



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:23 am BST

PDB ID : 9FJF / pdb_00009fjf
EMDB ID : EMD-50502
Title : Lysosomal transporting complex of beta-glucocerebrosidase (GCase) and lysosomal integral membrane protein 2 (LIMP-2) with bound Pro-macrobodies (Combined focus map)
Authors : Dobert, J.P.; Schaefer, J.H.S.; Dal Maso, T.; Socher, E.; Versees, W.; Moeller, A.; Zunke, F.; Arnold, P.
Deposited on : 2024-05-31
Resolution : 3.70 Å(reported)
Based on initial models : 9ENA, 4Q4F, 6TN1

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev117
Mogul : ?? (???), CSD ??CSD?? (???)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

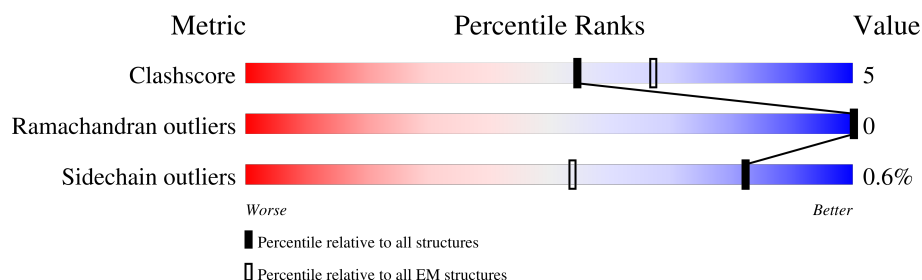
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	391	90% 10%
2	B	497	90% 8% .
3	C	130	82% 18%
4	D	121	72% 23% . .
5	E	3	33% 67%
6	F	2	100%
6	G	2	100%
6	H	2	100%
6	J	2	50% 50%

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Mol	Chain	Length	Quality of chain
7	I	5	 <div>80%20%</div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9307 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	391	Total	C	N	O	S	0	0
			3166	2044	513	597	12		

- Molecule 2 is a protein called Lysosomal acid glucosylceramidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3854	2482	661	696	15		

- Molecule 3 is a protein called Nanobody Nb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			1014	636	172	201	5		

- Molecule 4 is a protein called Nanobody Nb6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	116	Total	C	N	O	S	0	0
			888	560	150	172	6		

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



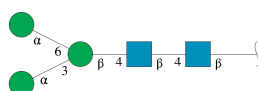
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



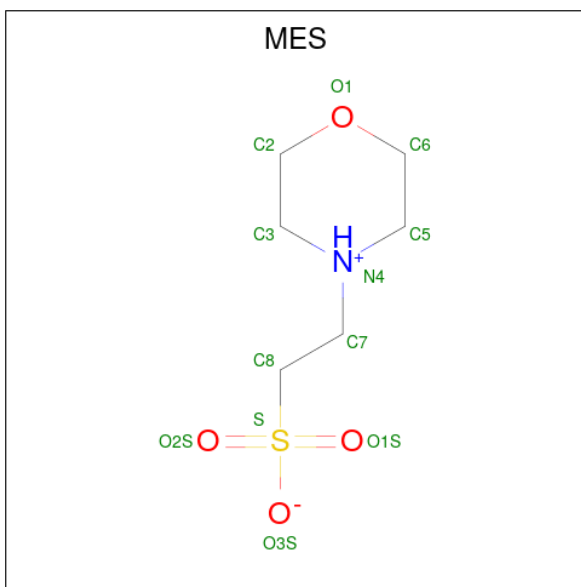
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	S	0
			12	6	1	4	1	
9	B	1	Total	C	N	O	S	0
			12	6	1	4	1	
9	B	1	Total	C	N	O	S	0
			12	6	1	4	1	
9	B	1	Total	C	N	O	S	0
			12	6	1	4	1	

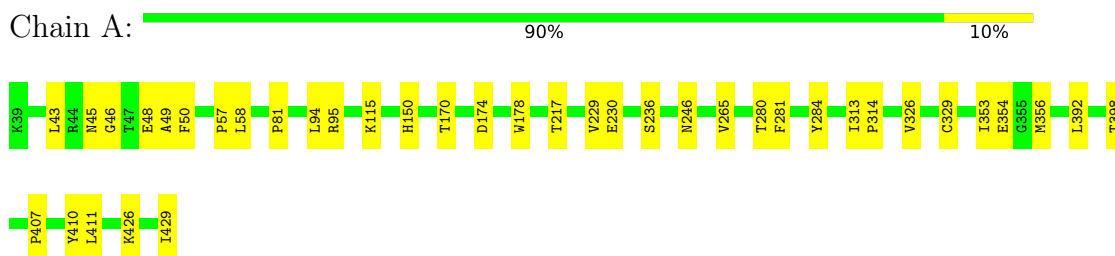
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	11	Total	O	0
			11	11	
10	B	11	Total	O	0
			11	11	
10	C	1	Total	O	0
			1	1	
10	D	4	Total	O	0
			4	4	

