



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:20 PM UTC

PDB ID : 9D7I / pdb_00009d7i
EMDB ID : EMD-46606
Title : Cryo-EM structure of BG505 DS-SOSIP.664 with 2 CH103 KN Fabs bound
Authors : Parsons, R.J.; Acharya, P.
Deposited on : 2024-08-16
Resolution : 3.68 Å(reported)

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:

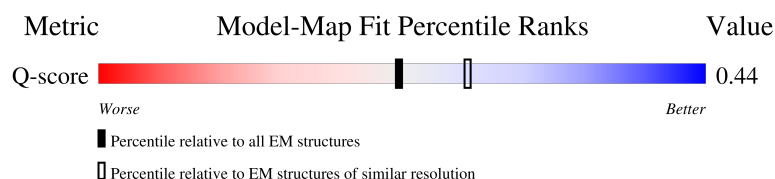
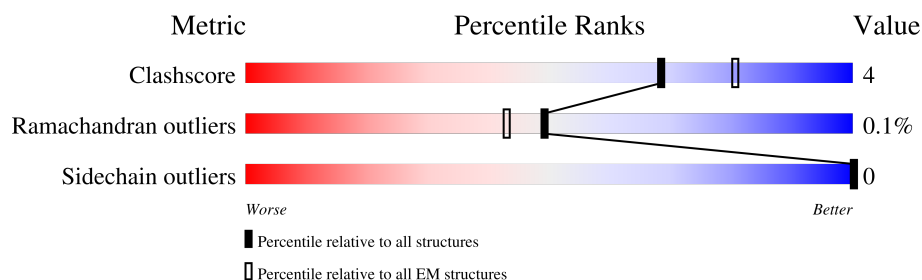
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11376 (3.18 - 4.18)

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	496	19% 78% 9% 14%
1	C	496	8% 80% 8% 12%
1	E	496	7% 76% 11% 12%
2	B	162	33% 69% 9% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	162	
2	F	162	
3	G	229	
3	I	229	
4	H	245	
4	J	245	
5	K	2	
5	M	2	
5	N	2	
5	P	2	
5	Q	2	
5	T	2	
5	U	2	
5	W	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	e	2	
5	f	2	
6	L	3	
6	O	3	
6	R	3	
6	S	3	
6	V	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	X	3	100%
6	c	3	33% 100%
6	d	3	100%
6	g	3	67% 33%
6	h	3	67% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19675 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 Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3373	2121	594	629	29		
1	C	438	Total	C	N	O	S	0	0
			3447	2162	609	646	30		
1	E	438	Total	C	N	O	S	0	0
			3447	2162	609	646	30		

- Molecule 2 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	127	Total	C	N	O	S	0	0
			1008	636	175	191	6		
2	D	121	Total	C	N	O	S	0	0
			963	607	167	183	6		
2	F	121	Total	C	N	O	S	0	0
			963	607	167	183	6		

- Molecule 3 is a protein called CH103 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	192	Total	C	N	O	S	0	0
			1447	915	237	290	5		
3	I	192	Total	C	N	O	S	0	0
			1447	915	237	290	5		

- Molecule 4 is a protein called CH103 K75 N76 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	158	Total	C	N	O	S	0	0
			1189	760	201	225	3		
4	J	158	Total	C	N	O	S	0	0
			1189	760	201	225	3		

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



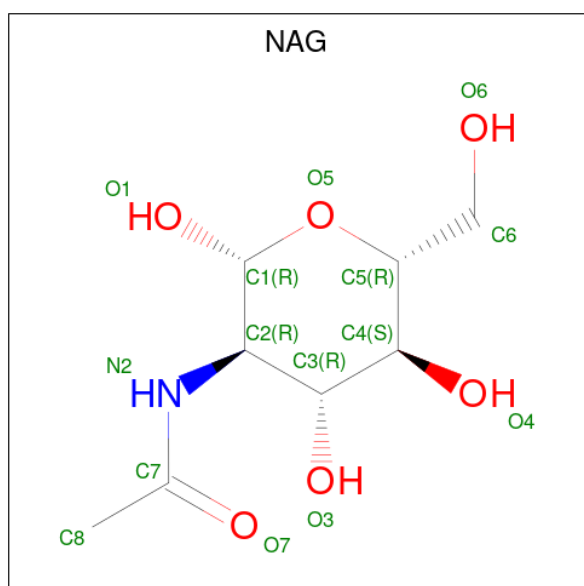
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	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		

- Molecule 6 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
6	L	3	Total	C	N	O	0	0
			39	22	2	15		
6	O	3	Total	C	N	O	0	0
			39	22	2	15		
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	V	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		
6	c	3	Total	C	N	O	0	0
			39	22	2	15		
6	d	3	Total	C	N	O	0	0
			39	22	2	15		
6	g	3	Total	C	N	O	0	0
			39	22	2	15		
6	h	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

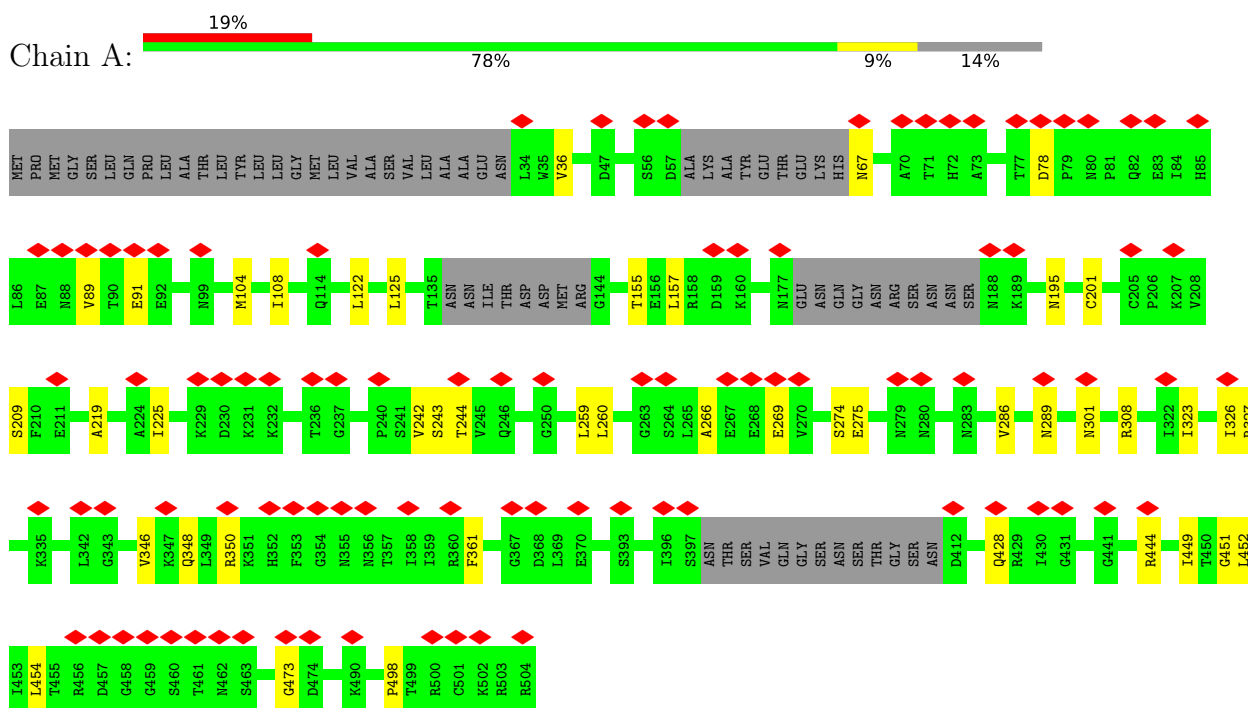
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	F	1	Total	C	N	O	0
			14	8	1	5	
7	F	1	Total	C	N	O	0
			14	8	1	5	

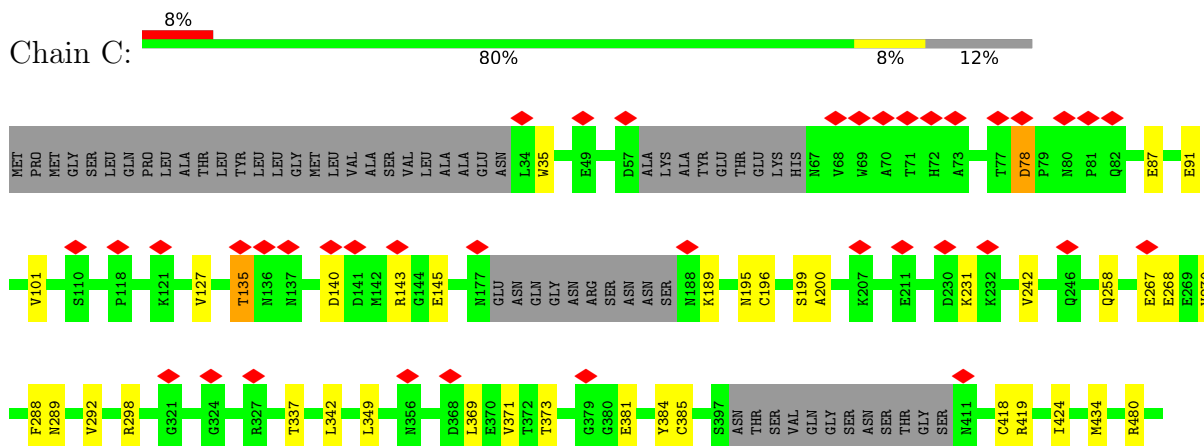
3 Residue-property plots

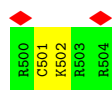
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Surface protein gp120

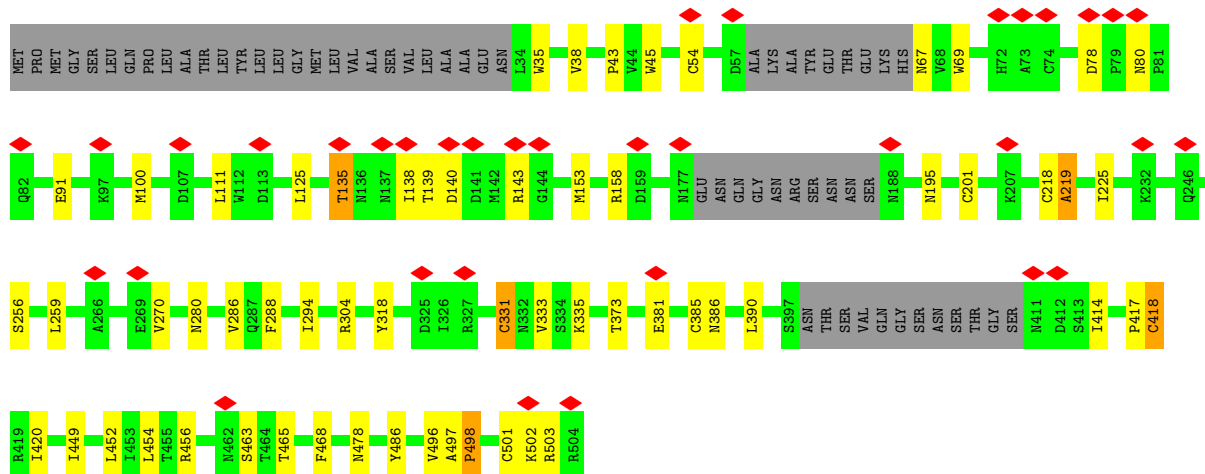
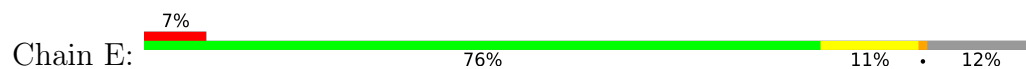


• Molecule 1: Surface protein gp120

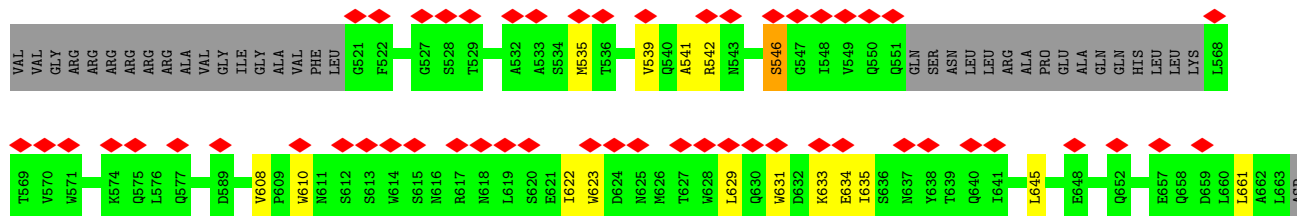




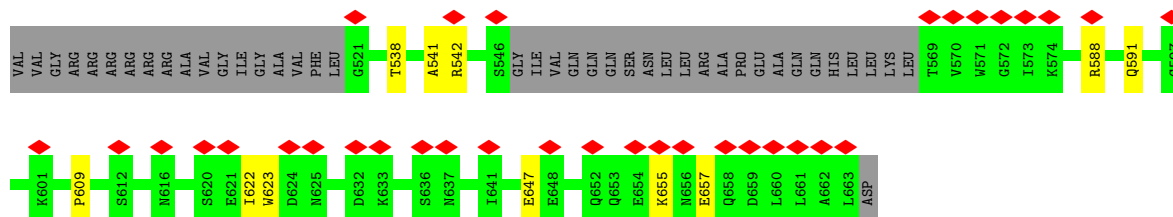
• Molecule 1: Surface protein gp120



• Molecule 2: Transmembrane protein gp41

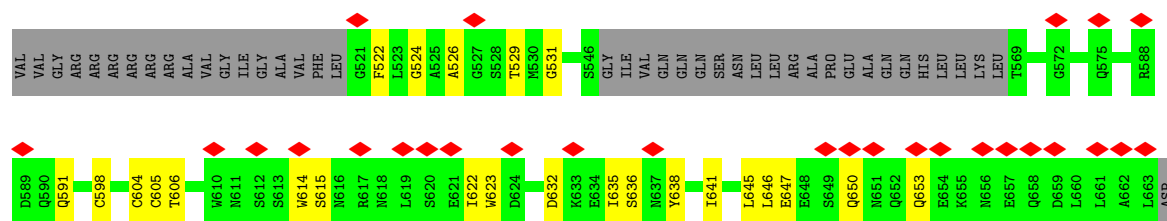


• Molecule 2: Transmembrane protein gp41

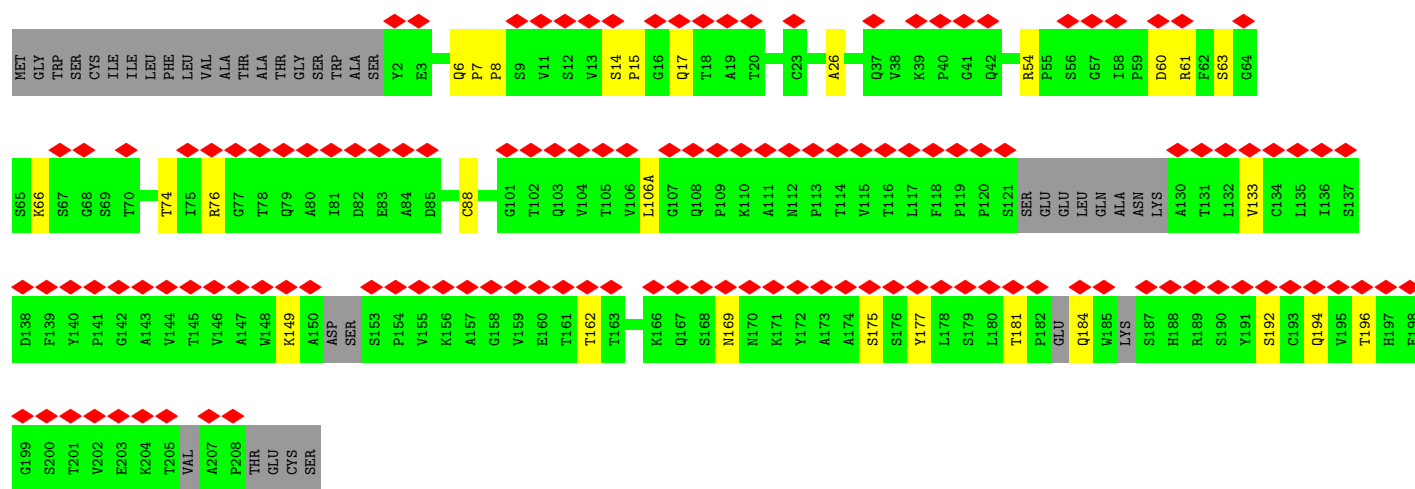
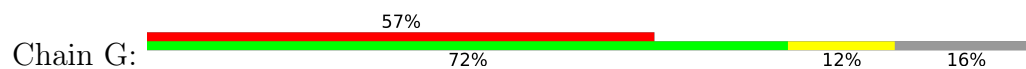


• Molecule 2: Transmembrane protein gp41

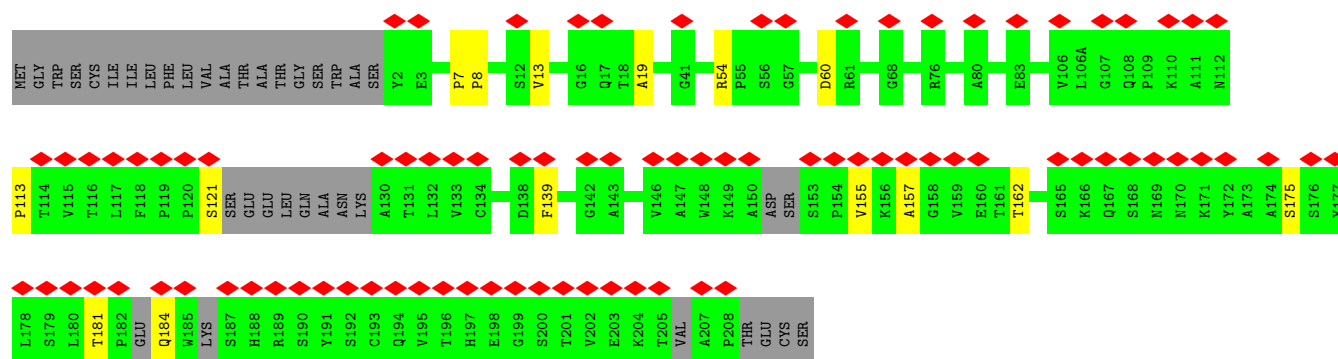
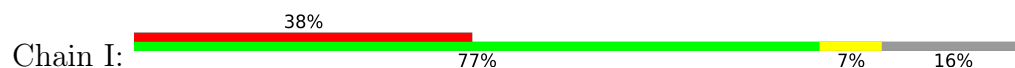




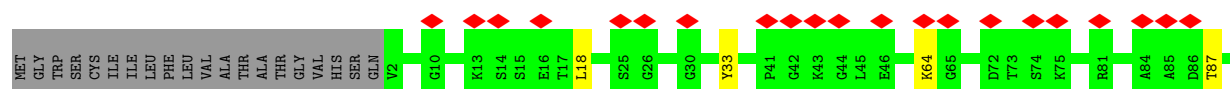
• Molecule 3: CH103 Fab light chain

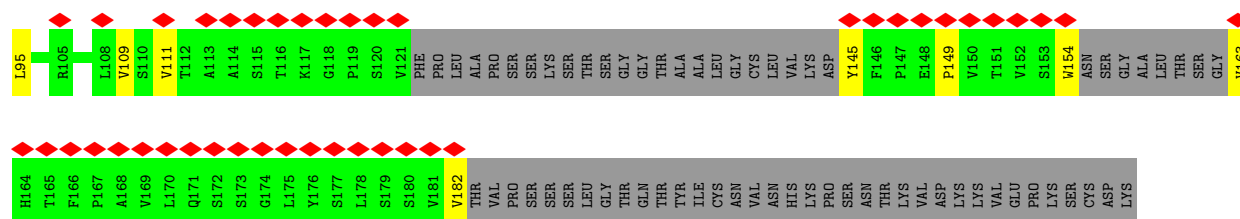


• Molecule 3: CH103 Fab light chain

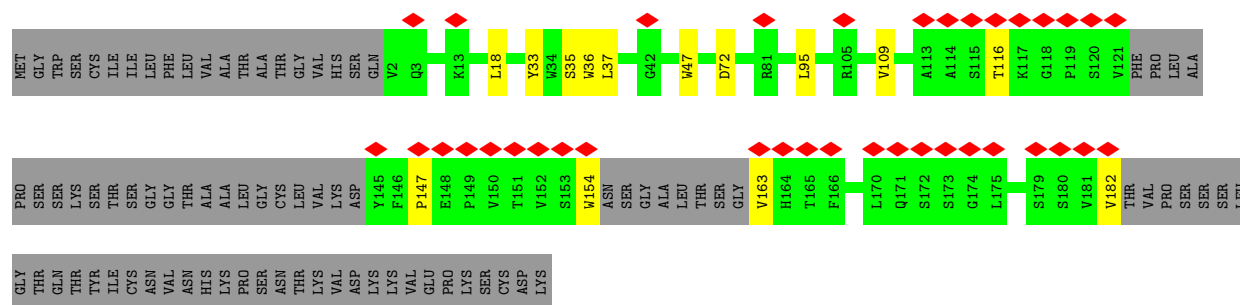


• Molecule 4: CH103 K75 N76 Fab heavy chain





• Molecule 4: CH103 K75 N76 Fab heavy chain



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



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





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



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



- Molecule 6: beta-D-mannopyranose-(1-4)-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, Not provided	
Number of particles used	73518	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CryoSPARCv4.01 Patch motion correction and CTF estimation jobs	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.1	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.972	Depositor
Minimum map value	-0.635	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.22	0/3443	0.51	0/4671
1	C	0.28	1/3518 (0.0%)	0.58	3/4774 (0.1%)
1	E	0.34	0/3518	0.85	7/4774 (0.1%)
2	B	0.24	0/1025	0.52	0/1390
2	D	0.22	0/980	0.60	0/1329
2	F	0.28	0/980	0.86	1/1329 (0.1%)
3	G	0.23	0/1483	0.58	2/2026 (0.1%)
3	I	0.18	0/1483	0.50	0/2026
4	H	0.18	0/1219	0.43	0/1662
4	J	0.20	0/1219	0.47	0/1662
All	All	0.26	1/18868 (0.0%)	0.62	13/25643 (0.1%)

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	1
1	C	0	2
1	E	0	3
2	B	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	ASP	C-N	8.43	1.44	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	635	ILE	N-CA-C	-6.80	106.50	113.10
1	E	135	THR	O-C-N	-6.34	114.43	123.06
1	C	135	THR	O-C-N	-6.04	116.58	123.40
1	E	496	VAL	CA-C-N	5.99	136.41	121.80
1	E	496	VAL	C-N-CA	5.99	136.41	121.80
1	E	418	CYS	CA-CB-SG	5.96	128.10	114.40
3	G	169	ASN	CA-C-N	5.70	132.43	121.54
3	G	169	ASN	C-N-CA	5.70	132.43	121.54
1	C	127	VAL	N-CA-C	-5.55	104.00	110.05
1	E	219	ALA	N-CA-C	-5.31	100.93	109.58
1	E	497	ALA	N-CA-C	5.24	121.39	109.81
1	C	189	LYS	CB-CG-CD	5.11	123.06	111.30
1	E	80	ASN	CB-CA-C	5.05	120.12	110.17

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	ASP	Mainchain
2	B	546	SER	Peptide,Mainchain
1	C	135	THR	Mainchain
1	C	78	ASP	Mainchain
1	E	135	THR	Mainchain
1	E	331	CYS	Peptide
1	E	78	ASP	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3373	0	3316	24	0
1	C	3447	0	3386	22	0
1	E	3447	0	3386	34	0
2	B	1008	0	994	12	0
2	D	963	0	940	11	0
2	F	963	0	942	18	0
3	G	1447	0	1390	13	0
3	I	1447	0	1390	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1189	0	1163	8	0
4	J	1189	0	1163	8	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	W	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	e	28	0	25	0	0
5	f	28	0	25	0	0
6	L	39	0	34	0	0
6	O	39	0	34	0	0
6	R	39	0	34	0	0
6	S	39	0	34	0	0
6	V	39	0	34	0	0
6	X	39	0	34	0	0
6	c	39	0	34	0	0
6	d	39	0	34	0	0
6	g	39	0	34	1	0
6	h	39	0	34	1	0
7	A	126	0	117	1	0
7	B	14	0	13	0	0
7	C	98	0	91	0	0
7	D	28	0	26	0	0
7	E	126	0	117	0	0
7	F	28	0	26	1	0
All	All	19675	0	19150	145	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 4.

