



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:47 AM UTC

PDB ID : 7T9B / pdb_00007t9b
EMDB ID : EMD-25755
Title : ApexGT5 in complex with GT5-d42.16 and RM20A3 Fabs
Authors : Berndsen, Z.T.; Ward, A.B.
Deposited on : 2021-12-18
Resolution : 3.72 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:

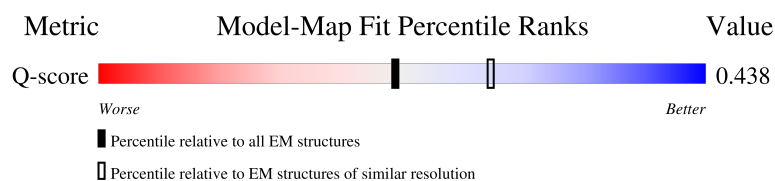
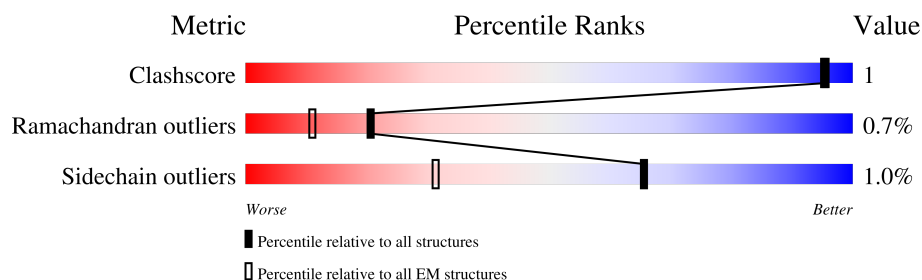
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.72 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.



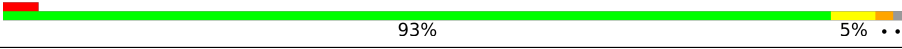
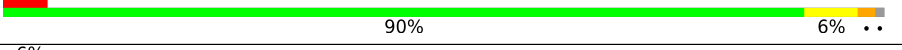
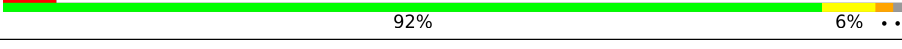
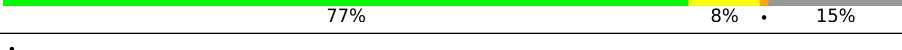
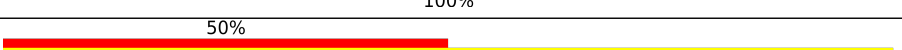
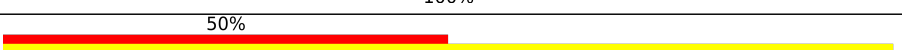
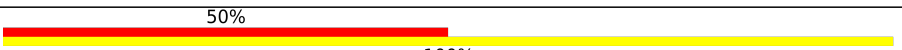
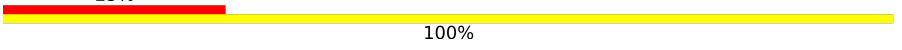
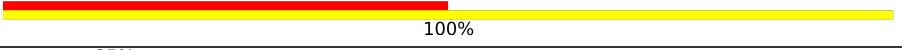
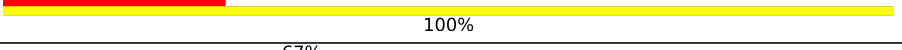
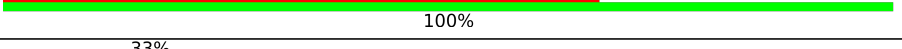
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10474 (3.22 - 4.22)

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	473	 6% 85% 7% 8%
1	C	473	 5% 84% 7% 8%
1	E	473	 1% 84% 7% 9%
2	B	153	 1% 75% 22%

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Mol	Chain	Length	Quality of chain
2	D	153	
2	F	153	
3	J	125	
3	M	125	
3	O	125	
4	K	128	
4	N	128	
4	P	128	
5	H	134	
6	L	107	
7	G	2	
7	I	2	
7	V	2	
7	W	2	
7	X	2	
7	Z	2	
7	c	2	
7	d	2	
7	f	2	
7	g	2	
8	Q	4	
8	Y	4	
8	e	4	
9	R	3	
9	h	3	

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Mol	Chain	Length	Quality of chain
10	S	7	
11	T	2	
11	a	2	
11	i	2	
12	U	3	
12	b	3	
12	j	3	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21592 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 HIV-1 Envelope ApexGT5 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	435	Total	C	N	O	S	0	0
			3433	2166	601	639	27		
1	C	434	Total	C	N	O	S	0	0
			3425	2162	599	637	27		
1	E	429	Total	C	N	O	S	0	0
			3387	2136	593	631	27		

- Molecule 2 is a protein called HIV-1 Envelope ApexGT5 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	D	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	F	120	Total	C	N	O	S	0	0
			958	604	167	181	6		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	517	SER	PHE	conflict	UNP Q2N0S6
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	PRO	ALA	conflict	UNP Q2N0S6
B	568	ASP	LEU	conflict	UNP Q2N0S6
B	570	HIS	VAL	conflict	UNP Q2N0S6
B	585	HIS	ARG	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	517	SER	PHE	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	561	PRO	ALA	conflict	UNP Q2N0S6
D	568	ASP	LEU	conflict	UNP Q2N0S6
D	570	HIS	VAL	conflict	UNP Q2N0S6
D	585	HIS	ARG	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	605	CYS	THR	conflict	UNP Q2N0S6
F	517	SER	PHE	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	PRO	ALA	conflict	UNP Q2N0S6
F	568	ASP	LEU	conflict	UNP Q2N0S6
F	570	HIS	VAL	conflict	UNP Q2N0S6
F	585	HIS	ARG	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called RM20A3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
3	M	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
3	O	124	Total	C	N	O	S	0	0
			943	595	161	182	5		

- Molecule 4 is a protein called RM20A3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
4	N	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
4	P	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

- Molecule 5 is a protein called GT5-d42.16 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			1051	663	171	211	6		

- Molecule 6 is a protein called GT5-d42.16 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			809	514	134	159	2		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	4	Total	C	N	O	0	0
			50	28	2	20		
8	Y	4	Total	C	N	O	0	0
			50	28	2	20		
8	e	4	Total	C	N	O	0	0
			50	28	2	20		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	3	Total 39	C 22	N 2	O 15	0	0
9	h	3	Total 39	C 22	N 2	O 15	0	0

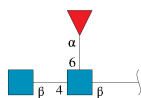
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Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	7	Total	C	N	O	0	0
			83	46	2	35		

