



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 04:17 PM JST

PDB ID : 8YVM / pdb_00008yvm
EMDB ID : EMD-39608
Title : Neuraminidase of A/Switzerland/9715293/2013 H3N2 in complex with CAV-F34 Fab
Authors : Wang, X.; Ge, J.; Li, X.
Deposited on : 2024-03-28
Resolution : 3.02 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

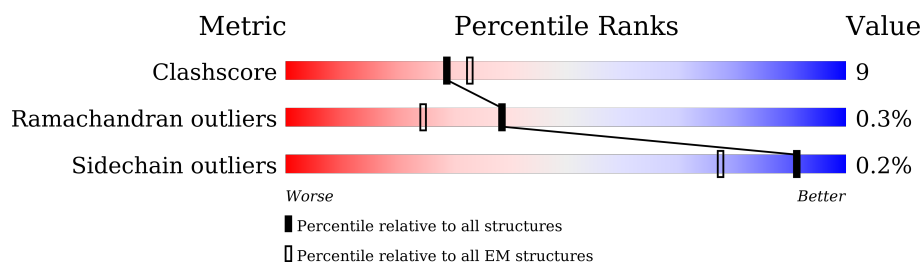
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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	387	
1	B	387	
1	C	387	
1	D	387	
2	E	107	
3	F	123	
4	G	3	
4	K	3	

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Mol	Chain	Length	Quality of chain
4	O	3	 67% 33%
4	S	3	 100%
5	H	2	 100%
5	I	2	 50% 50%
5	L	2	 50% 50%
5	M	2	 50% 50%
5	P	2	 50% 50%
5	Q	2	 100%
5	T	2	 50% 50%
5	U	2	 50% 50%
6	J	8	 12% 62% 38%
6	N	8	 50% 50%
6	R	8	 38% 62%
6	V	8	 38% 50% 12%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14579 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 Neuraminidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	387	Total	C	N	O	S	0	0
			2990	1852	529	587	22		
1	B	387	Total	C	N	O	S	0	0
			2990	1852	529	587	22		
1	C	387	Total	C	N	O	S	0	0
			2990	1852	529	587	22		
1	D	387	Total	C	N	O	S	0	0
			2990	1852	529	587	22		

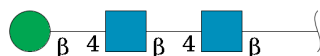
- Molecule 2 is a protein called CAV-F34 kappa chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			808	509	135	161	3		

- Molecule 3 is a protein called CAV-F34 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	123	Total	C	N	O	S	0	0
			939	587	159	188	5		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

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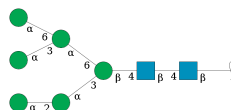
Mol	Chain	Residues	Atoms				AltConf	Trace
4	O	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	L	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	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		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



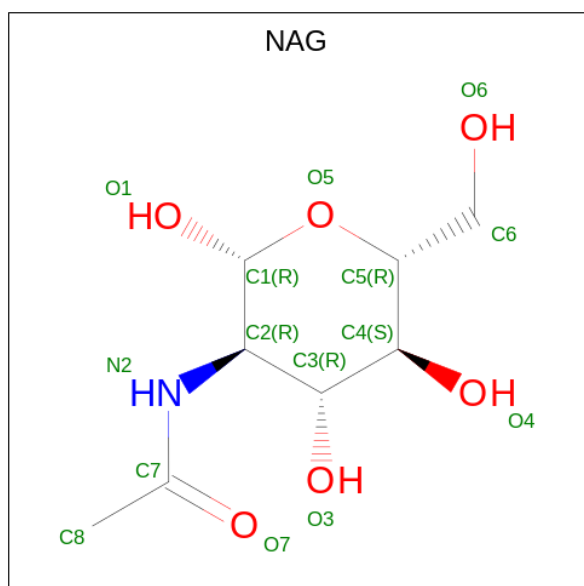
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	8	Total	C	N	O	0	0
			94	52	2	40		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	8	Total	C	N	O	0	0
			94	52	2	40		
6	R	8	Total	C	N	O	0	0
			94	52	2	40		
6	V	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

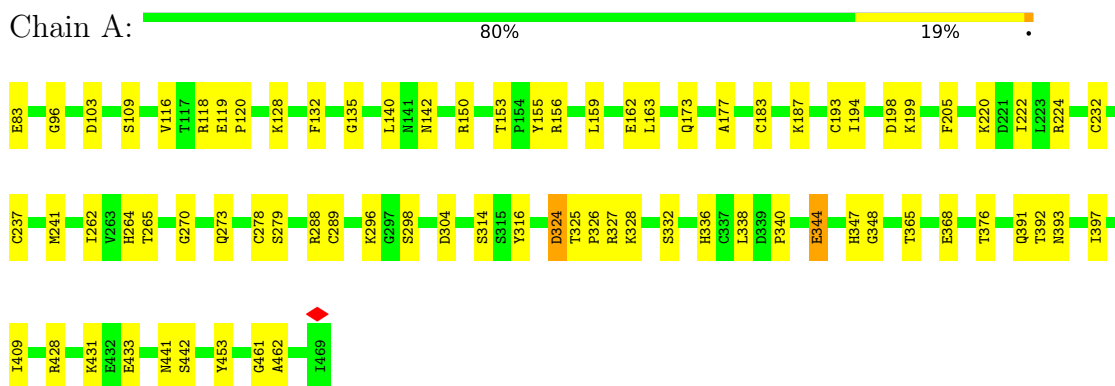
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total 1	Ca 1	0
8	B	1	Total 1	Ca 1	0
8	C	1	Total 1	Ca 1	0
8	D	1	Total 1	Ca 1	0

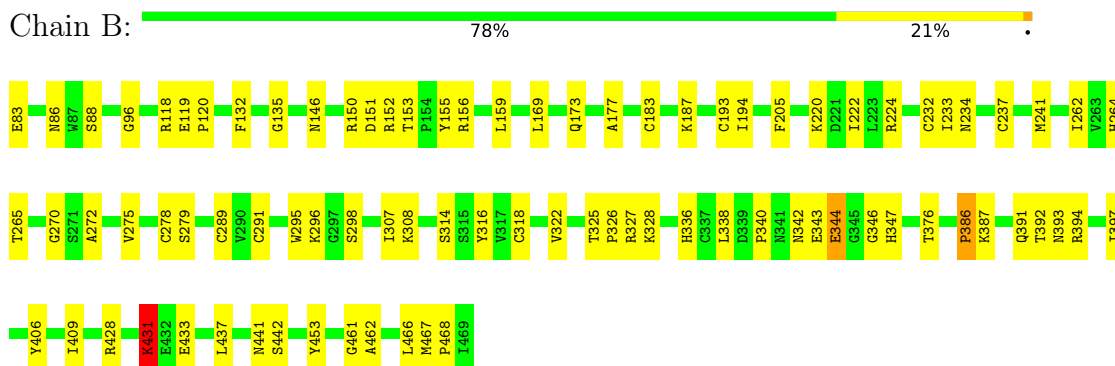
3 Residue-property plots

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.

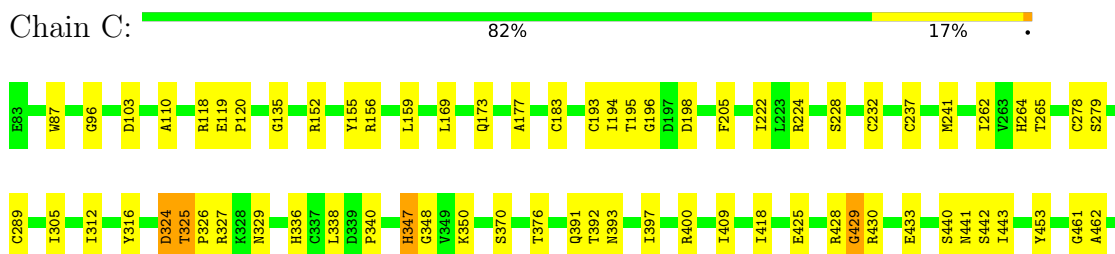
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



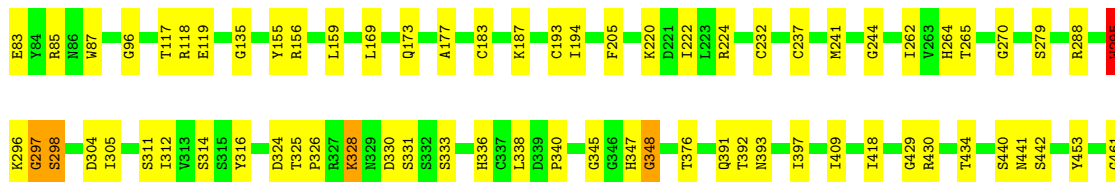
• Molecule 1: Neuraminidase





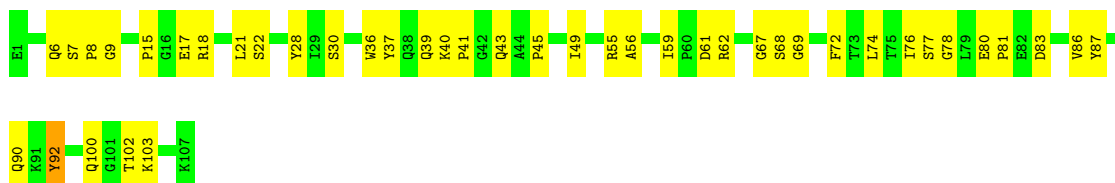
• Molecule 1: Neuraminidase

Chain D: 81% 17%



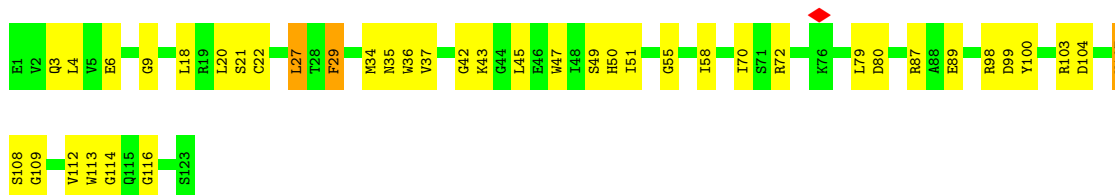
• Molecule 2: CAV-F34 kappa chain

Chain E: 61% 38%



• Molecule 3: CAV-F34 heavy chain

Chain F: 67% 31%



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

Chain G: 33% 67%



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

Chain K: 33% 67%



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

Chain O: 67% 33%



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

Chain S: 100%



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

Chain H: 100%



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

Chain I: 50% 50%



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

Chain L: 50% 50%



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

Chain M: 50% 50%



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

Chain P:  50% 50%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain J:  12% 62% 38%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain N:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain R:  38% 62%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

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

Chain V:  38% 50% 12%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.889	Depositor
Minimum map value	-1.820	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.232	Depositor
Map size (\AA)	335.15042, 335.15042, 335.15042	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, MAN, 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	0.59	0/3057	0.87	9/4147 (0.2%)
1	B	0.59	0/3057	0.85	6/4147 (0.1%)
1	C	0.61	1/3057 (0.0%)	0.88	14/4147 (0.3%)
1	D	0.65	2/3057 (0.1%)	0.89	14/4147 (0.3%)
2	E	0.55	0/826	0.97	3/1120 (0.3%)
3	F	0.68	1/958 (0.1%)	1.14	5/1298 (0.4%)
All	All	0.61	4/14012 (0.0%)	0.90	51/19006 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	468	PRO	N-CD	-12.05	1.30	1.47
1	D	440	SER	CA-CB	-5.66	1.46	1.53
3	F	108	SER	CA-CB	-5.22	1.45	1.53
1	C	440	SER	CA-CB	-5.20	1.47	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	98	ARG	CB-CA-C	-8.15	93.28	109.33
1	C	468	PRO	N-CA-C	8.14	123.83	111.14
1	B	431	LYS	CB-CA-C	7.81	117.56	109.83
1	B	386	PRO	N-CA-C	-7.61	100.56	111.22
1	D	244	GLY	CA-C-O	-7.21	116.25	122.16
1	B	325	THR	CB-CA-C	-7.13	96.13	110.17
1	B	346	GLY	N-CA-C	6.92	120.53	112.50
1	D	331	SER	N-CA-C	-6.79	104.63	113.12
1	C	429	GLY	N-CA-C	6.70	120.53	110.75
1	B	468	PRO	CB-CA-C	-6.68	102.84	111.46
1	D	330	ASP	N-CA-C	-6.66	103.37	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	107	TYR	CB-CA-C	-6.57	100.94	110.06
1	C	325	THR	CB-CA-C	-6.52	100.38	110.62
1	D	325	THR	CB-CA-C	-6.51	100.39	110.62
2	E	9	GLY	N-CA-C	-6.39	105.06	112.73
3	F	29	PHE	N-CA-C	-6.30	105.34	113.16
1	A	325	THR	CB-CA-C	-6.24	100.82	110.62
1	D	429	GLY	N-CA-C	6.22	119.53	110.63
1	C	336	HIS	CB-CA-C	6.13	118.54	109.29
3	F	27	LEU	N-CA-C	-5.96	101.46	110.70
1	A	324	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	324	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	324	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	344	GLU	CB-CA-C	5.76	120.58	111.95
1	C	430	ARG	CA-C-N	-5.75	112.96	120.44
1	C	430	ARG	C-N-CA	-5.75	112.96	120.44
2	E	92	TYR	CB-CA-C	-5.71	99.03	109.54
1	C	196	GLY	CA-C-O	-5.68	117.08	122.13
1	A	325	THR	CA-C-O	-5.60	115.22	119.59
1	D	442	SER	N-CA-C	-5.58	101.66	109.69
1	D	295	TRP	CA-C-O	-5.55	115.39	121.89
1	D	297	GLY	CA-C-O	-5.53	114.89	121.08
1	D	325	THR	CA-C-O	-5.52	115.28	119.59
1	C	325	THR	CA-C-O	-5.52	115.29	119.59
1	A	365	THR	O-C-N	-5.50	116.52	123.01
1	D	468	PRO	CB-CA-C	-5.45	104.72	111.64
1	A	442	SER	N-CA-C	-5.37	101.95	109.69
1	B	442	SER	N-CA-C	-5.37	101.96	109.69
1	C	195	THR	CA-C-N	-5.32	115.03	122.85
1	C	195	THR	C-N-CA	-5.32	115.03	122.85
3	F	29	PHE	CA-CB-CG	5.32	119.12	113.80
2	E	15	PRO	CB-CA-C	-5.32	104.26	111.12
1	D	348	GLY	CA-C-O	-5.31	116.59	121.63
1	C	429	GLY	CA-C-O	-5.29	116.36	121.75
1	A	298	SER	N-CA-C	-5.28	105.69	113.61
1	A	326	PRO	N-CD-CG	-5.27	97.48	103.80
1	D	326	PRO	N-CD-CG	-5.18	97.59	103.80
1	C	326	PRO	N-CD-CG	-5.17	97.60	103.80
1	D	468	PRO	N-CA-CB	-5.13	98.57	103.19
1	A	198	ASP	CB-CA-C	-5.12	102.85	110.88
1	C	442	SER	N-CA-C	-5.05	101.73	109.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2990	0	2838	49	0
1	B	2990	0	2840	63	0
1	C	2990	0	2840	44	0
1	D	2990	0	2840	49	0
2	E	808	0	792	33	0
3	F	939	0	890	36	0
4	G	39	0	34	0	0
4	K	39	0	34	0	0
4	O	39	0	34	0	0
4	S	39	0	34	0	0
5	H	28	0	25	0	0
5	I	28	0	25	1	0
5	L	28	0	25	0	0
5	M	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	2	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
6	J	94	0	79	0	0
6	N	94	0	79	0	0
6	R	94	0	79	0	0
6	V	94	0	79	1	0
7	A	28	0	26	0	0
7	B	28	0	26	3	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	14579	0	13796	260	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 9.