All (145) 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:E:195:ASN:ND2	1:E:201:CYS:SG	2.63	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:CYS:HA	1:E:418:CYS:HA	1.73	0.69
1:E:69:TRP:HA	1:E:111:LEU:HD21	1.73	0.69
1:A:67:ASN:HA	1:A:209:SER:H	1.62	0.65
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.79	0.64
3:G:14:SER:HB2	3:G:17:GLN:HE22	1.62	0.64
1:A:269:GLU:HB2	1:A:348:GLN:HE22	1.62	0.63
3:G:61:ARG:HG2	3:G:76:ARG:HB2	1.81	0.62
3:G:149:LYS:HB3	3:G:192:SER:HB2	1.81	0.62
1:E:498:PRO:HB3	2:F:623:TRP:HZ2	1.64	0.61
4:J:33:TYR:HB2	4:J:95:LEU:HB2	1.84	0.60
1:E:335:LYS:HG3	1:E:414:ILE:HD11	1.81	0.60
2:B:541:ALA:O	2:D:591:GLN:NE2	2.35	0.58
3:I:113:PRO:HB3	3:I:139:PHE:HB3	1.85	0.58
1:E:333:VAL:HG11	1:E:390:LEU:HD21	1.86	0.57
1:E:373:THR:OG1	1:E:385:CYS:O	2.22	0.56
2:B:634:GLU:HG2	2:B:635:ILE:HG13	1.88	0.56
1:C:501:CYS:SG	1:C:502:LYS:N	2.78	0.56
2:D:542:ARG:NH2	2:F:647:GLU:OE2	2.39	0.56
2:B:629:LEU:O	2:B:633:LYS:NZ	2.38	0.55
3:G:6:GLN:NE2	3:G:88:CYS:SG	2.79	0.55
1:E:280:ASN:OD1	1:E:456:ARG:NH1	2.40	0.54
3:I:181:THR:O	3:I:184:GLN:N	2.40	0.54
3:G:194:GLN:HE22	3:G:196:THR:HG1	1.55	0.54
1:E:256:SER:O	1:E:478:ASN:ND2	2.39	0.54
1:A:301:ASN:HB3	1:A:323:ILE:HB	1.89	0.53
3:G:54:ARG:HH12	3:G:60:ASP:HA	1.74	0.53
2:B:546:SER:OG	2:D:588:ARG:NH2	2.41	0.52
1:C:258:GLN:NE2	1:C:371:VAL:O	2.40	0.52
4:H:33:TYR:HB2	4:H:95:LEU:HB2	1.92	0.52
2:D:622:ILE:HG23	2:D:623:TRP:HD1	1.74	0.52
3:I:54:ARG:HH12	3:I:60:ASP:HA	1.76	0.51
1:E:386:ASN:HD22	1:E:417:PRO:HG2	1.74	0.51
1:A:308:ARG:NH2	4:J:72:ASP:OD1	2.44	0.50
1:C:231:LYS:HD2	1:C:267:GLU:HG3	1.93	0.50
1:E:498:PRO:HB3	2:F:623:TRP:CZ2	2.46	0.50
3:G:181:THR:OG1	3:G:184:GLN:OE1	2.26	0.50
1:C:369:LEU:O	1:C:373:THR:OG1	2.29	0.49
4:H:87:THR:HB	4:H:111:VAL:HG22	1.94	0.49
1:A:444:ARG:NH1	7:A:606:NAG:O6	2.45	0.49
2:B:535:MET:SD	2:B:535:MET:N	2.86	0.49
4:H:18:LEU:HD11	4:H:109:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PRO:HB2	2:F:526:ALA:HB2	1.93	0.49
2:B:661:LEU:HD21	1:E:503:ARG:HA	1.93	0.49
1:C:140:ASP:OD1	1:C:143:ARG:NH2	2.45	0.49
1:C:91:GLU:HB2	1:C:242:VAL:HG21	1.95	0.49
1:E:454:LEU:HD23	1:E:468:PHE:HB3	1.93	0.49
4:J:163:VAL:HA	4:J:182:VAL:HA	1.94	0.49
1:C:424:ILE:HB	1:C:434:MET:HB3	1.93	0.48
1:E:158:ARG:O	1:E:158:ARG:NH1	2.46	0.48
2:B:542:ARG:NH1	2:D:647:GLU:OE2	2.46	0.48
1:C:101:VAL:HG21	1:C:480:ARG:HD3	1.96	0.48
1:C:267:GLU:N	1:C:267:GLU:OE1	2.47	0.48
1:C:298:ARG:NH1	1:C:381:GLU:OE2	2.46	0.48
1:E:125:LEU:HA	1:E:153:MET:HE1	1.95	0.48
3:G:162:THR:HB	3:G:175:SER:H	1.79	0.48
1:C:87:GLU:N	1:C:87:GLU:OE1	2.47	0.48
2:F:632:ASP:O	2:F:636:SER:OG	2.28	0.48
3:I:155:VAL:HG22	3:I:157:ALA:H	1.79	0.48
1:A:219:ALA:HB2	1:A:225:ILE:HG23	1.95	0.48
1:A:361:PHE:HE1	1:A:454:LEU:HD21	1.79	0.47
1:A:195:ASN:ND2	1:A:201:CYS:SG	2.76	0.47
3:G:63:SER:OG	3:G:74:THR:OG1	2.31	0.47
4:H:154:TRP:HB2	4:H:163:VAL:HG11	1.96	0.47
1:E:381:GLU:HG3	1:E:420:ILE:HD11	1.95	0.47
1:E:463:SER:OG	1:E:465:THR:O	2.33	0.47
1:A:36:VAL:HG12	2:B:610:TRP:HE3	1.79	0.47
1:C:35:TRP:HD1	2:D:609:PRO:HA	1.80	0.47
1:A:326:ILE:O	1:A:327:ARG:NE	2.47	0.47
1:C:292:VAL:HG12	1:C:337:THR:HG22	1.97	0.47
1:E:35:TRP:CE2	1:E:502:LYS:HD3	2.50	0.47
4:J:154:TRP:HB2	4:J:163:VAL:HG11	1.95	0.46
6:g:3:BMA:HO2	6:h:2:NAG:HO6	1.64	0.46
1:A:243:SER:OG	1:A:244:THR:N	2.49	0.46
2:F:522:PHE:O	2:F:524:GLY:N	2.47	0.46
2:B:608:VAL:HG21	2:B:645:LEU:HB3	1.97	0.46
2:F:529:THR:HG22	2:F:531:GLY:H	1.81	0.46
2:B:622:ILE:HG13	2:B:623:TRP:HD1	1.81	0.45
2:F:606:THR:HG21	2:F:646:LEU:HD21	1.98	0.45
1:E:331:CYS:HB2	1:E:418:CYS:HB3	1.87	0.45
3:G:15:PRO:HD3	3:G:106(A):LEU:H	1.80	0.45
1:E:139:THR:OG1	1:E:140:ASP:N	2.49	0.45
1:E:294:ILE:HD12	1:E:449:ILE:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:HG23	1:A:157:LEU:H	1.82	0.45
1:A:266:ALA:HB3	1:A:289:ASN:HA	1.99	0.45
4:H:163:VAL:HA	4:H:182:VAL:HA	1.98	0.45
4:J:37:LEU:HD23	4:J:47:TRP:HA	1.98	0.45
2:D:655:LYS:HB3	2:D:655:LYS:HE3	1.73	0.45
1:A:122:LEU:HD13	1:A:125:LEU:HD22	2.00	0.45
2:D:541:ALA:O	2:F:591:GLN:NE2	2.50	0.45
1:A:428:GLN:NE2	1:A:473:GLY:O	2.50	0.44
1:E:219:ALA:HB2	1:E:225:ILE:HG13	1.99	0.44
2:F:598:CYS:HB2	2:F:604:CYS:HB2	1.26	0.44
3:I:162:THR:OG1	3:I:175:SER:OG	2.32	0.44
2:F:622:ILE:HG13	2:F:623:TRP:HD1	1.83	0.44
1:E:153:MET:HE2	1:E:153:MET:HB2	1.82	0.44
1:E:501:CYS:HB3	2:F:605:CYS:HB2	1.99	0.43
2:F:641:ILE:O	2:F:645:LEU:N	2.47	0.43
2:F:614:TRP:HD1	2:F:638:TYR:HB3	1.83	0.43
3:I:7:PRO:HA	3:I:8:PRO:HD3	1.89	0.43
3:G:133:VAL:HG23	3:G:177:TYR:HE1	1.84	0.43
1:A:286:VAL:HB	1:A:452:LEU:HB2	2.01	0.43
1:C:145:GLU:OE2	1:C:419:ARG:NH2	2.47	0.43
1:E:259:LEU:HD22	1:E:449:ILE:HD13	2.01	0.43
3:I:13:VAL:HG21	3:I:19:ALA:HB2	2.01	0.43
2:B:539:VAL:HA	2:B:542:ARG:HH21	1.84	0.42
1:A:498:PRO:HD2	2:B:631:TRP:HZ2	1.84	0.42
1:C:385:CYS:HA	1:C:418:CYS:HA	2.01	0.42
1:C:270:VAL:HG12	1:C:288:PHE:HA	2.00	0.42
3:G:26:ALA:O	3:G:66:LYS:NZ	2.44	0.42
1:A:104:MET:O	1:A:108:ILE:HG12	2.20	0.42
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.92	0.42
1:A:346:VAL:O	1:A:350:ARG:HG3	2.20	0.42
1:C:195:ASN:OD1	1:C:196:CYS:N	2.51	0.42
1:E:304:ARG:HD3	1:E:318:TYR:HD1	1.84	0.42
4:H:64:LYS:HE2	4:H:64:LYS:HB2	1.82	0.42
4:J:18:LEU:HD11	4:J:109:VAL:HG11	2.00	0.42
2:F:622:ILE:HG13	2:F:623:TRP:CD1	2.55	0.41
4:J:35:SER:OG	4:J:36:TRP:N	2.53	0.41
4:J:116:THR:HG23	4:J:147:PRO:HG3	2.02	0.41
1:C:268:GLU:O	1:C:289:ASN:ND2	2.53	0.41
1:E:138:ILE:HG21	1:E:143:ARG:HD2	2.02	0.41
1:C:199:SER:OG	1:C:200:ALA:N	2.53	0.41
2:D:538:THR:HA	2:D:541:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:650:GLN:HA	2:F:653:GLN:HG2	2.02	0.41
1:A:89:VAL:HG11	1:A:242:VAL:HB	2.02	0.41
1:E:67:ASN:ND2	1:E:69:TRP:O	2.53	0.41
1:C:349:LEU:HD23	1:C:349:LEU:HA	1.91	0.41
4:H:163:VAL:HG12	4:H:182:VAL:HB	2.03	0.41
1:A:91:GLU:HB3	1:A:242:VAL:HG21	2.03	0.41
1:E:54:CYS:HB2	1:E:218:CYS:SG	2.60	0.41
3:G:7:PRO:HA	3:G:8:PRO:HD3	1.93	0.41
1:A:274:SER:OG	1:A:275:GLU:N	2.53	0.41
1:E:45:TRP:NE1	1:E:91:GLU:OE1	2.53	0.41
2:D:657:GLU:OE1	2:D:657:GLU:N	2.54	0.41
1:E:270:VAL:HG12	1:E:288:PHE:HA	2.03	0.40
1:A:260:LEU:HD12	1:A:451:GLY:HA3	2.03	0.40
2:F:614:TRP:CD1	2:F:638:TYR:HB3	2.56	0.40
1:C:384:TYR:HB2	1:C:419:ARG:HG2	2.02	0.40
1:E:100:MET:HE1	1:E:486:TYR:HB3	2.04	0.40
1:A:259:LEU:HD11	1:A:449:ILE:HD13	2.02	0.40
2:D:538:THR:O	2:D:542:ARG:N	2.55	0.40
2:F:614:TRP:HZ3	7:F:701:NAG:HN2	1.70	0.40
4:H:145:TYR:HD2	4:H:149:PRO:HA	1.86	0.40
3:I:121:SER:O	3:I:121:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	419/496 (84%)	393 (94%)	26 (6%)	0	100	100
1	C	430/496 (87%)	412 (96%)	18 (4%)	0	100	100
1	E	430/496 (87%)	373 (87%)	55 (13%)	2 (0%)	24	56
2	B	123/162 (76%)	118 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	117/162 (72%)	114 (97%)	3 (3%)	0	100	100
2	F	117/162 (72%)	105 (90%)	11 (9%)	1 (1%)	14	45
3	G	180/229 (79%)	170 (94%)	10 (6%)	0	100	100
3	I	180/229 (79%)	171 (95%)	9 (5%)	0	100	100
4	H	152/245 (62%)	149 (98%)	3 (2%)	0	100	100
4	J	152/245 (62%)	151 (99%)	1 (1%)	0	100	100
All	All	2300/2922 (79%)	2156 (94%)	141 (6%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	498	PRO
1	E	38	VAL
2	F	615	SER

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	384/440 (87%)	384 (100%)	0	100	100
1	C	393/440 (89%)	393 (100%)	0	100	100
1	E	393/440 (89%)	393 (100%)	0	100	100
2	B	109/137 (80%)	109 (100%)	0	100	100
2	D	104/137 (76%)	104 (100%)	0	100	100
2	F	104/137 (76%)	104 (100%)	0	100	100
3	G	165/196 (84%)	165 (100%)	0	100	100
3	I	165/196 (84%)	165 (100%)	0	100	100
4	H	132/207 (64%)	132 (100%)	0	100	100
4	J	132/207 (64%)	132 (100%)	0	100	100
All	All	2081/2537 (82%)	2081 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	72	HIS
1	A	203	GLN
1	A	249	HIS
1	A	348	GLN
1	A	432	GLN
2	B	543	ASN
2	B	550	GLN
2	B	616	ASN
2	B	650	GLN
1	C	130	GLN
1	C	177	ASN
1	C	188	ASN
1	C	328	GLN
1	C	352	HIS
2	D	591	GLN
1	E	99	ASN
1	E	114	GLN
1	E	293	GLN
2	F	575	GLN
3	G	17	GLN
3	I	169	ASN
3	I	170	ASN
3	I	188	HIS
3	I	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

58 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	$\# Z > 2$
5	NAG	K	1	1,5	14,14,15	0.69	0	17,19,21	1.26	2 (11%)
5	NAG	K	2	5	14,14,15	0.71	0	17,19,21	0.98	2 (11%)
6	NAG	L	1	1,6	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
6	NAG	L	2	6	14,14,15	0.71	0	17,19,21	1.75	3 (17%)
6	BMA	L	3	6	11,11,12	0.89	1 (9%)	15,15,17	2.66	4 (26%)
5	NAG	M	1	1,5	14,14,15	0.71	0	17,19,21	1.26	1 (5%)
5	NAG	M	2	5	14,14,15	0.71	0	17,19,21	1.66	2 (11%)
5	NAG	N	1	1,5	14,14,15	0.69	0	17,19,21	1.30	2 (11%)
5	NAG	N	2	5	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
6	NAG	O	1	1,6	14,14,15	0.70	0	17,19,21	1.26	2 (11%)
6	NAG	O	2	6	14,14,15	0.73	0	17,19,21	0.97	0
6	BMA	O	3	6	11,11,12	0.92	1 (9%)	15,15,17	2.52	5 (33%)
5	NAG	P	1	1,5	14,14,15	0.66	0	17,19,21	1.24	1 (5%)
5	NAG	P	2	5	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
5	NAG	Q	1	1,5	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
5	NAG	Q	2	5	14,14,15	0.77	0	17,19,21	1.70	3 (17%)
6	NAG	R	1	1,6	14,14,15	0.76	0	17,19,21	1.23	2 (11%)
6	NAG	R	2	6	14,14,15	0.73	0	17,19,21	1.70	3 (17%)
6	BMA	R	3	6	11,11,12	0.91	1 (9%)	15,15,17	2.55	5 (33%)
6	NAG	S	1	1,6	14,14,15	0.71	0	17,19,21	1.28	1 (5%)
6	NAG	S	2	6	14,14,15	0.68	0	17,19,21	1.10	2 (11%)
6	BMA	S	3	6	11,11,12	0.87	0	15,15,17	2.89	6 (40%)
5	NAG	T	1	1,5	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
5	NAG	T	2	5	14,14,15	0.73	0	17,19,21	1.35	2 (11%)
5	NAG	U	1	1,5	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
5	NAG	U	2	5	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
6	NAG	V	1	1,6	14,14,15	0.73	0	17,19,21	1.30	2 (11%)
6	NAG	V	2	6	14,14,15	0.71	0	17,19,21	1.70	3 (17%)
6	BMA	V	3	6	11,11,12	0.92	1 (9%)	15,15,17	2.65	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	W	1	1,5	14,14,15	0.71	0	17,19,21	2.43	8 (47%)
5	NAG	W	2	5	14,14,15	0.74	0	17,19,21	1.17	1 (5%)
6	NAG	X	1	1,6	14,14,15	0.71	0	17,19,21	1.33	2 (11%)
6	NAG	X	2	6	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
6	BMA	X	3	6	11,11,12	0.90	1 (9%)	15,15,17	2.63	5 (33%)
5	NAG	Y	1	1,5	14,14,15	0.69	0	17,19,21	1.21	2 (11%)
5	NAG	Y	2	5	14,14,15	0.69	0	17,19,21	0.90	1 (5%)
5	NAG	Z	1	1,5	14,14,15	0.84	0	17,19,21	3.43	7 (41%)
5	NAG	Z	2	5	14,14,15	0.85	1 (7%)	17,19,21	3.22	5 (29%)
5	NAG	a	1	1,5	14,14,15	0.68	0	17,19,21	1.64	3 (17%)
5	NAG	a	2	5	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
5	NAG	b	1	1,5	14,14,15	0.67	0	17,19,21	1.19	1 (5%)
5	NAG	b	2	5	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
6	NAG	c	1	1,6	14,14,15	0.66	0	17,19,21	3.15	5 (29%)
6	NAG	c	2	6	14,14,15	0.73	0	17,19,21	1.18	2 (11%)
6	BMA	c	3	6	11,11,12	0.88	1 (9%)	15,15,17	2.84	6 (40%)
6	NAG	d	1	6	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
6	NAG	d	2	6	14,14,15	0.79	0	17,19,21	1.79	3 (17%)
6	BMA	d	3	6	11,11,12	0.83	0	15,15,17	2.88	5 (33%)
5	NAG	e	1	1,5	14,14,15	0.69	0	17,19,21	1.36	2 (11%)
5	NAG	e	2	5	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
5	NAG	f	1	1,5	14,14,15	0.71	0	17,19,21	1.14	3 (17%)
5	NAG	f	2	5	14,14,15	0.69	0	17,19,21	1.17	1 (5%)
6	NAG	g	1	1,6	14,14,15	0.69	0	17,19,21	1.05	1 (5%)
6	NAG	g	2	6	14,14,15	0.69	0	17,19,21	1.08	1 (5%)
6	BMA	g	3	6	11,11,12	0.91	1 (9%)	15,15,17	2.77	6 (40%)
6	NAG	h	1	1,6	14,14,15	0.82	0	17,19,21	1.91	5 (29%)
6	NAG	h	2	6	14,14,15	0.81	0	17,19,21	1.73	3 (17%)
6	BMA	h	3	6	11,11,12	0.77	0	15,15,17	3.38	5 (33%)