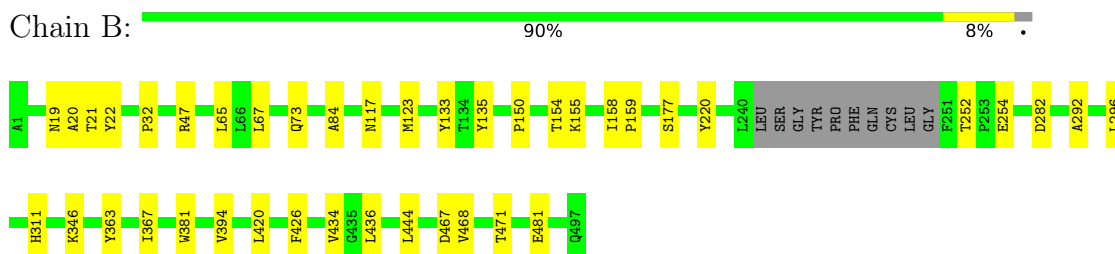
3 Residue-property plots

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.

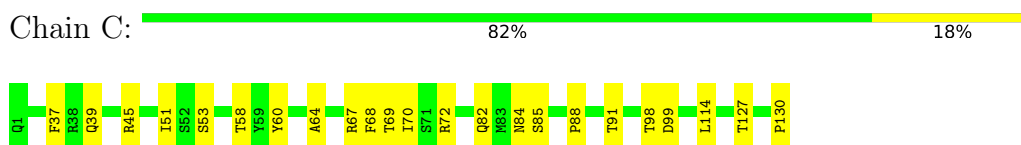
- Molecule 1: Lysosome membrane protein 2



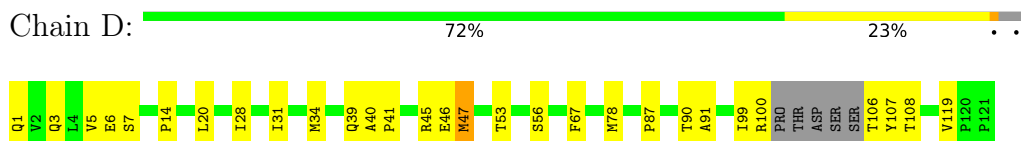
- Molecule 2: Lysosomal acid glucosylceramidase



- Molecule 3: Nanobody Nb1



- Molecule 4: Nanobody Nb6



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





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

Chain F:  100%



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

Chain G:  100%



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

Chain H:  100%




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

Chain J:  50% 50%



- Molecule 7: 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 I:  80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	397385	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: NAG, BMA, MES, 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	0.49	0/3249	0.55	0/4416
2	B	0.38	0/3970	0.53	0/5411
3	C	0.43	0/1040	0.55	0/1412
4	D	0.36	0/908	0.54	0/1233
All	All	0.43	0/9167	0.54	0/12472

There are no bond length outliers.

There are no bond angle outliers.

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	3166	0	3072	28	0
2	B	3854	0	3778	25	0
3	C	1014	0	946	15	0
4	D	888	0	854	21	0
5	E	39	0	34	2	0
6	F	28	0	25	0	0
6	G	28	0	25	1	0
6	H	28	0	25	0	0
6	J	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	61	0	52	1	0
8	A	56	0	52	2	0
8	B	42	0	39	0	0
9	A	12	0	13	0	0
9	B	36	0	39	1	0
10	A	11	0	0	0	0
10	B	11	0	0	0	0
10	C	1	0	0	0	0
10	D	4	0	0	0	0
All	All	9307	0	8979	90	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 5.