All (260) 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)
3:F:6:GLU:OE2	3:F:116:GLY:N	2.05	0.89
3:F:4:LEU:HD13	3:F:112:VAL:CG1	2.05	0.86
1:D:297:GLY:H	1:D:345:GLY:HA3	1.40	0.85
1:A:109:SER:CB	1:A:140:LEU:HD22	2.12	0.80
3:F:4:LEU:HD13	3:F:112:VAL:HG11	1.67	0.75
1:C:305:ILE:HG23	1:C:312:ILE:HD11	1.67	0.75
1:C:222:ILE:O	1:C:224:ARG:NH1	2.25	0.70
1:A:222:ILE:O	1:A:224:ARG:NH1	2.25	0.69
1:C:347:HIS:CG	1:C:348:GLY:H	2.11	0.69
1:B:222:ILE:O	1:B:224:ARG:NH1	2.25	0.69
1:D:222:ILE:O	1:D:224:ARG:NH1	2.25	0.69
1:D:305:ILE:HG23	1:D:312:ILE:CD1	2.24	0.68
3:F:4:LEU:HD13	3:F:112:VAL:HG12	1.73	0.68
1:B:151:ASP:OD2	3:F:103:ARG:HG2	1.94	0.67
1:D:467:MET:HB3	1:D:468:PRO:HD2	1.76	0.67
1:C:467:MET:HB3	1:C:468:PRO:HD2	1.76	0.67
2:E:92:TYR:HB2	3:F:107:TYR:CD1	2.31	0.66
1:B:428:ARG:NH1	1:B:433:GLU:OE2	2.30	0.65
1:B:392:THR:HG22	1:B:393:ASN:N	2.09	0.65
1:C:305:ILE:HA	1:C:312:ILE:HD13	1.79	0.65
1:A:347:HIS:CG	1:A:348:GLY:H	2.15	0.65
1:C:425:GLU:HG3	1:C:441:ASN:HD22	1.62	0.65
1:D:135:GLY:O	1:D:156:ARG:HA	1.97	0.65
1:C:135:GLY:O	1:C:156:ARG:HA	1.97	0.64
1:C:400:ARG:O	1:C:400:ARG:HG2	1.96	0.64
1:A:428:ARG:NH1	1:A:433:GLU:OE2	2.30	0.64
1:C:305:ILE:HG23	1:C:312:ILE:CD1	2.28	0.64
1:B:392:THR:HG22	1:B:393:ASN:OD1	1.98	0.64
1:A:135:GLY:O	1:A:156:ARG:HA	1.97	0.64
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.81	0.63
1:B:135:GLY:O	1:B:156:ARG:HA	1.97	0.63
1:D:177:ALA:HB2	1:D:193:CYS:HB3	1.81	0.61
3:F:104:ASP:OD1	3:F:104:ASP:O	2.17	0.61
1:A:273:GLN:OE1	1:A:296:LYS:HD2	2.00	0.61
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.81	0.61
1:C:177:ALA:HB2	1:C:193:CYS:HB3	1.81	0.61
1:A:109:SER:HB3	1:A:140:LEU:HD22	1.80	0.60
1:A:150:ARG:HH11	1:A:153:THR:HG22	1.67	0.60
2:E:83:ASP:O	2:E:87:TYR:OH	2.20	0.59
1:C:325:THR:HG21	1:C:370:SER:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:HB2	1:B:342:ASN:OD1	2.02	0.59
1:A:264:HIS:CD2	1:A:265:THR:H	2.22	0.58
1:C:264:HIS:CD2	1:C:265:THR:H	2.22	0.58
1:C:103:ASP:OD2	1:C:443:ILE:HG22	2.03	0.58
2:E:18:ARG:HA	2:E:76:ILE:O	2.03	0.58
1:B:264:HIS:CD2	1:B:265:THR:H	2.21	0.58
2:E:45:PRO:HG2	3:F:45:LEU:HD21	1.84	0.58
3:F:70:ILE:HD11	3:F:79:LEU:HD12	1.86	0.57
1:D:347:HIS:CG	1:D:348:GLY:H	2.21	0.57
1:D:264:HIS:CD2	1:D:265:THR:H	2.22	0.57
3:F:36:TRP:CD1	3:F:70:ILE:HD13	2.39	0.56
1:B:159:LEU:HD23	1:B:173:GLN:HB3	1.88	0.56
1:D:305:ILE:HG23	1:D:312:ILE:HD11	1.86	0.56
3:F:6:GLU:HA	3:F:22:CYS:HA	1.87	0.56
1:C:347:HIS:CG	1:C:348:GLY:N	2.70	0.55
1:A:159:LEU:HD23	1:A:173:GLN:HB3	1.88	0.55
1:C:159:LEU:HD23	1:C:173:GLN:HB3	1.88	0.55
1:D:159:LEU:HD23	1:D:173:GLN:HB3	1.88	0.54
1:A:116:VAL:HG23	1:A:140:LEU:HD12	1.88	0.54
1:A:288:ARG:NE	1:A:304:ASP:OD1	2.32	0.54
1:D:288:ARG:NE	1:D:304:ASP:OD1	2.32	0.54
1:C:305:ILE:HG12	1:C:312:ILE:HD12	1.90	0.54
1:A:194:ILE:HD11	1:A:241:MET:HE3	1.91	0.53
1:B:295:TRP:CE3	2:E:30:SER:HB2	2.43	0.53
1:D:467:MET:HE2	1:D:468:PRO:HD2	1.91	0.53
1:C:194:ILE:HD11	1:C:241:MET:HE3	1.91	0.53
1:D:194:ILE:HD11	1:D:241:MET:HE3	1.91	0.53
3:F:6:GLU:OE2	3:F:116:GLY:CA	2.56	0.53
3:F:36:TRP:HB2	3:F:49:SER:OG	2.09	0.53
1:B:194:ILE:HD11	1:B:241:MET:HE3	1.91	0.52
1:A:150:ARG:NH1	1:A:153:THR:HG22	2.24	0.52
1:C:232:CYS:HA	1:C:237:CYS:HA	1.92	0.52
1:C:400:ARG:O	1:C:400:ARG:CG	2.57	0.52
1:B:152:ARG:HB2	3:F:100:TYR:OH	2.09	0.52
1:D:311:SER:O	1:D:312:ILE:HD13	2.11	0.51
1:D:328:LYS:HB2	1:D:333:SER:HB3	1.93	0.51
1:B:146:ASN:OD1	1:B:437:LEU:HB3	2.10	0.51
2:E:17:GLU:HG2	2:E:18:ARG:H	1.77	0.50
2:E:68:SER:OG	2:E:69:GLY:N	2.45	0.50
1:A:162:GLU:O	1:A:163:LEU:C	2.54	0.50
2:E:80:GLU:HB2	2:E:81:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:70:ILE:HD12	3:F:80:ASP:O	2.12	0.50
1:A:120:PRO:HG3	1:A:441:ASN:ND2	2.27	0.50
2:E:55:ARG:NE	2:E:61:ASP:HA	2.26	0.50
3:F:34:MET:HB2	3:F:51:ILE:CG2	2.42	0.50
1:A:116:VAL:CG2	1:A:140:LEU:HD12	2.42	0.49
1:A:347:HIS:CD2	1:A:348:GLY:H	2.29	0.49
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.94	0.49
2:E:37:TYR:HE1	2:E:90:GLN:HB3	1.77	0.49
3:F:35:ASN:OD1	3:F:50:HIS:ND1	2.33	0.49
2:E:39:GLN:NE2	2:E:43:GLN:O	2.46	0.49
3:F:27:LEU:N	3:F:27:LEU:HD22	2.27	0.49
2:E:28:TYR:CE1	2:E:69:GLY:HA2	2.47	0.49
1:B:152:ARG:NH2	3:F:100:TYR:CE1	2.81	0.49
1:A:155:TYR:CE1	1:C:461:GLY:HA3	2.47	0.49
1:A:327:ARG:NE	1:A:368:GLU:HG2	2.27	0.49
2:E:83:ASP:OD1	2:E:87:TYR:OH	2.31	0.49
2:E:86:VAL:HG22	2:E:103:LYS:HG2	1.95	0.49
1:B:392:THR:CG2	1:B:393:ASN:N	2.75	0.48
3:F:51:ILE:HG13	3:F:58:ILE:CD1	2.43	0.48
1:A:118:ARG:NH1	1:A:119:GLU:OE2	2.46	0.48
1:B:461:GLY:HA3	1:D:155:TYR:CE1	2.48	0.48
2:E:7:SER:HB2	2:E:22:SER:HB2	1.94	0.48
1:B:326:PRO:HD2	1:B:347:HIS:O	2.14	0.48
1:C:152:ARG:HE	1:C:198:ASP:CG	2.21	0.48
2:E:62:ARG:HD2	2:E:78:GLY:O	2.13	0.48
1:D:118:ARG:NH1	1:D:119:GLU:OE2	2.46	0.48
1:D:392:THR:HG22	1:D:393:ASN:OD1	2.14	0.48
1:A:461:GLY:HA3	1:B:155:TYR:CE1	2.48	0.48
1:C:118:ARG:NH1	1:C:119:GLU:OE2	2.46	0.47
1:C:120:PRO:HD3	1:C:441:ASN:ND2	2.29	0.47
1:D:430:ARG:O	1:D:430:ARG:HG3	2.13	0.47
1:B:118:ARG:NH1	1:B:119:GLU:OE2	2.46	0.47
1:C:155:TYR:CE1	1:D:461:GLY:HA3	2.48	0.47
1:A:128:LYS:HD2	1:A:162:GLU:OE1	2.15	0.47
1:B:406:TYR:OH	3:F:104:ASP:CG	2.57	0.47
1:D:467:MET:HB3	1:D:467:MET:HE2	1.76	0.47
2:E:55:ARG:CZ	2:E:61:ASP:HA	2.44	0.47
2:E:8:PRO:HG2	2:E:21:LEU:HA	1.96	0.47
1:A:431:LYS:O	1:A:431:LYS:HG3	2.15	0.47
1:C:392:THR:HG22	1:C:393:ASN:OD1	2.14	0.47
2:E:45:PRO:HD2	3:F:113:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:THR:HG22	1:A:393:ASN:OD1	2.14	0.47
1:B:318:CYS:O	1:B:386:PRO:HA	2.15	0.47
1:B:298:SER:O	1:B:322:VAL:HB	2.16	0.46
1:C:467:MET:HE2	1:C:468:PRO:HD2	1.97	0.46
2:E:6:GLN:N	2:E:100:GLN:HE22	2.12	0.46
1:A:142:ASN:OD1	1:C:110:ALA:HB3	2.15	0.46
1:B:296:LYS:HG3	1:B:340:PRO:HB2	1.96	0.46
2:E:21:LEU:HD13	2:E:74:LEU:HD23	1.96	0.46
1:B:205:PHE:CE1	1:B:262:ILE:HD11	2.51	0.46
1:A:428:ARG:NH2	1:A:462:ALA:O	2.49	0.46
1:B:120:PRO:HG3	1:B:441:ASN:ND2	2.31	0.46
1:B:343:GLU:O	1:B:344:GLU:C	2.59	0.46
1:D:85:ARG:HD3	1:D:87:TRP:CE2	2.51	0.46
1:D:467:MET:HB3	1:D:468:PRO:CD	2.44	0.46
1:B:392:THR:O	1:B:393:ASN:C	2.58	0.46
3:F:36:TRP:HB2	3:F:49:SER:HG	1.80	0.46
1:C:205:PHE:CE1	1:C:262:ILE:HD11	2.51	0.46
1:B:308:LYS:HD3	7:B:502:NAG:C8	2.45	0.45
1:B:275:VAL:HG13	1:B:291:CYS:SG	2.56	0.45
1:A:205:PHE:CE1	1:A:262:ILE:HD11	2.51	0.45
1:D:205:PHE:CE1	1:D:262:ILE:HD11	2.51	0.45
1:A:347:HIS:CG	1:A:348:GLY:N	2.80	0.45
2:E:67:GLY:HA3	2:E:72:PHE:HA	1.98	0.45
1:B:308:LYS:HB2	7:B:502:NAG:H81	1.98	0.45
1:D:85:ARG:HD3	1:D:87:TRP:CZ2	2.52	0.45
1:D:305:ILE:HG12	1:D:312:ILE:HD12	1.99	0.45
1:A:336:HIS:C	1:A:338:LEU:H	2.24	0.45
1:D:117:THR:OG1	1:D:441:ASN:ND2	2.50	0.45
1:D:316:TYR:OH	1:D:340:PRO:HG3	2.17	0.45
3:F:55:GLY:HA3	3:F:72:ARG:HD2	1.99	0.45
2:E:36:TRP:HB2	2:E:49:ILE:HB	1.99	0.44
2:E:40:LYS:HD2	2:E:41:PRO:HD2	2.00	0.44
1:A:324:ASP:O	1:A:327:ARG:HB3	2.17	0.44
1:B:272:ALA:CB	1:B:314:SER:HB3	2.47	0.44
1:D:297:GLY:O	1:D:298:SER:HB3	2.17	0.44
1:D:467:MET:CE	1:D:468:PRO:HD2	2.47	0.44
1:B:88:SER:HB2	7:B:501:NAG:HN2	1.81	0.44
1:D:169:LEU:HD23	1:D:169:LEU:HA	1.83	0.44
1:D:467:MET:CB	1:D:468:PRO:CD	2.95	0.44
1:D:430:ARG:NH2	1:D:434:THR:HB	2.32	0.44
1:A:220:LYS:HA	1:A:220:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TYR:OH	1:A:340:PRO:HG3	2.17	0.44
1:C:316:TYR:OH	1:C:340:PRO:HG3	2.17	0.44
1:C:324:ASP:O	1:C:327:ARG:HB3	2.18	0.44
1:C:347:HIS:CD2	1:C:348:GLY:H	2.34	0.44
1:B:279:SER:HB3	1:B:409:ILE:HG22	2.00	0.44
2:E:92:TYR:HD1	3:F:107:TYR:HE1	1.64	0.44
1:A:332:SER:HB3	5:I:1:NAG:O7	2.18	0.44
1:B:391:GLN:HE22	1:B:394:ARG:HD2	1.83	0.43
1:D:336:HIS:C	1:D:338:LEU:H	2.26	0.43
1:B:316:TYR:OH	1:B:340:PRO:HG3	2.17	0.43
1:B:428:ARG:NH2	1:B:462:ALA:O	2.49	0.43
1:D:391:GLN:O	1:D:392:THR:OG1	2.32	0.43
1:A:279:SER:HB3	1:A:409:ILE:HG22	2.00	0.43
1:B:336:HIS:C	1:B:338:LEU:H	2.26	0.43
1:D:279:SER:HB3	1:D:409:ILE:HG22	2.00	0.43
2:E:37:TYR:HE1	2:E:90:GLN:CB	2.32	0.43
3:F:107:TYR:CE2	3:F:109:GLY:HA2	2.53	0.43
1:B:296:LYS:HG3	1:B:340:PRO:CB	2.49	0.43
1:B:431:LYS:HD3	1:B:431:LYS:HA	1.54	0.43
1:D:295:TRP:O	1:D:296:LYS:C	2.62	0.43
1:B:392:THR:HG22	1:B:393:ASN:H	1.82	0.43
1:D:297:GLY:N	1:D:345:GLY:HA3	2.20	0.43
3:F:99:ASP:OD1	3:F:100:TYR:N	2.52	0.43
1:D:83:GLU:HB3	1:D:187:LYS:HE2	2.01	0.43
1:A:96:GLY:HA3	1:A:453:TYR:CE2	2.54	0.43
1:A:391:GLN:O	1:A:392:THR:OG1	2.32	0.43
1:B:387:LYS:HB2	1:B:387:LYS:HE2	1.71	0.43
1:C:183:CYS:HB3	1:C:232:CYS:SG	2.59	0.43
1:D:220:LYS:HA	1:D:220:LYS:HD3	1.82	0.43
3:F:27:LEU:HD22	3:F:27:LEU:H	1.84	0.43
1:C:428:ARG:NH2	1:C:462:ALA:O	2.50	0.43
1:D:183:CYS:HB3	1:D:232:CYS:SG	2.59	0.43
1:B:96:GLY:HA3	1:B:453:TYR:CE2	2.54	0.42
1:B:183:CYS:HB3	1:B:232:CYS:SG	2.59	0.42
1:D:232:CYS:HA	1:D:237:CYS:HA	2.01	0.42
2:E:45:PRO:CG	3:F:45:LEU:HD21	2.47	0.42
1:A:183:CYS:HB3	1:A:232:CYS:SG	2.59	0.42
2:E:21:LEU:HD23	2:E:102:THR:CG2	2.49	0.42
1:B:327:ARG:HG3	1:B:328:LYS:O	2.18	0.42
1:C:279:SER:HB3	1:C:409:ILE:HG22	2.00	0.42
6:V:4:MAN:H2	6:V:5:MAN:H2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:HIS:O	1:B:347:HIS:CG	2.71	0.42
1:D:87:TRP:HE3	1:D:418:ILE:HD12	1.85	0.42
1:C:169:LEU:HA	1:C:169:LEU:HD23	1.83	0.42
1:A:328:LYS:HG3	1:A:344:GLU:HG3	2.01	0.42
1:C:429:GLY:O	1:C:433:GLU:HB2	2.19	0.42
1:D:96:GLY:HA3	1:D:453:TYR:CE2	2.54	0.42
3:F:87:ARG:HH21	3:F:89:GLU:CD	2.26	0.42
1:A:83:GLU:HB3	1:A:187:LYS:HE2	2.01	0.42
1:C:96:GLY:HA3	1:C:453:TYR:CE2	2.54	0.42
1:C:376:THR:HG23	1:C:397:ILE:HD13	2.01	0.42
1:C:391:GLN:O	1:C:392:THR:OG1	2.32	0.42
1:C:103:ASP:CG	1:C:443:ILE:HG22	2.44	0.42
1:C:87:TRP:HE3	1:C:418:ILE:HD12	1.85	0.42
3:F:6:GLU:OE1	3:F:114:GLY:HA3	2.20	0.42
1:B:270:GLY:HA3	1:B:314:SER:HB2	2.02	0.42
2:E:17:GLU:HG2	2:E:18:ARG:N	2.34	0.42
1:D:376:THR:HG23	1:D:397:ILE:HD13	2.01	0.41
1:A:270:GLY:HA3	1:A:314:SER:HB2	2.02	0.41
1:B:83:GLU:HB3	1:B:187:LYS:HE2	2.01	0.41
1:B:220:LYS:HD3	1:B:220:LYS:HA	1.82	0.41
1:A:376:THR:HG23	1:A:397:ILE:HD13	2.01	0.41
1:B:232:CYS:HA	1:B:237:CYS:HA	2.01	0.41
1:D:347:HIS:CG	1:D:348:GLY:N	2.88	0.41
1:B:233:ILE:HB	1:B:307:ILE:HG12	2.02	0.41
1:B:376:THR:HG23	1:B:397:ILE:HD13	2.01	0.41
1:A:132:PHE:HA	1:A:159:LEU:O	2.21	0.41
1:A:232:CYS:HA	1:A:237:CYS:HA	2.01	0.41
1:B:308:LYS:HB3	1:B:308:LYS:HE2	1.80	0.41
1:D:270:GLY:HA3	1:D:314:SER:HB2	2.03	0.41
2:E:56:ALA:HB3	2:E:59:ILE:HG13	2.01	0.41
2:E:76:ILE:HG21	2:E:83:ASP:OD2	2.20	0.41
3:F:42:GLY:C	3:F:43:LYS:HD2	2.46	0.41
1:C:329:ASN:HD22	5:Q:1:NAG:C7	2.33	0.41
3:F:20:LEU:HD23	3:F:20:LEU:HA	1.94	0.41
3:F:37:VAL:HG23	3:F:47:TRP:HA	2.02	0.41
1:A:83:GLU:HG3	1:A:187:LYS:HG2	2.03	0.41
1:B:467:MET:HE2	1:B:467:MET:HB3	1.56	0.41
1:B:466:LEU:O	1:B:467:MET:C	2.64	0.41
1:B:295:TRP:O	1:B:296:LYS:HG2	2.21	0.41
1:D:296:LYS:HE3	1:D:296:LYS:HB2	1.86	0.41
3:F:6:GLU:HA	3:F:21:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:ARG:HG3	2:E:77:SER:OG	2.22	0.40
1:B:132:PHE:HA	1:B:159:LEU:O	2.21	0.40
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.83	0.40
2:E:76:ILE:HD13	2:E:83:ASP:OD2	2.21	0.40
5:Q:1:NAG:H61	5:Q:2:NAG:O7	2.21	0.40
1:B:278:CYS:HB3	1:B:289:CYS:HB3	2.03	0.40
1:B:86:ASN:HB3	1:B:234:ASN:OD1	2.22	0.40
1:C:278:CYS:HB3	1:C:289:CYS:HB3	2.03	0.40
3:F:9:GLY:HA2	3:F:18:LEU:HD21	2.02	0.40
1:A:103:ASP:HA	1:B:173:GLN:NE2	2.37	0.40
1:A:199:LYS:HA	1:A:199:LYS:HD3	1.90	0.40
1:A:278:CYS:HB3	1:A:289:CYS:HB3	2.03	0.40
1:B:83:GLU:HG3	1:B:187:LYS:HG2	2.03	0.40
1:B:150:ARG:NH1	1:B:153:THR:HG22	2.37	0.40
1:D:295:TRP:HA	1:D:295:TRP:CE3	2.57	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	385/387 (100%)	359 (93%)	26 (7%)	0	100	100
1	B	385/387 (100%)	357 (93%)	27 (7%)	1 (0%)	37	69
1	C	385/387 (100%)	361 (94%)	22 (6%)	2 (0%)	25	59
1	D	385/387 (100%)	359 (93%)	24 (6%)	2 (0%)	25	59
2	E	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
3	F	121/123 (98%)	119 (98%)	1 (1%)	1 (1%)	16	49
All	All	1766/1778 (99%)	1652 (94%)	108 (6%)	6 (0%)	38	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	298	SER
3	F	3	GLN
1	C	347	HIS
1	D	328	LYS
1	B	344	GLU
1	C	338	LEU

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	337/337 (100%)	337 (100%)	0	100	100
1	B	337/337 (100%)	336 (100%)	1 (0%)	91	96
1	C	337/337 (100%)	337 (100%)	0	100	100
1	D	337/337 (100%)	336 (100%)	1 (0%)	91	96
2	E	88/88 (100%)	88 (100%)	0	100	100
3	F	99/100 (99%)	98 (99%)	1 (1%)	73	88
All	All	1535/1536 (100%)	1532 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	LYS
1	D	295	TRP
3	F	29	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	HIS
1	A	310	HIS
1	A	347	HIS
1	B	391	GLN
1	B	465	ASN

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Mol	Chain	Res	Type
1	C	161	ASN
1	C	336	HIS
1	C	441	ASN
1	D	161	ASN
1	D	342	ASN
1	D	441	ASN
2	E	90	GLN
3	F	77	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](#)

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.60	0	17,19,21	1.40	4 (23%)
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	1.16	1 (5%)
4	BMA	G	3	4	11,11,12	0.24	0	15,15,17	0.60	0
5	NAG	H	1	5,1	14,14,15	0.55	0	17,19,21	1.90	3 (17%)
5	NAG	H	2	5	14,14,15	0.38	0	17,19,21	1.03	1 (5%)
5	NAG	I	1	5,1	14,14,15	0.41	0	17,19,21	1.32	2 (11%)
5	NAG	I	2	5	14,14,15	0.29	0	17,19,21	0.86	0
6	NAG	J	1	1,6	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
6	NAG	J	2	6	14,14,15	0.68	0	17,19,21	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	J	3	6	11,11,12	0.73	0	15,15,17	1.06	0
6	MAN	J	4	6	11,11,12	0.35	0	15,15,17	1.35	2 (13%)
6	MAN	J	5	6	11,11,12	0.35	0	15,15,17	0.83	0
6	MAN	J	6	6	11,11,12	0.28	0	15,15,17	1.00	0
6	MAN	J	7	6	11,11,12	0.26	0	15,15,17	0.94	0
6	MAN	J	8	6	11,11,12	0.30	0	15,15,17	0.64	0
4	NAG	K	1	1,4	14,14,15	0.41	0	17,19,21	1.37	3 (17%)
4	NAG	K	2	4	14,14,15	0.35	0	17,19,21	1.54	3 (17%)
4	BMA	K	3	4	11,11,12	0.32	0	15,15,17	0.97	0
5	NAG	L	1	5,1	14,14,15	0.55	0	17,19,21	0.82	0
5	NAG	L	2	5	14,14,15	0.36	0	17,19,21	1.56	3 (17%)
5	NAG	M	1	5,1	14,14,15	0.62	0	17,19,21	0.89	0
5	NAG	M	2	5	14,14,15	0.40	0	17,19,21	1.04	1 (5%)
6	NAG	N	1	1,6	14,14,15	0.63	0	17,19,21	1.03	0
6	NAG	N	2	6	14,14,15	0.86	0	17,19,21	1.54	3 (17%)
6	BMA	N	3	6	11,11,12	0.68	0	15,15,17	1.09	1 (6%)
6	MAN	N	4	6	11,11,12	0.43	0	15,15,17	1.68	4 (26%)
6	MAN	N	5	6	11,11,12	0.34	0	15,15,17	0.84	0
6	MAN	N	6	6	11,11,12	0.39	0	15,15,17	1.45	2 (13%)
6	MAN	N	7	6	11,11,12	0.32	0	15,15,17	0.87	0
6	MAN	N	8	6	11,11,12	0.19	0	15,15,17	0.73	0
4	NAG	O	1	1,4	14,14,15	0.48	0	17,19,21	1.03	2 (11%)
4	NAG	O	2	4	14,14,15	0.33	0	17,19,21	0.83	0
4	BMA	O	3	4	11,11,12	0.24	0	15,15,17	0.68	0
5	NAG	P	1	5,1	14,14,15	0.48	0	17,19,21	0.78	0
5	NAG	P	2	5	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
5	NAG	Q	1	5,1	14,14,15	0.48	0	17,19,21	0.98	1 (5%)
5	NAG	Q	2	5	14,14,15	0.37	0	17,19,21	1.35	3 (17%)
6	NAG	R	1	1,6	14,14,15	0.56	0	17,19,21	1.39	2 (11%)
6	NAG	R	2	6	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
6	BMA	R	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.46	3 (20%)
6	MAN	R	4	6	11,11,12	0.59	0	15,15,17	1.70	5 (33%)
6	MAN	R	5	6	11,11,12	0.33	0	15,15,17	1.19	1 (6%)
6	MAN	R	6	6	11,11,12	0.35	0	15,15,17	0.89	0
6	MAN	R	7	6	11,11,12	0.29	0	15,15,17	0.81	0
6	MAN	R	8	6	11,11,12	0.27	0	15,15,17	0.65	0
4	NAG	S	1	1,4	14,14,15	0.53	0	17,19,21	0.86	1 (5%)
4	NAG	S	2	4	14,14,15	0.32	0	17,19,21	1.10	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	S	3	4	11,11,12	0.29	0	15,15,17	1.14	1 (6%)
5	NAG	T	1	5,1	14,14,15	0.50	0	17,19,21	0.64	0
5	NAG	T	2	5	14,14,15	0.26	0	17,19,21	1.21	2 (11%)
5	NAG	U	1	5,1	14,14,15	0.50	0	17,19,21	1.12	2 (11%)
5	NAG	U	2	5	14,14,15	0.41	0	17,19,21	0.74	0
6	NAG	V	1	1,6	14,14,15	0.54	0	17,19,21	1.27	3 (17%)
6	NAG	V	2	6	14,14,15	0.85	0	17,19,21	1.35	4 (23%)
6	BMA	V	3	6	11,11,12	0.79	0	15,15,17	1.47	1 (6%)
6	MAN	V	4	6	11,11,12	0.61	0	15,15,17	1.38	2 (13%)
6	MAN	V	5	6	11,11,12	0.46	0	15,15,17	0.65	0
6	MAN	V	6	6	11,11,12	0.43	0	15,15,17	0.85	0
6	MAN	V	7	6	11,11,12	0.23	0	15,15,17	0.77	0
6	MAN	V	8	6	11,11,12	0.20	0	15,15,17	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	1/2/19/22	0/1/1/1
6	MAN	J	6	6	-	2/2/19/22	0/1/1/1
6	MAN	J	7	6	-	0/2/19/22	0/1/1/1
6	MAN	J	8	6	-	0/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
5	NAG	L	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	MAN	N	6	6	-	0/2/19/22	0/1/1/1
6	MAN	N	7	6	-	2/2/19/22	0/1/1/1
6	MAN	N	8	6	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	5/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
6	MAN	R	4	6	-	0/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1
6	MAN	R	6	6	-	0/2/19/22	0/1/1/1
6	MAN	R	7	6	-	0/2/19/22	0/1/1/1
6	MAN	R	8	6	-	0/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	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	5,1	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
6	MAN	V	4	6	-	2/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	V	6	6	-	2/2/19/22	0/1/1/1
6	MAN	V	7	6	-	0/2/19/22	0/1/1/1
6	MAN	V	8	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	3	BMA	C2-C3	-2.04	1.49	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-O5-C5	5.66	119.86	112.19
6	V	3	BMA	O3-C3-C2	-4.32	101.72	109.99
6	R	1	NAG	C1-O5-C5	4.08	117.72	112.19
6	R	3	BMA	O3-C3-C2	-4.02	102.30	109.99
6	N	4	MAN	O5-C1-C2	3.91	116.81	110.77
6	N	2	NAG	O4-C4-C3	-3.91	101.32	110.35
4	K	2	NAG	O5-C1-C2	-3.80	105.29	111.29
4	S	3	BMA	C1-O5-C5	3.71	117.21	112.19
6	J	1	NAG	C1-O5-C5	3.63	117.11	112.19
5	L	2	NAG	C2-N2-C7	3.63	128.07	122.90
5	L	2	NAG	C1-C2-N2	3.56	116.57	110.49
5	Q	2	NAG	C2-N2-C7	3.39	127.72	122.90
5	H	1	NAG	O5-C5-C6	-3.32	102.00	107.20
6	R	4	MAN	O5-C1-C2	3.28	115.83	110.77
4	K	2	NAG	C4-C3-C2	-3.23	106.28	111.02
5	H	1	NAG	O5-C1-C2	-3.18	106.26	111.29
6	V	1	NAG	C1-O5-C5	3.17	116.48	112.19
5	M	2	NAG	C1-O5-C5	3.14	116.45	112.19
5	I	1	NAG	C4-C3-C2	-3.14	106.41	111.02
4	K	1	NAG	O4-C4-C3	-2.93	103.57	110.35
6	R	2	NAG	O4-C4-C3	-2.87	103.72	110.35
5	T	2	NAG	C2-N2-C7	2.86	126.98	122.90
6	V	4	MAN	O5-C5-C6	2.85	111.67	107.20
5	U	1	NAG	C1-O5-C5	2.84	116.04	112.19
4	G	1	NAG	C2-N2-C7	-2.79	118.94	122.90
6	N	2	NAG	C1-O5-C5	2.75	115.92	112.19
6	N	2	NAG	C1-C2-N2	-2.75	105.80	110.49
4	S	2	NAG	C2-N2-C7	2.74	126.80	122.90
6	R	4	MAN	C1-O5-C5	2.71	115.86	112.19
5	H	2	NAG	C4-C3-C2	-2.62	107.18	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	4	MAN	O5-C1-C2	2.61	114.80	110.77
6	J	4	MAN	C1-O5-C5	2.60	115.72	112.19
4	G	2	NAG	O4-C4-C3	-2.58	104.37	110.35
5	T	2	NAG	C1-O5-C5	2.58	115.69	112.19
5	I	1	NAG	O5-C5-C6	2.56	111.22	107.20
5	L	2	NAG	C4-C3-C2	-2.53	107.31	111.02
4	O	1	NAG	O5-C1-C2	2.53	115.28	111.29
6	V	2	NAG	O5-C1-C2	-2.52	107.31	111.29
6	J	2	NAG	C2-N2-C7	2.50	126.46	122.90
4	G	1	NAG	O5-C1-C2	-2.49	107.36	111.29
6	R	2	NAG	C1-O5-C5	2.47	115.54	112.19
4	K	1	NAG	O5-C1-C2	-2.41	107.47	111.29
6	N	6	MAN	O3-C3-C2	2.40	114.59	109.99
6	N	4	MAN	C1-O5-C5	2.33	115.34	112.19
6	R	1	NAG	O3-C3-C2	-2.31	104.69	109.47
4	K	1	NAG	C2-N2-C7	-2.30	119.62	122.90
4	K	2	NAG	C2-N2-C7	-2.30	119.62	122.90
4	S	2	NAG	C1-C2-N2	2.30	114.42	110.49
5	Q	2	NAG	C1-C2-N2	2.26	114.35	110.49
6	N	4	MAN	O2-C2-C1	-2.25	104.55	109.15
6	R	3	BMA	C2-C3-C4	-2.23	107.04	110.89
6	V	2	NAG	C2-N2-C7	-2.22	119.74	122.90
6	V	4	MAN	O2-C2-C1	2.19	113.64	109.15
6	N	6	MAN	O5-C1-C2	-2.17	107.42	110.77
6	R	5	MAN	C3-C4-C5	-2.15	106.40	110.24
6	V	1	NAG	O5-C1-C2	-2.14	107.90	111.29
6	R	4	MAN	O2-C2-C1	2.14	113.52	109.15
6	R	4	MAN	C3-C4-C5	2.12	114.02	110.24
4	S	1	NAG	O4-C4-C3	-2.12	105.45	110.35
6	J	1	NAG	O5-C1-C2	-2.11	107.96	111.29
5	U	1	NAG	O5-C5-C6	-2.10	103.91	107.20
6	R	4	MAN	O3-C3-C4	-2.09	105.51	110.35
5	Q	1	NAG	C4-C3-C2	-2.09	107.96	111.02
6	J	2	NAG	O4-C4-C3	-2.08	105.53	110.35
4	G	1	NAG	C1-O5-C5	2.07	115.00	112.19
4	G	1	NAG	O4-C4-C5	-2.07	104.17	109.30
5	Q	2	NAG	C1-O5-C5	2.07	114.99	112.19
6	V	2	NAG	C1-O5-C5	2.05	114.97	112.19
6	N	3	BMA	C6-C5-C4	-2.05	108.20	113.00
6	R	3	BMA	C6-C5-C4	-2.04	108.23	113.00
6	V	1	NAG	O3-C3-C2	-2.04	105.25	109.47
5	P	2	NAG	C4-C3-C2	-2.02	108.06	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	4	MAN	O3-C3-C4	-2.01	105.69	110.35
4	O	1	NAG	O4-C4-C3	-2.01	105.71	110.35
6	V	2	NAG	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
5	Q	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C8-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
6	N	7	MAN	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	J	6	MAN	C4-C5-C6-O6
4	G	2	NAG	O7-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	T	1	NAG	C8-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
6	V	4	MAN	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
5	L	2	NAG	C1-C2-N2-C7
6	J	4	MAN	O5-C5-C6-O6
6	V	6	MAN	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
5	T	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	V	6	MAN	C4-C5-C6-O6
6	J	6	MAN	O5-C5-C6-O6
6	N	7	MAN	C4-C5-C6-O6
4	S	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
6	V	4	MAN	O5-C5-C6-O6
6	R	1	NAG	O7-C7-N2-C2
4	S	3	BMA	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
5	I	2	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
6	V	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O7-C7-N2-C2
6	N	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C1-C2-N2-C7
6	N	1	NAG	C8-C7-N2-C2
5	Q	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
4	S	3	BMA	C4-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
4	O	2	NAG	O7-C7-N2-C2