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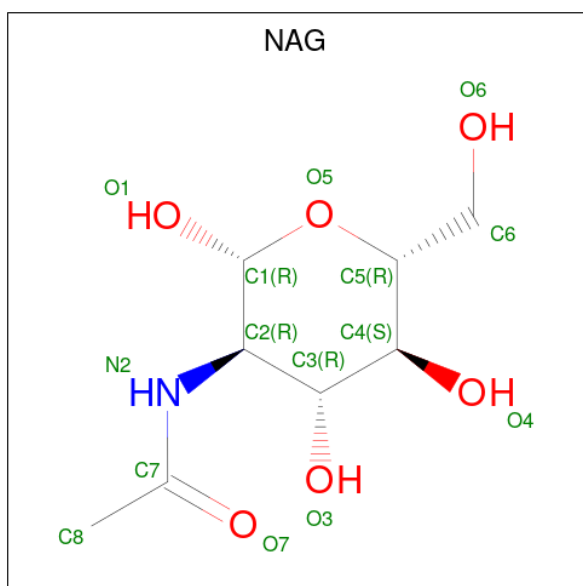
Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	2	Total 24	C 14	N 1	O 9	0	0
11	a	2	Total 24	C 14	N 1	O 9	0	0
11	i	2	Total 24	C 14	N 1	O 9	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	3	Total	C	N	O	0	0
			38	22	2	14		
12	b	3	Total	C	N	O	0	0
			38	22	2	14		
12	j	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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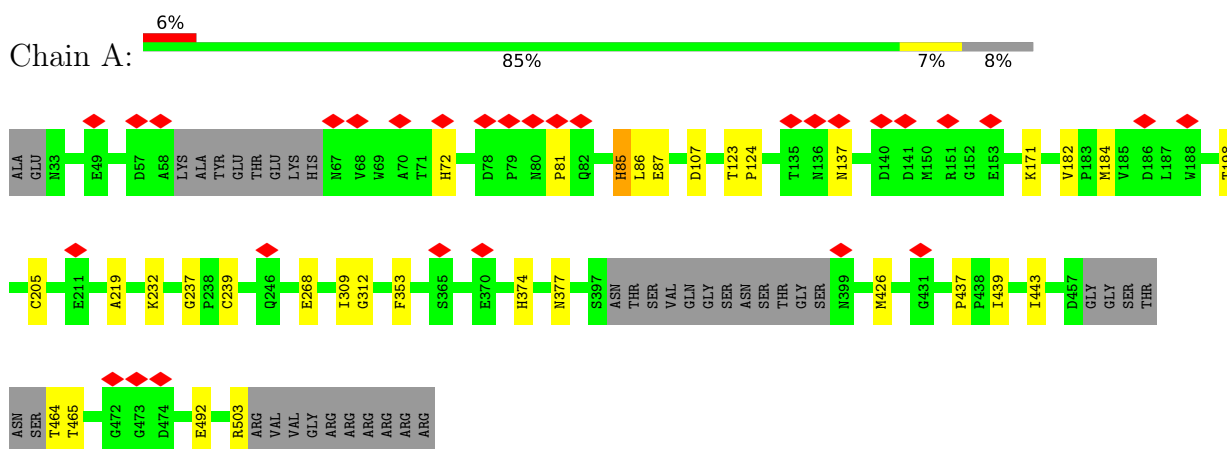
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Mol	Chain	Residues	Atoms				AltConf
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13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total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

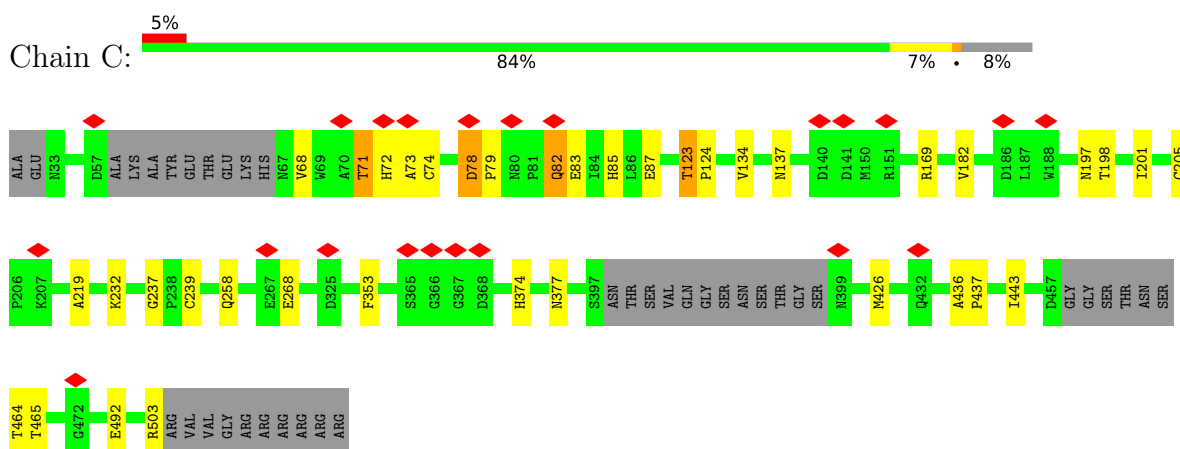
3 Residue-property plots

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.

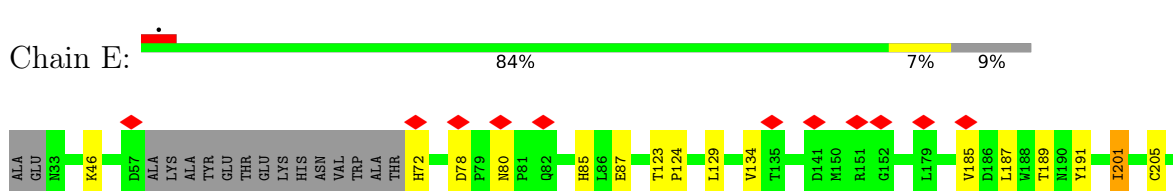
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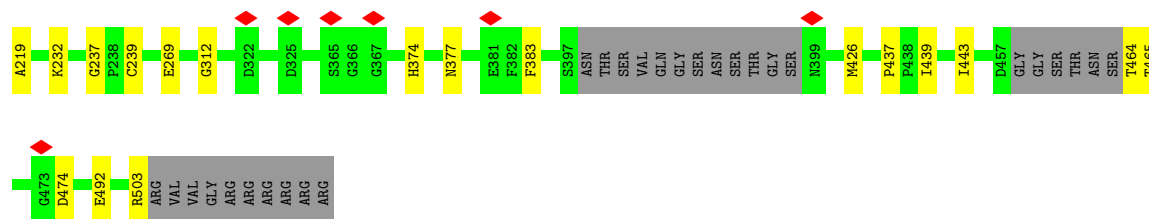


