



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 1KKT / pdb_00001kkt
Title : Structure of P. citrinum alpha 1,2-mannosidase reveals the basis for differences in specificity of the ER and Golgi Class I enzymes
Authors : Lobsanov, Y.D.; Vallee, F.; Imberty, A.; Yoshida, T.; Yip, P.; Herscovics, A.; Howell, P.L.
Deposited on : 2001-12-10
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

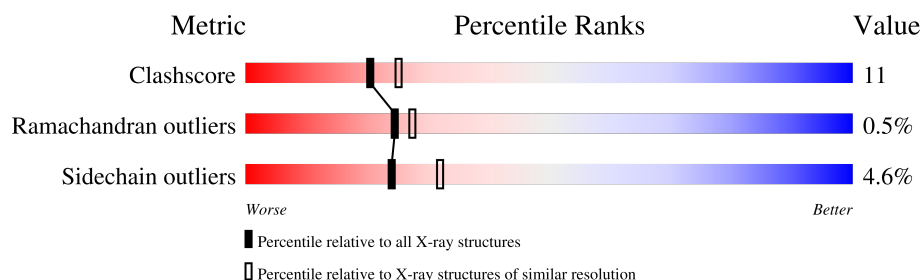
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	72% 18% • 7%
1	B	511	65% 26% • 7%
2	C	2	50% 50%
2	E	2	100%
2	F	2	100%
2	H	2	50% 50%
3	D	5	40% 60%
3	G	5	80% 20%

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
2	NAG	C	2	X	-	-	-
2	NAG	E	2	X	-	-	-
2	NAG	F	2	X	-	-	-
2	NAG	H	2	X	-	-	-
3	NAG	D	2	X	-	-	-
3	MAN	D	3	X	-	-	-
3	NAG	G	2	X	-	-	-
3	MAN	G	3	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7885 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.

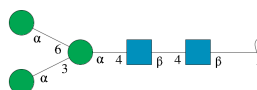
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3724	2359	619	738	8			
1	B	475	Total	C	N	O	S	0	0	0
			3724	2359	619	738	8			

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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-beta-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			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is water.

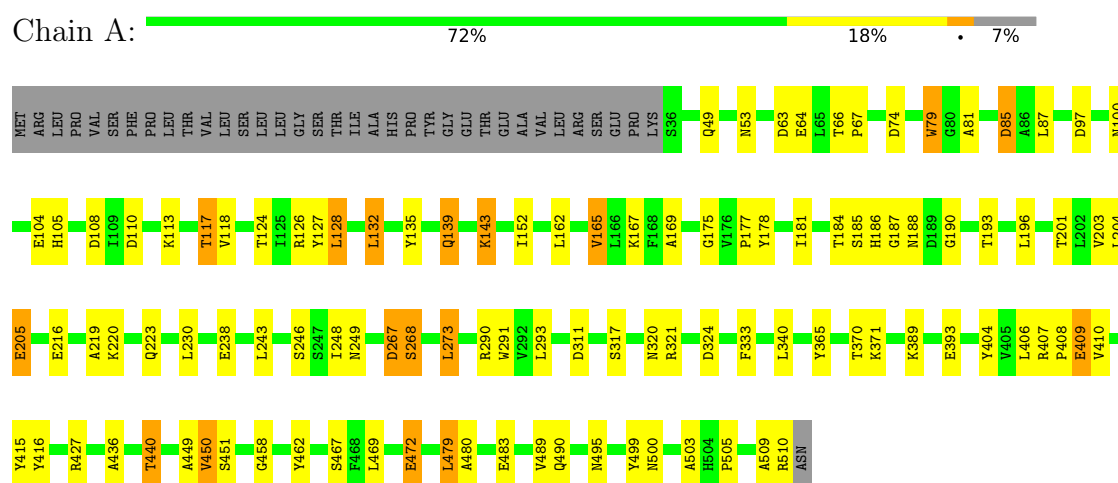
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	58	Total	O	0	0
			58	58		

3 Residue-property plots

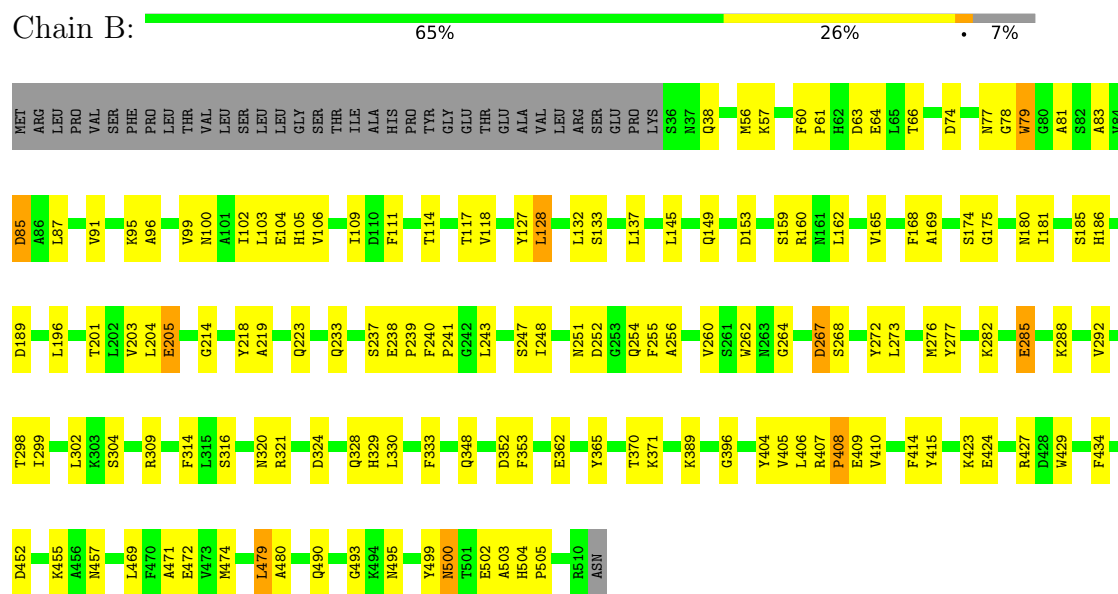
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- 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

Chain C:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain D:  40% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain G:  80% 20%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