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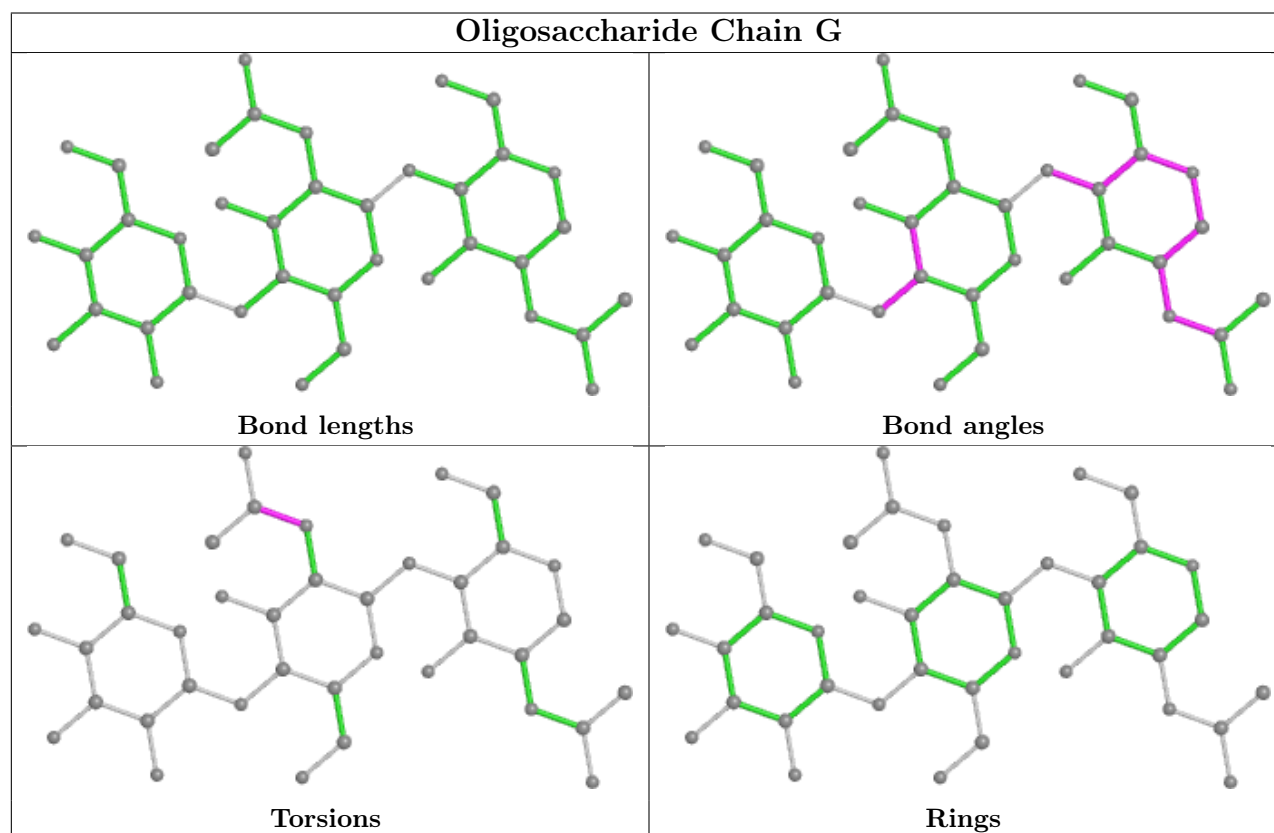
Mol	Chain	Res	Type	Atoms
6	V	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C4-C5-C6-O6

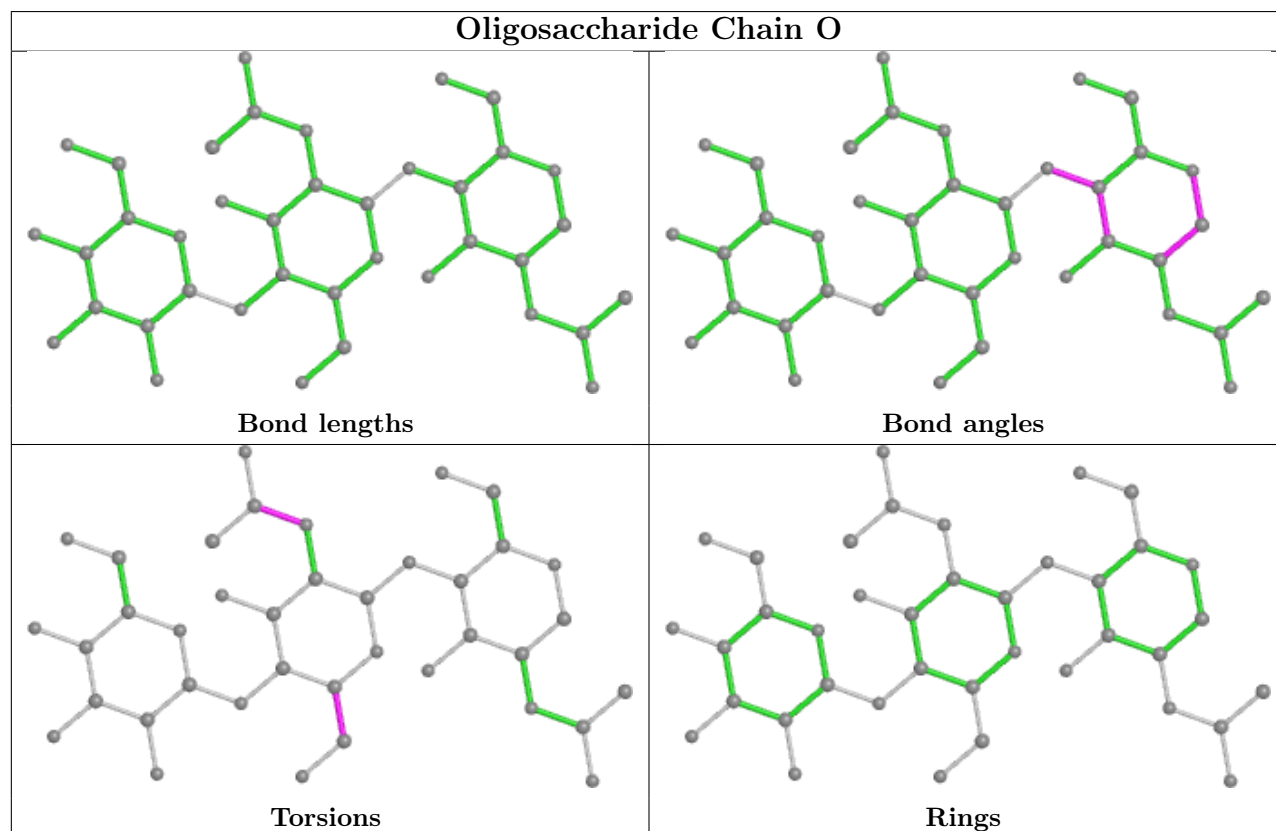
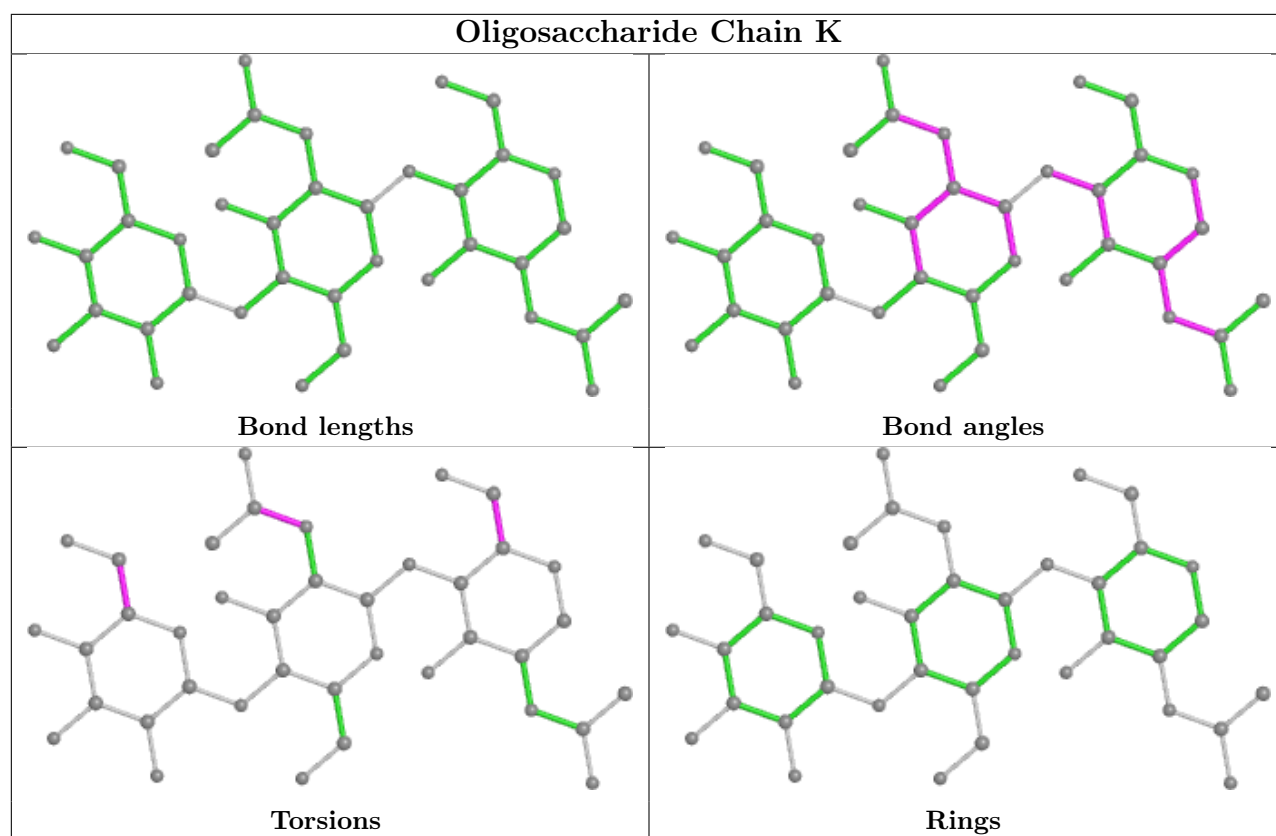
There are no ring outliers.

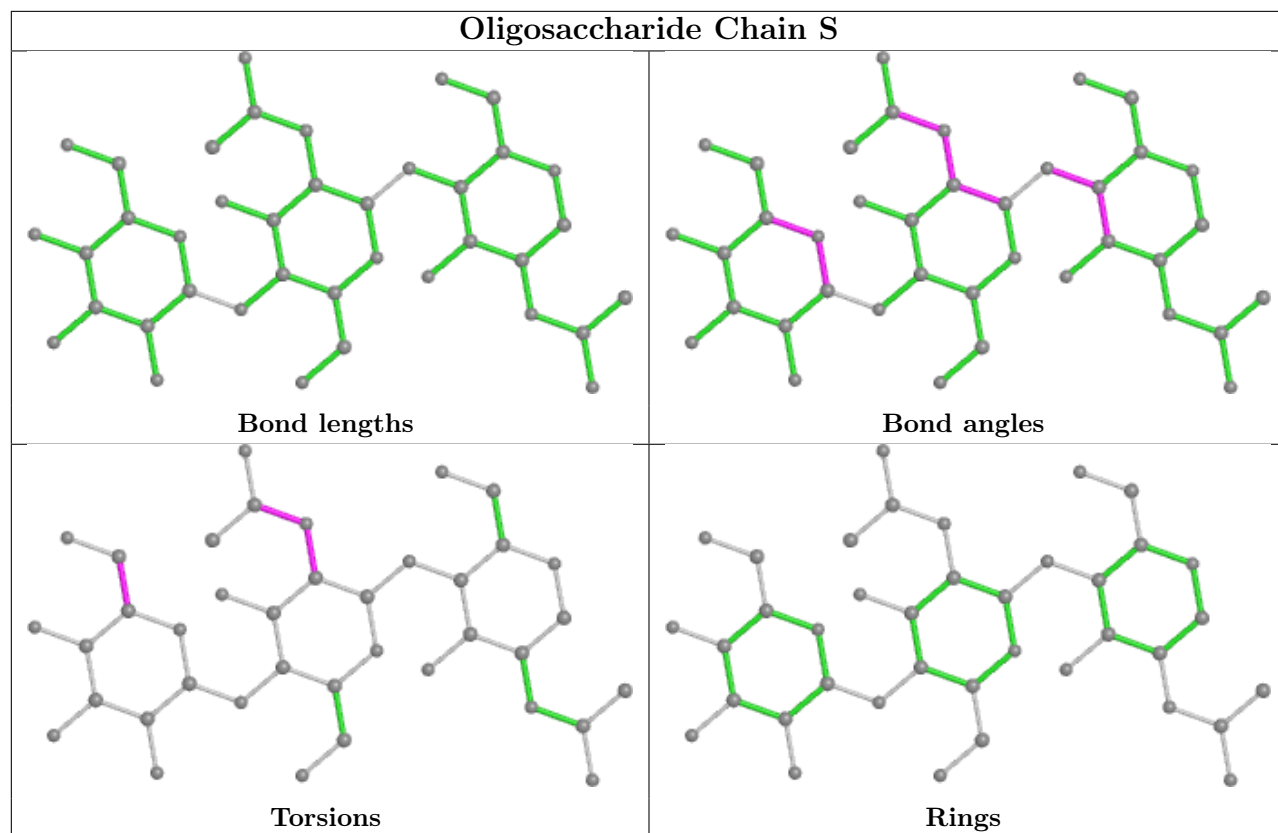
5 monomers are involved in 4 short contacts:

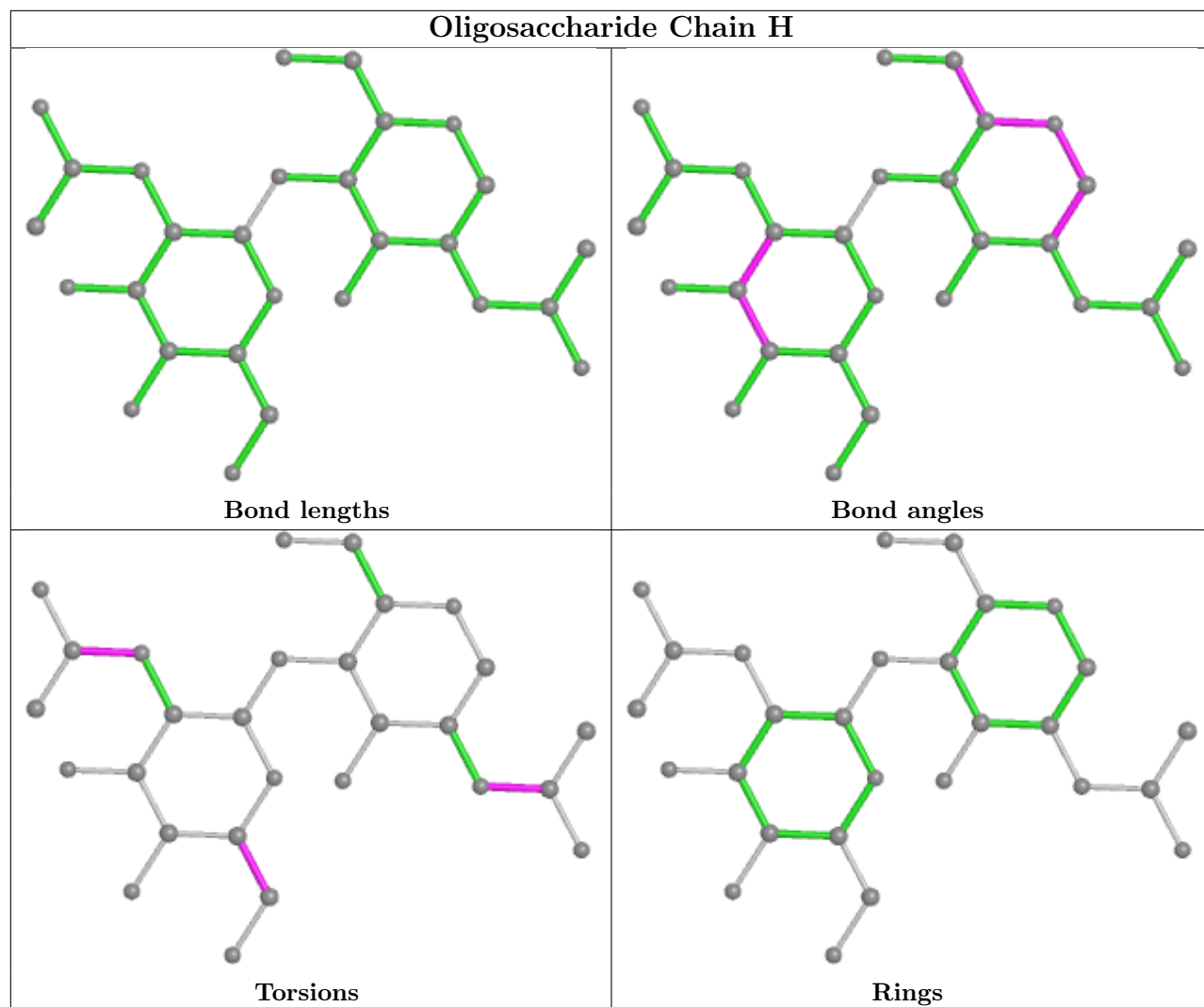
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0
6	V	5	MAN	1	0
5	Q	2	NAG	1	0
5	Q	1	NAG	2	0
6	V	4	MAN	1	0