All (90) 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:313:ILE:HG23	1:A:314:PRO:HA	1.57	0.85
3:C:69:THR:HB	3:C:82:GLN:HB3	1.64	0.79
2:B:47:ARG:NH2	4:D:56:SER:OG	2.25	0.70
2:B:394:VAL:HG12	2:B:394:VAL:O	1.92	0.69
2:B:444:LEU:HD11	2:B:468:VAL:HG21	1.77	0.66
3:C:53:SER:HA	3:C:72:ARG:HH12	1.61	0.64
3:C:64:ALA:HB3	3:C:68:PHE:CE2	2.32	0.64
1:A:57:PRO:C	1:A:58:LEU:HD12	2.18	0.64
1:A:313:ILE:CG2	1:A:314:PRO:HA	2.26	0.63
3:C:91:THR:HG23	3:C:127:THR:HG22	1.82	0.61
3:C:88:PRO:CB	3:C:130:PRO:HA	2.30	0.61
4:D:1:GLN:NE2	4:D:3:GLN:O	2.32	0.61
4:D:100:ARG:HA	4:D:107:TYR:HA	1.83	0.59
4:D:39:GLN:HB2	4:D:45:ARG:HG2	1.83	0.59
2:B:22:TYR:CD2	6:J:1:NAG:H61	2.37	0.59
1:A:57:PRO:O	1:A:58:LEU:HD12	2.04	0.58
5:E:1:NAG:H61	5:E:2:NAG:HN2	1.68	0.57
1:A:57:PRO:HG2	1:A:58:LEU:HD13	1.84	0.57
4:D:14:PRO:HG2	4:D:20:LEU:HA	1.88	0.55
2:B:292:ALA:HB1	2:B:296:LEU:HD12	1.88	0.55
3:C:67:ARG:HG3	3:C:84:ASN:HB3	1.87	0.55
2:B:363:TYR:HD2	2:B:420:LEU:HD11	1.72	0.55
1:A:95:ARG:HB3	1:A:115:LYS:HG2	1.90	0.54
3:C:51:ILE:HB	3:C:70:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:O	1:A:354:GLU:HG2	2.08	0.53
4:D:39:GLN:O	4:D:91:ALA:HB1	2.08	0.52
4:D:31:ILE:HG22	4:D:99:ILE:HG23	1.90	0.52
3:C:98:THR:HG22	3:C:99:ASP:H	1.75	0.52
2:B:65:LEU:HD12	2:B:65:LEU:H	1.76	0.51
1:A:57:PRO:HG2	1:A:58:LEU:CD1	2.41	0.50
4:D:34:MET:HB2	4:D:78:MET:HE3	1.94	0.50
1:A:43:LEU:HD12	1:A:217:THR:HA	1.93	0.50
4:D:100:ARG:HA	4:D:107:TYR:HD1	1.76	0.50
1:A:170:THR:HG21	5:E:2:NAG:H82	1.94	0.49
1:A:426:LYS:HA	1:A:429:ILE:HG22	1.94	0.49
2:B:394:VAL:O	2:B:394:VAL:CG1	2.59	0.49
1:A:94:LEU:O	1:A:94:LEU:HD12	2.13	0.49
1:A:313:ILE:CG2	1:A:314:PRO:CA	2.91	0.49
1:A:326:VAL:HG22	1:A:329:CYS:HB2	1.95	0.49
1:A:94:LEU:HD12	1:A:94:LEU:C	2.33	0.48
4:D:31:ILE:HG13	4:D:53:THR:HG21	1.95	0.48
4:D:67:PHE:HZ	4:D:87:PRO:HB3	1.78	0.48
8:A:501:NAG:O7	8:A:501:NAG:O3	2.30	0.47
3:C:67:ARG:HD2	3:C:85:SER:O	2.14	0.47
4:D:6:GLU:HG2	4:D:7:SER:H	1.80	0.47
6:G:1:NAG:H61	6:G:2:NAG:HN2	1.80	0.47
1:A:174:ASP:OD1	1:A:178:TRP:HD1	1.97	0.47
3:C:58:THR:HG22	3:C:60:TYR:CE2	2.50	0.47
3:C:39:GLN:NE2	3:C:45:ARG:HG2	2.30	0.46
2:B:154:THR:HG23	2:B:155:LYS:HG3	1.97	0.46
2:B:32:PRO:HA	4:D:106:THR:OG1	2.15	0.46
2:B:158:ILE:N	2:B:159:PRO:HD2	2.31	0.46
1:A:392:LEU:HB2	1:A:398:THR:HG21	1.98	0.46
4:D:100:ARG:C	4:D:108:THR:H	2.19	0.46
4:D:5:VAL:HG13	4:D:28:ILE:HG22	1.98	0.46
4:D:90:THR:HG21	4:D:119:VAL:H	1.81	0.46
1:A:265:VAL:HG12	1:A:280:THR:HG22	1.97	0.46
1:A:313:ILE:HG23	1:A:314:PRO:CA	2.38	0.46
1:A:45:ASN:OD1	1:A:46:GLY:N	2.48	0.45
2:B:123:MET:O	2:B:135:TYR:OH	2.25	0.45
1:A:229:VAL:HG22	1:A:230:GLU:HG3	1.98	0.45
2:B:471:THR:HG23	2:B:481:GLU:HG2	1.97	0.45
1:A:411:LEU:HD12	1:A:411:LEU:C	2.37	0.45
1:A:236:SER:HB2	1:A:246:ASN:O	2.16	0.45
1:A:410:TYR:HE2	7:I:1:NAG:H81	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:TYR:CE2	2:B:150:PRO:HG3	2.52	0.45
1:A:353:ILE:HD12	1:A:407:PRO:HD3	1.98	0.44
2:B:252:THR:C	2:B:254:GLU:H	2.19	0.44
1:A:281:PHE:HZ	1:A:284:TYR:CE1	2.36	0.44
2:B:363:TYR:O	2:B:367:ILE:HG13	2.18	0.44
1:A:48:GLU:HG2	1:A:49:ALA:N	2.34	0.43
2:B:67:LEU:HD23	2:B:436:LEU:HD21	1.99	0.43
2:B:73:GLN:HB2	2:B:434:VAL:O	2.18	0.43
2:B:20:ALA:O	2:B:21:THR:OG1	2.35	0.43
4:D:46:GLU:HG2	4:D:47:MET:N	2.33	0.43
2:B:84:ALA:HB3	2:B:381:TRP:O	2.19	0.43
2:B:123:MET:HG3	2:B:177:SER:O	2.18	0.43
3:C:88:PRO:HB2	3:C:130:PRO:HA	2.01	0.43
3:C:88:PRO:CA	3:C:130:PRO:HA	2.49	0.43
4:D:67:PHE:CZ	4:D:87:PRO:HB3	2.53	0.42
2:B:346:LYS:HB3	2:B:346:LYS:HE2	1.90	0.42
2:B:426:PHE:HA	9:B:506:MES:H22	2.01	0.42
2:B:282:ASP:OD1	2:B:311:HIS:NE2	2.52	0.42
2:B:19:ASN:OD1	6:J:1:NAG:N2	2.51	0.42
3:C:37:PHE:CE2	3:C:114:LEU:HD21	2.54	0.42
1:A:50:PHE:CZ	8:A:501:NAG:H82	2.56	0.41
4:D:106:THR:OG1	4:D:107:TYR:N	2.54	0.41
3:C:64:ALA:HB1	3:C:67:ARG:HB3	2.02	0.40
4:D:5:VAL:HG21	4:D:99:ILE:HG22	2.03	0.40
4:D:40:ALA:HB1	4:D:41:PRO:HD2	2.03	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 PDB entries followed by that with respect to all EM entries.