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)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7885	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, 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	0.43	0/3819	0.93	21/5190 (0.4%)
1	B	0.34	0/3819	0.88	15/5190 (0.3%)
All	All	0.38	0/7638	0.91	36/10380 (0.3%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	THR	CA-C-N	8.26	127.98	119.56
1	B	66	THR	C-N-CA	8.26	127.98	119.56
1	A	178	TYR	N-CA-C	-6.81	98.15	109.46
1	B	64	GLU	N-CA-C	6.49	118.71	108.79
1	A	190	GLY	N-CA-C	-6.33	106.59	115.32
1	A	66	THR	CA-C-N	6.33	126.01	119.56
1	A	66	THR	C-N-CA	6.33	126.01	119.56
1	A	175	GLY	N-CA-C	-6.30	106.34	114.85
1	B	214	GLY	N-CA-C	-6.19	106.88	114.92
1	B	469	LEU	N-CA-C	-6.16	104.49	111.14
1	A	67	PRO	N-CA-C	6.11	121.78	113.84
1	A	167	LYS	N-CA-C	6.06	119.77	112.38
1	A	333	PHE	N-CA-C	-5.94	105.30	112.54
1	A	64	GLU	N-CA-C	5.89	118.02	109.07
1	A	472	GLU	N-CA-C	5.89	120.76	112.93
1	A	238	GLU	CA-C-N	5.67	125.78	119.32
1	A	238	GLU	C-N-CA	5.67	125.78	119.32
1	A	203	VAL	N-CA-C	5.64	118.10	111.05
1	A	469	LEU	N-CA-C	-5.57	105.11	111.07
1	B	66	THR	N-CA-C	-5.53	97.75	108.59
1	B	333	PHE	N-CA-C	-5.46	106.12	112.89
1	A	188	ASN	N-CA-C	5.45	115.31	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	GLY	N-CA-C	-5.42	107.54	114.37
1	A	66	THR	N-CA-C	-5.37	97.89	109.01
1	A	409	GLU	N-CA-C	5.35	117.80	111.33
1	B	471	ALA	N-CA-C	5.30	117.14	111.36
1	A	246	SER	N-CA-C	5.30	119.89	113.38
1	B	57	LYS	N-CA-C	5.29	117.13	111.36
1	B	78	GLY	N-CA-C	5.28	122.39	115.36
1	B	285	GLU	N-CA-C	-5.13	105.81	111.71
1	A	177	PRO	N-CA-C	5.06	118.66	111.13
1	B	500	ASN	N-CA-C	-5.05	103.38	110.35
1	B	414	PHE	N-CA-C	-5.03	105.88	111.36
1	A	451	SER	N-CA-C	5.02	118.56	112.23
1	B	329	HIS	N-CA-C	-5.01	105.81	111.28
1	A	81	ALA	N-CA-C	5.00	117.38	111.33