• Molecule 1: HIV-1 Envelope ApexGT5 gp120

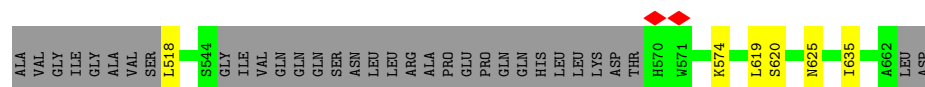
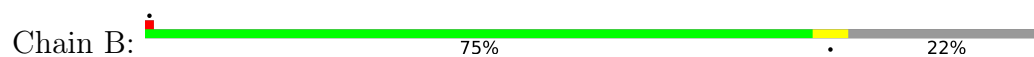


• Molecule 1: HIV-1 Envelope ApexGT5 gp120

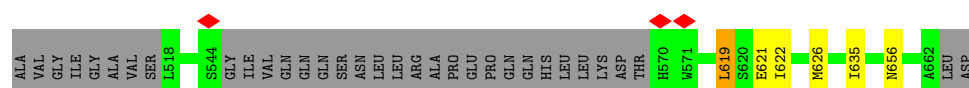




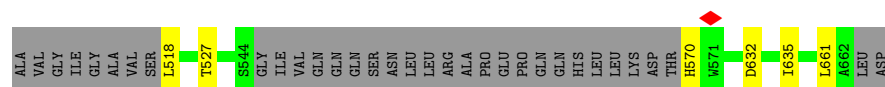
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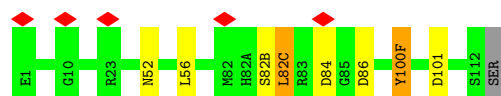
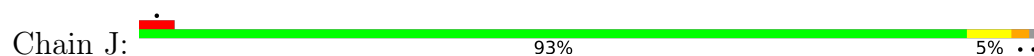
• Molecule 2: HIV-1 Envelope ApexGT5 gp41



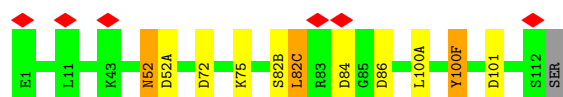
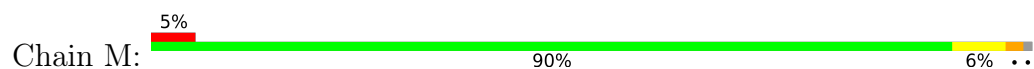
• Molecule 2: HIV-1 Envelope ApexGT5 gp41



• Molecule 3: RM20A3 Fab Heavy Chain

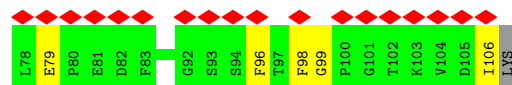
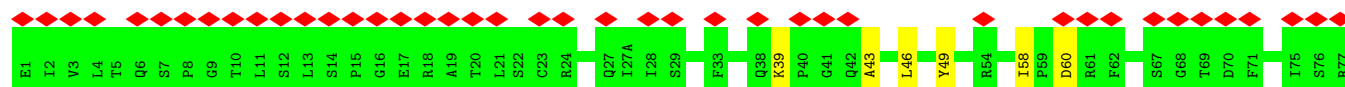
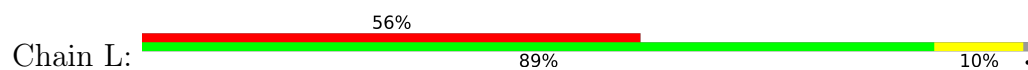
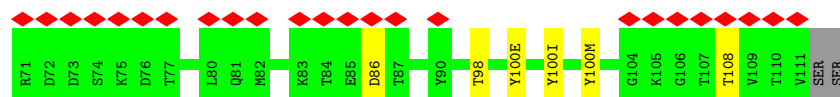
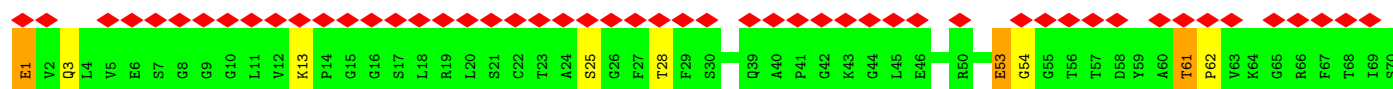
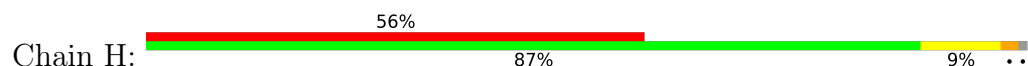
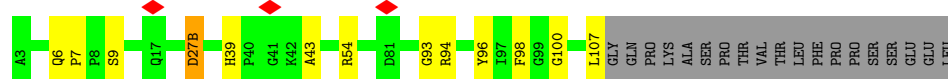
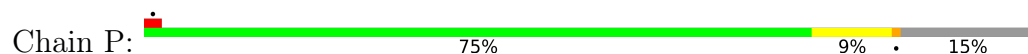
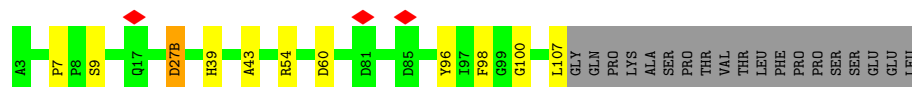
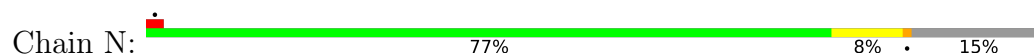
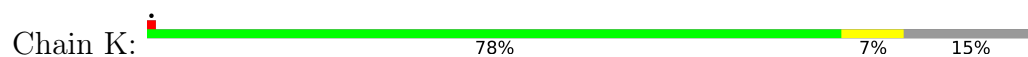
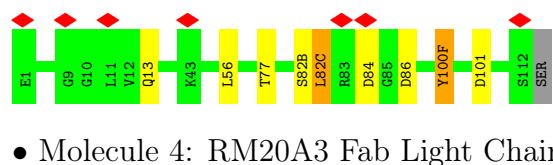


• Molecule 3: RM20A3 Fab Heavy Chain



• Molecule 3: RM20A3 Fab Heavy Chain





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



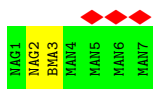
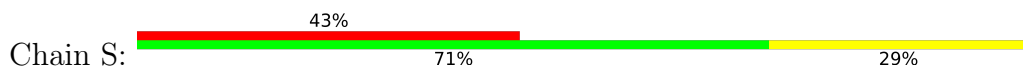
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]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	35763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.310	Depositor
Minimum map value	-0.477	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.293	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYS, MAN, NAG, FUC, BMA