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	389/391 (100%)	371 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	483/497 (97%)	459 (95%)	24 (5%)	0	100	100
3	C	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
4	D	112/121 (93%)	106 (95%)	6 (5%)	0	100	100
All	All	1112/1139 (98%)	1059 (95%)	53 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	352/352 (100%)	350 (99%)	2 (1%)	84	90
2	B	416/424 (98%)	413 (99%)	3 (1%)	81	88
3	C	106/106 (100%)	106 (100%)	0	100	100
4	D	94/99 (95%)	93 (99%)	1 (1%)	70	80
All	All	968/981 (99%)	962 (99%)	6 (1%)	82	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	356	MET
2	B	117	ASN
2	B	220	TYR
2	B	467	ASP
4	D	47	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	357	HIS

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 ⓘ

16 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

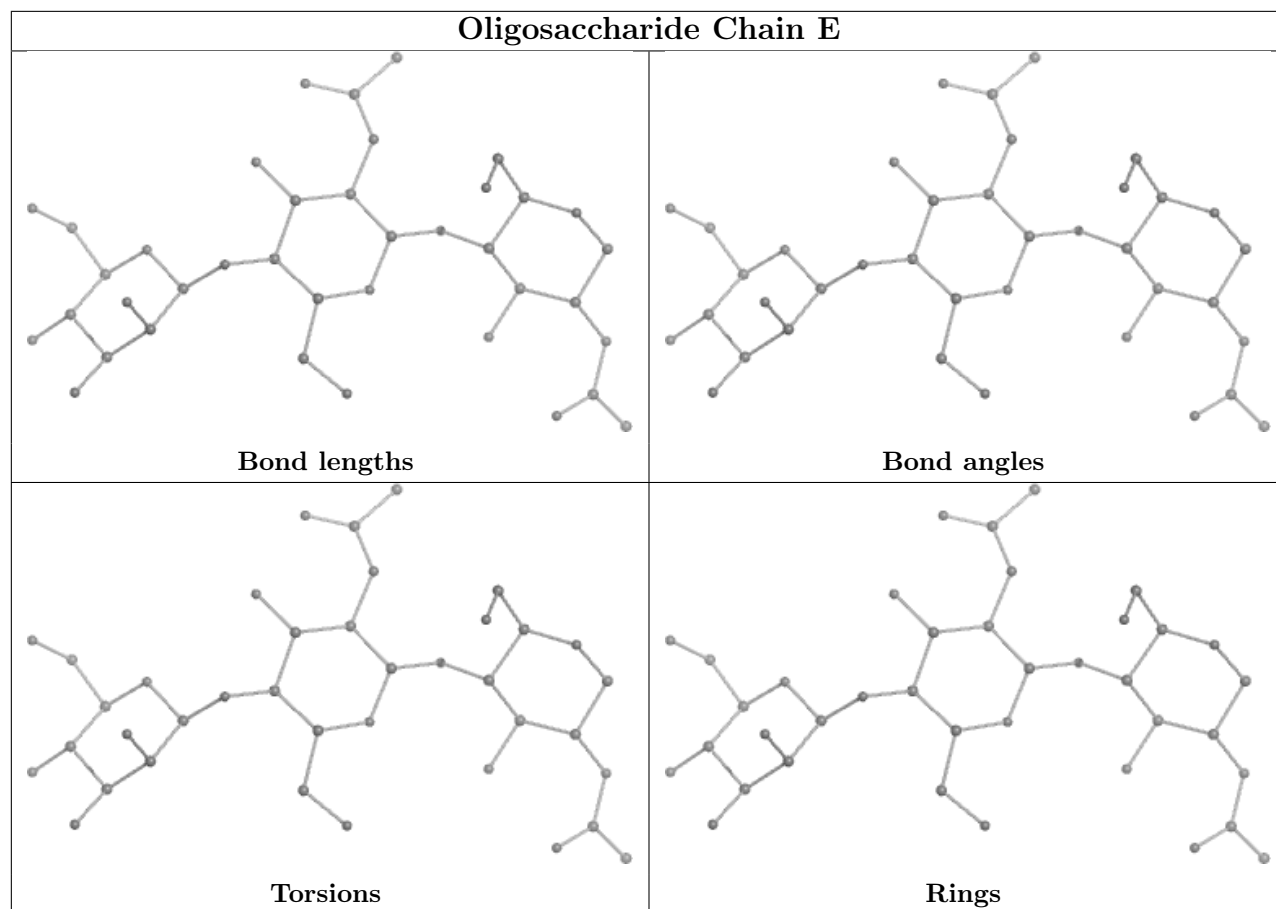
There are no chirality outliers.