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
5	NAG	K	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	3/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	3/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	c	2	6	-	0/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	NAG	d	1	6	-	1/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
5	NAG	e	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	1/6/23/26	0/1/1/1
5	NAG	f	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
6	NAG	g	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	0/2/19/22	0/1/1/1
6	NAG	h	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
6	BMA	h	3	6	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	2	NAG	C1-C2	2.19	1.55	1.52
6	V	3	BMA	C2-C3	2.17	1.55	1.52
6	O	3	BMA	C2-C3	2.12	1.55	1.52
6	R	3	BMA	C2-C3	2.12	1.55	1.52
6	L	3	BMA	C2-C3	2.10	1.55	1.52
6	c	3	BMA	C2-C3	2.09	1.55	1.52
6	X	3	BMA	C2-C3	2.08	1.55	1.52
6	g	3	BMA	C2-C3	2.07	1.55	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	1	NAG	C2-N2-C7	11.33	138.09	122.90
5	Z	2	NAG	C2-N2-C7	11.20	137.91	122.90
6	h	3	BMA	C1-O5-C5	11.11	127.08	112.19
6	c	1	NAG	C1-O5-C5	10.12	125.75	112.19
6	S	3	BMA	C1-O5-C5	9.08	124.36	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	d	3	BMA	C1-O5-C5	8.85	124.05	112.19
6	c	3	BMA	C1-O5-C5	8.51	123.59	112.19
6	V	3	BMA	C1-O5-C5	8.42	123.47	112.19
6	L	3	BMA	C1-O5-C5	8.40	123.45	112.19
6	g	3	BMA	C1-O5-C5	8.24	123.23	112.19
6	X	3	BMA	C1-O5-C5	8.23	123.22	112.19
6	R	3	BMA	C1-O5-C5	7.89	122.76	112.19
6	O	3	BMA	C1-O5-C5	7.80	122.64	112.19
6	c	1	NAG	C2-N2-C7	5.61	130.42	122.90
5	W	1	NAG	C1-O5-C5	5.54	119.62	112.19
5	W	1	NAG	C2-N2-C7	5.27	129.96	122.90
5	a	1	NAG	C1-O5-C5	5.17	119.12	112.19
6	L	2	NAG	C2-N2-C7	5.16	129.81	122.90
6	V	2	NAG	C2-N2-C7	5.12	129.76	122.90
6	h	1	NAG	C2-N2-C7	5.11	129.74	122.90
5	M	2	NAG	C2-N2-C7	5.06	129.68	122.90
6	d	2	NAG	C2-N2-C7	5.03	129.64	122.90
6	R	2	NAG	C2-N2-C7	4.98	129.57	122.90
6	h	2	NAG	C2-N2-C7	4.92	129.50	122.90
5	Q	2	NAG	C2-N2-C7	4.88	129.44	122.90
5	Z	1	NAG	C8-C7-N2	4.68	123.88	116.12
5	Z	2	NAG	C8-C7-N2	3.95	122.68	116.12
6	g	3	BMA	C2-C3-C4	3.83	117.59	110.86
6	c	3	BMA	C2-C3-C4	3.73	117.42	110.86
5	W	1	NAG	C1-C2-N2	3.73	116.30	110.43
5	Z	1	NAG	C4-C3-C2	3.68	116.41	111.02
5	Z	2	NAG	C1-O5-C5	3.61	117.02	112.19
6	d	3	BMA	C3-C4-C5	3.58	116.72	110.23
5	e	1	NAG	C1-O5-C5	3.50	116.88	112.19
6	V	3	BMA	C2-C3-C4	3.44	116.92	110.86
6	L	3	BMA	C2-C3-C4	3.42	116.88	110.86
6	X	1	NAG	C2-N2-C7	3.41	127.47	122.90
6	S	3	BMA	C2-C3-C4	3.38	116.81	110.86
6	h	3	BMA	C3-C4-C5	3.37	116.34	110.23
6	X	3	BMA	C2-C3-C4	3.35	116.75	110.86
5	U	1	NAG	C2-N2-C7	3.32	127.35	122.90
5	M	1	NAG	C2-N2-C7	3.32	127.35	122.90
6	c	3	BMA	C1-C2-C3	3.32	114.48	109.64
5	T	2	NAG	C2-N2-C7	3.31	127.33	122.90
6	R	3	BMA	C2-C3-C4	3.31	116.68	110.86
5	Z	1	NAG	C1-C2-N2	3.30	115.63	110.43
6	O	1	NAG	C2-N2-C7	3.29	127.31	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	BMA	C2-C3-C4	3.25	116.58	110.86
5	T	2	NAG	C1-O5-C5	3.23	116.51	112.19
5	f	2	NAG	C2-N2-C7	3.23	127.22	122.90
5	N	1	NAG	C2-N2-C7	3.22	127.21	122.90
6	d	3	BMA	C2-C3-C4	3.20	116.48	110.86
5	b	1	NAG	C2-N2-C7	3.15	127.12	122.90
5	K	1	NAG	C2-N2-C7	3.14	127.11	122.90
6	h	1	NAG	C1-O5-C5	3.10	116.34	112.19
5	T	1	NAG	C2-N2-C7	3.08	127.03	122.90
6	g	3	BMA	C1-C2-C3	3.08	114.13	109.64
6	h	3	BMA	C2-C3-C4	3.06	116.24	110.86
6	S	3	BMA	C3-C4-C5	3.05	115.77	110.23
5	W	2	NAG	C1-O5-C5	3.05	116.27	112.19
5	e	1	NAG	C2-N2-C7	3.01	126.94	122.90
5	b	2	NAG	C1-O5-C5	2.99	116.19	112.19
5	Z	2	NAG	C1-C2-N2	2.91	115.01	110.43
6	g	2	NAG	C1-O5-C5	2.90	116.07	112.19
5	P	2	NAG	C1-O5-C5	2.89	116.06	112.19
5	P	1	NAG	C2-N2-C7	2.88	126.76	122.90
6	S	2	NAG	C1-O5-C5	2.84	116.00	112.19
5	Y	1	NAG	C2-N2-C7	2.83	126.69	122.90
5	U	2	NAG	C1-O5-C5	2.80	115.93	112.19
5	e	2	NAG	C1-O5-C5	2.77	115.89	112.19
6	V	1	NAG	C1-O5-C5	2.69	115.79	112.19
6	c	1	NAG	O7-C7-N2	2.66	126.68	121.98
6	h	3	BMA	O5-C5-C4	2.65	117.26	110.83
6	R	1	NAG	C1-O5-C5	2.62	115.69	112.19
5	Q	1	NAG	C1-O5-C5	2.59	115.66	112.19
6	d	3	BMA	O4-C4-C3	-2.59	104.27	110.38
6	X	1	NAG	C1-O5-C5	2.56	115.61	112.19
5	f	1	NAG	O5-C1-C2	-2.54	107.36	111.29
6	X	3	BMA	C3-C4-C5	2.54	114.84	110.23
5	N	1	NAG	C1-O5-C5	2.54	115.59	112.19
6	O	3	BMA	C3-C4-C5	2.54	114.83	110.23
6	c	1	NAG	C1-C2-N2	2.53	114.41	110.43
5	U	1	NAG	C1-O5-C5	2.51	115.55	112.19
5	Z	2	NAG	O7-C7-C8	-2.49	117.62	122.05
5	Z	1	NAG	O7-C7-C8	-2.48	117.64	122.05
5	a	1	NAG	C1-C2-N2	2.47	114.32	110.43
6	d	2	NAG	C1-O5-C5	2.46	115.49	112.19
5	Q	2	NAG	C1-O5-C5	2.46	115.49	112.19
6	S	3	BMA	O4-C4-C3	-2.46	104.57	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	d	3	BMA	O5-C5-C4	2.44	116.78	110.83
6	L	1	NAG	C1-O5-C5	2.44	115.45	112.19
6	c	2	NAG	C1-O5-C5	2.43	115.45	112.19
6	R	2	NAG	C1-O5-C5	2.41	115.42	112.19
6	h	3	BMA	O4-C4-C3	-2.41	104.69	110.38
5	K	1	NAG	C1-O5-C5	2.40	115.40	112.19
5	W	1	NAG	O3-C3-C4	2.38	115.99	110.38
6	h	2	NAG	O7-C7-N2	2.37	126.17	121.98
6	S	1	NAG	C4-C3-C2	2.37	114.48	111.02
6	h	1	NAG	O5-C1-C2	-2.36	107.64	111.29
6	R	3	BMA	C3-C4-C5	2.34	114.47	110.23
6	d	2	NAG	O7-C7-N2	2.32	126.09	121.98
6	L	2	NAG	O5-C1-C2	-2.32	107.70	111.29
6	L	2	NAG	O7-C7-N2	2.31	126.06	121.98
6	h	2	NAG	C4-C3-C2	2.31	114.40	111.02
6	V	3	BMA	C3-C4-C5	2.30	114.40	110.23
5	Q	2	NAG	O7-C7-N2	2.29	126.03	121.98
5	a	1	NAG	O5-C1-C2	-2.28	107.76	111.29
6	h	1	NAG	O7-C7-N2	2.27	126.00	121.98
6	g	3	BMA	C3-C4-C5	2.26	114.33	110.23
6	V	1	NAG	O4-C4-C3	-2.26	105.06	110.38
6	V	2	NAG	O7-C7-N2	2.25	125.96	121.98
5	W	1	NAG	O7-C7-N2	2.25	125.95	121.98
5	M	2	NAG	O7-C7-N2	2.24	125.94	121.98
6	S	2	NAG	O5-C1-C2	-2.24	107.83	111.29
6	g	3	BMA	O4-C4-C3	-2.23	105.12	110.38
6	L	3	BMA	C3-C4-C5	2.23	114.27	110.23
6	c	2	NAG	C4-C3-C2	2.22	114.28	111.02
5	f	1	NAG	C1-O5-C5	2.22	115.16	112.19
5	K	2	NAG	C1-O5-C5	2.21	115.15	112.19
5	a	2	NAG	C1-O5-C5	2.18	115.11	112.19
5	Z	1	NAG	C1-O5-C5	2.18	115.11	112.19
6	h	1	NAG	C4-C3-C2	2.18	114.21	111.02
6	L	3	BMA	O3-C3-C2	-2.18	105.61	110.05
5	N	2	NAG	C1-O5-C5	2.17	115.09	112.19
5	Y	1	NAG	C1-O5-C5	2.16	115.08	112.19
5	f	1	NAG	O4-C4-C3	-2.16	105.28	110.38
6	g	1	NAG	C1-O5-C5	2.16	115.08	112.19
6	c	3	BMA	C3-C4-C5	2.15	114.14	110.23
5	Z	1	NAG	O4-C4-C3	-2.15	105.30	110.38
6	R	2	NAG	O7-C7-N2	2.15	125.78	121.98
6	R	1	NAG	C4-C3-C2	2.14	114.15	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	3	BMA	O3-C3-C2	-2.14	105.69	110.05
6	V	2	NAG	O5-C1-C2	-2.13	107.99	111.29
6	c	3	BMA	O4-C4-C3	-2.13	105.36	110.38
6	X	3	BMA	O4-C4-C3	-2.12	105.37	110.38
6	c	3	BMA	O3-C3-C2	-2.12	105.72	110.05
6	O	3	BMA	O4-C4-C3	-2.12	105.38	110.38
6	S	3	BMA	O5-C5-C4	2.12	115.98	110.83
5	W	1	NAG	O5-C1-C2	-2.11	108.02	111.29
6	R	3	BMA	O3-C3-C2	-2.11	105.75	110.05
6	c	1	NAG	C3-C4-C5	-2.10	106.42	110.23
6	O	1	NAG	C1-O5-C5	2.09	114.99	112.19
6	V	3	BMA	O3-C3-C2	-2.08	105.81	110.05
6	g	3	BMA	O3-C3-C2	-2.07	105.82	110.05
5	K	2	NAG	O5-C1-C2	-2.07	108.09	111.29
6	O	3	BMA	O3-C3-C2	-2.06	105.84	110.05
5	W	1	NAG	C3-C4-C5	-2.05	106.52	110.23
5	Y	2	NAG	O5-C1-C2	-2.05	108.12	111.29
5	W	1	NAG	O3-C3-C2	-2.04	105.16	109.40
6	S	3	BMA	O3-C3-C2	-2.04	105.88	110.05
6	d	1	NAG	O3-C3-C4	2.04	115.18	110.38
6	R	3	BMA	O4-C4-C3	-2.03	105.59	110.38
6	X	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	2	NAG	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	e	1	NAG	C8-C7-N2-C2
5	e	1	NAG	O7-C7-N2-C2
5	f	2	NAG	C8-C7-N2-C2
5	f	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	L	2	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	C3-C2-N2-C7
5	Z	2	NAG	C3-C2-N2-C7
6	L	2	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	c	1	NAG	C3-C2-N2-C7
6	h	1	NAG	C3-C2-N2-C7
6	h	2	NAG	C3-C2-N2-C7
5	M	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

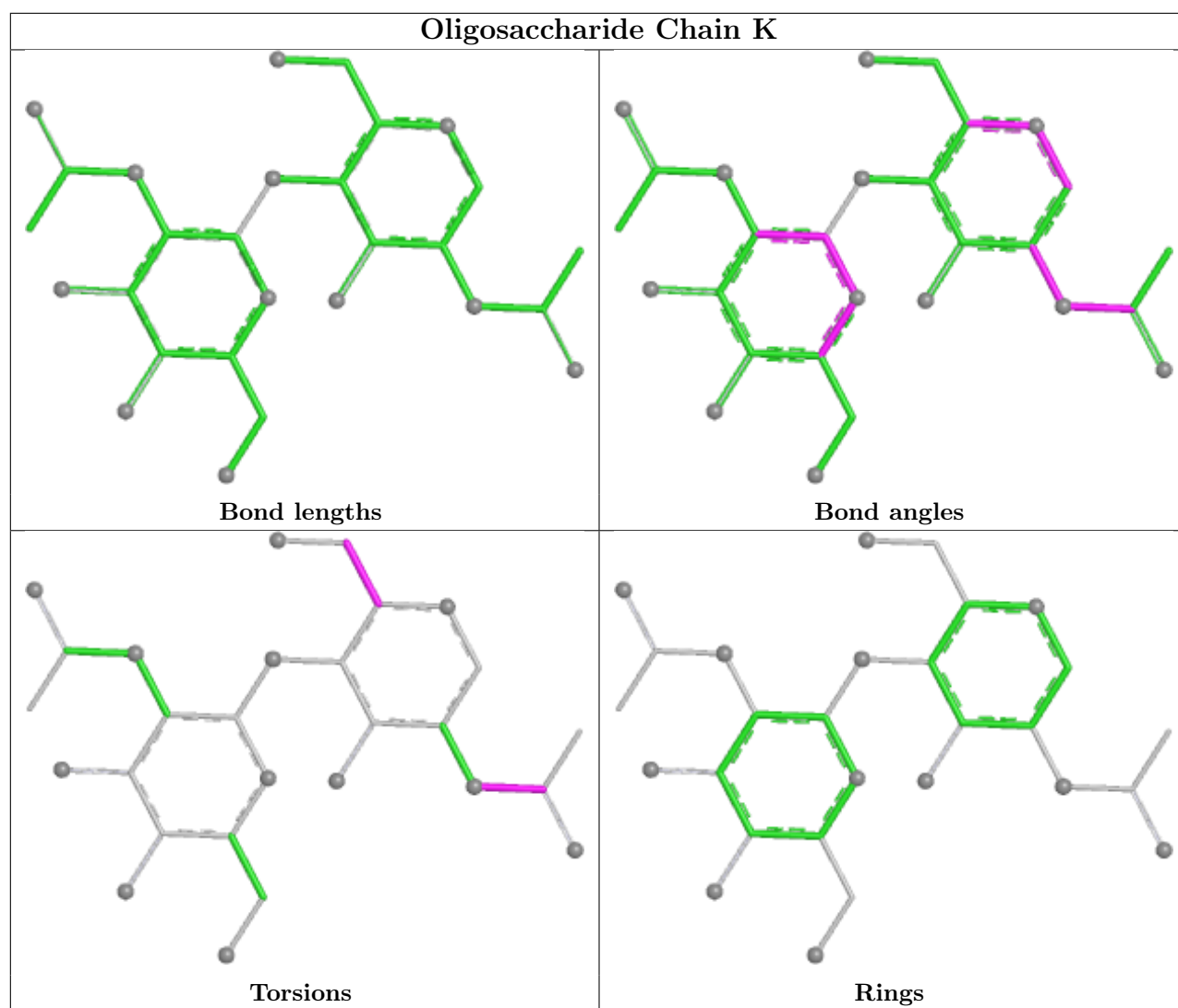
Mol	Chain	Res	Type	Atoms
5	Q	2	NAG	C1-C2-N2-C7
5	W	1	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7
5	Z	2	NAG	C1-C2-N2-C7
6	L	2	NAG	C1-C2-N2-C7
6	R	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7
6	d	2	NAG	C1-C2-N2-C7
6	g	1	NAG	C1-C2-N2-C7
6	h	1	NAG	C1-C2-N2-C7
6	h	2	NAG	C1-C2-N2-C7
5	M	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	W	1	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
6	d	2	NAG	C3-C2-N2-C7
5	W	1	NAG	C4-C5-C6-O6

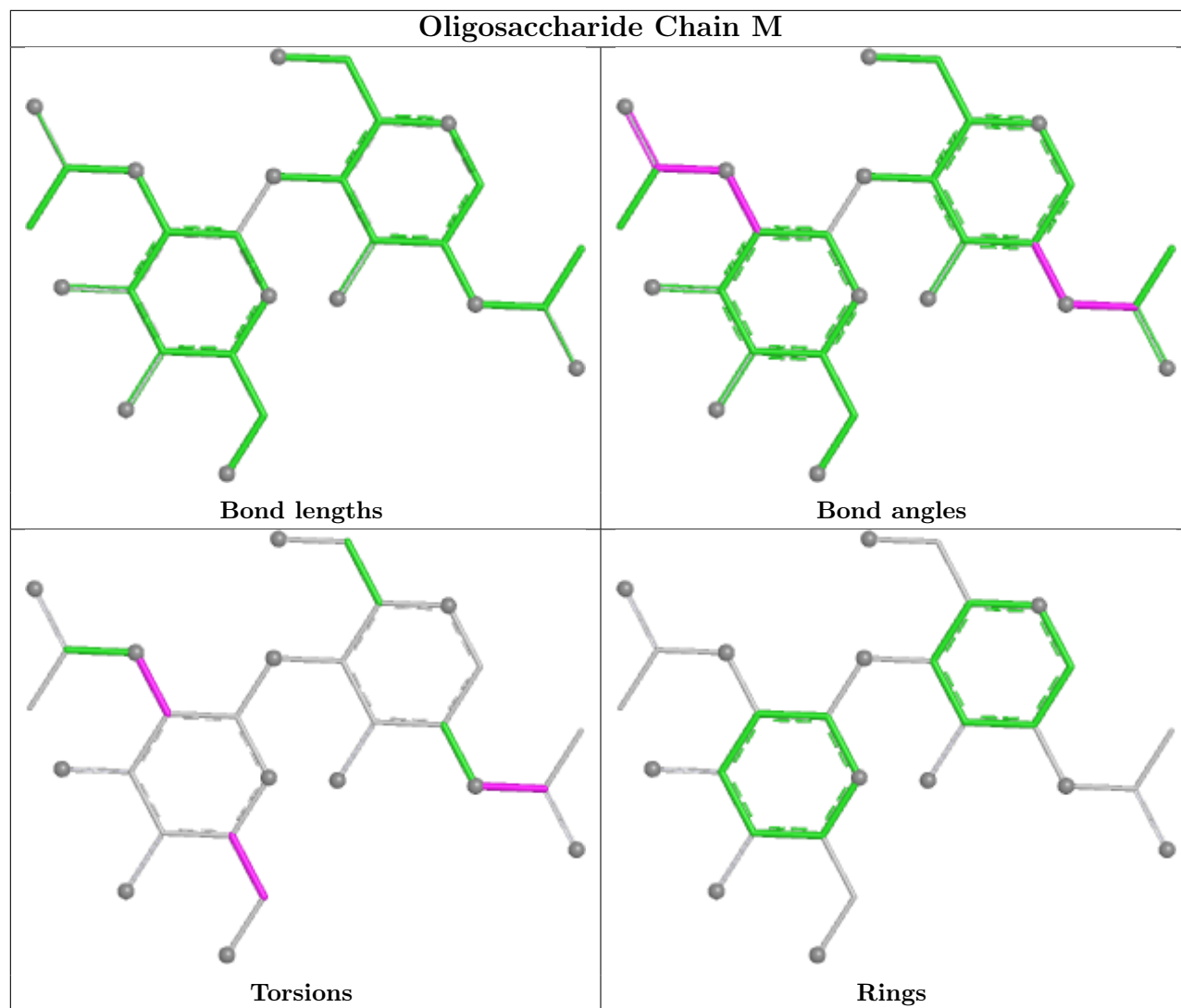
There are no ring outliers.

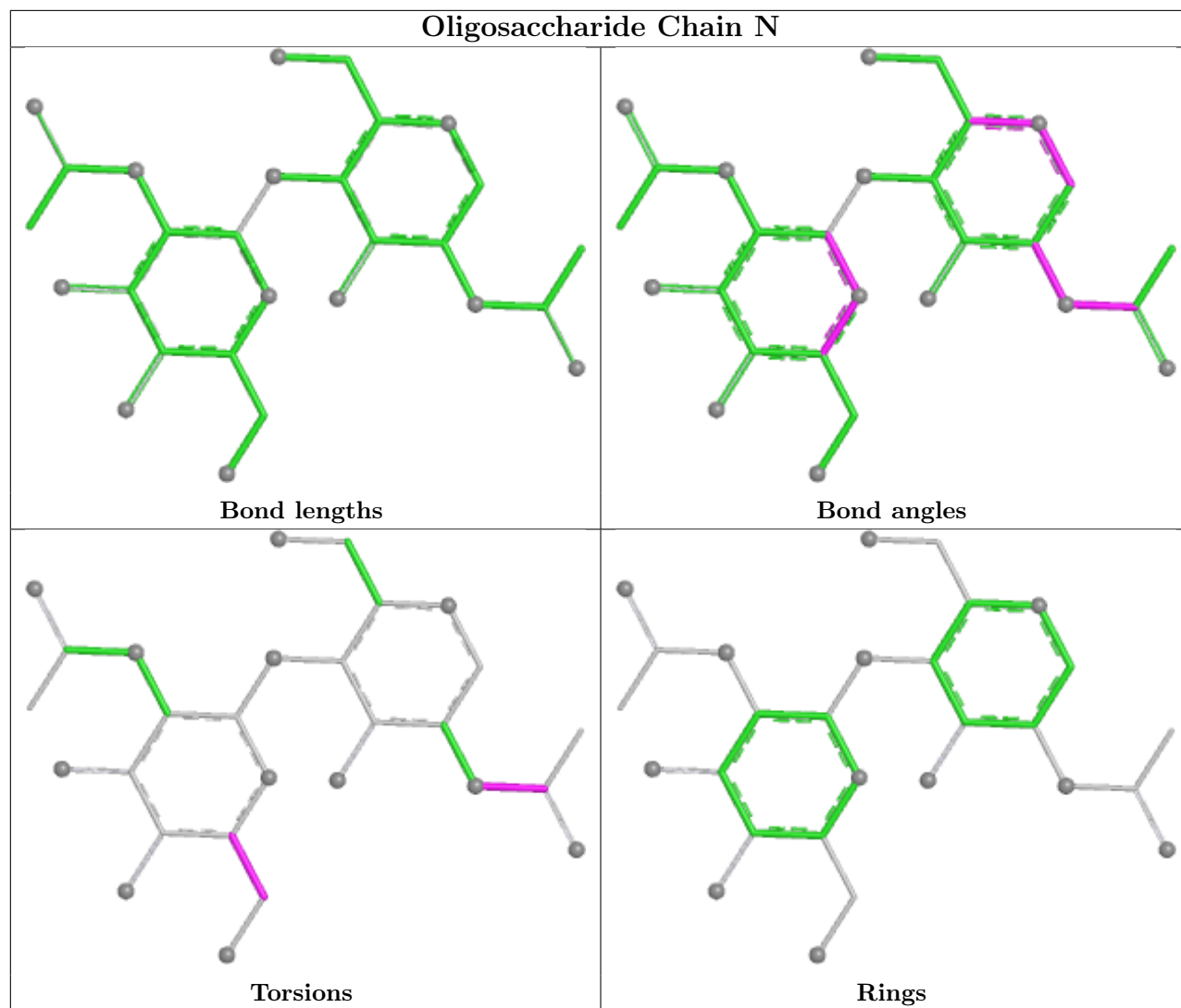
2 monomers are involved in 1 short contact:

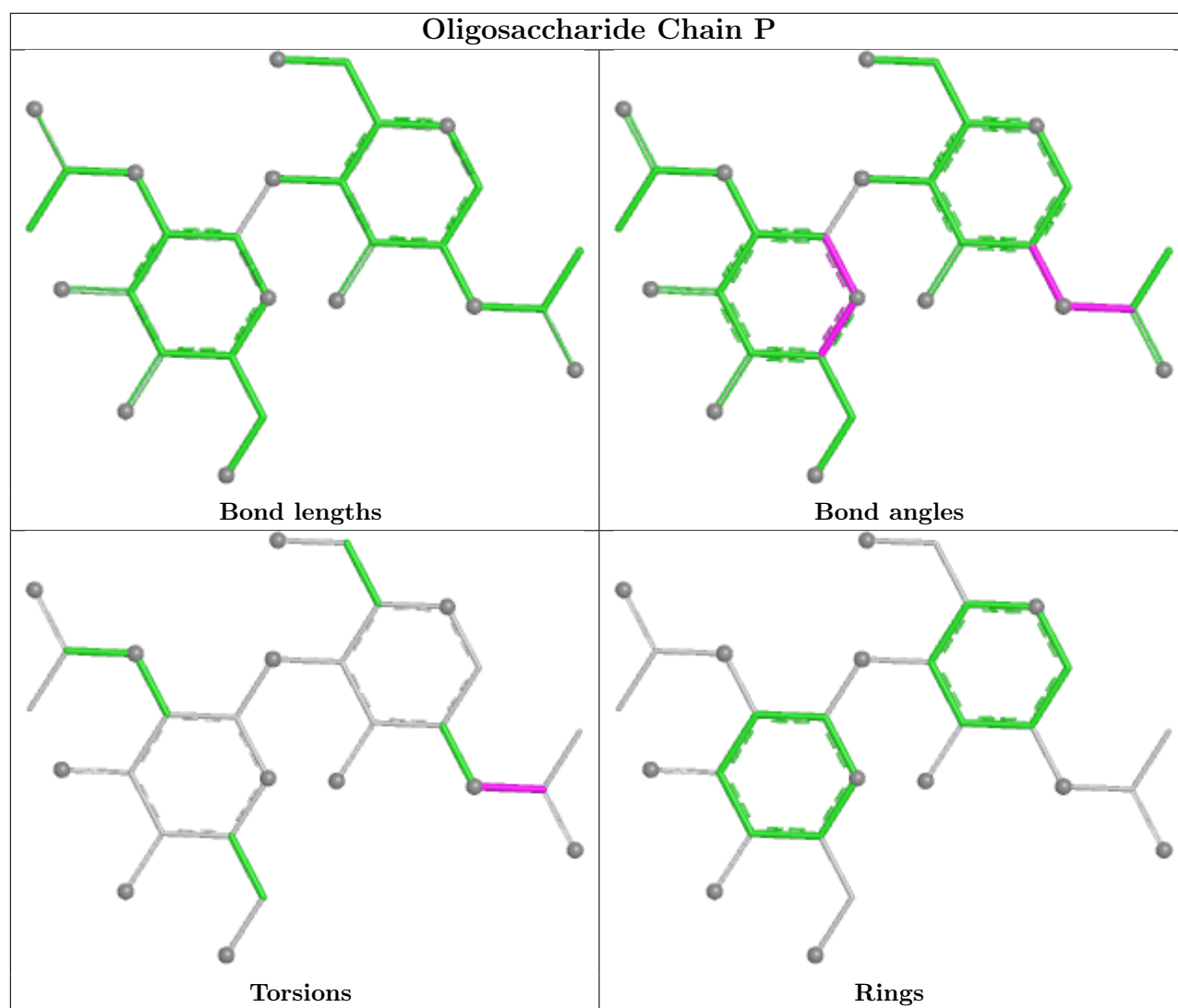
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	h	2	NAG	1	0
6	g	3	BMA	1	0

