



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:34 PM JST

PDB ID : 7XU0
EMDB ID : EMD-33454
Title : Structure of SARS-CoV-2 Spike Protein with Engineered x3 Disulfide (x3(D427C, V987C) and single Arg S1/S2 cleavage site), Locked-211 Conformation
Authors : Qu, K.; Chen, Q.; Ciazynska, K.A.; Liu, B.; Zhang, X.; Wang, J.; He, Y.; Guan, J.; He, J.; Liu, T.; Zhang, X.; Carter, A.P.; Xiong, X.; Briggs, J.A.G.
Deposited on : 2022-05-18
Resolution : 2.90 Å(reported)
Based on initial model : 6ZP2

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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

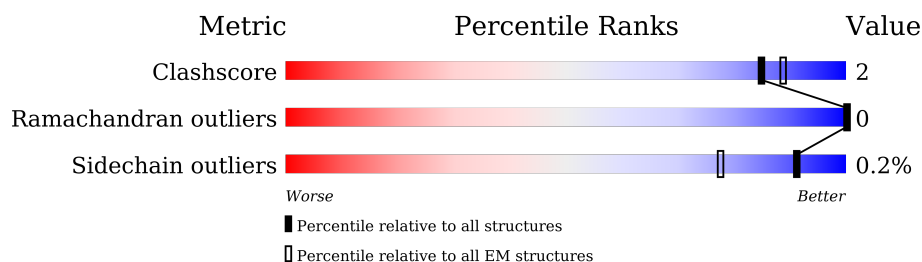
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



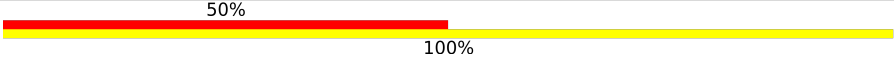
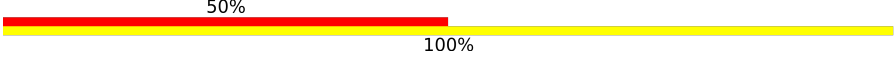
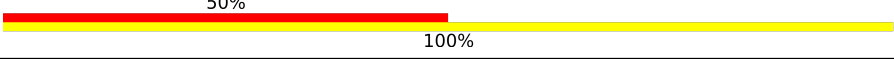
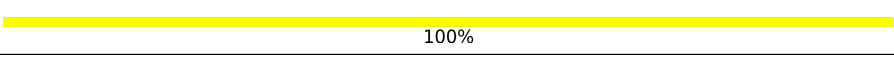

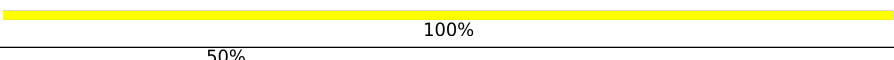
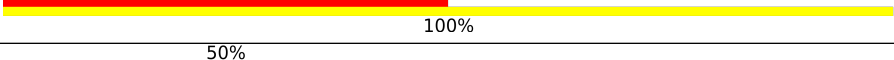
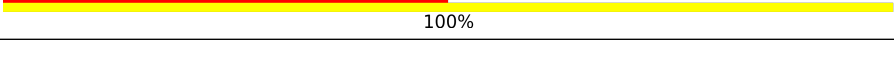
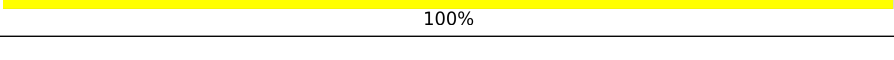
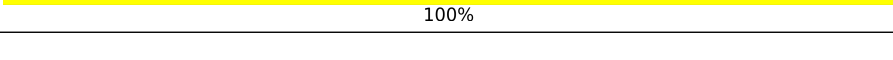
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	A	1128	 90% 8%
1	B	1128	 92% 5%
1	C	1128	 93%
2	D	2	 100%
2	E	2	 100%
2	F	2	 50% 100%
2	G	2	 50% 100%

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Mol	Chain	Length	Quality of chain
2	H	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 53028 atoms, of which 26135 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	A	1110	Total	C	H	N	O	S	0	0
			17100	5525	8434	1450	1649	42		
1	B	1097	Total	C	H	N	O	S	0	0
			16916	5465	8345	1434	1630	42		
1	C	1093	Total	C	H	N	O	S	0	0
			16866	5447	8323	1430	1624	42		

There are 30 discrepancies between the modelled and reference sequences:

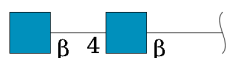
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	427	CYS	ASP	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	987	CYS	VAL	engineered mutation	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	427	CYS	ASP	engineered mutation	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	987	CYS	VAL	engineered mutation	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	427	CYS	ASP	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	987	CYS	VAL	engineered mutation	UNP P0DTC2

- 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					AltConf	Trace
2	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	E	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	J	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	L	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	M	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	N	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	P	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

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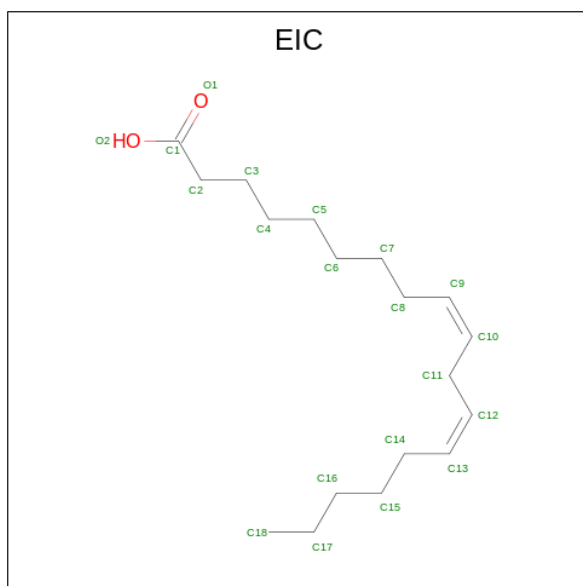
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

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Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 4 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			51	18	31	2	
4	A	1	Total	C	H	O	0
			51	18	31	2	
4	B	1	Total	C	H	O	0
			51	18	31	2	

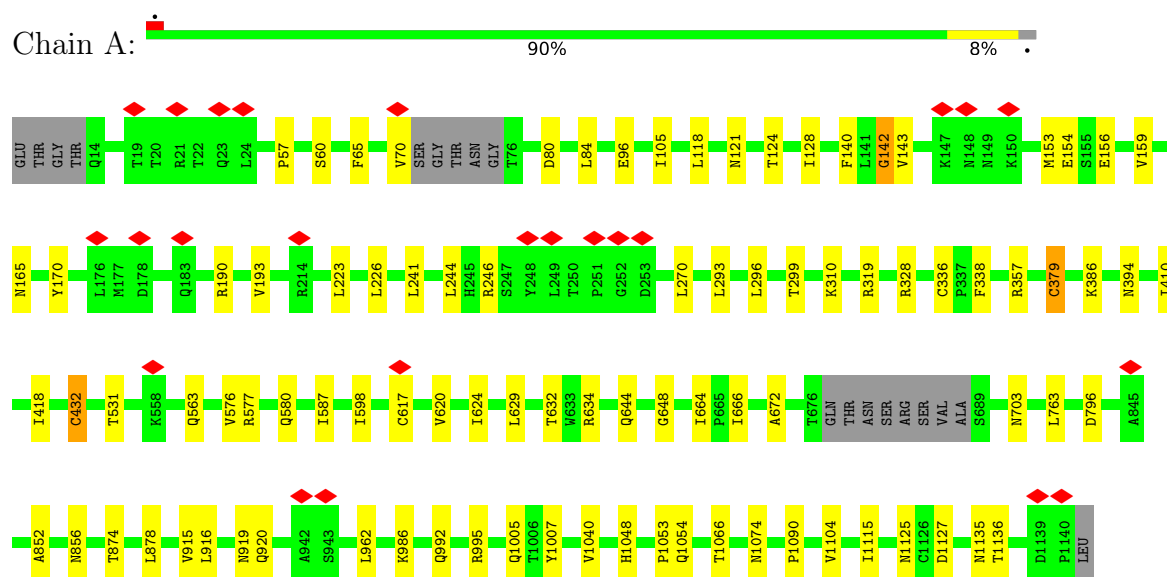
- Molecule 5 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



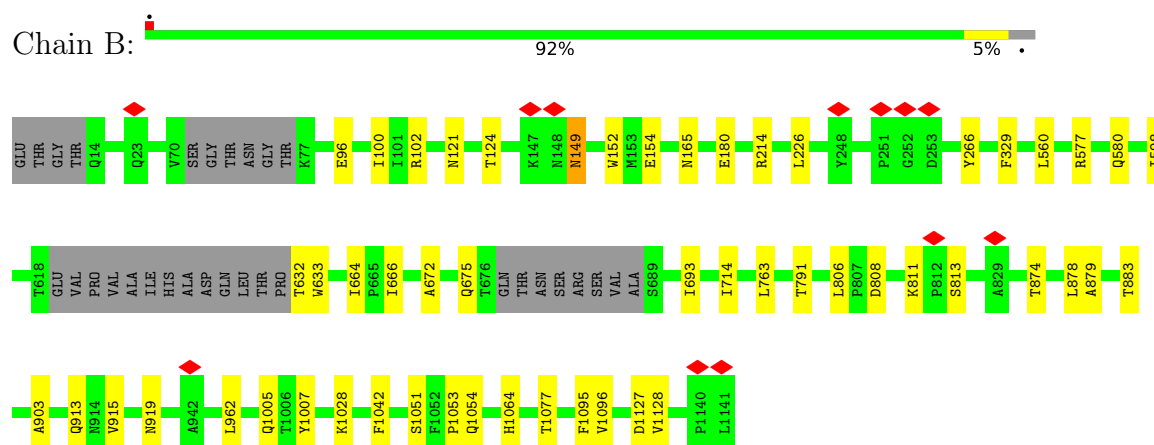
3 Residue-property plots

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

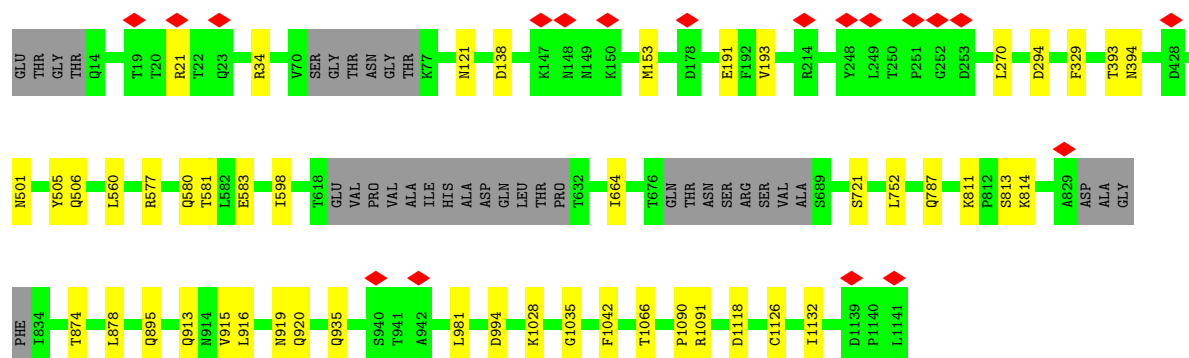


• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein





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

Chain D: 100%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

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

Chain F: 50%
100%

NAG1
NAG2

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

Chain G: 50%
100%

NAG1
NAG2

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

Chain H: 50%
100%



- 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 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

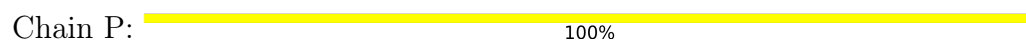




- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138382	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EIC, NAG, BLA

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	0.31	2/8868 (0.0%)	0.57	1/12071 (0.0%)
1	B	0.28	0/8769	0.54	0/11929
1	C	0.28	0/8739	0.53	0/11887
All	All	0.29	2/26376 (0.0%)	0.55	1/35887 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	CYS	CB-SG	-6.43	1.71	1.82
1	A	379	CYS	CB-SG	5.17	1.91	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	CYS	CA-CB-SG	11.48	134.66	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	GLY	Peptide
1	A	165	ASN	Peptide
1	A	617	CYS	Peptide
1	B	165	ASN	Peptide

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	8666	8434	8440	56	0
1	B	8571	8345	8345	30	0
1	C	8543	8323	8323	29	0
2	D	28	25	25	0	0
2	E	28	25	25	0	0
2	F	28	25	25	0	0
2	G	28	25	25	0	0
2	H	28	25	25	0	0
2	I	28	25	25	0	0
2	J	28	25	25	0	0
2	K	28	25	25	0	0
2	L	28	25	25	1	0
2	M	28	25	25	0	0
2	N	28	25	25	0	0
2	O	28	25	25	0	0
2	P	28	25	25	0	0
2	Q	28	25	25	0	0
3	A	168	156	156	2	0
3	B	182	169	169	0	0
3	C	182	169	169	1	0
4	A	40	62	62	0	0
4	B	20	31	31	0	0
5	A	43	32	32	2	0
5	B	43	32	32	2	0
5	C	43	32	32	1	0
All	All	26893	26135	26141	110	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 2.

All (110) 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:811:LYS:NZ	1:B:813:SER:OG	2.24	0.71
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.24	0.70
1:B:879:ALA:O	1:B:883:THR:OG1	2.09	0.69
1:A:96:GLU:OE2	1:A:190:ARG:NH1	2.27	0.68
1:A:629:LEU:O	1:A:634:ARG:NH2	2.28	0.67
1:B:102:ARG:NH1	1:B:154:GLU:OE2	2.27	0.67
1:A:319:ARG:HE	1:A:624:ILE:HD11	1.59	0.66
1:C:811:LYS:NZ	1:C:813:SER:OG	2.31	0.63
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.30	0.62
1:B:560:LEU:O	1:B:577:ARG:NH2	2.32	0.61
1:A:563:GLN:O	1:A:577:ARG:NH2	2.33	0.61
1:A:142:GLY:HA3	1:A:143:VAL:HG23	1.83	0.61
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.37	0.58
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.85	0.57
1:C:329:PHE:O	1:C:580:GLN:NE2	2.37	0.57
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.37	0.57
1:A:915:VAL:O	1:A:919:ASN:ND2	2.37	0.57
1:B:124:THR:OG1	2:L:1:NAG:N2	2.38	0.57
1:B:121:ASN:ND2	5:B:1215:BLA:OB	2.39	0.56
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.88	0.56
1:A:386:LYS:NZ	1:C:981:LEU:O	2.39	0.56
1:A:666:ILE:HD11	1:A:672:ALA:CB	2.35	0.55
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.38	0.55
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.41	0.54
1:C:153:MET:SD	3:C:1213:NAG:O6	2.52	0.53
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.89	0.53
1:A:1125:ASN:ND2	1:A:1127:ASP:OD2	2.42	0.53
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.41	0.53
1:B:96:GLU:OE1	1:B:100:ILE:N	2.41	0.53
1:C:916:LEU:O	1:C:920:GLN:N	2.42	0.53
1:A:598:ILE:HG12	1:A:666:ILE:HD12	1.91	0.53
1:B:913:GLN:NE2	1:C:1090:PRO:O	2.43	0.52
1:B:915:VAL:O	1:B:919:ASN:ND2	2.42	0.52
1:C:501:ASN:ND2	1:C:505:TYR:O	2.42	0.52
1:B:329:PHE:O	1:B:580:GLN:NE2	2.43	0.52
1:C:21:ARG:NH2	1:C:138:ASP:OD2	2.41	0.52
1:A:328:ARG:NH2	1:A:531:THR:O	2.43	0.52
1:A:666:ILE:HD11	1:A:672:ALA:HB3	1.92	0.51
1:B:1127:ASP:OD1	1:B:1128:VAL:N	2.43	0.51
1:A:620:VAL:O	1:A:624:ILE:HG22	2.11	0.51
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.43	0.50
1:A:379:CYS:HA	1:A:432:CYS:CB	2.42	0.50
1:B:763:LEU:HD21	1:B:1005:GLN:HG2	1.94	0.50
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.93	0.50
1:A:796:ASP:N	1:A:796:ASP:OD1	2.45	0.49
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	1.93	0.49
1:A:121:ASN:ND2	5:A:1314:BLA:OB	2.40	0.49
1:A:128:ILE:HD12	1:A:170:TYR:HD2	1.77	0.49
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	1.94	0.49
1:C:752:LEU:HD22	1:C:994:ASP:OD1	2.13	0.49
1:B:632:THR:OG1	1:B:633:TRP:N	2.43	0.48
1:C:811:LYS:O	1:C:814:LYS:NZ	2.42	0.48
1:B:791:THR:HG21	1:B:806:LEU:HD22	1.94	0.48
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.96	0.48
1:C:915:VAL:O	1:C:919:ASN:ND2	2.46	0.47
1:A:852:ALA:O	1:A:856:ASN:ND2	2.47	0.47
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.48	0.47
1:A:156:GLU:OE2	1:A:246:ARG:NH1	2.48	0.47
1:A:1074:ASN:OD1	1:C:895:GLN:NE2	2.48	0.46
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.46	0.46
1:A:57:PRO:O	1:A:60:SER:OG	2.22	0.46
1:A:763:LEU:HD21	1:A:1005:GLN:CG	2.47	0.45
1:A:410:ILE:HD11	1:A:418:ILE:HG21	1.97	0.45
1:B:874:THR:O	1:B:878:LEU:HD23	2.17	0.45
1:A:293:LEU:O	1:A:632:THR:OG1	2.18	0.45
1:A:916:LEU:O	1:A:920:GLN:N	2.49	0.45
1:C:193:VAL:HG13	1:C:270:LEU:HD11	1.99	0.45
1:A:193:VAL:HG13	1:A:270:LEU:HD11	2.00	0.44
1:A:874:THR:O	1:A:878:LEU:HD23	2.16	0.44
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.46	0.44
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.50	0.44
1:A:65:PHE:CZ	1:A:84:LEU:HD21	2.54	0.43
1:C:874:THR:O	1:C:878:LEU:HD23	2.18	0.43
1:A:644:GLN:NE2	1:A:648:GLY:O	2.51	0.43
1:A:124:THR:OG1	3:A:1302:NAG:O5	2.36	0.43
1:C:721:SER:OG	1:C:1066:THR:OG1	2.36	0.43
1:A:140:PHE:CD2	1:A:244:LEU:HD12	2.54	0.43
1:A:763:LEU:HD21	1:A:1005:GLN:HG2	2.00	0.43
1:B:152:TRP:NE1	1:B:180:GLU:OE2	2.52	0.43
1:C:121:ASN:ND2	5:C:1214:BLA:OB	2.51	0.43
1:B:666:ILE:HD11	1:B:672:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:CYS:O	1:A:338:PHE:N	2.52	0.42
1:A:576:VAL:HG12	1:A:587:ILE:HD11	2.01	0.42
1:A:666:ILE:HD11	1:A:672:ALA:HB2	2.01	0.42
1:B:808:ASP:N	1:B:808:ASP:OD1	2.49	0.42
1:A:310:LYS:HG3	1:A:664:ILE:HD11	2.00	0.42
1:B:1077:THR:OG1	1:B:1095:PHE:O	2.22	0.42
1:A:319:ARG:NE	1:A:624:ILE:HD11	2.32	0.42
1:A:118:LEU:HD11	1:A:159:VAL:HG11	2.02	0.42
1:A:992:GLN:OE1	1:A:995:ARG:NH2	2.52	0.42
1:A:962:LEU:HD13	1:A:1007:TYR:HB2	2.02	0.41
1:C:393:THR:OG1	1:C:394:ASN:N	2.54	0.41
1:A:128:ILE:HD12	1:A:170:TYR:CD2	2.54	0.41
1:A:226:LEU:HD21	5:A:1314:BLA:HMB2	2.01	0.41
1:A:1104:VAL:HG23	1:A:1115:ILE:HD13	2.03	0.41
1:B:149:ASN:OD1	1:B:149:ASN:N	2.53	0.41
1:B:962:LEU:HD13	1:B:1007:TYR:HB2	2.01	0.41
1:C:501:ASN:O	1:C:506:GLN:NE2	2.51	0.41
1:A:105:ILE:CD1	1:A:241:LEU:HD21	2.50	0.41
1:C:560:LEU:O	1:C:577:ARG:NH2	2.53	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:B:214:ARG:O	1:B:266:TYR:OH	2.39	0.41
1:C:294:ASP:OD1	1:C:294:ASP:N	2.53	0.41
1:C:581:THR:O	1:C:583:GLU:N	2.54	0.40
1:A:296:LEU:O	1:A:299:THR:OG1	2.32	0.40
1:B:675:GLN:HG3	1:B:693:ILE:HD11	2.03	0.40
3:A:1302:NAG:O7	3:A:1302:NAG:O3	2.31	0.40
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.04	0.40
1:B:226:LEU:HD21	5:B:1215:BLA:HMB2	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 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	1104/1128 (98%)	1060 (96%)	44 (4%)	0	100	100
1	B	1089/1128 (96%)	1061 (97%)	28 (3%)	0	100	100
1	C	1083/1128 (96%)	1053 (97%)	30 (3%)	0	100	100
All	All	3276/3384 (97%)	3174 (97%)	102 (3%)	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	965/979 (99%)	960 (100%)	5 (0%)	86	96
1	B	954/979 (97%)	953 (100%)	1 (0%)	92	98
1	C	952/979 (97%)	951 (100%)	1 (0%)	92	98
All	All	2871/2937 (98%)	2864 (100%)	7 (0%)	91	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	80	ASP
1	A	153	MET
1	A	154	GLU
1	A	986	LYS
1	B	149	ASN
1	C	935	GLN

