



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:39 PM UTC

PDB ID : 2RI9 / pdb_00002ri9
Title : Penicillium citrinum alpha-1,2-mannosidase in complex with a substrate analog
Authors : Lobsanov, Y.D.; Yoshida, T.; Desmet, T.; Nerinckx, W.; Yip, P.; Claeysens, M.; Herscovics, A.; Howell, P.L.
Deposited on : 2007-10-10
Resolution : 1.95 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

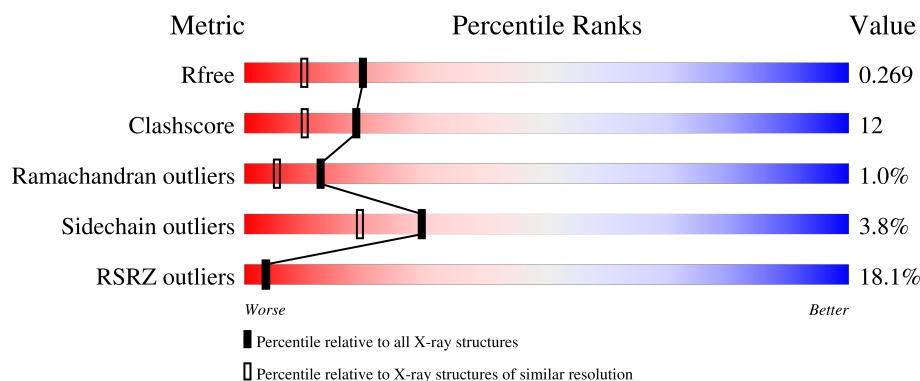
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	475	81% 17% .
1	B	475	35% 63% 32% .
2	C	2	50% 50%
2	E	2	100%
2	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	D	5	 60%20%20%
3	H	5	 60%40%
4	F	2	 50%50%
4	J	2	 50%50%
5	I	2	 50%50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	D	3	X	-	-	-
3	MAN	H	3	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8503 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

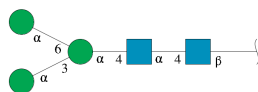
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	2	0
			3744	2370	624	741	9			
1	B	475	Total	C	N	O	S	0	1	0
			3736	2365	623	740	8			

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



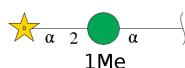
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

- Molecule 4 is an oligosaccharide called alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	O		0	2	0
			22	12	10				
4	J	2	Total	C	O		0	2	0
			22	12	10				

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



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			6	3	3		
7	A	1	Total	C	O	0	1
			6	3	3		
7	B	1	Total	C	O	0	1
			6	3	3		
7	B	1	Total	C	O	0	1
			6	3	3		

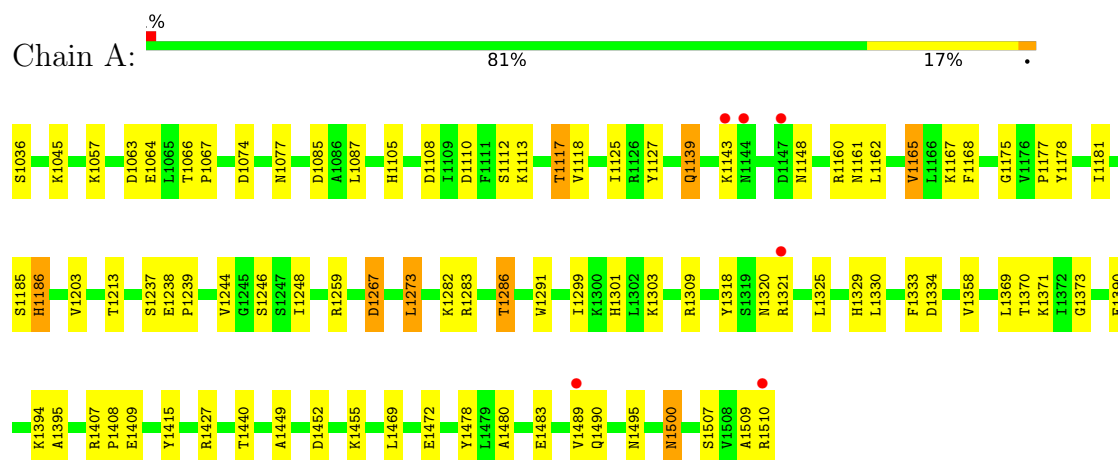
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	482	Total	O	0	1
			483	483		
8	B	235	Total	O	0	1
			236	236		

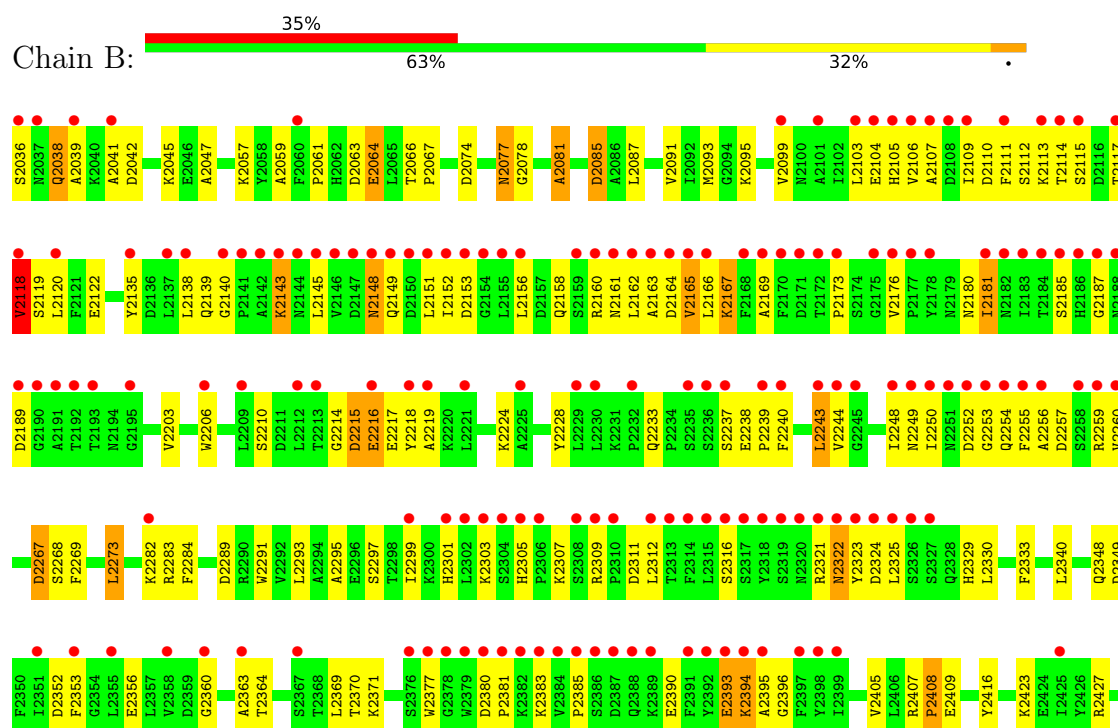
3 Residue-property plots

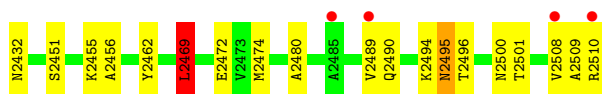
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mannosyl-oligosaccharide alpha-1,2-mannosidase



- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase





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



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



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



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



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



- Molecule 4: alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside



- Molecule 4: alpha-D-lyxopyranose-(1-2)-methyl alpha-D-mannopyranoside

Chain J:  50% 50%

MDA1
LDY2

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

Chain I:  50% 50%

MDG1
MDG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.49Å 111.00Å 86.23Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	49.83 – 1.95 49.83 – 1.97	Depositor EDS
% Data completeness (in resolution range)	93.9 (49.83-1.95) 94.0 (49.83-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.97Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.260 0.220 , 0.269	Depositor DCC
R_{free} test set	5018 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MMA, NDG, LDY, CA, MAN, NAG

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	0.81	0/3839	1.07	37/5215 (0.7%)
1	B	0.52	0/3831	1.02	31/5205 (0.6%)
All	All	0.68	0/7670	1.05	68/10420 (0.7%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2253	GLY	N-CA-C	-8.56	102.68	115.00
1	B	2067	PRO	N-CA-C	8.00	124.23	113.84
1	A	1167	LYS	N-CA-C	7.78	122.45	112.34
1	B	2409	GLU	N-CA-C	7.72	120.67	111.33
1	B	2333	PHE	N-CA-C	-7.61	103.25	112.54
1	B	2203	VAL	N-CA-C	7.61	119.29	110.62
1	B	2167	LYS	N-CA-C	7.55	120.46	111.33
1	A	1067	PRO	N-CA-C	7.54	123.65	113.84
1	A	1238	GLU	CA-C-N	7.33	127.68	119.32
1	A	1238	GLU	C-N-CA	7.33	127.68	119.32
1	A	1066	THR	CA-C-N	7.29	126.99	119.56
1	A	1066	THR	C-N-CA	7.29	126.99	119.56
1	B	2284	PHE	N-CA-C	7.22	121.63	111.30
1	B	2495	ASN	N-CA-C	7.03	120.44	109.96
1	B	2469	LEU	N-CA-C	-6.84	103.76	111.14
1	B	2064	GLU	N-CA-C	6.71	119.06	108.79
1	A	1177	PRO	N-CA-C	6.70	120.59	111.22
1	A	1409	GLU	N-CA-C	6.67	119.38	111.71
1	A	1333	PHE	N-CA-C	-6.66	104.41	112.54
1	A	1246	SER	N-CA-C	6.64	121.40	113.16
1	B	2118	VAL	N-CA-C	6.60	119.02	108.85
1	A	1066	THR	N-CA-C	-6.55	95.45	109.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1509	ALA	N-CA-C	6.46	118.63	110.24
1	A	1064	GLU	N-CA-C	6.40	118.80	109.07
1	B	2059	ALA	N-CA-C	6.34	121.42	113.43
1	B	2066	THR	N-CA-C	-6.30	96.25	108.59
1	B	2472	GLU	N-CA-C	6.01	120.36	112.13
1	A	1244	VAL	N-CA-C	6.00	117.48	108.96
1	B	2145	LEU	N-CA-C	-5.98	105.90	113.43
1	B	2267	ASP	N-CA-C	5.92	123.42	110.80
1	B	2066	THR	CA-C-N	5.90	125.58	119.56
1	B	2066	THR	C-N-CA	5.90	125.58	119.56
1	A	1087	LEU	N-CA-C	5.88	117.36	111.07
1	B	2329	HIS	N-CA-C	-5.88	104.96	111.36
1	A	1118	VAL	N-CA-C	5.87	116.39	108.17
1	A	1329	HIS	N-CA-C	-5.82	104.93	111.28
1	B	2057	LYS	N-CA-C	5.78	117.66	111.36
1	A	1175	GLY	N-CA-C	-5.71	106.64	114.64
1	A	1283	ARG	N-CA-C	5.71	118.28	111.71
1	A	1057	LYS	N-CA-C	5.63	117.50	111.36
1	B	2078	GLY	N-CA-C	5.62	122.83	115.36
1	B	2509	ALA	N-CA-C	5.60	117.77	110.43
1	A	1178	TYR	N-CA-C	-5.57	100.11	108.96
1	A	1301	HIS	N-CA-C	5.52	120.51	113.55
1	A	1500	ASN	N-CA-C	-5.47	102.81	110.35
1	A	1440	THR	N-CA-C	5.44	118.39	111.69
1	A	1203	VAL	N-CA-C	5.42	118.64	111.17
1	A	1267	ASP	N-CA-C	5.42	122.34	110.80
1	B	2462	TYR	CB-CA-C	-5.41	100.26	109.51
1	A	1334	ASP	N-CA-C	5.38	117.56	111.11
1	A	1127	TYR	N-CA-C	5.37	116.94	111.14
1	A	1449	ALA	N-CA-C	-5.35	102.96	110.50
1	B	2077	ASN	N-CA-C	5.34	119.62	113.38
1	A	1309	ARG	CA-C-N	5.27	124.93	119.56
1	A	1309	ARG	C-N-CA	5.27	124.93	119.56
1	A	1077	ASN	N-CA-C	5.22	121.65	113.72
1	B	2269	PHE	N-CA-C	-5.19	105.52	111.07
1	A	1125	ILE	N-CA-C	5.17	117.56	111.09
1	B	2451	SER	N-CA-C	5.16	118.72	112.23
1	A	1469	LEU	N-CA-C	-5.13	105.58	111.07
1	B	2268	SER	N-CA-C	5.12	119.02	112.87
1	A	1472	GLU	N-CA-C	5.12	119.74	112.93
1	B	2380	ASP	CA-C-N	5.12	126.24	119.84
1	B	2380	ASP	C-N-CA	5.12	126.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2408	PRO	N-CA-C	5.09	122.95	112.47
1	B	2081	ALA	N-CA-C	5.07	117.46	111.33
1	A	1373	GLY	CA-C-N	5.05	125.03	120.03
1	A	1373	GLY	C-N-CA	5.05	125.03	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3744	0	3543	44	0
1	B	3736	0	3536	132	0
2	C	28	0	25	1	0
2	E	28	0	25	0	0
2	G	28	0	25	2	0
3	D	61	0	51	1	0
3	H	61	0	51	7	0
4	F	22	0	13	1	0
4	J	22	0	14	0	0
5	I	28	0	24	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	3	0	0
7	B	12	0	3	0	0
8	A	483	0	0	14	0
8	B	236	0	0	17	0
All	All	8503	0	7313	181	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 12.

