



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 09:19 AM EST

PDB ID : 7THT
EMDB ID : EMD-25904
Title : CryoEM structure of SARS-CoV-2 S protein in complex with Receptor Binding Domain antibody DH1042
Authors : Manne, K.; May, A.; Acharya, P.
Deposited on : 2022-01-12
Resolution : 3.42 Å (reported)
Based on initial models : 6VYB, 7EAN

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

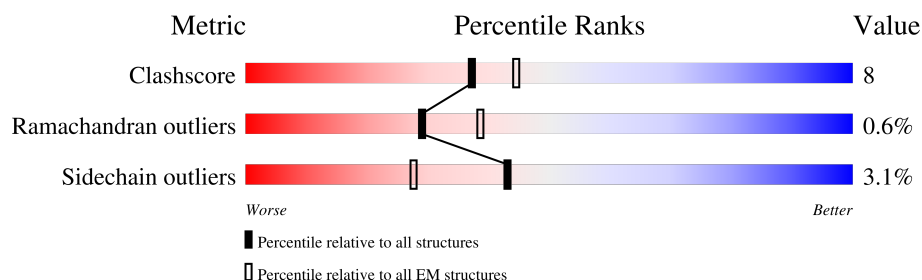
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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.



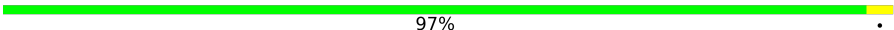
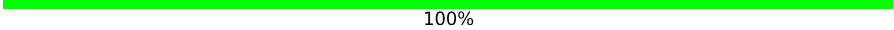
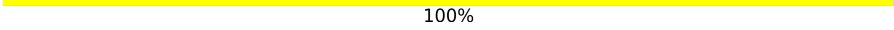
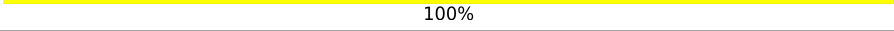
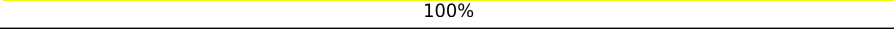
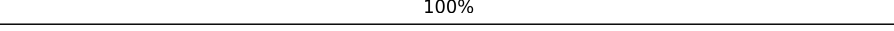
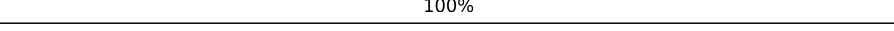
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	1121	
1	S	1121	
1	V	1121	
2	H	122	
2	a	122	
2	d	122	
3	L	106	
3	b	106	

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Mol	Chain	Length	Quality of chain
3	c	106	 97%
4	A	3	 67% 33%
5	B	2	 100%
5	D	2	 100%
5	E	2	 100%
5	F	2	 100%
5	G	2	 100%
5	I	2	 100%
5	J	2	 100%
5	K	2	 100%
5	M	2	 100%
5	N	2	 100%
5	O	2	 100%
5	W	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28900 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	991	Total	C	N	O	S	0	0
			7620	4877	1268	1441	34		
1	V	986	Total	C	N	O	S	0	0
			7587	4856	1260	1437	34		
1	C	990	Total	C	N	O	S	0	0
			7606	4872	1270	1430	34		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	607	GLU	GLN	conflict	UNP P0DTC2
S	986	PRO	LYS	conflict	UNP P0DTC2
S	987	PRO	VAL	conflict	UNP P0DTC2
V	607	GLU	GLN	conflict	UNP P0DTC2
V	986	PRO	LYS	conflict	UNP P0DTC2
V	987	PRO	VAL	conflict	UNP P0DTC2
C	607	GLU	GLN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

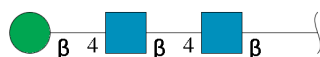
- Molecule 2 is a protein called DH1042 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total	C	N	O	S	0	0
			946	597	159	184	6		
2	a	122	Total	C	N	O	S	0	0
			946	597	159	184	6		
2	d	122	Total	C	N	O	S	0	0
			946	597	159	184	6		

- Molecule 3 is a protein called DH1042 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			804	504	132	165	3		
3	c	106	Total	C	N	O	S	0	0
			804	504	132	165	3		
3	b	106	Total	C	N	O	S	0	0
			804	504	132	165	3		

- Molecule 4 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
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

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



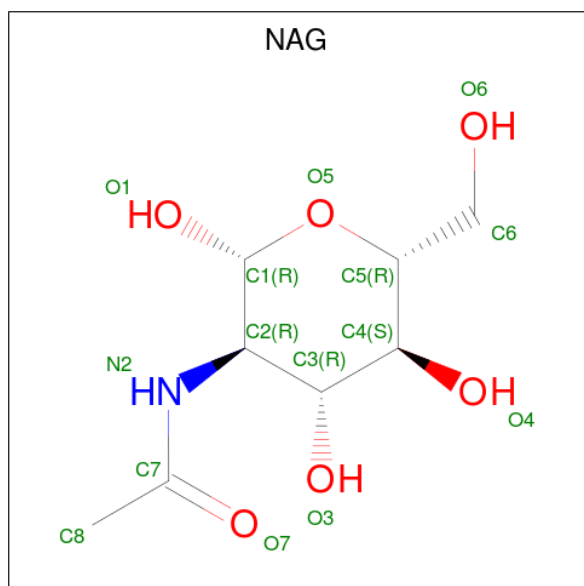
Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	S	1	Total	C	N	O	0
			140	80	10	50	
6	S	1	Total	C	N	O	0
			140	80	10	50	
6	S	1	Total	C	N	O	0
			140	80	10	50	
6	S	1	Total	C	N	O	0
			140	80	10	50	
6	S	1	Total	C	N	O	0
			140	80	10	50	
6	S	1	Total	C	N	O	0
			140	80	10	50	

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Mol	Chain	Residues	Atoms				AltConf
6	S	1	Total 140	C 80	N 10	O 50	0
6	S	1	Total 140	C 80	N 10	O 50	0
6	S	1	Total 140	C 80	N 10	O 50	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	V	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 154	C 88	N 11	O 55	0
6	C	1	Total 154	C 88	N 11	O 55	0
6	C	1	Total 154	C 88	N 11	O 55	0
6	C	1	Total 154	C 88	N 11	O 55	0
6	C	1	Total 154	C 88	N 11	O 55	0
6	C	1	Total 154	C 88	N 11	O 55	0

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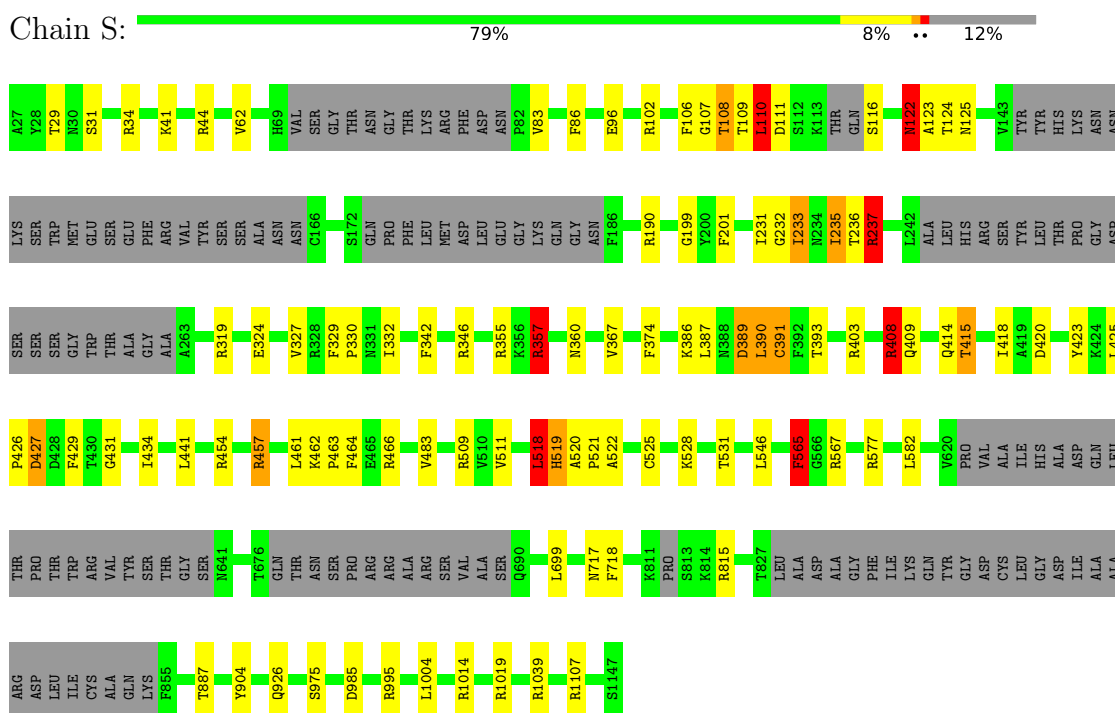
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			154	88	11	55	
6	C	1	Total	C	N	O	0
			154	88	11	55	
6	C	1	Total	C	N	O	0
			154	88	11	55	
6	C	1	Total	C	N	O	0
			154	88	11	55	
6	C	1	Total	C	N	O	0
			154	88	11	55	

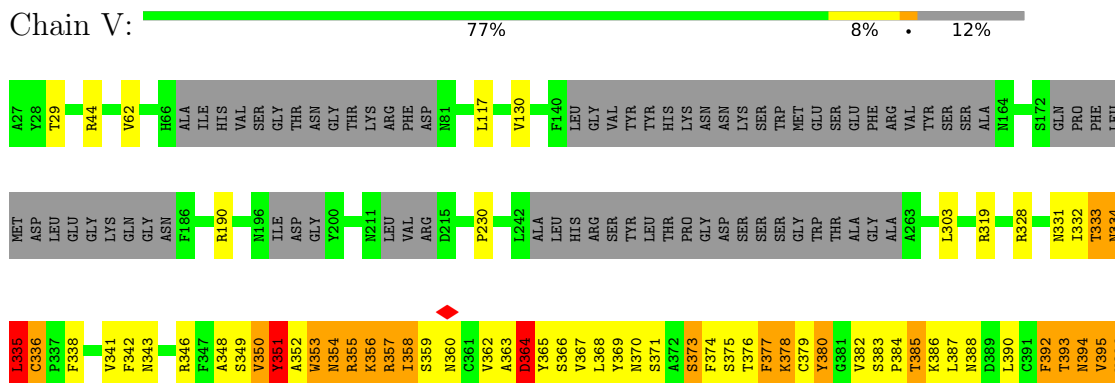
3 Residue-property plots

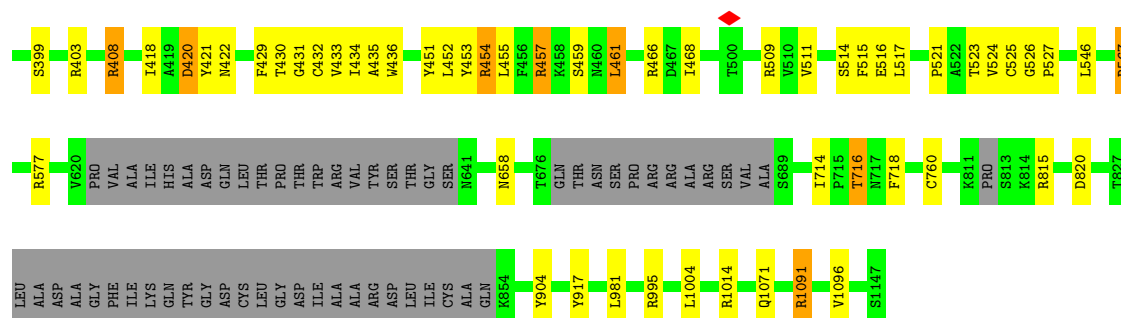
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Spike glycoprotein