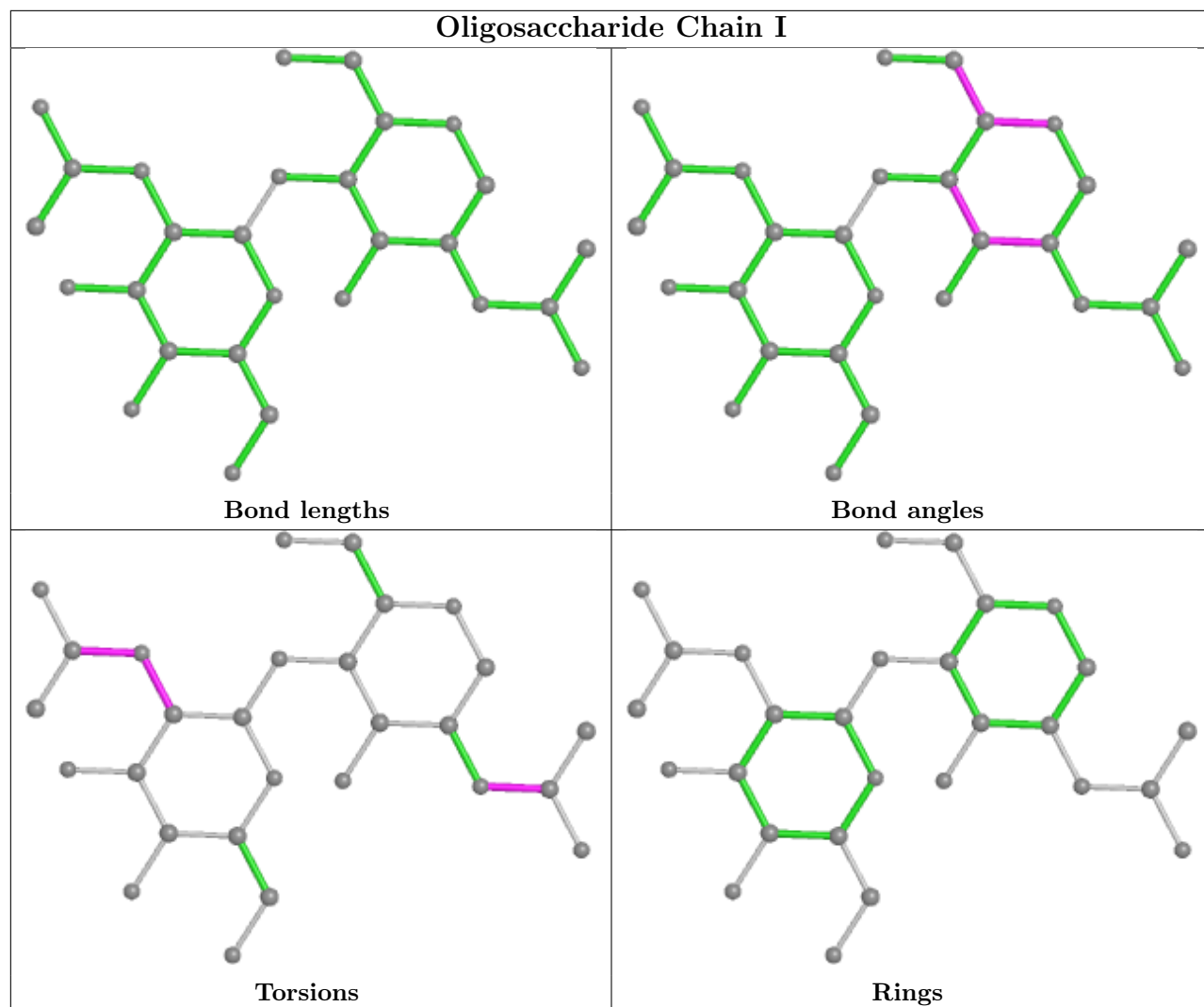
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