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	1.04	2/3507 (0.1%)	1.25	28/4770 (0.6%)
1	C	1.06	2/3499 (0.1%)	1.26	31/4759 (0.7%)
1	E	1.07	4/3458 (0.1%)	1.25	25/4699 (0.5%)
2	B	1.05	1/977 (0.1%)	1.06	1/1325 (0.1%)
2	D	1.05	0/977	1.05	2/1325 (0.2%)
2	F	1.04	2/977 (0.2%)	1.07	1/1325 (0.1%)
3	J	1.08	0/963	1.25	3/1300 (0.2%)
3	M	1.08	0/963	1.27	5/1300 (0.4%)
3	O	1.10	0/963	1.24	6/1300 (0.5%)
4	K	1.14	1/830 (0.1%)	1.27	11/1129 (1.0%)
4	N	1.12	2/830 (0.2%)	1.27	13/1129 (1.2%)
4	P	1.10	2/830 (0.2%)	1.29	14/1129 (1.2%)
5	H	0.99	0/1043	1.22	10/1411 (0.7%)
6	L	0.98	1/829 (0.1%)	1.34	10/1126 (0.9%)
All	All	1.06	17/20646 (0.1%)	1.23	160/28027 (0.6%)

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	C	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	503	ARG	NE-CZ	6.33	1.40	1.33
4	N	27(B)	ASP	CB-CG	-6.20	1.36	1.52
1	C	503	ARG	NE-CZ	6.13	1.39	1.33
1	A	503	ARG	NE-CZ	6.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	107	LEU	CB-CG	5.97	1.65	1.53
4	K	107	LEU	CB-CG	5.88	1.65	1.53
4	P	107	LEU	CB-CG	5.85	1.65	1.53
1	E	72	HIS	CB-CG	5.63	1.58	1.50
4	P	27(B)	ASP	CB-CG	-5.56	1.38	1.52
2	F	570	HIS	CB-CG	5.47	1.57	1.50
1	E	187	LEU	N-CA	5.32	1.49	1.46
1	C	374	HIS	CB-CG	-5.32	1.42	1.50
1	E	374	HIS	CB-CG	-5.31	1.42	1.50
1	A	374	HIS	CB-CG	-5.30	1.42	1.50
6	L	106	ILE	CB-CG1	5.25	1.64	1.53
2	B	518	LEU	CB-CG	5.19	1.63	1.53
2	F	518	LEU	CB-CG	5.14	1.63	1.53