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

Mol	Chain	Res	Type
1	A	69	HIS
1	A	146	HIS
1	A	787	GLN

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 ⓘ

28 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	D	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	1.09	1 (5%)
2	NAG	D	2	2	14,14,15	2.14	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	E	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	0.95	1 (5%)
2	NAG	E	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.98	1 (5%)
2	NAG	F	1	1,2	14,14,15	2.18	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	F	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.08	1 (5%)
2	NAG	G	1	1,2	14,14,15	2.13	4 (28%)	17,19,21	1.09	1 (5%)
2	NAG	G	2	2	14,14,15	2.19	4 (28%)	17,19,21	1.11	1 (5%)
2	NAG	H	1	1,2	14,14,15	2.15	4 (28%)	17,19,21	0.96	1 (5%)
2	NAG	H	2	2	14,14,15	2.18	4 (28%)	17,19,21	0.93	1 (5%)
2	NAG	I	1	1,2	14,14,15	2.22	4 (28%)	17,19,21	1.12	1 (5%)
2	NAG	I	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.18	1 (5%)
2	NAG	J	1	1,2	14,14,15	2.20	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	J	2	2	14,14,15	2.18	4 (28%)	17,19,21	1.01	1 (5%)
2	NAG	K	1	1,2	14,14,15	2.14	4 (28%)	17,19,21	1.00	1 (5%)
2	NAG	K	2	2	14,14,15	2.16	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	L	1	1,2	14,14,15	2.16	4 (28%)	17,19,21	1.05	1 (5%)
2	NAG	L	2	2	14,14,15	2.23	4 (28%)	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	M	1	1,2	14,14,15	2.15	4 (28%)	17,19,21	0.97	1 (5%)
2	NAG	M	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.97	1 (5%)
2	NAG	N	1	1,2	14,14,15	2.20	4 (28%)	17,19,21	1.11	1 (5%)
2	NAG	N	2	2	14,14,15	2.14	4 (28%)	17,19,21	1.08	1 (5%)
2	NAG	O	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	0.94	1 (5%)
2	NAG	O	2	2	14,14,15	2.18	4 (28%)	17,19,21	0.97	1 (5%)
2	NAG	P	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	P	2	2	14,14,15	2.16	4 (28%)	17,19,21	1.04	1 (5%)
2	NAG	Q	1	1,2	14,14,15	2.15	4 (28%)	17,19,21	1.09	1 (5%)
2	NAG	Q	2	2	14,14,15	2.20	4 (28%)	17,19,21	1.31	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	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
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	5.59	1.52	1.43
2	N	1	NAG	O5-C1	5.53	1.52	1.43
2	F	1	NAG	O5-C1	5.50	1.52	1.43
2	G	2	NAG	O5-C1	5.39	1.52	1.43
2	J	1	NAG	O5-C1	5.37	1.52	1.43
2	L	2	NAG	O5-C1	5.37	1.52	1.43
2	J	2	NAG	O5-C1	5.36	1.52	1.43
2	Q	1	NAG	O5-C1	5.28	1.52	1.43
2	L	1	NAG	O5-C1	5.27	1.52	1.43
2	F	2	NAG	O5-C1	5.27	1.52	1.43
2	H	2	NAG	O5-C1	5.27	1.52	1.43
2	K	2	NAG	O5-C1	5.27	1.52	1.43
2	M	1	NAG	O5-C1	5.27	1.52	1.43
2	Q	2	NAG	O5-C1	5.27	1.52	1.43
2	O	1	NAG	O5-C1	5.25	1.52	1.43
2	H	1	NAG	O5-C1	5.25	1.52	1.43
2	P	2	NAG	O5-C1	5.25	1.52	1.43
2	M	2	NAG	O5-C1	5.23	1.52	1.43
2	O	2	NAG	O5-C1	5.23	1.52	1.43
2	E	2	NAG	O5-C1	5.21	1.52	1.43
2	I	2	NAG	O5-C1	5.20	1.52	1.43
2	N	2	NAG	O5-C1	5.16	1.52	1.43
2	G	1	NAG	O5-C1	5.15	1.51	1.43
2	D	2	NAG	O5-C1	5.14	1.51	1.43
2	E	1	NAG	O5-C1	5.14	1.51	1.43
2	K	1	NAG	O5-C1	5.09	1.51	1.43
2	D	1	NAG	O5-C1	5.08	1.51	1.43
2	P	1	NAG	O5-C1	4.92	1.51	1.43
2	L	2	NAG	C7-N2	4.11	1.48	1.34
2	Q	2	NAG	C7-N2	4.06	1.48	1.34
2	O	1	NAG	C7-N2	4.00	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	NAG	C7-N2	3.99	1.48	1.34
2	M	2	NAG	C7-N2	3.99	1.48	1.34
2	J	1	NAG	C7-N2	3.98	1.48	1.34
2	H	2	NAG	C7-N2	3.97	1.48	1.34
2	E	2	NAG	C7-N2	3.97	1.48	1.34
2	P	2	NAG	C7-N2	3.96	1.48	1.34
2	G	2	NAG	C7-N2	3.95	1.47	1.34
2	K	1	NAG	C7-N2	3.95	1.47	1.34
2	H	1	NAG	C7-N2	3.94	1.47	1.34
2	J	2	NAG	C7-N2	3.94	1.47	1.34
2	I	2	NAG	C7-N2	3.94	1.47	1.34
2	F	2	NAG	C7-N2	3.94	1.47	1.34
2	N	2	NAG	C7-N2	3.94	1.47	1.34
2	P	1	NAG	C7-N2	3.93	1.47	1.34
2	K	2	NAG	C7-N2	3.93	1.47	1.34
2	D	1	NAG	C7-N2	3.92	1.47	1.34
2	D	2	NAG	C7-N2	3.92	1.47	1.34
2	L	1	NAG	C7-N2	3.92	1.47	1.34
2	G	1	NAG	C7-N2	3.91	1.47	1.34
2	E	1	NAG	C7-N2	3.91	1.47	1.34
2	Q	1	NAG	C7-N2	3.91	1.47	1.34
2	M	1	NAG	C7-N2	3.91	1.47	1.34
2	F	1	NAG	C7-N2	3.90	1.47	1.34
2	N	1	NAG	C7-N2	3.90	1.47	1.34
2	I	1	NAG	C7-N2	3.88	1.47	1.34
2	Q	2	NAG	C2-N2	3.29	1.51	1.46
2	L	2	NAG	C2-N2	3.26	1.51	1.46
2	M	2	NAG	C2-N2	3.21	1.51	1.46
2	O	2	NAG	C2-N2	3.20	1.51	1.46
2	H	2	NAG	C2-N2	3.19	1.51	1.46
2	K	1	NAG	C2-N2	3.17	1.51	1.46
2	E	2	NAG	C2-N2	3.16	1.51	1.46
2	J	1	NAG	C2-N2	3.15	1.51	1.46
2	G	2	NAG	C2-N2	3.14	1.51	1.46
2	G	1	NAG	C2-N2	3.12	1.51	1.46
2	D	1	NAG	C2-N2	3.11	1.51	1.46
2	O	1	NAG	C2-N2	3.11	1.51	1.46
2	Q	1	NAG	C2-N2	3.10	1.51	1.46
2	E	1	NAG	C2-N2	3.10	1.51	1.46
2	P	1	NAG	C2-N2	3.10	1.51	1.46
2	P	2	NAG	C2-N2	3.10	1.51	1.46
2	I	2	NAG	C2-N2	3.08	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	NAG	C2-N2	3.08	1.51	1.46
2	M	1	NAG	C2-N2	3.06	1.51	1.46
2	K	2	NAG	C2-N2	3.06	1.51	1.46
2	D	2	NAG	C2-N2	3.06	1.51	1.46
2	L	1	NAG	C2-N2	3.06	1.51	1.46
2	F	2	NAG	C2-N2	3.05	1.51	1.46
2	N	2	NAG	C2-N2	3.05	1.51	1.46
2	H	1	NAG	C2-N2	3.03	1.51	1.46
2	N	1	NAG	C2-N2	3.02	1.51	1.46
2	F	1	NAG	C2-N2	3.02	1.51	1.46
2	I	1	NAG	C2-N2	3.02	1.51	1.46
2	P	1	NAG	O7-C7	-2.19	1.18	1.23
2	D	1	NAG	O7-C7	-2.17	1.18	1.23
2	K	1	NAG	O7-C7	-2.17	1.18	1.23
2	E	2	NAG	O7-C7	-2.17	1.18	1.23
2	F	1	NAG	O7-C7	-2.16	1.18	1.23
2	L	2	NAG	O7-C7	-2.15	1.18	1.23
2	N	1	NAG	O7-C7	-2.14	1.18	1.23
2	I	1	NAG	O7-C7	-2.14	1.18	1.23
2	H	1	NAG	O7-C7	-2.14	1.18	1.23
2	J	1	NAG	O7-C7	-2.14	1.18	1.23
2	H	2	NAG	O7-C7	-2.14	1.18	1.23
2	D	2	NAG	O7-C7	-2.13	1.18	1.23
2	M	1	NAG	O7-C7	-2.13	1.18	1.23
2	G	1	NAG	O7-C7	-2.13	1.18	1.23
2	E	1	NAG	O7-C7	-2.13	1.18	1.23
2	O	2	NAG	O7-C7	-2.13	1.18	1.23
2	J	2	NAG	O7-C7	-2.13	1.18	1.23
2	I	2	NAG	O7-C7	-2.12	1.18	1.23
2	N	2	NAG	O7-C7	-2.12	1.18	1.23
2	G	2	NAG	O7-C7	-2.12	1.18	1.23
2	L	1	NAG	O7-C7	-2.12	1.18	1.23
2	O	1	NAG	O7-C7	-2.12	1.18	1.23
2	Q	1	NAG	O7-C7	-2.11	1.18	1.23
2	K	2	NAG	O7-C7	-2.11	1.18	1.23
2	F	2	NAG	O7-C7	-2.11	1.18	1.23
2	M	2	NAG	O7-C7	-2.11	1.18	1.23
2	Q	2	NAG	O7-C7	-2.09	1.18	1.23
2	P	2	NAG	O7-C7	-2.08	1.18	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	NAG	C8-C7-N2	3.89	122.69	116.10
2	Q	2	NAG	C8-C7-N2	3.79	122.52	116.10
2	K	2	NAG	C8-C7-N2	2.32	120.03	116.10
2	F	1	NAG	C8-C7-N2	2.31	120.01	116.10
2	N	1	NAG	C8-C7-N2	2.27	119.95	116.10
2	G	1	NAG	C8-C7-N2	2.26	119.92	116.10
2	P	2	NAG	C8-C7-N2	2.25	119.92	116.10
2	F	2	NAG	C8-C7-N2	2.24	119.89	116.10
2	N	2	NAG	C8-C7-N2	2.24	119.89	116.10
2	M	1	NAG	C8-C7-N2	2.22	119.86	116.10
2	G	2	NAG	C8-C7-N2	2.22	119.85	116.10
2	Q	1	NAG	C8-C7-N2	2.21	119.84	116.10
2	I	2	NAG	C8-C7-N2	2.19	119.81	116.10
2	I	1	NAG	C8-C7-N2	2.18	119.78	116.10
2	D	2	NAG	C8-C7-N2	2.17	119.78	116.10
2	J	2	NAG	C8-C7-N2	2.17	119.78	116.10
2	H	1	NAG	C8-C7-N2	2.17	119.78	116.10
2	L	1	NAG	C8-C7-N2	2.12	119.68	116.10
2	O	1	NAG	C8-C7-N2	2.10	119.65	116.10
2	H	2	NAG	C8-C7-N2	2.09	119.64	116.10
2	E	2	NAG	C8-C7-N2	2.09	119.63	116.10
2	E	1	NAG	C8-C7-N2	2.08	119.62	116.10
2	M	2	NAG	C8-C7-N2	2.08	119.62	116.10
2	D	1	NAG	C8-C7-N2	2.08	119.62	116.10
2	O	2	NAG	C8-C7-N2	2.06	119.58	116.10
2	K	1	NAG	C8-C7-N2	2.05	119.57	116.10
2	J	1	NAG	C8-C7-N2	2.03	119.53	116.10
2	P	1	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6

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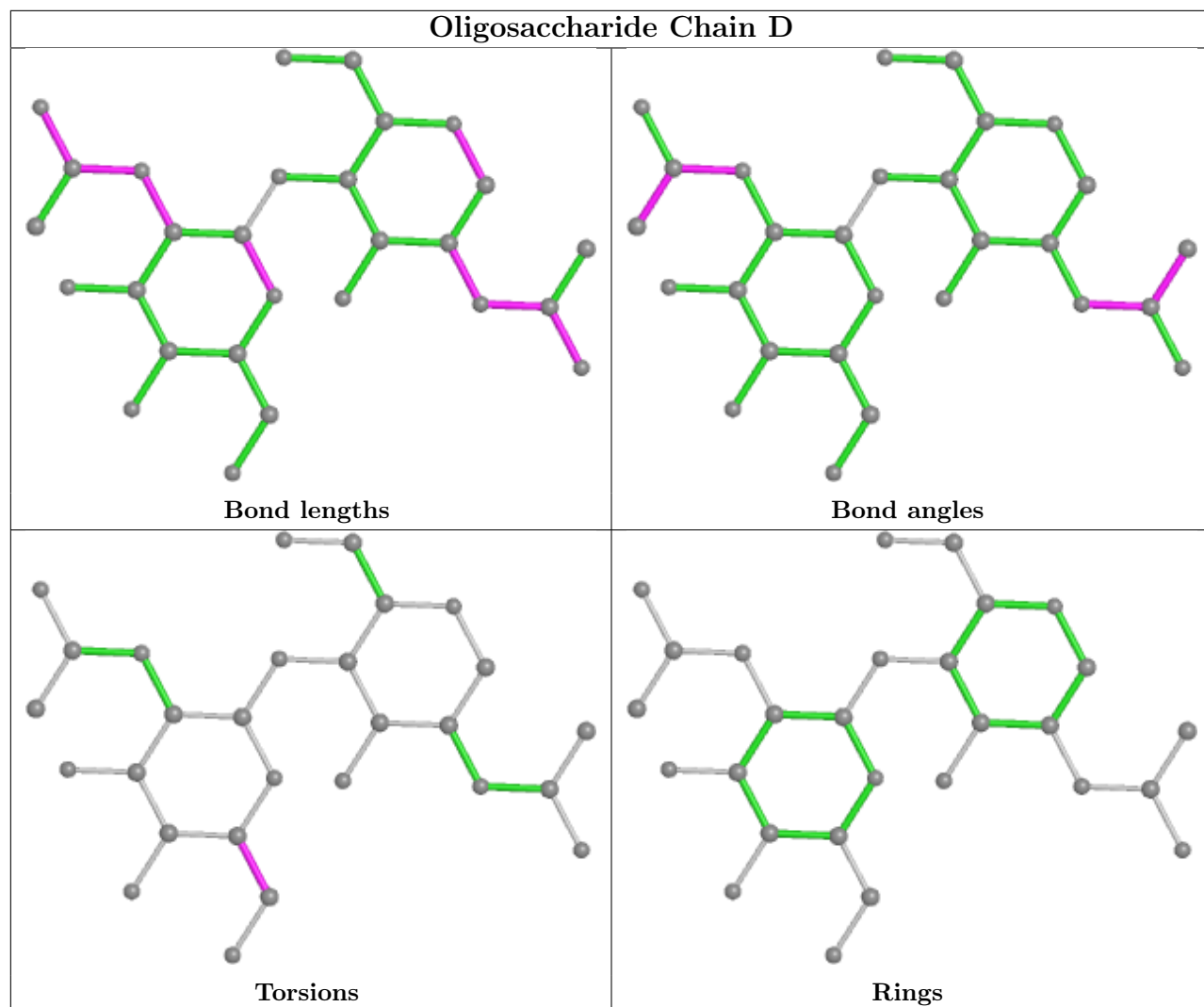
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6

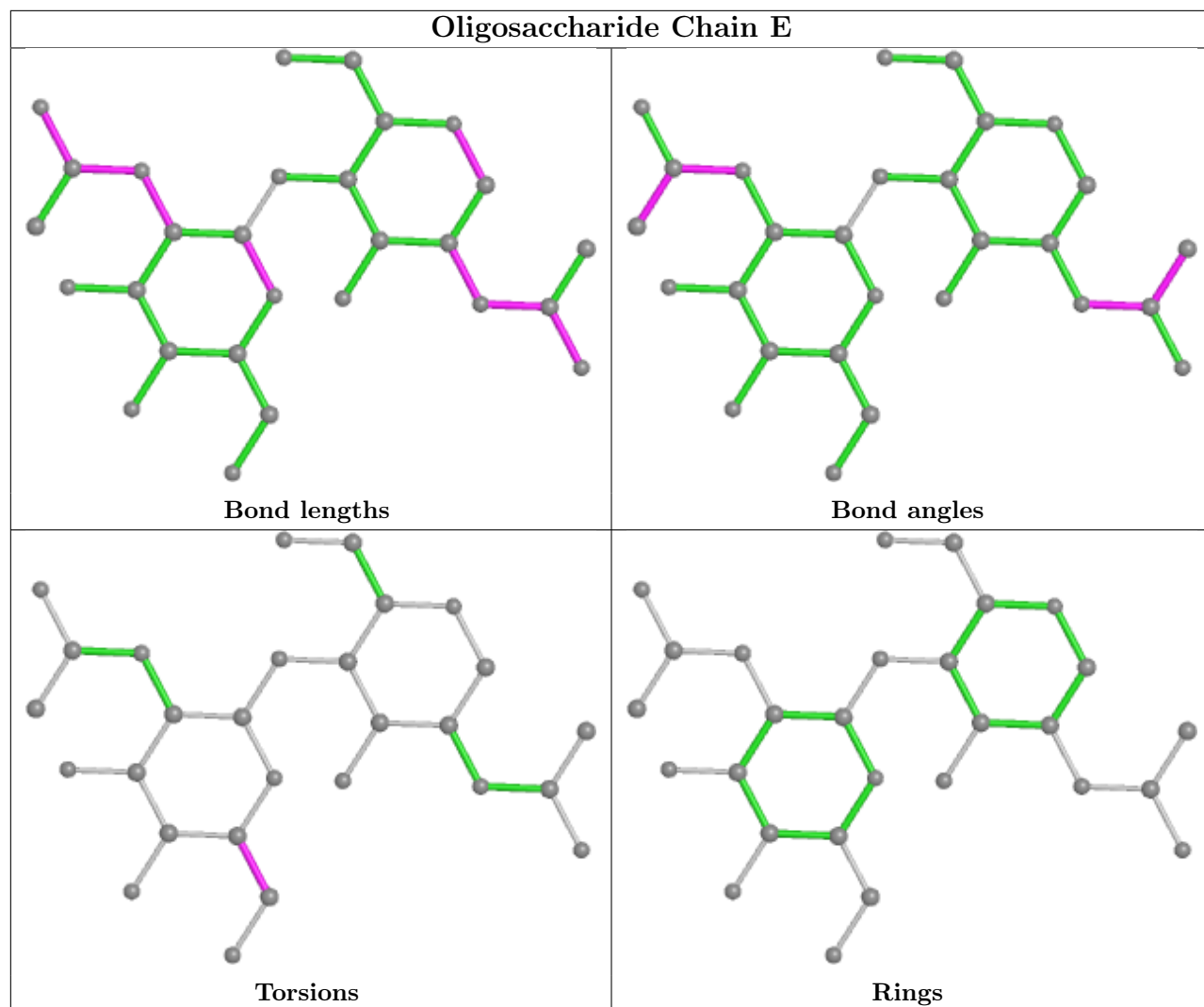
There are no ring outliers.