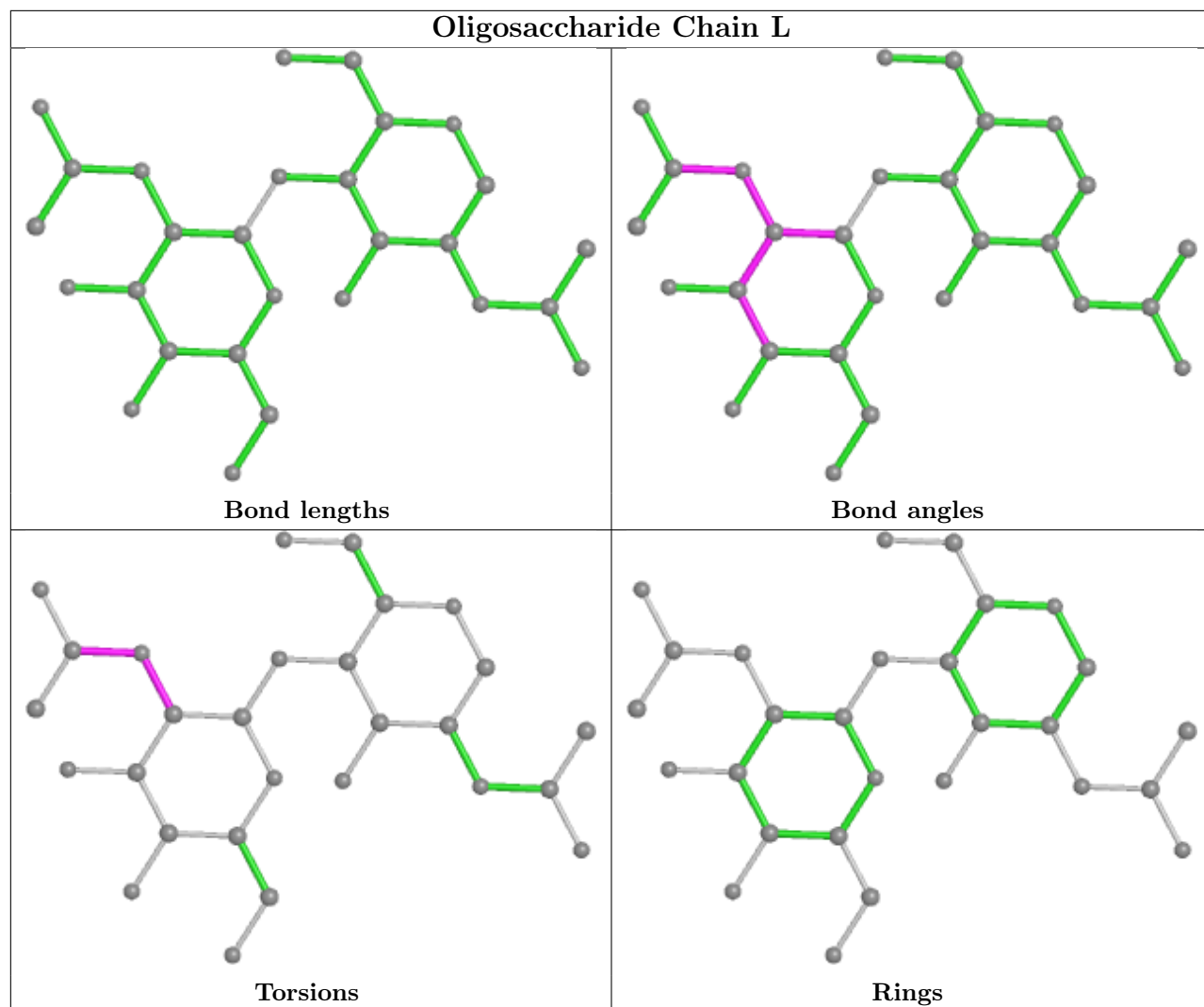


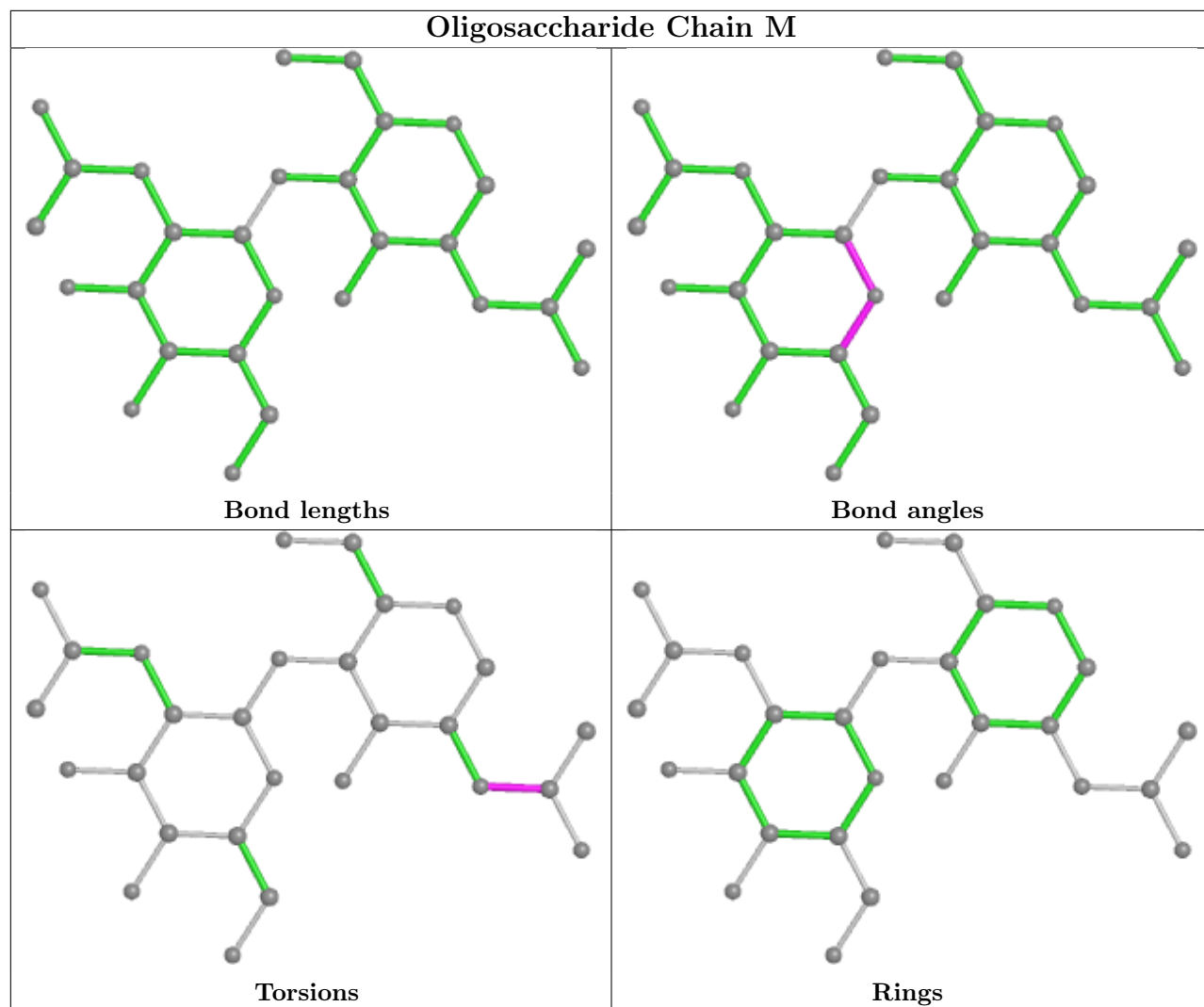


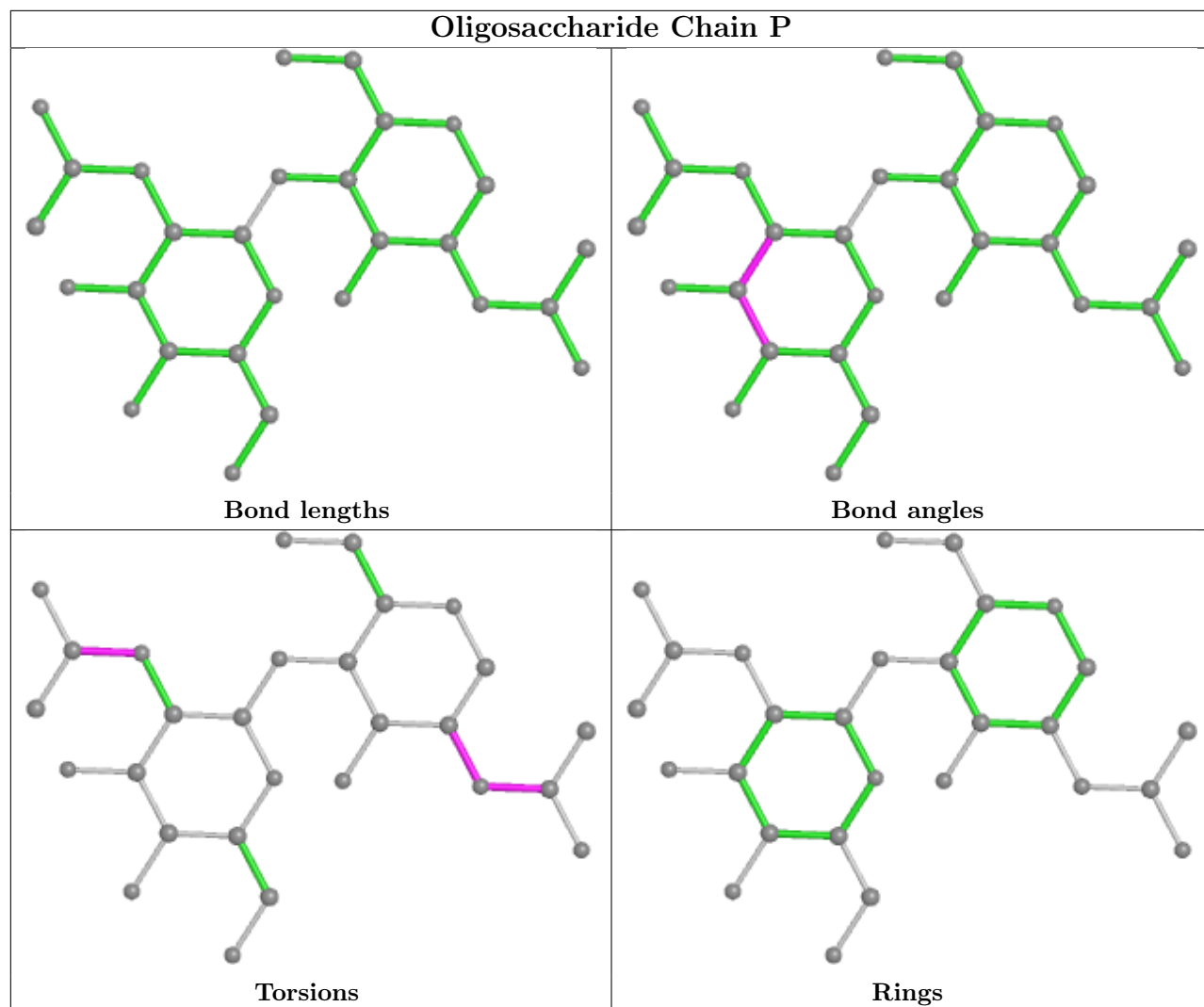


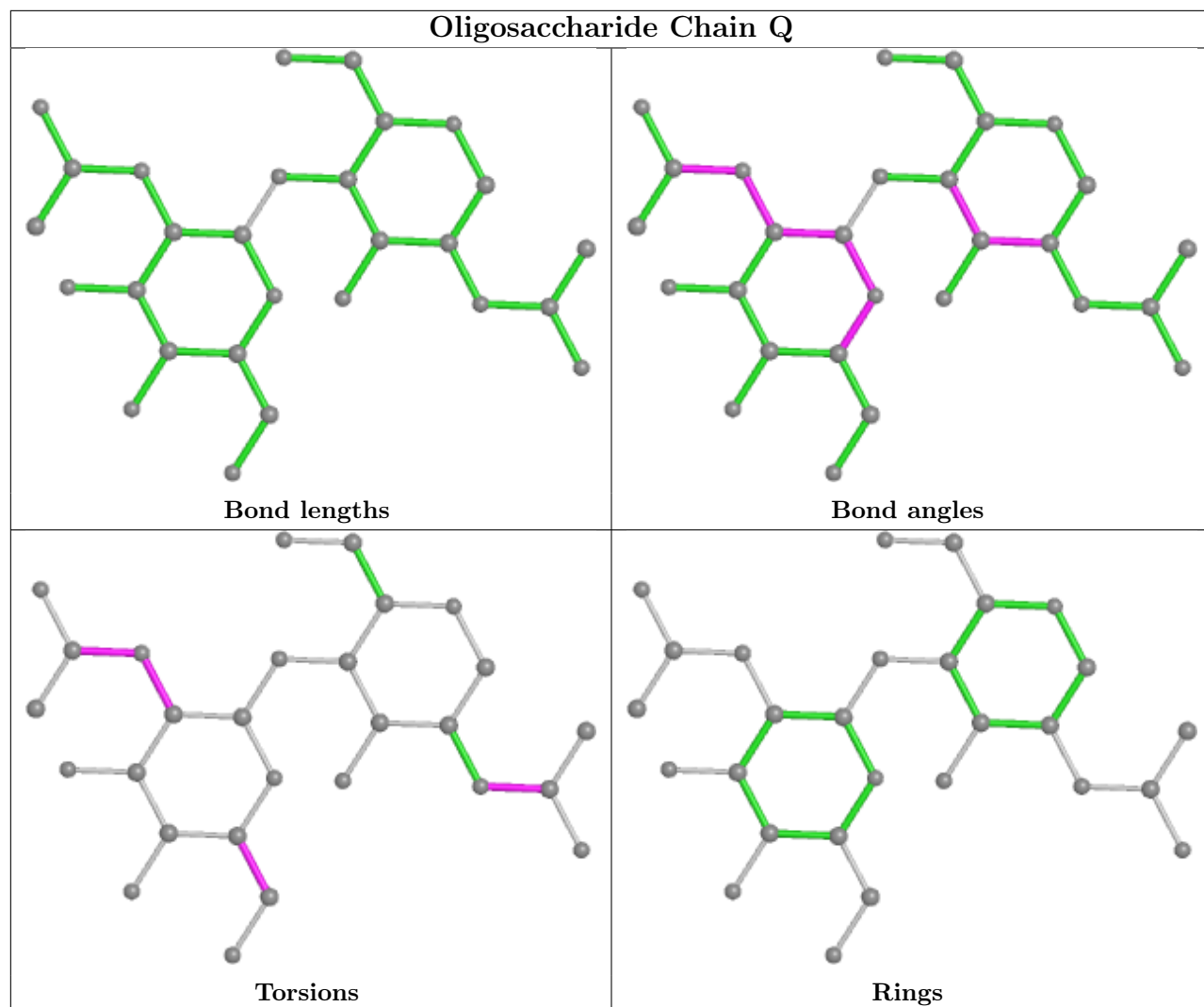


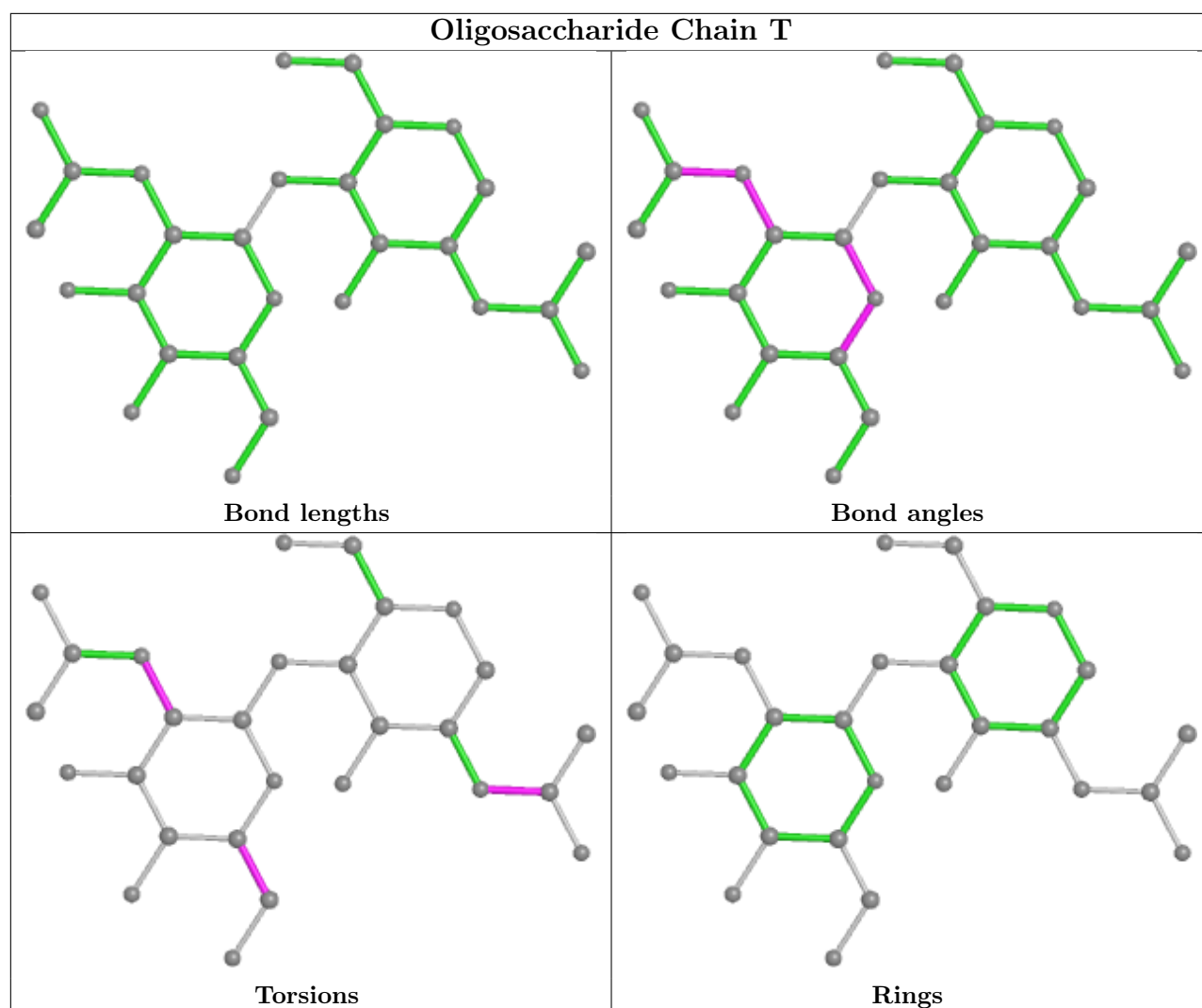


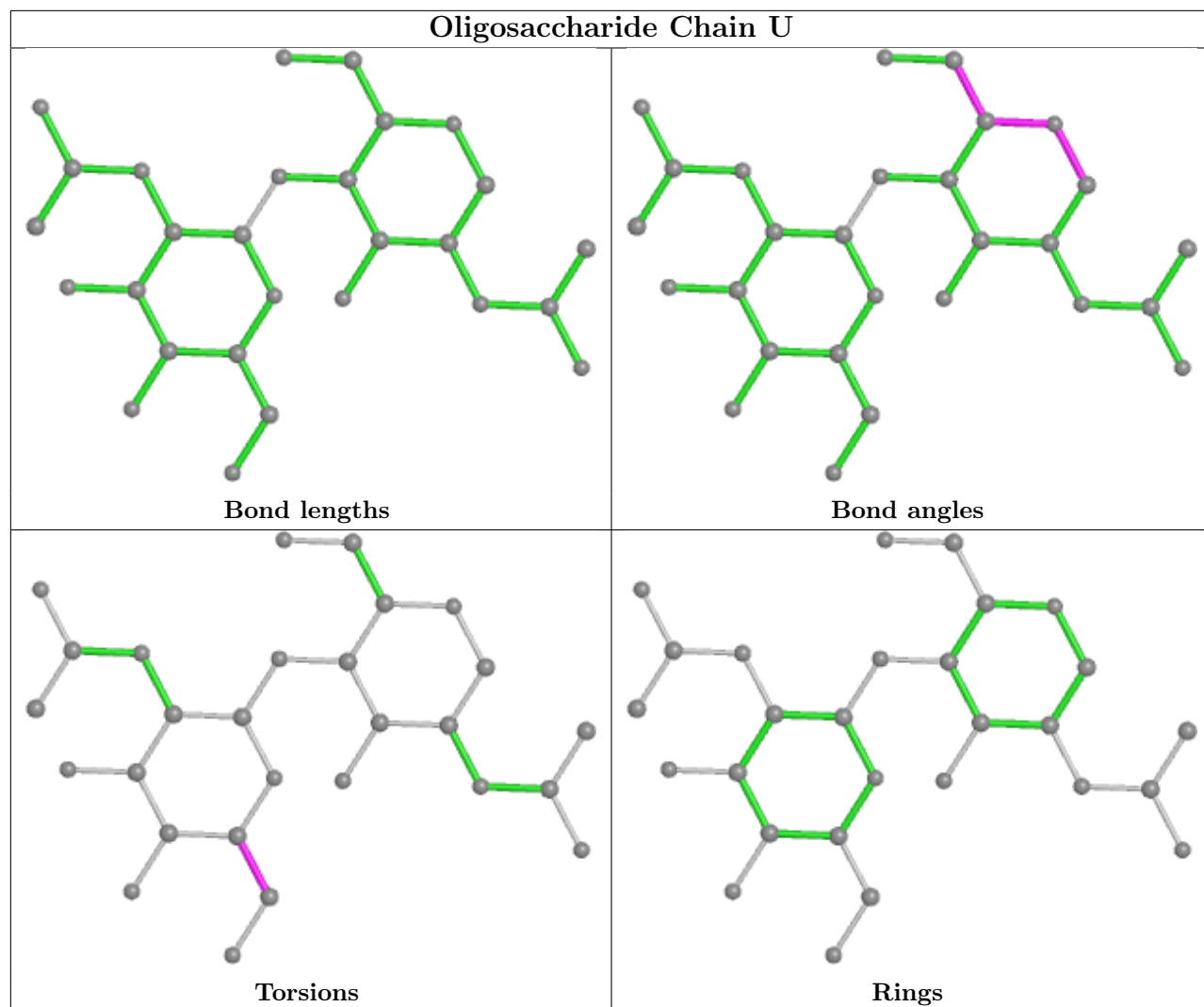


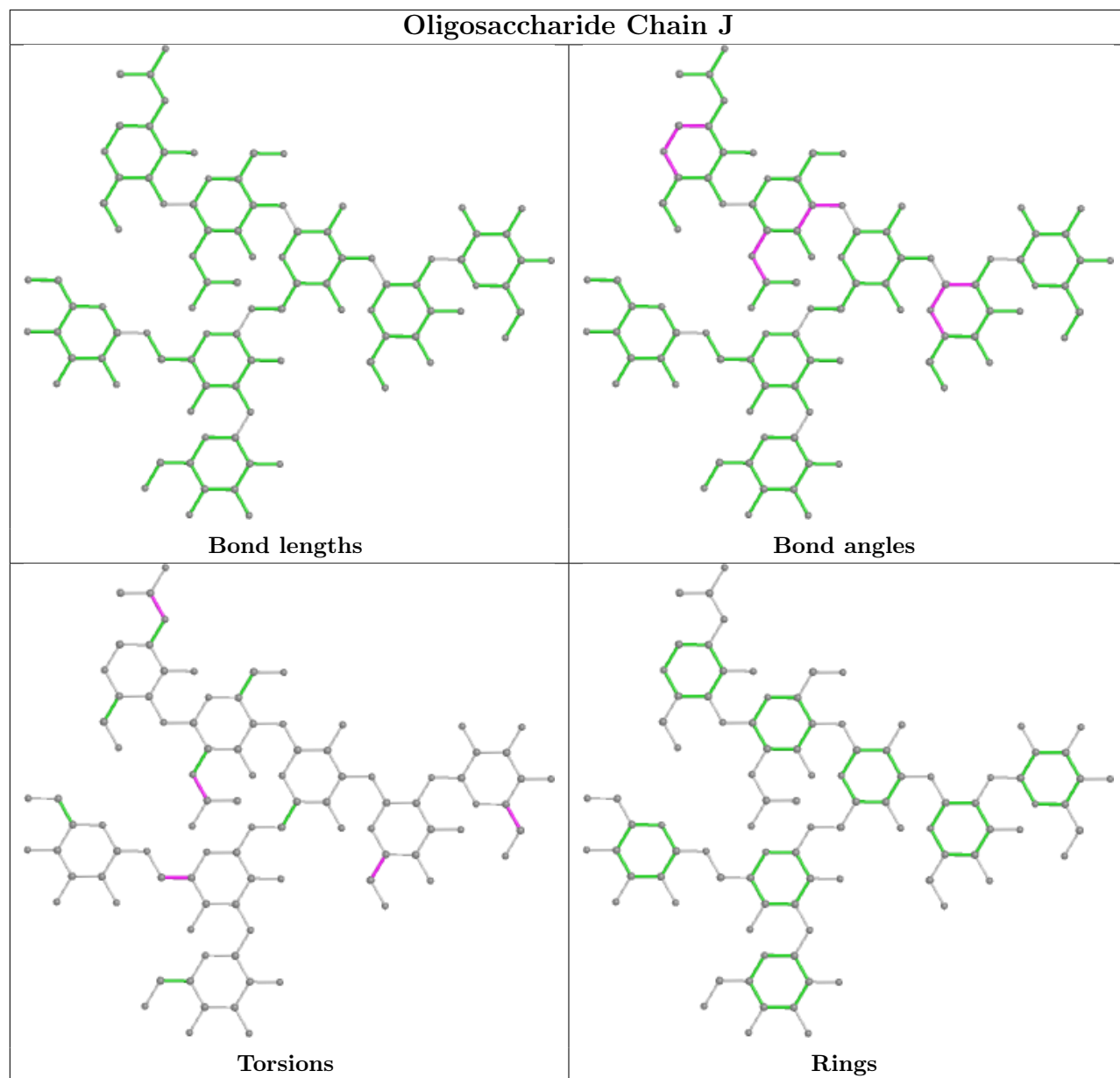


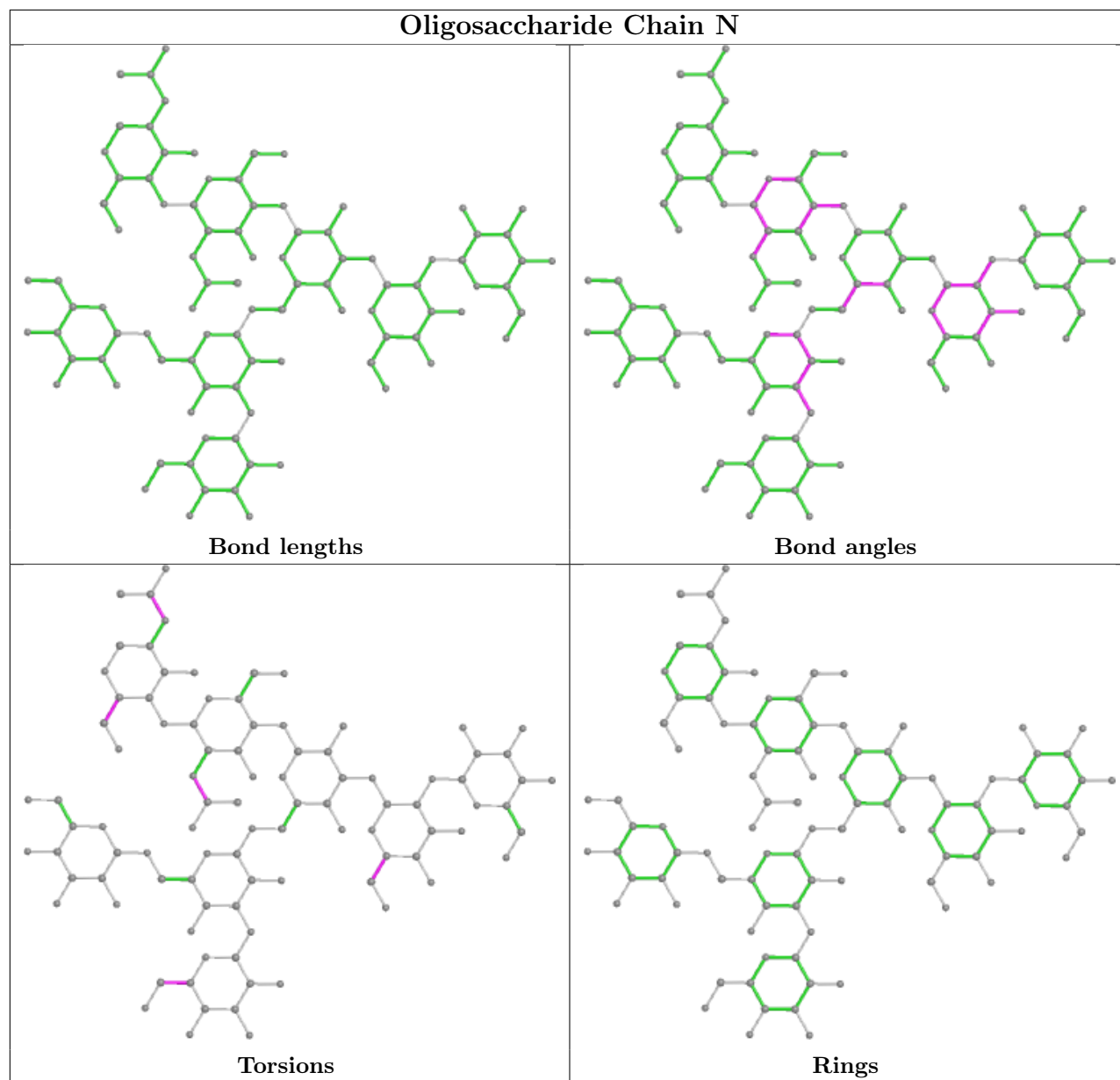


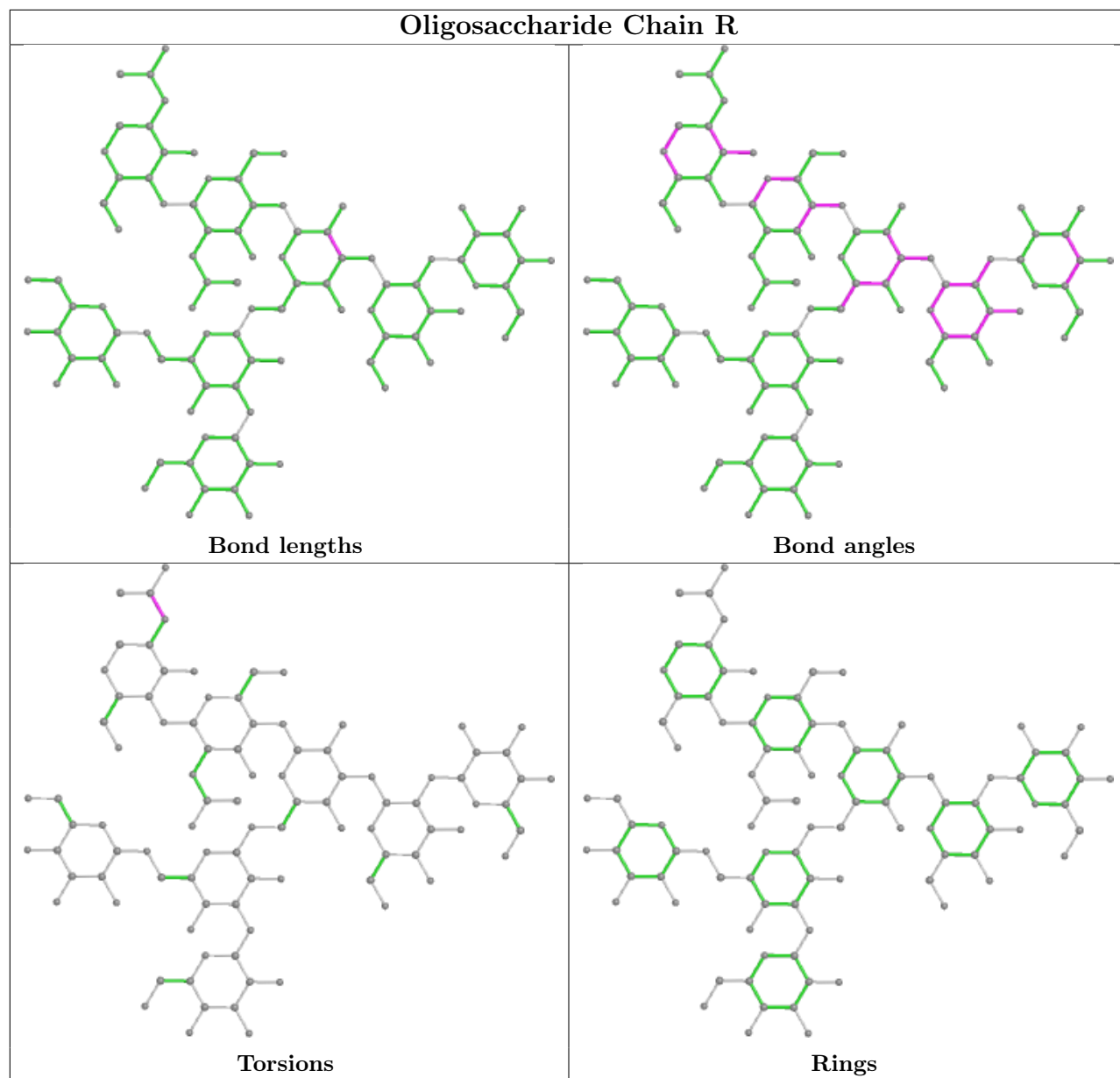


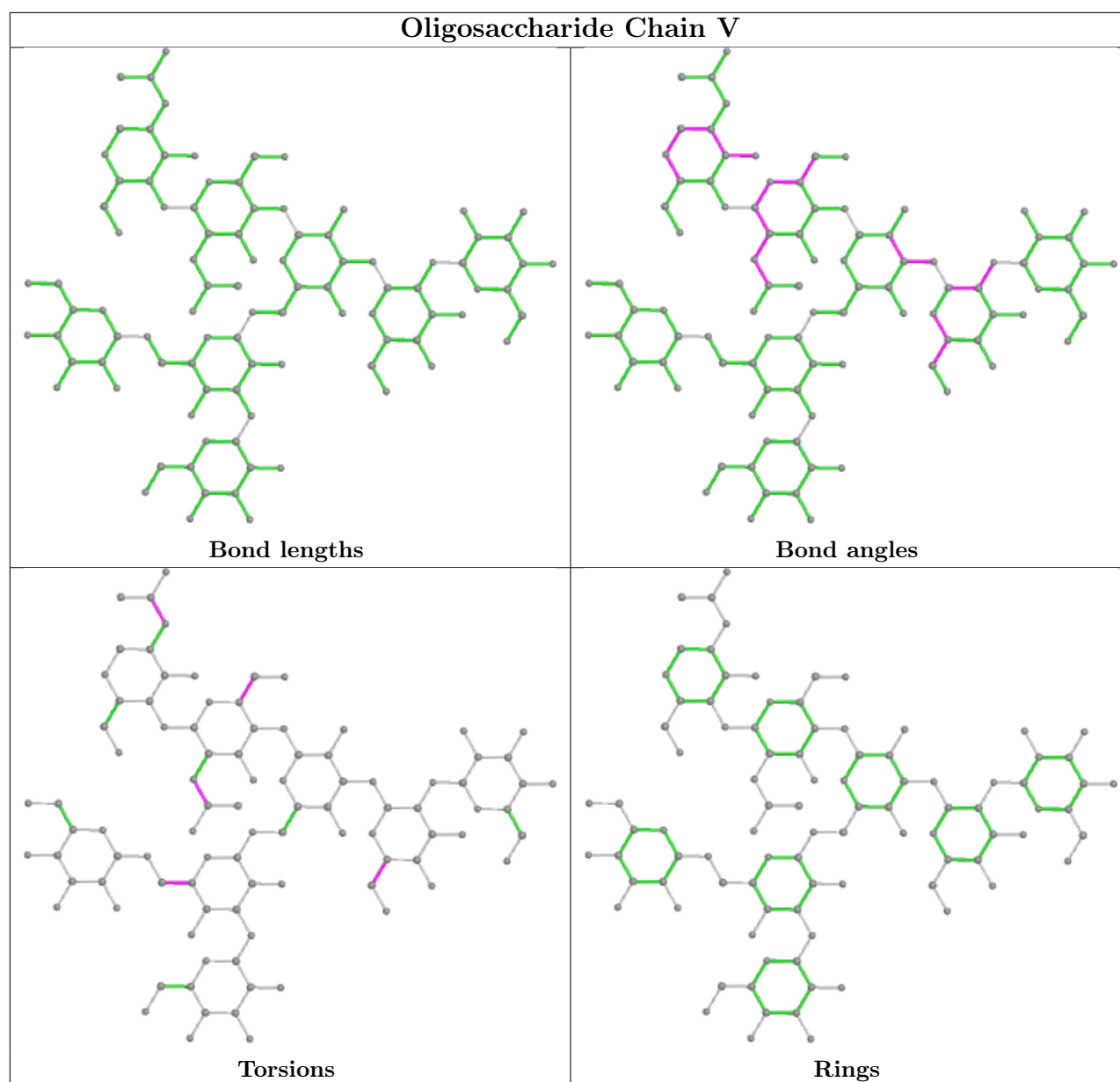












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	502	1	14,14,15	0.43	0	17,19,21	0.93	1 (5%)
7	NAG	D	501	1	14,14,15	0.48	0	17,19,21	0.98	2 (11%)
7	NAG	B	502	1	14,14,15	0.35	0	17,19,21	1.26	1 (5%)
7	NAG	D	502	1	14,14,15	0.39	0	17,19,21	0.72	1 (5%)
7	NAG	C	501	1	14,14,15	0.37	0	17,19,21	0.77	1 (5%)
7	NAG	A	501	1	14,14,15	0.32	0	17,19,21	0.68	0
7	NAG	B	501	1	14,14,15	0.40	0	17,19,21	0.90	0
7	NAG	C	502	1	14,14,15	0.35	0	17,19,21	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	502	1	-	2/6/23/26	0/1/1/1
7	NAG	D	501	1	-	4/6/23/26	0/1/1/1
7	NAG	B	502	1	-	2/6/23/26	0/1/1/1
7	NAG	D	502	1	-	2/6/23/26	0/1/1/1
7	NAG	C	501	1	-	2/6/23/26	0/1/1/1
7	NAG	A	501	1	-	2/6/23/26	0/1/1/1
7	NAG	B	501	1	-	2/6/23/26	0/1/1/1
7	NAG	C	502	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	NAG	C1-O5-C5	4.18	117.85	112.19
7	A	502	NAG	C2-N2-C7	-2.33	119.59	122.90
7	D	501	NAG	C1-O5-C5	2.31	115.32	112.19
7	C	501	NAG	C6-C5-C4	-2.10	108.08	113.00
7	D	502	NAG	O5-C5-C6	2.07	110.46	107.20
7	D	501	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