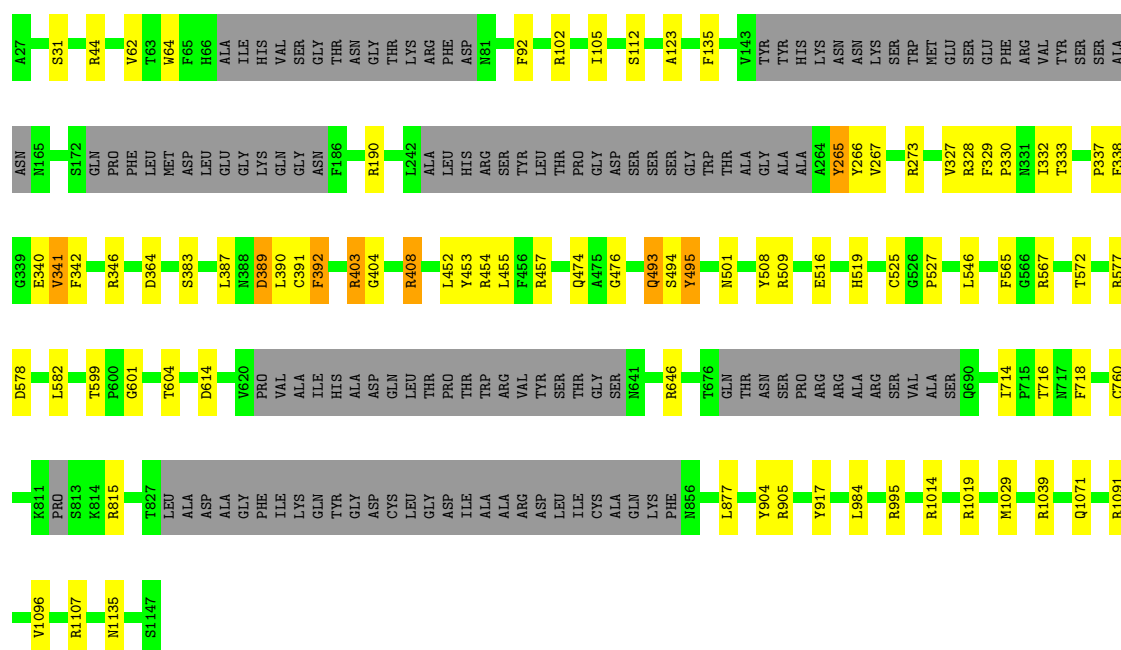
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

Chain C: 81% 7% 12%



• Molecule 2: DH1042 heavy chain

Chain H: 97%

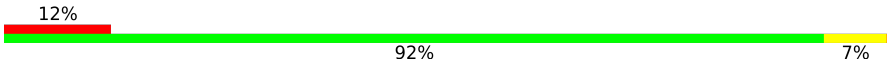


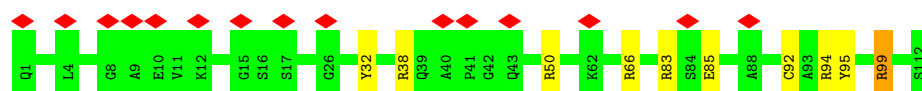
• Molecule 2: DH1042 heavy chain

Chain a: 95% 5%



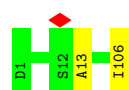
• Molecule 2: DH1042 heavy chain

Chain d:  12% 92% 7%



- Molecule 3: DH1042 light chain

Chain L:  98%



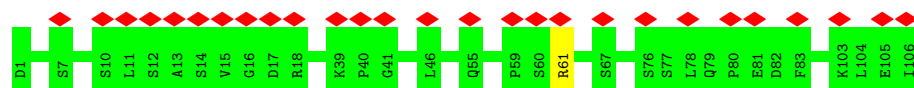
- Molecule 3: DH1042 light chain

Chain c:  97%



- Molecule 3: DH1042 light chain

Chain b:  25% 99%



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

Chain A:  67% 33%



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

Chain B:  100%



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

Chain D:  100%



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain M:  100%MAG1
MAG2

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

Chain N:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.02	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.997	Depositor
Minimum map value	-1.602	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.1321	Depositor
Map size (Å)	338.56, 338.56, 338.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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: BMA, 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	C	0.65	0/7777	0.99	27/10596 (0.3%)
1	S	0.65	0/7790	1.00	33/10611 (0.3%)
1	V	0.65	0/7757	0.96	22/10565 (0.2%)
2	H	0.74	0/966	1.08	3/1307 (0.2%)
2	a	0.74	0/966	1.06	3/1307 (0.2%)
2	d	0.75	0/966	1.09	5/1307 (0.4%)
3	L	0.71	0/823	0.96	0/1118
3	b	0.70	0/823	0.98	1/1118 (0.1%)
3	c	0.70	0/823	0.97	1/1118 (0.1%)
All	All	0.67	0/28691	0.99	95/39047 (0.2%)

There are no bond length outliers.

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	190	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	V	403	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	C	403	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	S	357	ARG	CG-CD-NE	-8.14	94.71	111.80
1	C	495	TYR	CB-CA-C	-8.10	94.19	110.40

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	C	7606	0	7342	73	0
1	S	7620	0	7364	105	0
1	V	7587	0	7307	247	0
2	H	946	0	926	0	0
2	a	946	0	926	0	0
2	d	946	0	924	0	0
3	L	804	0	781	1	0
3	b	804	0	781	0	0
3	c	804	0	781	0	0
4	A	39	0	34	5	0
5	B	28	0	25	3	0
5	D	28	0	25	0	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	W	28	0	25	0	0
6	C	154	0	143	0	0
6	S	140	0	130	4	0
6	V	168	0	156	4	0
All	All	28900	0	27895	420	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 8.

The worst 5 of 420 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:V:380:TYR:CD2	1:V:429:PHE:HE2	1.16	1.64
1:V:353:TRP:CZ3	1:V:466:ARG:CD	1.81	1.61
1:V:353:TRP:CZ3	1:V:466:ARG:HD2	1.35	1.58
1:S:357:ARG:HH22	1:V:230:PRO:CB	0.98	1.56
1:S:83:VAL:CG1	1:S:237:ARG:HD3	1.25	1.56

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	C	972/1121 (87%)	904 (93%)	62 (6%)	6 (1%)	25	61
1	S	971/1121 (87%)	899 (93%)	65 (7%)	7 (1%)	22	58
1	V	964/1121 (86%)	895 (93%)	64 (7%)	5 (0%)	29	65
2	H	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
2	a	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
2	d	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	19	56
3	L	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
3	b	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
3	c	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	15	51
All	All	3579/4047 (88%)	3320 (93%)	239 (7%)	20 (1%)	29	61

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	110	LEU
1	S	122	ASN
1	S	518	LEU
1	S	528	LYS
1	V	364	ASP

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 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	C	827/972 (85%)	810 (98%)	17 (2%)	53	79
1	S	833/972 (86%)	805 (97%)	28 (3%)	37	68
1	V	830/972 (85%)	790 (95%)	40 (5%)	25	59
2	H	101/101 (100%)	100 (99%)	1 (1%)	76	88
2	a	101/101 (100%)	98 (97%)	3 (3%)	41	71
2	d	101/101 (100%)	96 (95%)	5 (5%)	24	57
3	L	92/92 (100%)	92 (100%)	0	100	100
3	b	92/92 (100%)	92 (100%)	0	100	100
3	c	92/92 (100%)	91 (99%)	1 (1%)	73	87
All	All	3069/3495 (88%)	2974 (97%)	95 (3%)	43	70

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	396	TYR
1	C	341	VAL
1	V	455	LEU
1	V	760	CYS
1	C	408	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	926	GLN
1	V	370	ASN
1	V	422	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 ⓘ

27 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$
4	NAG	A	1	4,1	14,14,15	2.52	5 (35%)	17,19,21	2.54	5 (29%)
4	NAG	A	2	4	14,14,15	0.72	0	17,19,21	2.19	5 (29%)
4	BMA	A	3	4	11,11,12	0.44	0	15,15,17	2.21	6 (40%)
5	NAG	B	1	5,1	14,14,15	0.53	0	17,19,21	2.32	6 (35%)
5	NAG	B	2	5	14,14,15	0.44	0	17,19,21	1.21	2 (11%)
5	NAG	D	1	5,1	14,14,15	0.28	0	17,19,21	0.68	0
5	NAG	D	2	5	14,14,15	0.28	0	17,19,21	0.72	0
5	NAG	E	1	5,1	14,14,15	0.27	0	17,19,21	0.74	0
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.66	0
5	NAG	F	1	5,1	14,14,15	1.20	2 (14%)	17,19,21	0.68	0
5	NAG	F	2	5	14,14,15	1.21	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	G	1	5,1	14,14,15	1.22	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	G	2	5	14,14,15	1.19	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	I	1	5,1	14,14,15	1.16	1 (7%)	17,19,21	0.67	0
5	NAG	I	2	5	14,14,15	1.23	2 (14%)	17,19,21	0.75	0
5	NAG	J	1	5,1	14,14,15	1.27	3 (21%)	17,19,21	1.01	1 (5%)
5	NAG	J	2	5	14,14,15	1.22	2 (14%)	17,19,21	0.79	0
5	NAG	K	1	5,1	14,14,15	1.20	2 (14%)	17,19,21	0.70	0
5	NAG	K	2	5	14,14,15	1.19	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	M	1	5,1	14,14,15	1.19	2 (14%)	17,19,21	0.75	0
5	NAG	M	2	5	14,14,15	1.23	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	N	1	5,1	14,14,15	1.25	2 (14%)	17,19,21	0.85	0
5	NAG	N	2	5	14,14,15	1.20	1 (7%)	17,19,21	0.77	0
5	NAG	O	1	5,1	14,14,15	1.22	2 (14%)	17,19,21	0.68	0
5	NAG	O	2	5	14,14,15	1.26	2 (14%)	17,19,21	0.77	1 (5%)
5	NAG	W	1	5,1	14,14,15	1.18	2 (14%)	17,19,21	0.78	0
5	NAG	W	2	5	14,14,15	1.26	2 (14%)	17,19,21	1.03	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	3/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	B	2	5	-	3/6/23/26	0/1/1/1
5	NAG	D	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	-5.60	1.34	1.43
4	A	1	NAG	C1-C2	-4.23	1.46	1.52
4	A	1	NAG	O5-C5	-3.59	1.36	1.43
4	A	1	NAG	C2-N2	-3.06	1.41	1.46
5	J	2	NAG	O5-C5	2.73	1.49	1.43

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	O4-C4-C3	6.47	125.32	110.35
4	A	1	NAG	O5-C5-C6	-5.43	98.69	107.20
4	A	3	BMA	O5-C1-C2	-5.18	102.77	110.77
4	A	2	NAG	O3-C3-C4	-5.03	98.73	110.35
5	B	1	NAG	C1-C2-N2	-4.99	101.97	110.49

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

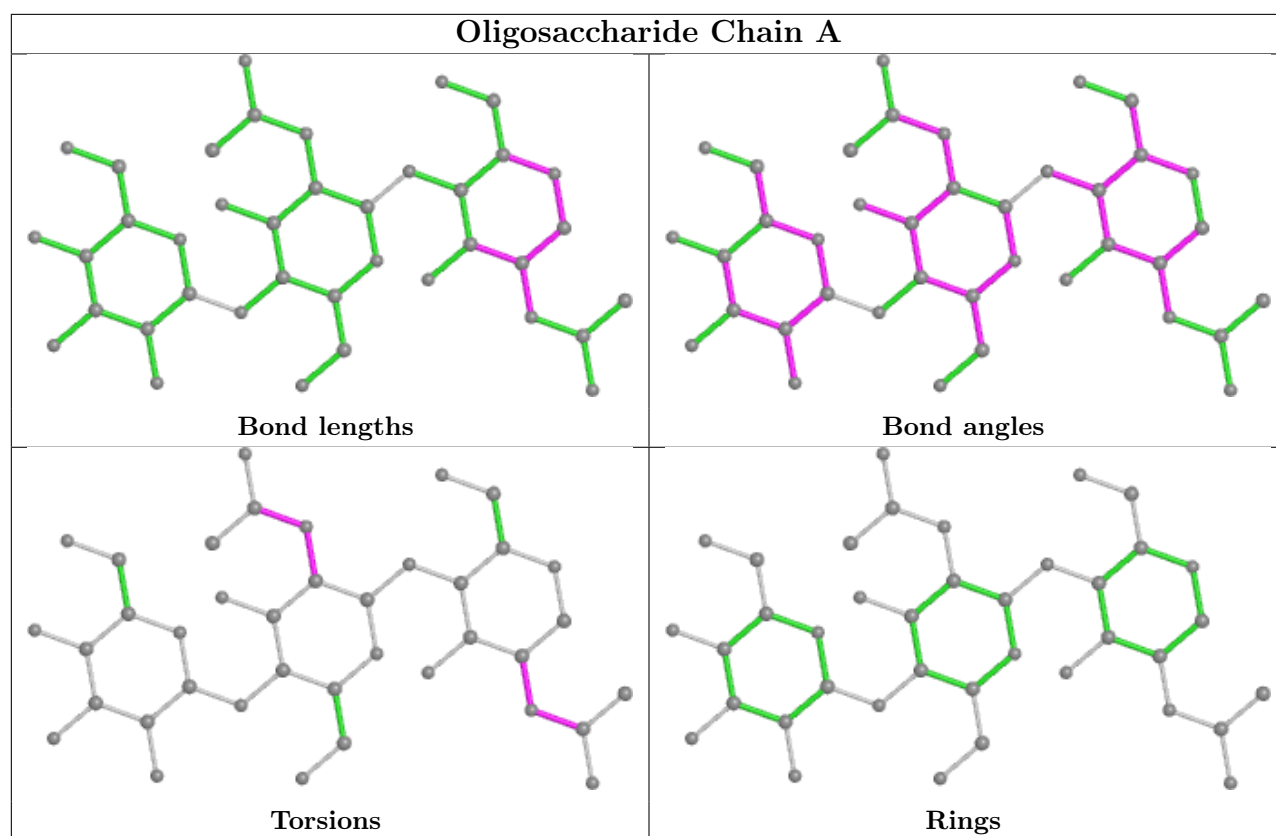
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
5	B	1	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
5	B	1	NAG	C1-C2-N2-C7