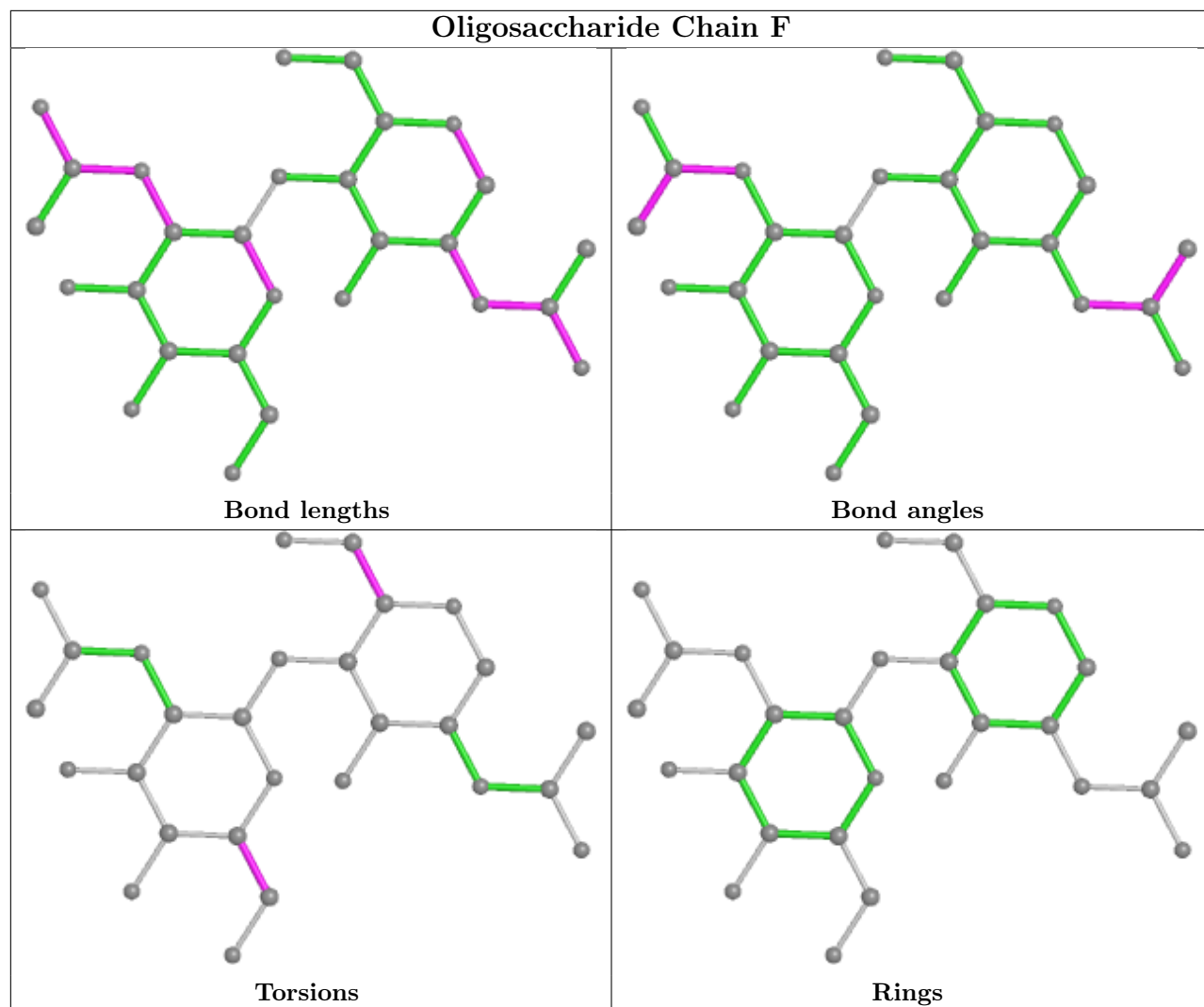
1 monomer is involved in 1 short contact:

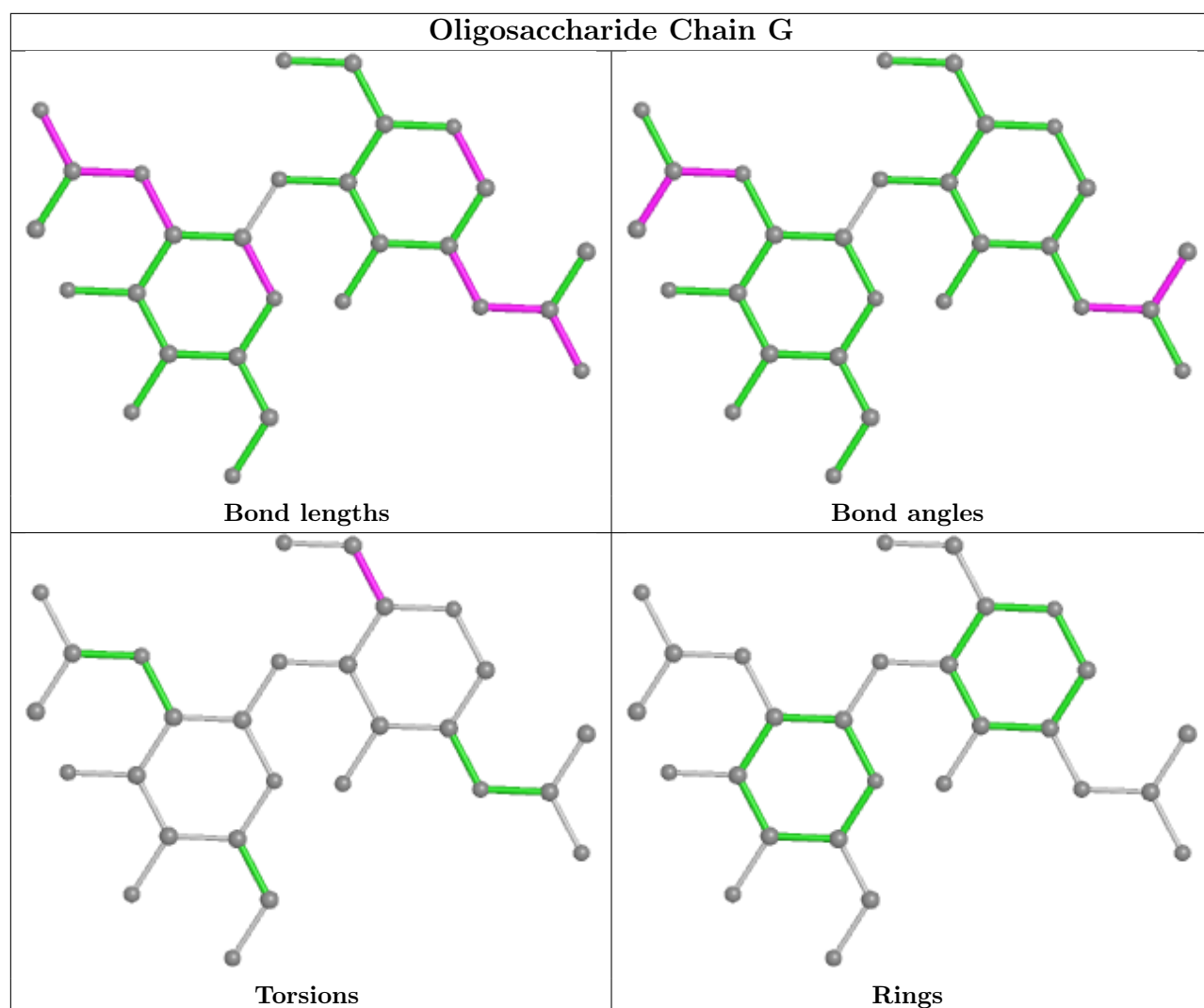
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	1	0

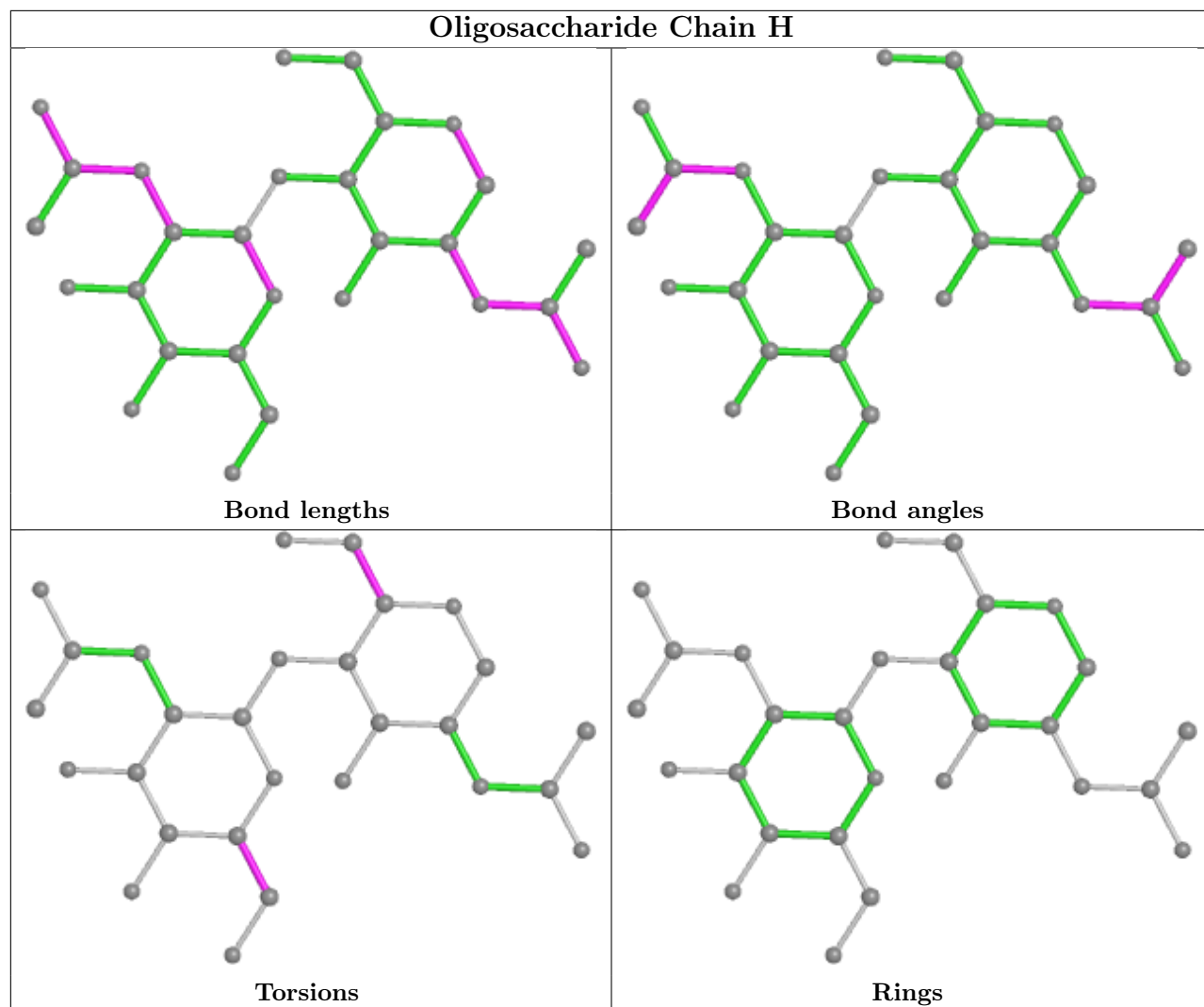
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