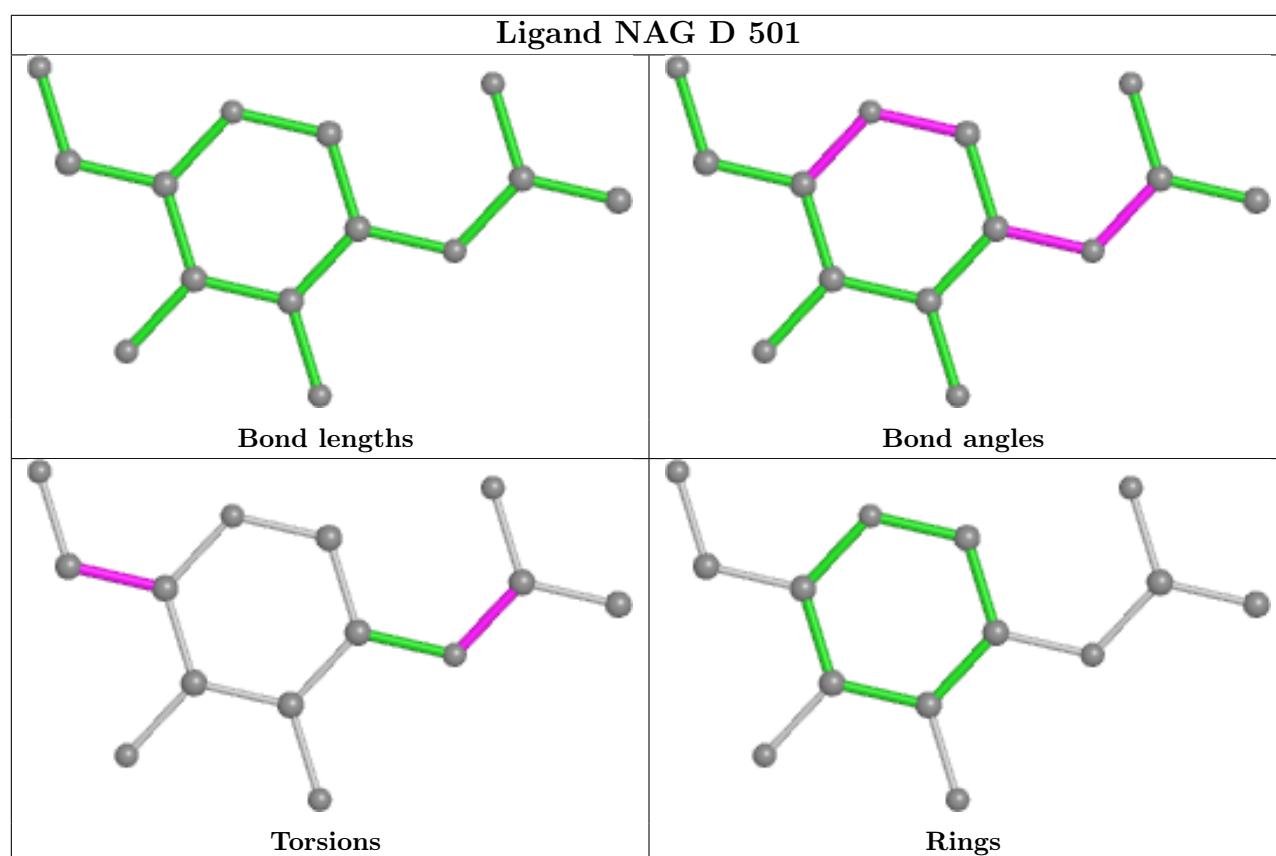
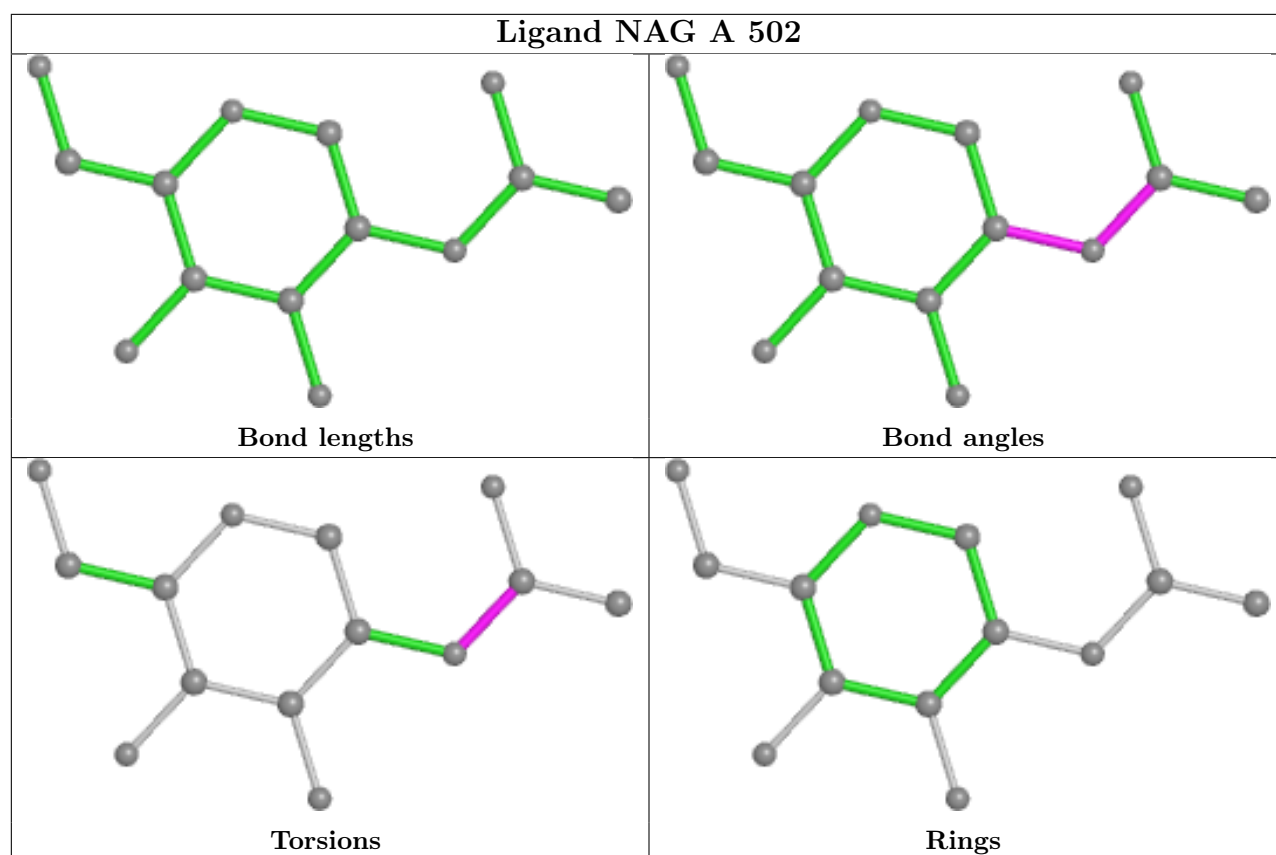
Mol	Chain	Res	Type	Atoms
7	A	501	NAG	C8-C7-N2-C2
7	A	501	NAG	O7-C7-N2-C2
7	A	502	NAG	C8-C7-N2-C2
7	A	502	NAG	O7-C7-N2-C2
7	B	501	NAG	C8-C7-N2-C2
7	B	501	NAG	O7-C7-N2-C2
7	B	502	NAG	C8-C7-N2-C2
7	B	502	NAG	O7-C7-N2-C2
7	C	502	NAG	C8-C7-N2-C2
7	C	502	NAG	O7-C7-N2-C2
7	D	502	NAG	C8-C7-N2-C2
7	D	502	NAG	O7-C7-N2-C2
7	D	501	NAG	C8-C7-N2-C2
7	C	501	NAG	C8-C7-N2-C2
7	D	501	NAG	O7-C7-N2-C2
7	C	501	NAG	O7-C7-N2-C2
7	D	501	NAG	O5-C5-C6-O6
7	C	502	NAG	O5-C5-C6-O6
7	D	501	NAG	C4-C5-C6-O6

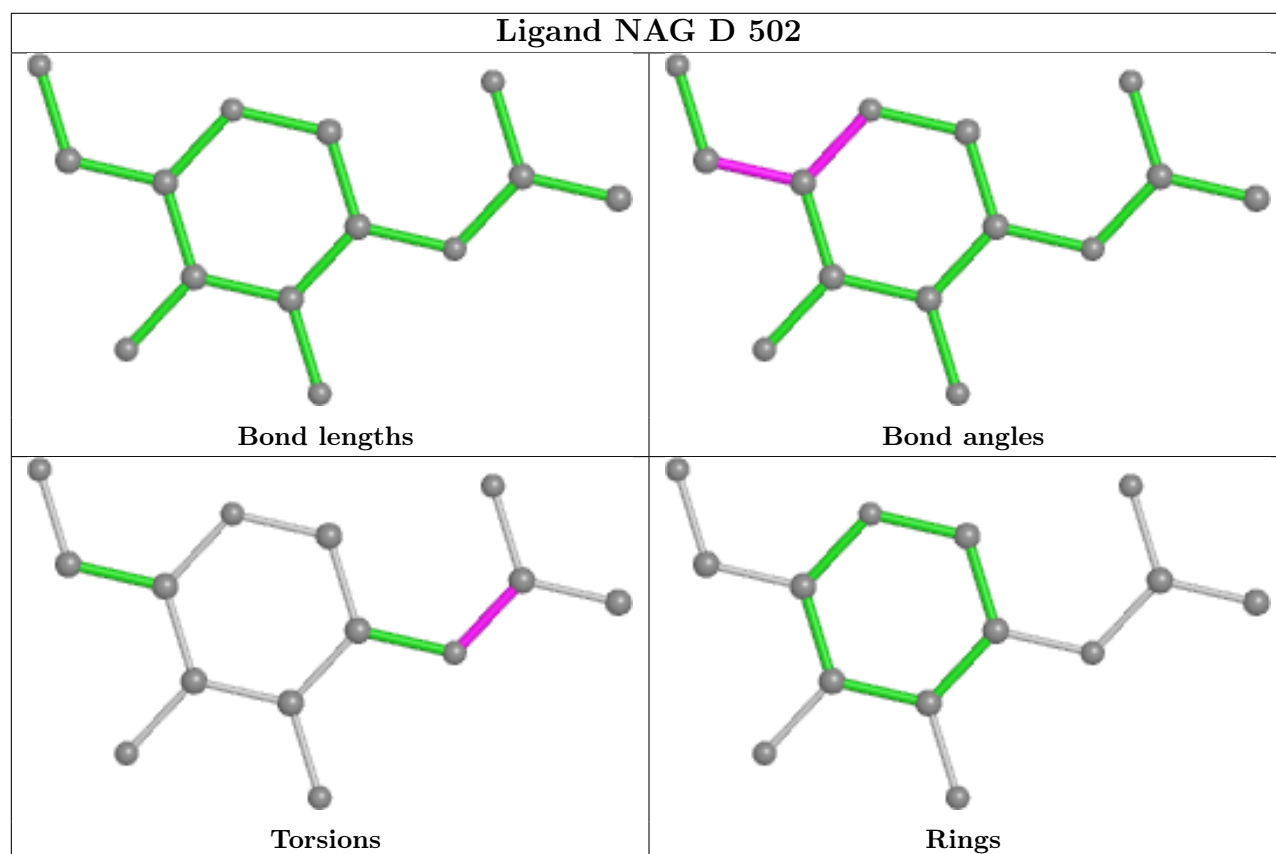
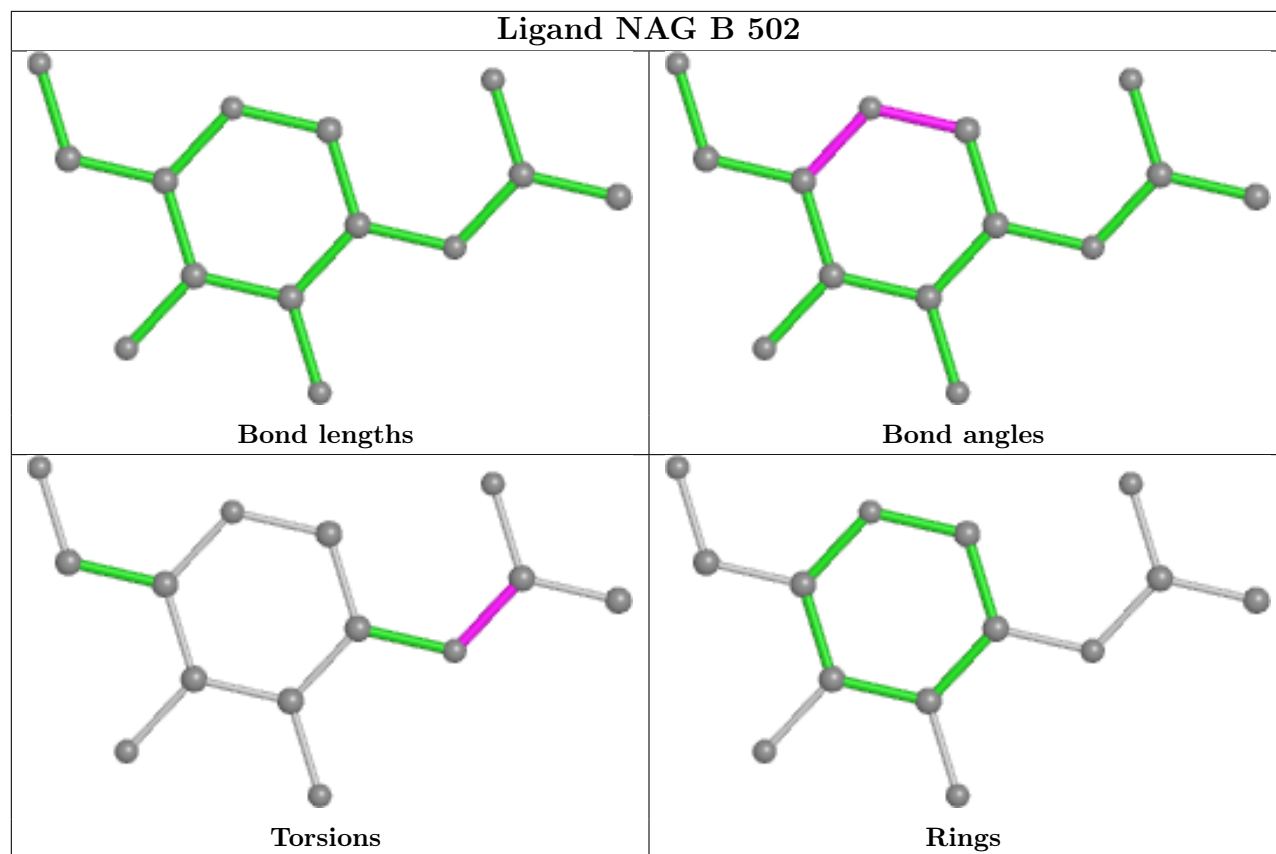
There are no ring outliers.

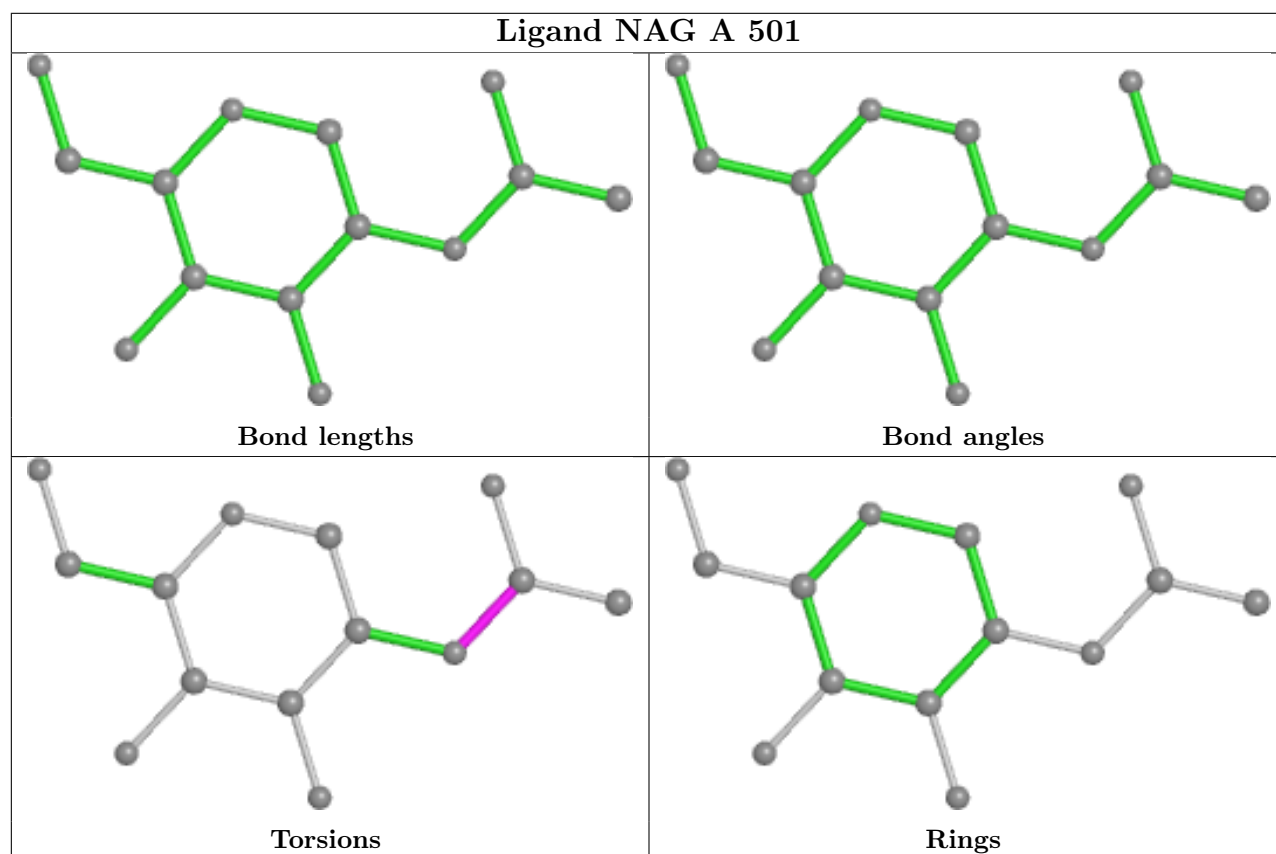
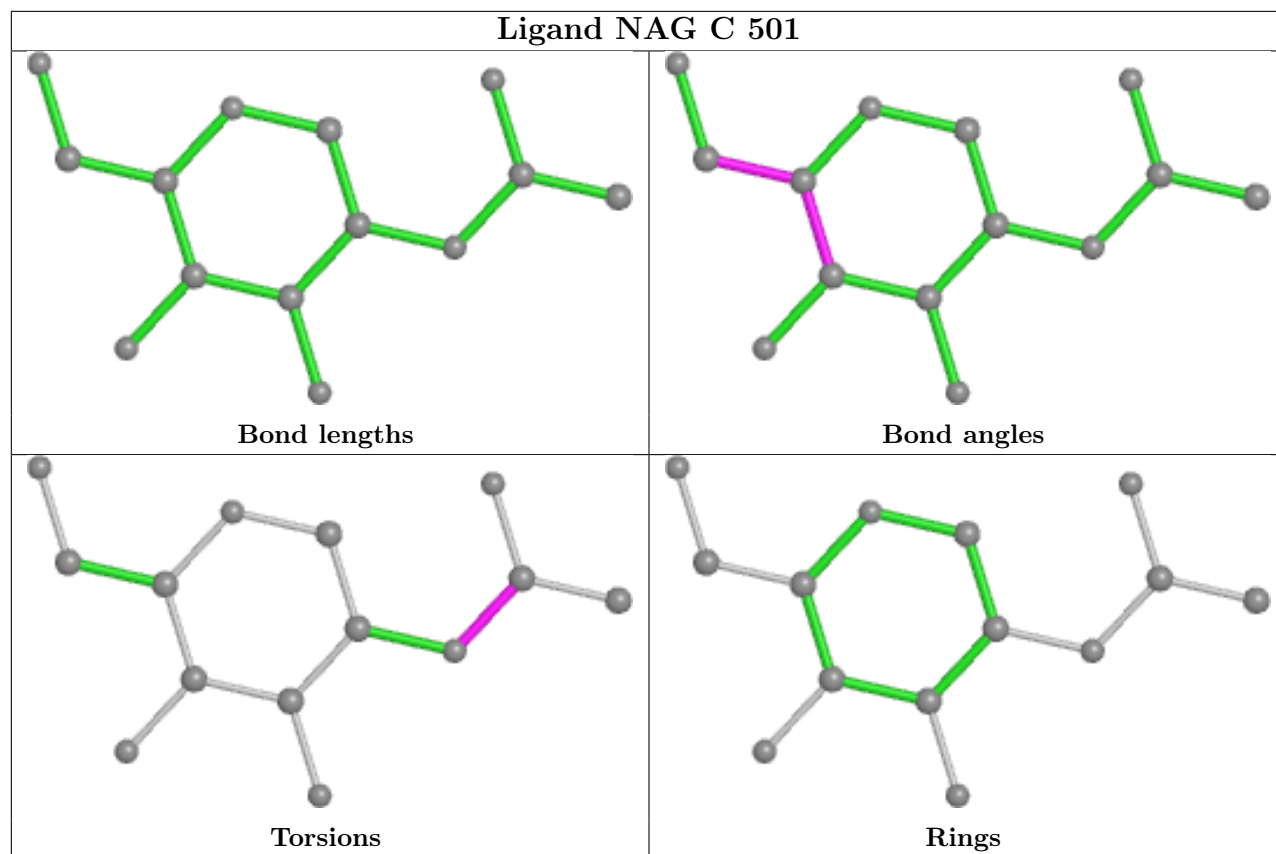
2 monomers are involved in 3 short contacts:

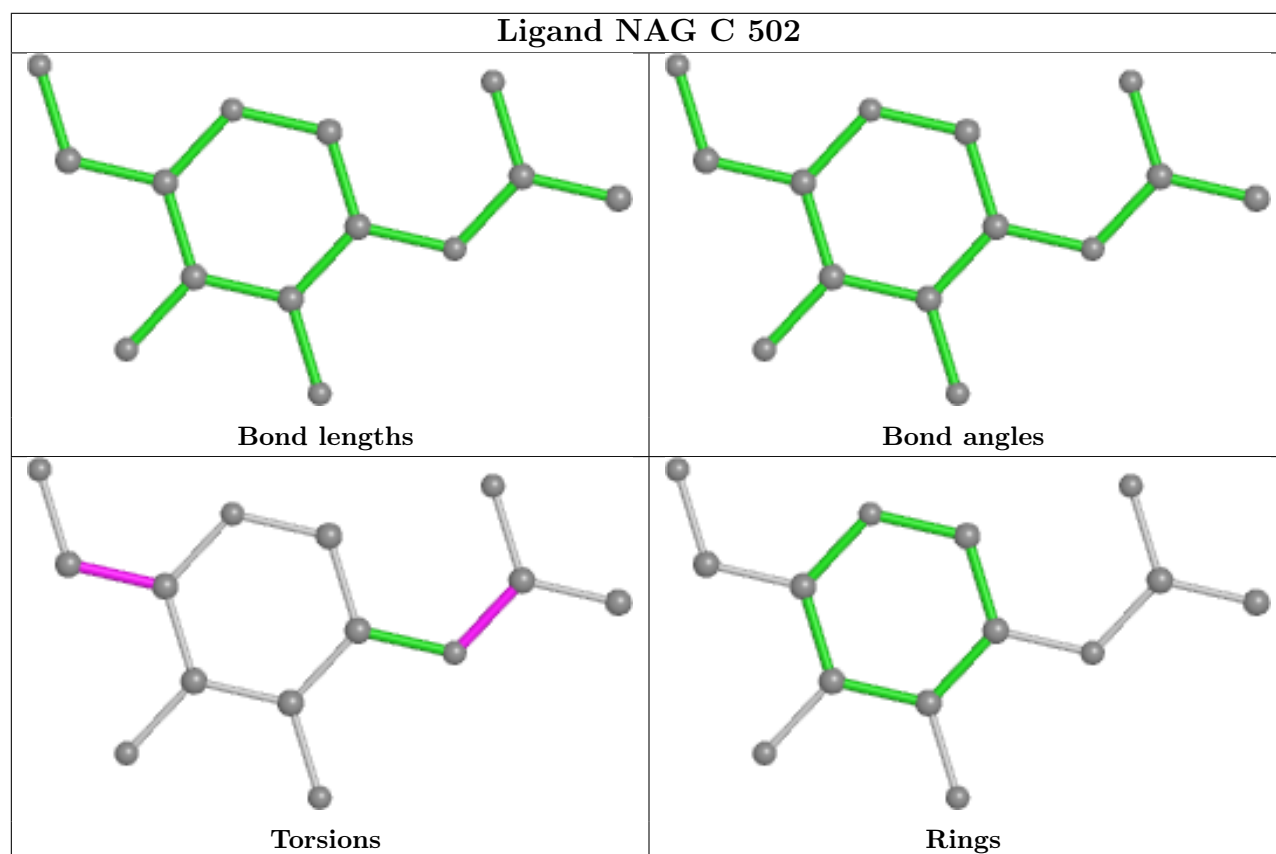
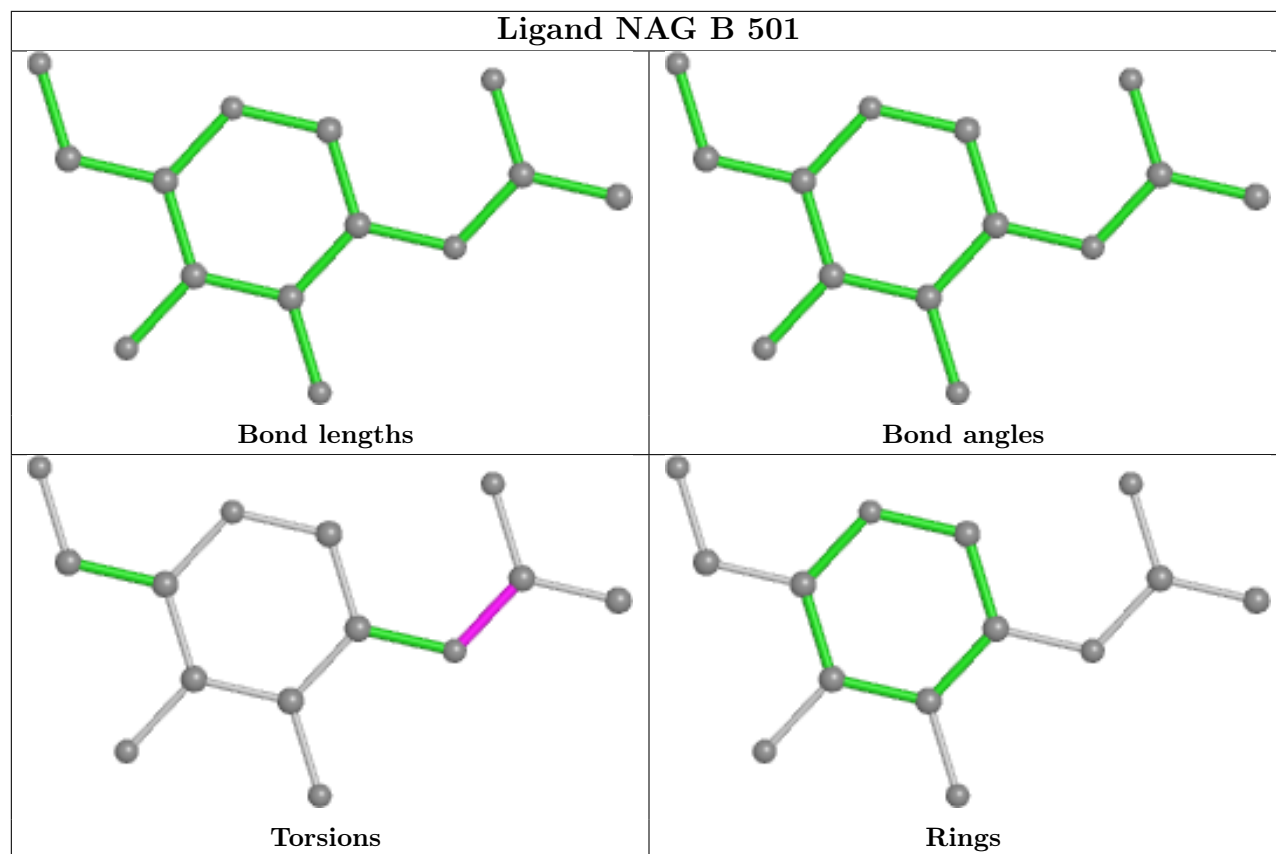
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	NAG	2	0
7	B	501	NAG	1	0

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

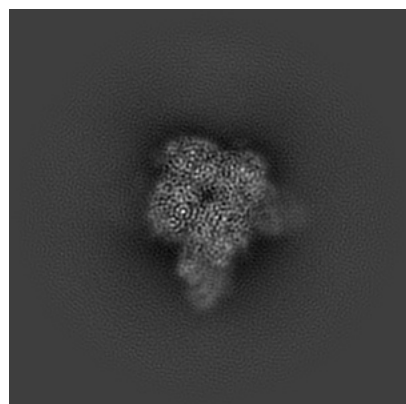
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39608. These allow visual inspection of the internal detail of the map and identification of artifacts.

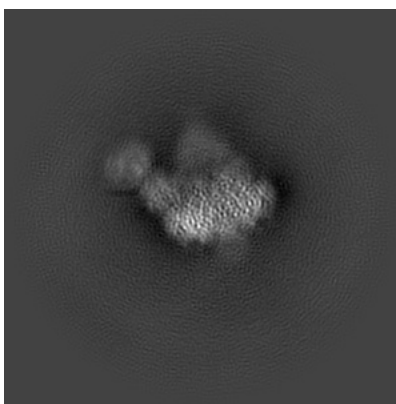
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

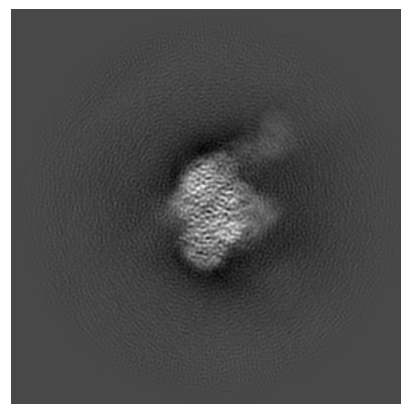
6.1.1 Primary map



X

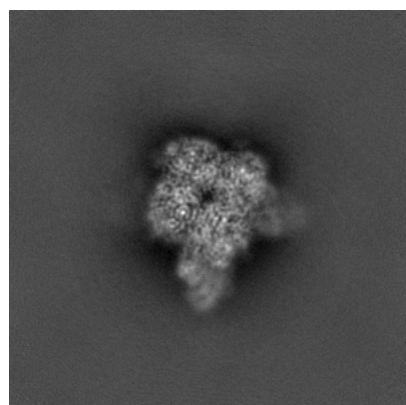


Y

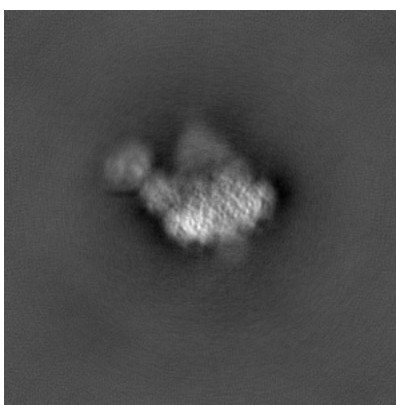


Z

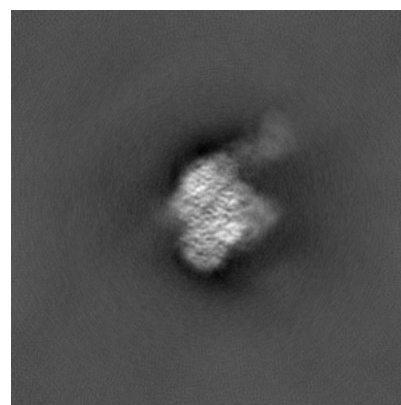
6.1.2 Raw map



X



Y

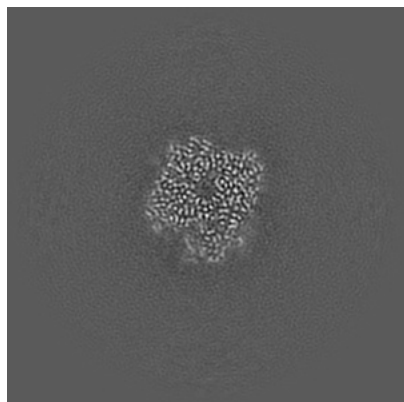


Z

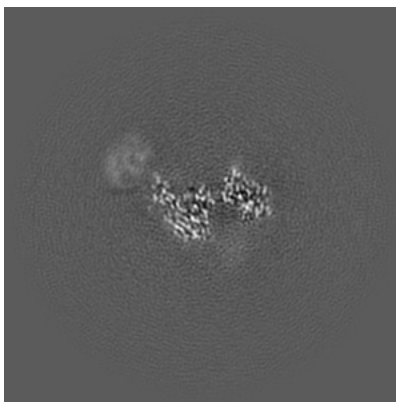
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

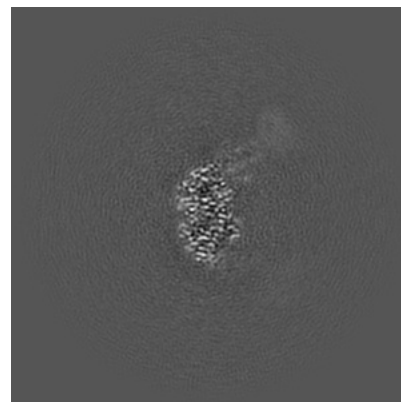
6.2.1 Primary map



X Index: 156

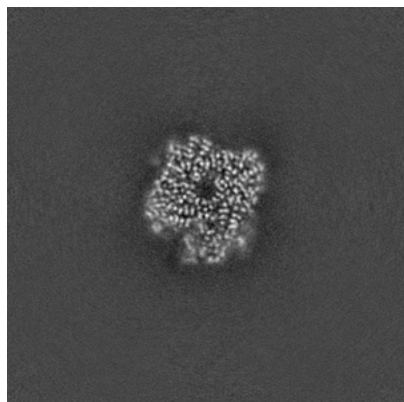


Y Index: 156

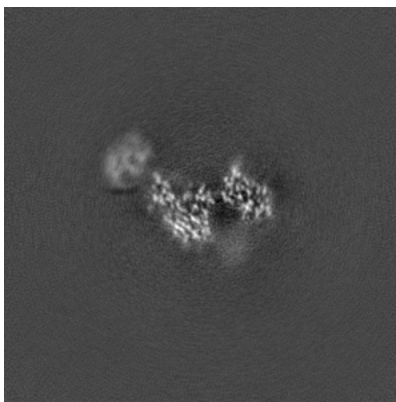


Z Index: 156

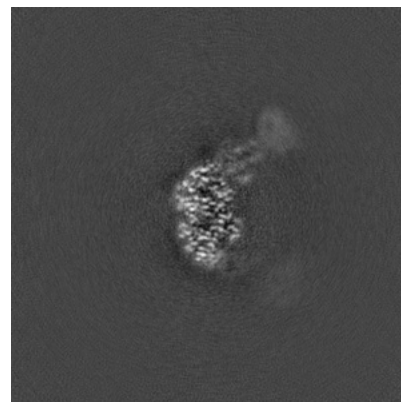
6.2.2 Raw map



X Index: 156



Y Index: 156

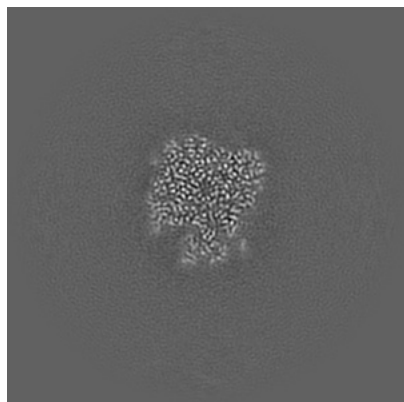


Z Index: 156

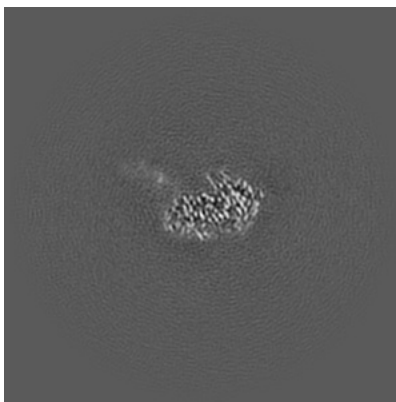
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

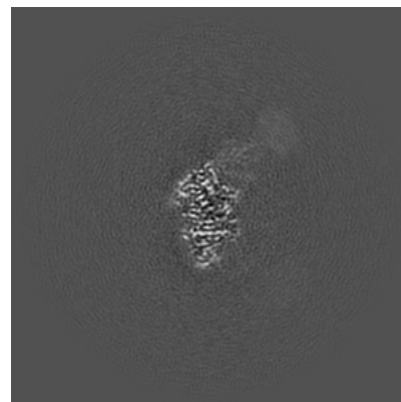
6.3.1 Primary map



X Index: 159

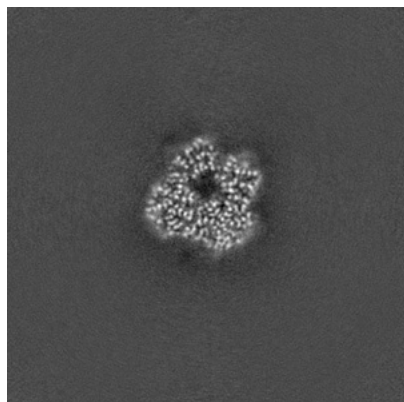


Y Index: 174

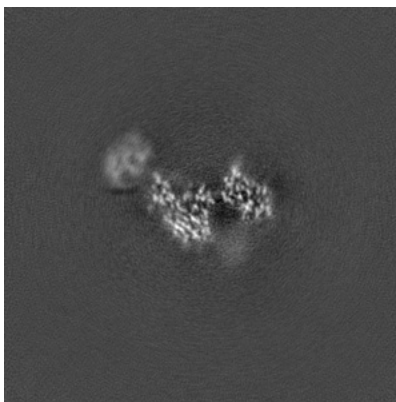


Z Index: 153

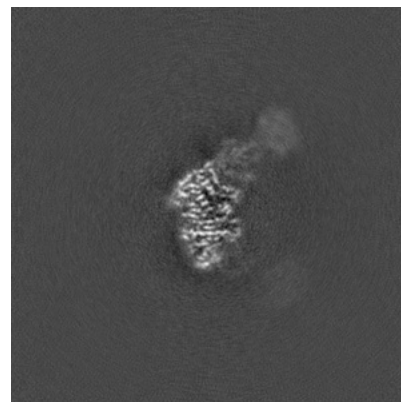
6.3.2 Raw map



X Index: 149



Y Index: 156

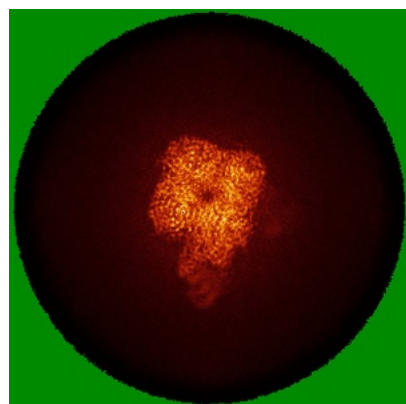


Z Index: 153

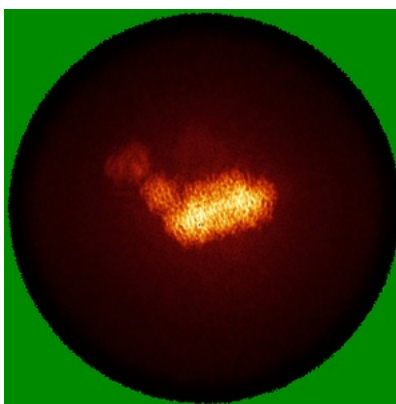
The images above show the largest variance slices of the map in three orthogonal directions.

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

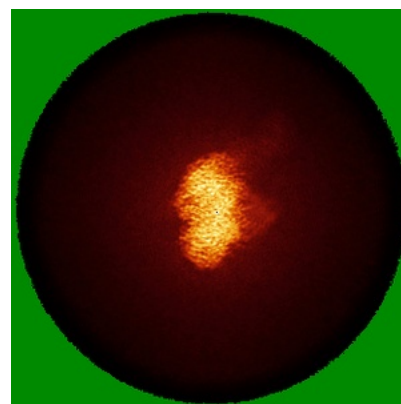
6.4.1 Primary map



X

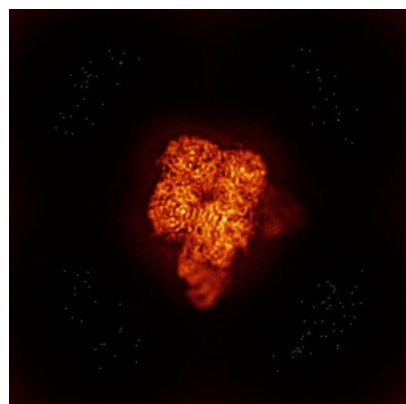


Y

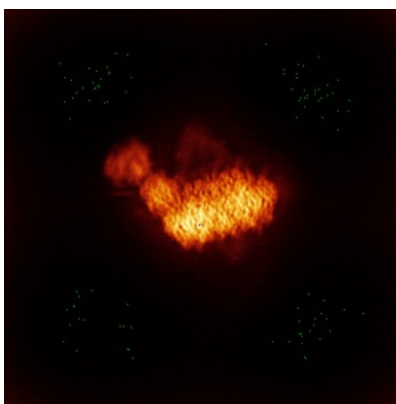


Z

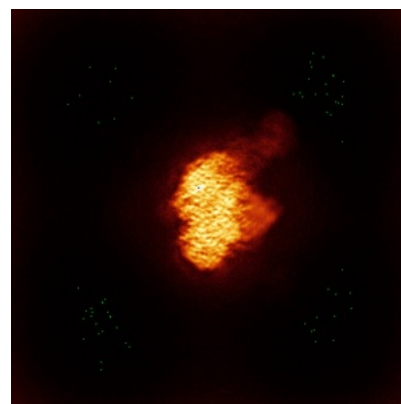
6.4.2 Raw map



X



Y

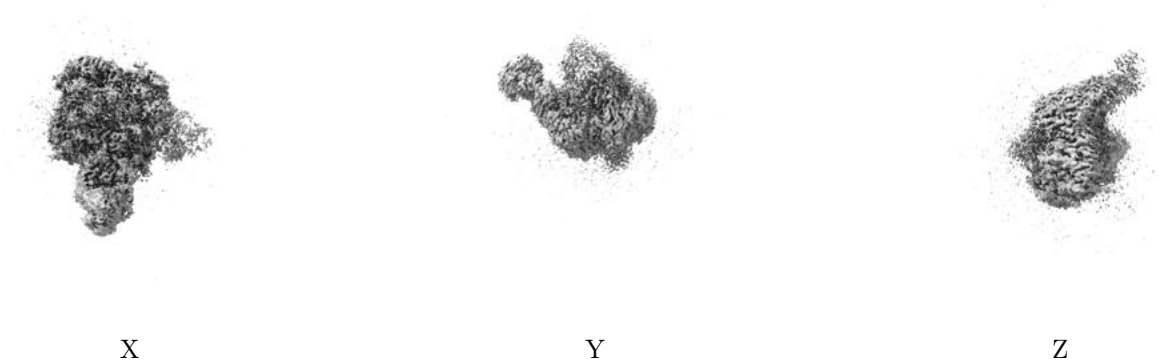


Z

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.

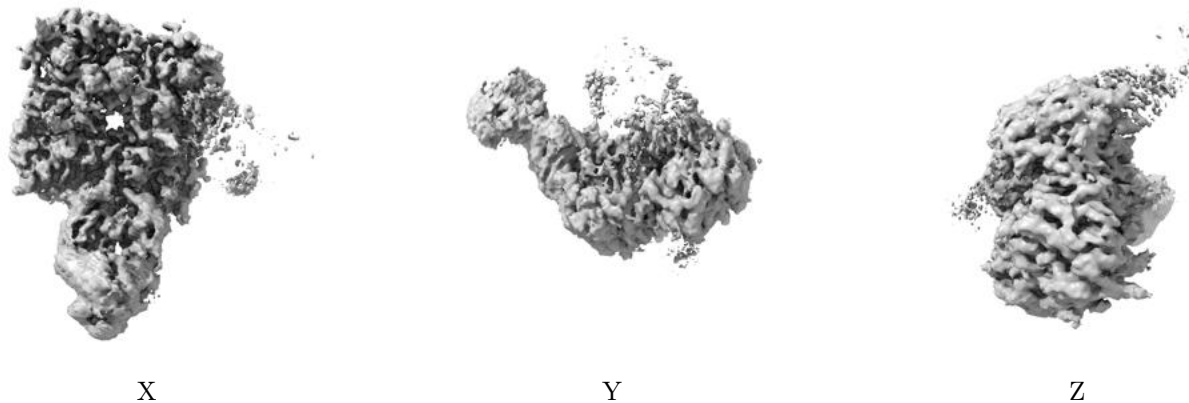
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.232. 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.