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	HIS	N-CA-C	7.89	120.98	111.82
1	C	83	GLU	N-CA-C	7.83	121.71	109.96
1	C	78	ASP	CA-C-N	7.54	127.20	119.82
1	C	78	ASP	C-N-CA	7.54	127.20	119.82
1	C	239	CYS	CA-C-N	7.05	126.68	119.56
1	C	239	CYS	C-N-CA	7.05	126.68	119.56
1	A	87	GLU	N-CA-C	6.88	119.65	111.33
1	E	205	CYS	CA-C-N	6.75	126.44	119.56
1	E	205	CYS	C-N-CA	6.75	126.44	119.56
1	A	239	CYS	CA-C-N	6.74	126.88	119.87
1	A	239	CYS	C-N-CA	6.74	126.88	119.87
1	C	87	GLU	N-CA-C	6.72	119.46	111.33
4	K	7	PRO	CA-C-N	6.65	126.82	120.31
4	K	7	PRO	C-N-CA	6.65	126.82	120.31
1	E	492	GLU	CA-C-N	6.61	126.75	119.87
1	E	492	GLU	C-N-CA	6.61	126.75	119.87
1	E	87	GLU	N-CA-C	6.59	119.31	111.33
1	E	85	HIS	N-CA-C	6.58	119.27	111.71
3	J	101	ASP	CA-CB-CG	6.52	119.12	112.60
1	C	205	CYS	CA-C-N	6.50	126.13	119.56
1	C	205	CYS	C-N-CA	6.50	126.13	119.56
6	L	58	ILE	CA-C-N	6.49	126.47	119.78
6	L	58	ILE	C-N-CA	6.49	126.47	119.78
3	M	101	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	492	GLU	CA-C-N	6.45	126.58	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	GLU	C-N-CA	6.45	126.58	119.87
6	L	99	GLY	CA-C-N	6.45	126.07	119.56
6	L	99	GLY	C-N-CA	6.45	126.07	119.56
1	E	239	CYS	CA-C-N	6.43	126.55	119.87
1	E	239	CYS	C-N-CA	6.43	126.55	119.87
1	C	492	GLU	CA-C-N	6.36	126.48	119.87
1	C	492	GLU	C-N-CA	6.36	126.48	119.87
1	A	205	CYS	CA-C-N	6.35	125.97	119.56
1	A	205	CYS	C-N-CA	6.35	125.97	119.56
1	E	80	ASN	CA-C-N	6.32	125.94	119.56
1	E	80	ASN	C-N-CA	6.32	125.94	119.56
1	E	78	ASP	CA-C-N	6.29	125.97	119.56
1	E	78	ASP	C-N-CA	6.29	125.97	119.56
4	N	7	PRO	CA-C-N	6.27	126.45	120.31
4	N	7	PRO	C-N-CA	6.27	126.45	120.31
1	E	443	ILE	N-CA-C	6.27	116.95	108.17
5	H	108	THR	N-CA-C	6.12	119.69	109.95
1	E	219	ALA	CA-C-N	6.07	126.26	120.31
1	E	219	ALA	C-N-CA	6.07	126.26	120.31
6	L	43	ALA	CA-C-N	6.04	126.00	119.78
6	L	43	ALA	C-N-CA	6.04	126.00	119.78
4	P	7	PRO	CA-C-N	5.99	126.18	120.31
4	P	7	PRO	C-N-CA	5.99	126.18	120.31
1	A	443	ILE	N-CA-C	5.97	116.53	108.17
4	P	39	HIS	N-CA-C	-5.92	102.31	109.83
4	N	39	HIS	N-CA-C	-5.87	102.65	109.93
1	A	437	PRO	CA-C-N	5.84	125.75	119.85
1	A	437	PRO	C-N-CA	5.84	125.75	119.85
1	A	85	HIS	N-CA-C	5.83	118.41	111.71
1	A	439	ILE	N-CA-C	5.80	116.29	108.17
5	H	100(M)	TYR	CA-C-O	-5.79	114.45	120.70
1	C	443	ILE	N-CA-C	5.75	116.22	108.17
2	B	620	SER	N-CA-C	-5.75	104.99	113.61
1	E	439	ILE	N-CA-C	5.69	116.13	108.17
3	O	101	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	182	VAL	CA-C-N	5.63	125.57	119.78
1	C	182	VAL	C-N-CA	5.63	125.57	119.78
1	C	219	ALA	CA-C-N	5.62	125.60	120.03
1	C	219	ALA	C-N-CA	5.62	125.60	120.03
6	L	98	PHE	CA-CB-CG	5.61	119.41	113.80
4	P	43	ALA	CA-C-N	5.60	125.53	119.76
4	P	43	ALA	C-N-CA	5.60	125.53	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	54	ARG	CA-C-N	5.58	125.56	120.03
4	P	54	ARG	C-N-CA	5.58	125.56	120.03
1	C	437	PRO	CA-C-N	5.58	125.49	119.85
1	C	437	PRO	C-N-CA	5.58	125.49	119.85
4	P	100	GLY	N-CA-C	-5.56	104.09	112.60
1	E	437	PRO	CA-C-N	5.55	125.45	119.85
1	E	437	PRO	C-N-CA	5.55	125.45	119.85
3	M	100(A)	LEU	N-CA-C	-5.54	106.36	114.39
1	E	237	GLY	CA-C-N	5.53	125.46	119.76
1	E	237	GLY	C-N-CA	5.53	125.46	119.76
4	P	9	SER	N-CA-C	5.53	119.02	111.39
3	J	86	ASP	CA-CB-CG	5.53	118.13	112.60
6	L	39	LYS	N-CA-C	-5.53	102.81	109.83
1	C	237	GLY	CA-C-N	5.52	125.44	119.76
1	C	237	GLY	C-N-CA	5.52	125.44	119.76
1	A	219	ALA	CA-C-N	5.50	125.48	120.03
1	A	219	ALA	C-N-CA	5.50	125.48	120.03
1	A	437	PRO	N-CA-C	-5.50	105.19	110.47
4	P	6	GLN	CA-C-N	5.49	123.61	119.66
4	P	6	GLN	C-N-CA	5.49	123.61	119.66
3	M	86	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	123	THR	CA-C-N	5.41	125.12	119.82
1	C	123	THR	C-N-CA	5.41	125.12	119.82
4	N	54	ARG	CA-C-N	5.39	125.37	120.03
4	N	54	ARG	C-N-CA	5.39	125.37	120.03
5	H	86	ASP	N-CA-C	5.39	119.49	113.02
5	H	28	THR	N-CA-C	5.38	117.02	110.41
1	A	237	GLY	CA-C-N	5.37	125.29	119.76
1	A	237	GLY	C-N-CA	5.37	125.29	119.76
4	P	27(B)	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	169	ARG	NE-CZ-NH2	-5.36	114.38	119.20
4	N	100	GLY	N-CA-C	-5.36	103.98	112.66
4	K	54	ARG	CA-C-N	5.34	125.55	120.31
4	K	54	ARG	C-N-CA	5.34	125.55	120.31
4	N	9	SER	N-CA-C	5.34	118.76	111.39
4	K	61	ARG	N-CA-C	-5.32	106.74	113.18
3	M	52	ASN	CA-C-O	-5.32	116.02	121.87
1	E	464	THR	CA-C-N	5.30	131.67	121.54
1	E	464	THR	C-N-CA	5.30	131.67	121.54
4	P	93	GLY	CA-C-O	-5.29	118.50	122.37
5	H	1	GLU	CA-C-N	-5.29	114.40	121.80
5	H	1	GLU	C-N-CA	-5.29	114.40	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	100(F)	TYR	CA-C-O	-5.28	115.71	121.84
6	L	79	GLU	CA-C-N	5.27	125.59	119.47
6	L	79	GLU	C-N-CA	5.27	125.59	119.47
3	M	100(F)	TYR	CA-C-O	-5.26	115.44	121.54
1	A	72	HIS	CA-C-N	5.25	127.83	120.28
1	A	72	HIS	C-N-CA	5.25	127.83	120.28
4	K	43	ALA	CA-C-N	5.25	125.17	119.76
4	K	43	ALA	C-N-CA	5.25	125.17	119.76
1	A	184	MET	N-CA-C	5.24	117.15	109.24
2	D	622	ILE	N-CA-C	-5.21	106.60	111.45
1	A	182	VAL	CA-C-N	5.20	125.10	119.85
1	A	182	VAL	C-N-CA	5.20	125.10	119.85
5	H	13	LYS	CA-C-N	5.20	125.24	119.32
5	H	13	LYS	C-N-CA	5.20	125.24	119.32
1	E	383	PHE	CA-CB-CG	5.19	118.99	113.80
4	N	27(B)	ASP	CA-CB-CG	5.17	117.77	112.60
3	O	86	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	309	ILE	N-CA-C	-5.14	108.11	113.10