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	3724	0	3522	64	0
1	B	3724	0	3522	101	0
2	C	28	0	25	3	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	1	0
3	D	61	0	52	1	0
3	G	61	0	52	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	143	0	0	4	0
5	B	58	0	0	2	0
All	All	7885	0	7248	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (167) 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:423:LYS:HE3	3:G:4:MAN:H61	1.46	0.95
1:A:201:THR:OG1	1:A:268:SER:HB3	1.73	0.88
1:B:264:GLY:H	1:B:328:GLN:HE22	1.20	0.88
1:A:185:SER:O	1:A:187:GLY:N	2.09	0.85
1:B:243:LEU:HB3	1:B:260:VAL:HG21	1.56	0.85
1:B:264:GLY:H	1:B:328:GLN:NE2	1.79	0.79
1:A:436:ALA:O	1:A:440:THR:HG23	1.83	0.79
1:B:77:ASN:ND2	1:B:118:VAL:HG12	1.99	0.77
1:A:79:TRP:HD1	1:A:127:TYR:CZ	2.02	0.76
1:A:499:TYR:CE2	1:A:505:PRO:HG3	2.23	0.73
1:B:79:TRP:HD1	1:B:127:TYR:CZ	2.07	0.73
1:A:490:GLN:H	1:A:495:ASN:HD21	1.35	0.72
1:A:490:GLN:H	1:A:495:ASN:ND2	1.89	0.71
1:B:180:ASN:HB2	1:B:189:ASP:HB2	1.74	0.68
1:B:133:SER:O	1:B:137:LEU:HD23	1.95	0.66
1:A:273:LEU:HB3	1:A:291:TRP:HB2	1.77	0.66
1:A:128:LEU:HD22	1:A:132:LEU:HD22	1.78	0.65
1:A:193:THR:HG22	1:A:249:ASN:HD22	1.61	0.65
1:B:499:TYR:CE2	1:B:505:PRO:HG3	2.32	0.65
1:A:290:ARG:HD3	5:A:820:HOH:O	1.98	0.64
1:A:427:ARG:HD3	1:A:480:ALA:O	1.98	0.64
1:A:311:ASP:OD2	3:D:2:NAG:H81	1.98	0.63
1:B:427:ARG:HD3	1:B:480:ALA:O	1.98	0.63
1:B:370:THR:O	1:B:371:LYS:HB2	1.98	0.63
1:B:490:GLN:H	1:B:495:ASN:HD21	1.46	0.63
1:B:365:TYR:CE1	1:B:410:VAL:HG21	2.34	0.62
1:A:450:VAL:HG13	1:A:458:GLY:O	2.01	0.60
1:A:185:SER:C	1:A:187:GLY:H	2.08	0.59
1:B:95:LYS:O	1:B:99:VAL:HG23	2.03	0.59
1:A:389:LYS:O	1:A:393:GLU:HG3	2.03	0.59
1:A:509:ALA:O	1:A:510:ARG:HB2	2.03	0.59
1:B:111:PHE:HD2	1:B:162:LEU:HD13	1.68	0.59
1:B:452:ASP:CG	1:B:455:LYS:HG3	2.28	0.58
1:B:103:LEU:O	1:B:106:VAL:HG12	2.03	0.58
1:B:237:SER:OG	1:B:255:PHE:HB2	2.05	0.57
1:B:277:TYR:CE1	1:B:288:LYS:HD3	2.39	0.57
1:A:449:ALA:HB3	1:A:462:TYR:HB2	1.86	0.57
1:A:126:ARG:HH11	1:A:467:SER:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:OE1	1:B:288:LYS:HE3	2.05	0.56
1:A:117:THR:HG22	5:A:924:HOH:O	2.06	0.56
1:B:128:LEU:O	1:B:132:LEU:HD13	2.05	0.56
1:B:304:SER:HB3	1:B:314:PHE:O	2.06	0.56
1:A:185:SER:HB3	2:C:1:NAG:H61	1.87	0.56
1:B:288:LYS:O	1:B:292:VAL:HG23	2.06	0.56
1:B:472:GLU:HG2	1:B:503:ALA:HB3	1.87	0.56
2:H:2:NAG:O7	2:H:2:NAG:H3	2.06	0.55
1:B:106:VAL:HA	1:B:109:ILE:CD1	2.37	0.55
2:C:1:NAG:H62	2:C:2:NAG:H82	1.89	0.55
1:A:100:ASN:O	1:A:104:GLU:HG3	2.07	0.55
1:B:105:HIS:O	1:B:109:ILE:HG13	2.07	0.54
1:B:348:GLN:HE21	1:B:352:ASP:CG	2.16	0.54
1:B:63:ASP:HB2	1:B:74:ASP:HA	1.89	0.54
1:B:490:GLN:H	1:B:495:ASN:ND2	2.05	0.54
1:B:248:ILE:HD12	1:B:248:ILE:N	2.23	0.53
1:B:238:GLU:HG2	1:B:240:PHE:O	2.09	0.53
1:B:434:PHE:HE1	1:B:474:MET:HE1	1.74	0.53
1:A:472:GLU:HG2	1:A:503:ALA:HB3	1.90	0.53
1:A:185:SER:O	1:A:185:SER:OG	2.22	0.52
1:B:205:GLU:H	1:B:205:GLU:CD	2.17	0.52
1:B:264:GLY:N	1:B:328:GLN:HE22	1.98	0.52
1:A:110:ASP:OD1	1:A:113:LYS:NZ	2.42	0.52
1:B:219:ALA:O	1:B:223:GLN:HG3	2.09	0.52
1:B:174:SER:HB3	1:B:251:ASN:O	2.10	0.52
1:A:365:TYR:CE1	1:A:410:VAL:HG21	2.45	0.51
1:B:132:LEU:HD11	1:B:159:SER:HB3	1.92	0.51
1:B:247:SER:O	1:B:255:PHE:HA	2.10	0.51
1:B:238:GLU:OE2	1:B:241:PRO:HA	2.10	0.51
1:B:407:ARG:HB3	1:B:409:GLU:OE2	2.10	0.51
1:B:111:PHE:CD2	1:B:162:LEU:HD13	2.45	0.50
1:A:219:ALA:O	1:A:223:GLN:HG3	2.11	0.50
1:B:267:ASP:CG	1:B:268:SER:H	2.19	0.50
1:B:320:ASN:O	1:B:321:ARG:HB2	2.10	0.50
1:A:97:ASP:HB2	5:A:844:HOH:O	2.09	0.50
1:B:106:VAL:HA	1:B:109:ILE:HD12	1.93	0.50
1:B:79:TRP:CD1	1:B:127:TYR:CZ	2.95	0.50
1:B:247:SER:OG	1:B:256:ALA:HB3	2.12	0.50
1:A:139:GLN:HE22	1:A:152:ILE:HG21	1.77	0.50
1:B:302:LEU:HD22	1:B:316:SER:O	2.12	0.50
1:B:389:LYS:HD3	1:B:389:LYS:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TRP:CD1	1:A:127:TYR:CZ	2.93	0.49
1:B:409:GLU:H	1:B:409:GLU:CD	2.20	0.49
1:A:184:THR:HG23	5:A:878:HOH:O	2.13	0.48
1:B:99:VAL:O	1:B:103:LEU:HG	2.14	0.48
1:B:247:SER:C	1:B:248:ILE:HD12	2.37	0.48
1:A:79:TRP:O	1:A:105:HIS:HE1	1.97	0.48
1:B:405:VAL:HG23	1:B:407:ARG:HG3	1.95	0.48
1:B:162:LEU:O	1:B:165:VAL:HG22	2.13	0.48
1:A:370:THR:O	1:A:371:LYS:HB2	2.14	0.48
1:B:237:SER:C	1:B:239:PRO:HD3	2.38	0.48
1:B:404:TYR:CE2	1:B:406:LEU:HA	2.48	0.48