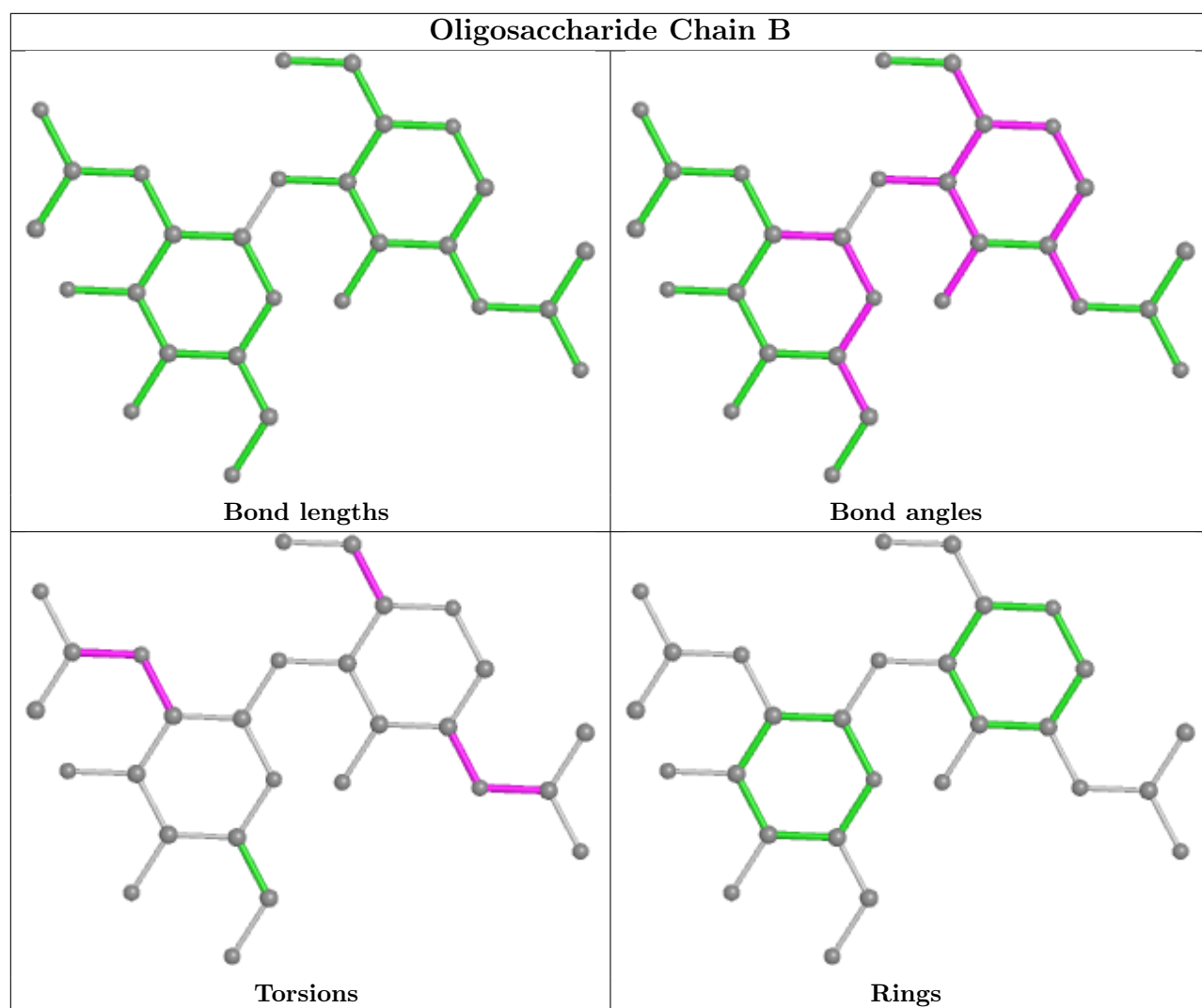
There are no ring outliers.

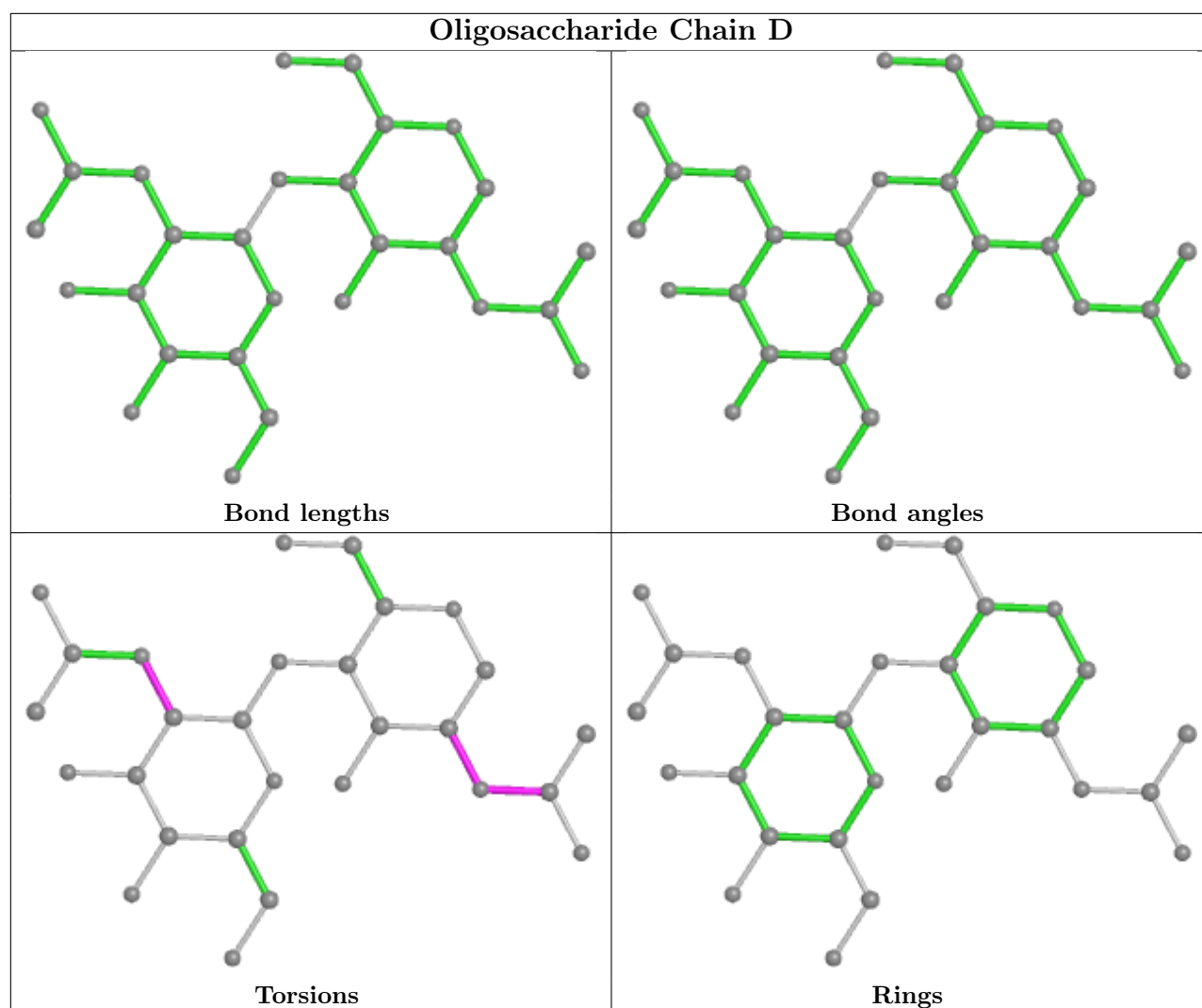
3 monomers are involved in 8 short contacts:

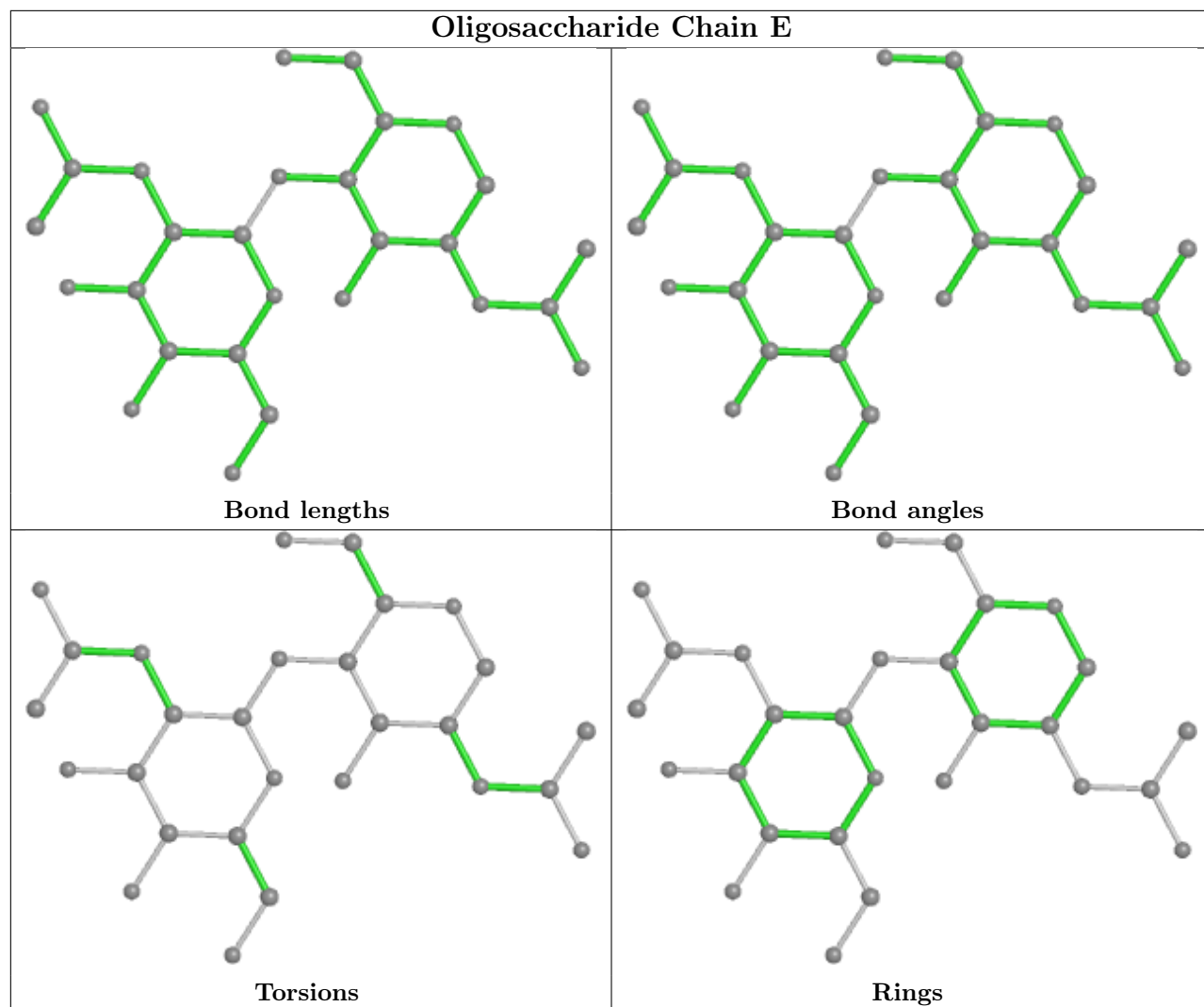
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	2	0
4	A	1	NAG	5	0
5	B	2	NAG	2	0