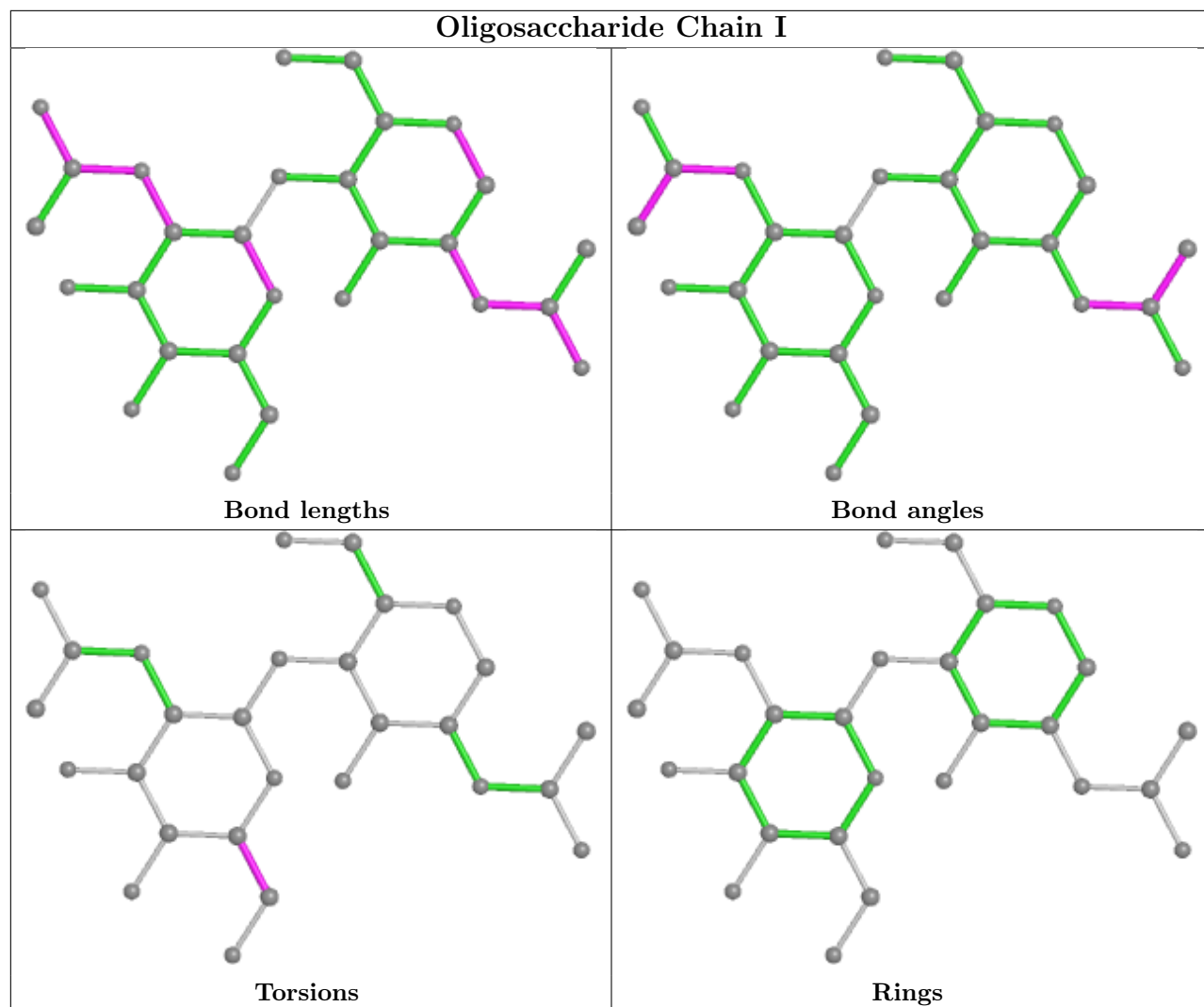


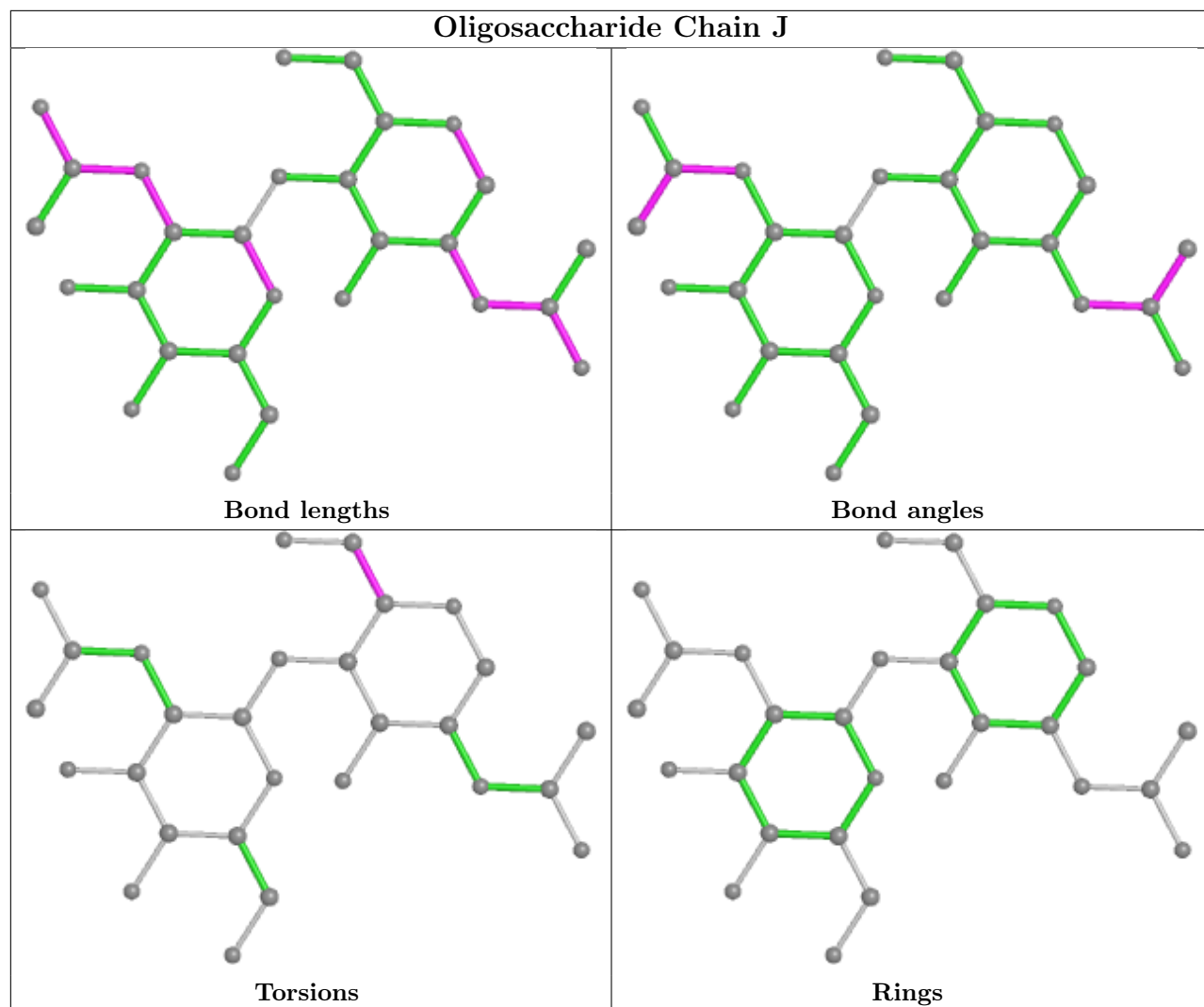


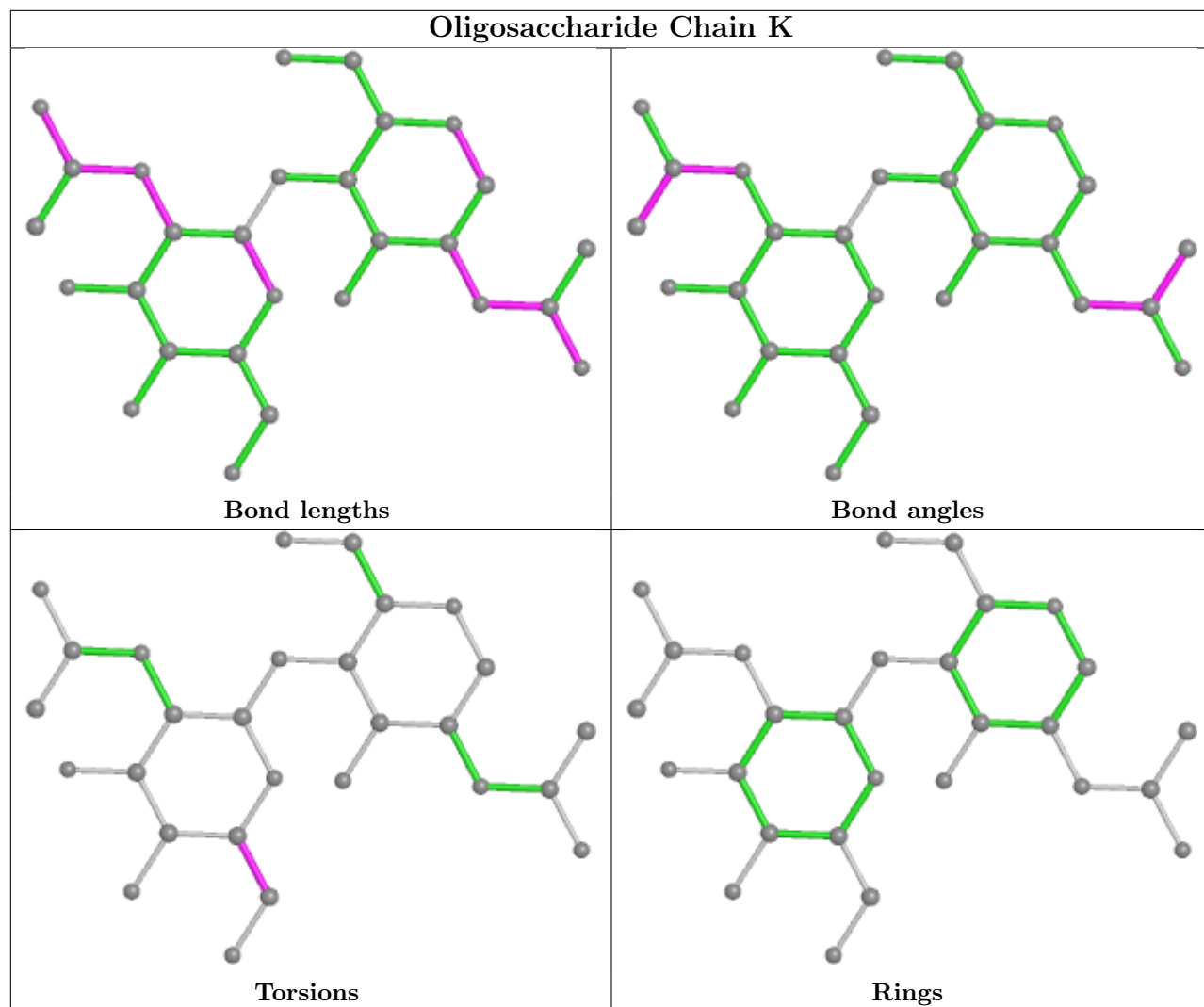


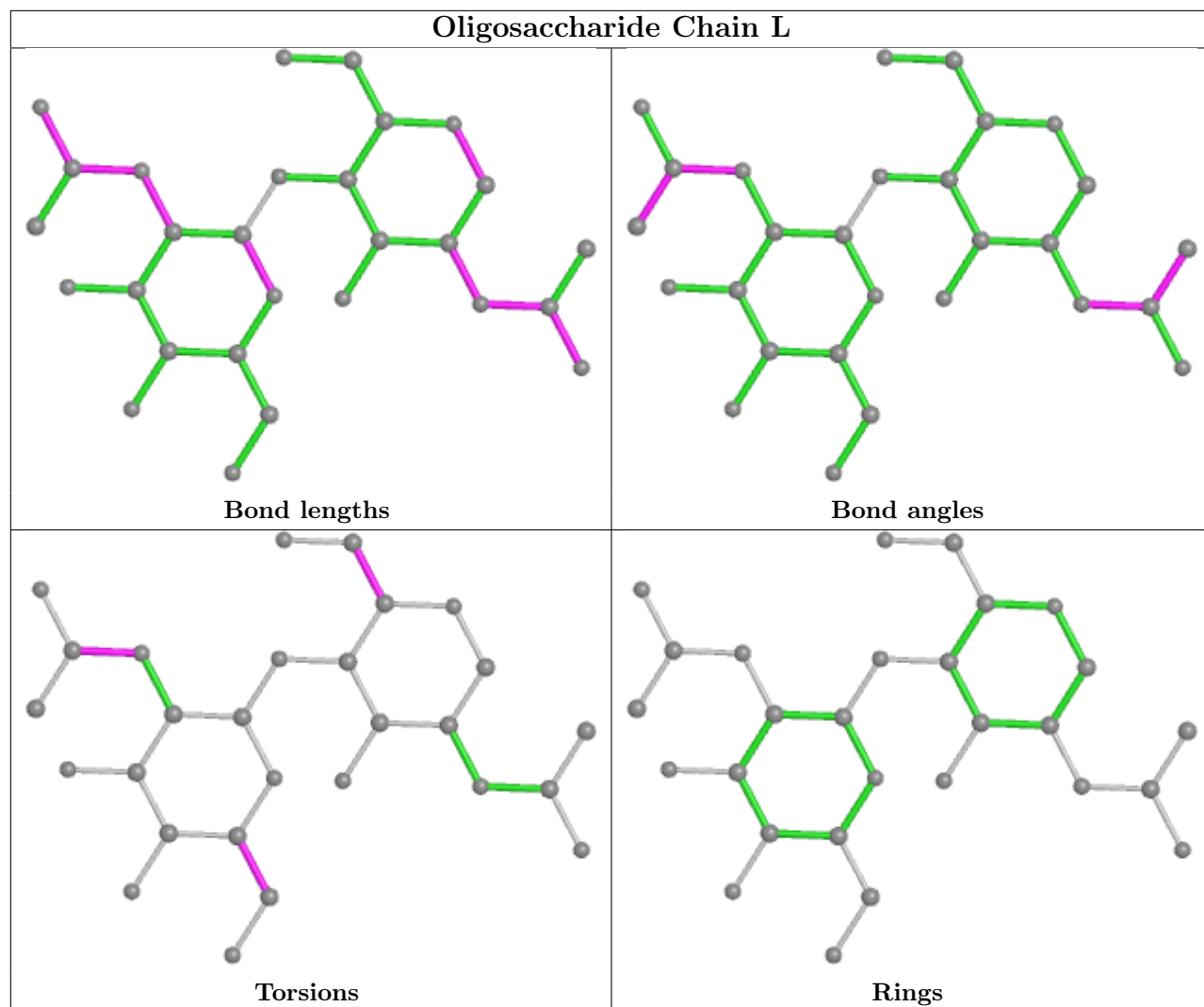


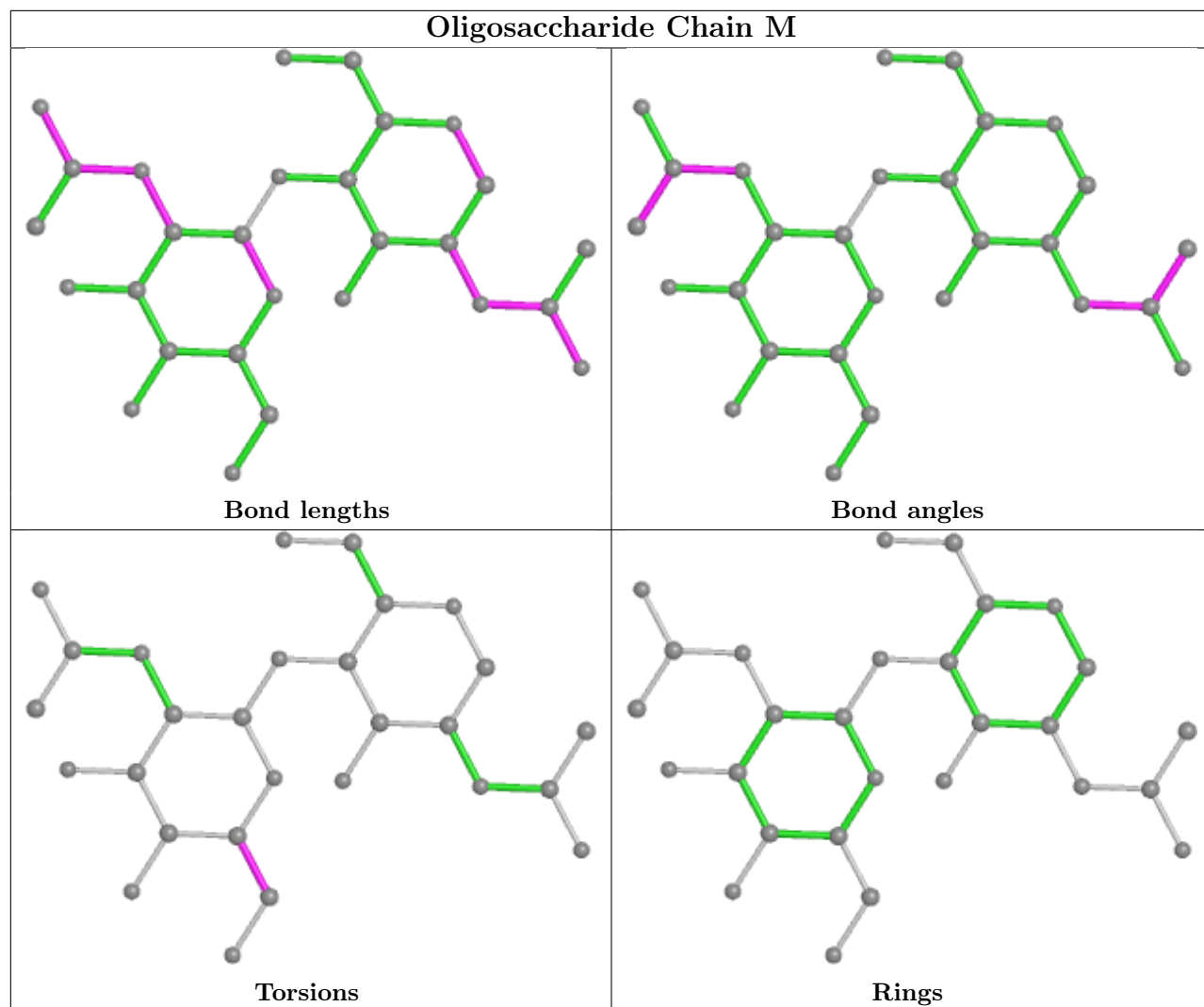


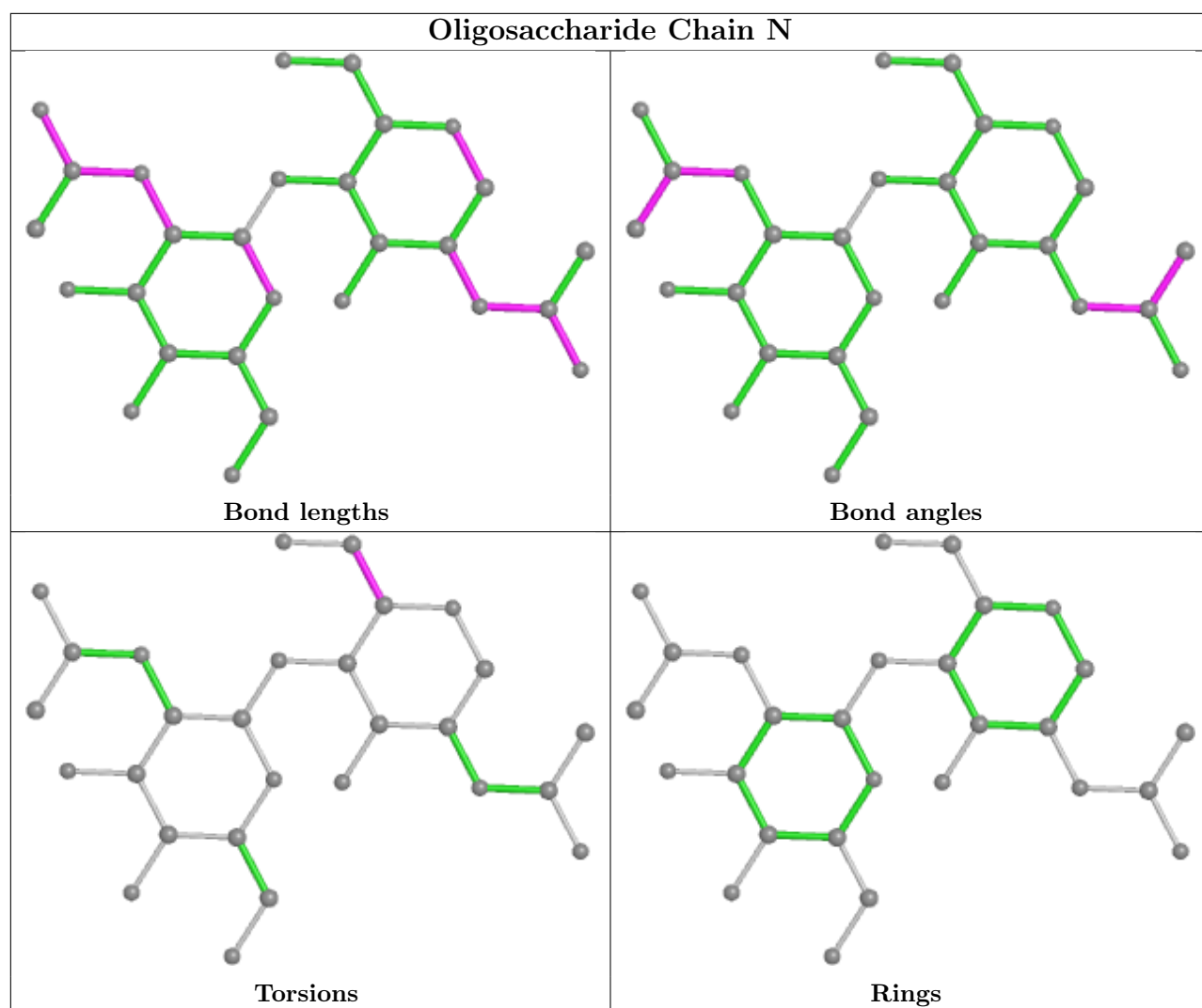


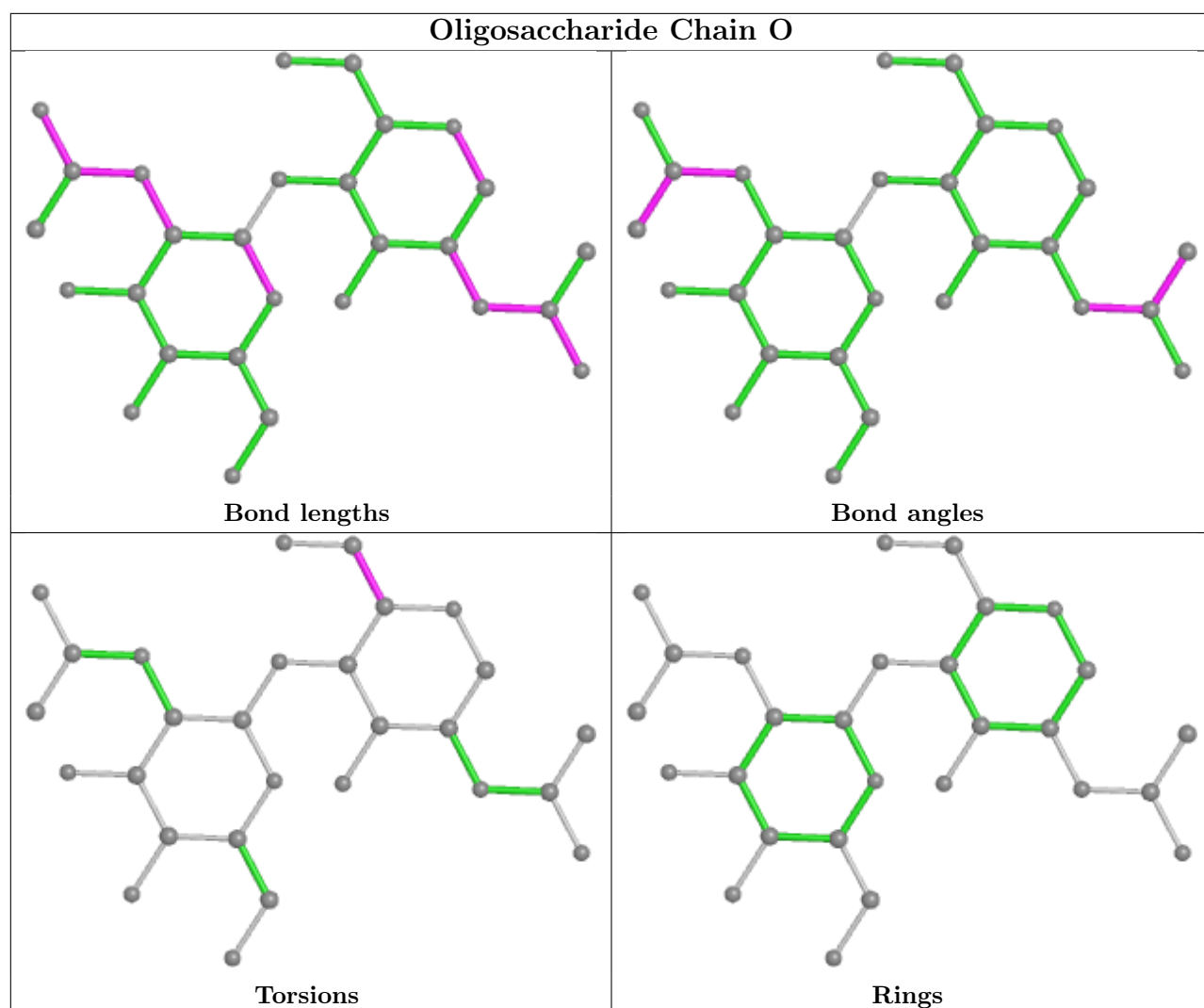


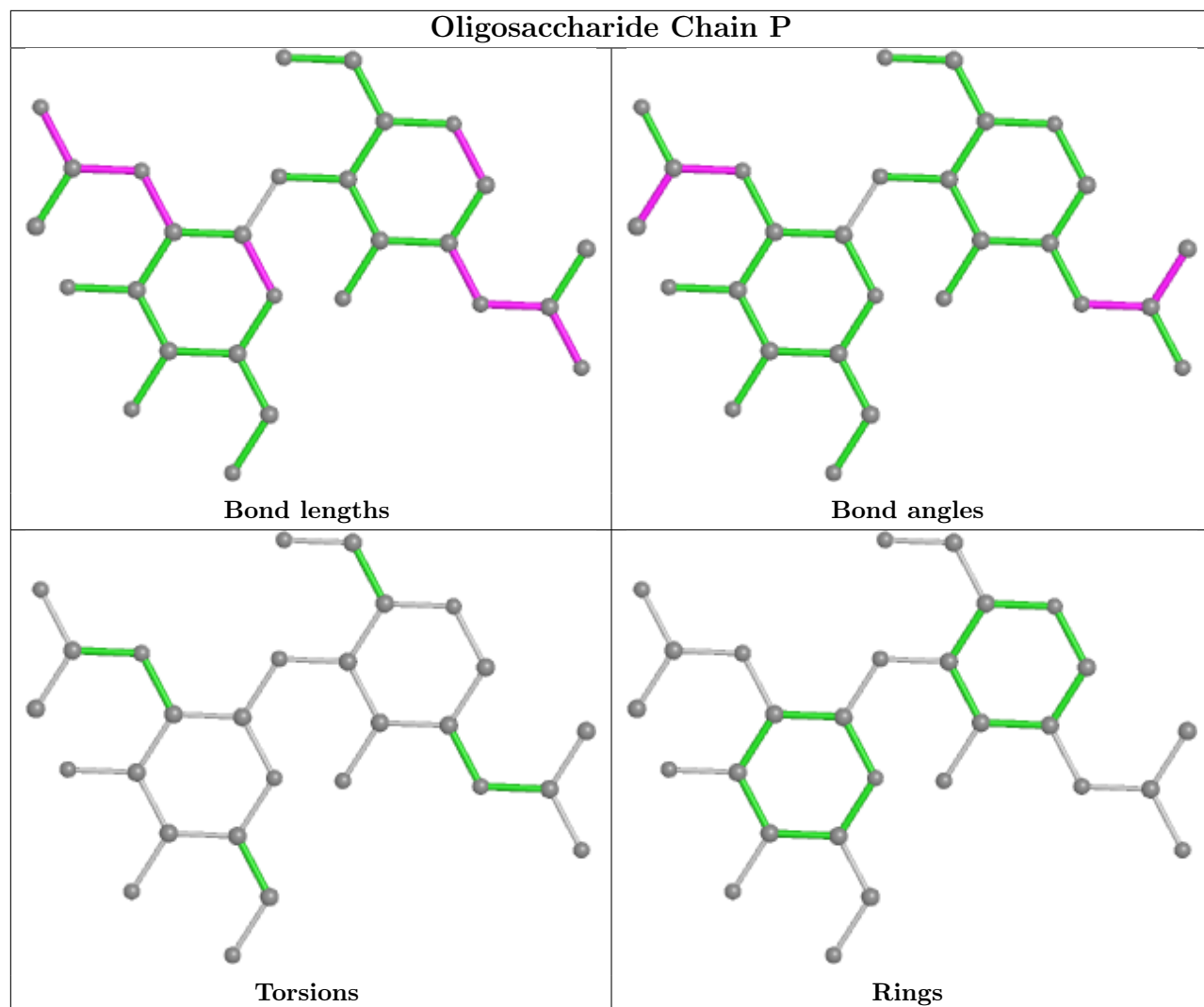


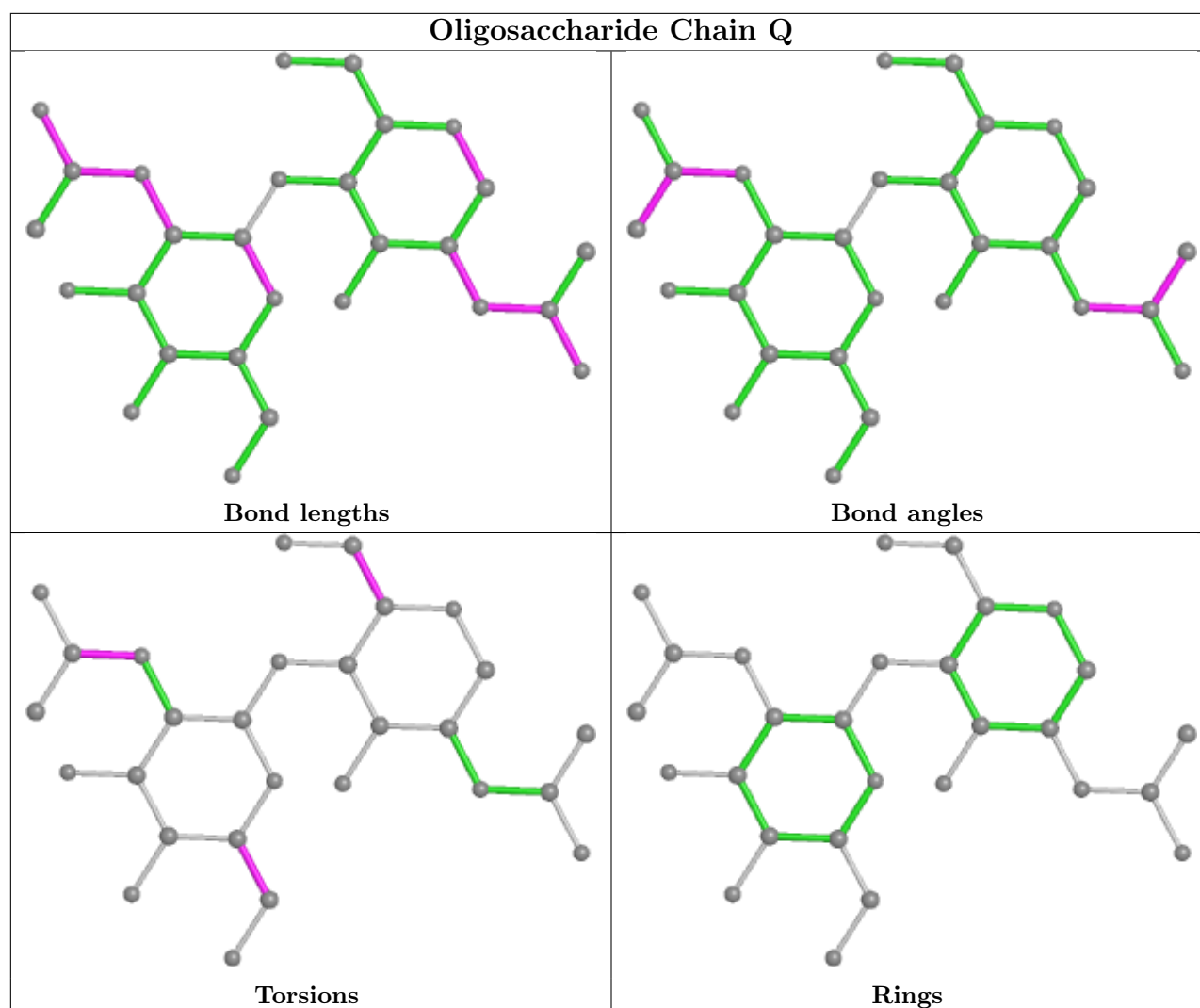












5.6 Ligand geometry [i](#)

44 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	$\# Z > 2$
3	NAG	B	1201	1	14,14,15	2.20	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	C	1212	1	14,14,15	2.19	4 (28%)	17,19,21	0.98	1 (5%)
3	NAG	C	1208	1	14,14,15	2.16	4 (28%)	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1306	1	14,14,15	2.16	4 (28%)	17,19,21	0.89	0
3	NAG	A	1310	1	14,14,15	2.15	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	C	1213	1	14,14,15	2.15	4 (28%)	17,19,21	1.04	2 (11%)
5	BLA	B	1215	-	42,46,46	3.57	20 (47%)	53,67,67	1.90	9 (16%)
5	BLA	C	1214	-	42,46,46	3.59	21 (50%)	53,67,67	1.96	10 (18%)
3	NAG	B	1206	1	14,14,15	2.17	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	B	1212	1	14,14,15	2.15	4 (28%)	17,19,21	1.05	1 (5%)
3	NAG	B	1203	1	14,14,15	2.13	4 (28%)	17,19,21	1.15	1 (5%)
5	BLA	A	1314	-	42,46,46	3.59	20 (47%)	53,67,67	1.95	10 (18%)
3	NAG	C	1209	1	14,14,15	2.16	4 (28%)	17,19,21	0.92	1 (5%)
3	NAG	C	1201	1	14,14,15	2.22	4 (28%)	17,19,21	1.08	1 (5%)
3	NAG	B	1202	1	14,14,15	2.15	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	A	1309	1	14,14,15	2.16	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	C	1202	1	14,14,15	2.13	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	B	1204	1	14,14,15	2.14	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	C	1210	1	14,14,15	2.18	4 (28%)	17,19,21	0.99	1 (5%)
3	NAG	C	1211	1	14,14,15	2.15	4 (28%)	17,19,21	1.10	1 (5%)
3	NAG	B	1214	1	14,14,15	2.16	4 (28%)	17,19,21	1.11	1 (5%)
3	NAG	C	1206	1	14,14,15	2.19	4 (28%)	17,19,21	0.90	1 (5%)
3	NAG	A	1308	1	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
3	NAG	C	1203	1	14,14,15	2.13	4 (28%)	17,19,21	1.05	1 (5%)
3	NAG	A	1304	1	14,14,15	2.16	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	B	1205	1	14,14,15	2.16	4 (28%)	17,19,21	0.92	0
4	EIC	A	1313	-	19,19,19	0.88	0	19,19,19	1.30	1 (5%)
3	NAG	A	1311	1	14,14,15	2.17	4 (28%)	17,19,21	0.95	1 (5%)
3	NAG	B	1210	1	14,14,15	2.19	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	A	1303	1	14,14,15	2.20	4 (28%)	17,19,21	0.94	0
3	NAG	C	1204	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	B	1208	1	14,14,15	2.15	4 (28%)	17,19,21	1.08	1 (5%)
4	EIC	B	1211	-	19,19,19	0.92	0	19,19,19	1.08	1 (5%)
3	NAG	A	1312	1	14,14,15	2.18	4 (28%)	17,19,21	1.06	1 (5%)
3	NAG	A	1307	1	14,14,15	2.16	4 (28%)	17,19,21	0.97	0
3	NAG	B	1209	1	14,14,15	2.15	4 (28%)	17,19,21	1.05	1 (5%)
3	NAG	B	1213	1	14,14,15	2.13	4 (28%)	17,19,21	1.08	1 (5%)
3	NAG	A	1301	1	14,14,15	2.15	4 (28%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1302	1	14,14,15	2.14	4 (28%)	17,19,21	1.35	2 (11%)
3	NAG	B	1207	1	14,14,15	2.16	4 (28%)	17,19,21	1.05	1 (5%)
3	NAG	A	1305	1	14,14,15	2.15	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	C	1207	1	14,14,15	2.17	4 (28%)	17,19,21	1.01	1 (5%)
4	EIC	A	1315	-	19,19,19	0.90	0	19,19,19	1.23	2 (10%)
3	NAG	C	1205	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	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
3	NAG	B	1201	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1212	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1213	1	-	2/6/23/26	0/1/1/1
5	BLA	B	1215	-	-	14/26/74/74	0/4/4/4
5	BLA	C	1214	-	-	14/26/74/74	0/4/4/4
3	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1212	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1203	1	-	3/6/23/26	0/1/1/1
5	BLA	A	1314	-	-	12/26/74/74	0/4/4/4
3	NAG	C	1209	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1201	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1202	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1202	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1210	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1211	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1214	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1203	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1205	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1313	-	-	7/17/17/17	-
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1210	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
4	EIC	B	1211	-	-	7/17/17/17	-
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1213	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1207	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1207	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1315	-	-	9/17/17/17	-
3	NAG	C	1205	1	-	2/6/23/26	0/1/1/1

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1214	BLA	C4C-NC	9.79	1.54	1.37
5	C	1214	BLA	C1B-NB	9.76	1.54	1.37
5	A	1314	BLA	C4C-NC	9.75	1.54	1.37
5	B	1215	BLA	C1B-NB	9.72	1.54	1.37
5	A	1314	BLA	C1B-NB	9.70	1.54	1.37
5	B	1215	BLA	C4C-NC	9.62	1.53	1.37
5	C	1214	BLA	C4B-NB	7.51	1.53	1.38
5	A	1314	BLA	C4B-NB	7.49	1.53	1.38
5	A	1314	BLA	C1C-NC	7.36	1.53	1.38
5	B	1215	BLA	C4B-NB	7.30	1.53	1.38
5	B	1215	BLA	C1C-NC	7.30	1.53	1.38
5	C	1214	BLA	C1C-NC	7.23	1.53	1.38
5	C	1214	BLA	C4D-ND	5.70	1.50	1.38
5	A	1314	BLA	C4D-ND	5.67	1.50	1.38
5	B	1215	BLA	C4D-ND	5.64	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1201	NAG	O5-C1	5.59	1.52	1.43
3	B	1201	NAG	O5-C1	5.54	1.52	1.43
5	A	1314	BLA	C3D-C2D	5.50	1.48	1.36
3	C	1206	NAG	O5-C1	5.43	1.52	1.43
5	B	1215	BLA	CHD-C1D	5.42	1.53	1.40
5	C	1214	BLA	C3D-C2D	5.42	1.48	1.36
3	A	1312	NAG	O5-C1	5.42	1.52	1.43
5	A	1314	BLA	CHD-C1D	5.41	1.53	1.40
5	C	1214	BLA	CHD-C1D	5.41	1.53	1.40
5	B	1215	BLA	C3D-C2D	5.39	1.48	1.36
3	C	1207	NAG	O5-C1	5.36	1.52	1.43
3	A	1308	NAG	O5-C1	5.35	1.52	1.43
3	A	1311	NAG	O5-C1	5.34	1.52	1.43
3	B	1210	NAG	O5-C1	5.34	1.52	1.43
3	C	1212	NAG	O5-C1	5.33	1.52	1.43
3	B	1214	NAG	O5-C1	5.33	1.52	1.43
3	A	1303	NAG	O5-C1	5.32	1.52	1.43
3	B	1206	NAG	O5-C1	5.32	1.52	1.43
3	C	1204	NAG	O5-C1	5.31	1.52	1.43
3	A	1302	NAG	O5-C1	5.30	1.52	1.43
3	C	1210	NAG	O5-C1	5.30	1.52	1.43
3	C	1205	NAG	O5-C1	5.30	1.52	1.43
3	A	1304	NAG	O5-C1	5.28	1.52	1.43
3	B	1209	NAG	O5-C1	5.28	1.52	1.43