All (181) 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:B:2330:LEU:HD21	1:B:2407[B]:ARG:NH2	1.86	0.89
1:A:1330:LEU:HD21	1:A:1407[B]:ARG:NH2	1.96	0.80
1:A:1139:GLN:HE21	1:A:1139:GLN:HA	1.49	0.78
1:A:1490:GLN:H	1:A:1495:ASN:HD21	1.32	0.78
1:B:2423:LYS:HE2	1:B:2423:LYS:HA	1.67	0.77
1:B:2394:LYS:HB2	1:B:2394:LYS:NZ	2.05	0.72
1:B:2427:ARG:HD3	1:B:2480:ALA:O	1.90	0.71
1:A:1162:LEU:O	1:A:1165:VAL:HG13	1.92	0.70
1:B:2119:SER:HB3	1:B:2122:GLU:HB2	1.74	0.69
1:B:2210:SER:OG	1:B:2218:TYR:HB2	1.93	0.69
1:A:1390:GLU:HG3	8:A:673:HOH:O	1.92	0.68
1:A:1490:GLN:H	1:A:1495:ASN:ND2	1.92	0.67
1:B:2181:ILE:H	1:B:2181:ILE:HD13	1.60	0.67
1:B:2330:LEU:HD21	1:B:2407[B]:ARG:HH21	1.57	0.66
1:B:2494:LYS:HB3	8:B:646:HOH:O	1.94	0.66
1:B:2370:THR:O	1:B:2371:LYS:HB2	1.94	0.66
1:B:2244:VAL:HB	1:B:2255:PHE:CE2	2.31	0.65
1:B:2303:LYS:HE2	1:B:2305:HIS:CE1	2.31	0.64
8:A:207:HOH:O	2:C:1:NAG:H61	1.96	0.64
1:B:2393:GLU:HG3	8:B:656:HOH:O	1.97	0.64
1:B:2161:ASN:O	1:B:2165:VAL:HG13	1.97	0.64
1:B:2135:TYR:CE2	1:B:2156:LEU:HB2	2.33	0.63
1:B:2164:ASP:HA	1:B:2167:LYS:HE2	1.81	0.63
1:B:2139:GLN:HA	8:B:605:HOH:O	2.00	0.62
1:A:1117:THR:HG22	8:A:152:HOH:O	1.98	0.62
1:A:1139:GLN:HG2	8:A:663:HOH:O	1.99	0.61
1:B:2149:GLN:HG3	1:B:2153:ASP:OD2	2.01	0.61
1:B:2113:LYS:HD2	1:B:2114:THR:N	2.16	0.60
1:A:1036:SER:N	8:A:658:HOH:O	2.34	0.60
1:B:2311:ASP:OD2	3:H:2:NDG:H8C2	2.02	0.60
1:B:2162:LEU:O	1:B:2165:VAL:HG22	2.01	0.60
8:A:453:HOH:O	3:D:2:NDG:H6C2	2.02	0.60
1:B:2105:HIS:O	1:B:2109:ILE:HG13	2.01	0.59
1:B:2307:LYS:HE2	1:B:2381:PRO:HG2	1.85	0.59
1:B:2394:LYS:HB2	1:B:2394:LYS:HZ2	1.66	0.59
1:B:2063:ASP:HB2	1:B:2074:ASP:HA	1.83	0.59
1:A:1139:GLN:HA	1:A:1139:GLN:NE2	2.18	0.58
1:B:2490:GLN:H	1:B:2495:ASN:HD21	1.51	0.58
1:A:1161:ASN:O	1:A:1165:VAL:HG12	2.04	0.58
1:B:2321:ARG:HB2	8:B:574:HOH:O	2.02	0.58
1:B:2356:GLU:HG3	8:B:336:HOH:O	2.03	0.58
1:B:2309:ARG:HG3	1:B:2396:GLY:CA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2103:LEU:HB3	1:B:2151:LEU:HB3	1.87	0.57
1:B:2348:GLN:HE21	1:B:2352:ASP:CG	2.12	0.56
1:A:1185:SER:O	1:A:1186:HIS:HB2	2.05	0.56
1:B:2114:THR:HA	8:B:332:HOH:O	2.05	0.56
1:B:2289:ASP:O	1:B:2293:LEU:HD13	2.05	0.56
1:B:2106:VAL:HA	1:B:2109:ILE:HD12	1.87	0.56
1:B:2252:ASP:HB3	1:B:2254:GLN:HG2	1.88	0.56
1:B:2047:ALA:HB1	1:B:2474:MET:HE1	1.89	0.55
1:B:2496:THR:O	1:B:2508:VAL:HG22	2.07	0.55
1:B:2283:ARG:NH2	1:B:2510:ARG:HH12	2.05	0.54
8:A:231[A]:HOH:O	4:F:2[A]:LDY:C5	2.56	0.54
1:A:1160:ARG:NH2	1:A:1213:THR:HB	2.23	0.54
1:B:2164:ASP:O	1:B:2167:LYS:HE2	2.08	0.54
1:B:2138:LEU:O	1:B:2143:LYS:HA	2.08	0.53
1:A:1369:LEU:HD12	1:A:1369:LEU:O	2.08	0.53
1:B:2164:ASP:HA	1:B:2167:LYS:CE	2.39	0.53
1:B:2316:SER:HB3	1:B:2324:ASP:O	2.09	0.53
1:B:2045:LYS:HA	1:B:2093:MET:CE	2.39	0.53
1:B:2180:ASN:HB2	1:B:2189:ASP:HB2	1.91	0.53
1:B:2237:SER:C	1:B:2239:PRO:HD3	2.34	0.53
1:A:1110:ASP:OD1	1:A:1113:LYS:NZ	2.25	0.52
1:A:1286:THR:HB	8:A:94:HOH:O	2.08	0.52
1:B:2312:LEU:HA	8:B:89:HOH:O	2.08	0.52
1:B:2405:VAL:HG22	1:B:2405:VAL:O	2.10	0.52
1:A:1299:ILE:O	1:A:1303:LYS:HE2	2.10	0.52
1:B:2214:GLY:O	1:B:2216:GLU:N	2.42	0.52
1:A:1286:THR:HG21	8:A:477:HOH:O	2.10	0.52
1:B:2148:ASN:HA	8:B:515:HOH:O	2.09	0.52
1:A:1394:LYS:HD3	8:A:615:HOH:O	2.10	0.51
1:B:2106:VAL:HA	1:B:2109:ILE:CD1	2.40	0.51
1:B:2105:HIS:CD2	1:B:2109:ILE:HD11	2.45	0.51
1:B:2185:SER:C	1:B:2187:GLY:N	2.67	0.51
1:B:2309:ARG:NH1	3:H:2:NDG:H8C3	2.26	0.51
1:B:2041:ALA:O	1:B:2045:LYS:HG3	2.11	0.51
1:B:2249:ASN:HD21	1:B:2256:ALA:HB2	1.76	0.51
1:B:2348:GLN:NE2	1:B:2352:ASP:OD1	2.44	0.51
1:A:1259:ARG:HG2	1:A:1259:ARG:HH11	1.76	0.51
1:B:2249:ASN:ND2	1:B:2256:ALA:HB2	2.26	0.51
1:B:2148:ASN:CG	1:B:2151:LEU:HG	2.36	0.51
1:B:2273:LEU:HB3	1:B:2291:TRP:HB2	1.93	0.50
1:B:2118:VAL:O	1:B:2180:ASN:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2369:LEU:C	1:B:2369:LEU:HD23	2.36	0.50
1:B:2248:ILE:N	1:B:2248:ILE:HD12	2.26	0.50
1:B:2038:GLN:O	1:B:2042:ASP:OD2	2.29	0.50
1:B:2390:GLU:HB3	8:B:126:HOH:O	2.12	0.50
1:A:1427:ARG:HD3	1:A:1480:ALA:O	2.11	0.49
1:A:1325:LEU:N	1:A:1325:LEU:HD22	2.26	0.49
1:B:2095:LYS:O	1:B:2099:VAL:HG23	2.12	0.49
1:B:2405:VAL:HG13	1:B:2407[A]:ARG:HG3	1.93	0.49
1:A:1160:ARG:HD2	8:A:316:HOH:O	2.11	0.49
1:B:2036:SER:O	1:B:2039:ALA:N	2.45	0.49
1:A:1452:ASP:OD2	1:A:1455:LYS:HD2	2.13	0.49
1:B:2110:ASP:C	1:B:2112:SER:H	2.21	0.49
1:B:2045:LYS:HA	1:B:2093:MET:HE2	1.95	0.48
1:B:2077:ASN:ND2	1:B:2118:VAL:HG12	2.28	0.48
1:B:2233:GLN:HB2	1:B:2254:GLN:HE22	1.78	0.48
1:B:2160:ARG:NH2	8:B:713:HOH:O	2.47	0.48
1:B:2312:LEU:CD2	3:H:2:NDG:H8C1	2.44	0.48
1:B:2364:THR:HG21	1:B:2377:TRP:CE2	2.49	0.48
8:B:375:HOH:O	3:H:4:MAN:H3	2.14	0.48
1:A:1370:THR:O	1:A:1371:LYS:HB2	2.13	0.48
1:B:2160:ARG:HG3	1:B:2218:TYR:OH	2.14	0.48
1:B:2210:SER:OG	1:B:2219:ALA:N	2.43	0.48
1:B:2349:ASP:N	1:B:2349:ASP:OD1	2.47	0.48
1:B:2407[B]:ARG:HD2	8:B:383[B]:HOH:O	2.13	0.47
1:B:2045:LYS:HG2	1:B:2093:MET:HE2	1.95	0.47
1:A:1273:LEU:HB3	1:A:1291:TRP:HB2	1.95	0.47
1:A:1105:HIS:HD2	8:A:55:HOH:O	1.97	0.47
1:B:2282:LYS:HG2	1:B:2283:ARG:N	2.28	0.47
1:B:2360:GLY:O	1:B:2363:ALA:HB3	2.14	0.47
1:B:2110:ASP:OD2	1:B:2112:SER:OG	2.31	0.47
1:B:2325:LEU:HD12	1:B:2325:LEU:N	2.29	0.47
1:A:1510:ARG:HB3	1:A:1510:ARG:NH1	2.29	0.47
1:B:2087:LEU:O	1:B:2091:VAL:HG23	2.14	0.47
1:B:2167:LYS:C	1:B:2169:ALA:N	2.73	0.47
1:B:2301:HIS:O	1:B:2323:TYR:HE2	1.97	0.46
1:A:1318:TYR:CE1	1:A:1321:ARG:HA	2.50	0.46
1:A:1415:TYR:HE1	1:A:1489:VAL:HG23	1.79	0.46
1:B:2312:LEU:HD23	3:H:2:NDG:H8C1	1.97	0.46
5:I:2:NDG:O7	5:I:2:NDG:H3	2.15	0.46
1:B:2181:ILE:HD13	1:B:2181:ILE:N	2.30	0.46
1:B:2243:LEU:HB3	1:B:2260:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:PHE:CZ	1:A:1181:ILE:HD12	2.51	0.45
1:B:2238:GLU:HG3	1:B:2240:PHE:O	2.16	0.45
1:B:2330:LEU:CD2	1:B:2407[B]:ARG:HH21	2.26	0.45
1:A:1407[A]:ARG:NH2	8:A:449:HOH:O	2.48	0.45
1:B:2490:GLN:H	1:B:2495:ASN:ND2	2.14	0.45
1:B:2138:LEU:C	1:B:2140:GLY:H	2.24	0.45
1:B:2176:VAL:O	1:B:2250:ILE:HG23	2.17	0.45
1:B:2036:SER:O	1:B:2039:ALA:HB3	2.16	0.45
1:B:2164:ASP:CA	1:B:2167:LYS:HE2	2.45	0.45
1:B:2045:LYS:NZ	1:B:2045:LYS:HB3	2.32	0.45
1:B:2311:ASP:CG	3:H:2:NDG:H8C2	2.42	0.45
1:B:2257:ASP:OD2	1:B:2259:ARG:HB3	2.17	0.44
1:A:1394:LYS:HG3	1:A:1395:ALA:N	2.33	0.44
1:B:2064:GLU:HB2	8:B:183:HOH:O	2.17	0.44
1:B:2432:ASN:OD1	8:B:704:HOH:O	2.21	0.44
1:A:1237:SER:C	1:A:1239:PRO:HD3	2.42	0.44
1:B:2416:TYR:CE2	1:B:2489:VAL:HG11	2.52	0.44
1:B:2394:LYS:HG3	1:B:2395:ALA:N	2.33	0.43
1:A:1325:LEU:HD22	1:A:1325:LEU:H	1.84	0.43
1:B:2250:ILE:O	1:B:2250:ILE:HG22	2.17	0.43
1:B:2322:ASN:HB2	8:B:280:HOH:O	2.18	0.43
1:B:2299:ILE:HG12	1:B:2353:PHE:CD2	2.53	0.43
1:A:1139:GLN:O	1:A:1143:LYS:HD3	2.18	0.43
1:A:1045:LYS:HE3	1:A:1478:TYR:CE1	2.54	0.43
1:B:2106:VAL:O	1:B:2158:GLN:NE2	2.52	0.43
1:B:2138:LEU:HD13	1:B:2152:ILE:HG12	2.01	0.43
1:A:1108:ASP:HB2	8:A:334:HOH:O	2.19	0.43
1:B:2224:LYS:NZ	1:B:2228:TYR:CE2	2.86	0.43
1:B:2321:ARG:N	1:B:2321:ARG:HD2	2.34	0.42
1:B:2077:ASN:HB3	1:B:2114:THR:OG1	2.19	0.42
1:B:2185:SER:C	1:B:2187:GLY:H	2.26	0.42
1:B:2243:LEU:HD22	1:B:2297:SER:CB	2.49	0.42
1:B:2185:SER:HB3	2:G:1:NAG:H61	2.01	0.42
1:B:2109:ILE:HG22	1:B:2110:ASP:N	2.33	0.42
1:B:2295:ALA:O	1:B:2299:ILE:HG13	2.20	0.42
1:B:2455:LYS:O	1:B:2456:ALA:C	2.63	0.42
1:B:2423:LYS:HE2	8:B:379:HOH:O	2.19	0.42
1:B:2237:SER:OG	1:B:2255:PHE:HB2	2.20	0.42
1:B:2427:ARG:CD	1:B:2480:ALA:O	2.62	0.42
1:A:1248:ILE:HD12	1:A:1248:ILE:N	2.36	0.41
1:A:1063:ASP:HB2	1:A:1074:ASP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2163:ALA:HB1	1:B:2206:TRP:CZ3	2.55	0.41
1:B:2104:GLU:O	1:B:2107:ALA:HB3	2.20	0.41
1:B:2259:ARG:HH11	1:B:2259:ARG:HG3	1.86	0.41
1:B:2469:LEU:C	1:B:2469:LEU:HD13	2.45	0.41
1:A:1320:ASN:HB3	1:A:1321:ARG:HH12	1.85	0.41
1:B:2081:ALA:O	1:B:2085:ASP:HB2	2.20	0.41
1:B:2167:LYS:C	1:B:2169:ALA:H	2.27	0.41
1:A:1110:ASP:OD2	1:A:1112:SER:OG	2.31	0.41
1:B:2215:ASP:O	1:B:2217:GLU:N	2.54	0.41
1:B:2216:GLU:HB3	8:B:689:HOH:O	2.19	0.41
1:A:1415:TYR:CE1	1:A:1489:VAL:HG23	2.56	0.40
1:B:2383:LYS:O	1:B:2385:PRO:HD3	2.21	0.40
1:A:1259:ARG:HG2	1:A:1259:ARG:NH1	2.35	0.40
1:B:2311:ASP:OD2	3:H:2:NDG:C8	2.68	0.40
1:B:2115:SER:O	2:G:1:NAG:H81	2.22	0.40
1:B:2120:LEU:HD12	1:B:2166:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/475 (100%)	457 (96%)	15 (3%)	3 (1%)	21	12
1	B	474/475 (100%)	429 (90%)	39 (8%)	6 (1%)	9	3
All	All	949/950 (100%)	886 (93%)	54 (6%)	9 (1%)	12	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2215	ASP
1	A	1267	ASP