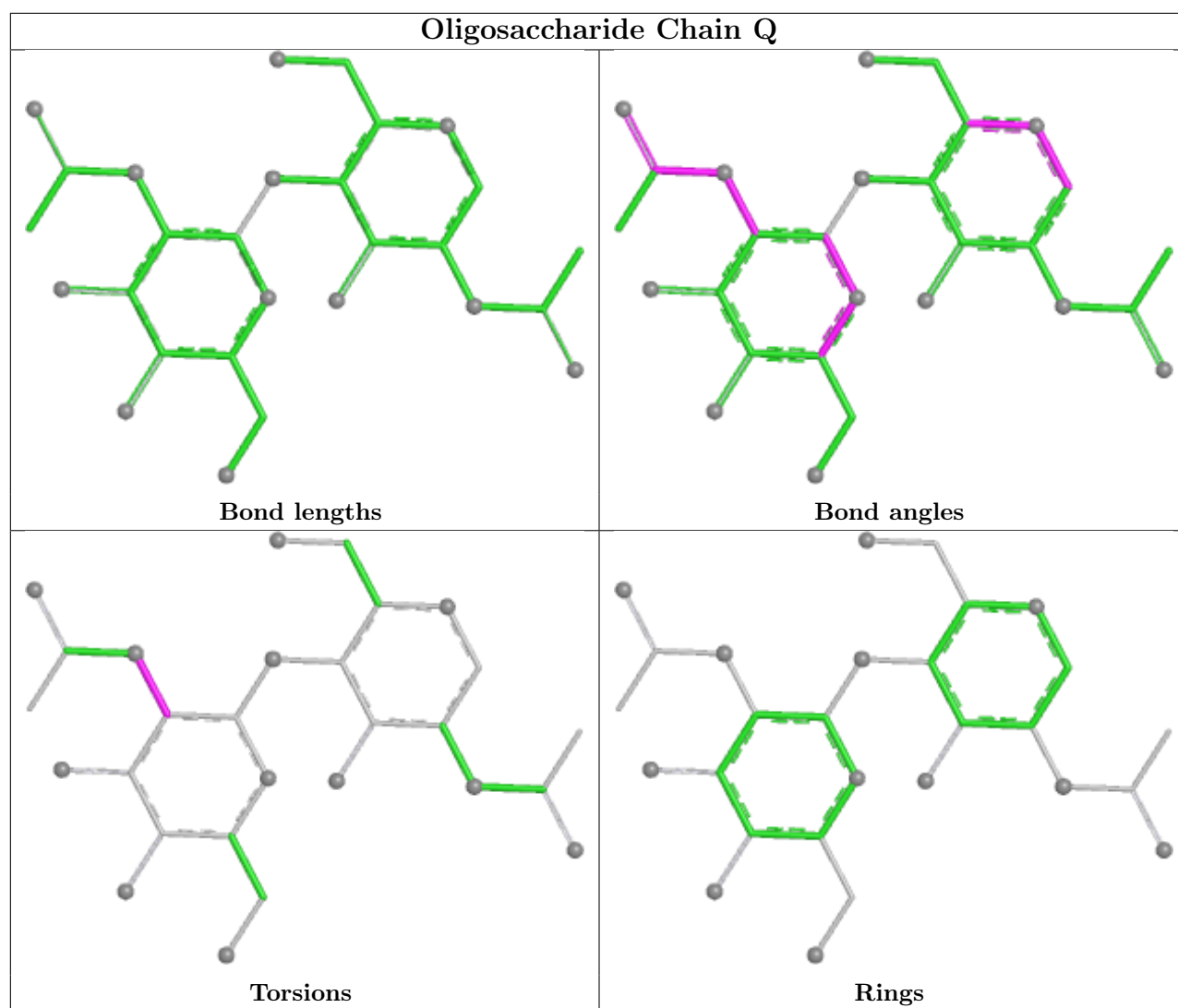
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