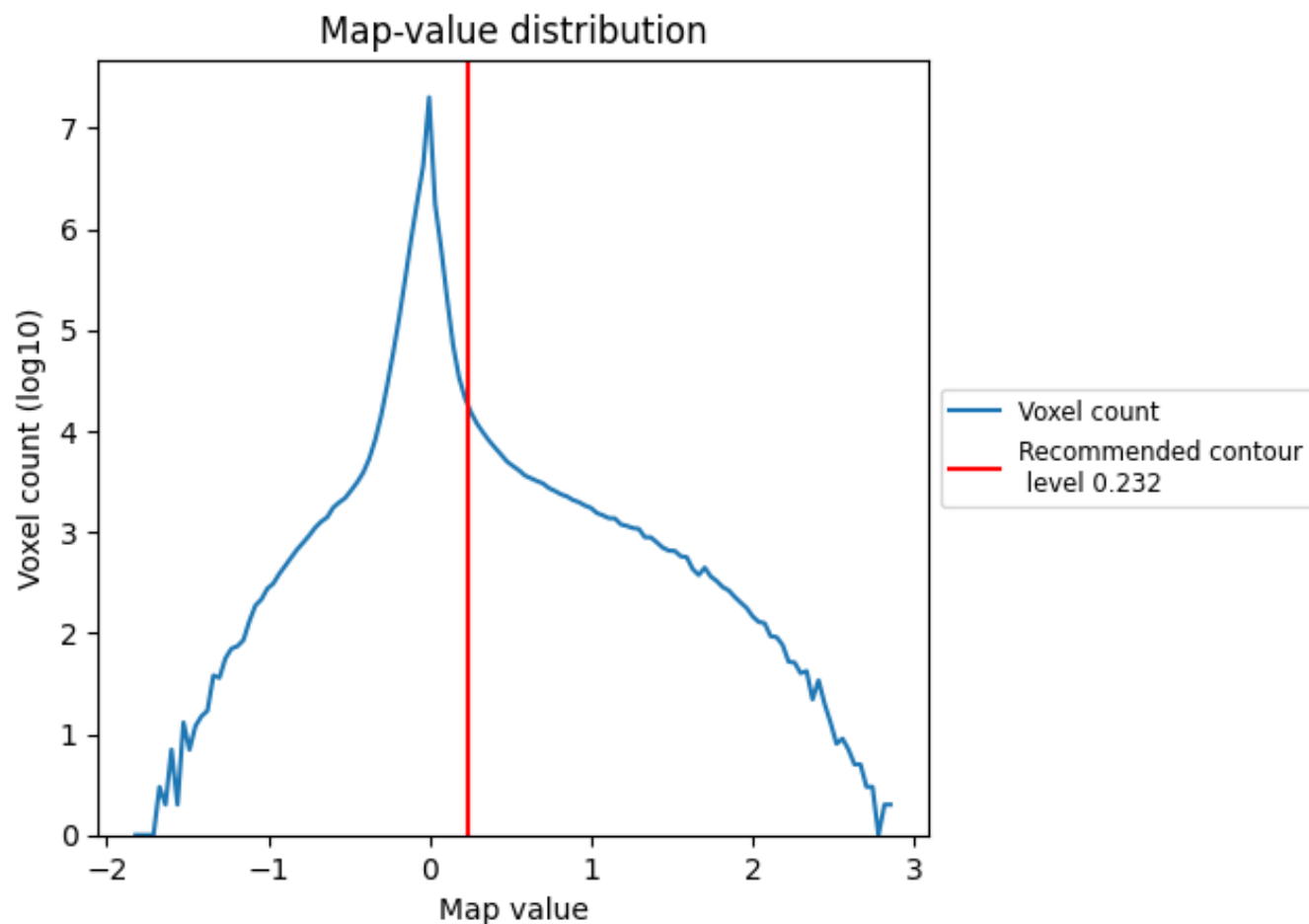
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

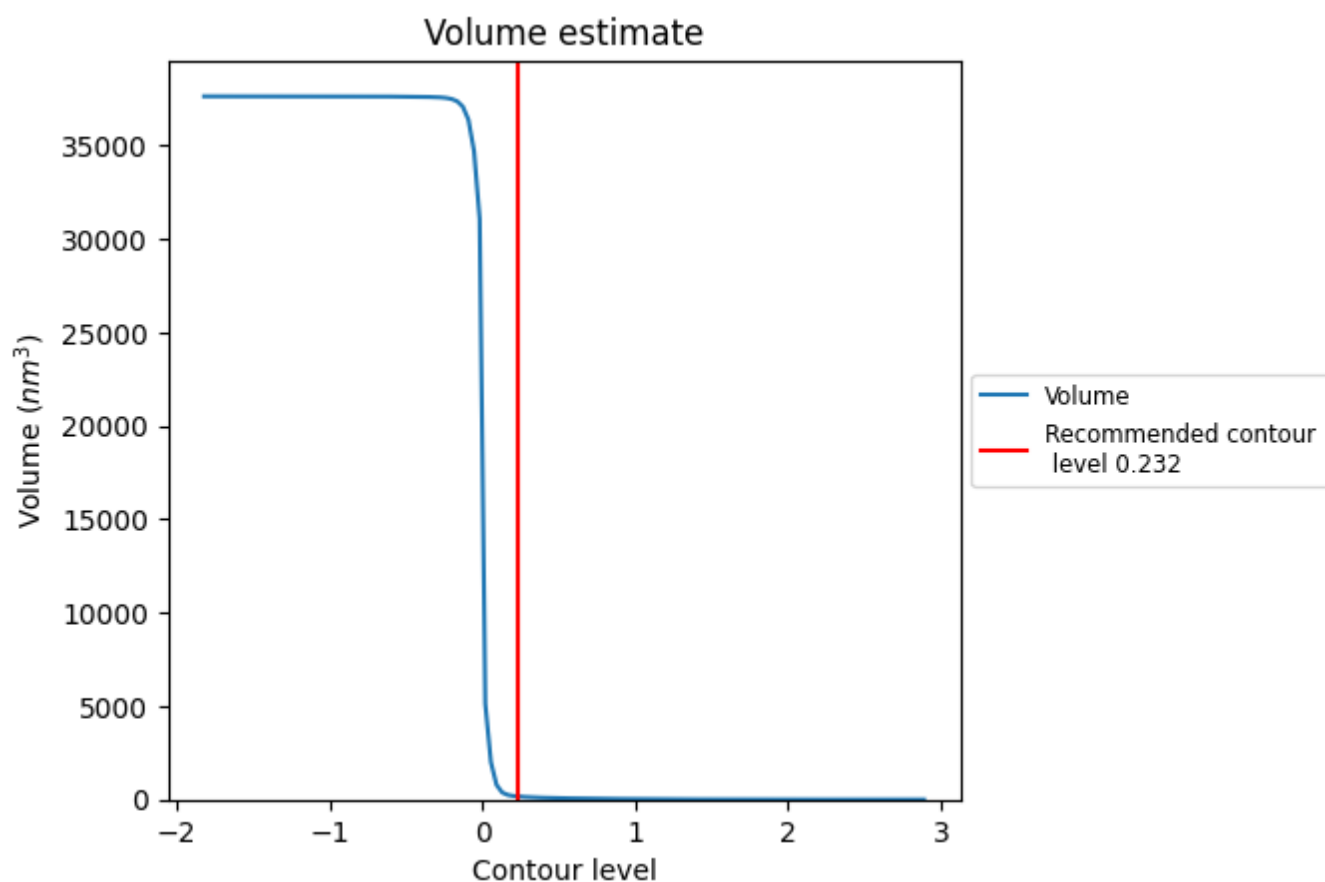
This section contains the results of statistical analysis of the map.

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.

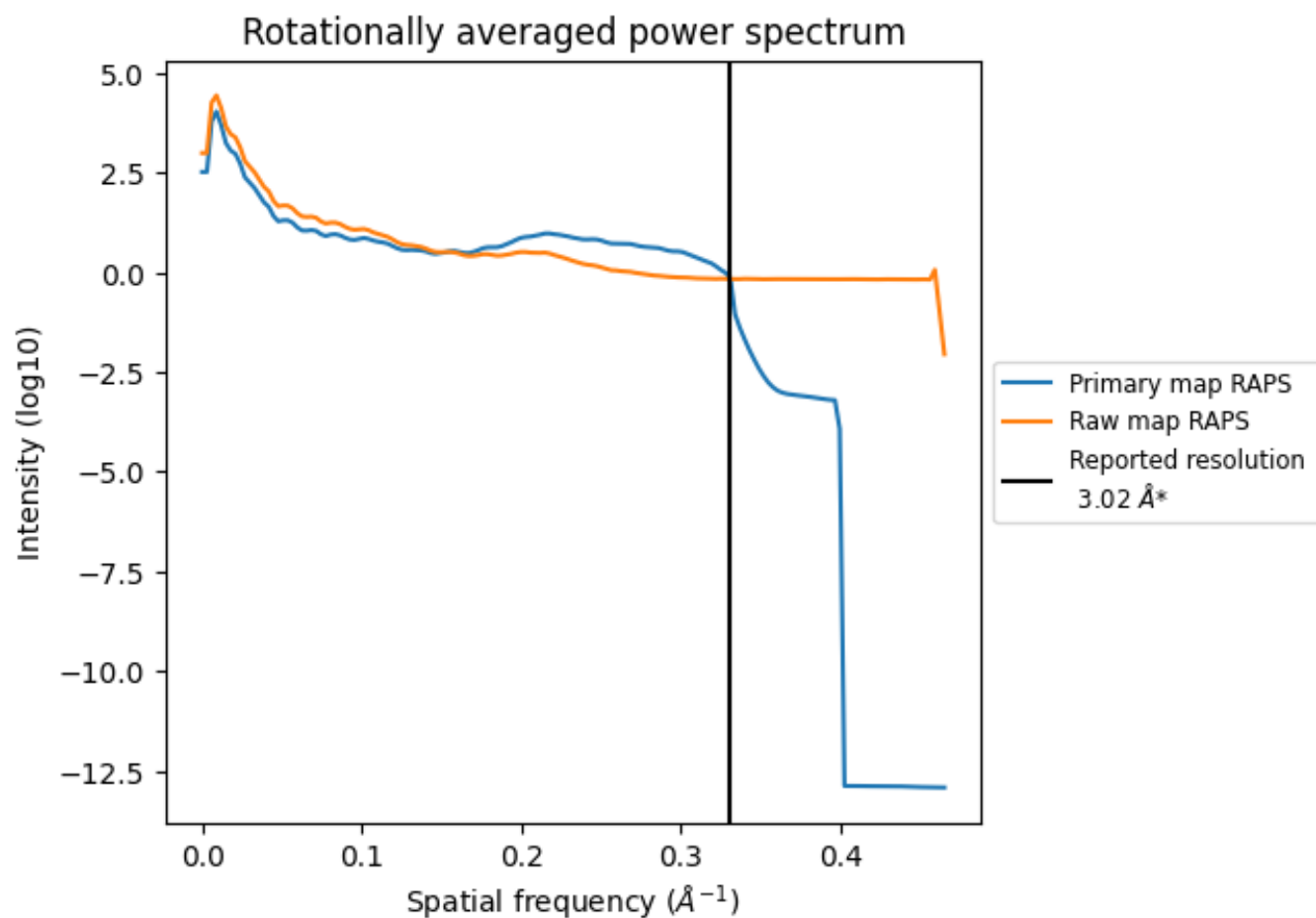
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 151 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 ⓘ

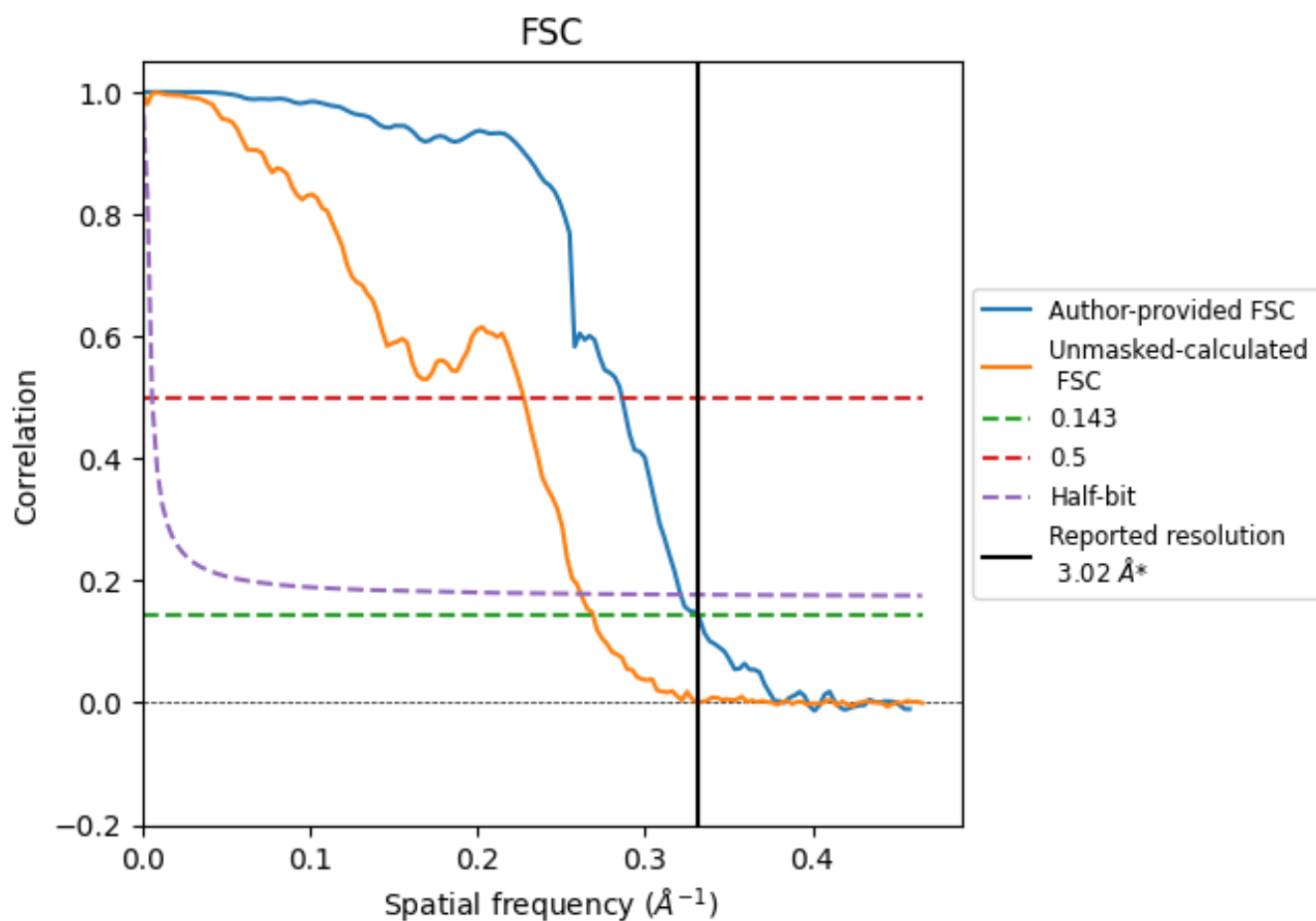


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

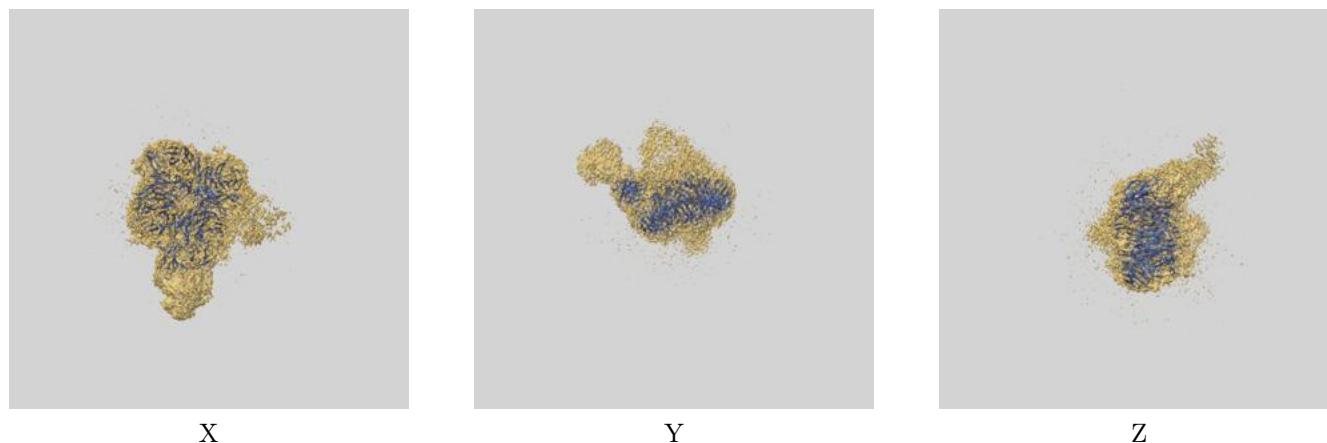
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.49	3.11
Unmasked-calculated*	3.72	4.40	3.82

*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 3.72 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

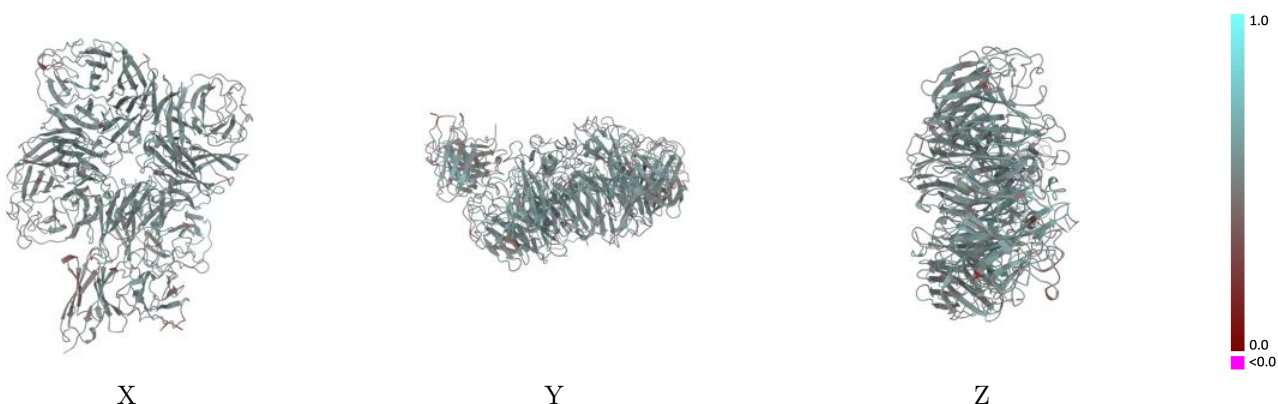
This section contains information regarding the fit between EMDB map EMD-39608 and PDB model 8YVM. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



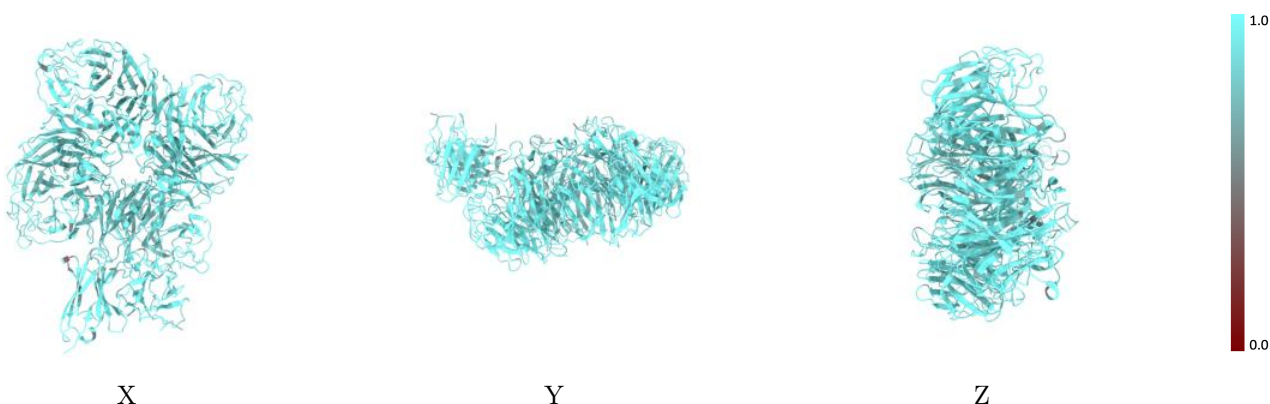
The images above show the 3D surface view of the map at the recommended contour level 0.232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



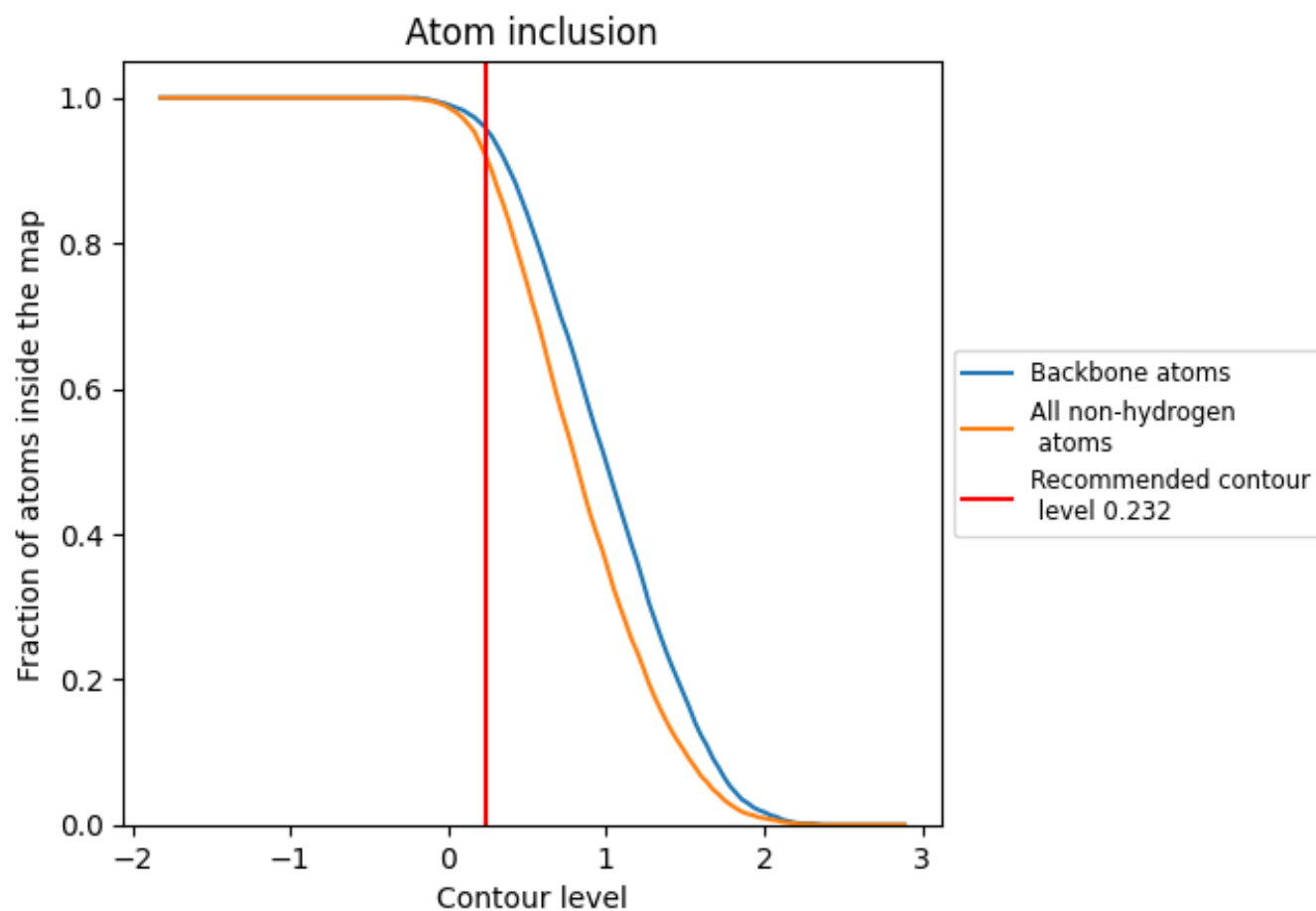
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.232).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.5250
A	 0.9240	 0.5270
B	 0.9380	 0.5350
C	 0.9230	 0.5370
D	 0.9280	 0.5300
E	 0.9320	 0.5000
F	 0.9000	 0.4920
G	 0.8720	 0.4580
H	 0.8930	 0.4630
I	 0.6430	 0.2620
J	 0.8620	 0.5030
K	 0.7440	 0.4410
L	 0.8570	 0.5070
M	 0.8570	 0.4630
N	 0.9470	 0.5350
O	 0.9490	 0.4770
P	 0.8210	 0.4820
Q	 0.7860	 0.3770
R	 0.8620	 0.5270
S	 0.8720	 0.5040
T	 0.9290	 0.4720
U	 0.7860	 0.4260
V	 0.8940	 0.4990