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Mol	Chain	Res	Type
1	B	2148	ASN
1	B	2267	ASP
1	B	2216	GLU
1	B	2111	PHE
1	B	2173	PRO
1	A	1186	HIS
1	A	1148	ASN

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	402/400 (100%)	390 (97%)	12 (3%)	36	27
1	B	401/400 (100%)	383 (96%)	18 (4%)	24	14
All	All	803/800 (100%)	773 (96%)	30 (4%)	29	20

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	ASP
1	A	1117	THR
1	A	1139	GLN
1	A	1165	VAL
1	A	1273	LEU
1	A	1282	LYS
1	A	1286	THR
1	A	1358	VAL
1	A	1408	PRO
1	A	1483	GLU
1	A	1500	ASN
1	A	1507	SER
1	B	2038	GLN
1	B	2061	PRO
1	B	2085	ASP
1	B	2117	THR

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Mol	Chain	Res	Type
1	B	2118	VAL
1	B	2143	LYS
1	B	2165	VAL
1	B	2181	ILE
1	B	2243	LEU
1	B	2273	LEU
1	B	2322	ASN
1	B	2340	LEU
1	B	2393	GLU
1	B	2394	LYS
1	B	2408	PRO
1	B	2469	LEU
1	B	2500	ASN
1	B	2501	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1037	ASN
1	A	1105	HIS
1	A	1139	GLN
1	A	1144	ASN
1	A	1148	ASN
1	A	1223	GLN
1	A	1233	GLN
1	A	1320	ASN
1	A	1432	ASN
1	A	1464	ASN
1	A	1490	GLN
1	A	1495	ASN
1	B	2053	ASN
1	B	2077	ASN
1	B	2139	GLN
1	B	2223	GLN
1	B	2249	ASN
1	B	2301	HIS
1	B	2348	GLN
1	B	2388	GLN
1	B	2432	ASN
1	B	2464	ASN
1	B	2490	GLN
1	B	2495	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 ⓘ

22 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	C	1	1,2	14,14,15	0.60	0	17,19,21	0.85	0
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	0.76	0
3	NAG	D	1	1,3	14,14,15	1.19	1 (7%)	17,19,21	0.88	0
3	NDG	D	2	3	14,14,15	1.11	2 (14%)	17,19,21	0.93	1 (5%)
3	MAN	D	3	3	11,11,12	0.48	0	15,15,17	0.47	0
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	0.59	0
3	MAN	D	5	3	11,11,12	0.47	0	15,15,17	0.63	0
2	NAG	E	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	0.80	0
2	NAG	E	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.70	0
4	MMA	F	1[A]	4	13,13,13	0.67	0	18,18,18	0.89	2 (11%)
4	LDY	F	2[A]	6,4	9,9,10	0.96	0	10,12,14	1.21	1 (10%)
2	NAG	G	1	1,2	14,14,15	0.68	0	17,19,21	0.72	1 (5%)
2	NAG	G	2	2	14,14,15	0.69	0	17,19,21	0.72	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.82	0	17,19,21	0.93	0
3	NDG	H	2	3	14,14,15	0.83	0	17,19,21	1.03	2 (11%)
3	MAN	H	3	3	11,11,12	0.52	0	15,15,17	0.45	0
3	MAN	H	4	3	11,11,12	0.43	0	15,15,17	0.66	1 (6%)
3	MAN	H	5	3	11,11,12	0.48	0	15,15,17	0.59	0
5	NAG	I	1	1,5	14,14,15	0.99	1 (7%)	17,19,21	0.71	0
5	NDG	I	2	5	14,14,15	0.81	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MMA	J	1[A]	4	13,13,13	0.64	0	18,18,18	0.76	0
4	LDY	J	2[A]	6,4	9,9,10	0.90	0	10,12,14	0.84	1 (10%)

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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NDG	D	2	3	-	3/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
4	MMA	F	1[A]	4	-	0/4/24/24	0/1/1/1
4	LDY	F	2[A]	6,4	-	-	0/1/1/1
2	NAG	G	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NDG	H	2	3	-	4/6/23/26	0/1/1/1
3	MAN	H	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NDG	I	2	5	-	3/6/23/26	0/1/1/1
4	MMA	J	1[A]	4	-	2/4/24/24	0/1/1/1
4	LDY	J	2[A]	6,4	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.91	1.56	1.52
3	D	2	NDG	C1-C2	2.86	1.56	1.52
5	I	1	NAG	C1-C2	2.46	1.55	1.52
2	E	1	NAG	C1-C2	2.39	1.55	1.52
3	D	2	NDG	O5-C5	2.18	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	2.16	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2[A]	LDY	C1-C2-C3	3.20	114.31	109.64
3	H	2	NDG	C2-N2-C7	-2.66	119.33	122.90
3	H	2	NDG	C4-C3-C2	-2.51	107.34	111.02
3	D	2	NDG	C2-N2-C7	-2.51	119.54	122.90
5	I	2	NDG	C2-N2-C7	-2.39	119.70	122.90
4	F	1[A]	MMA	C7-O1-C1	2.37	116.86	113.26
3	H	4	MAN	C1-O5-C5	2.26	115.22	112.19
2	G	1	NAG	C2-N2-C7	-2.11	120.07	122.90
4	F	1[A]	MMA	O1-C1-C2	2.08	110.53	108.14
2	G	2	NAG	C2-N2-C7	-2.04	120.17	122.90
4	J	2[A]	LDY	C1-C2-C3	2.01	112.58	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	3	MAN	C1
3	H	3	MAN	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
5	I	2	NDG	C3-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
3	H	2	NDG	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	D	2	NDG	C8-C7-N2-C2
5	I	2	NDG	C8-C7-N2-C2
4	J	1[A]	MMA	O5-C5-C6-O6
3	D	2	NDG	O7-C7-N2-C2
5	I	2	NDG	O7-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6