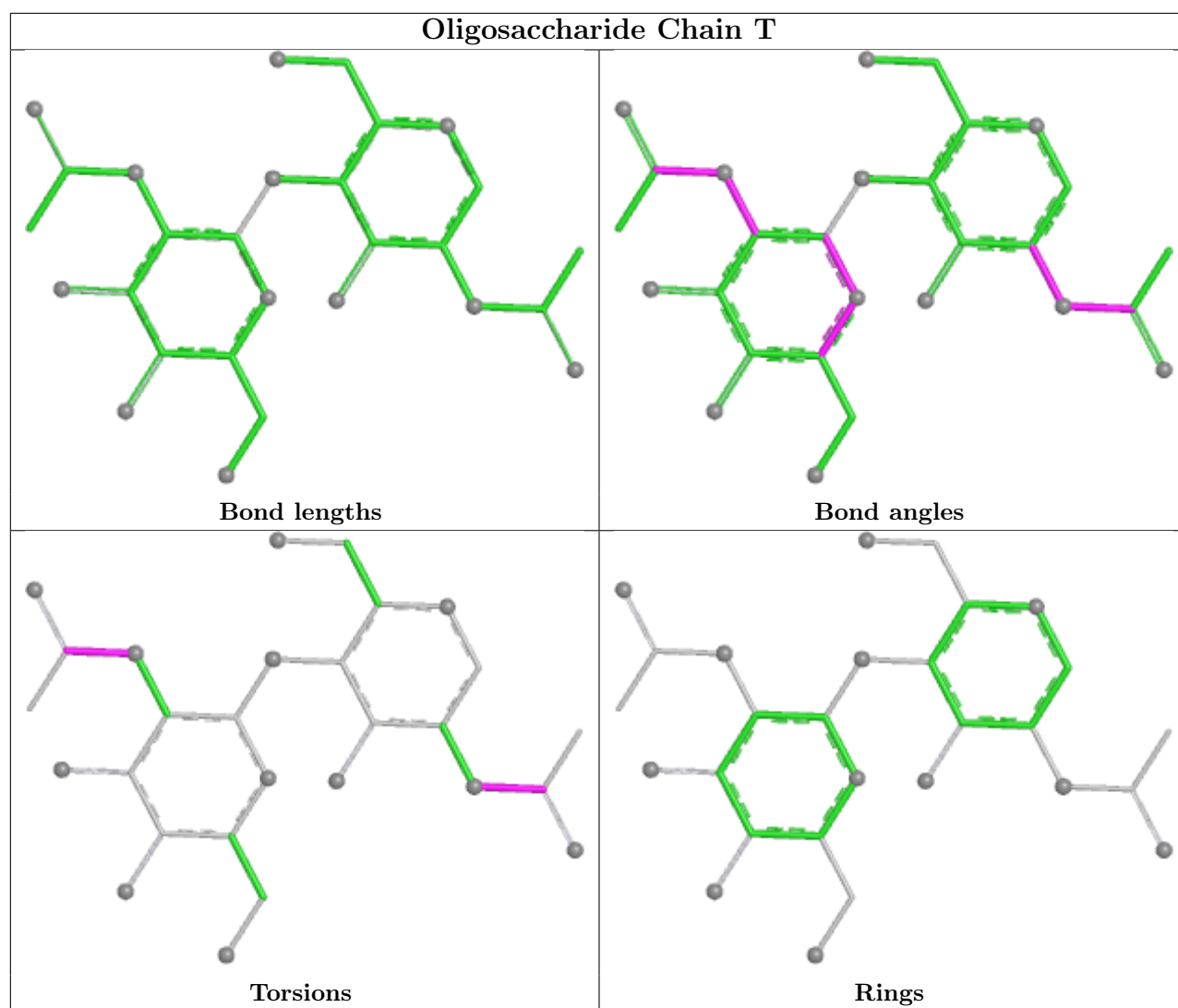


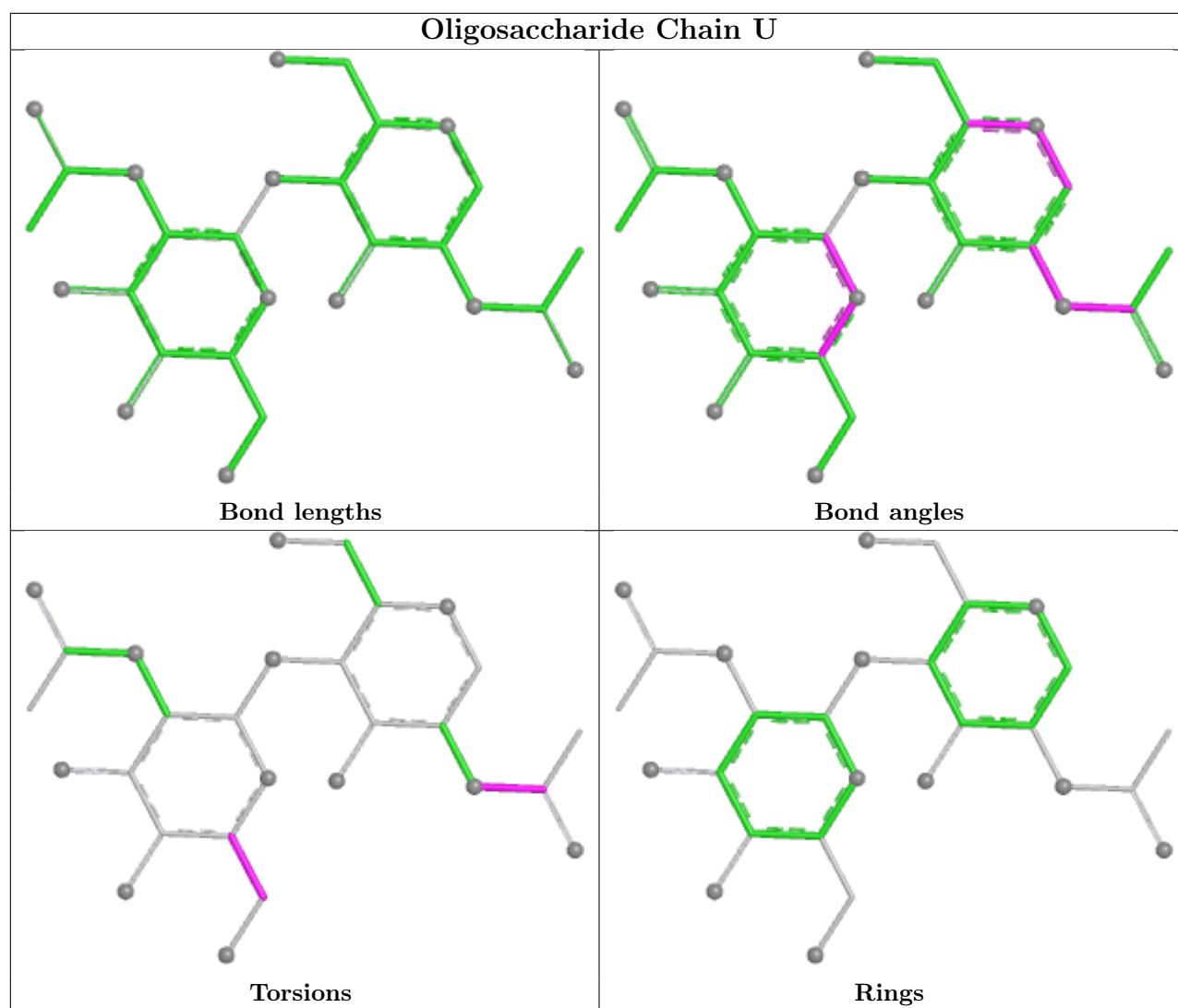


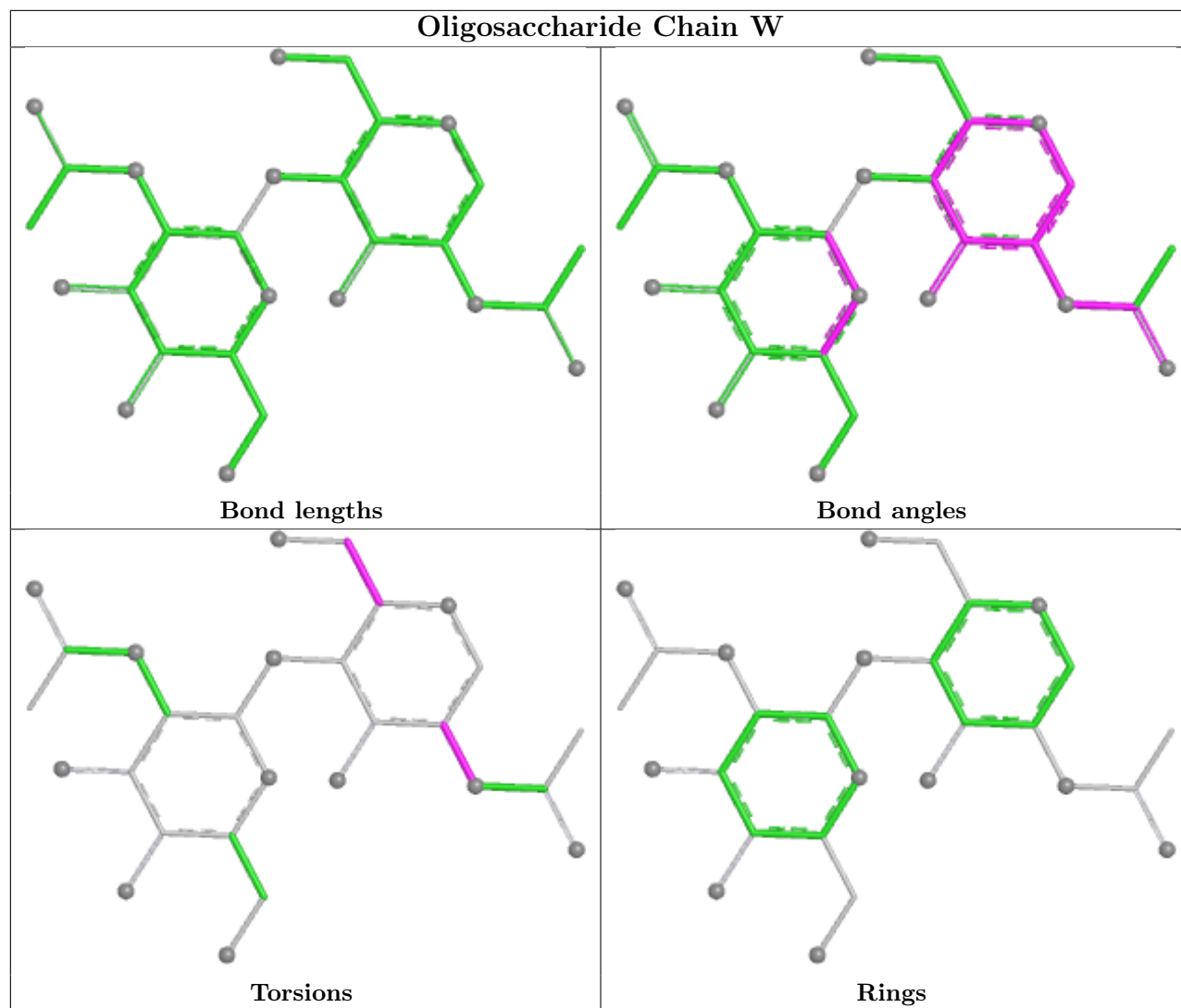


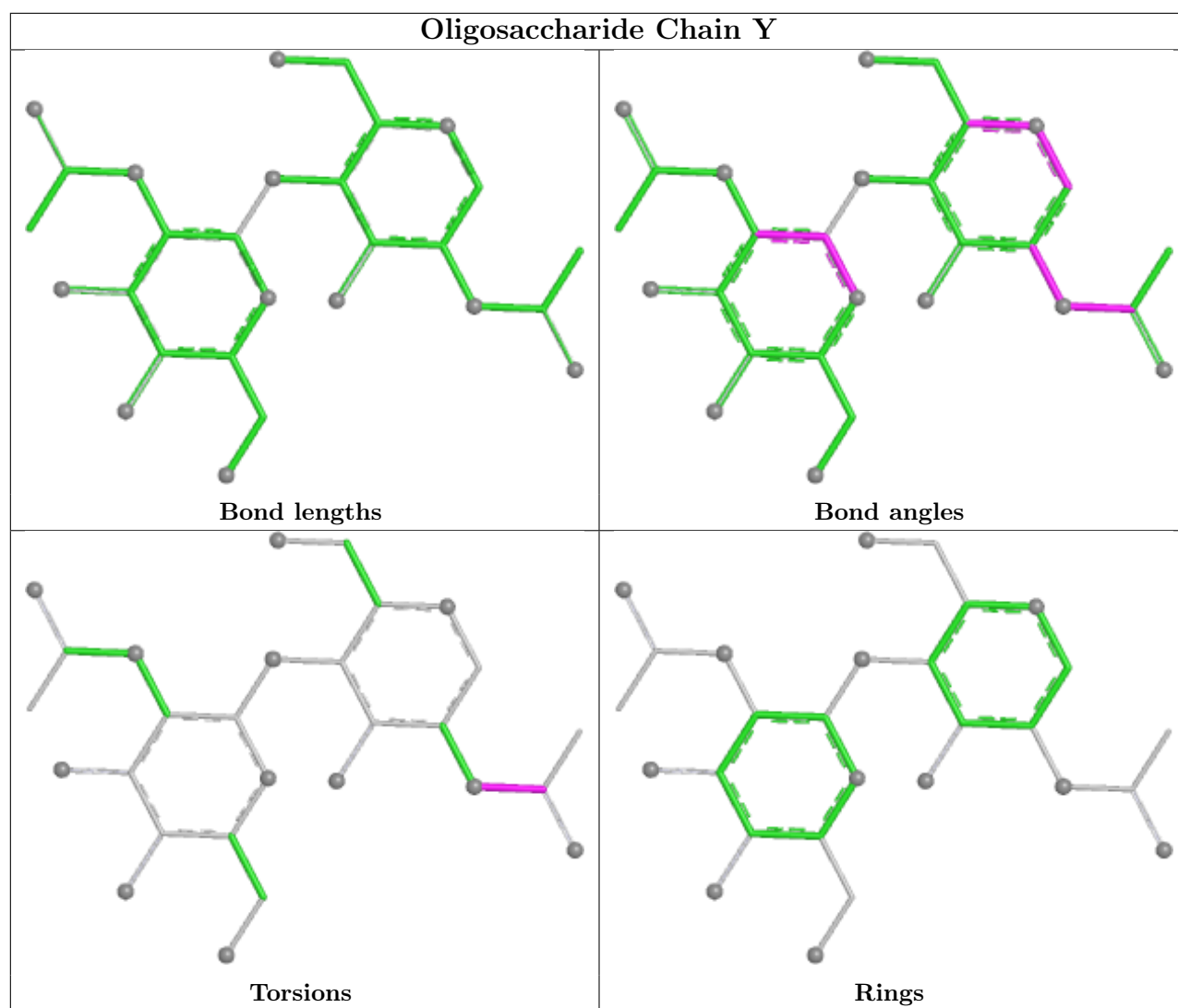


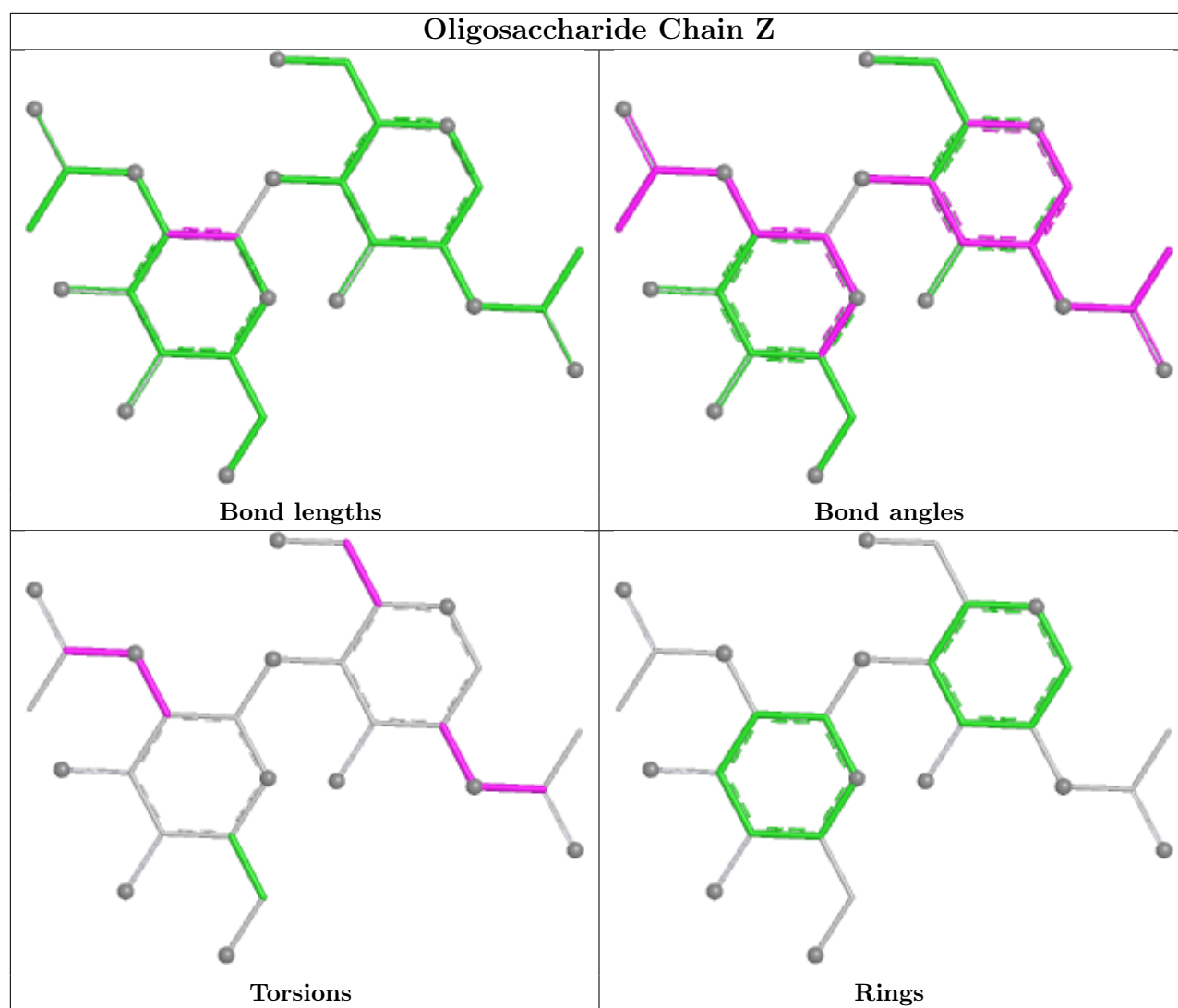


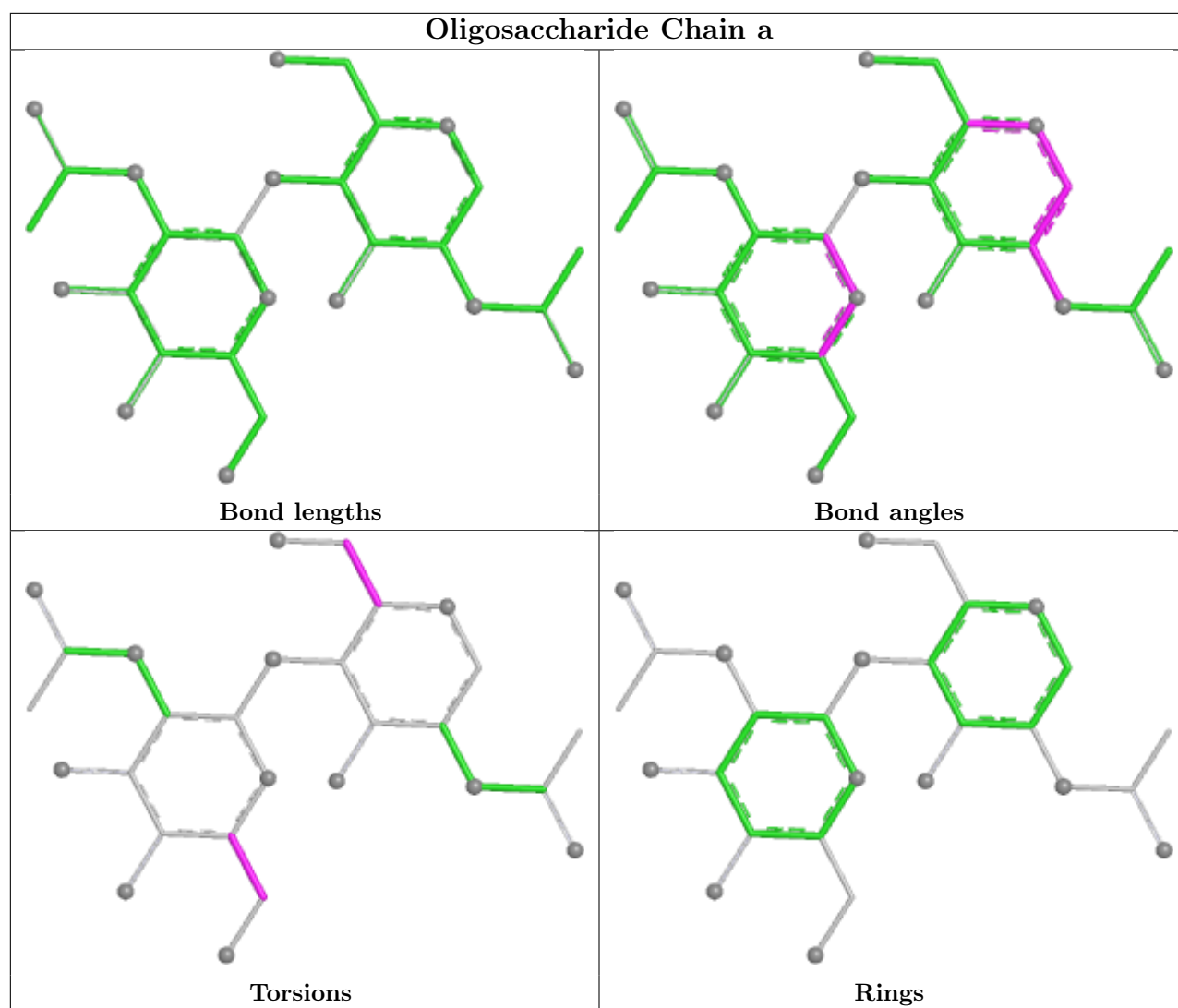


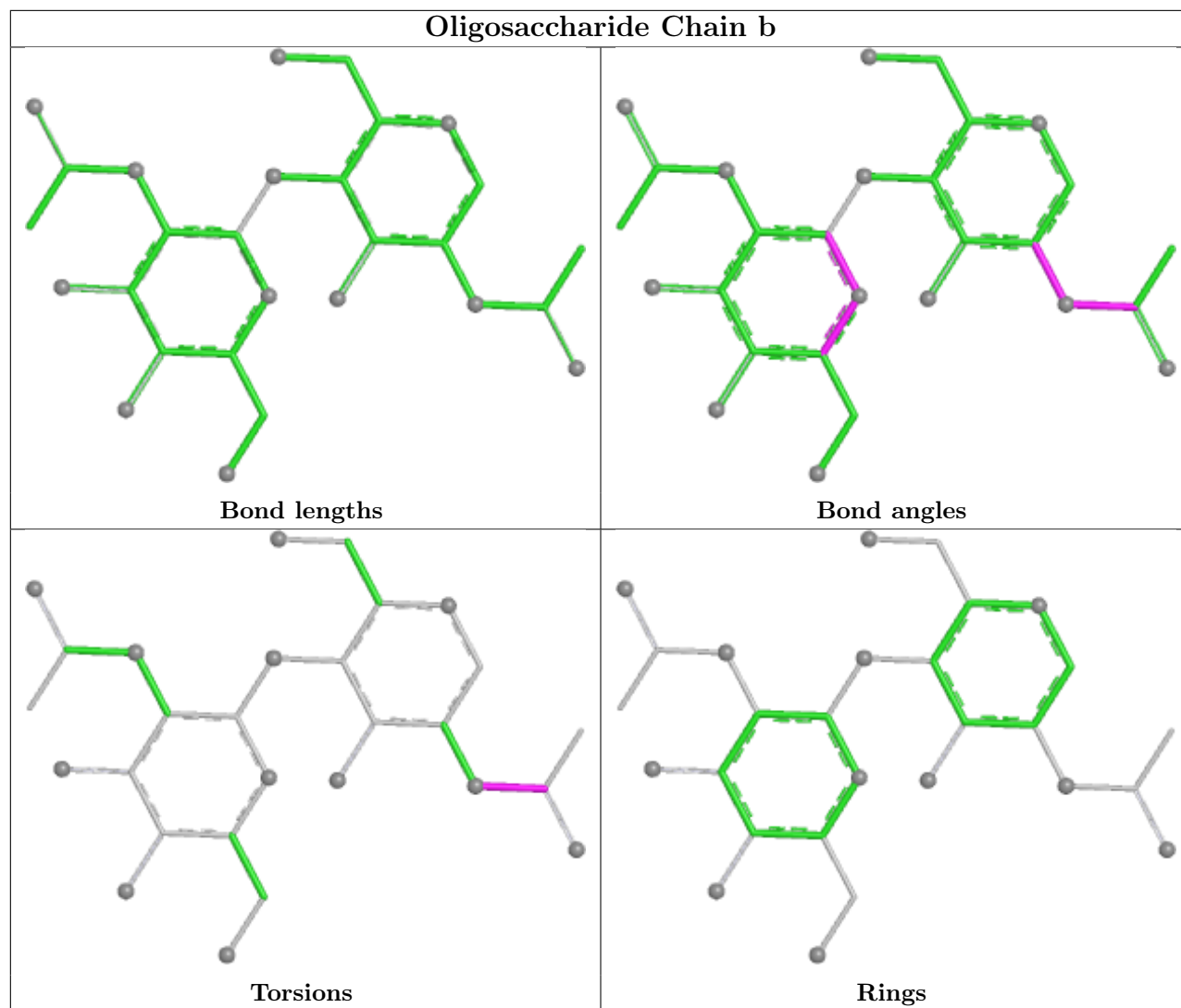


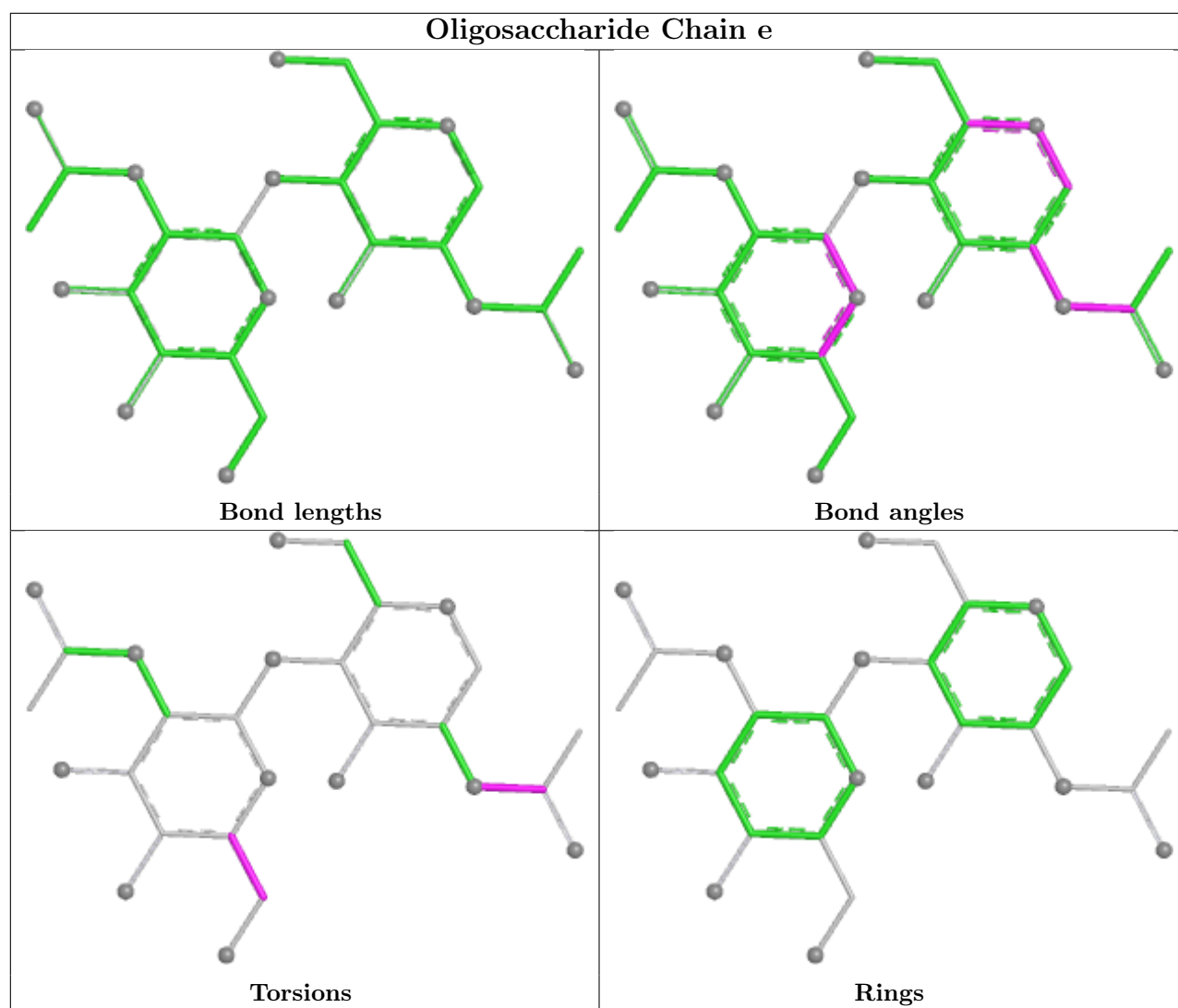


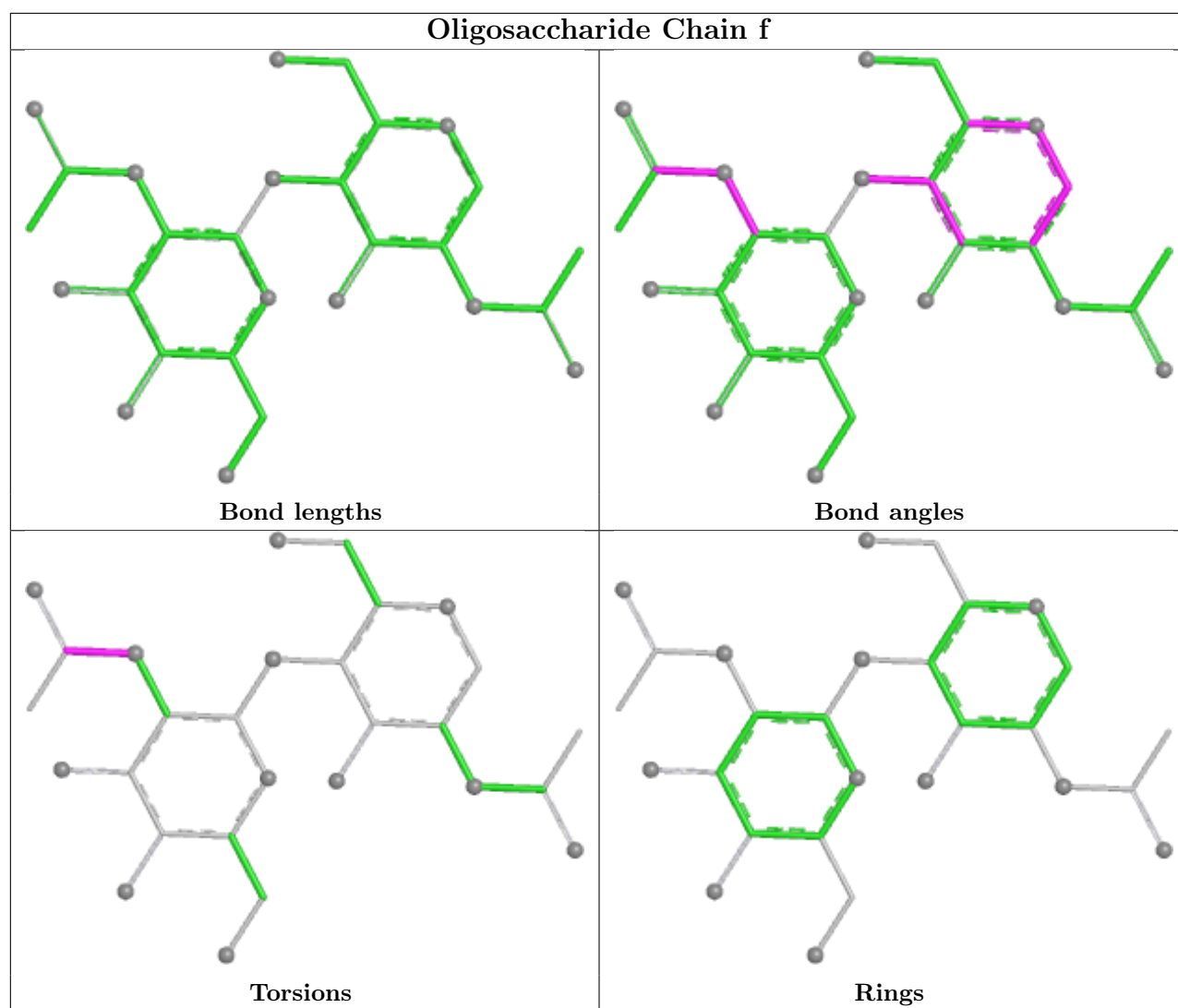


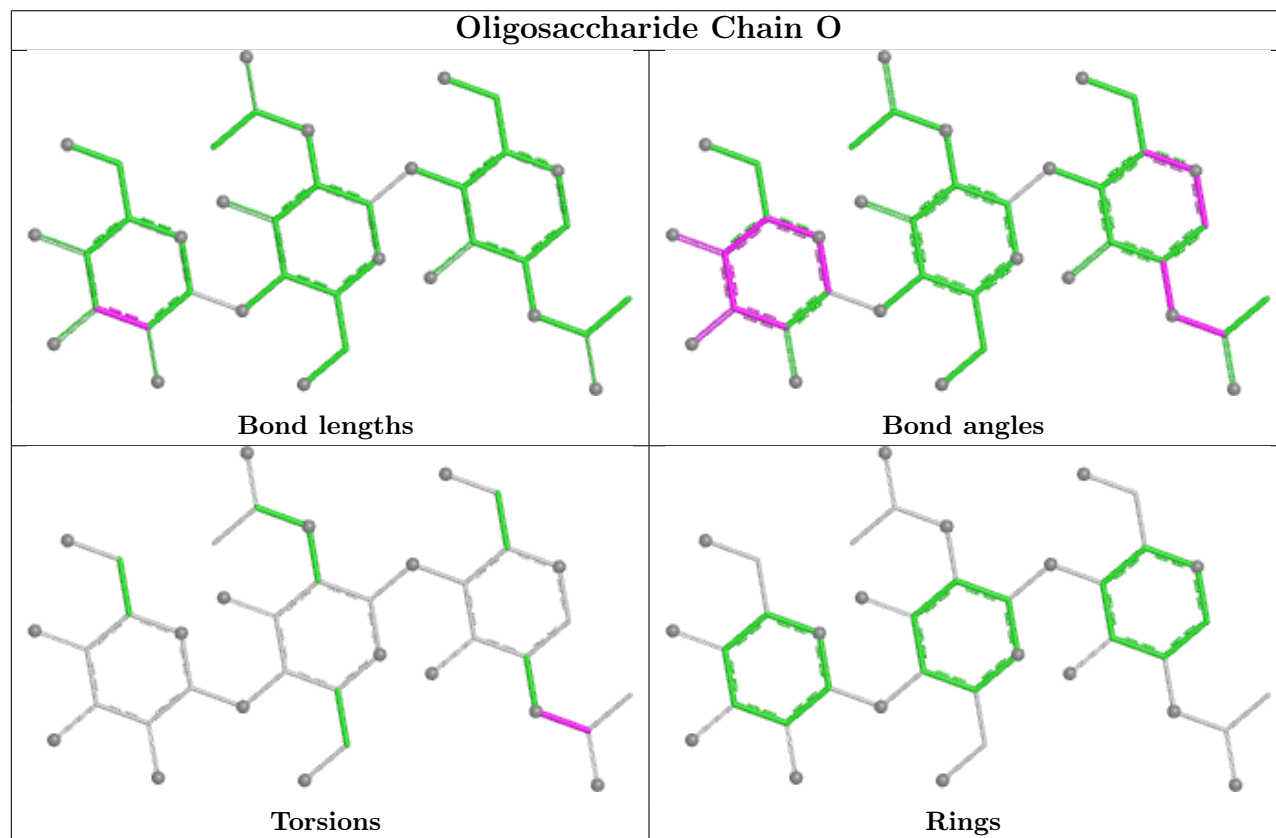
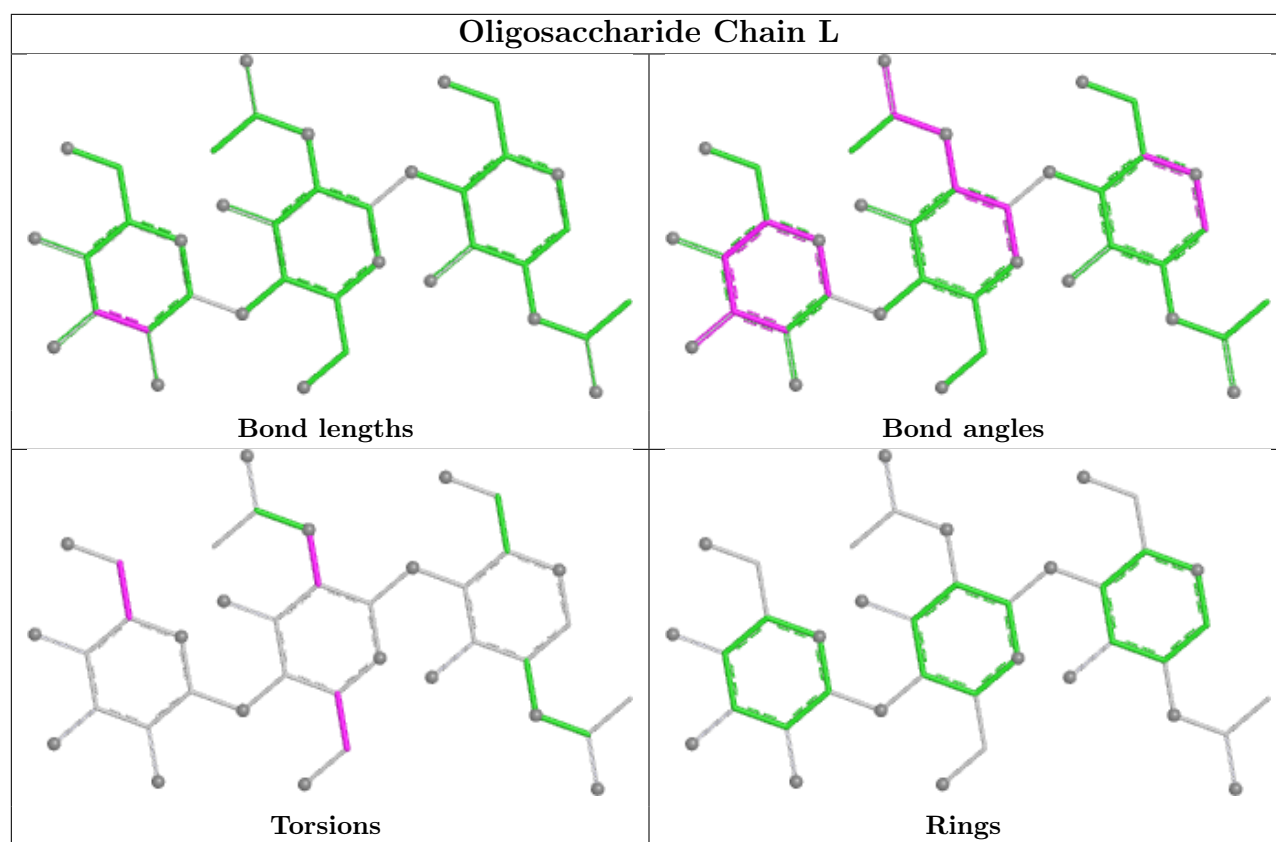


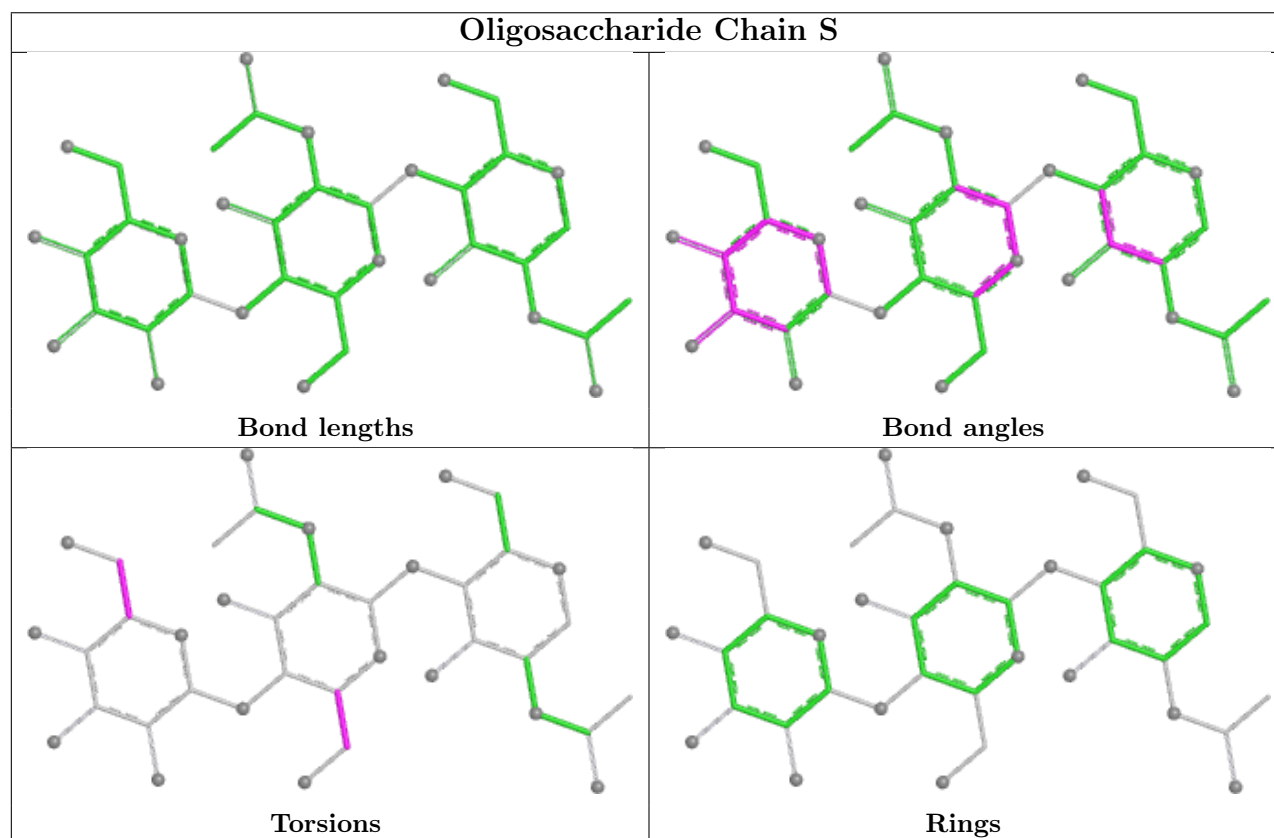
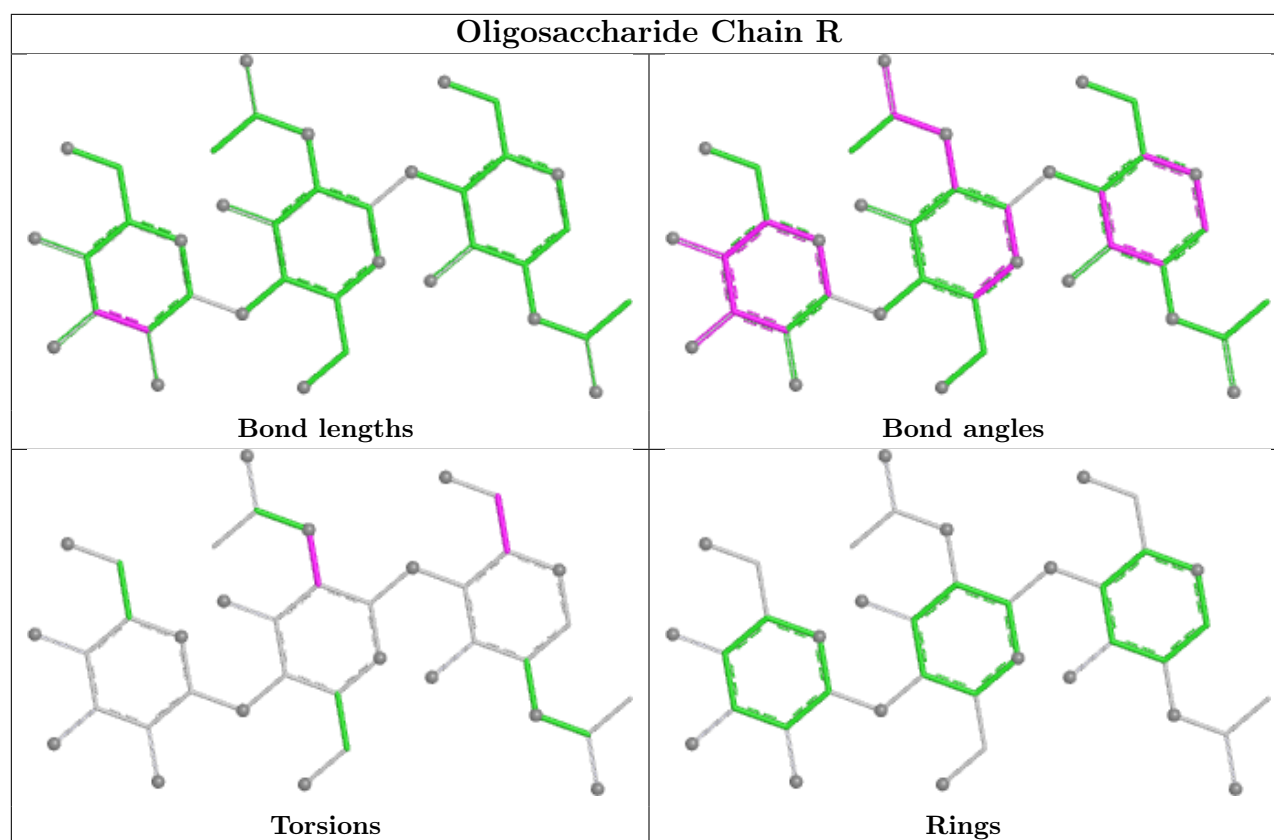