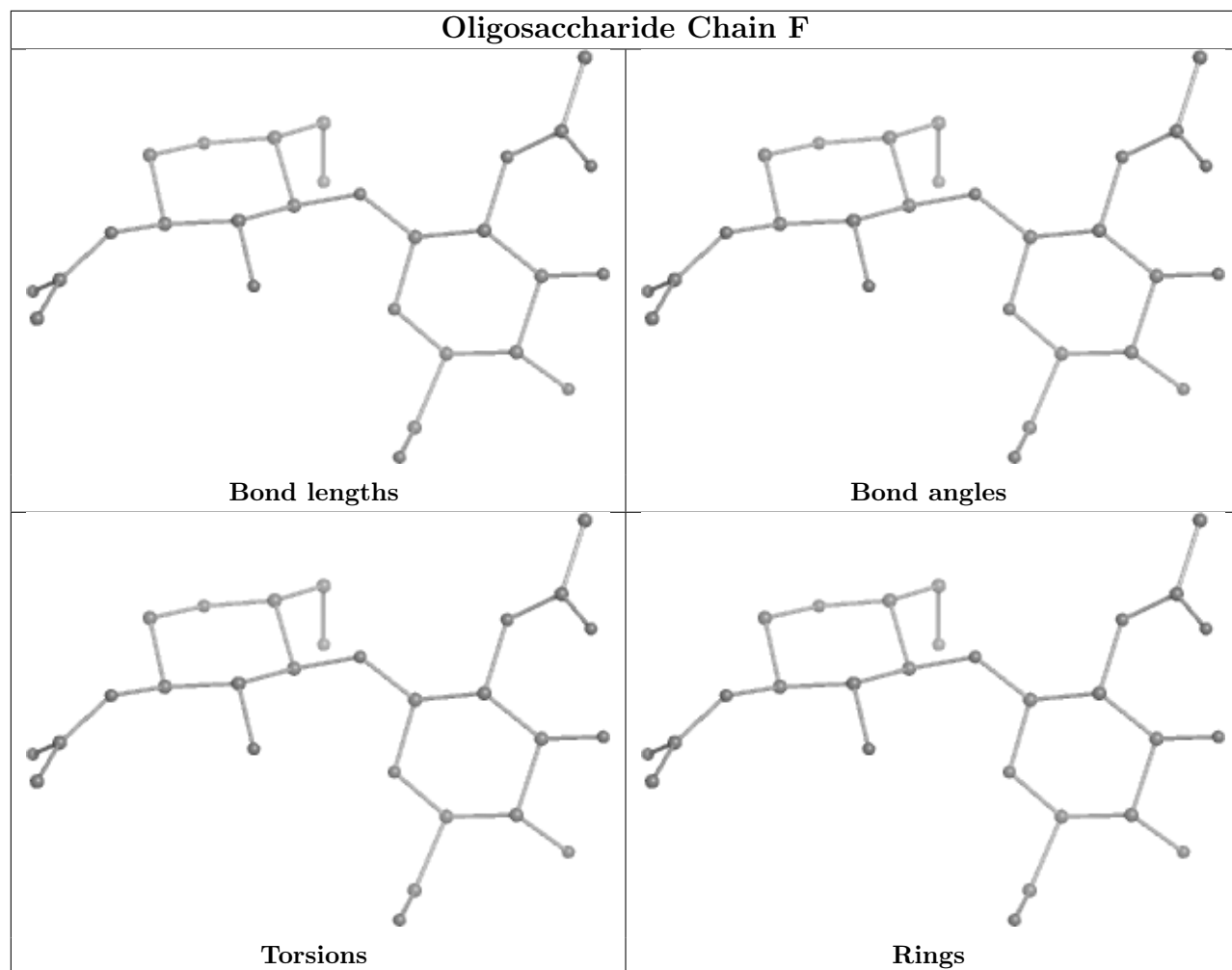
There are no torsion outliers.