1:B:185:SER:O	1:B:186:HIS:HB2	2.14	0.47
1:A:267:ASP:CG	1:A:268:SER:H	2.22	0.47
1:A:436:ALA:O	1:A:440:THR:CG2	2.59	0.47
1:B:309:ARG:HG3	1:B:396:GLY:HA3	1.95	0.47
1:A:79:TRP:HD1	1:A:127:TYR:CE1	2.33	0.47
1:B:415:TYR:CE2	1:B:479:LEU:HB3	2.49	0.47
1:B:299:ILE:HG12	1:B:353:PHE:CD2	2.49	0.47
1:B:203:VAL:HG13	5:B:811:HOH:O	2.14	0.46
1:A:79:TRP:CZ3	1:A:113:LYS:O	2.69	0.46
1:A:205:GLU:H	1:A:205:GLU:CD	2.22	0.46
1:A:79:TRP:HZ3	1:A:113:LYS:O	1.98	0.46
1:A:320:ASN:O	1:A:321:ARG:HB2	2.14	0.46
1:A:510:ARG:NE	1:A:510:ARG:HA	2.31	0.46
1:B:330:LEU:HA	1:B:409:GLU:HG2	1.98	0.46
1:B:237:SER:CB	1:B:255:PHE:HB2	2.46	0.46
1:B:299:ILE:HG12	1:B:353:PHE:CE2	2.51	0.46
1:A:185:SER:HB3	2:C:1:NAG:C6	2.46	0.46
1:B:38:GLN:HE21	1:B:38:GLN:HA	1.80	0.45
1:B:81:ALA:O	1:B:85:ASP:HB2	2.15	0.45
1:A:139:GLN:HE22	1:A:152:ILE:CG2	2.29	0.45
1:A:416:TYR:CE2	1:A:489:VAL:HG21	2.52	0.45
1:B:105:HIS:CE1	1:B:109:ILE:HD11	2.51	0.45
1:B:493:GLY:HA2	5:B:810:HOH:O	2.16	0.45
1:B:365:TYR:HE1	1:B:410:VAL:HG21	1.81	0.45
1:A:169:ALA:HB2	1:A:181:ILE:HD13	1.99	0.45
1:A:143:LYS:HB2	1:A:143:LYS:NZ	2.32	0.44
1:B:201:THR:HG21	1:B:268:SER:OG	2.17	0.44
1:A:49:GLN:HE21	1:A:53:ASN:ND2	2.15	0.44
1:B:298:THR:HG23	1:B:302:LEU:HD12	1.98	0.44
1:B:404:TYR:CZ	1:B:406:LEU:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:HE21	1:A:53:ASN:HD21	1.66	0.44
1:A:230:LEU:O	1:A:290:ARG:HD2	2.18	0.44
1:B:168:PHE:C	1:B:168:PHE:CD1	2.95	0.44
1:B:243:LEU:CB	1:B:260:VAL:HG21	2.38	0.44
1:A:407:ARG:HB3	1:A:409:GLU:OE2	2.18	0.43
1:A:415:TYR:CE2	1:A:479:LEU:HB3	2.54	0.43
1:B:233:GLN:O	1:B:254:GLN:HA	2.18	0.43
1:B:502:GLU:O	1:B:502:GLU:HG3	2.19	0.43
1:A:317:SER:HB2	1:A:324:ASP:HB3	2.01	0.43
1:B:118:VAL:CG2	1:B:181:ILE:HG13	2.48	0.43
1:B:169:ALA:HB2	1:B:181:ILE:HD13	2.01	0.43
1:B:149:GLN:HG3	1:B:153:ASP:OD2	2.19	0.42
1:B:472:GLU:HG2	1:B:503:ALA:CB	2.49	0.42
1:A:63:ASP:HB2	1:A:74:ASP:HA	2.00	0.42
1:B:133:SER:OG	1:B:505:PRO:HD2	2.19	0.42
1:B:201:THR:O	1:B:201:THR:HG22	2.20	0.42
1:B:285:GLU:O	1:B:288:LYS:HG2	2.18	0.42
1:A:105:HIS:HA	1:A:108:ASP:OD1	2.18	0.42
1:B:77:ASN:CG	1:B:118:VAL:HG12	2.43	0.42
1:B:424:GLU:OE2	1:B:427:ARG:NE	2.50	0.42
1:A:320:ASN:O	1:A:321:ARG:CB	2.67	0.42
1:A:321:ARG:HH11	1:A:321:ARG:HG3	1.85	0.42
1:B:100:ASN:O	1:B:104:GLU:HG2	2.19	0.42
1:B:56:MET:HA	1:B:60:PHE:HB2	2.01	0.42
1:B:96:ALA:HB2	1:B:145:LEU:CD1	2.50	0.42
1:A:216:GLU:O	1:A:220:LYS:HG3	2.19	0.42
1:A:321:ARG:HG3	1:A:321:ARG:NH1	2.34	0.42
1:B:83:ALA:O	1:B:102:ILE:HD13	2.20	0.42
1:B:87:LEU:HD23	1:B:91:VAL:HG23	2.02	0.42
1:B:160:ARG:HG3	1:B:218:TYR:OH	2.20	0.42
1:B:79:TRP:CH2	1:B:114:THR:HB	2.55	0.41
1:A:135:TYR:O	1:A:139:GLN:HB2	2.20	0.41
1:A:124:THR:HG22	1:A:205:GLU:HG3	2.02	0.41
1:A:320:ASN:HB3	1:A:321:ARG:NH1	2.35	0.41
1:A:162:LEU:O	1:A:165:VAL:CG1	2.69	0.41
1:B:60:PHE:HA	1:B:61:PRO:HA	1.88	0.41
1:B:133:SER:HB2	1:B:504:HIS:HB3	2.02	0.41
1:B:272:TYR:O	1:B:276:MET:HG2	2.21	0.41
1:A:404:TYR:CZ	1:A:406:LEU:HA	2.56	0.41
1:B:362:GLU:HG2	1:B:429:TRP:CZ3	2.56	0.41
1:B:474:MET:HA	1:B:474:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:HB2	1:A:467:SER:OG	2.21	0.41
1:B:262:TRP:O	1:B:267:ASP:HB3	2.21	0.41
1:B:316:SER:HB2	1:B:324:ASP:O	2.20	0.41
1:B:457:ASN:N	1:B:457:ASN:HD22	2.17	0.41
1:B:479:LEU:HD21	1:B:499:TYR:OH	2.21	0.40
1:B:38:GLN:HA	1:B:38:GLN:NE2	2.37	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	473/511 (93%)	457 (97%)	14 (3%)	2 (0%)	30	34
1	B	473/511 (93%)	440 (93%)	30 (6%)	3 (1%)	21	23
All	All	946/1022 (93%)	897 (95%)	44 (5%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	HIS
1	A	267	ASP
1	B	267	ASP
1	B	252	ASP
1	B	408	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/432 (93%)	375 (94%)	25 (6%)	16	19
1	B	400/432 (93%)	388 (97%)	12 (3%)	36	49
All	All	800/864 (93%)	763 (95%)	37 (5%)	24	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	TRP
1	A	85	ASP
1	A	87	LEU
1	A	117	THR
1	A	118	VAL
1	A	128	LEU
1	A	132	LEU
1	A	139	GLN
1	A	143	LYS
1	A	165	VAL
1	A	196	LEU
1	A	204	LEU
1	A	205	GLU
1	A	243	LEU
1	A	248	ILE
1	A	268	SER
1	A	273	LEU
1	A	293	LEU
1	A	340	LEU
1	A	408	PRO
1	A	440	THR
1	A	450	VAL
1	A	479	LEU
1	A	483	GLU
1	A	500	ASN
1	B	79	TRP
1	B	85	ASP
1	B	117	THR
1	B	128	LEU
1	B	196	LEU
1	B	204	LEU
1	B	205	GLU
1	B	273	LEU