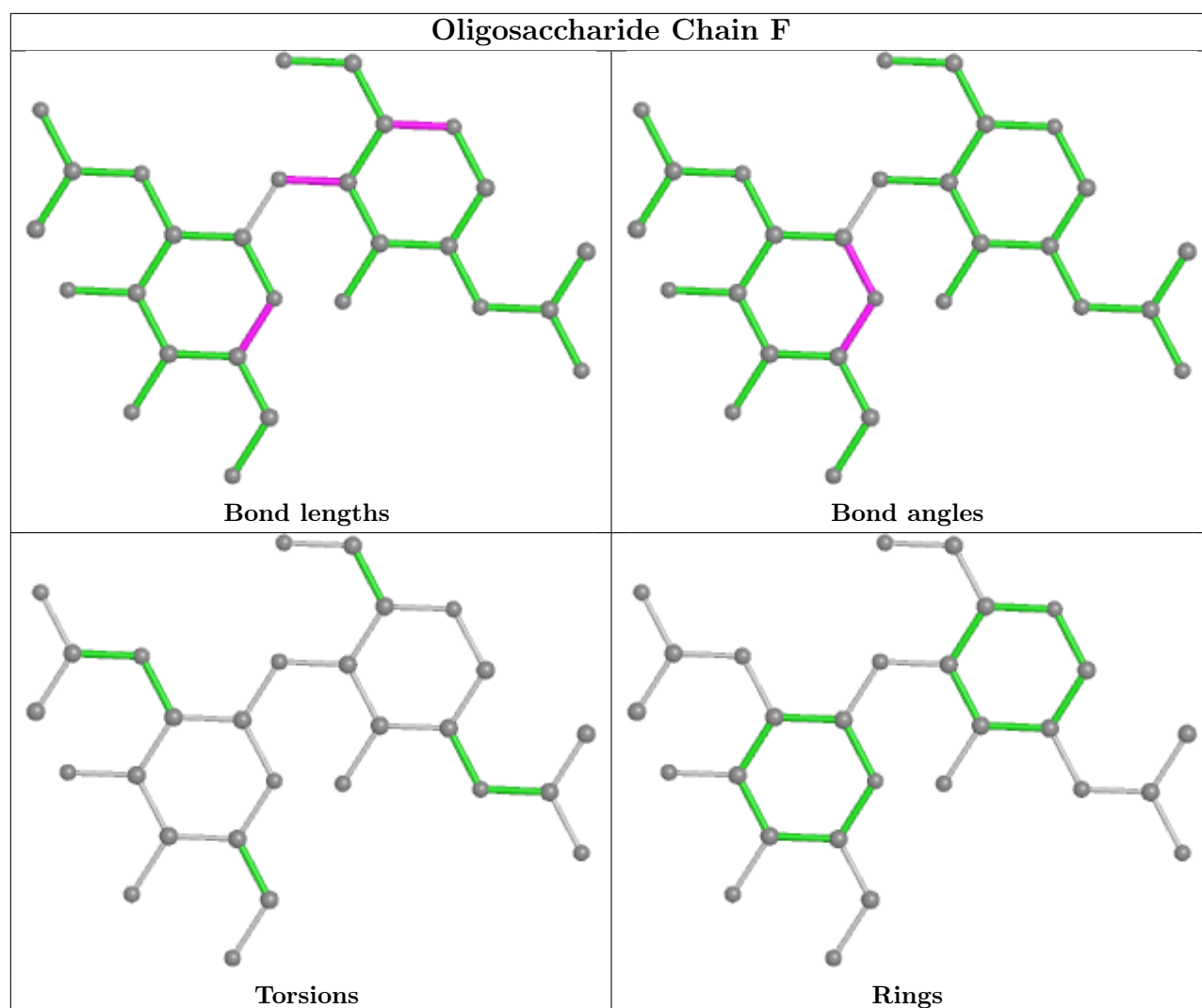
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