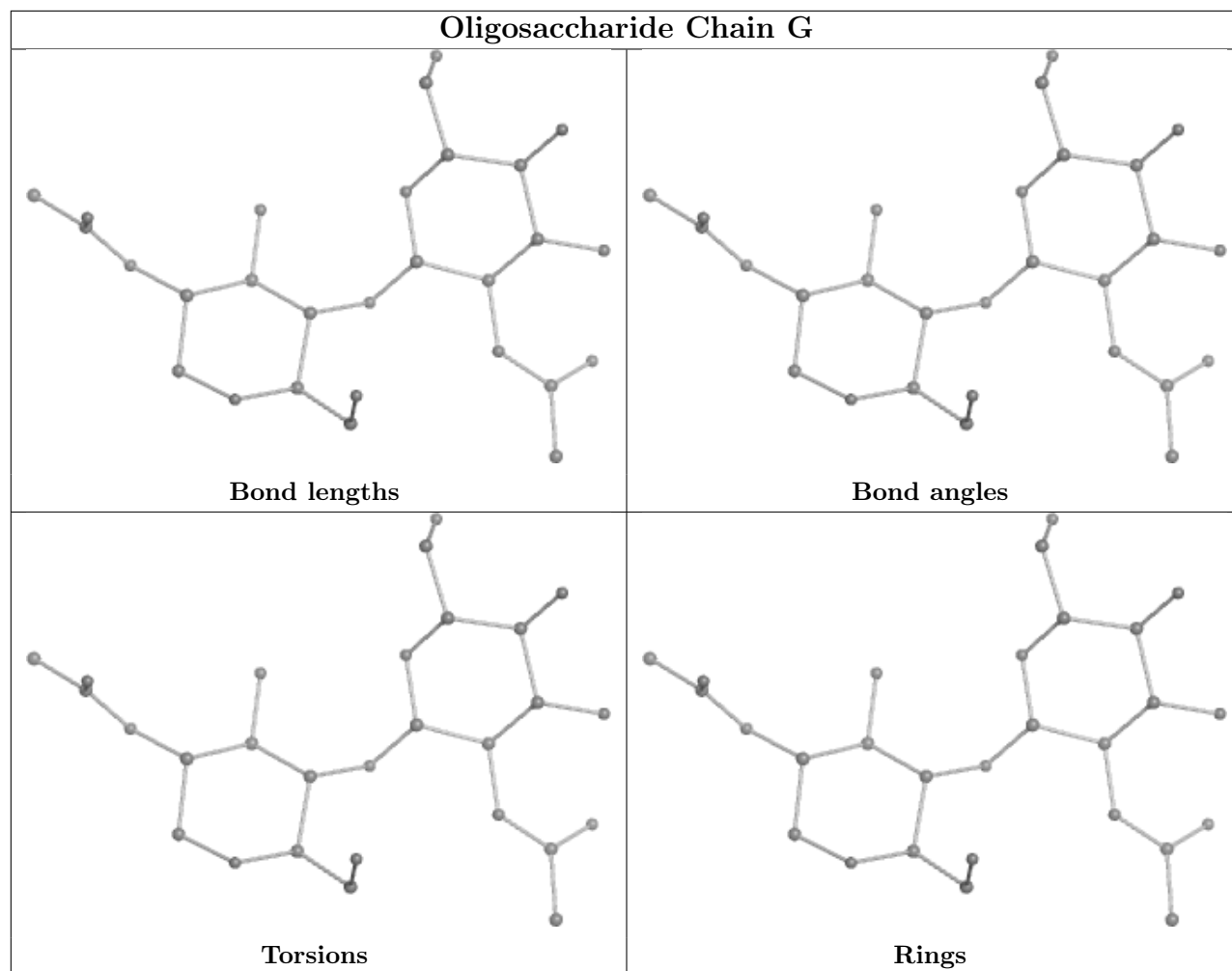
There are no ring outliers.