3	A	1306	NAG	O5-C1	5.28	1.52	1.43
3	C	1211	NAG	O5-C1	5.28	1.52	1.43
3	A	1307	NAG	O5-C1	5.27	1.52	1.43
3	A	1305	NAG	O5-C1	5.27	1.52	1.43
3	B	1202	NAG	O5-C1	5.27	1.52	1.43
3	C	1213	NAG	O5-C1	5.26	1.52	1.43
3	C	1209	NAG	O5-C1	5.26	1.52	1.43
3	B	1207	NAG	O5-C1	5.25	1.52	1.43
3	C	1208	NAG	O5-C1	5.25	1.52	1.43
3	B	1212	NAG	O5-C1	5.24	1.52	1.43
3	B	1205	NAG	O5-C1	5.24	1.52	1.43
3	B	1213	NAG	O5-C1	5.23	1.52	1.43
3	A	1310	NAG	O5-C1	5.21	1.52	1.43
3	A	1301	NAG	O5-C1	5.21	1.52	1.43
3	B	1204	NAG	O5-C1	5.20	1.52	1.43
3	C	1202	NAG	O5-C1	5.19	1.52	1.43
3	B	1203	NAG	O5-C1	5.18	1.52	1.43
3	A	1309	NAG	O5-C1	5.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1203	NAG	O5-C1	5.14	1.51	1.43
5	B	1215	BLA	C4D-C3D	5.14	1.53	1.45
3	B	1208	NAG	O5-C1	5.12	1.51	1.43
5	C	1214	BLA	C4D-C3D	5.11	1.53	1.45
5	A	1314	BLA	C4D-C3D	5.06	1.53	1.45
5	B	1215	BLA	C1D-ND	4.81	1.47	1.36
5	A	1314	BLA	C1D-ND	4.79	1.47	1.36
5	C	1214	BLA	C1D-ND	4.78	1.47	1.36
3	B	1208	NAG	C7-N2	4.00	1.48	1.34
3	A	1303	NAG	C7-N2	3.99	1.48	1.34
3	C	1210	NAG	C7-N2	3.99	1.48	1.34
3	A	1309	NAG	C7-N2	3.98	1.48	1.34
3	C	1209	NAG	C7-N2	3.97	1.48	1.34
3	A	1311	NAG	C7-N2	3.96	1.48	1.34
3	B	1205	NAG	C7-N2	3.96	1.48	1.34
3	C	1208	NAG	C7-N2	3.95	1.47	1.34
3	A	1302	NAG	C7-N2	3.95	1.47	1.34
3	A	1312	NAG	C7-N2	3.94	1.47	1.34
3	B	1212	NAG	C7-N2	3.94	1.47	1.34
3	C	1206	NAG	C7-N2	3.94	1.47	1.34
3	A	1307	NAG	C7-N2	3.94	1.47	1.34
3	B	1214	NAG	C7-N2	3.94	1.47	1.34
3	A	1301	NAG	C7-N2	3.94	1.47	1.34
3	C	1213	NAG	C7-N2	3.94	1.47	1.34
3	A	1310	NAG	C7-N2	3.93	1.47	1.34
3	C	1212	NAG	C7-N2	3.93	1.47	1.34
3	B	1202	NAG	C7-N2	3.93	1.47	1.34
3	A	1306	NAG	C7-N2	3.93	1.47	1.34
3	B	1204	NAG	C7-N2	3.93	1.47	1.34
3	B	1210	NAG	C7-N2	3.93	1.47	1.34
3	C	1204	NAG	C7-N2	3.93	1.47	1.34
3	A	1305	NAG	C7-N2	3.92	1.47	1.34
3	C	1203	NAG	C7-N2	3.92	1.47	1.34
3	A	1308	NAG	C7-N2	3.92	1.47	1.34
3	B	1203	NAG	C7-N2	3.92	1.47	1.34
3	C	1205	NAG	C7-N2	3.92	1.47	1.34
3	B	1206	NAG	C7-N2	3.91	1.47	1.34
3	C	1201	NAG	C7-N2	3.91	1.47	1.34
3	C	1211	NAG	C7-N2	3.91	1.47	1.34
3	B	1207	NAG	C7-N2	3.91	1.47	1.34
3	C	1202	NAG	C7-N2	3.91	1.47	1.34
3	C	1207	NAG	C7-N2	3.91	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	NAG	C7-N2	3.91	1.47	1.34
3	B	1209	NAG	C7-N2	3.90	1.47	1.34
3	B	1201	NAG	C7-N2	3.88	1.47	1.34
3	B	1213	NAG	C7-N2	3.86	1.47	1.34
5	C	1214	BLA	C1A-CHA	3.40	1.54	1.41
5	B	1215	BLA	C1A-CHA	3.40	1.54	1.41
5	A	1314	BLA	C1A-CHA	3.31	1.54	1.41
3	A	1303	NAG	C2-N2	3.28	1.51	1.46
3	C	1210	NAG	C2-N2	3.25	1.51	1.46
3	B	1210	NAG	C2-N2	3.21	1.51	1.46
5	C	1214	BLA	C4A-CHB	3.16	1.53	1.41
3	A	1311	NAG	C2-N2	3.14	1.51	1.46
3	A	1309	NAG	C2-N2	3.14	1.51	1.46
3	C	1206	NAG	C2-N2	3.12	1.51	1.46
3	C	1212	NAG	C2-N2	3.11	1.51	1.46
3	A	1304	NAG	C2-N2	3.11	1.51	1.46
3	C	1208	NAG	C2-N2	3.11	1.51	1.46
3	C	1204	NAG	C2-N2	3.11	1.51	1.46
3	B	1208	NAG	C2-N2	3.11	1.51	1.46
5	B	1215	BLA	C4A-CHB	3.11	1.53	1.41
3	B	1214	NAG	C2-N2	3.10	1.51	1.46
3	B	1206	NAG	C2-N2	3.10	1.51	1.46
3	C	1203	NAG	C2-N2	3.10	1.51	1.46
3	B	1204	NAG	C2-N2	3.10	1.51	1.46
3	C	1207	NAG	C2-N2	3.10	1.51	1.46
5	A	1314	BLA	C4A-CHB	3.09	1.53	1.41
3	C	1209	NAG	C2-N2	3.09	1.51	1.46
3	B	1212	NAG	C2-N2	3.08	1.51	1.46
3	B	1207	NAG	C2-N2	3.08	1.51	1.46
3	A	1308	NAG	C2-N2	3.08	1.51	1.46
3	B	1202	NAG	C2-N2	3.07	1.51	1.46
3	B	1205	NAG	C2-N2	3.07	1.51	1.46
3	A	1310	NAG	C2-N2	3.07	1.51	1.46
3	C	1201	NAG	C2-N2	3.07	1.51	1.46
3	C	1211	NAG	C2-N2	3.05	1.51	1.46
3	A	1302	NAG	C2-N2	3.05	1.51	1.46
3	A	1312	NAG	C2-N2	3.05	1.51	1.46
3	B	1203	NAG	C2-N2	3.05	1.51	1.46
3	C	1213	NAG	C2-N2	3.04	1.51	1.46
3	A	1301	NAG	C2-N2	3.04	1.51	1.46
3	C	1205	NAG	C2-N2	3.04	1.51	1.46
3	B	1209	NAG	C2-N2	3.03	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	NAG	C2-N2	3.02	1.51	1.46
3	A	1307	NAG	C2-N2	3.01	1.51	1.46
3	B	1201	NAG	C2-N2	3.00	1.51	1.46
3	A	1306	NAG	C2-N2	2.99	1.51	1.46
3	A	1305	NAG	C2-N2	2.99	1.51	1.46
3	B	1213	NAG	C2-N2	2.98	1.51	1.46
5	A	1314	BLA	CHA-C4D	-2.85	1.32	1.35
5	C	1214	BLA	C3C-C2C	2.81	1.43	1.37
5	B	1215	BLA	C3C-C2C	2.78	1.42	1.37
5	A	1314	BLA	C3C-C2C	2.78	1.42	1.37
5	B	1215	BLA	OC-C1C	-2.74	1.18	1.23
5	A	1314	BLA	OC-C1C	-2.73	1.18	1.23
5	B	1215	BLA	CHA-C4D	-2.70	1.32	1.35
5	C	1214	BLA	CHA-C4D	-2.67	1.32	1.35
5	C	1214	BLA	OC-C1C	-2.65	1.18	1.23
5	C	1214	BLA	C3B-C2B	2.65	1.42	1.37
5	B	1215	BLA	C1B-C2B	2.64	1.49	1.45
5	B	1215	BLA	C3B-C2B	2.59	1.42	1.37
5	A	1314	BLA	C1B-C2B	2.59	1.49	1.45
5	B	1215	BLA	OB-C4B	-2.56	1.18	1.23
5	A	1314	BLA	C3B-C2B	2.55	1.42	1.37
5	C	1214	BLA	C1B-C2B	2.54	1.49	1.45
5	C	1214	BLA	OB-C4B	-2.52	1.18	1.23
5	C	1214	BLA	C3C-C4C	2.52	1.49	1.45
5	A	1314	BLA	OB-C4B	-2.49	1.18	1.23
5	B	1215	BLA	C3C-C4C	2.47	1.49	1.45
5	A	1314	BLA	C3C-C4C	2.40	1.49	1.45
5	B	1215	BLA	CHD-C4C	-2.25	1.32	1.38
5	A	1314	BLA	CHD-C4C	-2.25	1.32	1.38
3	A	1309	NAG	O7-C7	-2.21	1.18	1.23
3	C	1201	NAG	O7-C7	-2.18	1.18	1.23
3	B	1208	NAG	O7-C7	-2.17	1.18	1.23
3	A	1307	NAG	O7-C7	-2.17	1.18	1.23
3	A	1302	NAG	O7-C7	-2.16	1.18	1.23
5	C	1214	BLA	CHD-C4C	-2.16	1.32	1.38
3	A	1310	NAG	O7-C7	-2.16	1.18	1.23
3	C	1206	NAG	O7-C7	-2.15	1.18	1.23
3	B	1209	NAG	O7-C7	-2.15	1.18	1.23
3	B	1202	NAG	O7-C7	-2.15	1.18	1.23
3	B	1206	NAG	O7-C7	-2.15	1.18	1.23
3	B	1203	NAG	O7-C7	-2.14	1.18	1.23
3	C	1212	NAG	O7-C7	-2.14	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	NAG	O7-C7	-2.14	1.18	1.23
3	C	1211	NAG	O7-C7	-2.14	1.18	1.23
3	B	1212	NAG	O7-C7	-2.14	1.18	1.23
3	C	1208	NAG	O7-C7	-2.13	1.18	1.23
3	C	1209	NAG	O7-C7	-2.13	1.18	1.23
3	C	1210	NAG	O7-C7	-2.13	1.18	1.23
3	B	1207	NAG	O7-C7	-2.13	1.18	1.23
3	A	1306	NAG	O7-C7	-2.13	1.18	1.23
3	A	1308	NAG	O7-C7	-2.13	1.18	1.23
3	C	1207	NAG	O7-C7	-2.13	1.18	1.23
3	C	1205	NAG	O7-C7	-2.13	1.18	1.23
3	A	1312	NAG	O7-C7	-2.13	1.18	1.23
3	C	1213	NAG	O7-C7	-2.13	1.18	1.23
3	C	1202	NAG	O7-C7	-2.12	1.18	1.23
3	B	1210	NAG	O7-C7	-2.12	1.18	1.23
3	B	1204	NAG	O7-C7	-2.11	1.18	1.23
3	A	1303	NAG	O7-C7	-2.11	1.18	1.23
3	A	1305	NAG	O7-C7	-2.11	1.18	1.23
3	C	1203	NAG	O7-C7	-2.11	1.18	1.23
3	B	1201	NAG	O7-C7	-2.11	1.18	1.23
3	A	1311	NAG	O7-C7	-2.11	1.18	1.23
3	B	1213	NAG	O7-C7	-2.11	1.18	1.23
3	B	1214	NAG	O7-C7	-2.10	1.18	1.23
3	C	1204	NAG	O7-C7	-2.10	1.18	1.23
3	B	1205	NAG	O7-C7	-2.09	1.18	1.23
3	A	1304	NAG	O7-C7	-2.09	1.18	1.23
5	B	1215	BLA	CAB-C3B	2.04	1.53	1.47
5	C	1214	BLA	CAB-C3B	2.04	1.53	1.47
5	A	1314	BLA	CAB-C3B	2.01	1.52	1.47
5	C	1214	BLA	CAC-C3C	2.00	1.52	1.47