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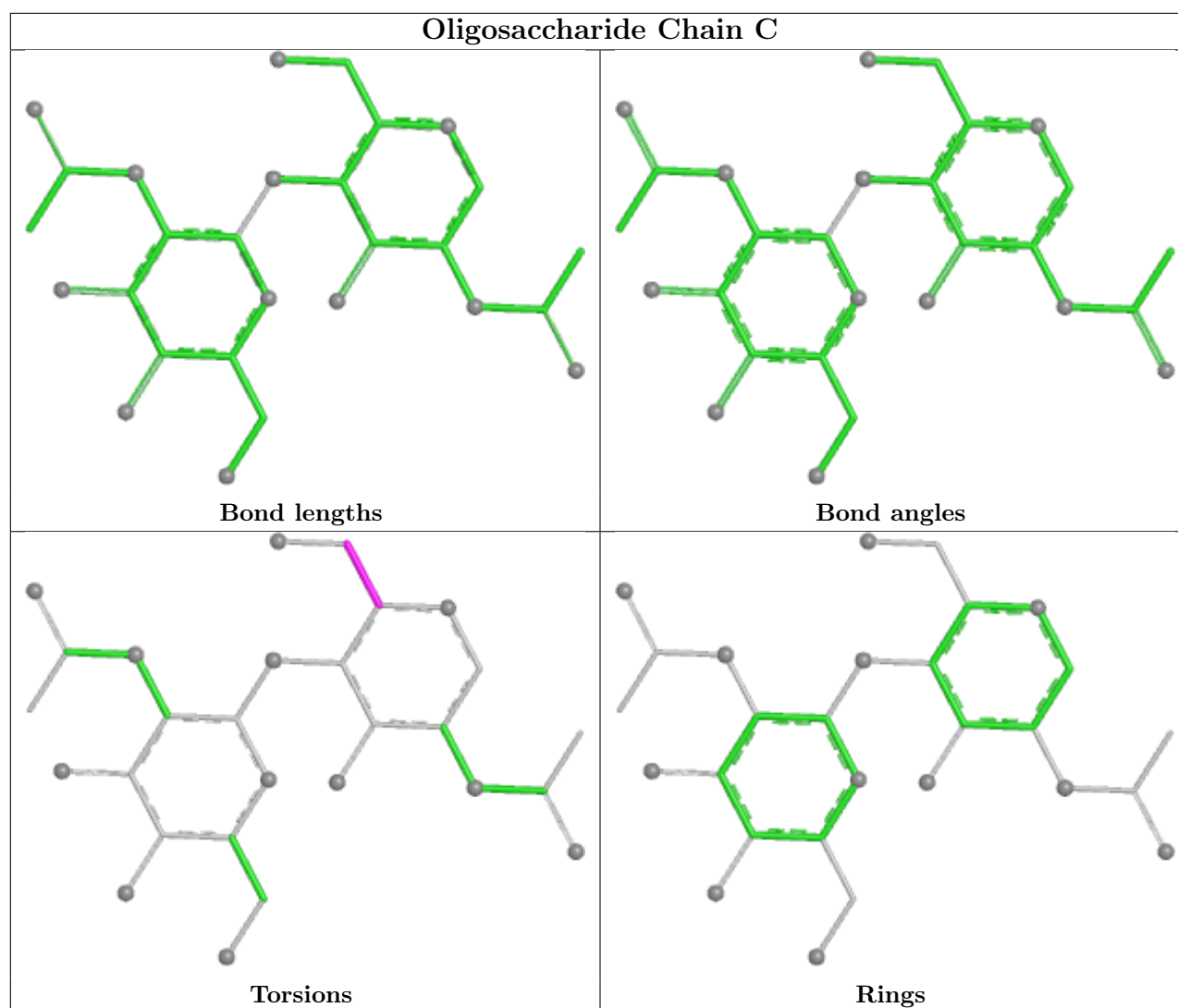
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
3	H	2	NDG	C4-C5-C6-O6
4	J	1[A]	MMA	C4-C5-C6-O6
3	H	2	NDG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NDG	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	H	2	NDG	O7-C7-N2-C2
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	H	5	MAN	O5-C5-C6-O6

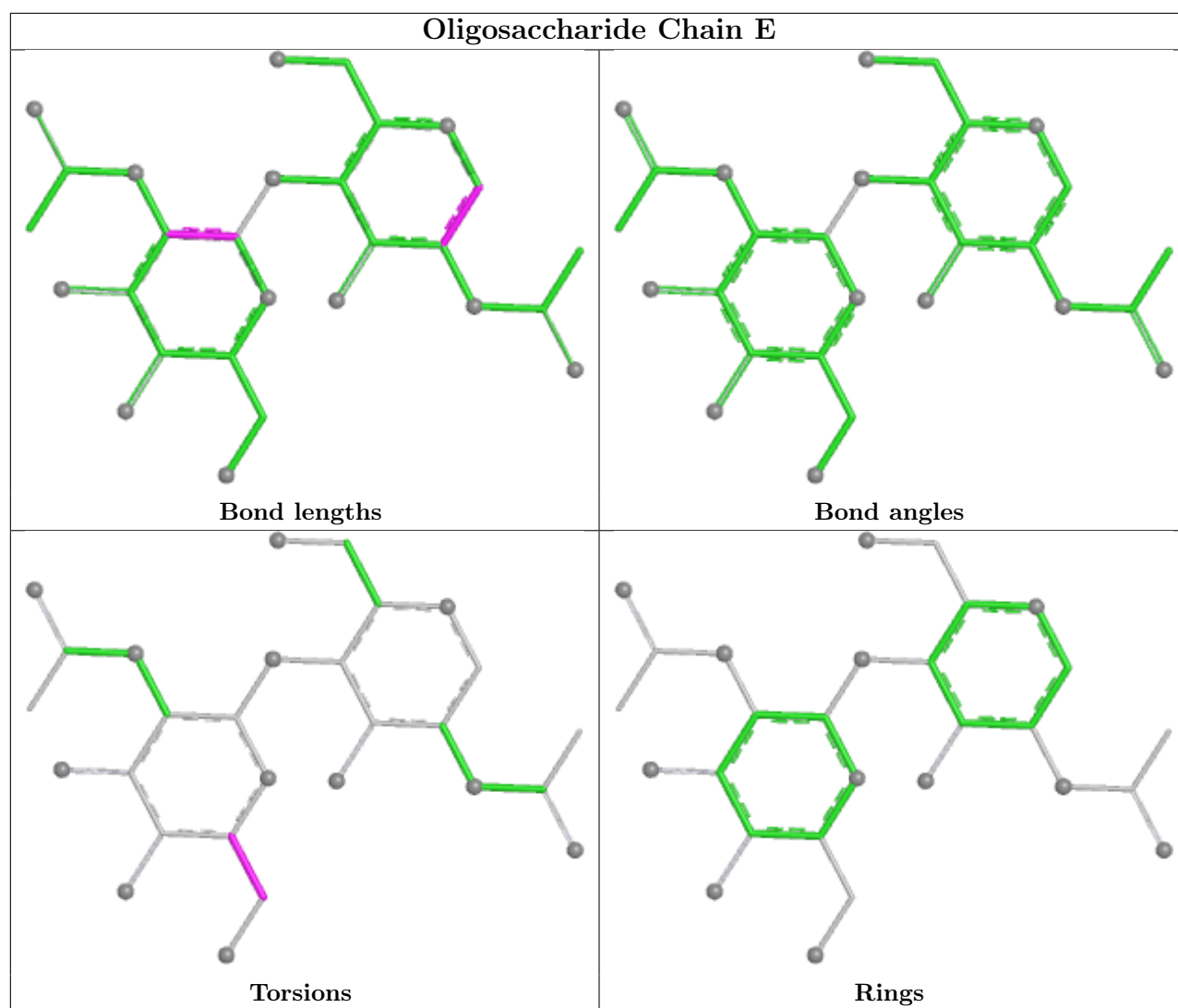
There are no ring outliers.

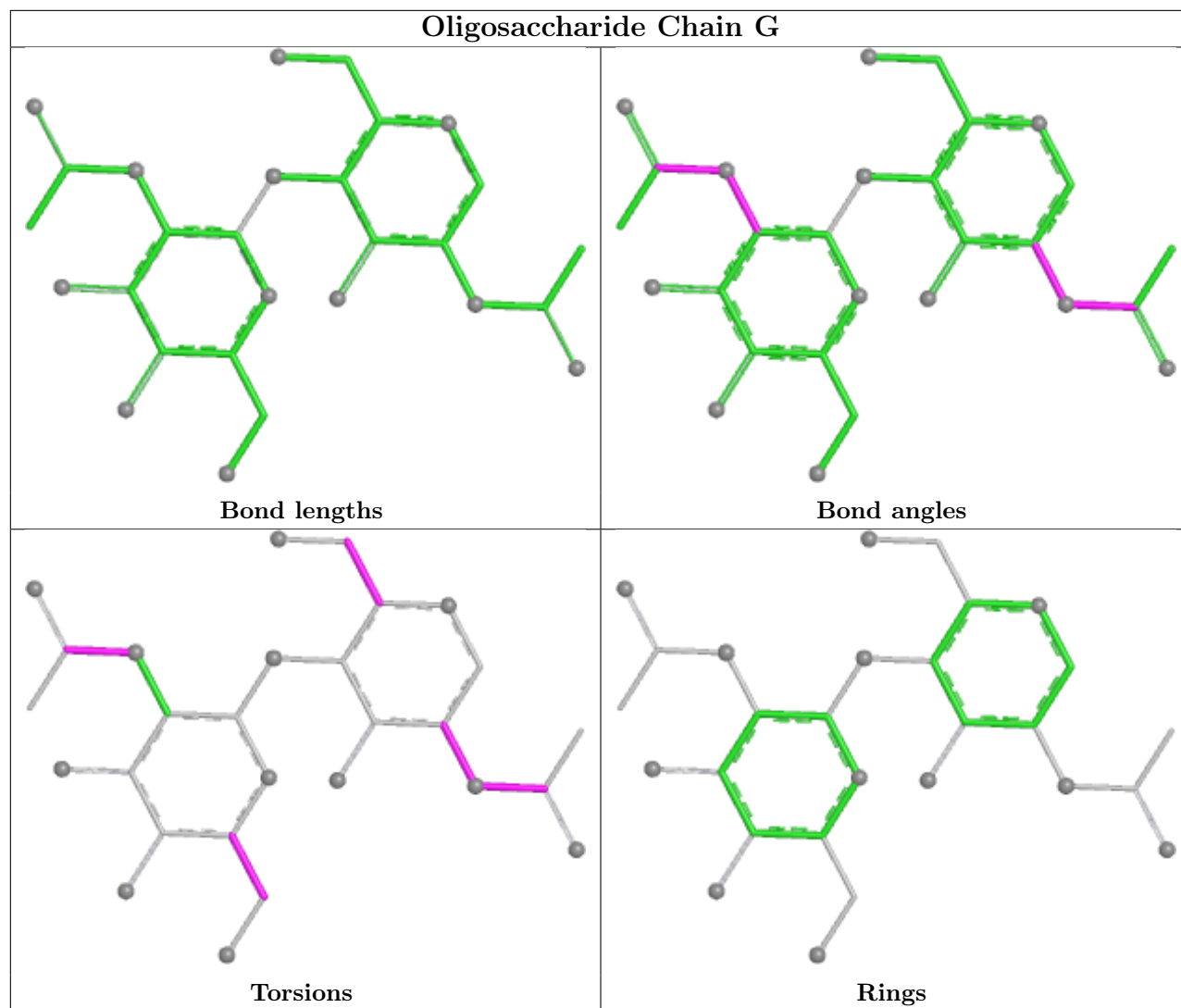
7 monomers are involved in 13 short contacts:

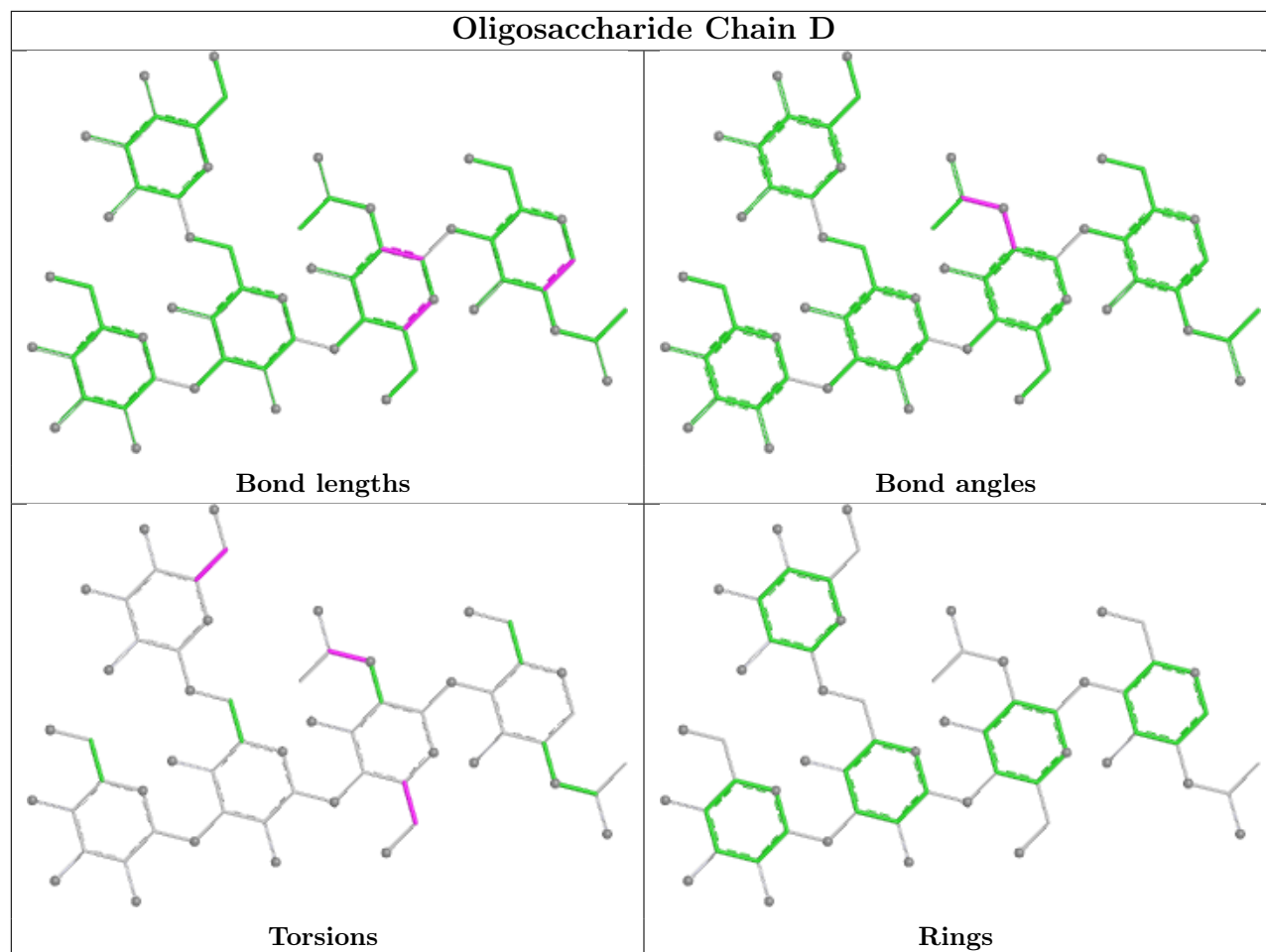
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
5	I	2	NDG	1	0
2	G	1	NAG	2	0
4	F	2[A]	LDY	1	0
3	H	4	MAN	1	0
3	H	2	NDG	6	0
3	D	2	NDG	1	0

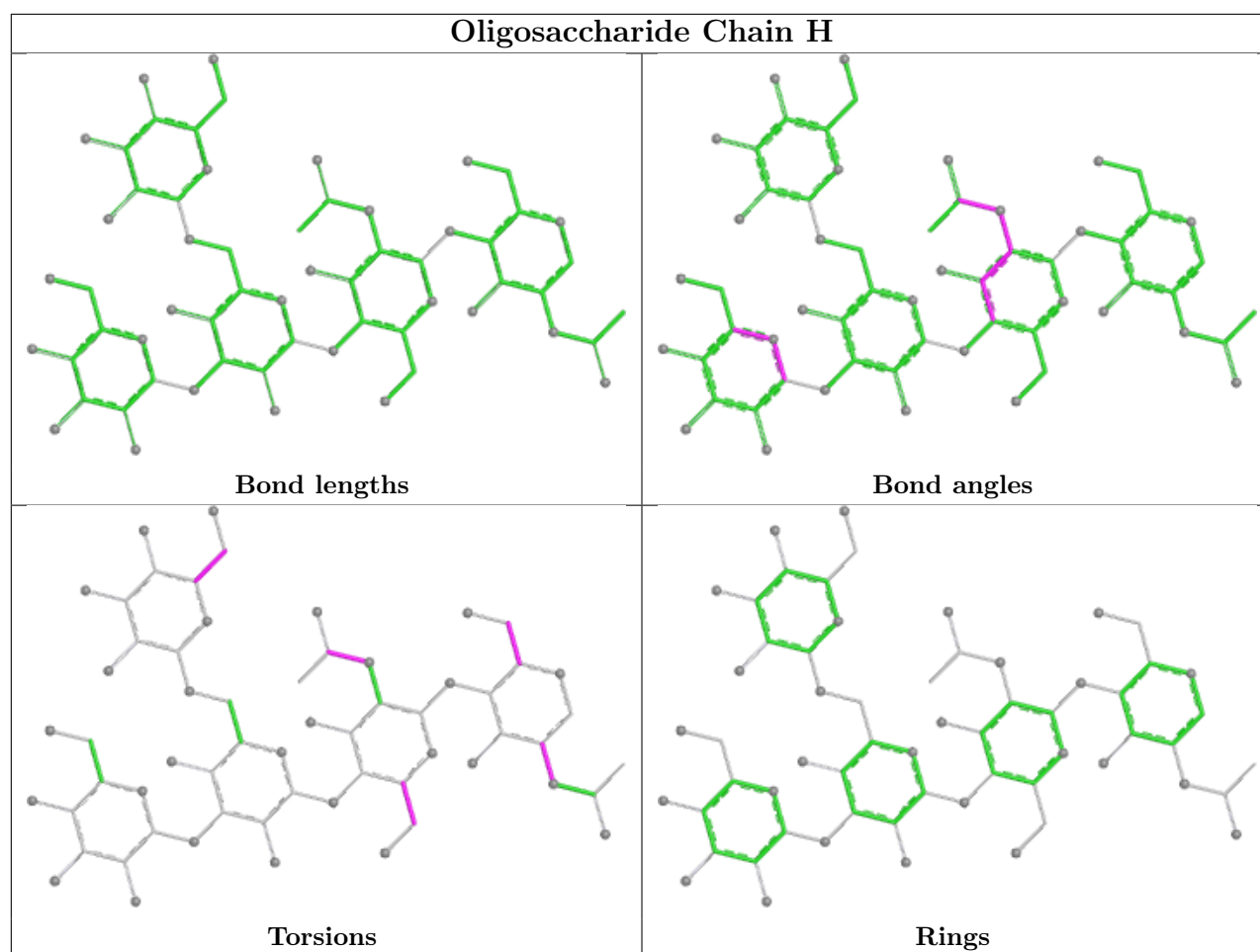
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