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Mol	Chain	Res	Type
1	B	282	LYS
1	B	408	PRO
1	B	479	LEU
1	B	500	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	53	ASN
1	A	105	HIS
1	A	139	GLN
1	A	144	ASN
1	A	180	ASN
1	A	223	GLN
1	A	249	ASN
1	A	301	HIS
1	A	305	HIS
1	A	418	HIS
1	A	432	ASN
1	A	490	GLN
1	A	495	ASN
1	B	38	GLN
1	B	77	ASN
1	B	139	GLN
1	B	149	GLN
1	B	223	GLN
1	B	249	ASN
1	B	263	ASN
1	B	305	HIS
1	B	328	GLN
1	B	348	GLN
1	B	432	ASN
1	B	457	ASN
1	B	464	ASN
1	B	490	GLN
1	B	495	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 ⓘ

18 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	0.48	0	17,19,21	0.72	1 (5%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	0.61	0
3	NAG	D	1	1,3	14,14,15	0.84	1 (7%)	17,19,21	0.68	0
3	NAG	D	2	3	14,14,15	0.83	0	17,19,21	0.70	0
3	MAN	D	3	3	11,11,12	0.58	0	15,15,17	0.40	0
3	MAN	D	4	3	11,11,12	0.45	0	15,15,17	0.60	1 (6%)
3	MAN	D	5	3	11,11,12	0.47	0	15,15,17	0.52	0
2	NAG	E	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.71	0
2	NAG	F	1	1,2	14,14,15	0.54	0	17,19,21	0.64	0
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.77	0
3	NAG	G	1	1,3	14,14,15	0.70	0	17,19,21	0.70	0
3	NAG	G	2	3	14,14,15	0.73	0	17,19,21	0.69	0
3	MAN	G	3	3	11,11,12	0.59	0	15,15,17	0.35	0
3	MAN	G	4	3	11,11,12	0.44	0	15,15,17	0.63	1 (6%)
3	MAN	G	5	3	11,11,12	0.51	0	15,15,17	0.57	0
2	NAG	H	1	1,2	14,14,15	0.60	0	17,19,21	0.68	0
2	NAG	H	2	2	14,14,15	0.70	0	17,19,21	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	1/1/5/7	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	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	F	2	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	3/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	1/1/5/7	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.05	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-2.16	120.01	122.90
3	G	4	MAN	C1-O5-C5	2.15	115.06	112.19
3	D	4	MAN	C1-O5-C5	2.05	114.94	112.19

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	NAG	C1
2	E	2	NAG	C1
2	F	2	NAG	C1
2	H	2	NAG	C1
3	D	2	NAG	C1
3	D	3	MAN	C1
3	G	2	NAG	C1

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Mol	Chain	Res	Type	Atom
3	G	3	MAN	C1

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6

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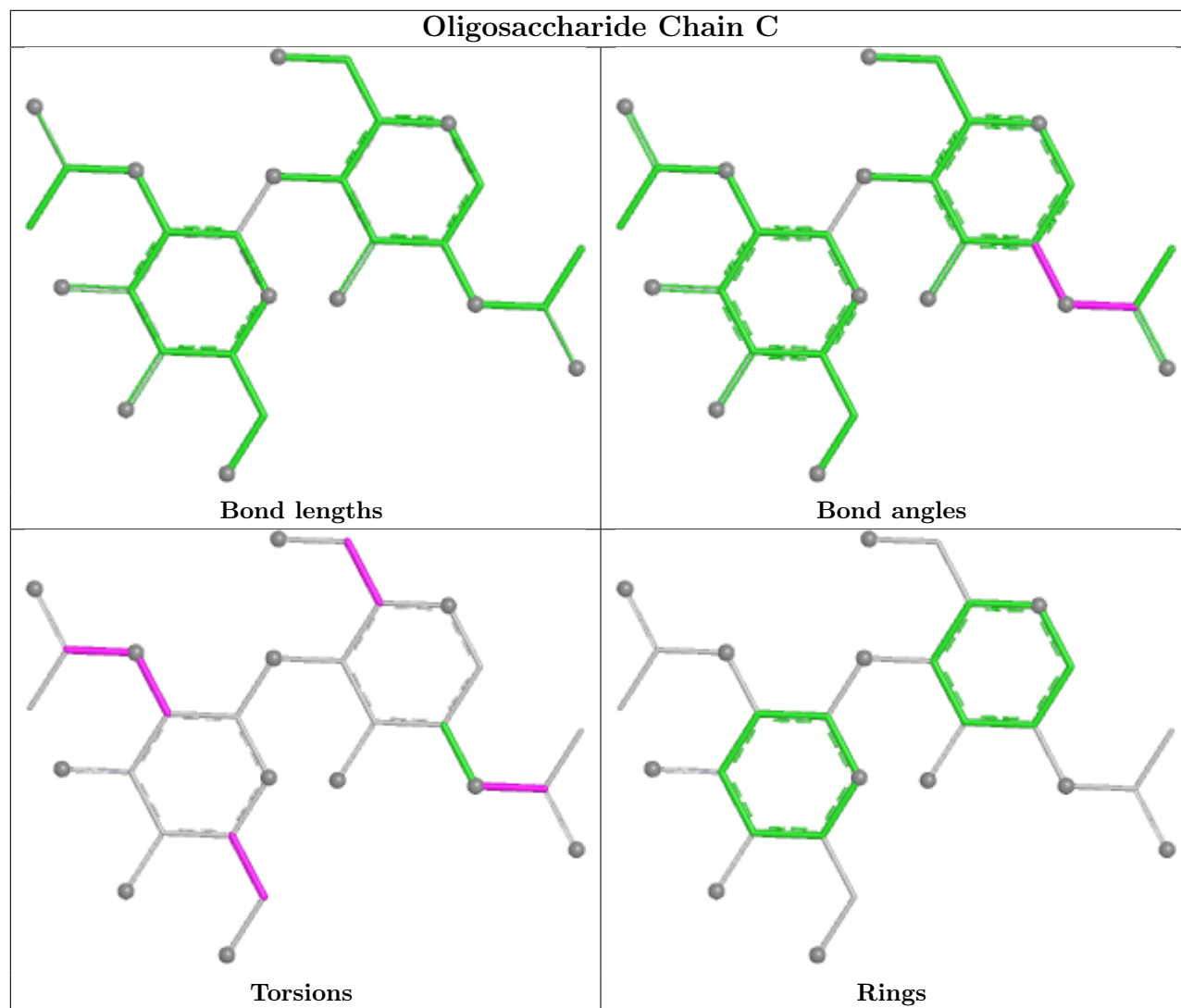
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6