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1314	BLA	C1A-CHA-C4D	-8.71	118.41	128.81
5	C	1214	BLA	C1A-CHA-C4D	-8.34	118.85	128.81
5	B	1215	BLA	C1A-CHA-C4D	-7.95	119.31	128.81
5	C	1214	BLA	C4C-CHD-C1D	-4.88	116.16	128.08
5	B	1215	BLA	C4C-CHD-C1D	-4.54	116.99	128.08
5	A	1314	BLA	C4C-CHD-C1D	-4.19	117.83	128.08
5	C	1214	BLA	C3D-C4D-ND	-3.87	104.42	110.05
5	B	1215	BLA	C3D-C4D-ND	-3.85	104.45	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1314	BLA	C3D-C4D-ND	-3.72	104.64	110.05
4	A	1313	EIC	C11-C10-C9	-3.34	95.36	123.57
4	A	1315	EIC	C11-C10-C9	-3.13	97.12	123.57
4	B	1211	EIC	C11-C10-C9	-2.98	98.44	123.57
5	A	1314	BLA	C1B-NB-C4B	-2.58	107.38	110.67
5	A	1314	BLA	CHA-C4D-ND	-2.54	125.30	128.83
4	A	1315	EIC	C3-C2-C1	-2.54	108.07	114.47
5	C	1214	BLA	C1B-NB-C4B	-2.53	107.45	110.67
5	C	1214	BLA	C4D-C3D-C2D	2.51	109.56	106.78
5	B	1215	BLA	C4C-NC-C1C	-2.48	107.50	110.67
5	A	1314	BLA	C4C-NC-C1C	-2.48	107.51	110.67
3	B	1208	NAG	C8-C7-N2	2.46	120.27	116.10
5	B	1215	BLA	C1B-NB-C4B	-2.45	107.55	110.67
5	B	1215	BLA	C4D-C3D-C2D	2.43	109.48	106.78
3	A	1309	NAG	C8-C7-N2	2.43	120.21	116.10
5	C	1214	BLA	C4C-NC-C1C	-2.38	107.64	110.67
3	C	1213	NAG	C8-C7-N2	2.38	120.12	116.10
3	B	1203	NAG	C8-C7-N2	2.37	120.12	116.10
3	A	1302	NAG	C1-O5-C5	-2.35	109.00	112.19
5	C	1214	BLA	CHA-C4D-ND	-2.35	125.56	128.83
3	A	1302	NAG	C8-C7-N2	2.35	120.08	116.10
5	A	1314	BLA	C4D-C3D-C2D	2.34	109.38	106.78
3	B	1212	NAG	C8-C7-N2	2.32	120.03	116.10
3	B	1210	NAG	C8-C7-N2	2.32	120.03	116.10
3	C	1208	NAG	C8-C7-N2	2.31	120.01	116.10
3	C	1211	NAG	C8-C7-N2	2.31	120.00	116.10
3	B	1209	NAG	C8-C7-N2	2.29	119.98	116.10
3	C	1203	NAG	C8-C7-N2	2.29	119.97	116.10
3	C	1210	NAG	C8-C7-N2	2.28	119.96	116.10
3	A	1301	NAG	C8-C7-N2	2.26	119.92	116.10
3	B	1214	NAG	C8-C7-N2	2.26	119.92	116.10
3	C	1205	NAG	C8-C7-N2	2.25	119.91	116.10
5	A	1314	BLA	C4B-C3B-C2B	2.24	110.81	107.92
5	C	1214	BLA	C4B-C3B-C2B	2.23	110.79	107.92
3	B	1207	NAG	C8-C7-N2	2.22	119.86	116.10
3	A	1312	NAG	C8-C7-N2	2.21	119.85	116.10
3	B	1213	NAG	C8-C7-N2	2.21	119.84	116.10
3	A	1304	NAG	C8-C7-N2	2.21	119.84	116.10
3	C	1201	NAG	C8-C7-N2	2.20	119.83	116.10
3	B	1206	NAG	C8-C7-N2	2.20	119.82	116.10
3	C	1207	NAG	C8-C7-N2	2.20	119.82	116.10
3	B	1204	NAG	C8-C7-N2	2.19	119.81	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1215	BLA	C4B-C3B-C2B	2.19	110.74	107.92
3	A	1308	NAG	C8-C7-N2	2.19	119.80	116.10
3	B	1201	NAG	C8-C7-N2	2.18	119.80	116.10
3	C	1204	NAG	C8-C7-N2	2.18	119.79	116.10
5	B	1215	BLA	CHA-C4D-ND	-2.17	125.82	128.83
3	A	1305	NAG	C8-C7-N2	2.16	119.76	116.10
5	C	1214	BLA	C3B-C2B-C1B	2.16	110.64	108.03
3	A	1310	NAG	C8-C7-N2	2.15	119.74	116.10
5	B	1215	BLA	C3B-C2B-C1B	2.14	110.61	108.03
3	A	1311	NAG	C8-C7-N2	2.13	119.71	116.10
3	C	1202	NAG	C8-C7-N2	2.13	119.70	116.10
3	B	1202	NAG	C8-C7-N2	2.12	119.70	116.10
5	A	1314	BLA	C3B-C2B-C1B	2.11	110.57	108.03
3	C	1213	NAG	C2-N2-C7	-2.10	119.91	122.90
3	C	1212	NAG	C8-C7-N2	2.10	119.66	116.10
3	C	1206	NAG	C8-C7-N2	2.07	119.61	116.10
5	A	1314	BLA	CHA-C4D-C3D	2.05	130.06	125.32
5	C	1214	BLA	CHA-C4D-C3D	2.03	130.01	125.32
3	C	1209	NAG	C8-C7-N2	2.02	119.53	116.10

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1314	BLA	NA-C1A-CHA-C4D
5	A	1314	BLA	C2A-C1A-CHA-C4D
5	A	1314	BLA	NA-C4A-CHB-C1B
5	A	1314	BLA	C3A-C4A-CHB-C1B
5	A	1314	BLA	C2C-C3C-CAC-CBC
5	A	1314	BLA	C4C-C3C-CAC-CBC
5	B	1215	BLA	NA-C1A-CHA-C4D
5	B	1215	BLA	C2A-C1A-CHA-C4D
5	B	1215	BLA	NA-C4A-CHB-C1B
5	B	1215	BLA	C3A-C4A-CHB-C1B
5	B	1215	BLA	C2C-C3C-CAC-CBC
5	B	1215	BLA	C4C-C3C-CAC-CBC
5	C	1214	BLA	NA-C1A-CHA-C4D
5	C	1214	BLA	C2A-C1A-CHA-C4D
5	C	1214	BLA	NA-C4A-CHB-C1B
5	C	1214	BLA	C3A-C4A-CHB-C1B
5	C	1214	BLA	C2B-C3B-CAB-CBB
5	C	1214	BLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	C	1214	BLA	C2C-C3C-CAC-CBC
5	C	1214	BLA	C4C-C3C-CAC-CBC
5	C	1214	BLA	ND-C1D-CHD-C4C
3	C	1212	NAG	O5-C5-C6-O6
3	B	1214	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1203	NAG	O5-C5-C6-O6
3	B	1205	NAG	O5-C5-C6-O6
3	B	1209	NAG	O5-C5-C6-O6
3	C	1213	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1208	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	C	1209	NAG	O5-C5-C6-O6
3	A	1312	NAG	C4-C5-C6-O6
3	B	1209	NAG	C4-C5-C6-O6
3	A	1312	NAG	O5-C5-C6-O6
3	B	1201	NAG	O5-C5-C6-O6
3	C	1211	NAG	O5-C5-C6-O6
3	C	1205	NAG	C4-C5-C6-O6
5	A	1314	BLA	ND-C1D-CHD-C4C
5	B	1215	BLA	ND-C1D-CHD-C4C
3	B	1214	NAG	O5-C5-C6-O6
3	B	1203	NAG	C4-C5-C6-O6
5	C	1214	BLA	C2D-C1D-CHD-C4C
3	A	1306	NAG	O5-C5-C6-O6
3	C	1206	NAG	O5-C5-C6-O6
3	A	1302	NAG	C1-C2-N2-C7
3	A	1308	NAG	O5-C5-C6-O6
3	C	1210	NAG	O5-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	C	1212	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1210	NAG	C4-C5-C6-O6
3	B	1201	NAG	C4-C5-C6-O6
3	C	1205	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	C	1206	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1205	NAG	C4-C5-C6-O6
3	C	1202	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1213	NAG	O5-C5-C6-O6
3	B	1208	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1212	NAG	O5-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1207	NAG	O5-C5-C6-O6
5	A	1314	BLA	C2D-C1D-CHD-C4C
5	B	1215	BLA	C2D-C1D-CHD-C4C
3	B	1213	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	C	1213	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	C	1211	NAG	C4-C5-C6-O6
3	B	1207	NAG	C4-C5-C6-O6
4	B	1211	EIC	C2-C3-C4-C5
3	B	1207	NAG	O5-C5-C6-O6
4	B	1211	EIC	C4-C5-C6-C7
4	A	1315	EIC	C13-C14-C15-C16
3	C	1202	NAG	O5-C5-C6-O6
5	B	1215	BLA	C4B-C3B-CAB-CBB
3	C	1209	NAG	C4-C5-C6-O6
5	B	1215	BLA	C2B-C3B-CAB-CBB
4	A	1315	EIC	C7-C8-C9-C10
4	A	1315	EIC	C2-C3-C4-C5
3	C	1201	NAG	O5-C5-C6-O6
4	B	1211	EIC	C5-C6-C7-C8
4	B	1211	EIC	C15-C16-C17-C18
4	A	1313	EIC	C1-C2-C3-C4
3	A	1308	NAG	C4-C5-C6-O6
4	A	1313	EIC	C9-C10-C11-C12
3	B	1212	NAG	C4-C5-C6-O6
4	A	1315	EIC	C5-C6-C7-C8
3	B	1212	NAG	C1-C2-N2-C7
3	A	1303	NAG	C1-C2-N2-C7
3	B	1203	NAG	C1-C2-N2-C7
3	A	1302	NAG	C3-C2-N2-C7
4	A	1313	EIC	C5-C6-C7-C8
5	A	1314	BLA	CAA-CBA-CGA-O1A
4	A	1315	EIC	O1-C1-C2-C3
5	A	1314	BLA	CAD-CBD-CGD-O1D
4	B	1211	EIC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	1315	EIC	C9-C10-C11-C12
4	B	1211	EIC	C9-C10-C11-C12
4	A	1315	EIC	C4-C5-C6-C7
4	B	1211	EIC	C3-C4-C5-C6
4	A	1315	EIC	O2-C1-C2-C3
5	A	1314	BLA	CAD-CBD-CGD-O2D
4	A	1313	EIC	C7-C8-C9-C10
4	A	1313	EIC	O1-C1-C2-C3
5	C	1214	BLA	CAA-CBA-CGA-O2A
4	A	1313	EIC	O2-C1-C2-C3
4	A	1315	EIC	C6-C7-C8-C9
5	A	1314	BLA	CAA-CBA-CGA-O2A
5	C	1214	BLA	CAD-CBD-CGD-O2D
5	B	1215	BLA	CAD-CBD-CGD-O2D
5	B	1215	BLA	CAA-CBA-CGA-O2A
5	B	1215	BLA	CAA-CBA-CGA-O1A
5	B	1215	BLA	CAD-CBD-CGD-O1D
3	C	1207	NAG	C4-C5-C6-O6
5	C	1214	BLA	CAA-CBA-CGA-O1A
4	A	1313	EIC	C12-C13-C14-C15
5	C	1214	BLA	CAD-CBD-CGD-O1D
3	A	1303	NAG	C3-C2-N2-C7
3	C	1203	NAG	C1-C2-N2-C7

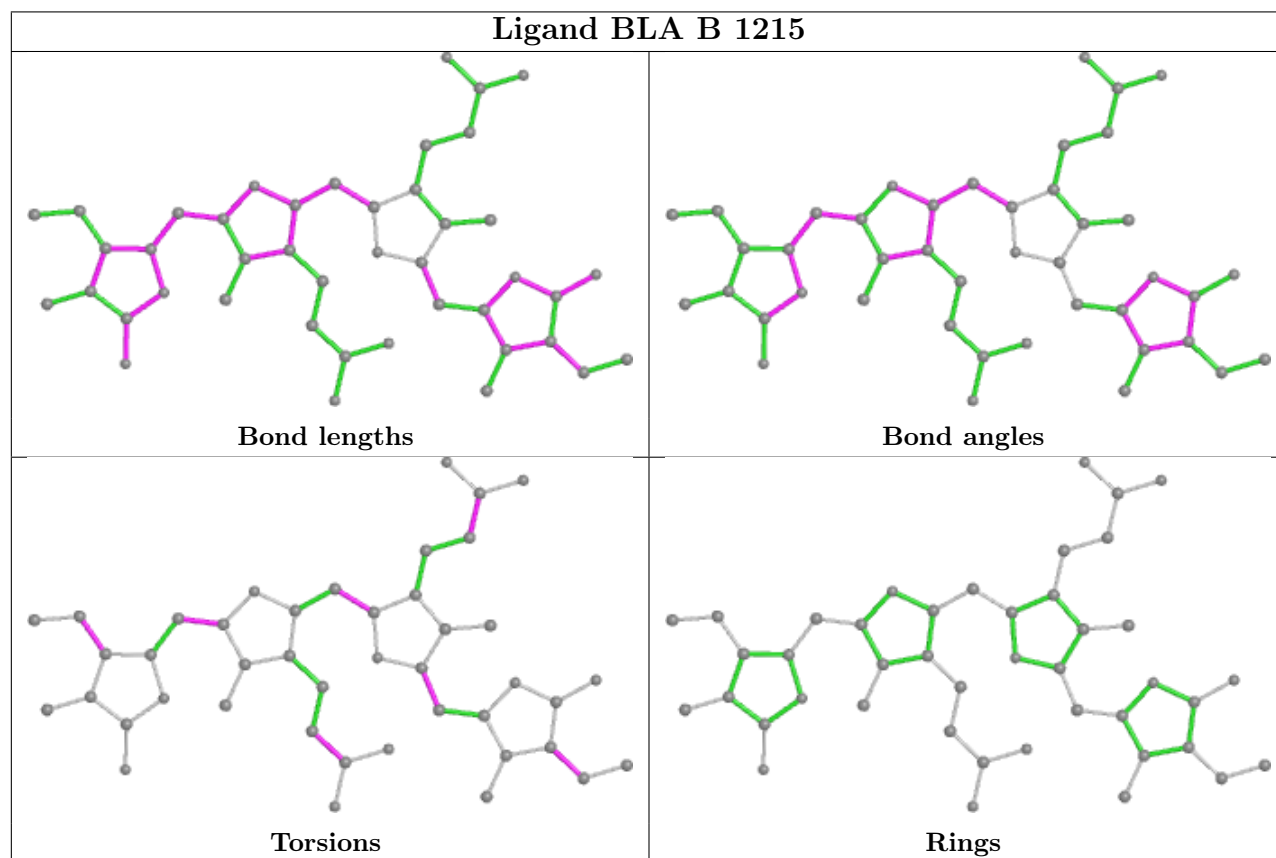
There are no ring outliers.

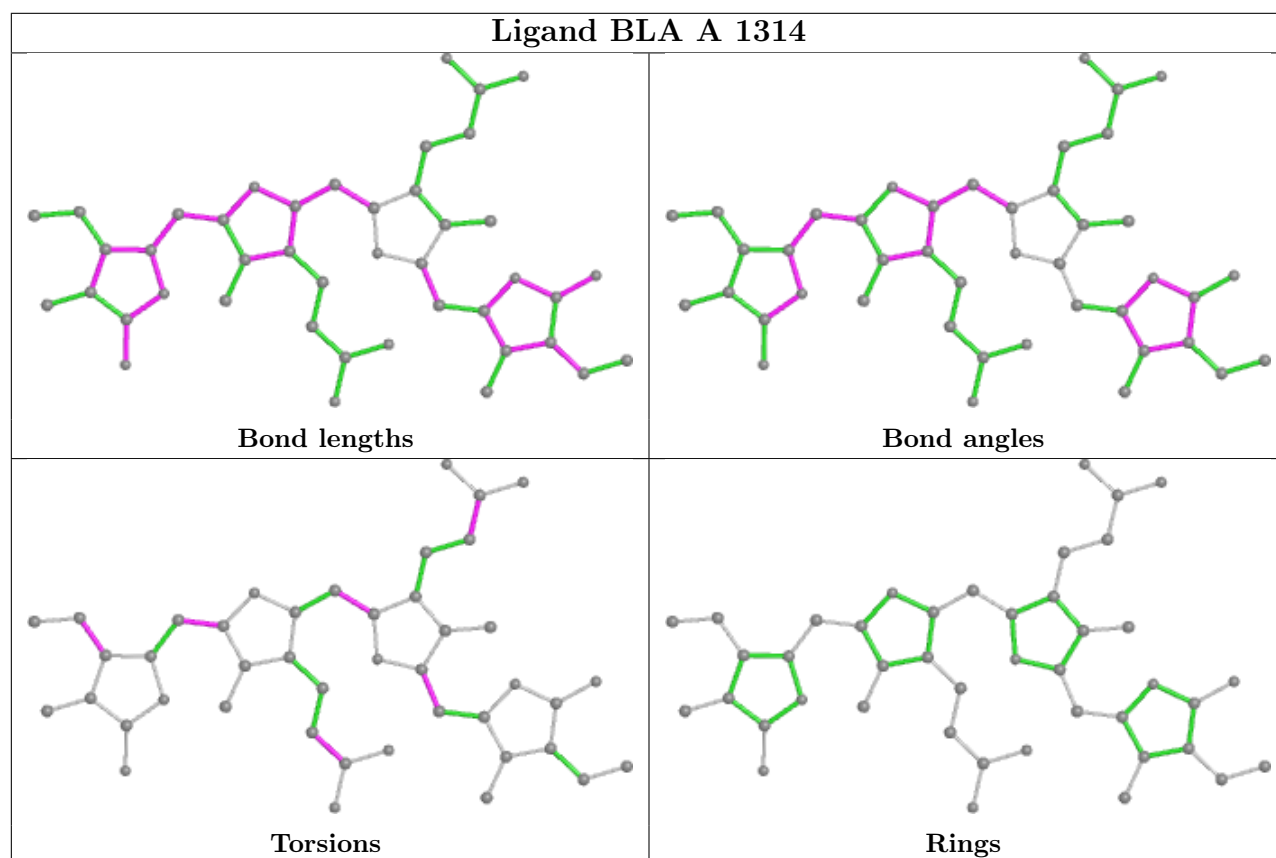
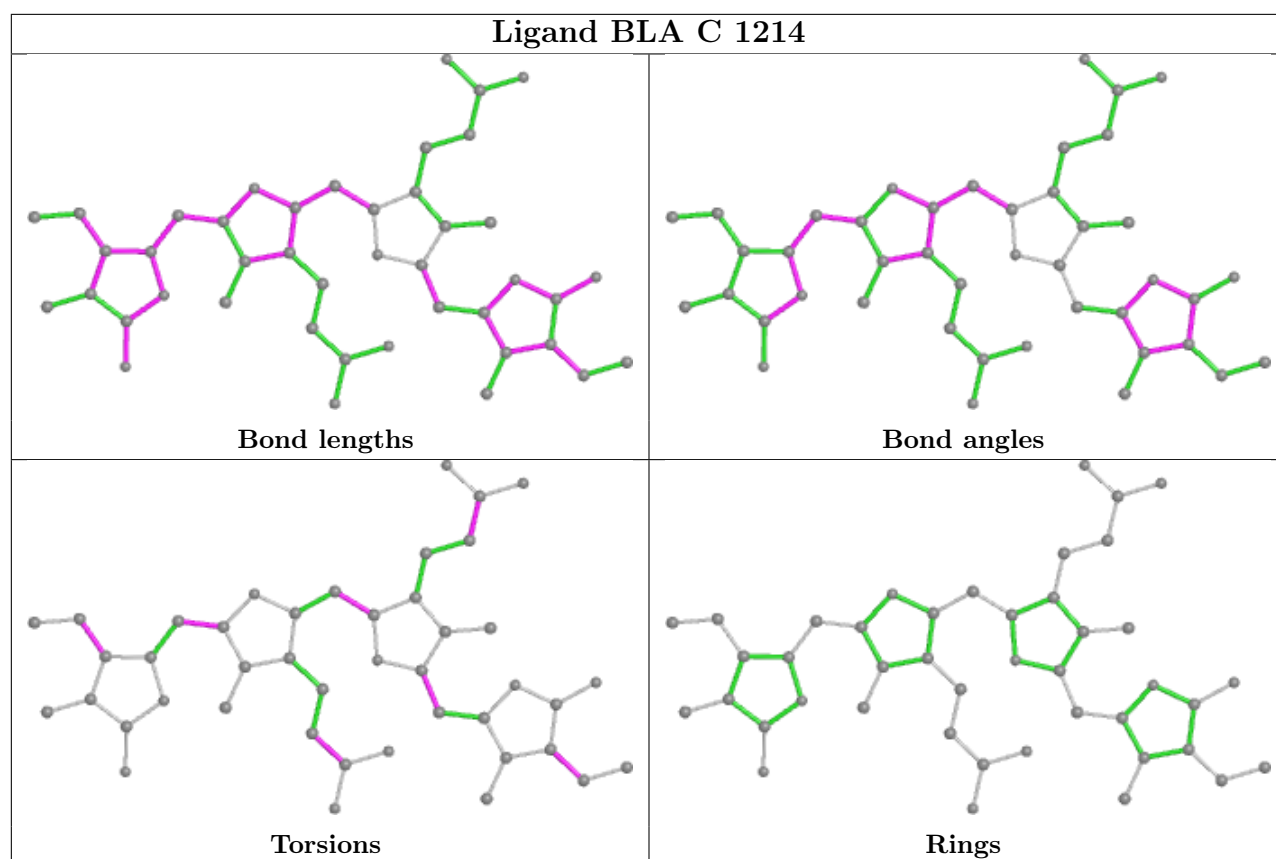
5 monomers are involved in 8 short contacts:

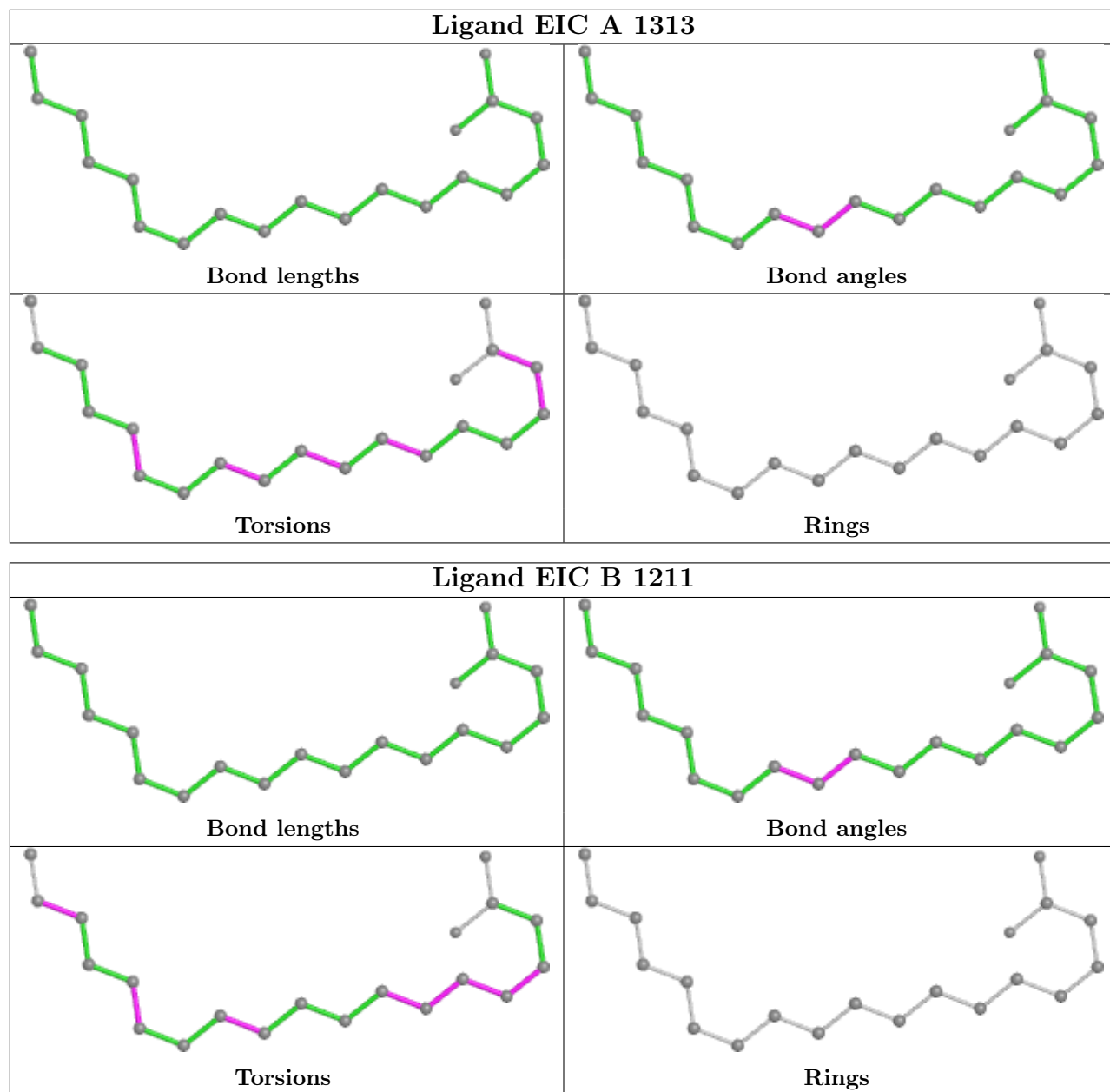
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1213	NAG	1	0
5	B	1215	BLA	2	0
5	C	1214	BLA	1	0
5	A	1314	BLA	2	0
3	A	1302	NAG	2	0