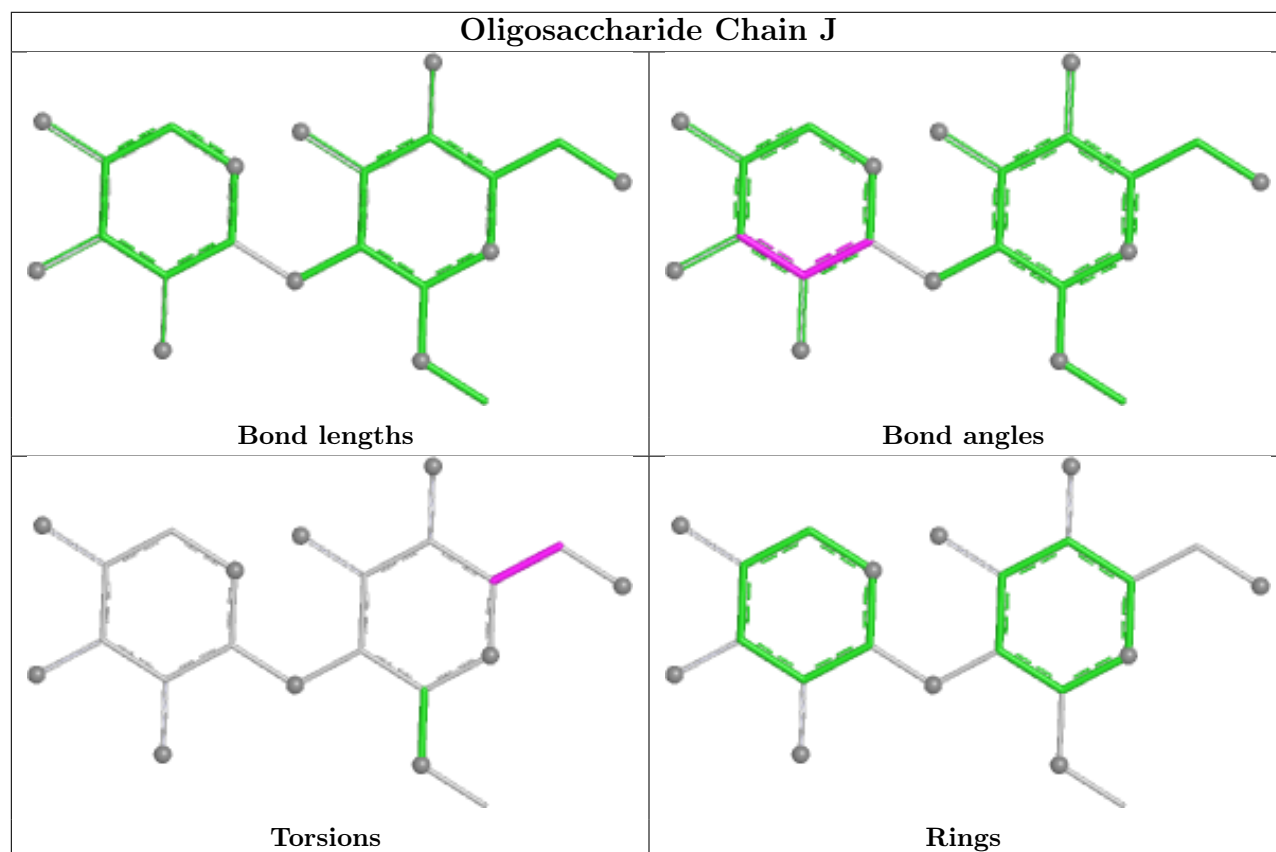
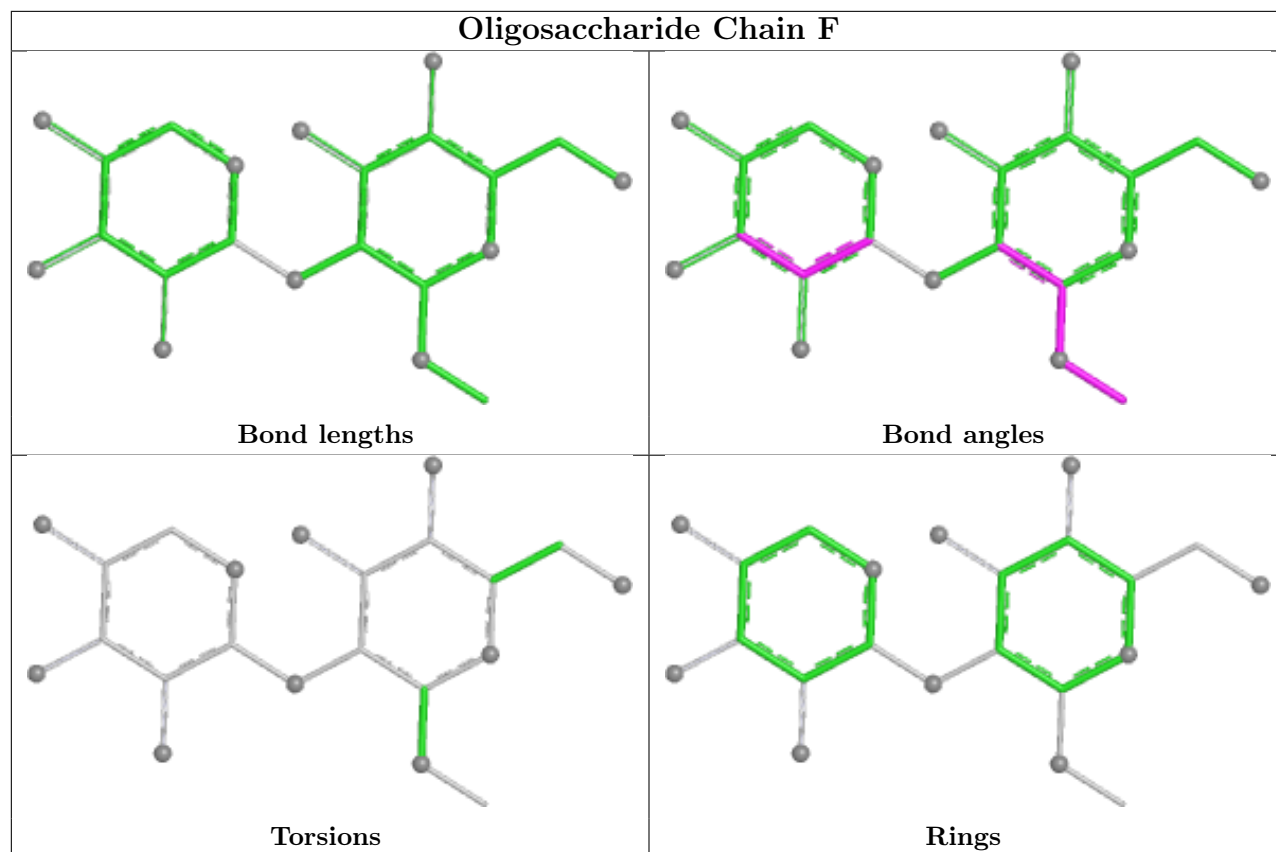


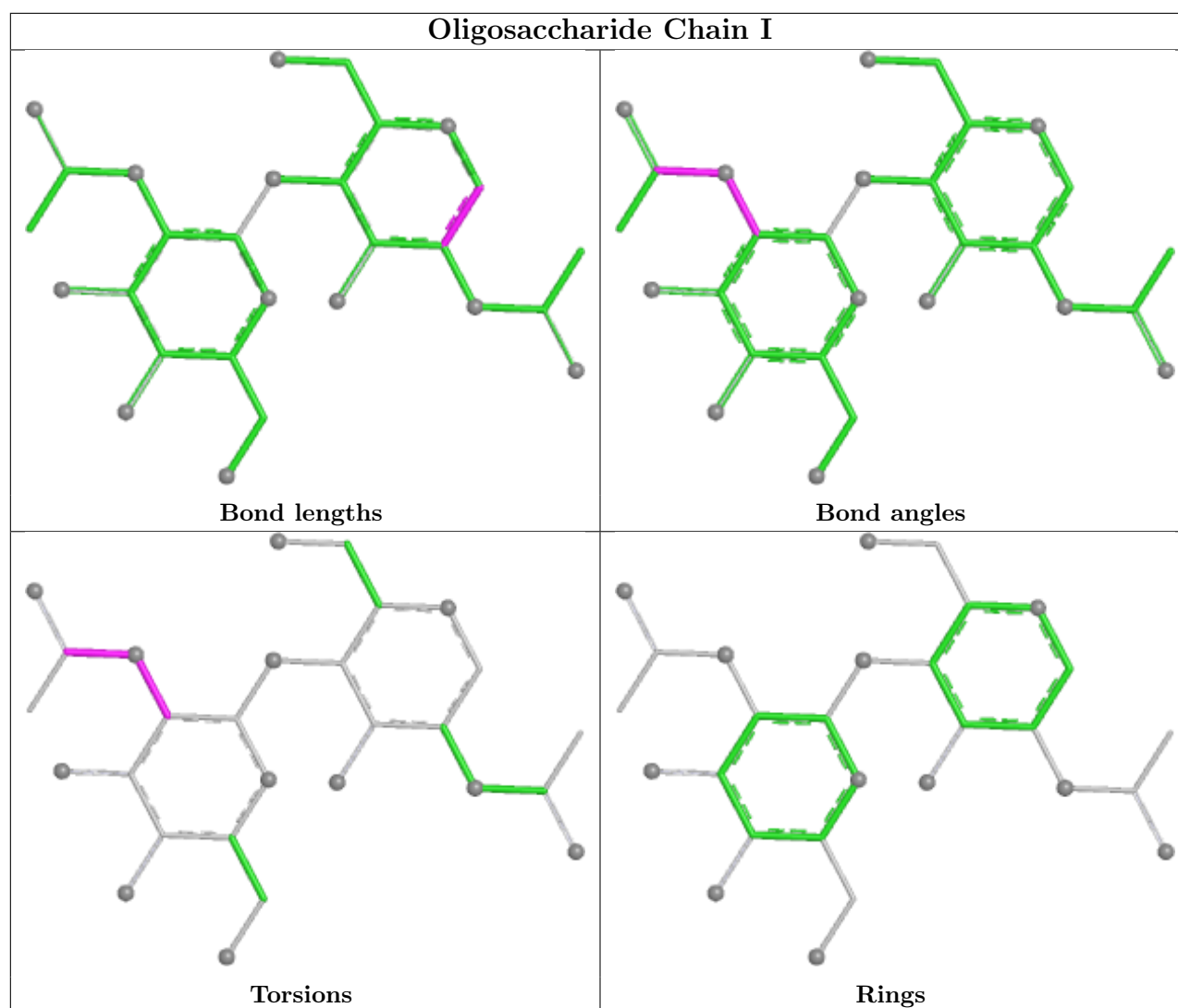












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	A	1903[B]	6	5,5,5	0.27	0	5,5,5	0.34	0
7	GOL	B	2903[B]	6	5,5,5	0.33	0	5,5,5	0.31	0
7	GOL	A	1902[B]	-	5,5,5	0.34	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	2902[B]	-	5,5,5	0.25	0	5,5,5	0.30	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
7	GOL	A	1903[B]	6	-	0/4/4/4	-
7	GOL	B	2903[B]	6	-	0/4/4/4	-
7	GOL	A	1902[B]	-	-	0/4/4/4	-
7	GOL	B	2902[B]	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	475/475 (100%)	-0.10	6 (1%) 75 81	5, 15, 32, 46	2 (0%)
1	B	475/475 (100%)	1.56	166 (34%) 1 0	8, 37, 62, 74	1 (0%)
All	All	950/950 (100%)	0.73	172 (18%) 3 3	5, 23, 58, 74	3 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2256	ALA	6.4
1	B	2379	TRP	5.7
1	B	2384	VAL	5.4
1	B	2145	LEU	4.9
1	B	2302	LEU	4.9
1	B	2323	TYR	4.8
1	B	2392	TYR	4.7
1	B	2146	VAL	4.5
1	B	2152	ILE	4.5
1	B	2165	VAL	4.5
1	B	2191	ALA	4.4
1	B	2190	GLY	4.3
1	B	2378	GLY	4.3
1	B	2178	TYR	4.2
1	B	2206	TRP	4.2
1	B	2181	ILE	4.1
1	B	2172	THR	4.1
1	B	2148	ASN	4.1
1	B	2039	ALA	4.1
1	B	2163	ALA	4.1
1	B	2255	PHE	4.0
1	B	2386	SER	4.0
1	B	2510	ARG	4.0
1	B	2304	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	2156	LEU	4.0
1	B	2118	VAL	4.0
1	B	2318	TYR	3.9
1	B	2385	PRO	3.9
1	B	2109	ILE	3.9
1	B	2425	ILE	3.9
1	B	2398	TYR	3.8
1	B	2391	PHE	3.8
1	B	2319	SER	3.8
1	B	2151	LEU	3.8
1	B	2381	PRO	3.8
1	B	2395	ALA	3.8
1	B	2250	ILE	3.8
1	B	2176	VAL	3.8
1	B	2325	LEU	3.7
1	B	2314	PHE	3.7
1	B	2138	LEU	3.6
1	B	2155	LEU	3.6
1	B	2177	PRO	3.6
1	B	2230	LEU	3.6
1	B	2170	PHE	3.6
1	B	2252	ASP	3.6
1	B	2111	PHE	3.6
1	B	2306	PRO	3.5
1	B	2142	ALA	3.5
1	B	2164	ASP	3.4
1	B	2149	GLN	3.4
1	B	2209	LEU	3.4
1	B	2162	LEU	3.4
1	B	2312	LEU	3.4
1	A	1321	ARG	3.3
1	B	2106	VAL	3.3
1	B	2166	LEU	3.3
1	B	2360	GLY	3.3
1	B	2248	ILE	3.3
1	B	2213	THR	3.3
1	B	2113	LYS	3.2
1	B	2189	ASP	3.2
1	B	2114	THR	3.2
1	B	2322	ASN	3.2
1	B	2388	GLN	3.2
1	B	2159	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	2316	SER	3.2
1	B	2321	ARG	3.2
1	B	2185	SER	3.1
1	B	2397	PHE	3.1
1	B	2377	TRP	3.1
1	A	1147	ASP	3.1
1	B	2168	PHE	3.1
1	B	2183	ILE	3.1
1	B	2249	ASN	3.1
1	B	2107	ALA	3.1
1	B	2173	PRO	3.0
1	B	2101	ALA	3.0
1	B	2310	PRO	3.0
1	B	2212	LEU	3.0
1	B	2260	VAL	3.0
1	B	2326	SER	3.0
1	B	2383	LYS	3.0
1	B	2258	SER	2.9
1	B	2299	ILE	2.9
1	B	2315	LEU	2.9
1	B	2489	VAL	2.9
1	B	2218	TYR	2.9
1	B	2150	ASP	2.9
1	B	2154	GLY	2.9
1	B	2184	THR	2.9
1	B	2225	ALA	2.9
1	B	2355	LEU	2.9
1	B	2187	GLY	2.9
1	B	2188	ASN	2.8
1	B	2301	HIS	2.8
1	B	2235	SER	2.8
1	B	2239	PRO	2.8
1	B	2135	TYR	2.8
1	B	2320	ASN	2.8
1	B	2171	ASP	2.8
1	B	2237	SER	2.7
1	B	2240	PHE	2.7
1	B	2229	LEU	2.7
1	B	2259	ARG	2.7
1	B	2317	SER	2.7
1	B	2327	SER	2.7
1	B	2244	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	2041	ALA	2.7
1	B	2305	HIS	2.7
1	B	2313	THR	2.6
1	B	2389	LYS	2.6
1	B	2108	ASP	2.6
1	B	2169	ALA	2.6
1	B	2485	ALA	2.6
1	B	2193	THR	2.6
1	B	2382	LYS	2.6
1	B	2036	SER	2.6
1	B	2182	ASN	2.6
1	B	2160	ARG	2.5
1	B	2309	ARG	2.5
1	B	2358	VAL	2.5
1	B	2232	PRO	2.5
1	B	2140	GLY	2.4
1	B	2308	SER	2.4
1	B	2380	ASP	2.4
1	A	1489	VAL	2.4
1	B	2175	GLY	2.4
1	B	2251	ASN	2.4
1	B	2147	ASP	2.4
1	B	2219	ALA	2.4
1	B	2103	LEU	2.4
1	B	2120	LEU	2.4
1	B	2324	ASP	2.4
1	B	2254	GLN	2.4
1	B	2117	THR	2.3
1	B	2351	ILE	2.3
1	B	2186	HIS	2.3
1	B	2221	LEU	2.3
1	B	2192	THR	2.3
1	B	2144	ASN	2.3
1	B	2141	PRO	2.3
1	B	2143	LYS	2.3
1	B	2253	GLY	2.3
1	B	2137	LEU	2.3
1	A	1510	ARG	2.3
1	A	1143	LYS	2.3
1	B	2060	PHE	2.2
1	B	2115	SER	2.2
1	B	2367	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2508	VAL	2.2
1	B	2161	ASN	2.2
1	B	2399	ILE	2.2
1	B	2394	LYS	2.2
1	B	2243	LEU	2.2
1	B	2037	ASN	2.2
1	B	2216	GLU	2.2
1	B	2303	LYS	2.2
1	B	2099	VAL	2.1
1	B	2376	SER	2.1
1	B	2245	GLY	2.1
1	B	2282	LYS	2.1
1	B	2393	GLU	2.1
1	B	2195	GLY	2.1
1	B	2105	HIS	2.1
1	B	2363	ALA	2.1
1	B	2153	ASP	2.1
1	B	2387	ASP	2.1
1	B	2104	GLU	2.0
1	B	2236	SER	2.0
1	B	2353	PHE	2.0
1	A	1144	ASN	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	2	14/15	0.58	0.16	70,71,72,73	0
2	NAG	G	1	14/15	0.59	0.19	60,62,65,68	0
3	MAN	H	5	11/12	0.66	0.15	58,59,60,60	11
3	MAN	D	5	11/12	0.67	0.17	42,46,48,48	11
3	NDG	H	2	14/15	0.74	0.16	53,54,56,56	0
3	NAG	H	1	14/15	0.74	0.18	47,49,53,54	0

