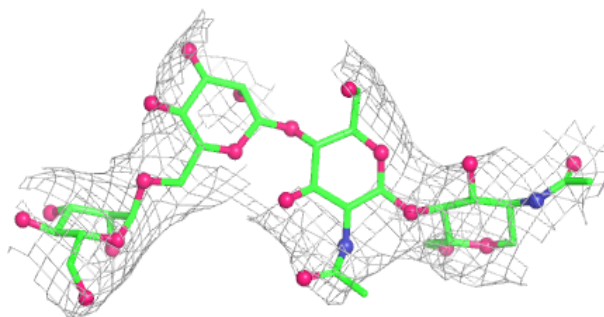


Electron density around Chain J:

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

**Electron density around Chain L:**

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



6.4 Ligands [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
12	NAG	A	1	14/15	0.64	0.10	149,152,154,158	0
12	NAG	A	2	14/15	0.77	0.17	158,161,164,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.