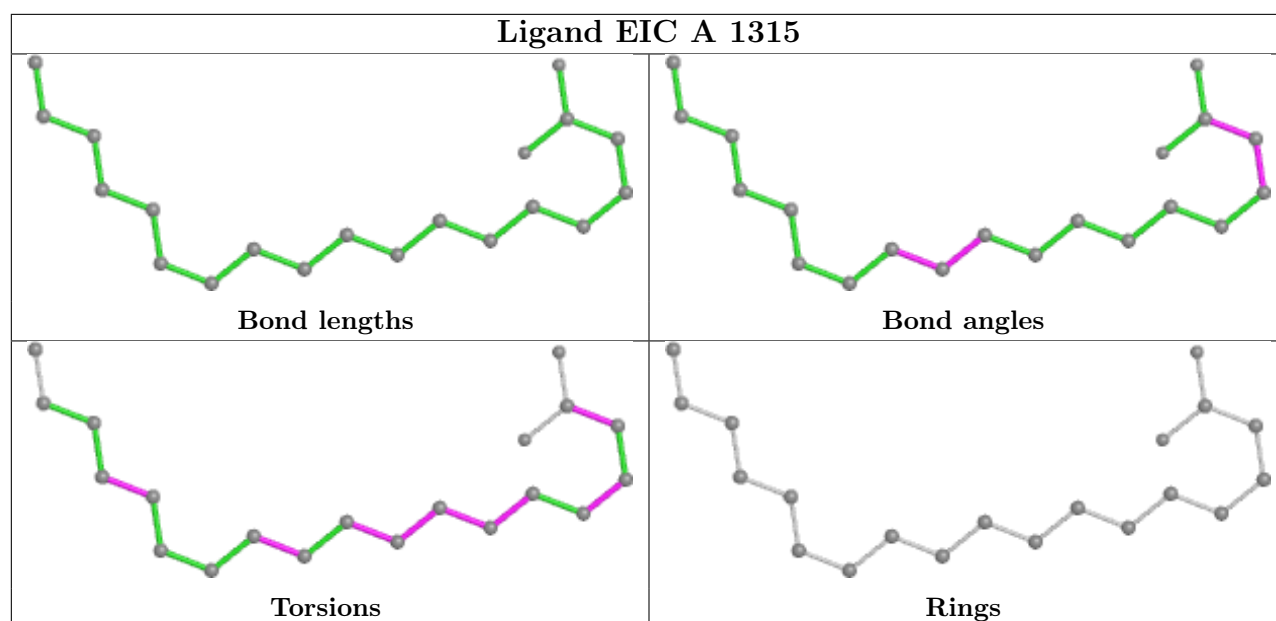
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

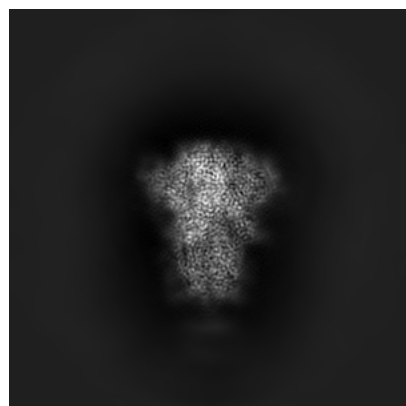
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33454. These allow visual inspection of the internal detail of the map and identification of artifacts.

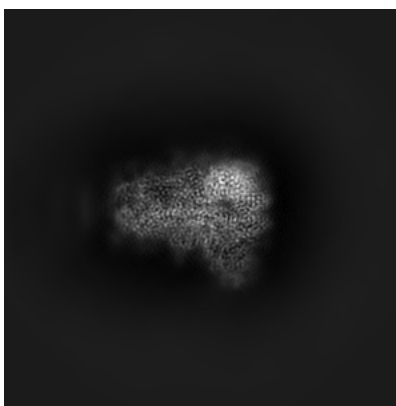
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

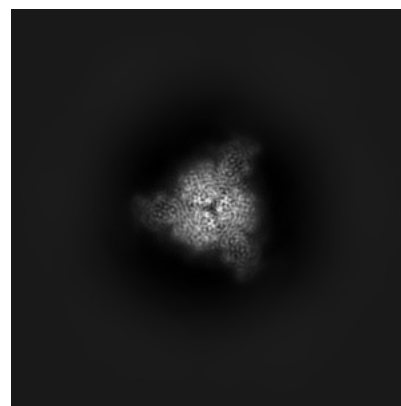
6.1.1 Primary map



X

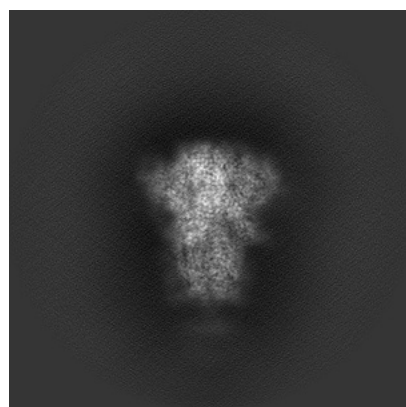


Y

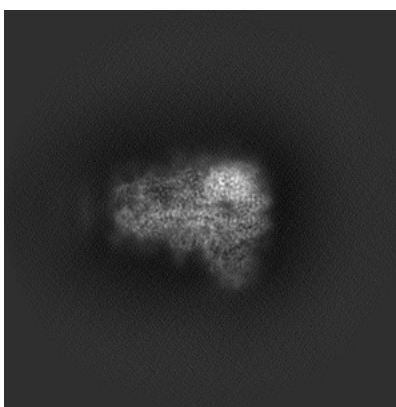


Z

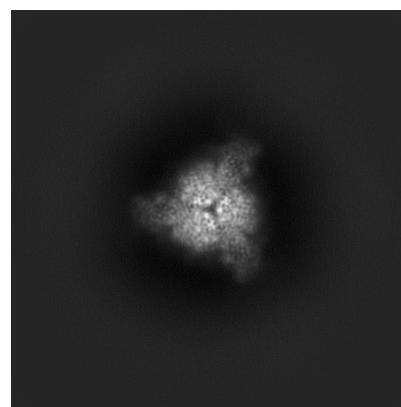
6.1.2 Raw map



X



Y

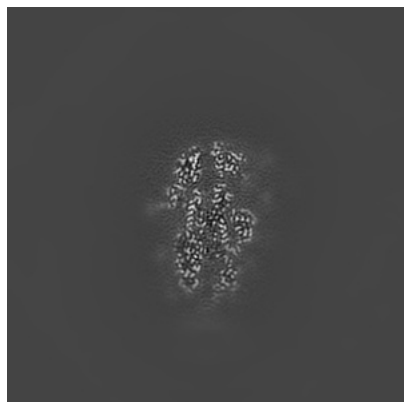


Z

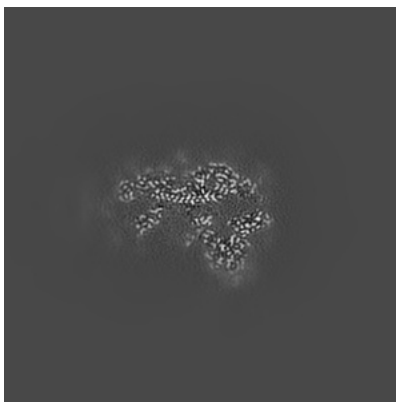
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

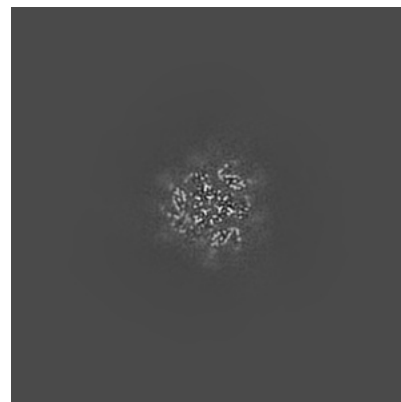
6.2.1 Primary map



X Index: 180

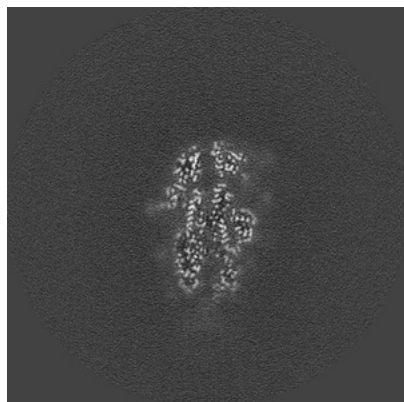


Y Index: 180

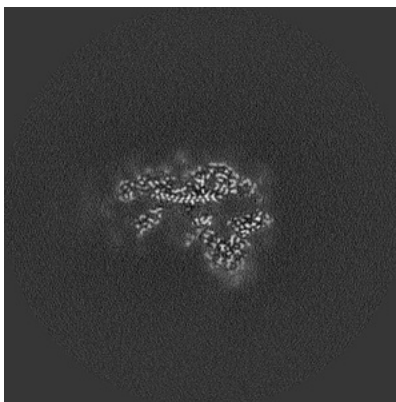


Z Index: 180

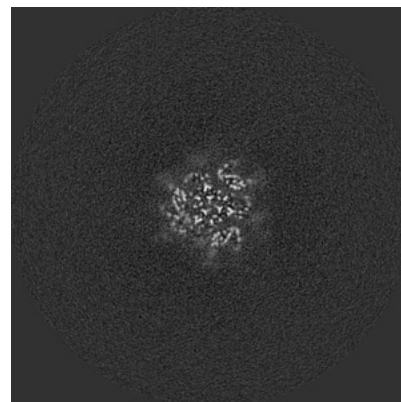
6.2.2 Raw map



X Index: 180



Y Index: 180

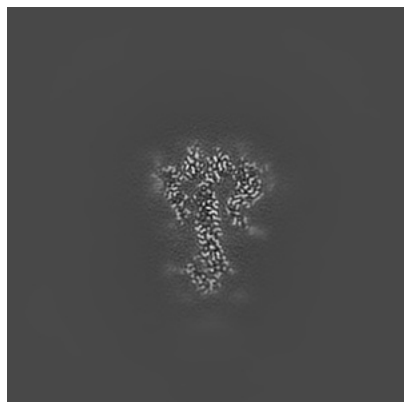


Z Index: 180

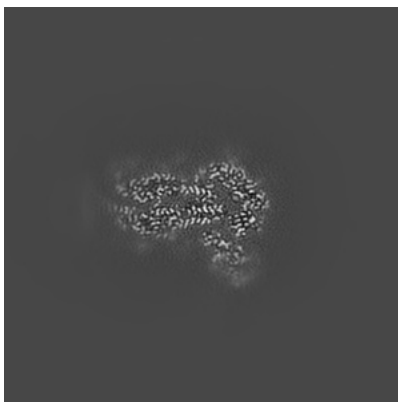
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

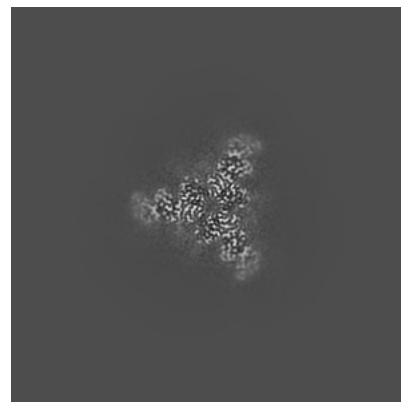
6.3.1 Primary map



X Index: 193

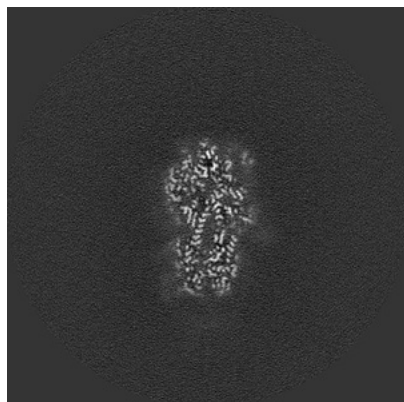


Y Index: 188

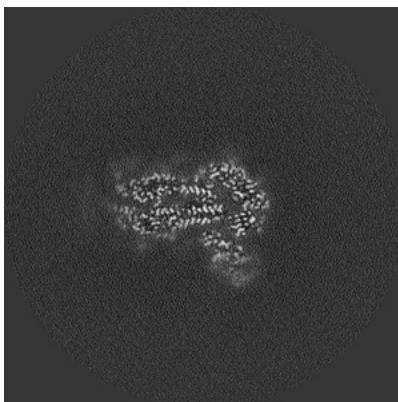


Z Index: 210

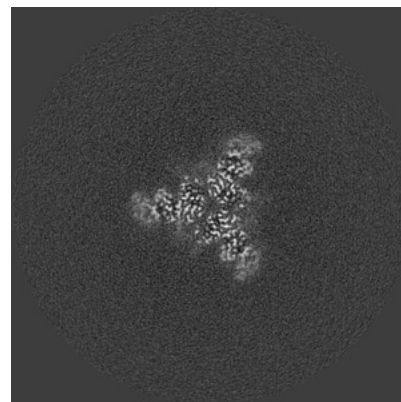
6.3.2 Raw map



X Index: 169



Y Index: 188



Z Index: 210

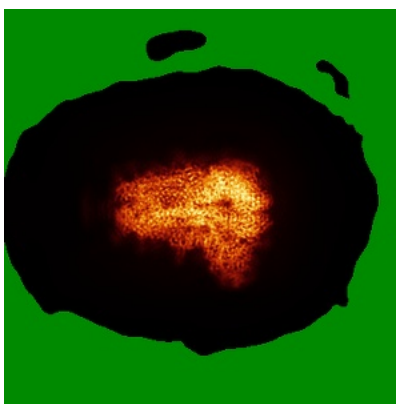
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

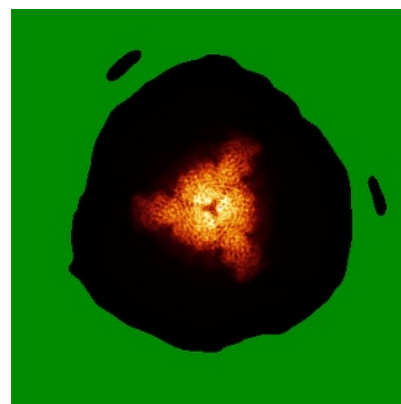
6.4.1 Primary map



X

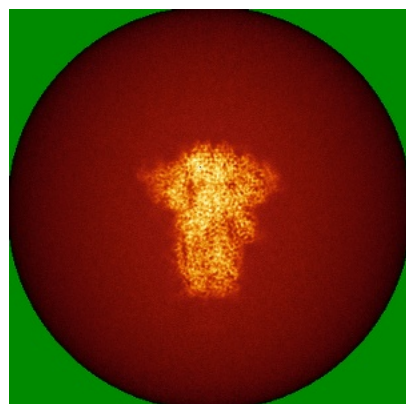


Y

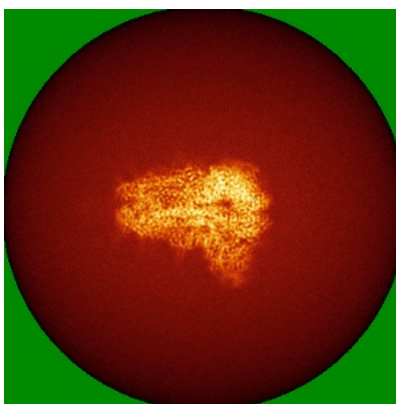


Z

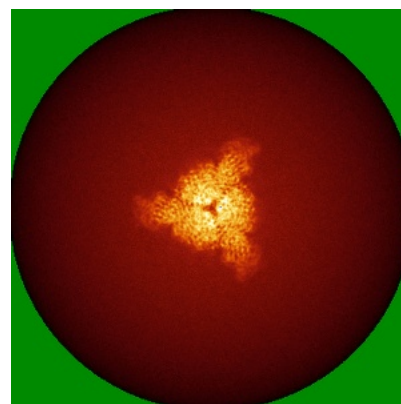
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

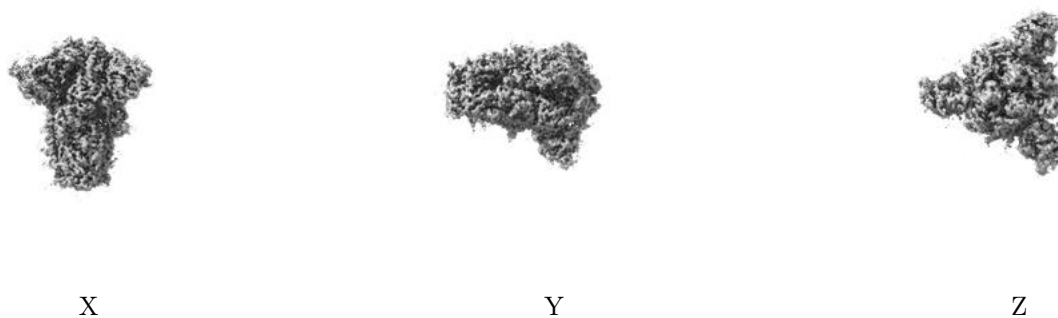
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

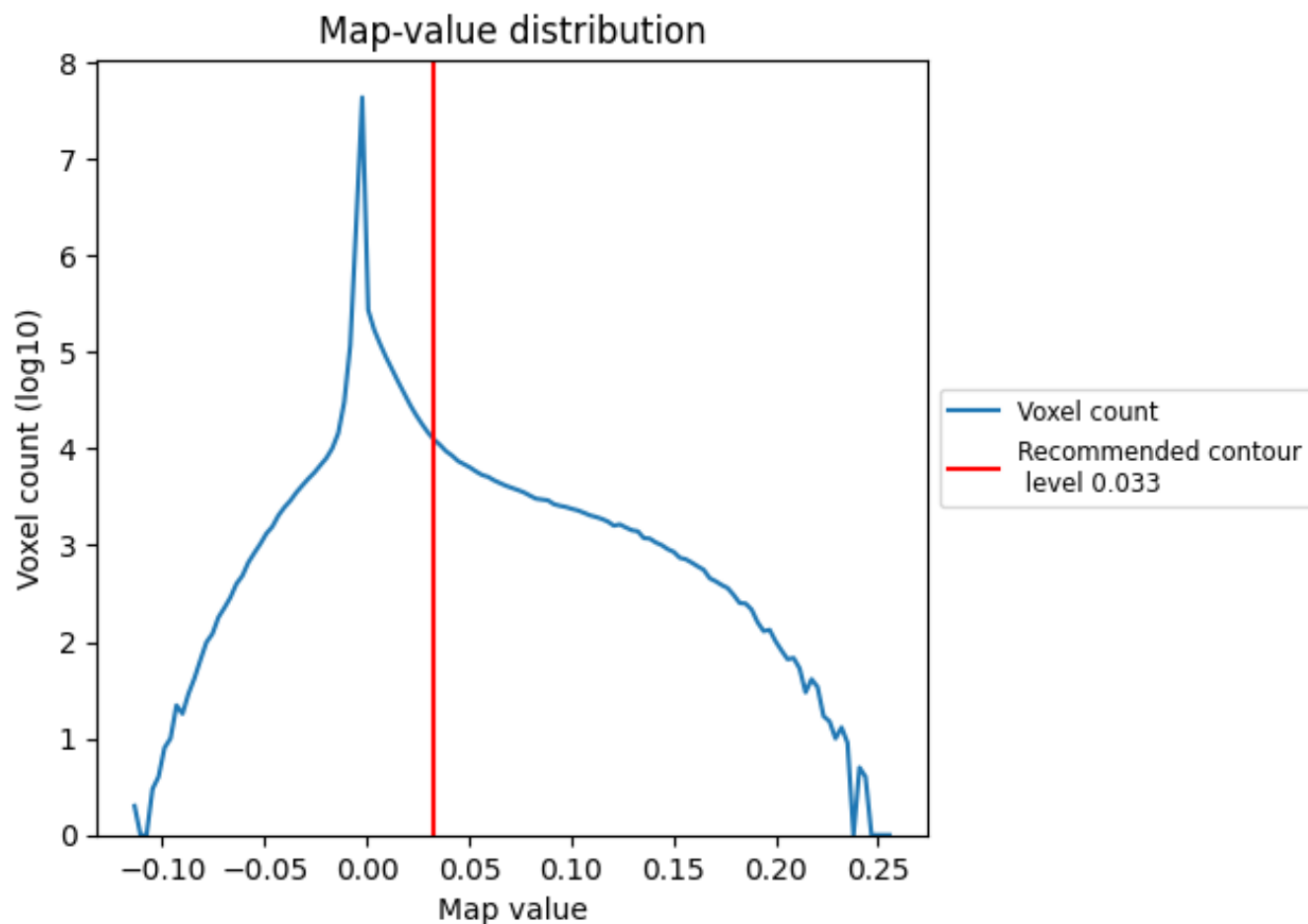
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