2	F	661	LEU	N-CA-C	-5.12	107.08	113.38
1	A	353	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	82	GLN	N-CA-C	5.11	121.68	110.80
3	O	77	THR	N-CA-C	5.11	117.23	108.90
4	K	100	GLY	N-CA-C	-5.10	104.40	112.66
1	C	436	ALA	CA-C-N	5.10	123.38	119.66
1	C	436	ALA	C-N-CA	5.10	123.38	119.66
1	C	437	PRO	N-CA-C	-5.10	105.58	110.47
5	H	61	THR	CA-C-N	5.09	124.81	119.82
5	H	61	THR	C-N-CA	5.09	124.81	119.82
4	N	100	GLY	CA-C-N	-5.09	116.06	121.45
4	N	100	GLY	C-N-CA	-5.09	116.06	121.45
1	C	353	PHE	CA-CB-CG	-5.07	108.73	113.80
2	D	621	GLU	N-CA-C	-5.07	107.48	113.97
4	P	98	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	464	THR	CA-C-N	5.07	131.22	121.54
1	A	464	THR	C-N-CA	5.07	131.22	121.54
4	K	39	HIS	N-CA-C	-5.07	102.84	110.24
1	A	312	GLY	CA-C-N	5.06	126.17	119.84
1	A	312	GLY	C-N-CA	5.06	126.17	119.84
1	C	258	GLN	N-CA-C	5.06	118.71	112.54
4	N	43	ALA	CA-C-N	5.05	124.96	119.76
4	N	43	ALA	C-N-CA	5.05	124.96	119.76
3	J	100(F)	TYR	CA-C-O	-5.05	116.12	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	GLY	CA-C-N	5.03	126.13	119.84
1	E	312	GLY	C-N-CA	5.03	126.13	119.84
4	K	100	GLY	CA-C-N	-5.02	116.13	121.45
4	K	100	GLY	C-N-CA	-5.02	116.13	121.45
1	C	464	THR	CA-C-N	5.01	131.12	121.54
1	C	464	THR	C-N-CA	5.01	131.12	121.54
3	O	13	GLN	CA-C-N	5.01	124.92	119.76
3	O	13	GLN	C-N-CA	5.01	124.92	119.76
4	N	98	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	197	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3375	6	0
1	C	3425	0	3365	8	0
1	E	3387	0	3331	8	0
2	B	958	0	924	1	0
2	D	958	0	923	3	0
2	F	958	0	923	1	0
3	J	943	0	915	4	0
3	M	943	0	915	4	0
3	O	943	0	915	4	0
4	K	811	0	767	1	0
4	N	811	0	767	2	0
4	P	811	0	767	1	0
5	H	1051	0	980	3	0
6	L	809	0	786	3	0
7	G	28	0	25	0	0
7	I	28	0	24	0	0
7	V	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	W	28	0	25	0	0
7	X	28	0	24	0	0
7	Z	28	0	25	1	0
7	c	28	0	25	0	0
7	d	28	0	24	0	0
7	f	28	0	25	0	0
7	g	28	0	25	1	0
8	Q	50	0	43	0	0
8	Y	50	0	43	0	0
8	e	50	0	43	0	0
9	R	39	0	34	0	0
9	h	39	0	34	0	0
10	S	83	0	70	0	0
11	T	24	0	22	0	0
11	a	24	0	22	0	0
11	i	24	0	22	0	0
12	U	38	0	34	0	0
12	b	38	0	34	0	0
12	j	38	0	34	0	0
13	A	168	0	156	1	0
13	B	28	0	26	0	0
13	C	168	0	156	1	0
13	D	28	0	26	0	0
13	E	154	0	143	0	0
13	F	28	0	26	0	0
All	All	21592	0	20868	43	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 1.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:HB	13:A:611:NAG:H82	1.83	0.60
1:A:123:THR:N	1:A:124:PRO:CD	2.66	0.58
3:J:84:ASP:N	3:J:84:ASP:OD1	2.37	0.58
3:M:84:ASP:N	3:M:84:ASP:OD1	2.37	0.57
3:O:84:ASP:OD1	3:O:84:ASP:N	2.37	0.57
1:C:123:THR:N	1:C:124:PRO:CD	2.67	0.57
1:E:123:THR:N	1:E:124:PRO:CD	2.68	0.56
1:E:134:VAL:HG13	7:g:1:NAG:H81	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:656:ASN:HB3	3:O:56:LEU:HD21	1.87	0.56
1:C:134:VAL:HG13	7:Z:1:NAG:H81	1.88	0.55
1:A:107:ASP:OD1	2:B:574:LYS:NZ	2.41	0.54
1:E:129:LEU:O	1:E:189:THR:HB	2.09	0.53
1:C:198:THR:HB	13:C:611:NAG:H82	1.94	0.50
1:C:71:THR:H	1:C:73:ALA:HB3	1.78	0.49
1:C:78:ASP:HB2	1:C:79:PRO:CD	2.42	0.49
6:L:96:PHE:CD1	6:L:96:PHE:N	2.79	0.49
1:E:232:LYS:NZ	1:E:269:GLU:OE2	2.47	0.48
1:C:232:LYS:NZ	1:C:268:GLU:OE1	2.48	0.46
3:M:72:ASP:OD2	3:M:75:LYS:NZ	2.43	0.46
1:A:232:LYS:NZ	1:A:268:GLU:OE1	2.48	0.46
6:L:46:LEU:HD21	6:L:49:TYR:HB3	1.98	0.46
1:E:474:ASP:OD1	1:E:474:ASP:C	2.58	0.46
3:J:82(B):SER:O	3:J:82(C):LEU:C	2.60	0.45
3:J:100(F):TYR:HA	4:K:96:TYR:OH	2.17	0.45
2:D:619:LEU:HD23	2:D:619:LEU:HA	1.67	0.44
2:D:626:MET:HE3	2:D:626:MET:HB2	1.81	0.44
3:M:82(B):SER:O	3:M:82(C):LEU:C	2.61	0.44
4:N:60:ASP:OD1	4:N:60:ASP:N	2.49	0.43
5:H:53:GLU:H	5:H:53:GLU:HG2	1.55	0.43
3:O:82(B):SER:O	3:O:82(C):LEU:C	2.62	0.43
1:C:377:ASN:C	1:C:377:ASN:OD1	2.63	0.42
6:L:60:ASP:N	6:L:60:ASP:OD1	2.48	0.42
3:J:52:ASN:HB2	3:J:56:LEU:HB2	2.02	0.42
1:E:46:LYS:NZ	2:F:632:ASP:OD2	2.47	0.42
1:E:201:ILE:H	1:E:201:ILE:HG13	1.47	0.42
1:A:377:ASN:OD1	1:A:377:ASN:C	2.62	0.42
3:M:100(F):TYR:HA	4:N:96:TYR:OH	2.20	0.42
1:E:377:ASN:OD1	1:E:377:ASN:C	2.62	0.42
3:O:100(F):TYR:HA	4:P:96:TYR:OH	2.20	0.41
1:A:85:HIS:O	1:A:86:LEU:C	2.64	0.41
5:H:61:THR:N	5:H:62:PRO:HD2	2.36	0.41
5:H:3:GLN:HB2	5:H:25:SER:HB3	2.02	0.41
1:C:78:ASP:HB2	1:C:79:PRO:HD2	2.02	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	427/473 (90%)	411 (96%)	13 (3%)	3 (1%)	18	49
1	C	426/473 (90%)	402 (94%)	21 (5%)	3 (1%)	18	49
1	E	419/473 (89%)	400 (96%)	15 (4%)	4 (1%)	12	43
2	B	116/153 (76%)	111 (96%)	5 (4%)	0	100	100
2	D	116/153 (76%)	112 (97%)	4 (3%)	0	100	100
2	F	116/153 (76%)	112 (97%)	4 (3%)	0	100	100
3	J	122/125 (98%)	119 (98%)	2 (2%)	1 (1%)	16	47
3	M	122/125 (98%)	116 (95%)	5 (4%)	1 (1%)	16	47
3	O	122/125 (98%)	119 (98%)	2 (2%)	1 (1%)	16	47
4	K	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	14	45
4	N	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	14	45
4	P	107/128 (84%)	100 (94%)	6 (6%)	1 (1%)	14	45
5	H	128/134 (96%)	124 (97%)	3 (2%)	1 (1%)	16	47
6	L	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
All	All	2539/2878 (88%)	2428 (96%)	94 (4%)	17 (1%)	20	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	82(C)	LEU
3	M	82(C)	LEU
3	O	82(C)	LEU
4	N	27(B)	ASP
1	E	191	TYR
1	A	426	MET
4	K	27(B)	ASP
1	E	465	THR
4	P	27(B)	ASP