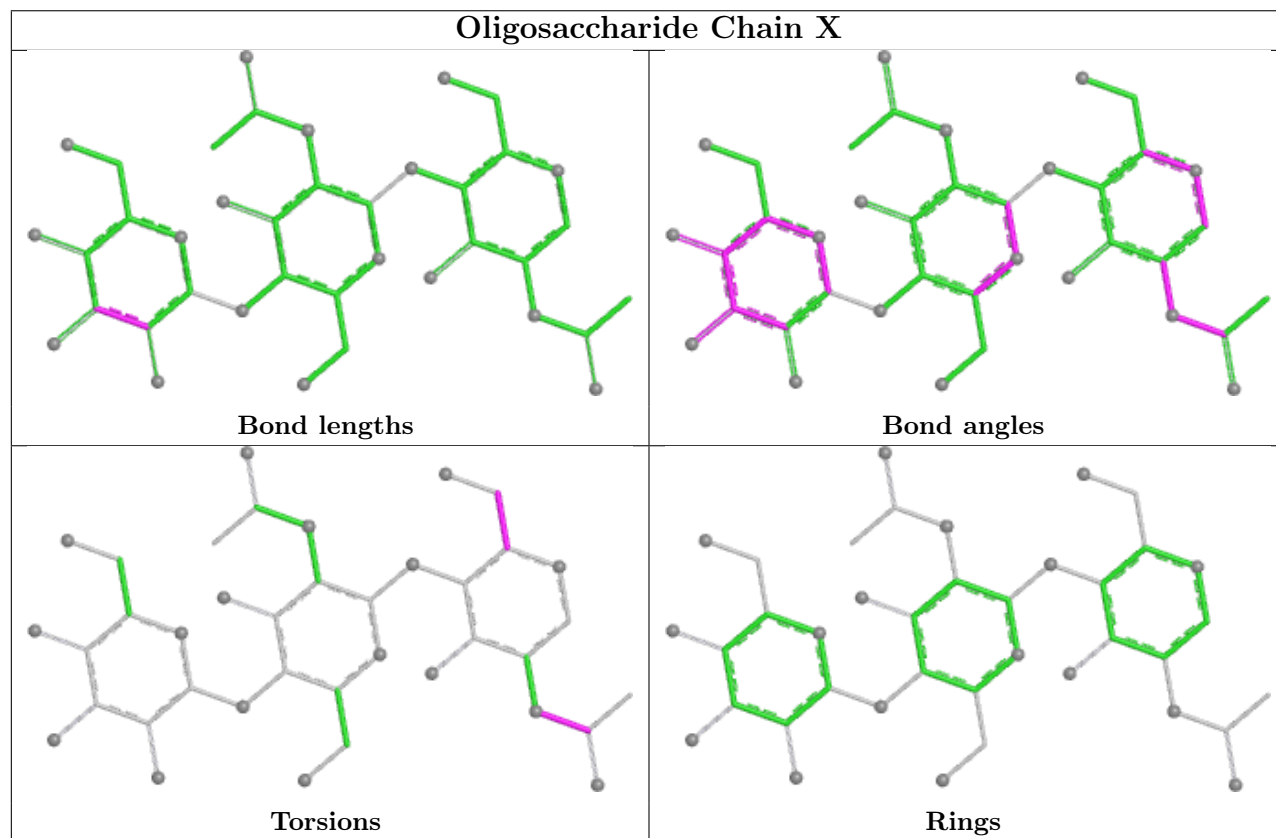
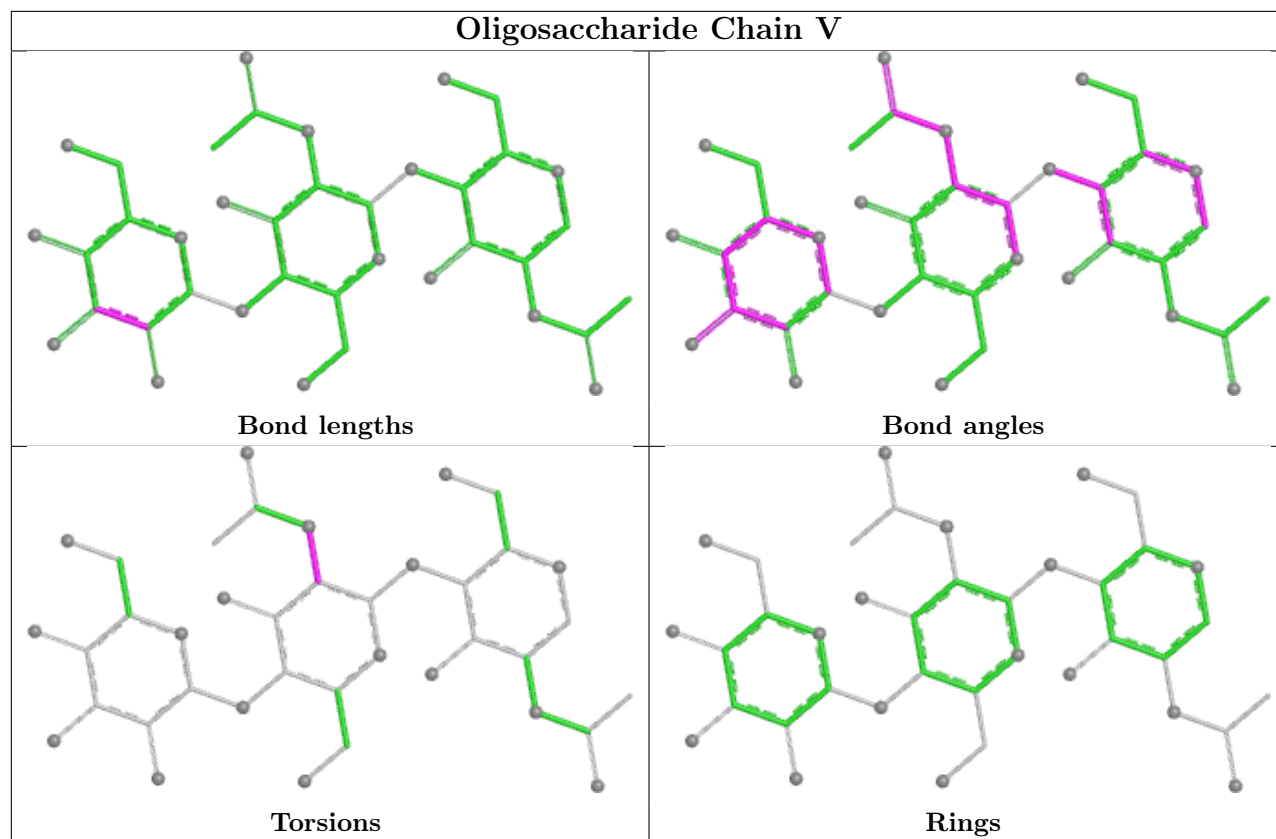


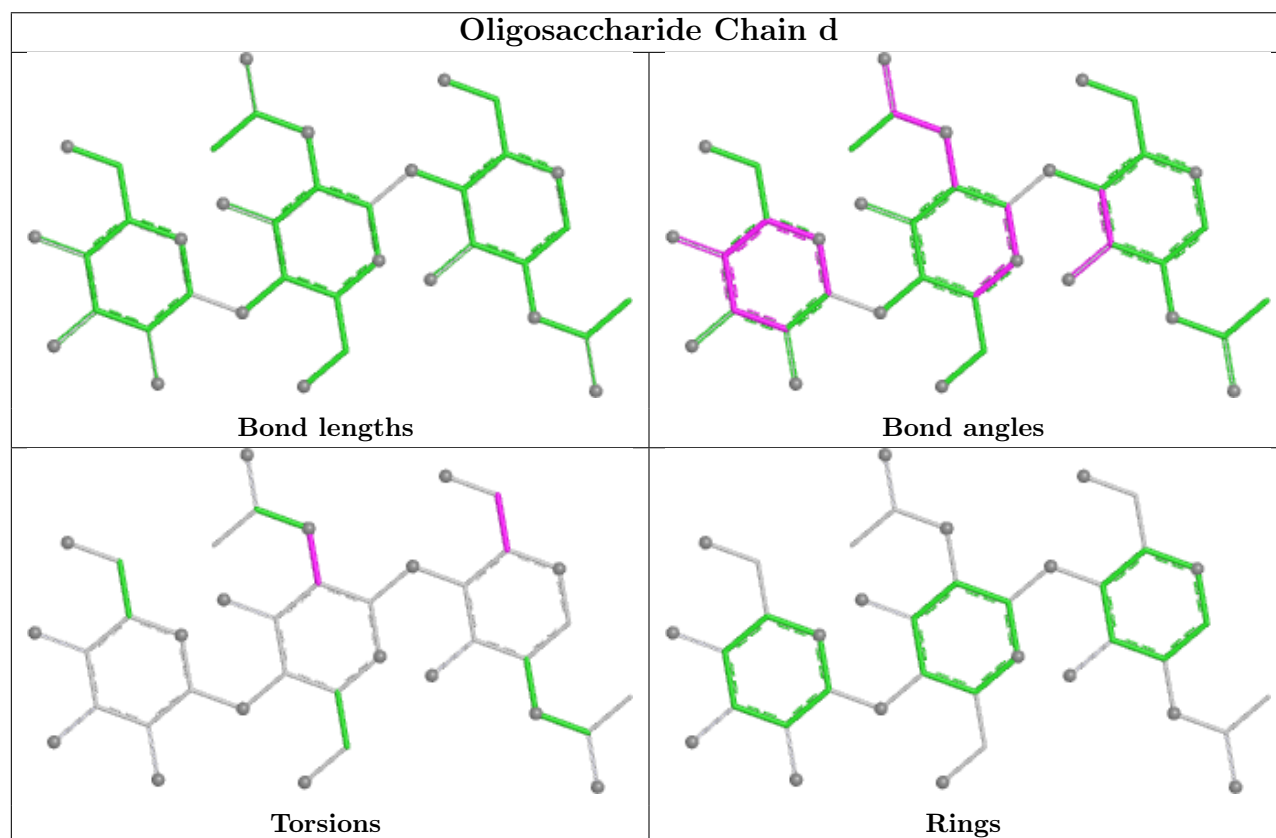
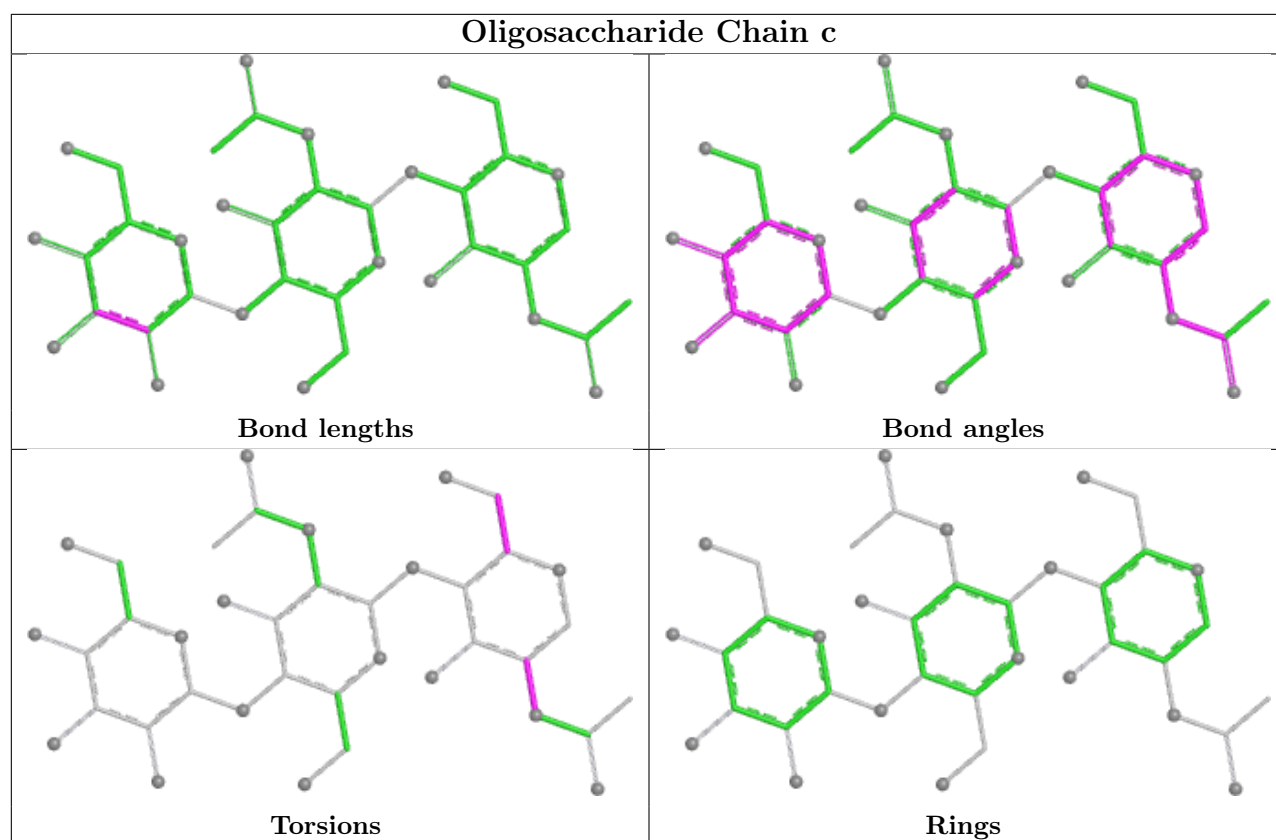


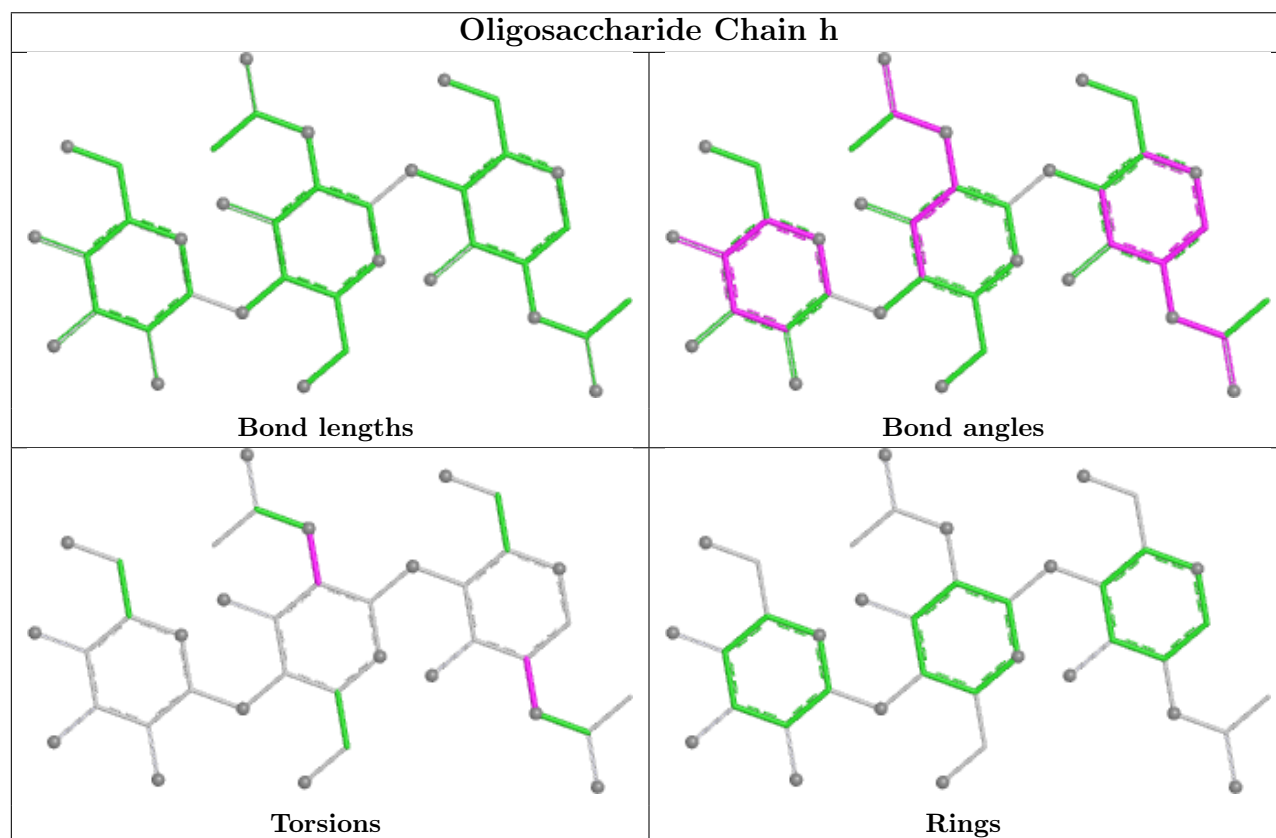
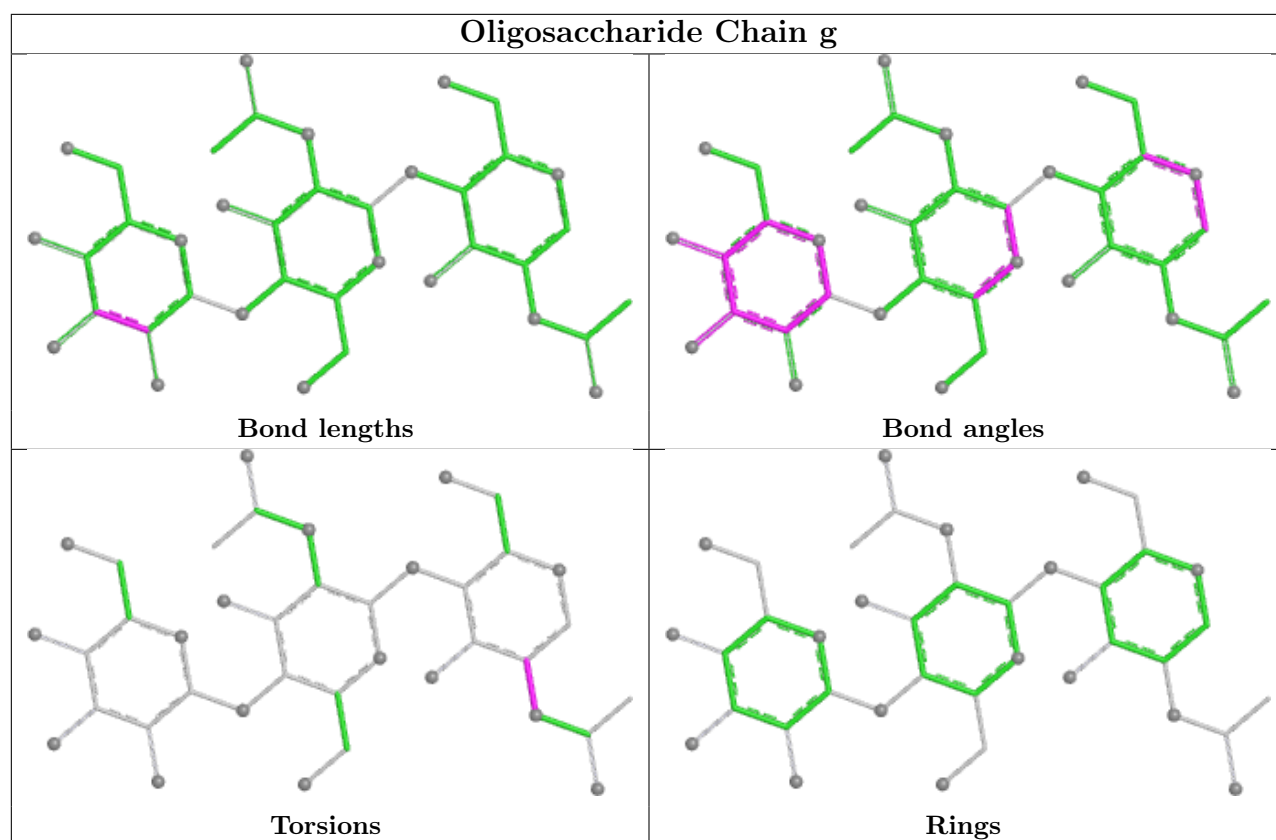