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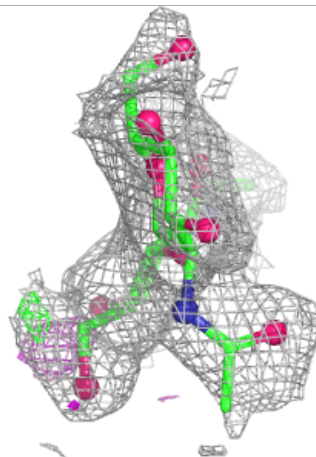
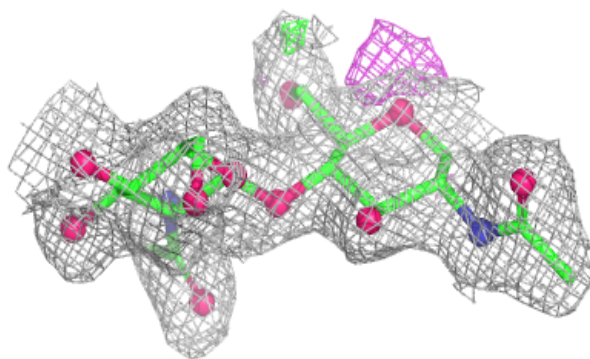
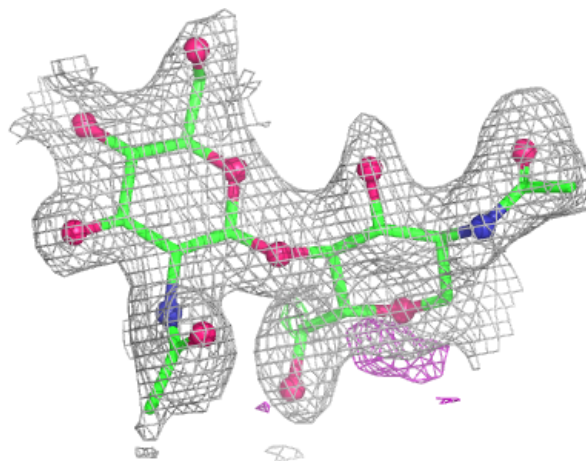
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	H	3	11/12	0.75	0.17	54,55,58,59	11
3	MAN	H	4	11/12	0.76	0.14	52,54,54,56	10
2	NAG	C	2	14/15	0.80	0.11	41,45,47,48	0
5	NDG	I	2	14/15	0.82	0.12	48,50,54,55	0
5	NAG	I	1	14/15	0.84	0.11	30,35,40,44	0
2	NAG	E	2	14/15	0.84	0.10	31,35,39,40	0
4	MMA	J	1[A]	13/13	0.85	0.11	24,26,29,29	13
3	MAN	D	4	11/12	0.86	0.11	25,29,31,33	10
2	NAG	C	1	14/15	0.86	0.11	26,29,32,35	0
3	NDG	D	2	14/15	0.89	0.10	21,25,30,30	0
4	MMA	F	1[A]	13/13	0.90	0.09	13,15,19,20	13
3	MAN	D	3	11/12	0.90	0.11	25,29,33,38	11
3	NAG	D	1	14/15	0.92	0.10	18,20,28,29	0
4	LDY	J	2[A]	9/10	0.92	0.10	15,18,20,22	9
2	NAG	E	1	14/15	0.95	0.06	15,18,21,25	0
4	LDY	F	2[A]	9/10	0.97	0.06	4,10,13,16	9

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.

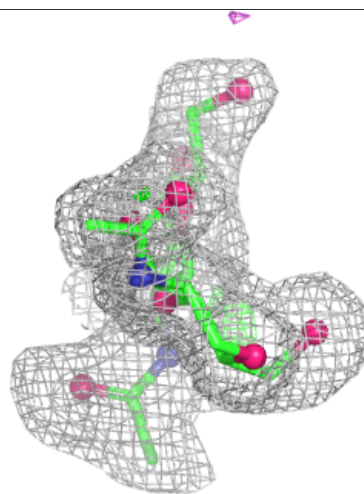
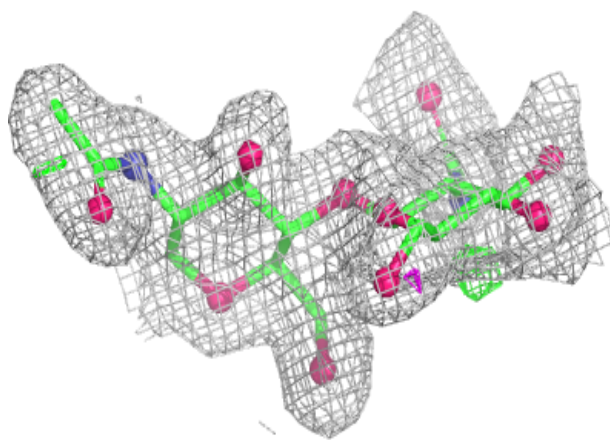
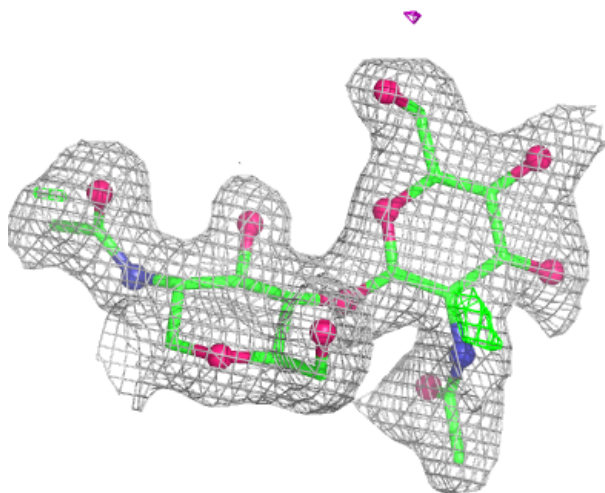
Electron density around Chain C:

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



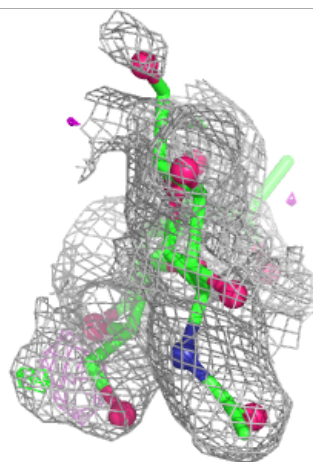
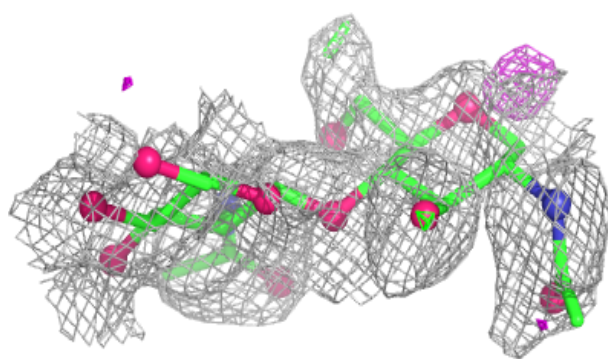
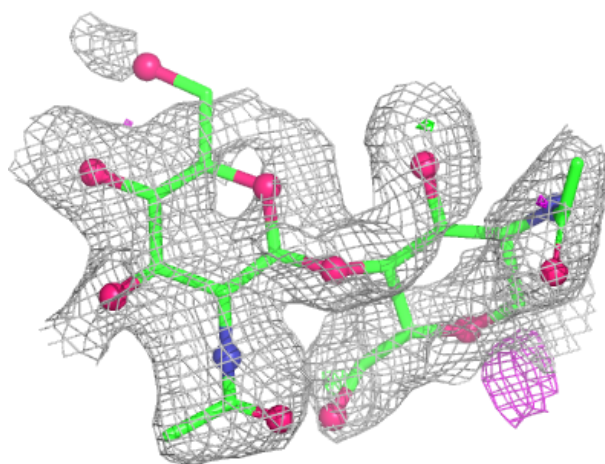
Electron density around Chain E:

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



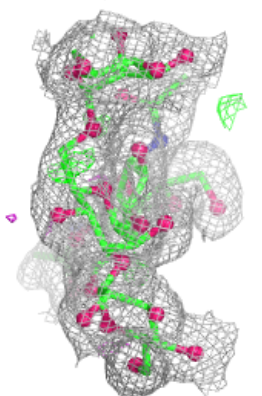
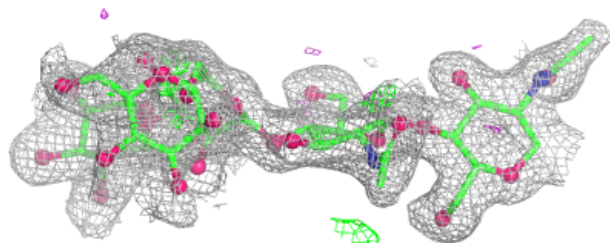
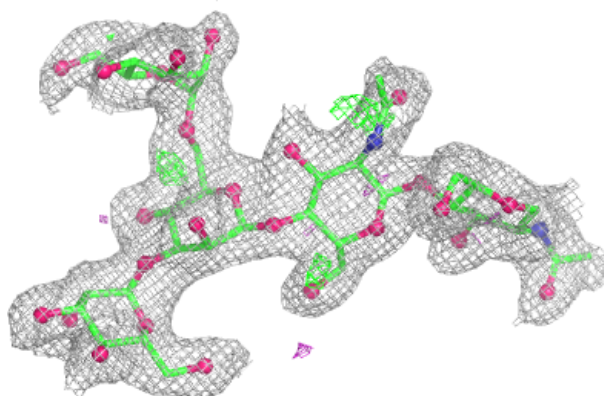
Electron density around Chain G:

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



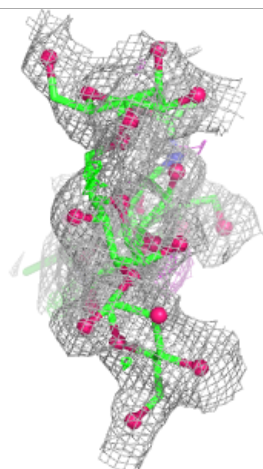
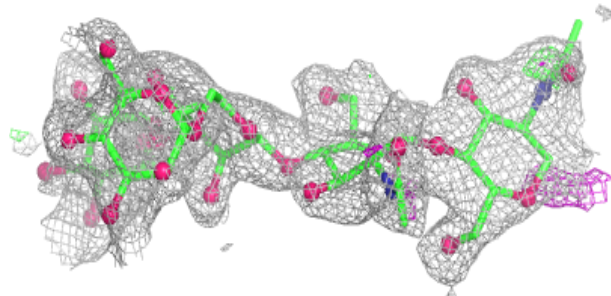
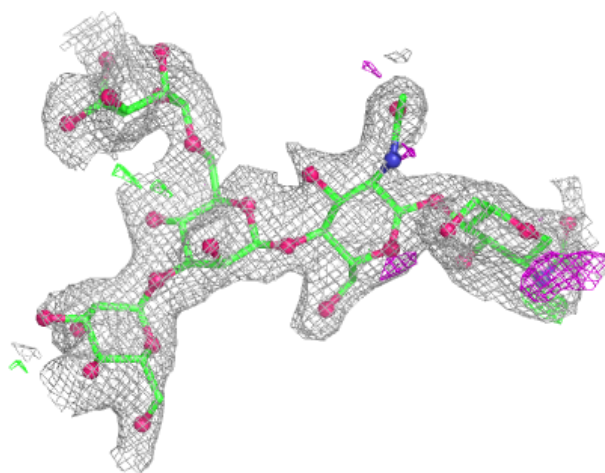
Electron density around Chain D:

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



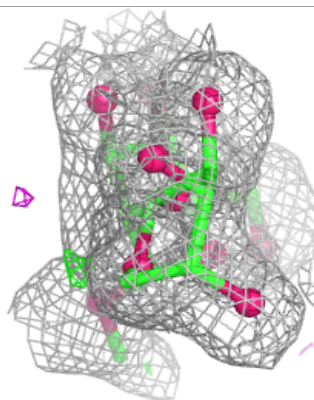
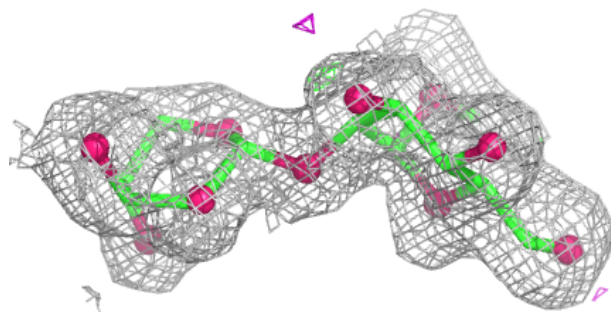
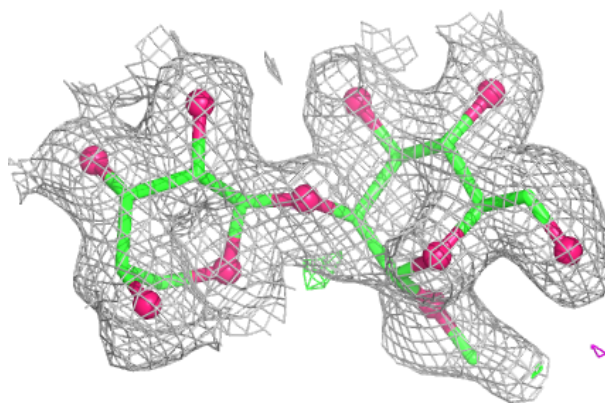
Electron density around Chain H:

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

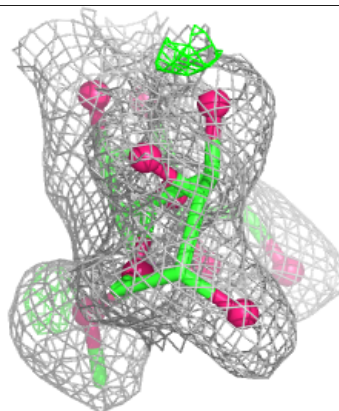
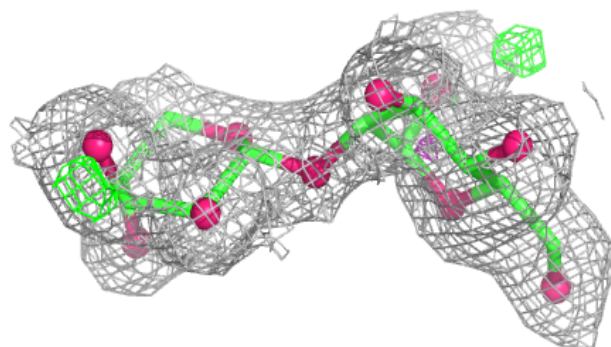
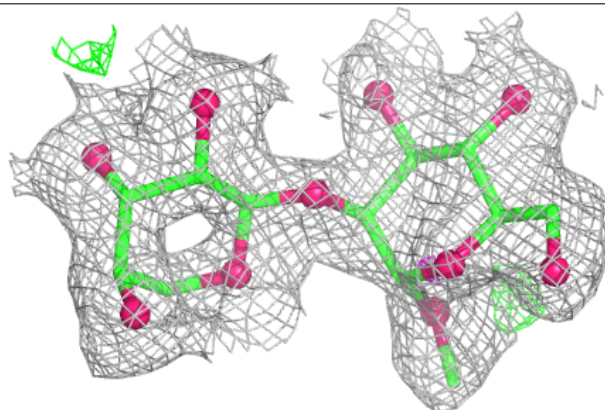


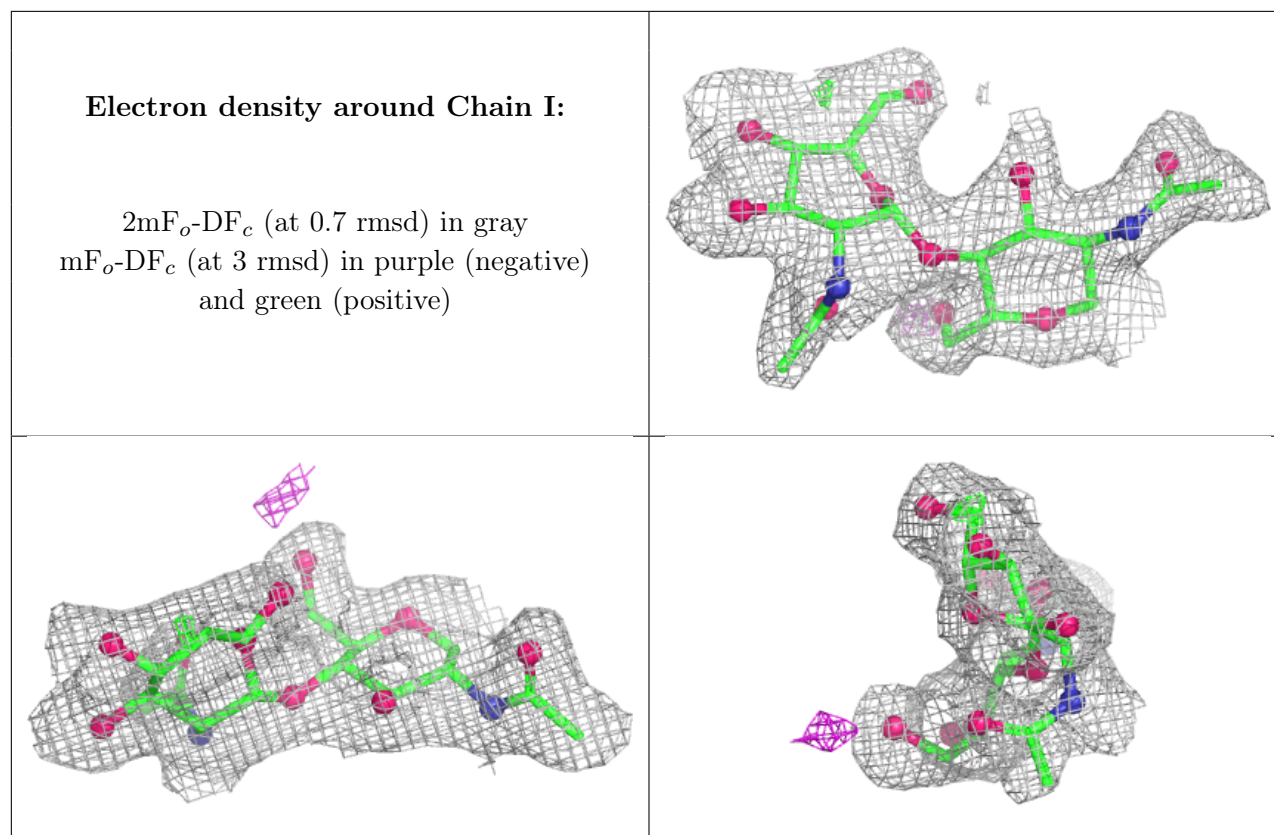
Electron density around Chain F:

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

**Electron density around Chain J:**

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





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
7	GOL	A	1902[B]	6/6	0.77	0.14	25,26,27,27	6
7	GOL	B	2902[B]	6/6	0.88	0.11	34,35,35,35	6
7	GOL	B	2903[B]	6/6	0.93	0.07	11,11,12,12	6
7	GOL	A	1903[B]	6/6	0.96	0.05	6,7,7,7	6
6	CA	B	2551	1/1	0.98	0.03	15,15,15,15	0
6	CA	A	1550	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.