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Mol	Chain	Res	Type
1	C	426	MET
1	E	426	MET
1	A	81	PRO
1	A	465	THR
1	C	82	GLN
1	C	465	THR
1	E	185	VAL
5	H	54	GLY

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	390/421 (93%)	388 (100%)	2 (0%)	81	80
1	C	389/421 (92%)	383 (98%)	6 (2%)	57	68
1	E	386/421 (92%)	385 (100%)	1 (0%)	86	83
2	B	103/130 (79%)	100 (97%)	3 (3%)	37	57
2	D	103/130 (79%)	101 (98%)	2 (2%)	50	65
2	F	103/130 (79%)	101 (98%)	2 (2%)	50	65
3	J	101/102 (99%)	101 (100%)	0	100	100
3	M	101/102 (99%)	99 (98%)	2 (2%)	48	64
3	O	101/102 (99%)	101 (100%)	0	100	100
4	K	89/106 (84%)	89 (100%)	0	100	100
4	N	89/106 (84%)	89 (100%)	0	100	100
4	P	89/106 (84%)	88 (99%)	1 (1%)	65	73
5	H	109/111 (98%)	106 (97%)	3 (3%)	38	58
6	L	88/89 (99%)	88 (100%)	0	100	100
All	All	2241/2477 (90%)	2219 (99%)	22 (1%)	65	74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	171	LYS
2	B	619	LEU
2	B	625	ASN
2	B	635	ILE
1	C	68	VAL
1	C	71	THR
1	C	72	HIS
1	C	74	CYS
1	C	137	ASN
1	C	201	ILE
2	D	619	LEU
2	D	635	ILE
3	M	52	ASN
3	M	52(A)	ASP
1	E	201	ILE
2	F	527	THR
2	F	635	ILE
4	P	94	ARG
5	H	1	GLU
5	H	53	GLU
5	H	98	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	302	ASN
1	A	328	GLN
1	A	425	ASN
2	B	658	GLN
3	J	39	GLN
3	J	82(A)	HIS
4	K	37	GLN
4	K	38	GLN
4	K	53	GLN
1	C	328	GLN
1	C	432	GLN
2	D	658	GLN
3	M	39	GLN
3	M	52	ASN
3	M	82(A)	HIS
4	N	37	GLN