5.6 Ligand geometry

30 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
7	NAG	A	603	1	14,14,15	0.78	0	17,19,21	1.35	2 (11%)
7	NAG	F	702	2	14,14,15	0.69	0	17,19,21	1.29	3 (17%)
7	NAG	A	609	1	14,14,15	0.68	0	17,19,21	1.30	2 (11%)
7	NAG	B	701	2	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
7	NAG	C	601	1	14,14,15	0.70	0	17,19,21	1.06	1 (5%)
7	NAG	A	608	1	14,14,15	0.69	0	17,19,21	1.19	2 (11%)
7	NAG	E	604	-	14,14,15	0.75	0	17,19,21	1.18	2 (11%)
7	NAG	A	602	1	14,14,15	0.71	0	17,19,21	0.91	0
7	NAG	C	606	1	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
7	NAG	D	702	2	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
7	NAG	D	701	2	14,14,15	0.70	0	17,19,21	1.27	2 (11%)
7	NAG	E	603	1	14,14,15	0.81	0	17,19,21	3.29	6 (35%)
7	NAG	A	604	1	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
7	NAG	C	605	1	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
7	NAG	C	607	1	14,14,15	0.99	1 (7%)	17,19,21	2.10	4 (23%)
7	NAG	E	602	1	14,14,15	0.67	0	17,19,21	1.72	2 (11%)
7	NAG	E	609	1	14,14,15	0.85	1 (7%)	17,19,21	3.19	5 (29%)
7	NAG	E	607	1	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
7	NAG	A	601	1	14,14,15	0.70	0	17,19,21	0.92	0
7	NAG	E	605	1	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
7	NAG	E	606	1	14,14,15	0.69	0	17,19,21	1.33	2 (11%)
7	NAG	A	606	1	14,14,15	0.73	0	17,19,21	1.31	2 (11%)
7	NAG	A	605	1	14,14,15	0.71	0	17,19,21	1.18	2 (11%)
7	NAG	C	603	1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
7	NAG	A	607	1	14,14,15	0.69	0	17,19,21	0.83	0
7	NAG	C	604	1	14,14,15	0.71	0	17,19,21	0.91	0
7	NAG	E	608	1	14,14,15	0.71	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	F	701	-	14,14,15	0.68	0	17,19,21	1.23	2 (11%)
7	NAG	E	601	1	14,14,15	0.69	0	17,19,21	0.93	1 (5%)
7	NAG	C	602	1	14,14,15	0.94	1 (7%)	17,19,21	3.31	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	603	1	-	0/6/23/26	0/1/1/1
7	NAG	F	702	2	-	2/6/23/26	0/1/1/1
7	NAG	A	609	1	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1
7	NAG	C	601	1	-	0/6/23/26	0/1/1/1
7	NAG	A	608	1	-	2/6/23/26	0/1/1/1
7	NAG	E	604	-	-	1/6/23/26	0/1/1/1
7	NAG	A	602	1	-	0/6/23/26	0/1/1/1
7	NAG	C	606	1	-	0/6/23/26	0/1/1/1
7	NAG	D	702	2	-	0/6/23/26	0/1/1/1
7	NAG	D	701	2	-	2/6/23/26	0/1/1/1
7	NAG	E	603	1	-	4/6/23/26	0/1/1/1
7	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	NAG	C	605	1	-	0/6/23/26	0/1/1/1
7	NAG	C	607	1	-	2/6/23/26	0/1/1/1
7	NAG	E	602	1	-	3/6/23/26	0/1/1/1
7	NAG	E	609	1	-	3/6/23/26	0/1/1/1
7	NAG	E	607	1	-	0/6/23/26	0/1/1/1
7	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	NAG	E	605	1	-	1/6/23/26	0/1/1/1
7	NAG	E	606	1	-	3/6/23/26	0/1/1/1
7	NAG	A	606	1	-	3/6/23/26	0/1/1/1
7	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	NAG	C	603	1	-	0/6/23/26	0/1/1/1
7	NAG	A	607	1	-	0/6/23/26	0/1/1/1
7	NAG	C	604	1	-	0/6/23/26	0/1/1/1
7	NAG	E	608	1	-	2/6/23/26	0/1/1/1
7	NAG	F	701	-	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	601	1	-	2/6/23/26	0/1/1/1
7	NAG	C	602	1	-	5/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	607	NAG	C1-C2	3.12	1.56	1.52
7	C	602	NAG	C1-C2	2.55	1.55	1.52
7	E	609	NAG	C1-C2	2.21	1.55	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	603	NAG	C2-N2-C7	11.42	138.21	122.90
7	C	602	NAG	C2-N2-C7	10.93	137.54	122.90
7	E	609	NAG	C2-N2-C7	10.92	137.53	122.90
7	E	602	NAG	C2-N2-C7	5.27	129.96	122.90
7	C	607	NAG	C1-O5-C5	5.04	118.94	112.19
7	C	607	NAG	C2-N2-C7	4.71	129.21	122.90
7	C	602	NAG	C1-O5-C5	4.67	118.45	112.19
7	E	603	NAG	C1-C2-N2	4.15	116.98	110.43
7	A	603	NAG	C1-O5-C5	4.04	117.60	112.19
7	E	609	NAG	C8-C7-N2	4.04	122.82	116.12
7	C	602	NAG	C8-C7-N2	4.03	122.81	116.12
7	E	603	NAG	C8-C7-N2	3.87	122.53	116.12
7	E	609	NAG	C1-O5-C5	3.68	117.12	112.19
7	E	606	NAG	C1-O5-C5	3.59	117.00	112.19
7	A	609	NAG	C2-N2-C7	3.45	127.52	122.90
7	F	701	NAG	C2-N2-C7	3.43	127.49	122.90
7	D	701	NAG	C2-N2-C7	3.31	127.33	122.90
7	A	606	NAG	C2-N2-C7	3.23	127.23	122.90
7	E	606	NAG	C2-N2-C7	3.09	127.04	122.90
7	F	702	NAG	C1-O5-C5	3.06	116.29	112.19
7	C	601	NAG	C1-O5-C5	3.06	116.29	112.19
7	A	604	NAG	C2-N2-C7	3.04	126.97	122.90
7	A	605	NAG	C2-N2-C7	3.03	126.96	122.90
7	A	608	NAG	C2-N2-C7	3.01	126.93	122.90
7	C	606	NAG	C1-O5-C5	3.00	116.21	112.19
7	F	702	NAG	C2-N2-C7	2.95	126.86	122.90
7	A	609	NAG	C1-O5-C5	2.88	116.05	112.19
7	E	607	NAG	C1-O5-C5	2.86	116.02	112.19
7	D	701	NAG	C1-O5-C5	2.84	115.99	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	602	NAG	C1-C2-N2	2.83	114.89	110.43
7	D	702	NAG	C1-O5-C5	2.53	115.57	112.19
7	C	602	NAG	O7-C7-C8	-2.53	117.56	122.05
7	E	609	NAG	C1-C2-N2	2.49	114.36	110.43
7	C	607	NAG	O7-C7-N2	2.45	126.32	121.98
7	E	609	NAG	O7-C7-C8	-2.45	117.69	122.05
7	C	603	NAG	C1-O5-C5	2.45	115.46	112.19
7	A	606	NAG	O5-C1-C2	-2.43	107.53	111.29
7	E	603	NAG	C1-O5-C5	2.42	115.43	112.19
7	A	605	NAG	C1-O5-C5	2.37	115.37	112.19
7	E	603	NAG	O7-C7-C8	-2.37	117.84	122.05
7	A	603	NAG	C2-N2-C7	2.32	126.02	122.90
7	E	603	NAG	O5-C1-C2	-2.31	107.71	111.29
7	A	608	NAG	C1-O5-C5	2.27	115.23	112.19
7	B	701	NAG	O5-C1-C2	-2.26	107.79	111.29
7	F	701	NAG	C1-O5-C5	2.25	115.20	112.19
7	E	604	NAG	C2-N2-C7	2.22	125.87	122.90
7	E	602	NAG	O7-C7-N2	2.12	125.73	121.98
7	E	605	NAG	C1-O5-C5	2.12	115.03	112.19
7	E	601	NAG	O5-C1-C2	-2.07	108.09	111.29
7	C	605	NAG	O5-C1-C2	-2.05	108.12	111.29
7	E	608	NAG	O5-C1-C2	-2.05	108.12	111.29
7	C	607	NAG	C4-C3-C2	2.05	114.02	111.02
7	E	604	NAG	C4-C3-C2	2.04	114.00	111.02
7	F	702	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	601	NAG	C4-C5-C6-O6
7	E	601	NAG	O5-C5-C6-O6
7	A	604	NAG	C8-C7-N2-C2
7	A	604	NAG	O7-C7-N2-C2
7	A	605	NAG	C8-C7-N2-C2
7	A	605	NAG	O7-C7-N2-C2
7	A	606	NAG	C8-C7-N2-C2
7	A	606	NAG	O7-C7-N2-C2
7	A	608	NAG	C8-C7-N2-C2
7	A	608	NAG	O7-C7-N2-C2
7	A	609	NAG	C8-C7-N2-C2
7	A	609	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	602	NAG	C8-C7-N2-C2
7	C	602	NAG	O7-C7-N2-C2
7	D	701	NAG	C8-C7-N2-C2
7	D	701	NAG	O7-C7-N2-C2
7	E	603	NAG	C8-C7-N2-C2
7	E	603	NAG	O7-C7-N2-C2
7	E	606	NAG	C8-C7-N2-C2
7	E	606	NAG	O7-C7-N2-C2
7	E	609	NAG	C8-C7-N2-C2
7	E	609	NAG	O7-C7-N2-C2
7	F	701	NAG	C8-C7-N2-C2
7	F	701	NAG	O7-C7-N2-C2
7	F	702	NAG	C8-C7-N2-C2
7	F	702	NAG	O7-C7-N2-C2
7	E	608	NAG	O5-C5-C6-O6
7	E	604	NAG	O5-C5-C6-O6
7	C	602	NAG	O5-C5-C6-O6
7	E	602	NAG	O5-C5-C6-O6
7	E	606	NAG	O5-C5-C6-O6
7	E	605	NAG	O5-C5-C6-O6
7	A	606	NAG	O5-C5-C6-O6
7	C	607	NAG	C1-C2-N2-C7
7	E	602	NAG	C1-C2-N2-C7
7	C	602	NAG	C3-C2-N2-C7
7	E	609	NAG	C3-C2-N2-C7
7	B	701	NAG	O5-C5-C6-O6
7	C	602	NAG	C1-C2-N2-C7
7	E	603	NAG	C1-C2-N2-C7
7	B	701	NAG	C4-C5-C6-O6
7	E	608	NAG	C4-C5-C6-O6
7	C	607	NAG	C3-C2-N2-C7
7	E	602	NAG	C3-C2-N2-C7
7	E	603	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	606	NAG	1	0
7	F	701	NAG	1	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.

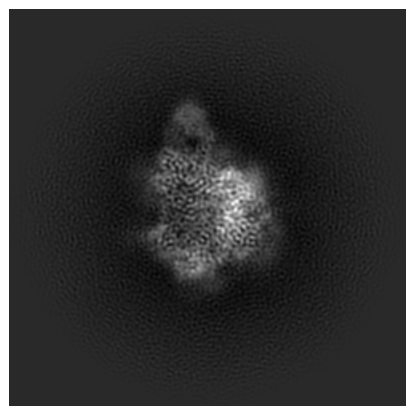
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46606. These allow visual inspection of the internal detail of the map and identification of artifacts.

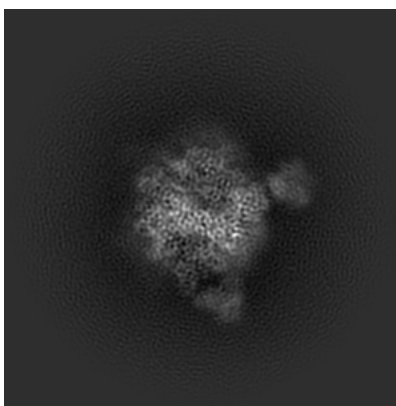
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

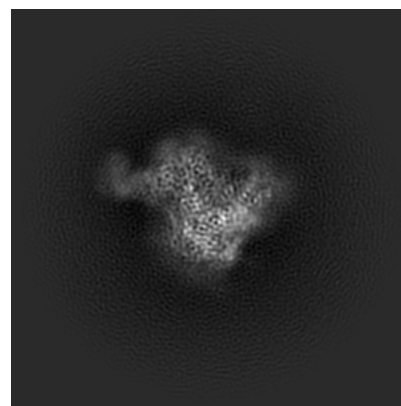
6.1.1 Primary map



X

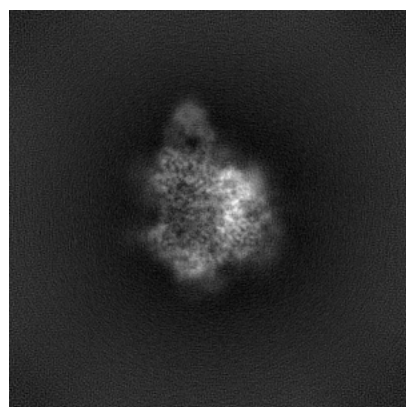


Y

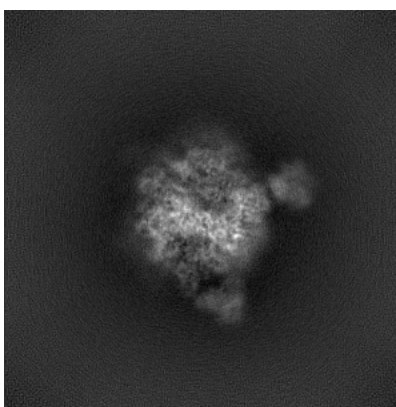


Z

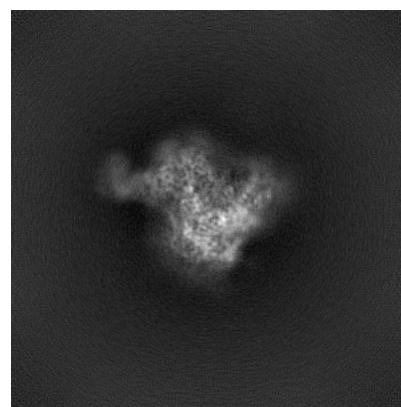
6.1.2 Raw map



X



Y

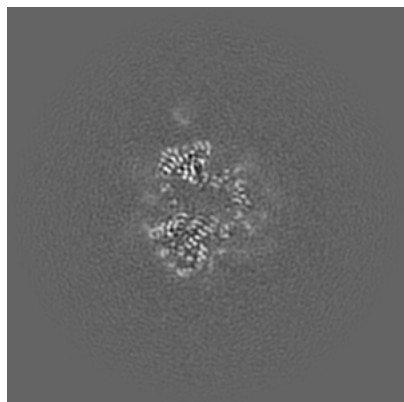


Z

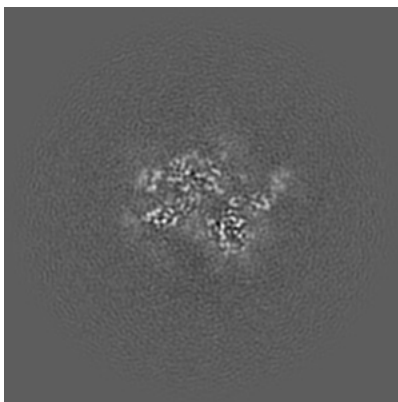
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

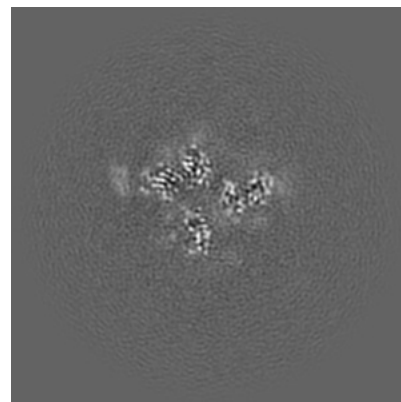
6.2.1 Primary map



X Index: 160

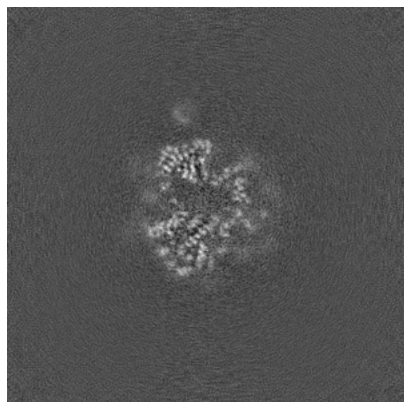


Y Index: 160

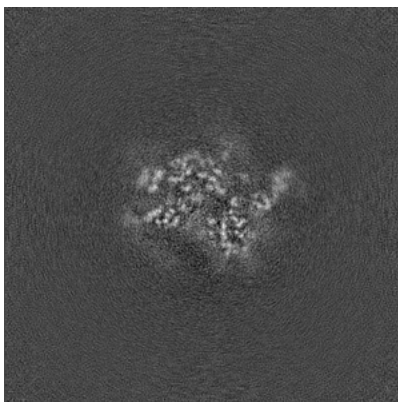


Z Index: 160

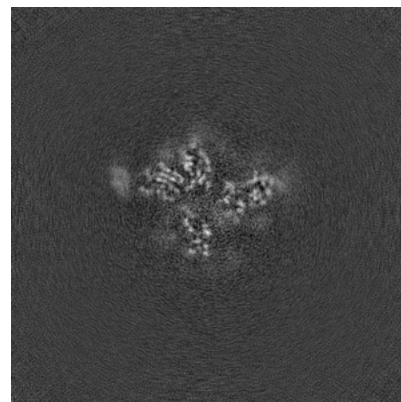
6.2.2 Raw map



X Index: 160



Y Index: 160

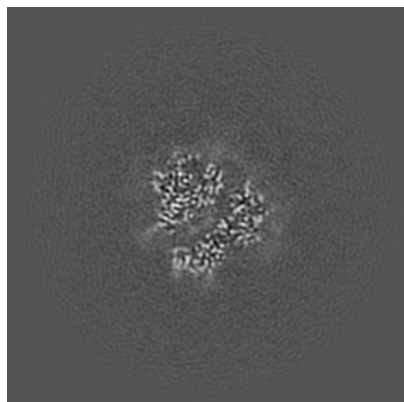


Z Index: 160

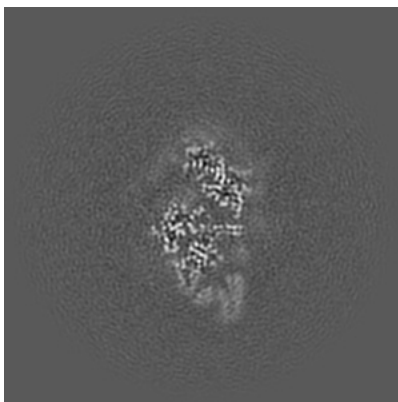
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

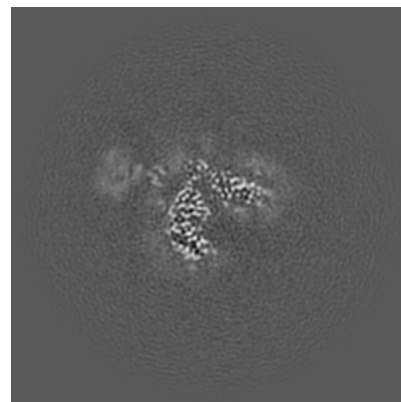
6.3.1 Primary map



X Index: 149

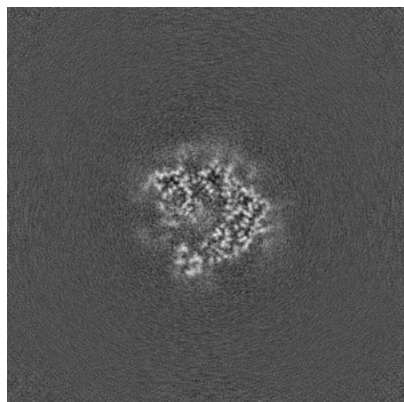


Y Index: 176

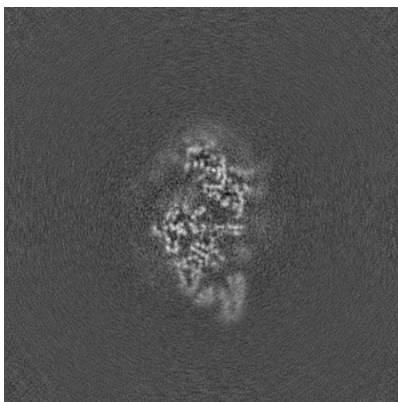


Z Index: 175

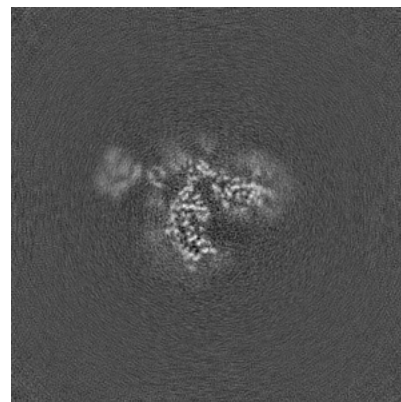
6.3.2 Raw map



X Index: 144



Y Index: 176

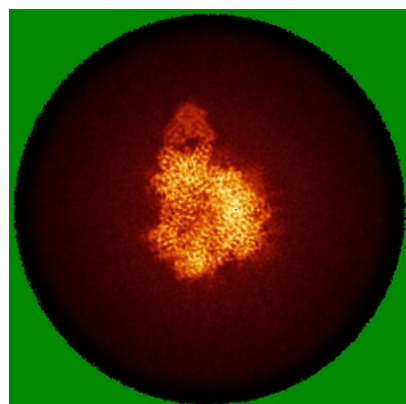


Z Index: 175

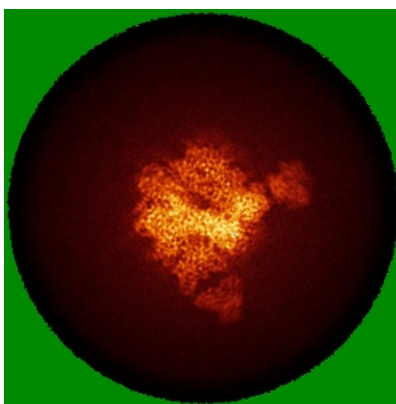
The images above show the largest variance slices of the map in three orthogonal directions.

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

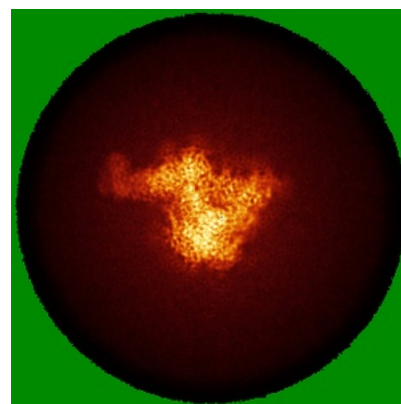
6.4.1 Primary map



X

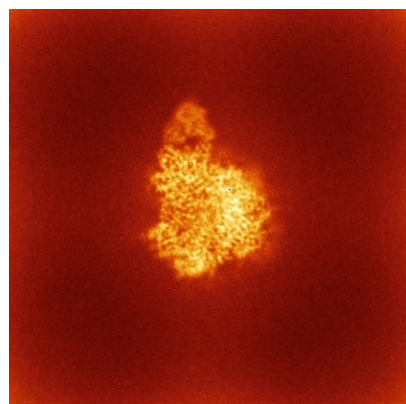


Y

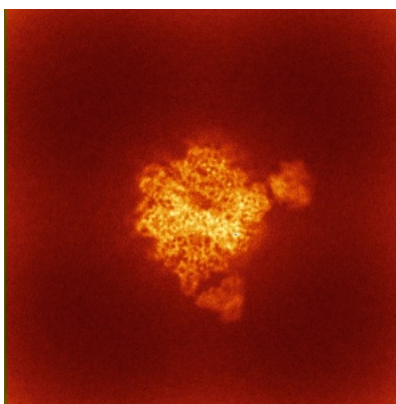


Z

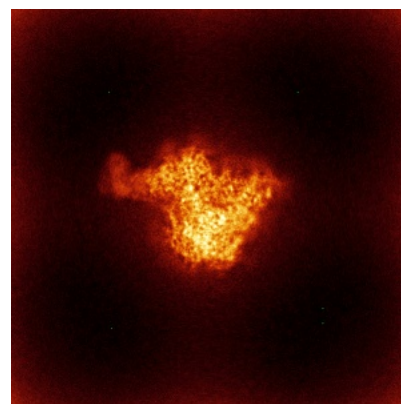
6.4.2 Raw map



X



Y

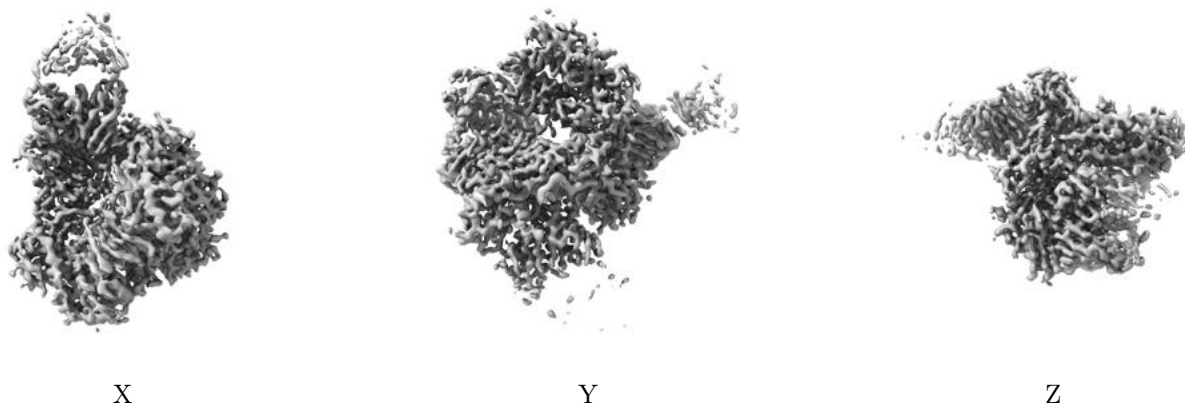


Z

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.