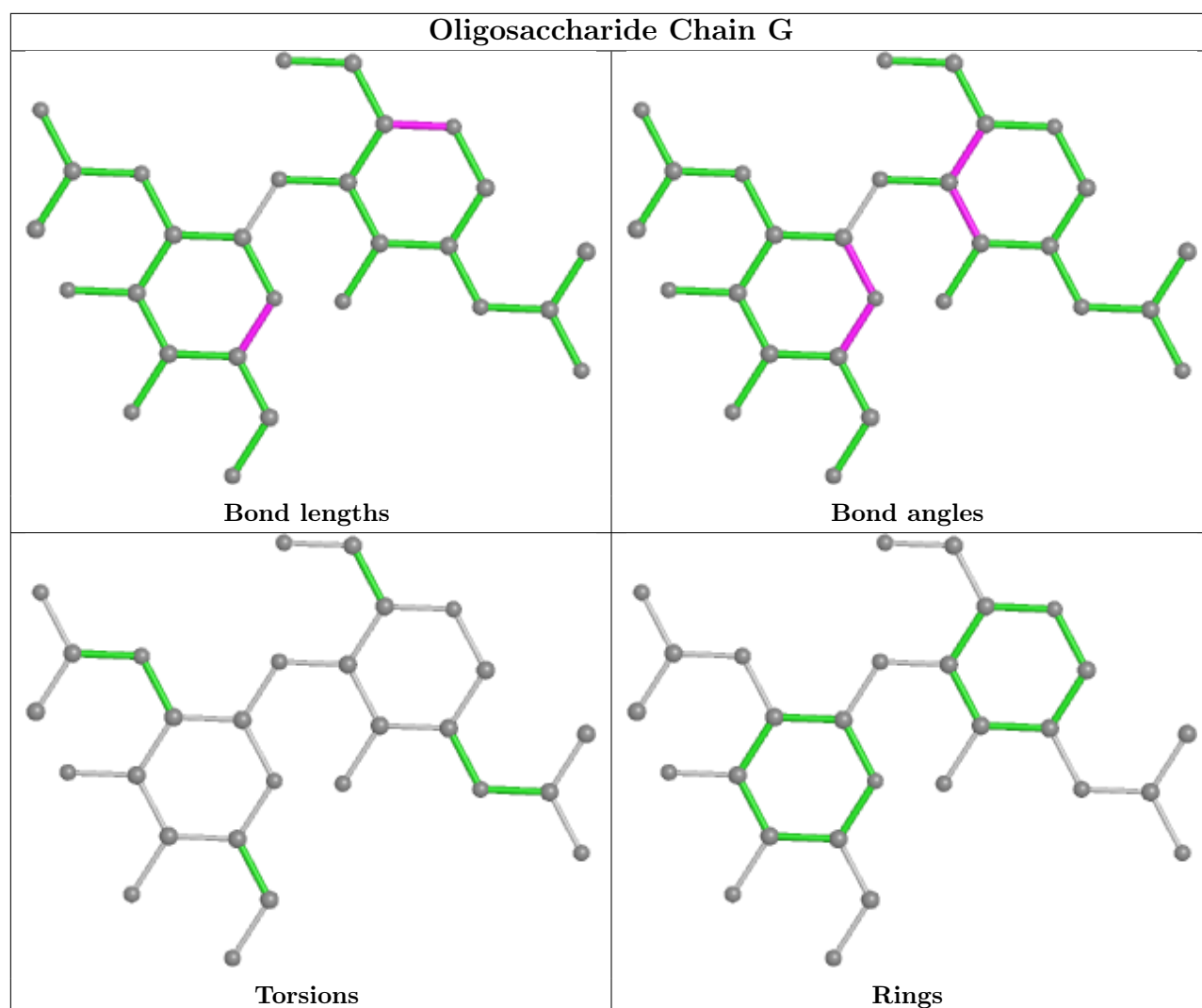


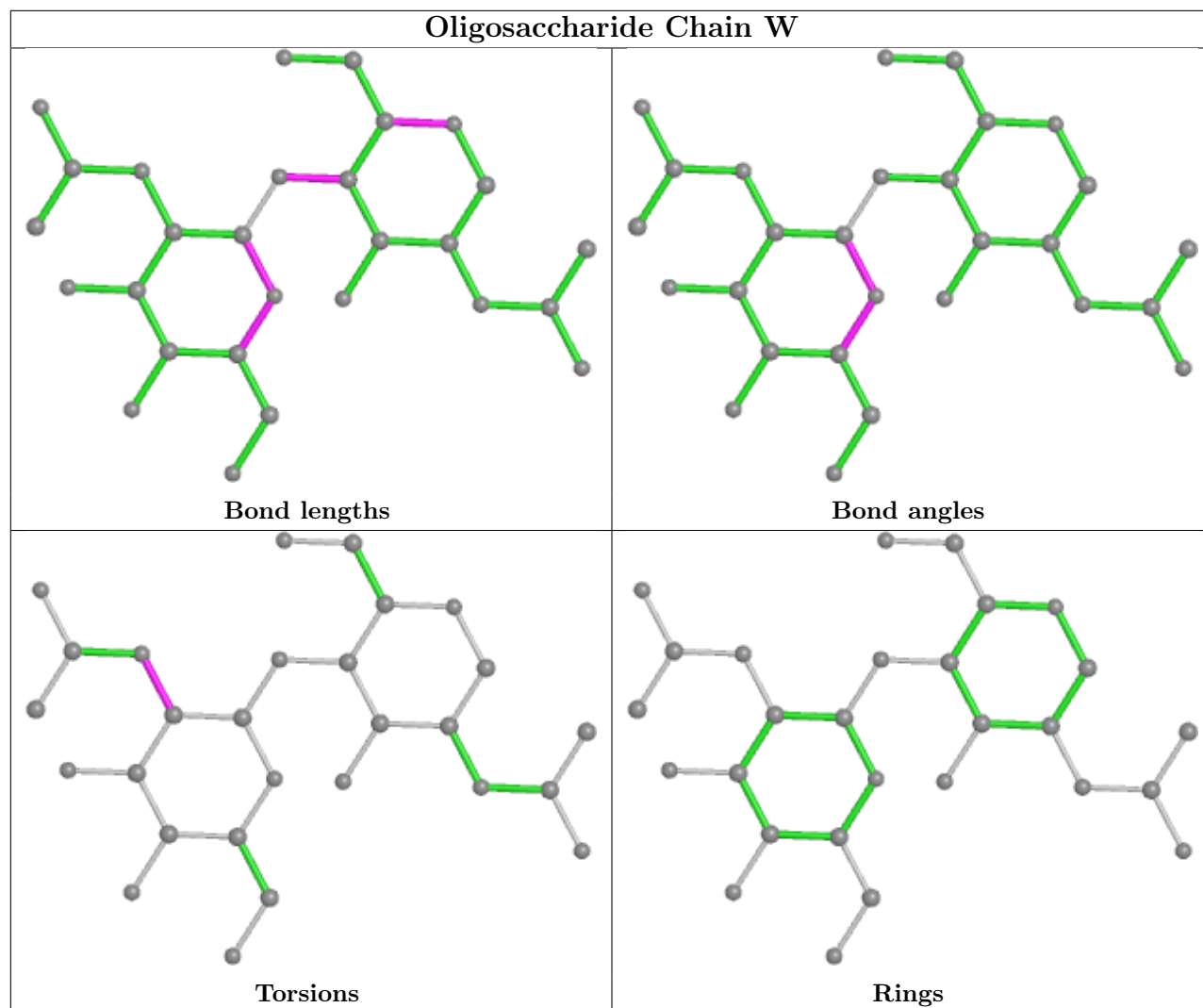


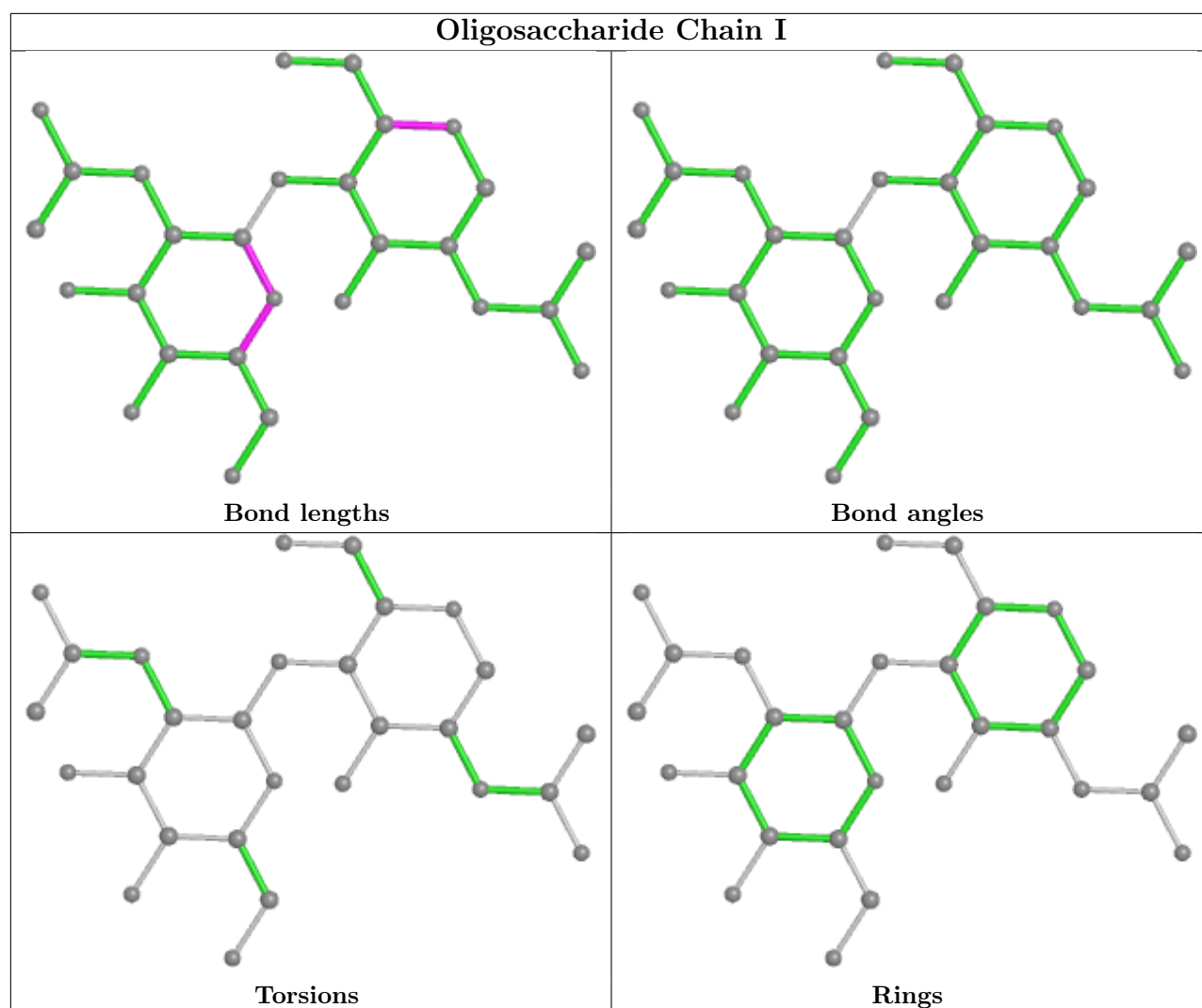


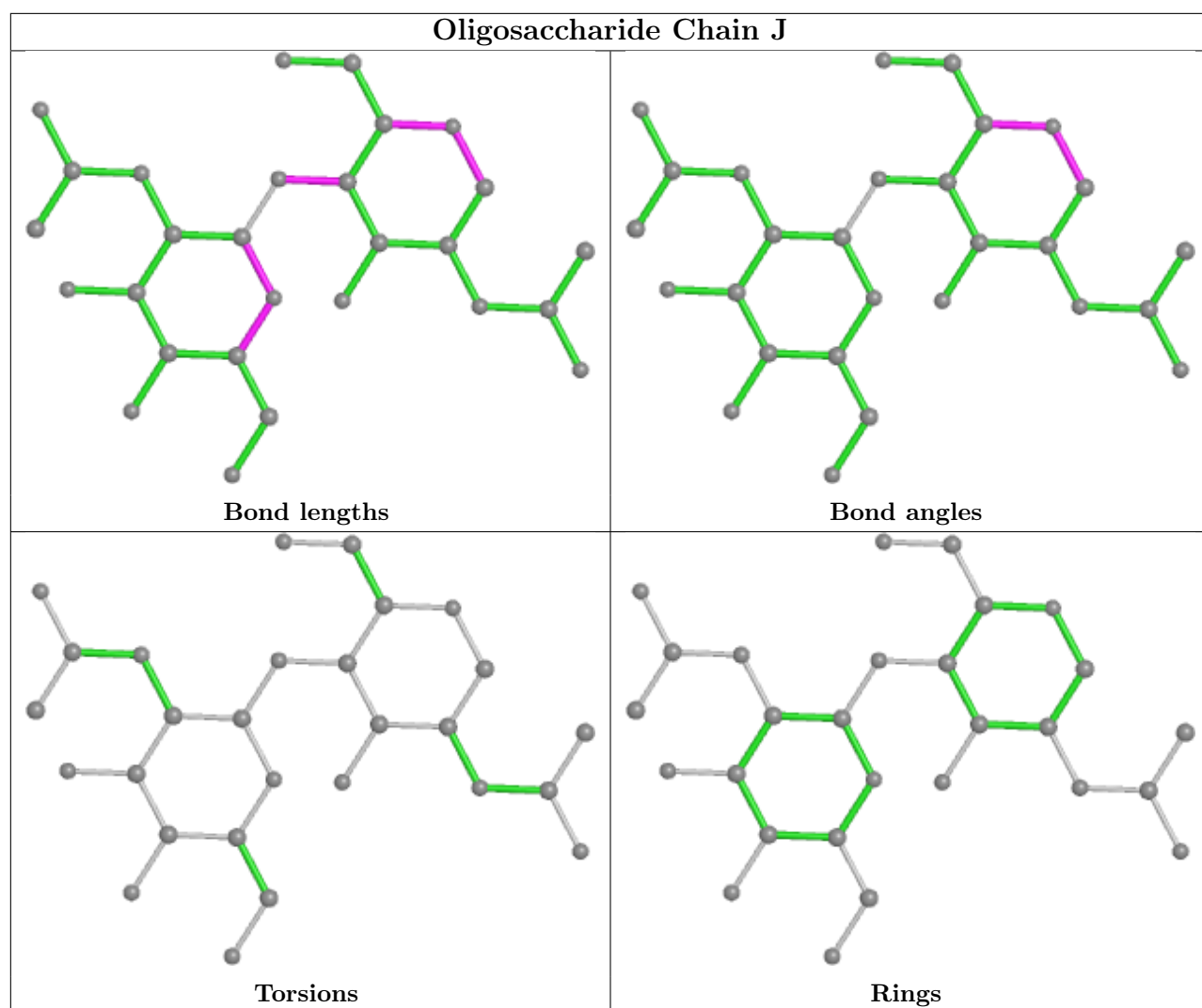


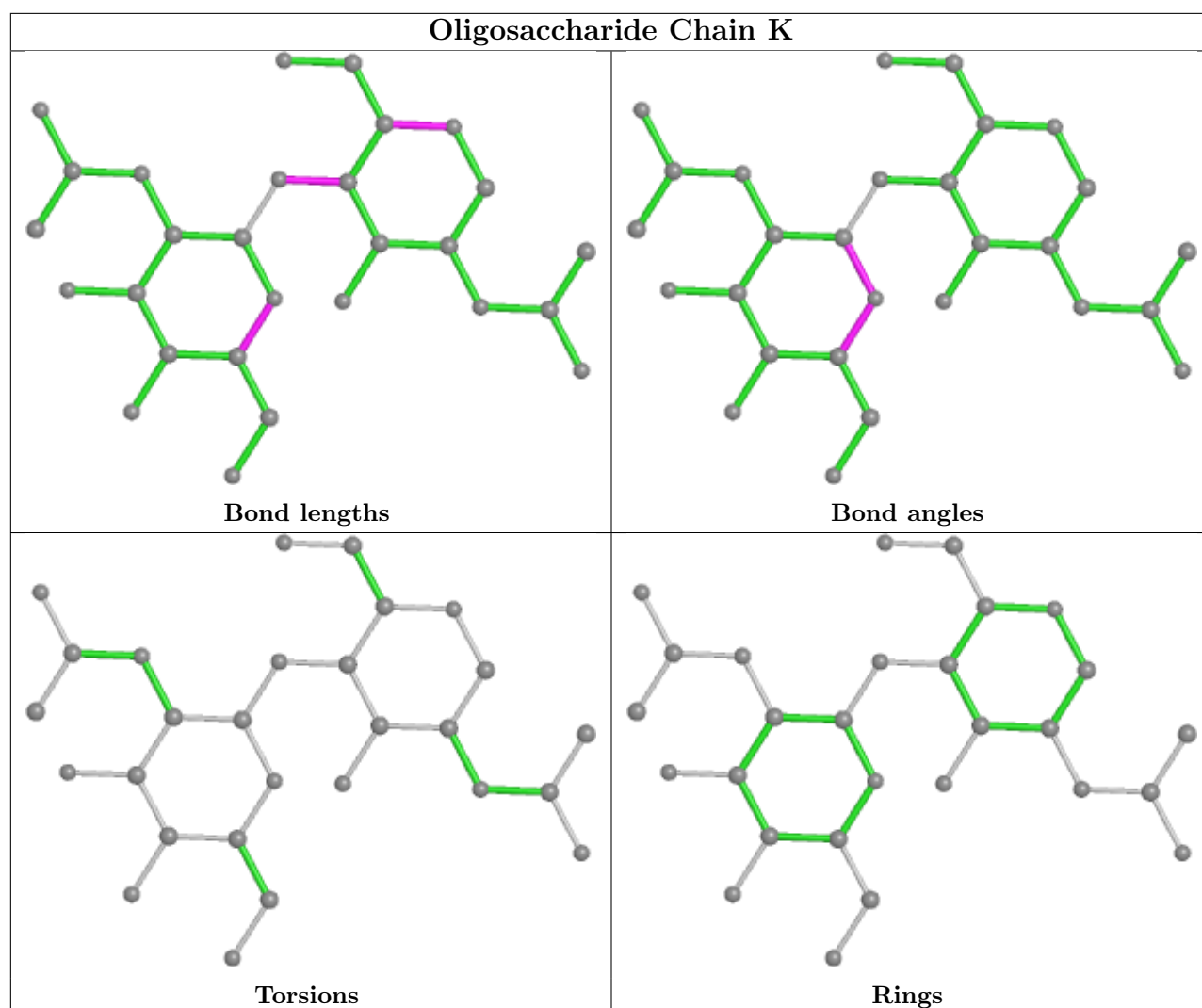


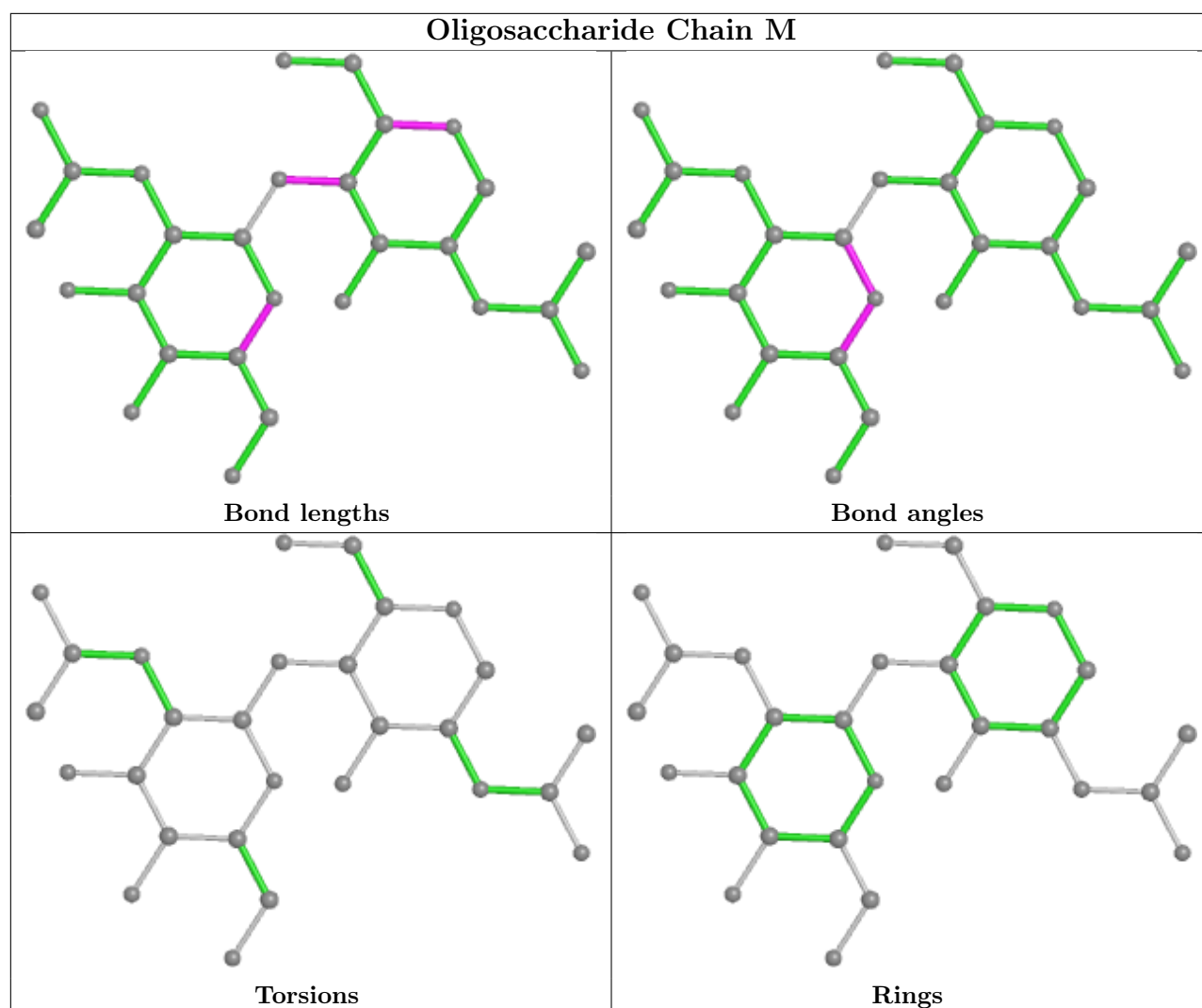


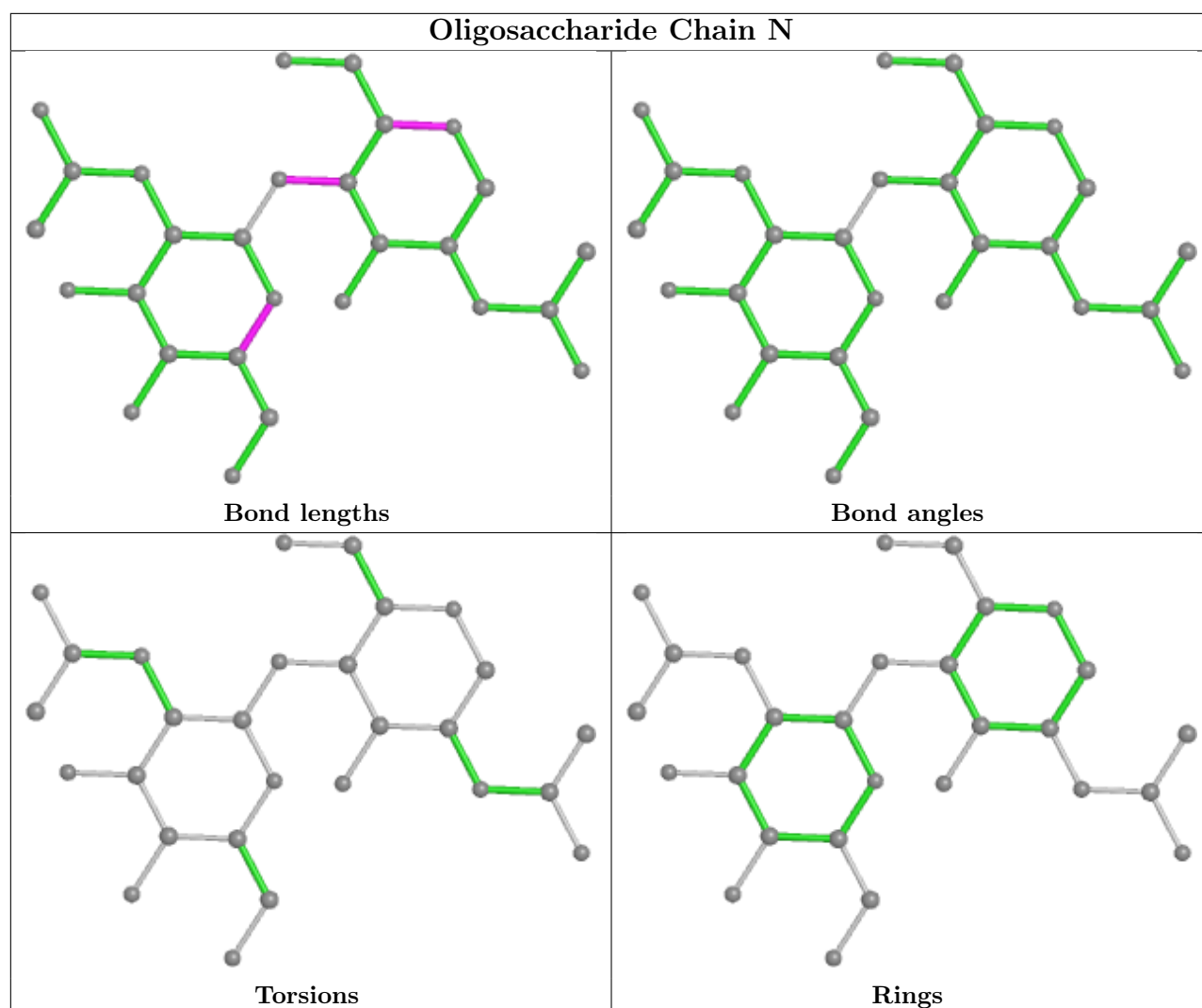


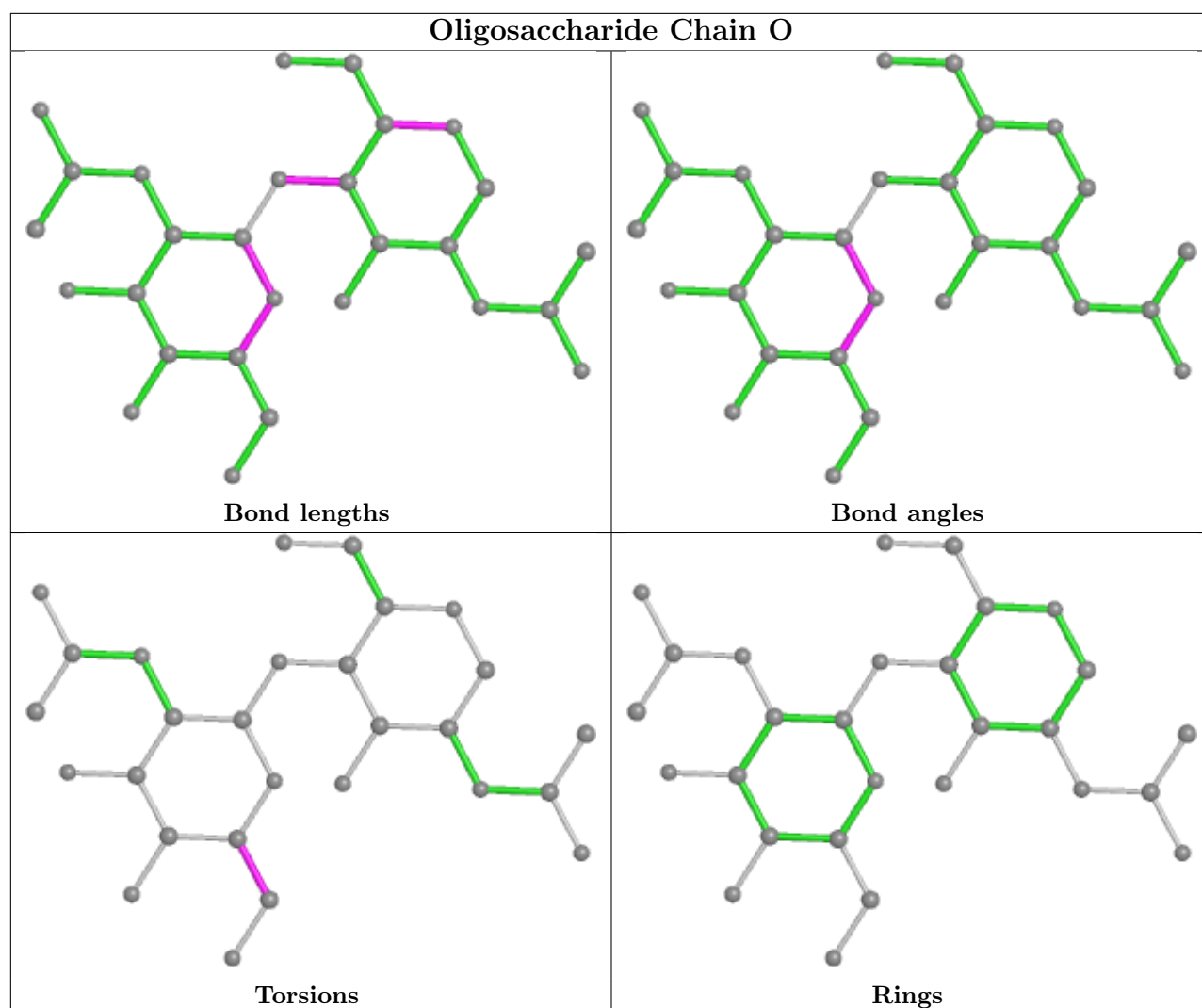












5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	1207	1	14,14,15	1.25	2 (14%)	17,19,21	0.75	0
6	NAG	C	1202	1	14,14,15	1.29	2 (14%)	17,19,21	0.60	0
6	NAG	S	1202	1	14,14,15	1.28	3 (21%)	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	V	1210	1	14,14,15	1.29	2 (14%)	17,19,21	0.63	0
6	NAG	S	1209	1	14,14,15	0.30	0	17,19,21	0.71	0
6	NAG	V	1207	1	14,14,15	1.29	3 (21%)	17,19,21	0.82	1 (5%)
6	NAG	C	1210	1	14,14,15	1.31	3 (21%)	17,19,21	0.88	1 (5%)
6	NAG	C	1203	1	14,14,15	1.34	2 (14%)	17,19,21	0.76	1 (5%)
6	NAG	V	1208	1	14,14,15	1.20	1 (7%)	17,19,21	0.76	1 (5%)
6	NAG	S	1205	1	14,14,15	1.18	1 (7%)	17,19,21	0.74	0
6	NAG	S	1204	1	14,14,15	1.29	3 (21%)	17,19,21	0.84	1 (5%)
6	NAG	C	1208	1	14,14,15	1.18	2 (14%)	17,19,21	1.04	1 (5%)
6	NAG	V	1206	1	14,14,15	1.24	2 (14%)	17,19,21	0.79	1 (5%)
6	NAG	V	1202	1	14,14,15	1.24	2 (14%)	17,19,21	0.74	1 (5%)
6	NAG	V	1212	1	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
6	NAG	C	1209	1	14,14,15	1.21	1 (7%)	17,19,21	1.01	1 (5%)
6	NAG	V	1203	1	14,14,15	1.23	1 (7%)	17,19,21	0.83	1 (5%)
6	NAG	S	1210	1	14,14,15	0.51	0	17,19,21	2.33	6 (35%)
6	NAG	C	1201	1	14,14,15	1.42	2 (14%)	17,19,21	0.70	0
6	NAG	C	1206	1	14,14,15	1.29	3 (21%)	17,19,21	0.97	1 (5%)
6	NAG	S	1207	1	14,14,15	0.30	0	17,19,21	0.96	0
6	NAG	V	1201	1	14,14,15	1.27	3 (21%)	17,19,21	1.08	1 (5%)
6	NAG	C	1211	1	14,14,15	0.30	0	17,19,21	0.72	0
6	NAG	S	1206	1	14,14,15	1.24	2 (14%)	17,19,21	1.07	1 (5%)
6	NAG	S	1208	1	14,14,15	0.27	0	17,19,21	0.73	0
6	NAG	V	1205	1	14,14,15	1.45	3 (21%)	17,19,21	0.74	0
6	NAG	V	1204	-	14,14,15	1.20	1 (7%)	17,19,21	0.76	1 (5%)
6	NAG	S	1201	1	14,14,15	1.23	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	C	1205	1	14,14,15	1.36	3 (21%)	17,19,21	0.92	1 (5%)
6	NAG	V	1209	1	14,14,15	1.21	1 (7%)	17,19,21	0.82	1 (5%)
6	NAG	V	1211	1	14,14,15	0.32	0	17,19,21	0.67	0