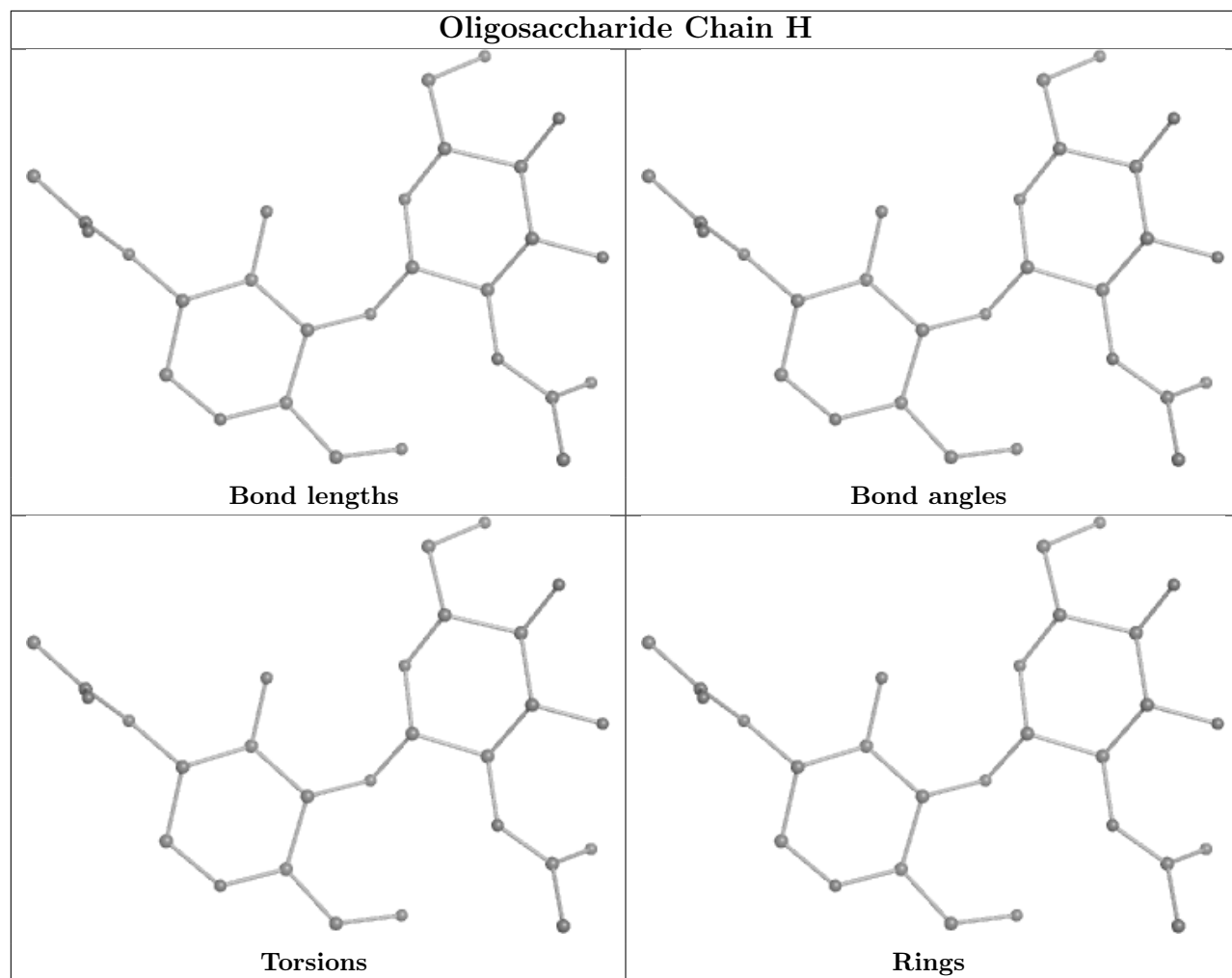
No monomer is involved in short contacts.

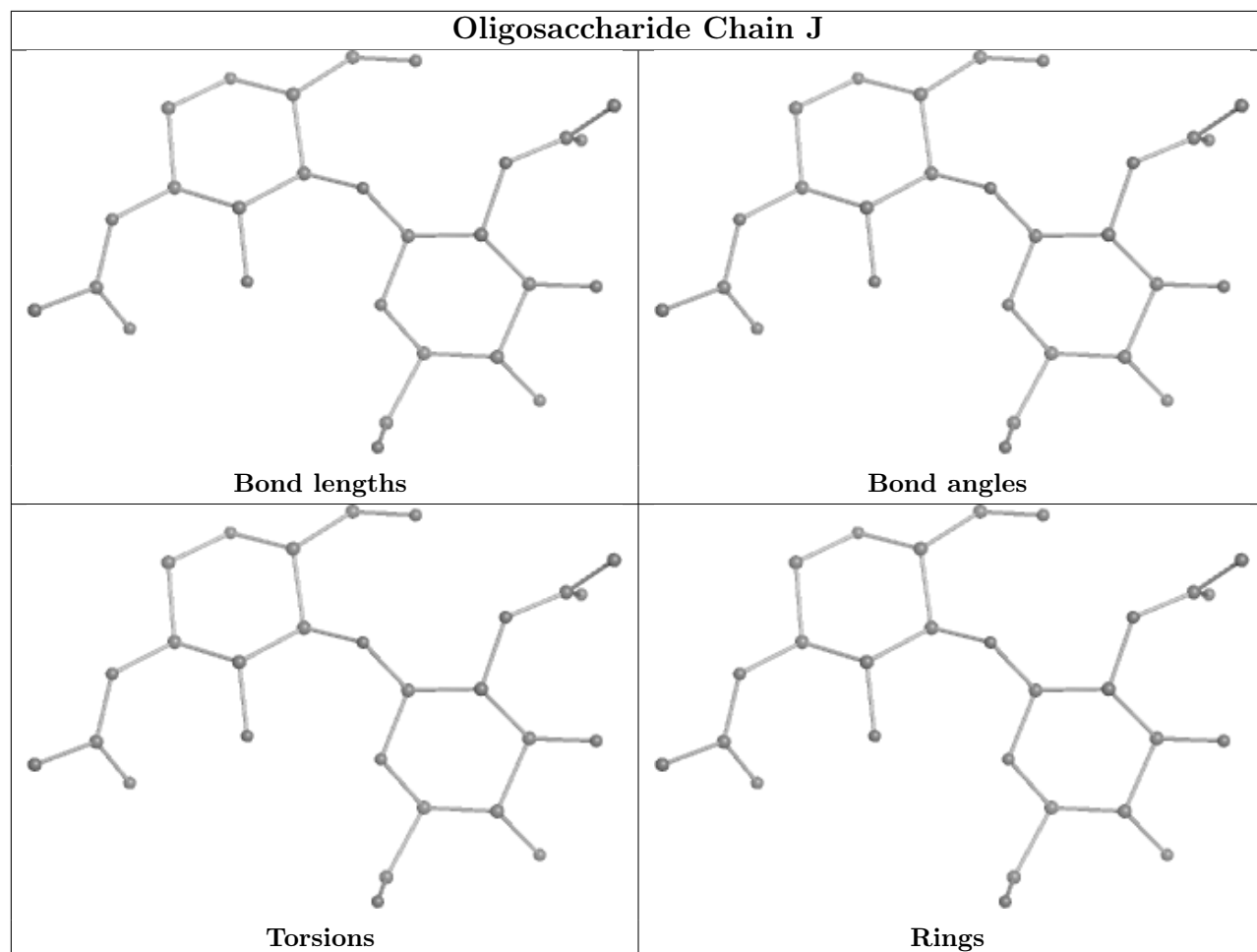
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