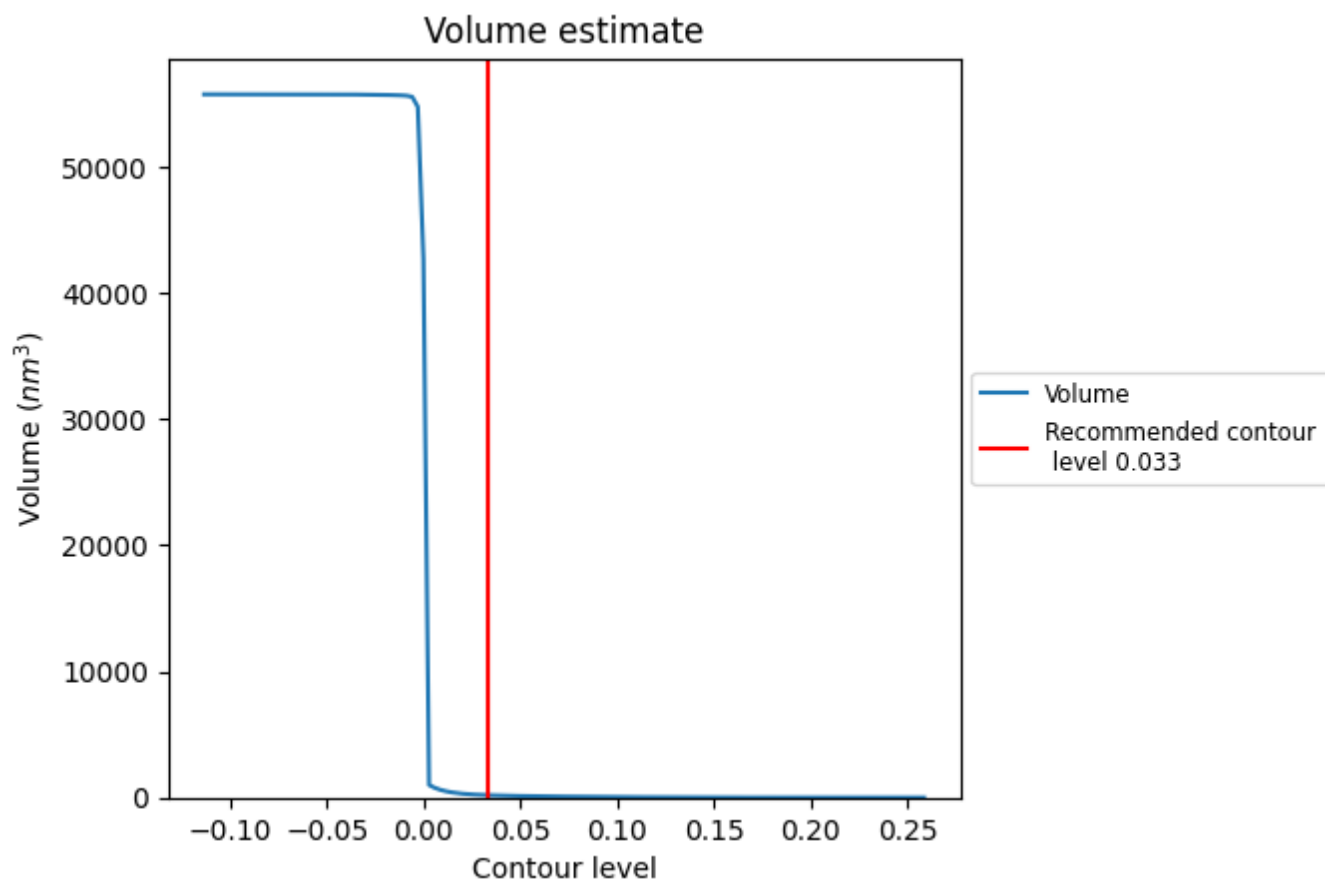
This section contains the results of statistical analysis of the map.

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.

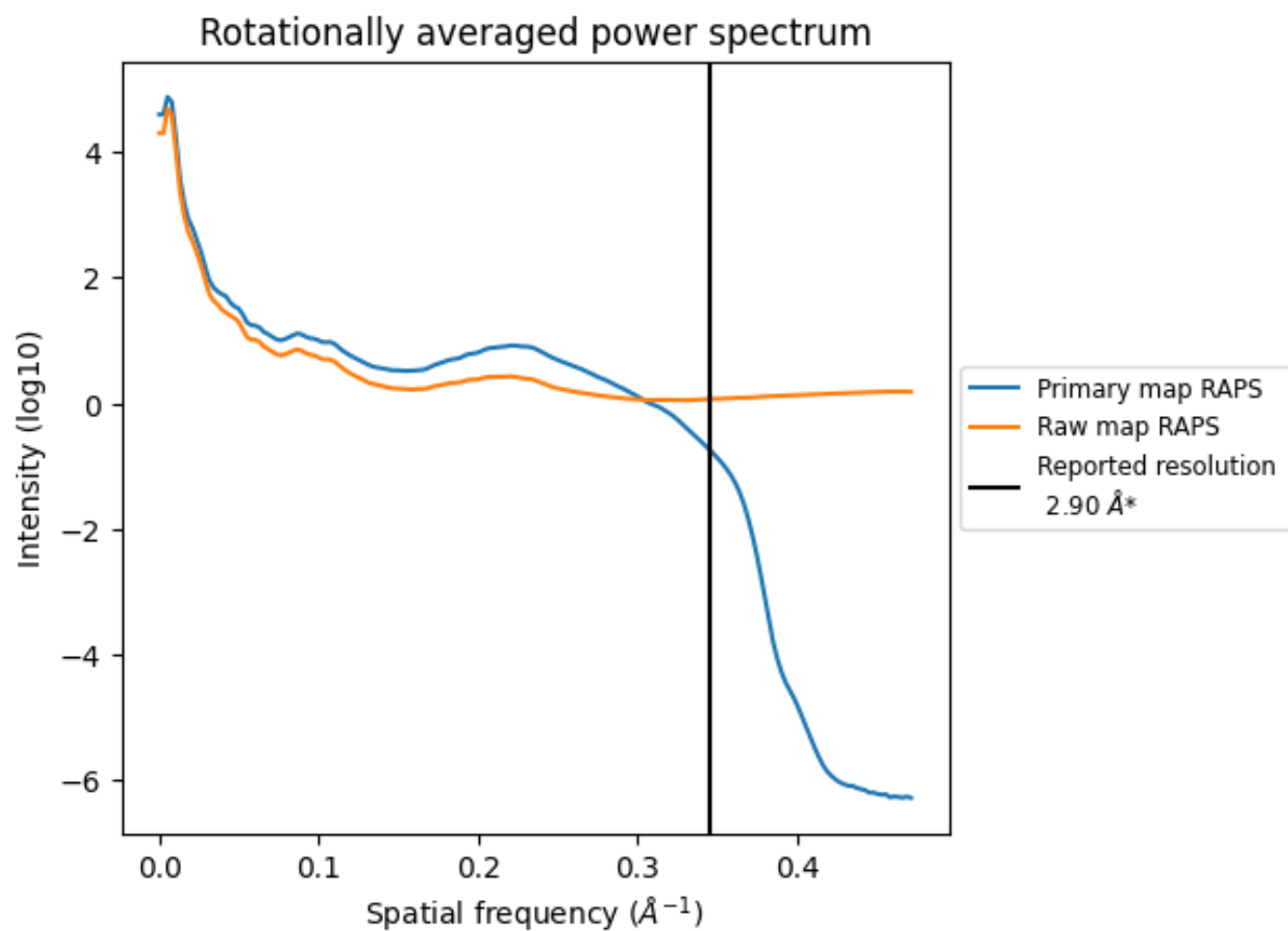
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm^3 ; this corresponds to an approximate mass of 170 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 ⓘ

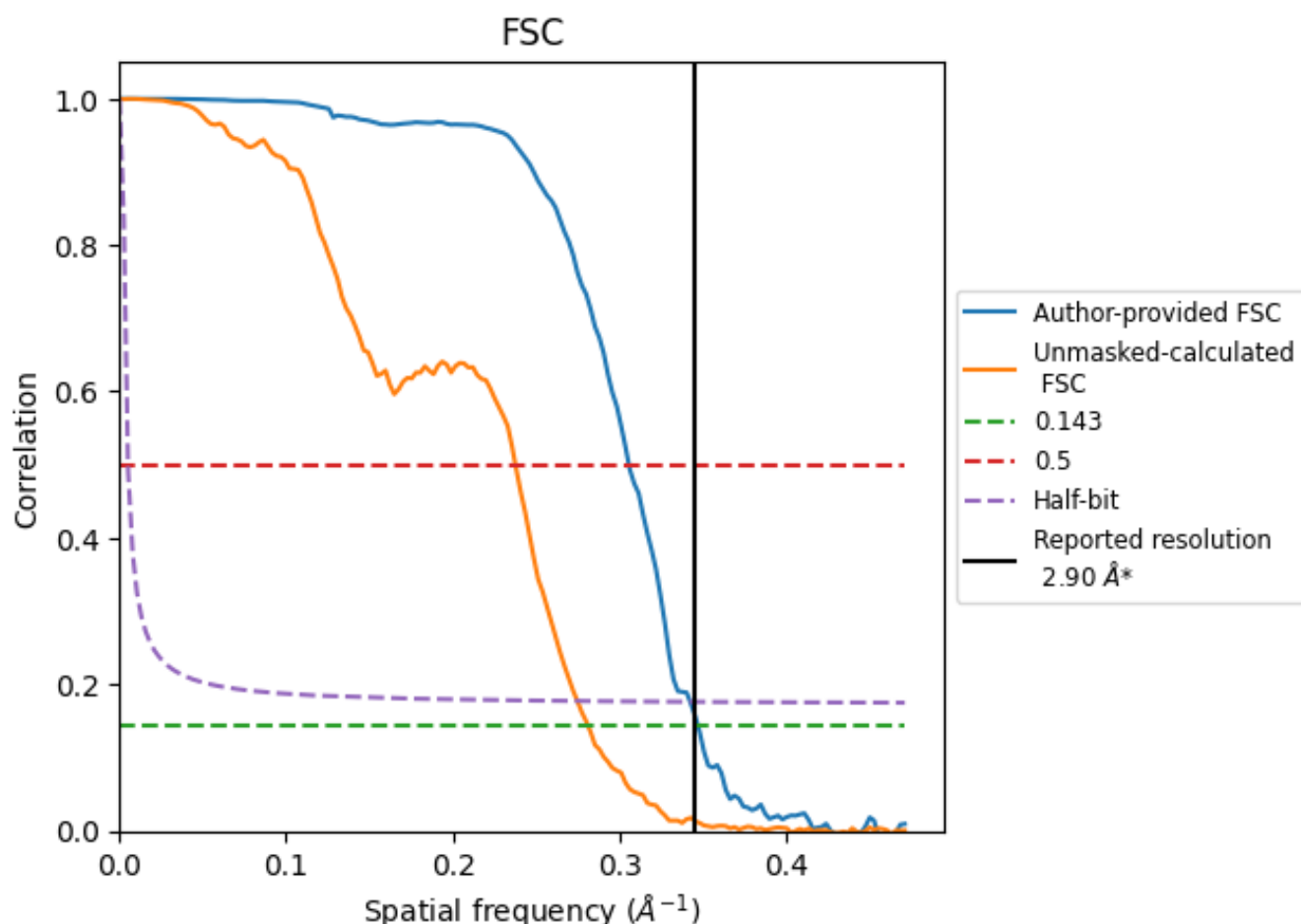


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

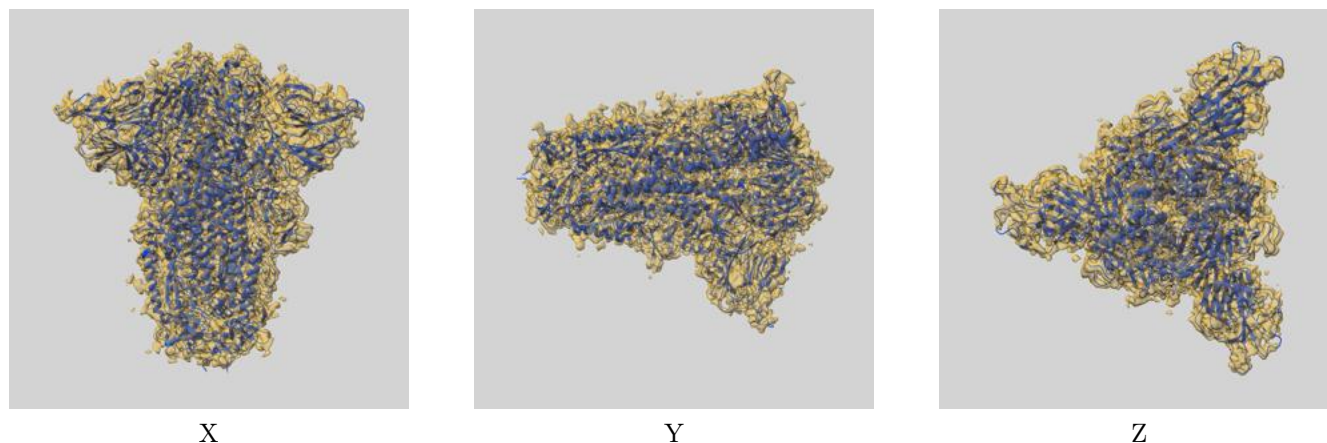
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.27	2.92
Unmasked-calculated*	3.55	4.21	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

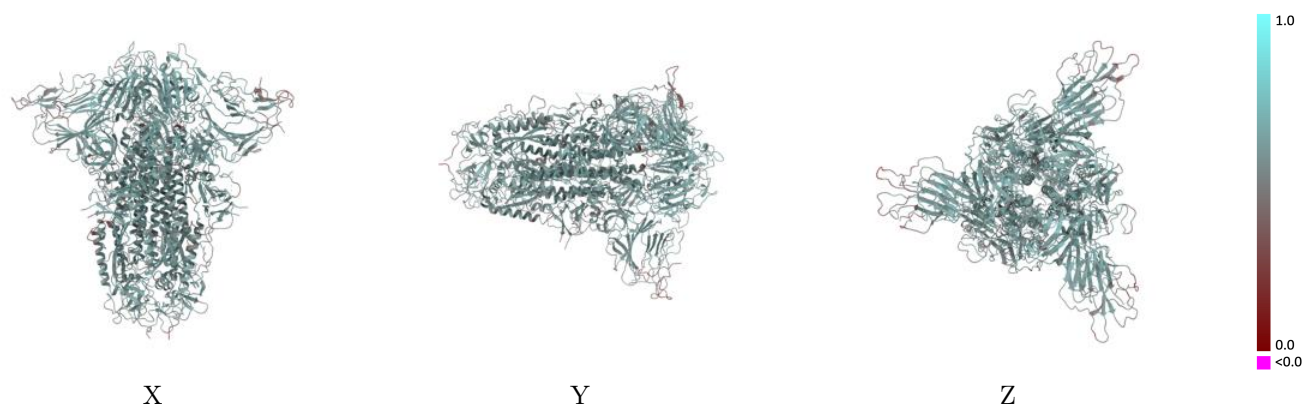
This section contains information regarding the fit between EMDB map EMD-33454 and PDB model 7XU0. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



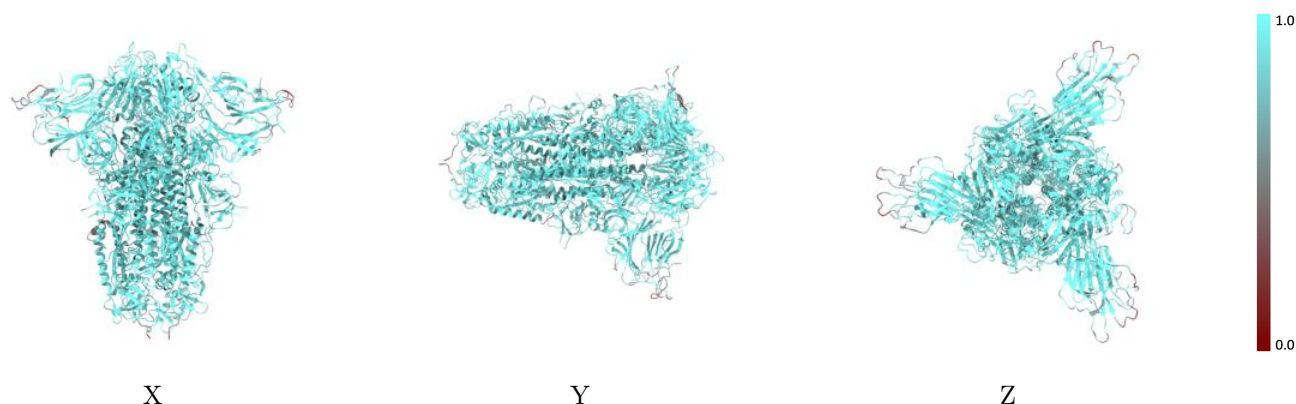
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



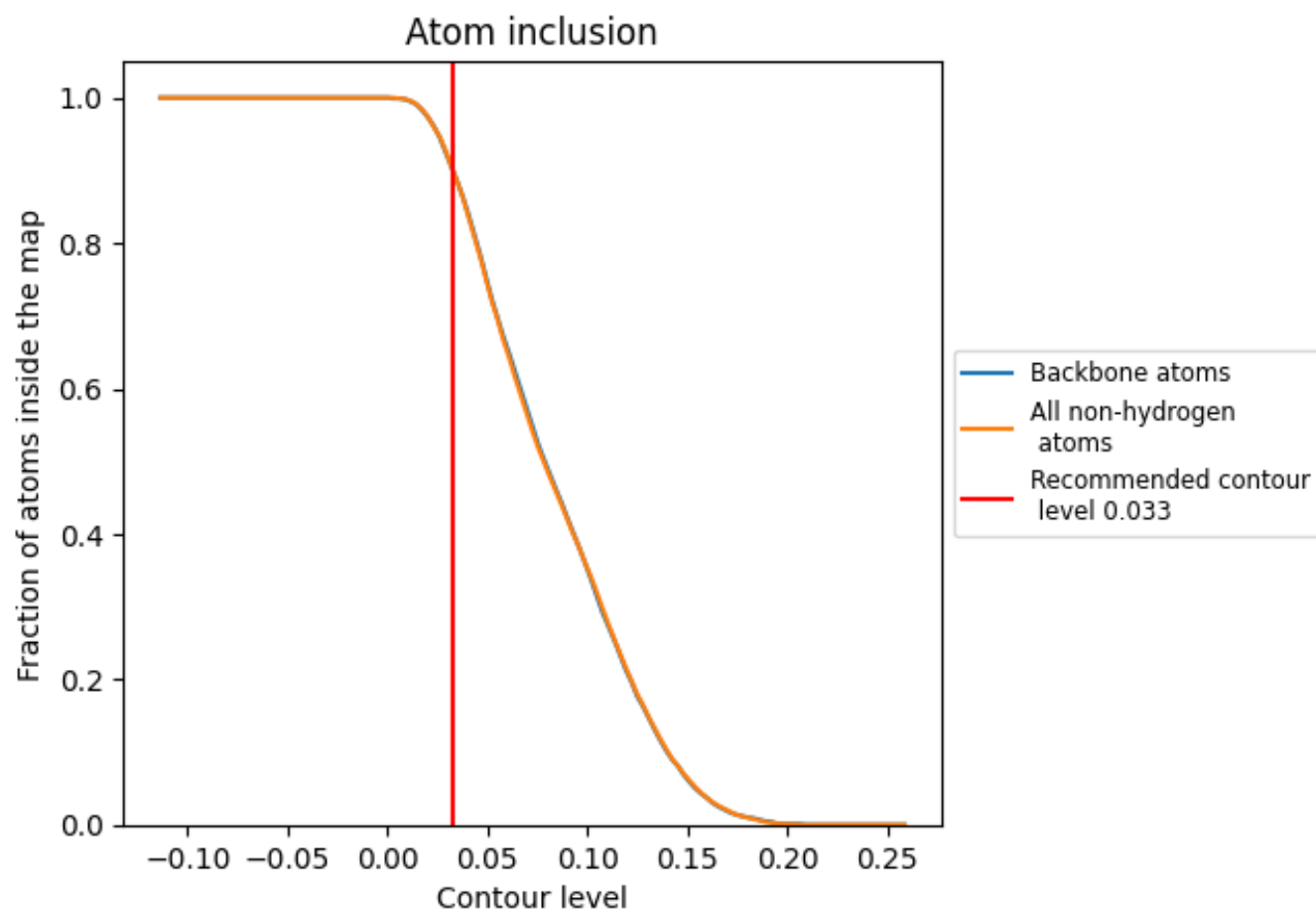
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.033).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.5690
A	 0.8960	 0.5630
B	 0.9110	 0.5750
C	 0.9050	 0.5750
D	 0.8570	 0.5020
E	 0.6430	 0.4530
F	 0.3570	 0.3080
G	 0.2500	 0.3910
H	 0.6070	 0.5020
I	 0.4640	 0.4040
J	 0.2860	 0.4290
K	 0.7860	 0.5420
L	 0.7140	 0.5030
M	 0.7500	 0.4980
N	 0.4640	 0.4740
O	 0.2500	 0.4390
P	 0.8210	 0.5600
Q	 0.6790	 0.4850