6	NAG	C	1204	1	14,14,15	1.25	1 (7%)	17,19,21	0.82	1 (5%)
6	NAG	S	1203	1	14,14,15	1.20	1 (7%)	17,19,21	0.68	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
6	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1202	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1210	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1209	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1207	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1210	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1208	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1205	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1208	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1202	1	-	1/6/23/26	0/1/1/1
6	NAG	V	1212	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1203	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1210	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1207	1	-	2/6/23/26	0/1/1/1
6	NAG	V	1201	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1211	1	-	3/6/23/26	0/1/1/1
6	NAG	S	1206	1	-	1/6/23/26	0/1/1/1
6	NAG	S	1208	1	-	6/6/23/26	0/1/1/1
6	NAG	V	1205	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1204	-	-	0/6/23/26	0/1/1/1
6	NAG	S	1201	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1205	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1209	1	-	0/6/23/26	0/1/1/1
6	NAG	V	1211	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
6	NAG	S	1203	1	-	1/6/23/26	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	1205	NAG	O5-C5	3.04	1.49	1.43
6	C	1203	NAG	O5-C5	3.01	1.49	1.43
6	C	1201	NAG	O5-C1	2.90	1.48	1.43
6	C	1201	NAG	O5-C5	2.79	1.49	1.43
6	C	1207	NAG	O5-C5	2.76	1.49	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1210	NAG	C2-N2-C7	-4.38	116.67	122.90
6	S	1210	NAG	C1-C2-N2	4.33	117.88	110.49
6	S	1210	NAG	O5-C1-C2	-4.15	104.73	111.29
6	S	1210	NAG	C4-C3-C2	-3.94	105.25	111.02
6	V	1201	NAG	C1-O5-C5	3.87	117.43	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	S	1208	NAG	C1-C2-N2-C7
6	S	1208	NAG	C8-C7-N2-C2
6	S	1208	NAG	O7-C7-N2-C2
6	V	1212	NAG	C8-C7-N2-C2
6	V	1212	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1210	NAG	1	0
6	S	1207	NAG	1	0
6	S	1208	NAG	2	0
6	V	1204	NAG	4	0

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.