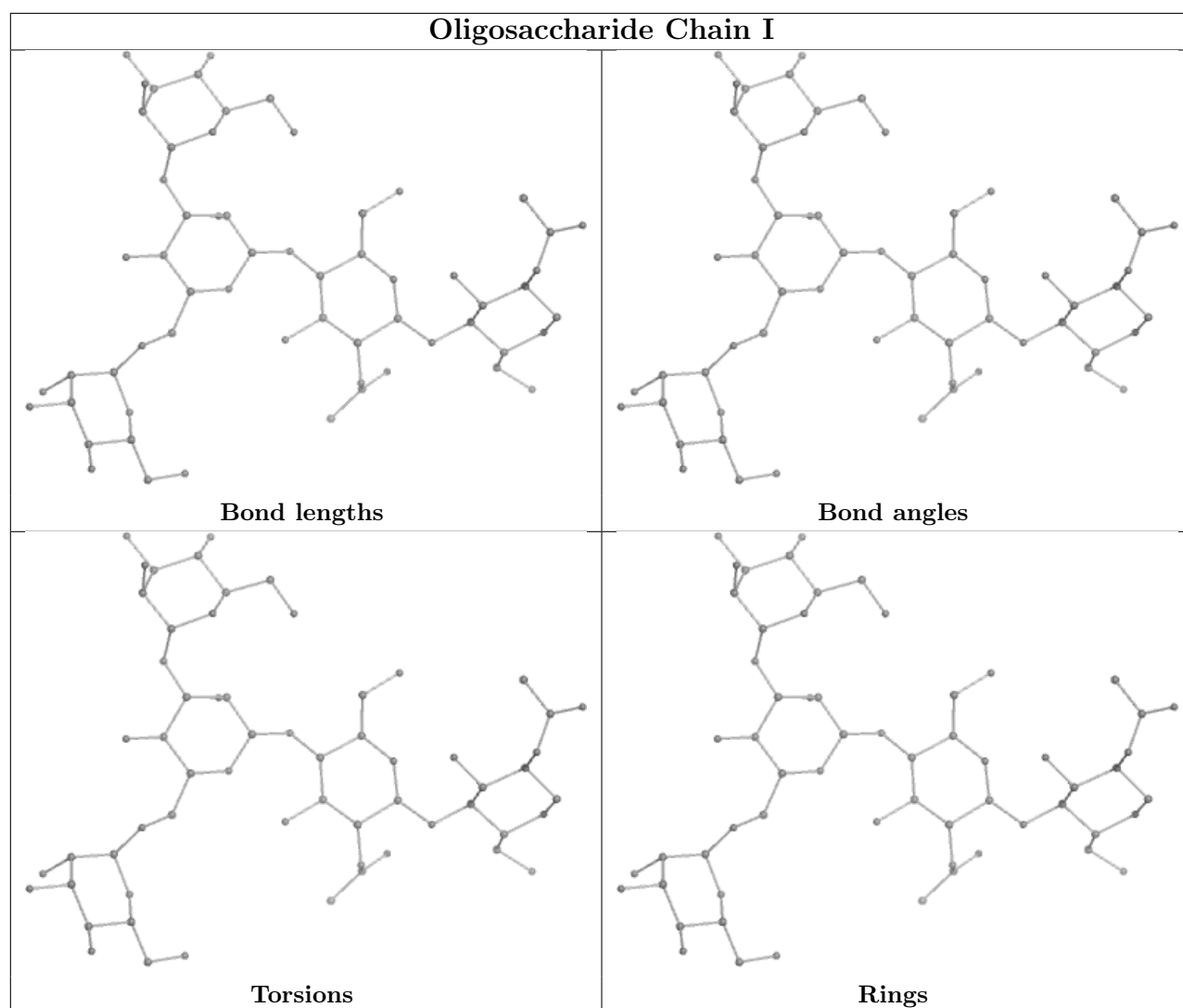












5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50502. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

This section was not generated.

6.2 Central slices [i](#)

This section was not generated.

6.3 Largest variance slices [i](#)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

This section was not generated.

6.5 Orthogonal surface views [i](#)

This section was not generated.

6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.