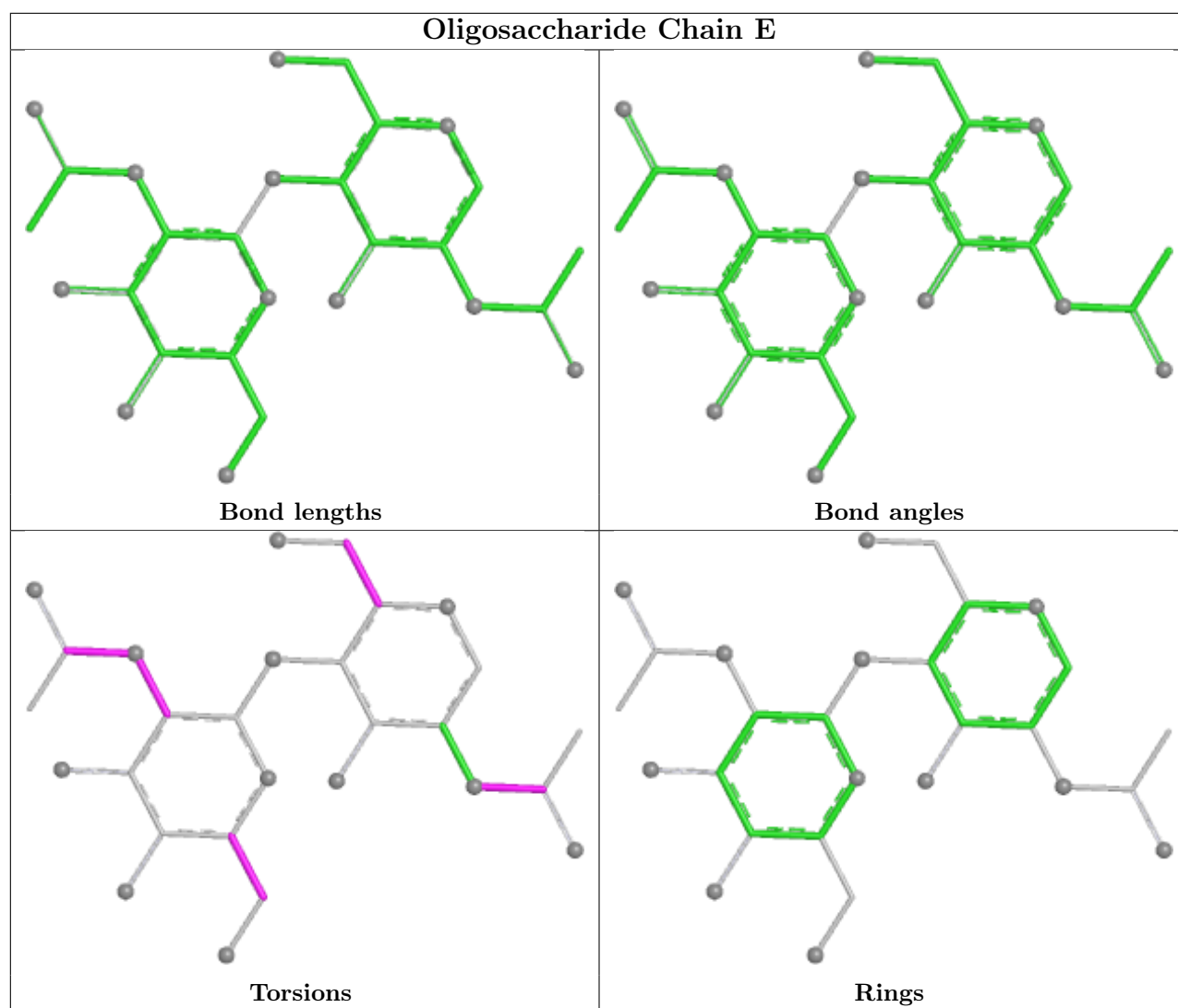
There are no ring outliers.

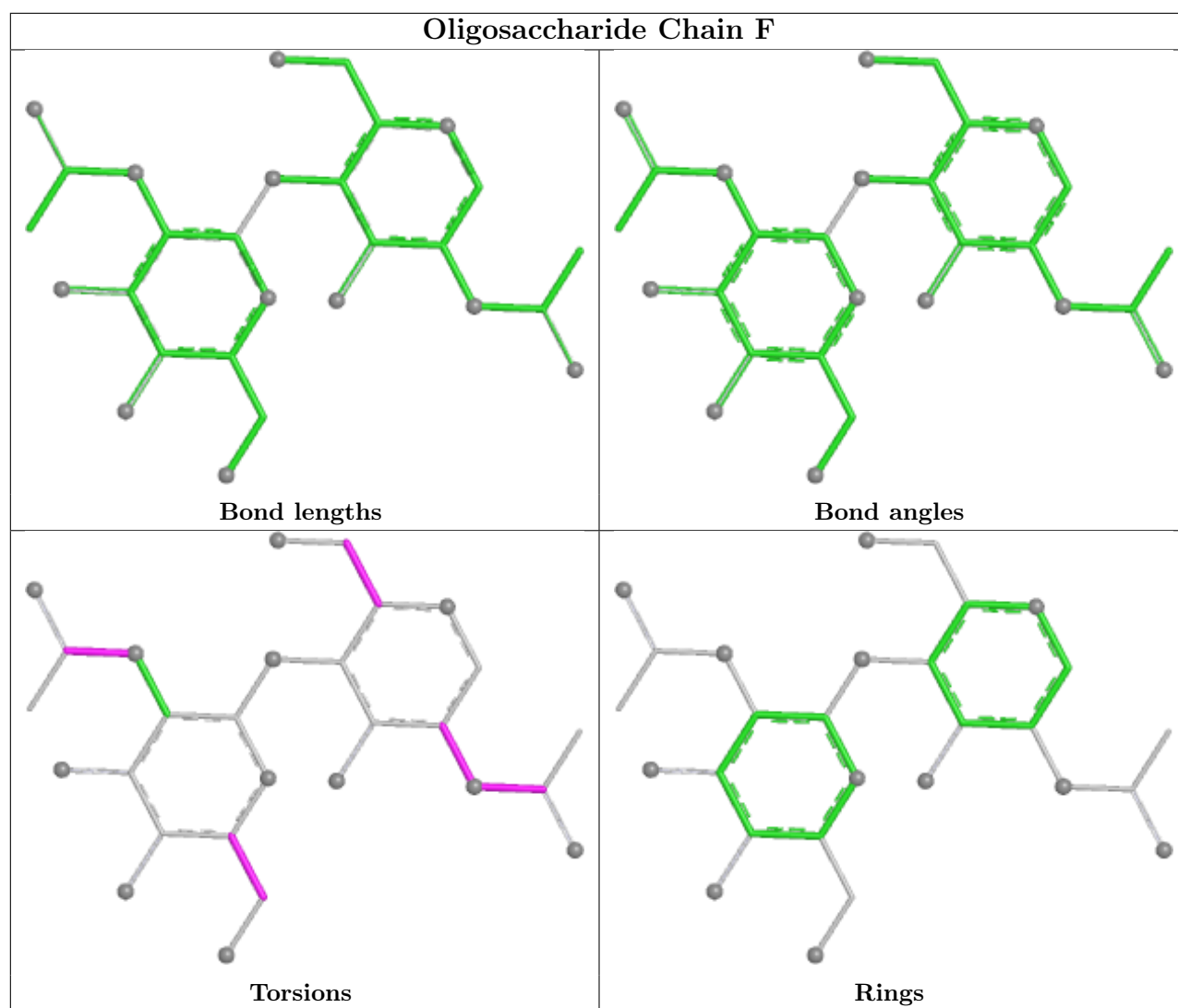
5 monomers are involved in 6 short contacts:

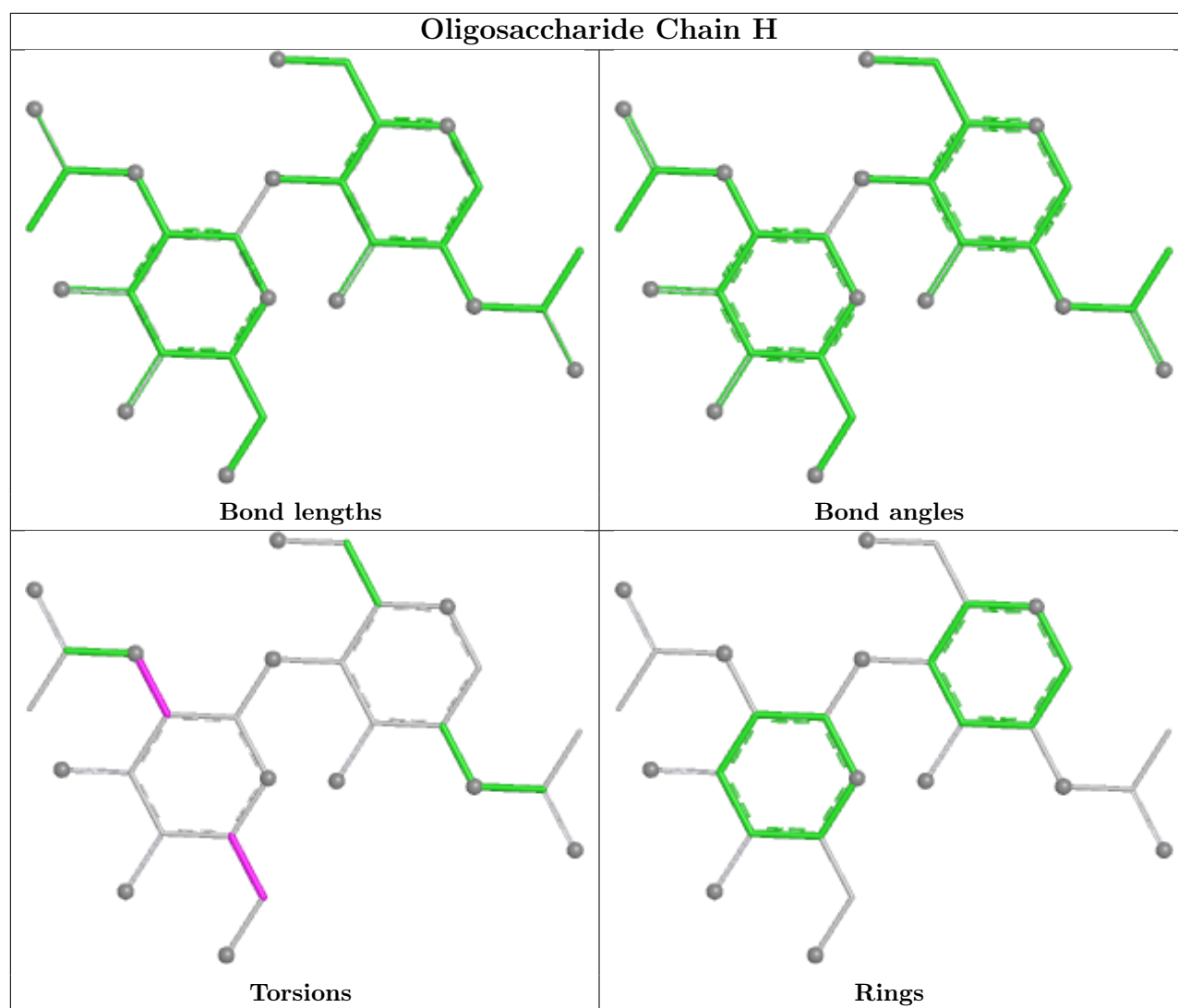
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	G	4	MAN	1	0
2	C	2	NAG	1	0
2	H	2	NAG	1	0
2	C	1	NAG	3	0