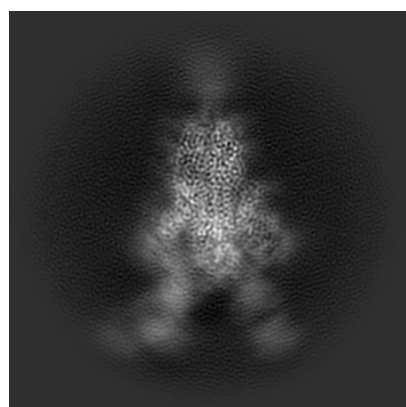
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25904. These allow visual inspection of the internal detail of the map and identification of artifacts.

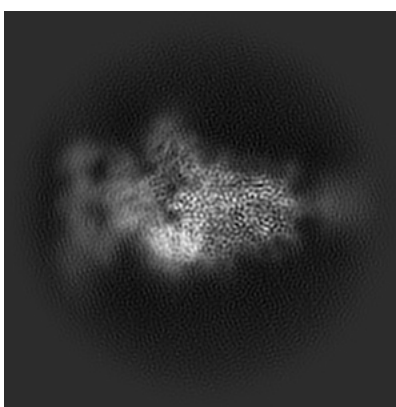
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

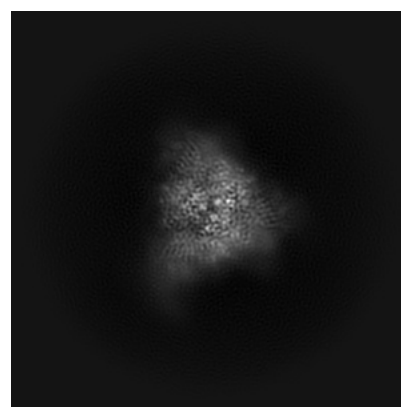
6.1.1 Primary map



X



Y

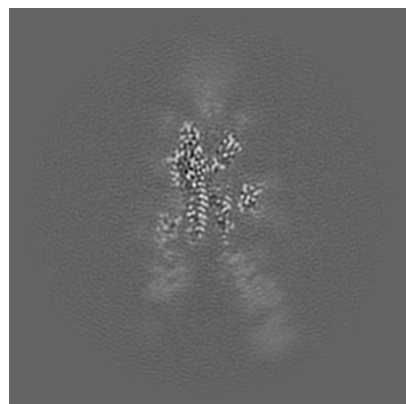


Z

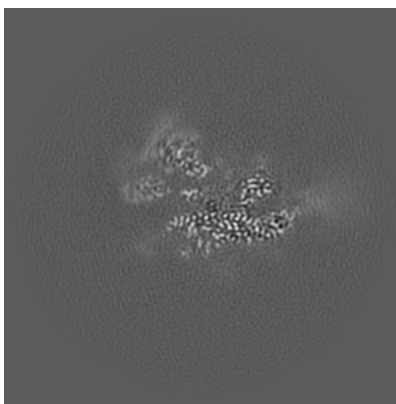
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

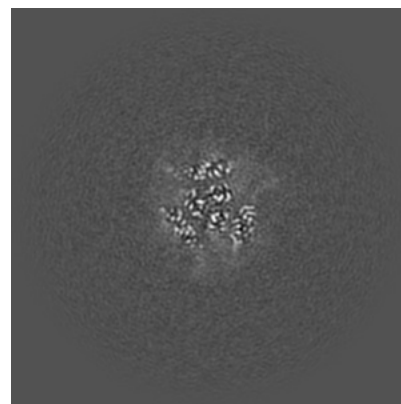
6.2.1 Primary map



X Index: 160



Y Index: 160

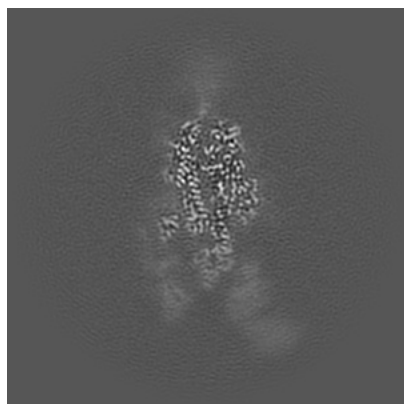


Z Index: 160

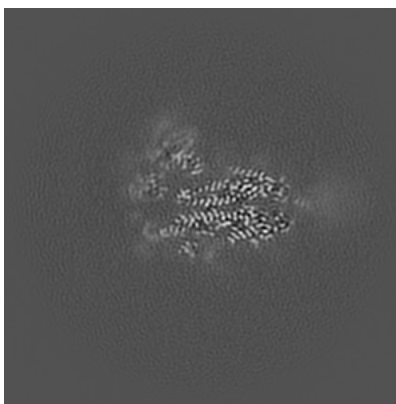
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

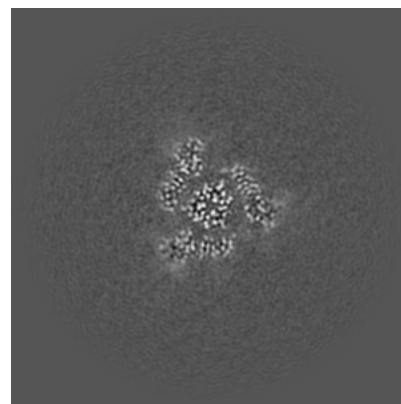
6.3.1 Primary map



X Index: 170



Y Index: 164



Z Index: 147

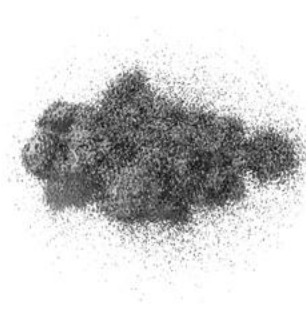
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1321. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

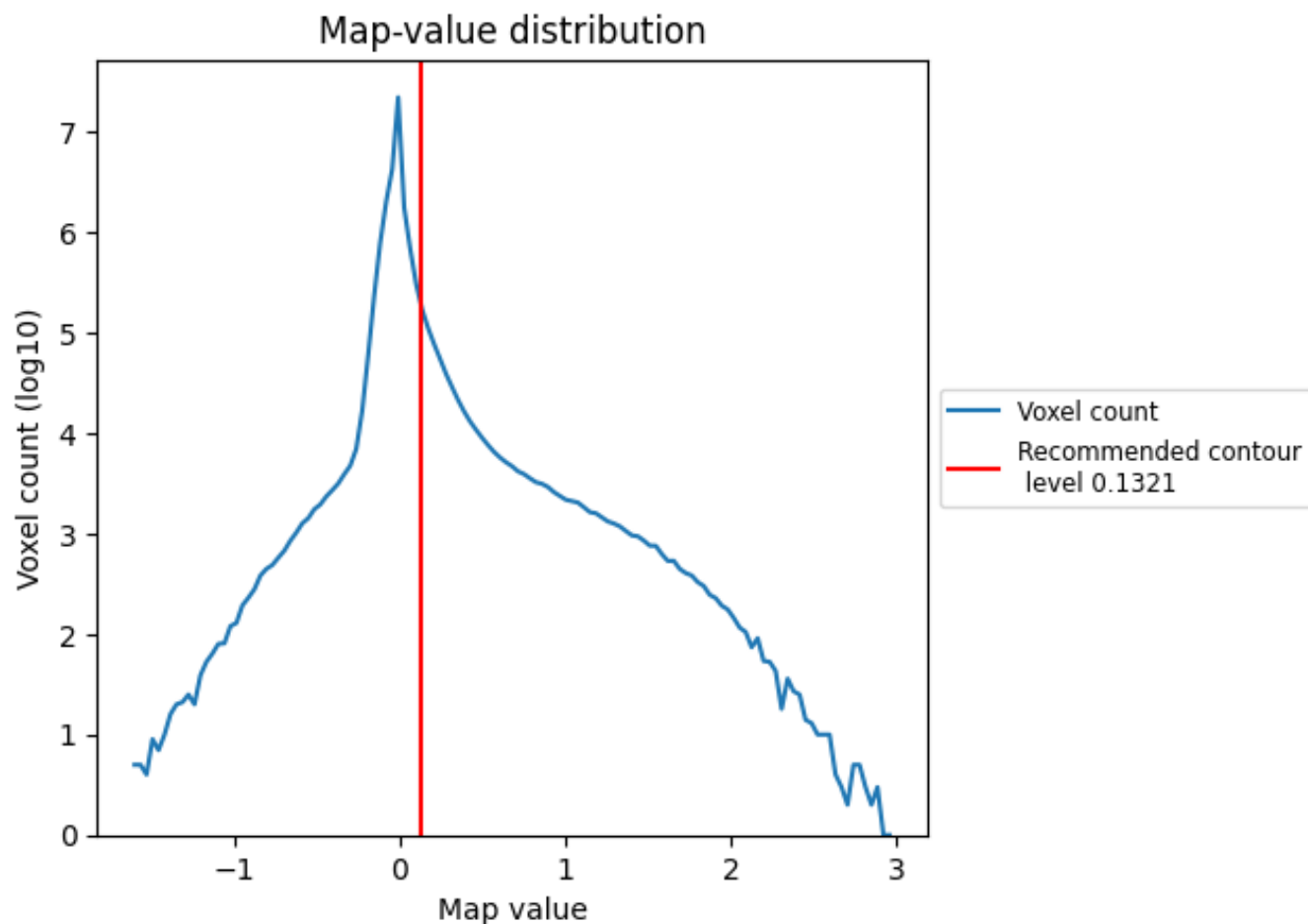
6.5 Mask visualisation

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

7 Map analysis [i](#)

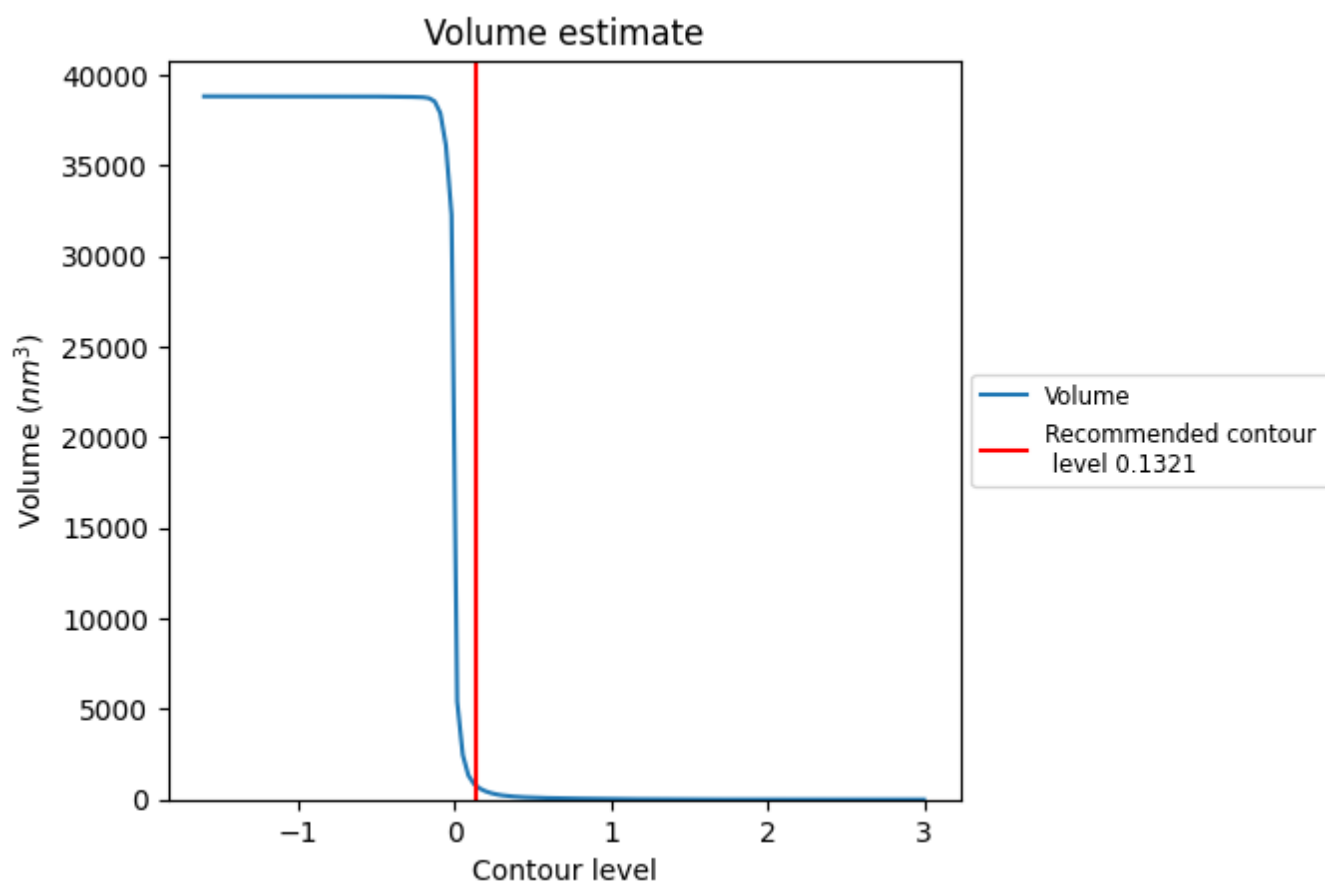
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