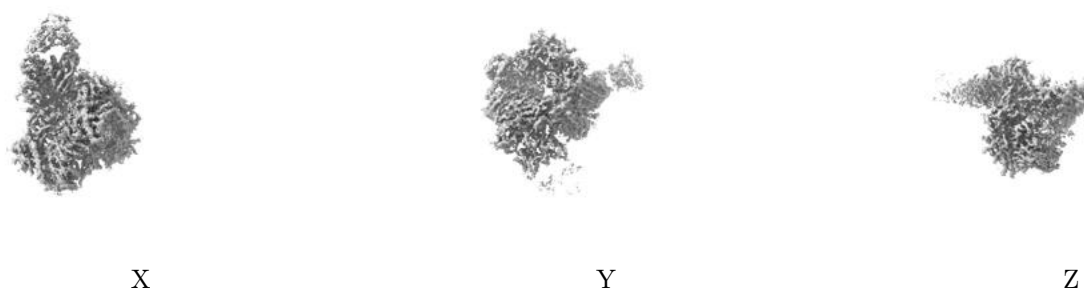
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

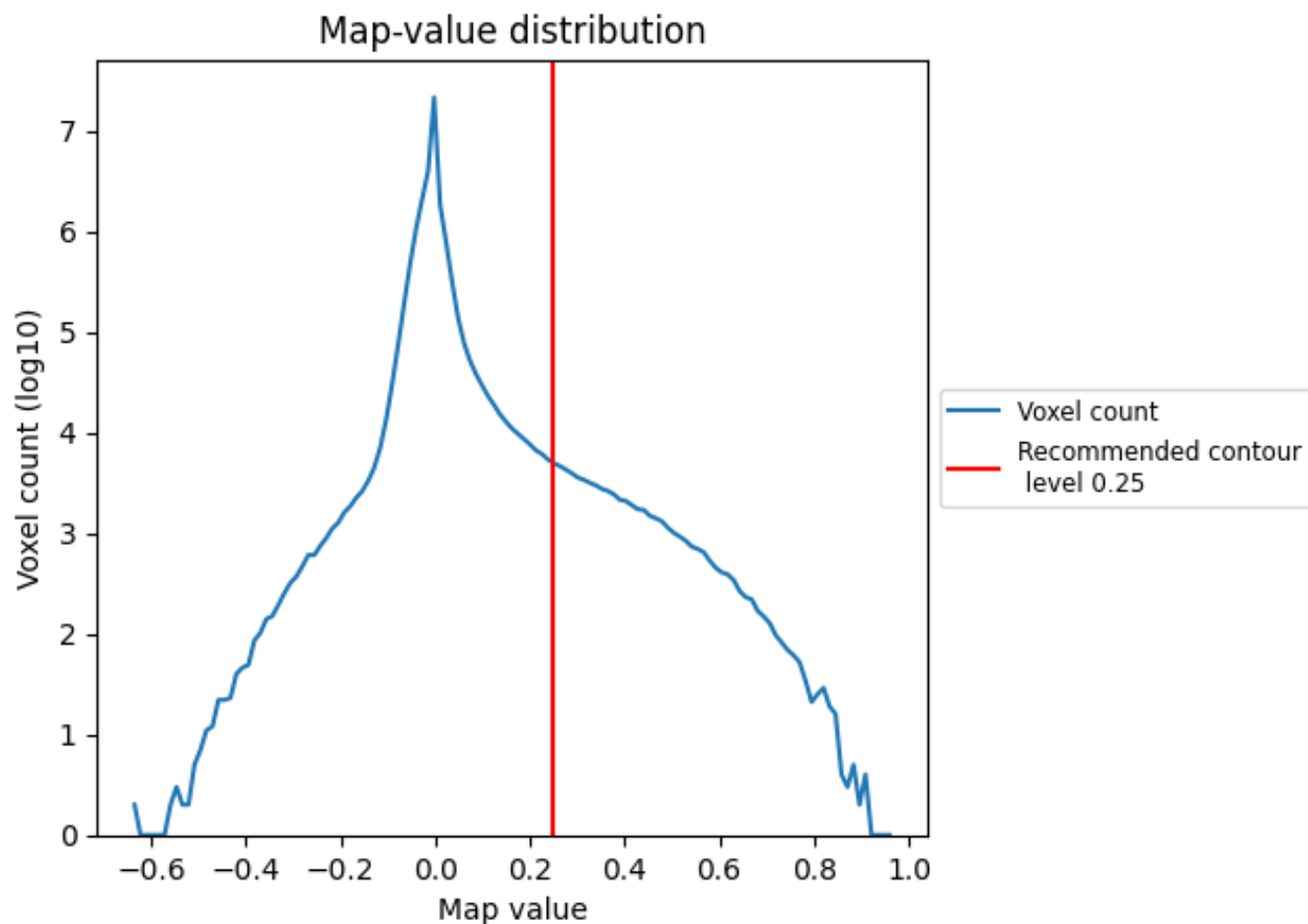
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

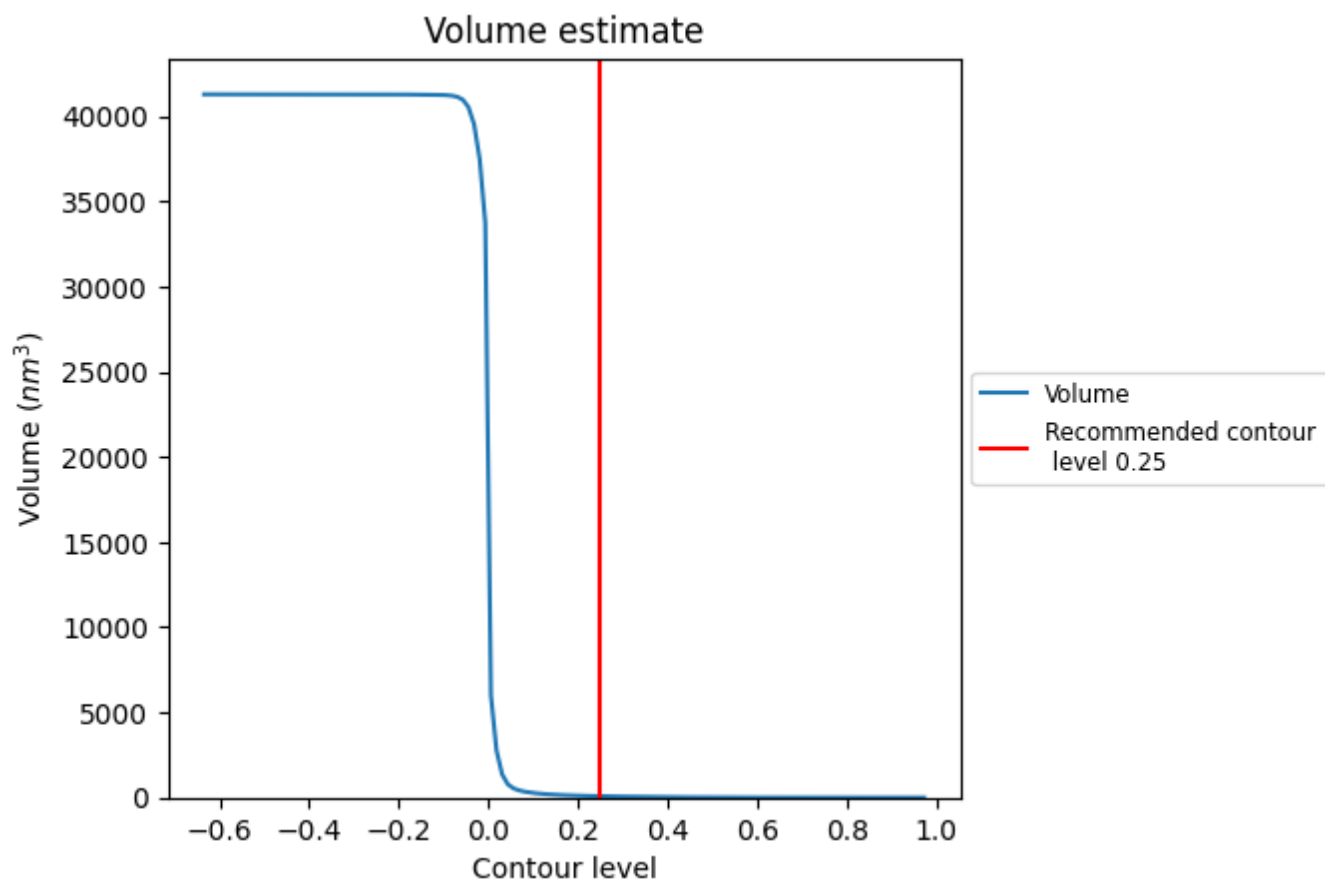
This section contains the results of statistical analysis of the map.

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.

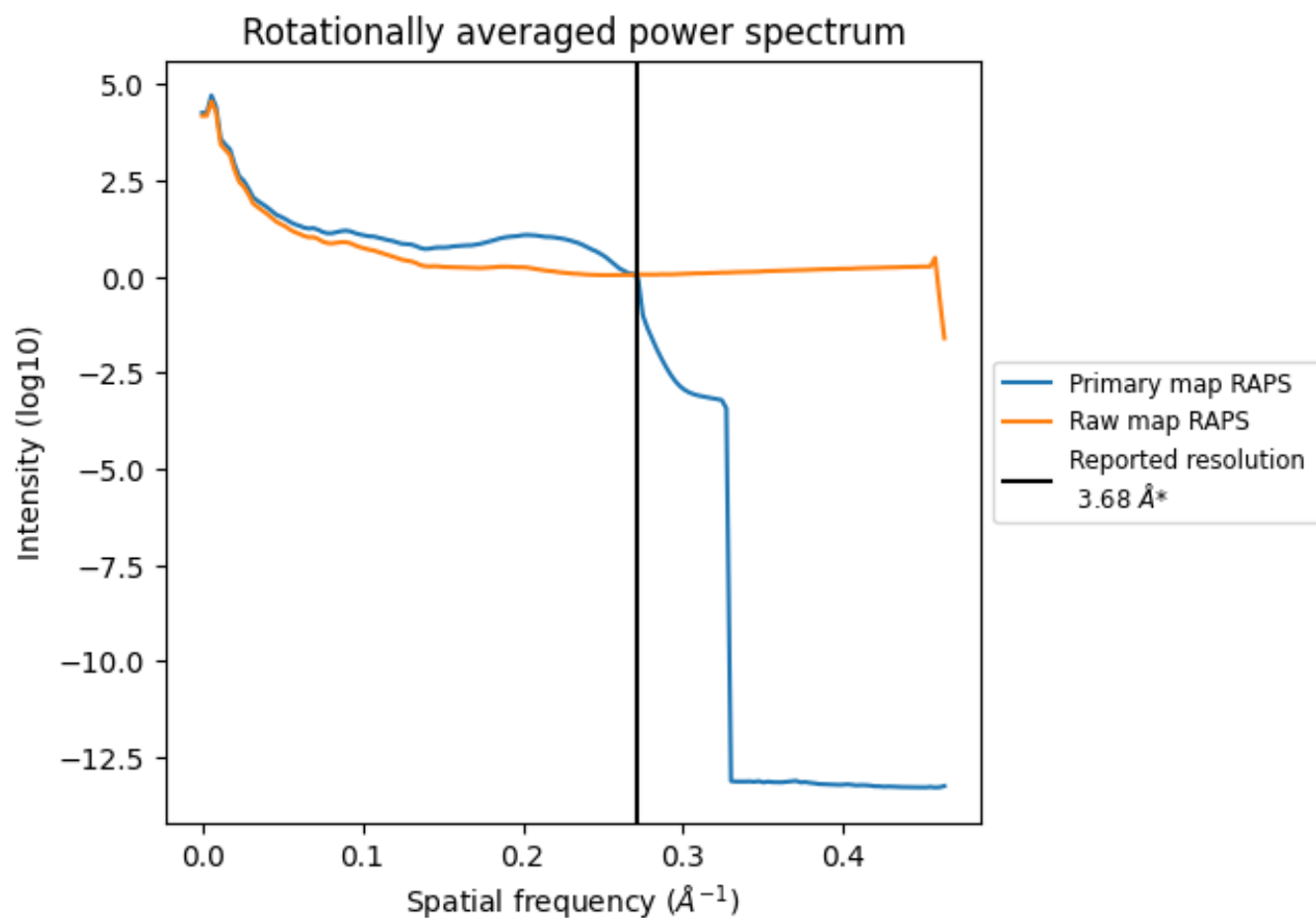
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; this corresponds to an approximate mass of 71 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 ⓘ

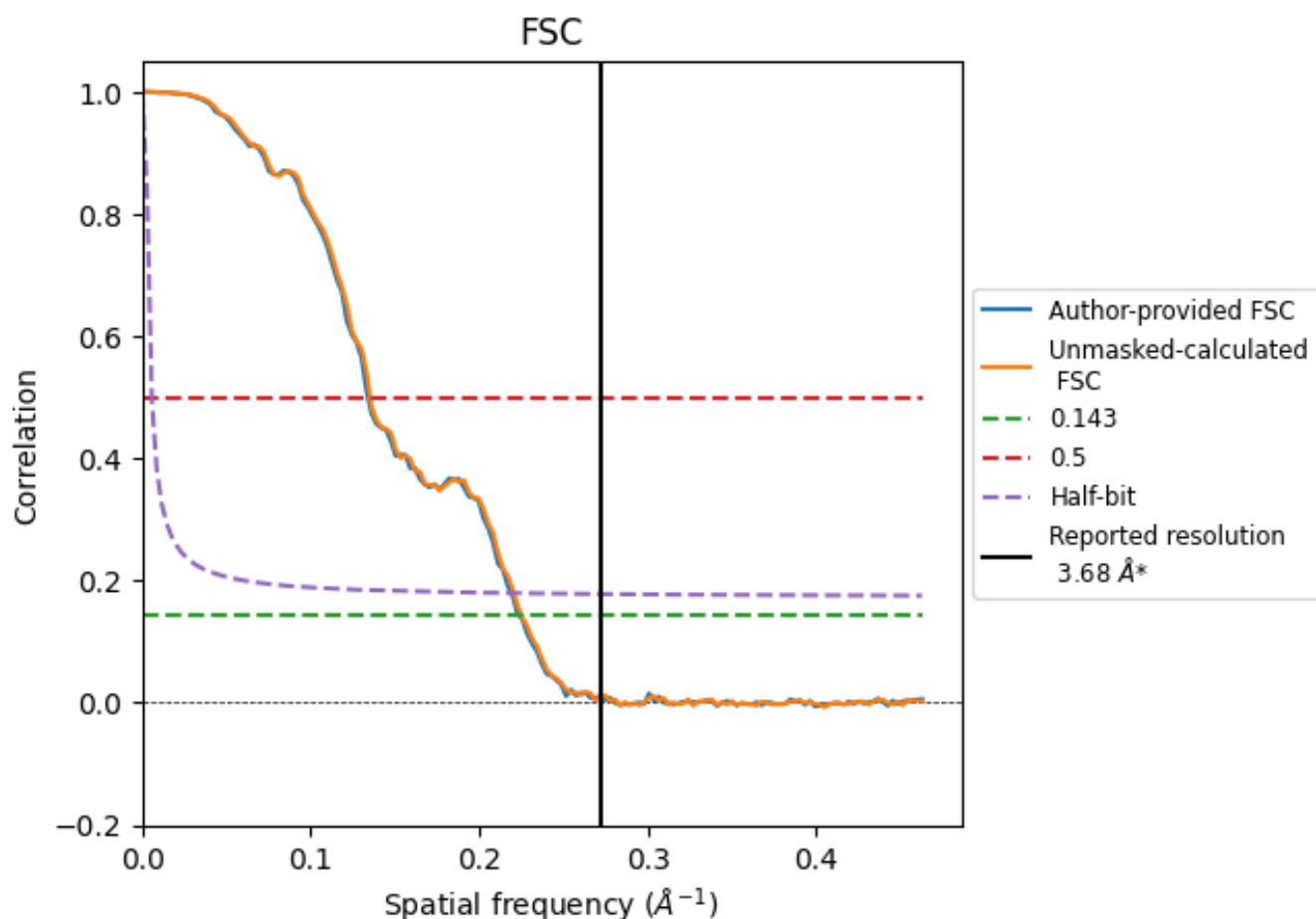


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.68	-
Author-provided FSC curve	4.47	7.46	4.56
Unmasked-calculated*	4.44	7.39	4.53

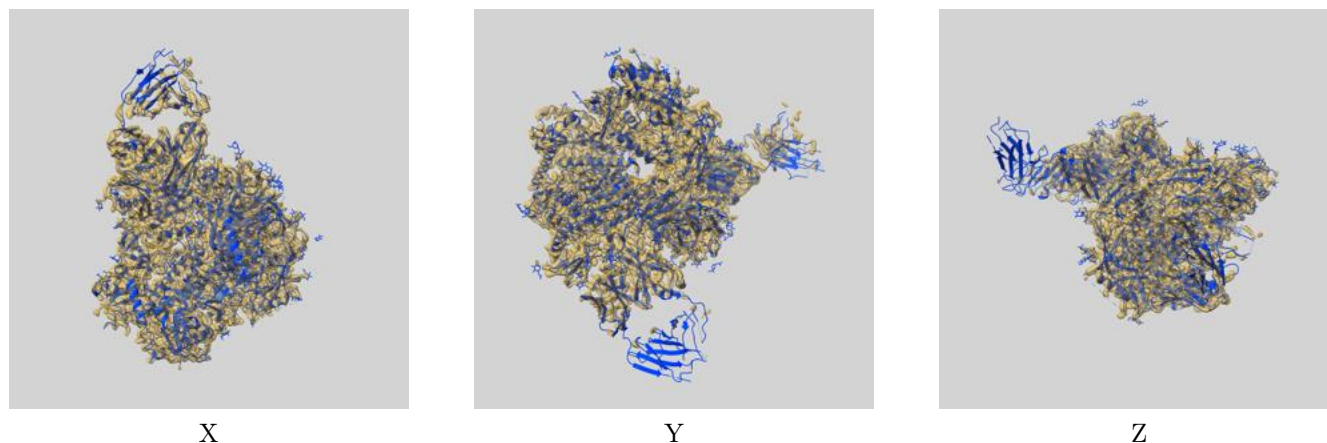
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 7.46 differs from the reported value 3.68 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 7.39 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

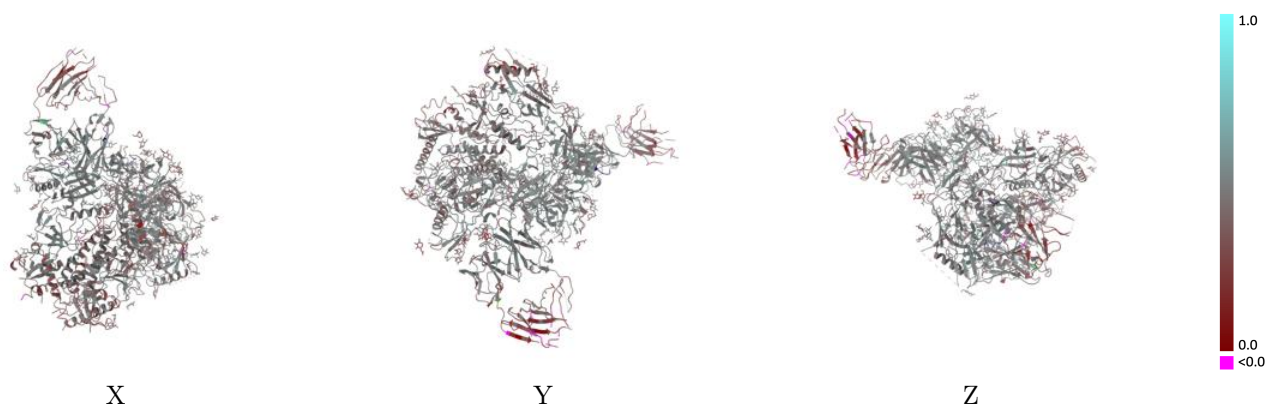
This section contains information regarding the fit between EMDB map EMD-46606 and PDB model 9D7I. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



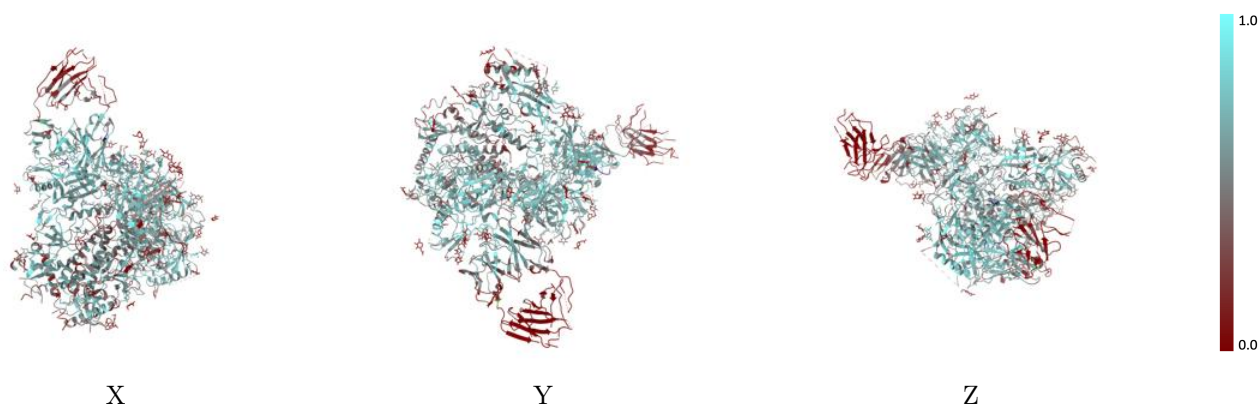
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



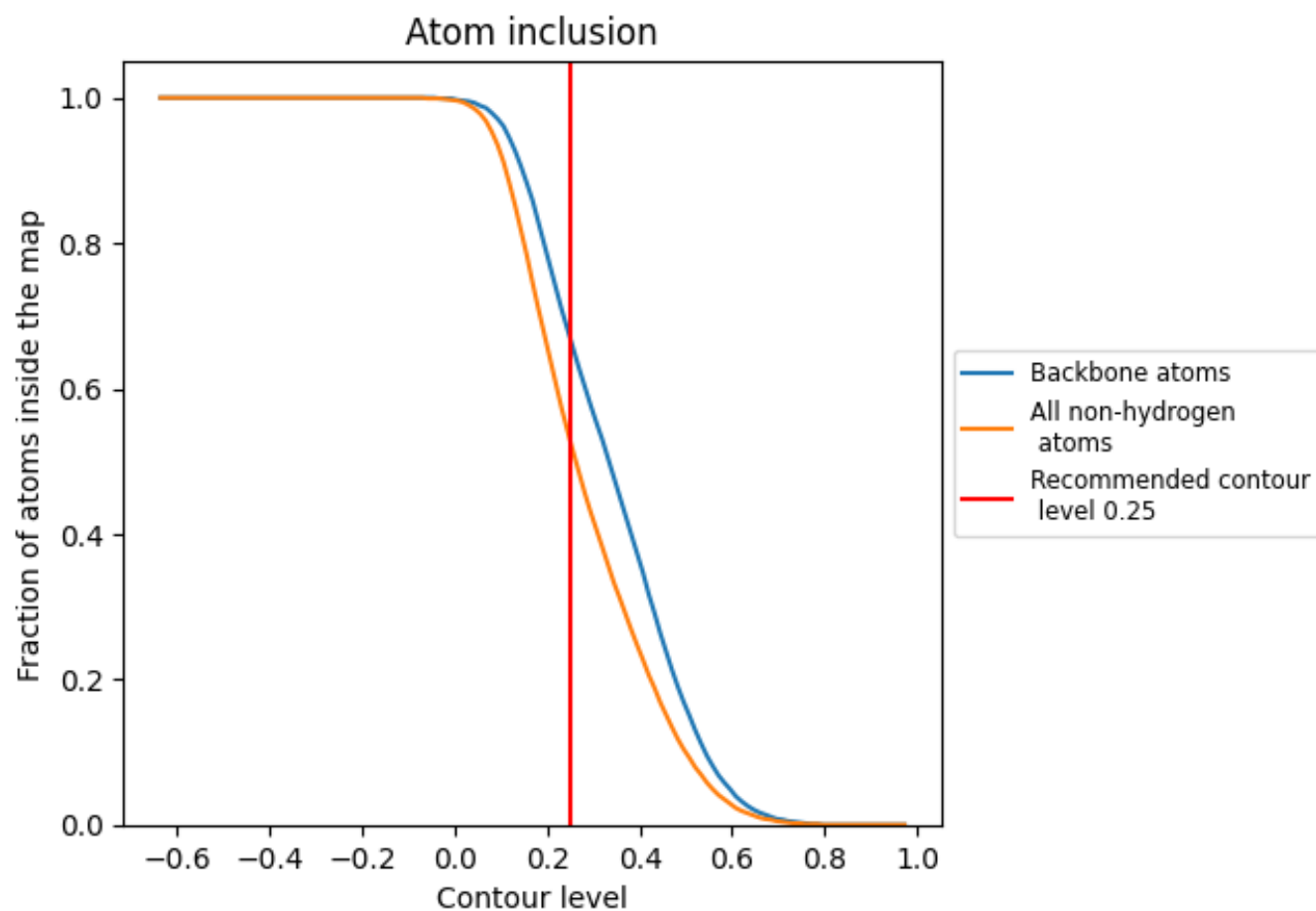
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 53% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5280	 0.4400
A	 0.5500	 0.4430
B	 0.4500	 0.3980
C	 0.6410	 0.4800
D	 0.5230	 0.4160
E	 0.6270	 0.4700
F	 0.5420	 0.4050
G	 0.2360	 0.3540
H	 0.4390	 0.4360
I	 0.4070	 0.4070
J	 0.5720	 0.4670
K	 0.0000	 0.3700
L	 0.2820	 0.3820
M	 0.2500	 0.3030
N	 0.3210	 0.4640
O	 0.4360	 0.4800
P	 0.2500	 0.4110
Q	 0.4640	 0.3900
R	 0.3590	 0.3890
S	 0.7690	 0.5160
T	 0.5000	 0.4110
U	 0.2860	 0.4070
V	 0.3080	 0.4190
W	 0.2500	 0.4050
X	 0.6670	 0.5330
Y	 0.3570	 0.4710
Z	 0.2860	 0.4460
a	 0.1790	 0.3370
b	 0.4290	 0.4670
c	 0.6150	 0.4500
d	 0.1030	 0.2690
e	 0.3570	 0.4090
f	 0.5000	 0.4660
g	 0.6410	 0.4710
h	 0.3080	 0.3050