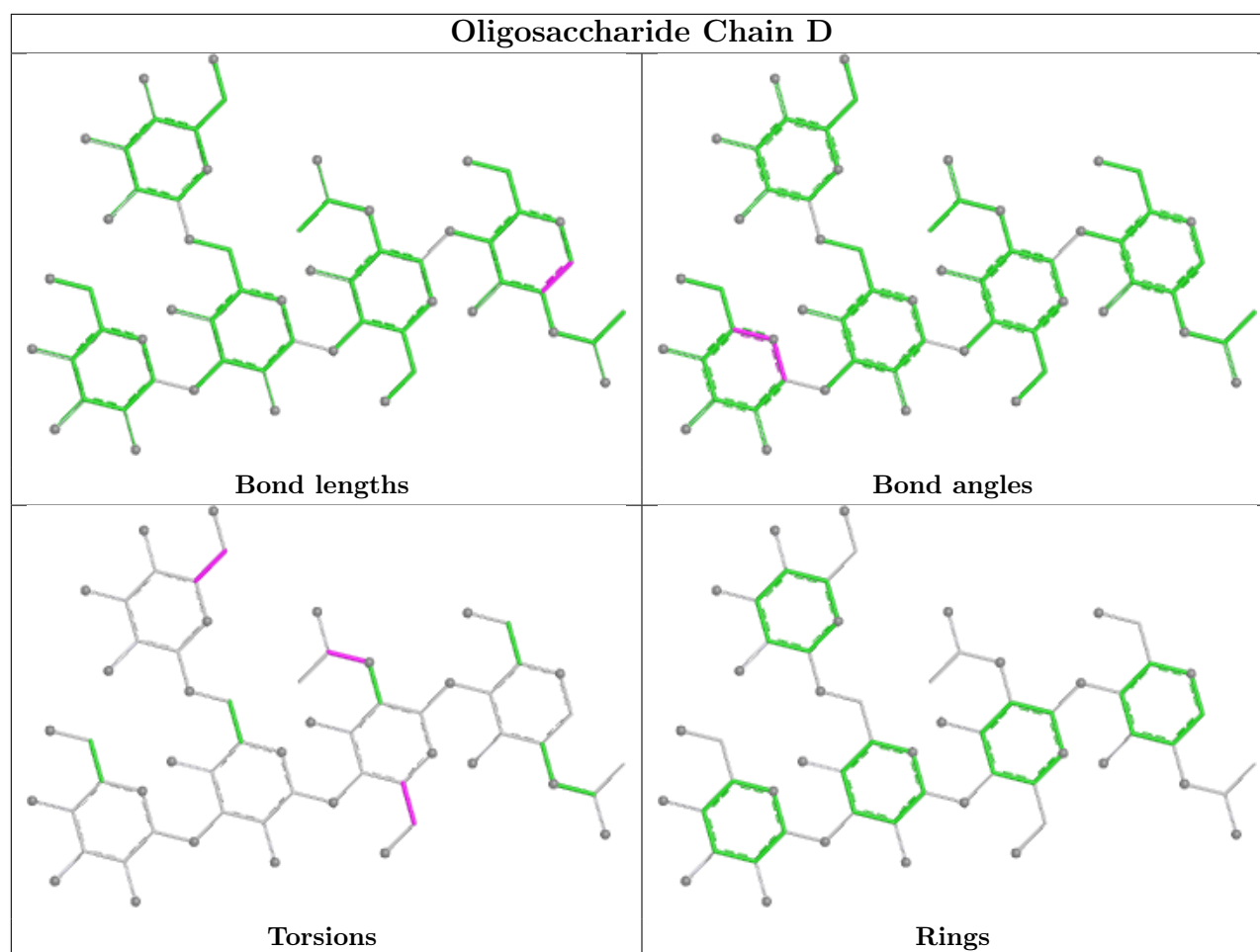
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

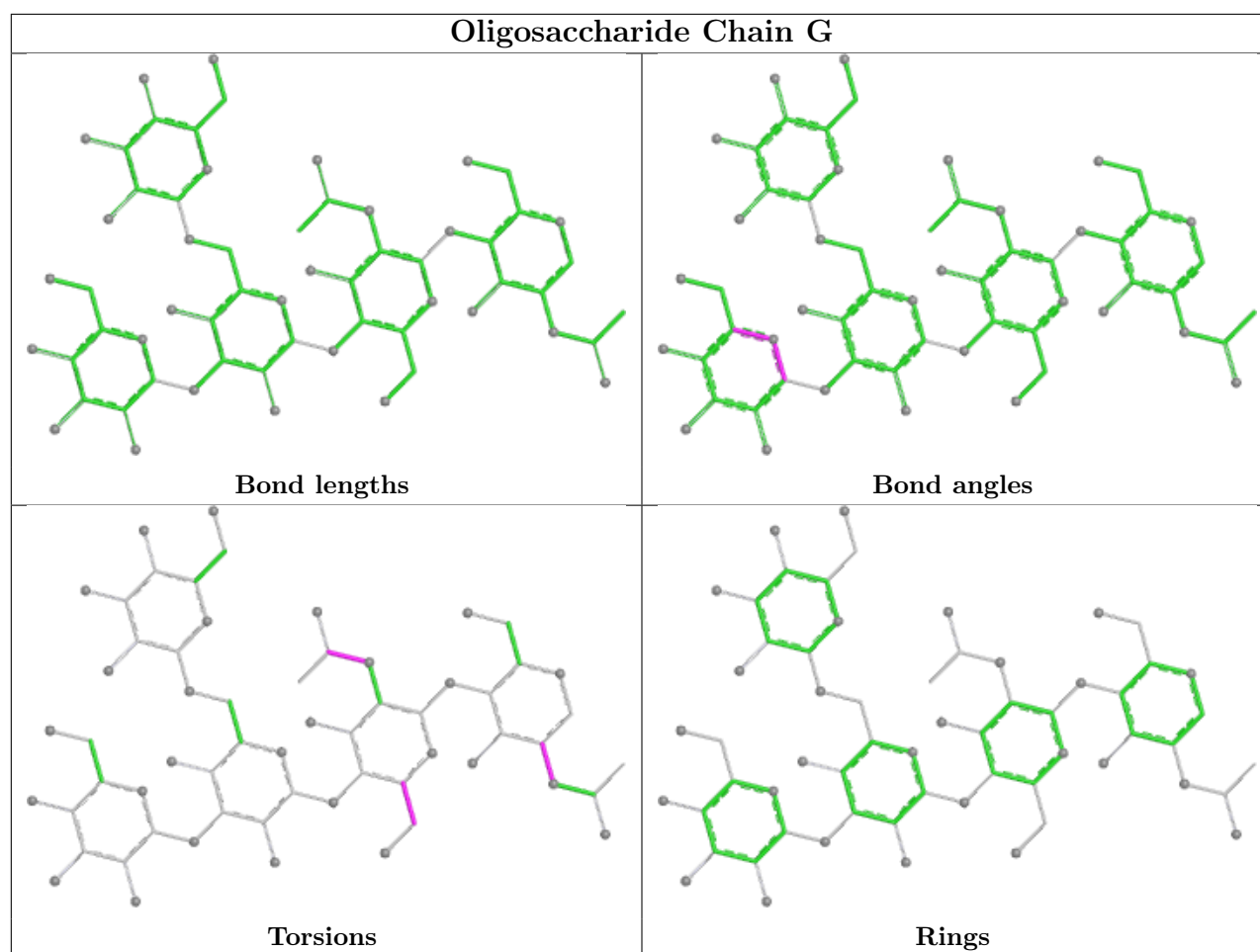












5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.