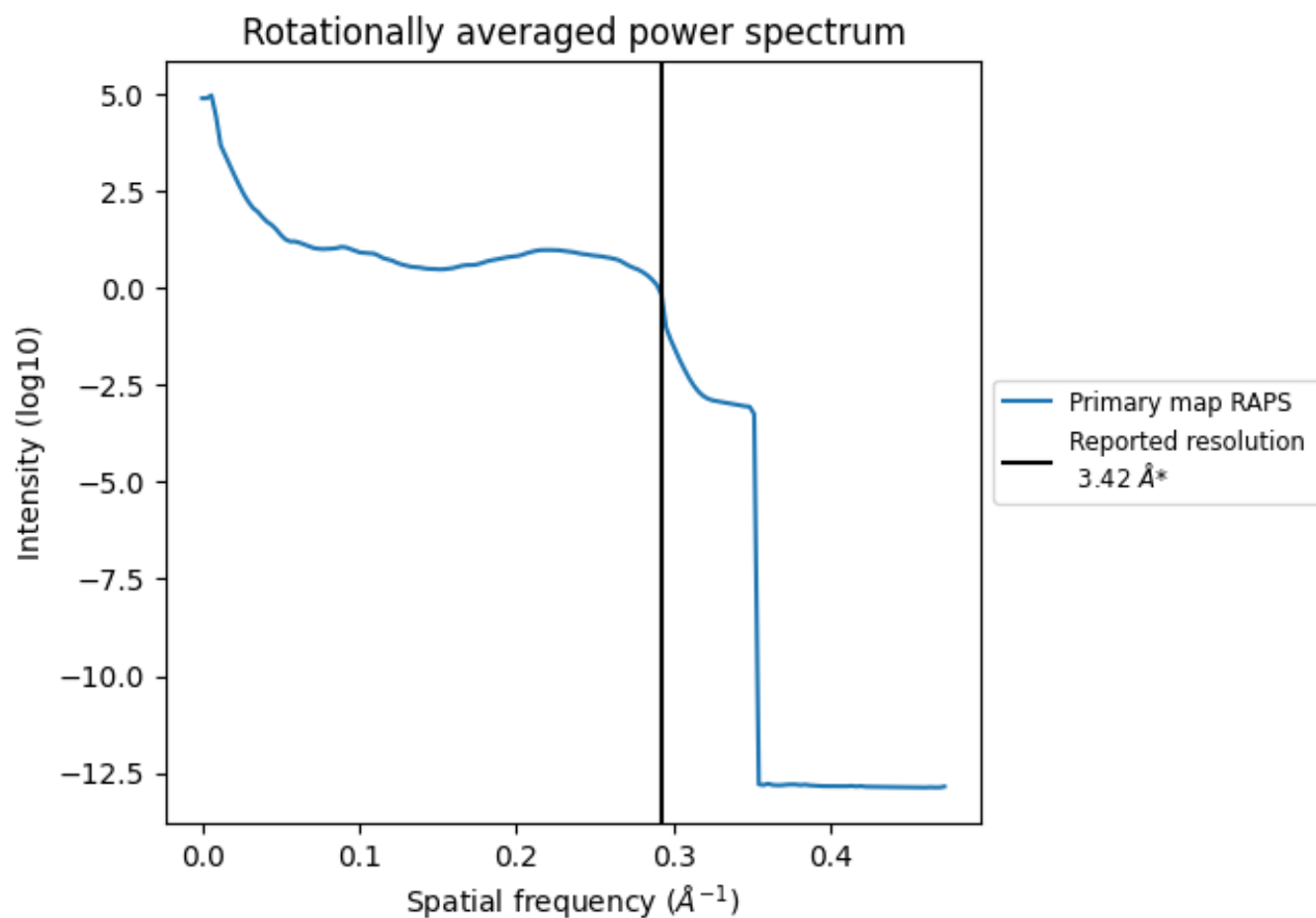
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 717 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

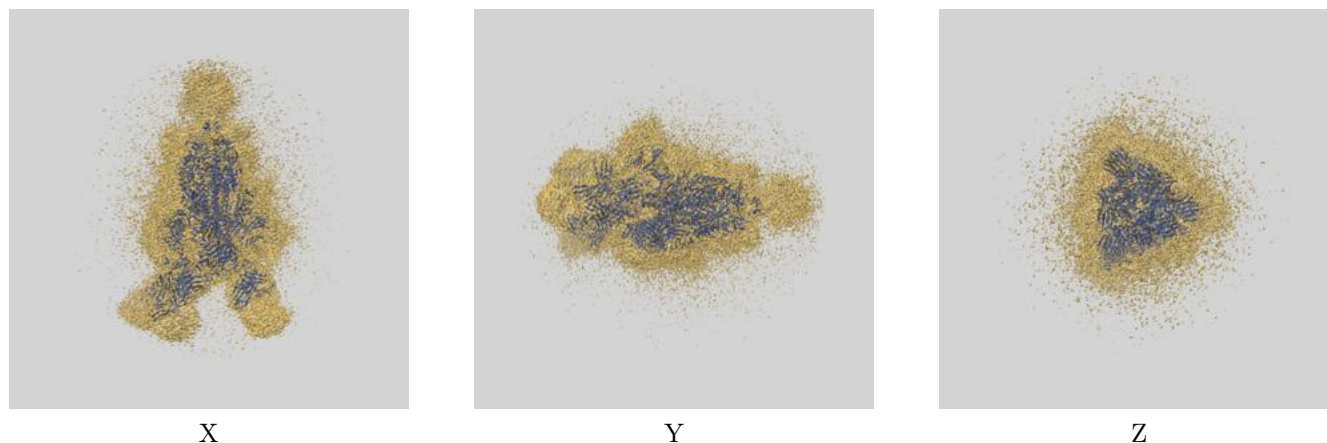
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

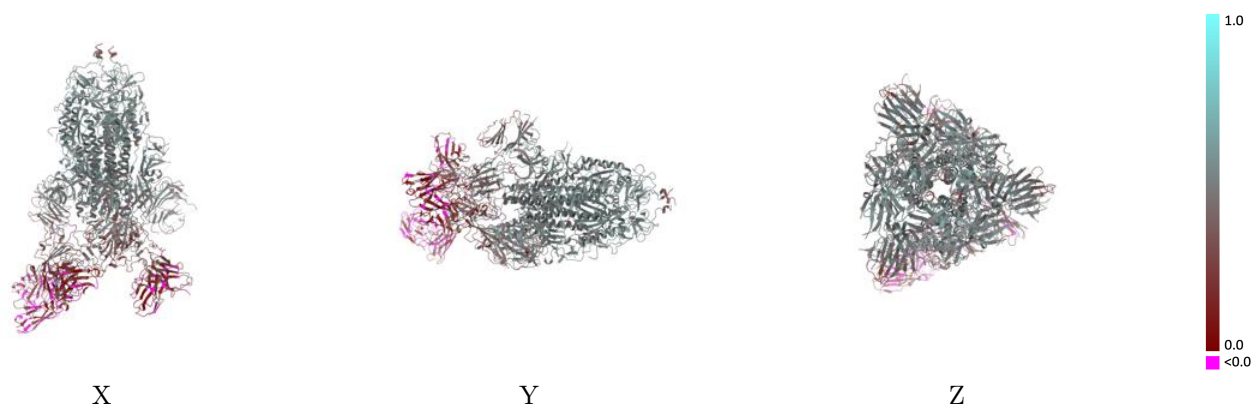
This section contains information regarding the fit between EMDB map EMD-25904 and PDB model 7THT. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1321 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



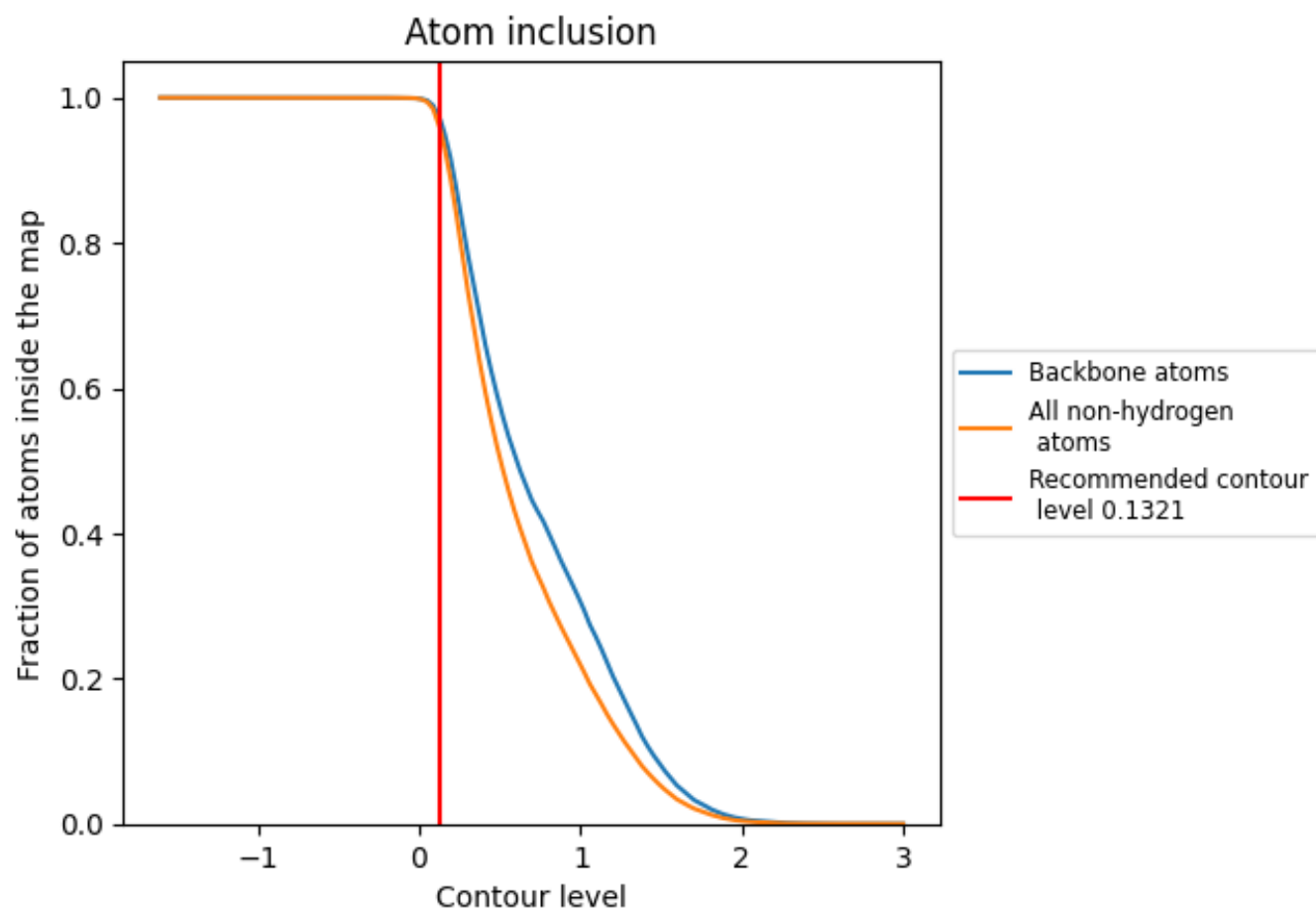
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1321).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1321) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9559	 0.4070
A	 1.0000	 0.5340
B	 0.9643	 0.4470
C	 0.9827	 0.4680
D	 1.0000	 0.4380
E	 1.0000	 0.3880
F	 1.0000	 0.4390
G	 1.0000	 0.4310
H	 0.9328	 0.1470
I	 1.0000	 0.4310
J	 1.0000	 0.4590
K	 1.0000	 0.4040
L	 0.8887	 0.1380
M	 1.0000	 0.4230
N	 1.0000	 0.4790
O	 1.0000	 0.4380
S	 0.9860	 0.4820
V	 0.9772	 0.4510
W	 1.0000	 0.4330
a	 0.9317	 0.2060
b	 0.6359	 0.0440
c	 0.9102	 0.2030
d	 0.7082	 0.0990