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Mol	Chain	Res	Type
4	N	38	GLN
4	N	53	GLN
4	N	69	ASN
1	E	105	HIS
1	E	114	GLN
1	E	130	GLN
1	E	432	GLN
3	O	39	GLN
3	O	52	ASN
4	P	38	GLN
4	P	53	GLN
4	P	69	ASN
5	H	81	GLN
5	H	82(A)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	TYS	H	100(I)	5	15,16,17	3.09	7 (46%)	15,22,24	0.78	0
5	TYS	H	100(E)	5	15,16,17	3.18	6 (40%)	15,22,24	0.58	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
5	TYS	H	100(I)	5	-	0/10/11/13	0/1/1/1
5	TYS	H	100(E)	5	-	0/10/11/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	100(I)	TYS	CE1-CZ	5.66	1.49	1.38
5	H	100(E)	TYS	CD1-CG	5.50	1.49	1.38
5	H	100(E)	TYS	CE1-CZ	5.11	1.48	1.38
5	H	100(I)	TYS	CD1-CG	5.03	1.48	1.38
5	H	100(I)	TYS	CD2-CG	5.00	1.48	1.38
5	H	100(I)	TYS	CE1-CD1	4.91	1.46	1.38
5	H	100(E)	TYS	CE2-CZ	4.85	1.47	1.38
5	H	100(E)	TYS	CE1-CD1	4.61	1.46	1.38
5	H	100(E)	TYS	CD2-CG	4.54	1.47	1.38
5	H	100(E)	TYS	CE2-CD2	4.38	1.45	1.38
5	H	100(I)	TYS	CE2-CZ	4.01	1.46	1.38
5	H	100(I)	TYS	CE2-CD2	2.97	1.43	1.38
5	H	100(I)	TYS	OH-CZ	-2.68	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
7	NAG	G	1	1,7	14,14,15	2.15	5 (35%)	17,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	2	7	14,14,15	2.00	6 (42%)	17,19,21	0.97	2 (11%)
7	NAG	I	1	1,7	14,14,15	2.22	5 (35%)	17,19,21	7.17	3 (17%)
7	NAG	I	2	7	14,14,15	1.96	5 (35%)	17,19,21	0.94	1 (5%)
8	NAG	Q	1	1,8	14,14,15	2.05	4 (28%)	17,19,21	1.15	2 (11%)
8	NAG	Q	2	8	14,14,15	1.94	5 (35%)	17,19,21	0.91	1 (5%)
8	BMA	Q	3	8	11,11,12	0.66	0	15,15,17	0.75	1 (6%)
8	MAN	Q	4	8	11,11,12	1.93	6 (54%)	15,15,17	0.75	0
9	NAG	R	1	9,1	14,14,15	0.40	0	17,19,21	0.78	0
9	NAG	R	2	9	14,14,15	0.38	0	17,19,21	0.81	0
9	BMA	R	3	9	11,11,12	0.26	0	15,15,17	0.59	0
10	NAG	S	1	1,10	14,14,15	0.50	0	17,19,21	0.84	0
10	NAG	S	2	10	14,14,15	0.42	0	17,19,21	0.95	1 (5%)
10	BMA	S	3	10	11,11,12	0.32	0	15,15,17	0.88	1 (6%)
10	MAN	S	4	10	11,11,12	0.26	0	15,15,17	0.90	0
10	MAN	S	5	10	11,11,12	0.19	0	15,15,17	0.54	0
10	MAN	S	6	10	11,11,12	0.24	0	15,15,17	0.65	0
10	MAN	S	7	10	11,11,12	0.20	0	15,15,17	0.56	0
11	NAG	T	1	2,11	14,14,15	2.08	5 (35%)	17,19,21	1.14	2 (11%)
11	FUC	T	2	11	10,10,11	2.04	4 (40%)	14,14,16	0.65	0
12	NAG	U	1	2,12	14,14,15	0.48	0	17,19,21	1.14	2 (11%)
12	NAG	U	2	12	14,14,15	0.24	0	17,19,21	0.98	1 (5%)
12	FUC	U	3	12	10,10,11	0.18	0	14,14,16	0.58	0
7	NAG	V	1	1,7	14,14,15	2.04	6 (42%)	17,19,21	1.14	3 (17%)
7	NAG	V	2	7	14,14,15	1.96	4 (28%)	17,19,21	0.85	1 (5%)
7	NAG	W	1	1,7	14,14,15	2.05	4 (28%)	17,19,21	1.22	2 (11%)
7	NAG	W	2	7	14,14,15	2.02	5 (35%)	17,19,21	0.92	1 (5%)
7	NAG	X	1	1,7	14,14,15	2.19	6 (42%)	17,19,21	7.07	3 (17%)
7	NAG	X	2	7	14,14,15	1.99	6 (42%)	17,19,21	0.94	1 (5%)
8	NAG	Y	1	1,8	14,14,15	2.07	4 (28%)	17,19,21	1.20	3 (17%)
8	NAG	Y	2	8	14,14,15	1.97	5 (35%)	17,19,21	0.95	1 (5%)
8	BMA	Y	3	8	11,11,12	0.76	0	15,15,17	0.77	1 (6%)
8	MAN	Y	4	8	11,11,12	1.95	6 (54%)	15,15,17	0.73	0
7	NAG	Z	1	1,7	14,14,15	2.00	4 (28%)	17,19,21	0.93	0
7	NAG	Z	2	7	14,14,15	1.96	5 (35%)	17,19,21	0.84	0
11	NAG	a	1	2,11	14,14,15	0.42	0	17,19,21	0.76	1 (5%)
11	FUC	a	2	11	10,10,11	0.25	0	14,14,16	0.94	0
12	NAG	b	1	2,12	14,14,15	0.43	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	b	2	12	14,14,15	0.32	0	17,19,21	0.63	0
12	FUC	b	3	12	10,10,11	0.18	0	14,14,16	0.67	0
7	NAG	c	1	1,7	14,14,15	2.07	4 (28%)	17,19,21	1.00	0
7	NAG	c	2	7	14,14,15	1.93	6 (42%)	17,19,21	1.01	1 (5%)
7	NAG	d	1	1,7	14,14,15	2.16	6 (42%)	17,19,21	7.41	3 (17%)
7	NAG	d	2	7	14,14,15	2.00	6 (42%)	17,19,21	0.94	1 (5%)
8	NAG	e	1	1,8	14,14,15	2.01	4 (28%)	17,19,21	1.24	3 (17%)
8	NAG	e	2	8	14,14,15	1.95	5 (35%)	17,19,21	0.95	1 (5%)
8	BMA	e	3	8	11,11,12	0.74	0	15,15,17	0.77	1 (6%)
8	MAN	e	4	8	11,11,12	1.95	6 (54%)	15,15,17	0.67	0
7	NAG	f	1	1,7	14,14,15	2.14	6 (42%)	17,19,21	1.21	1 (5%)
7	NAG	f	2	7	14,14,15	1.99	4 (28%)	17,19,21	0.84	0
7	NAG	g	1	1,7	14,14,15	2.04	4 (28%)	17,19,21	1.02	2 (11%)
7	NAG	g	2	7	14,14,15	2.02	5 (35%)	17,19,21	0.87	1 (5%)
9	NAG	h	1	9,1	14,14,15	0.51	0	17,19,21	1.07	2 (11%)
9	NAG	h	2	9	14,14,15	0.39	0	17,19,21	1.15	1 (5%)
9	BMA	h	3	9	11,11,12	0.30	0	15,15,17	0.69	0
11	NAG	i	1	2,11	14,14,15	0.42	0	17,19,21	1.07	1 (5%)
11	FUC	i	2	11	10,10,11	0.27	0	14,14,16	1.16	2 (14%)
12	NAG	j	1	2,12	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
12	NAG	j	2	12	14,14,15	0.28	0	17,19,21	1.06	1 (5%)
12	FUC	j	3	12	10,10,11	0.26	0	14,14,16	0.83	1 (7%)

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	G	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
9	NAG	R	1	9,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	BMA	R	3	9	-	0/2/19/22	0/1/1/1
10	NAG	S	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	BMA	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	2/2/19/22	0/1/1/1
10	MAN	S	5	10	-	0/2/19/22	0/1/1/1
10	MAN	S	6	10	-	0/2/19/22	0/1/1/1
10	MAN	S	7	10	-	0/2/19/22	0/1/1/1
11	NAG	T	1	2,11	-	0/6/23/26	0/1/1/1
11	FUC	T	2	11	-	-	0/1/1/1
12	NAG	U	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	U	2	12	-	3/6/23/26	0/1/1/1
12	FUC	U	3	12	-	-	0/1/1/1
7	NAG	V	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	1/2/19/22	0/1/1/1
7	NAG	Z	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	0/6/23/26	0/1/1/1
11	NAG	a	1	2,11	-	1/6/23/26	0/1/1/1
11	FUC	a	2	11	-	-	0/1/1/1
12	NAG	b	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	b	2	12	-	2/6/23/26	0/1/1/1
12	FUC	b	3	12	-	-	0/1/1/1
7	NAG	c	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	NAG	d	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
8	NAG	e	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
8	MAN	e	4	8	-	0/2/19/22	0/1/1/1
7	NAG	f	1	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	NAG	g	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
9	NAG	h	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
11	NAG	i	1	2,11	-	0/6/23/26	0/1/1/1
11	FUC	i	2	11	-	-	0/1/1/1
12	NAG	j	1	2,12	-	4/6/23/26	0/1/1/1
12	NAG	j	2	12	-	3/6/23/26	0/1/1/1
12	FUC	j	3	12	-	-	0/1/1/1

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	1	NAG	C1-C2	5.95	1.60	1.52
7	X	1	NAG	C1-C2	5.81	1.60	1.52
7	d	1	NAG	C1-C2	5.73	1.60	1.52
7	G	1	NAG	C1-C2	5.69	1.60	1.52
8	Q	1	NAG	C1-C2	5.52	1.59	1.52
8	Y	1	NAG	C1-C2	5.52	1.59	1.52
7	c	1	NAG	C1-C2	5.47	1.59	1.52
7	f	1	NAG	C1-C2	5.44	1.59	1.52
11	T	1	NAG	C1-C2	5.28	1.59	1.52
8	e	1	NAG	C1-C2	5.27	1.59	1.52
7	V	1	NAG	C1-C2	5.20	1.59	1.52
7	W	1	NAG	C1-C2	5.08	1.59	1.52
7	g	1	NAG	C1-C2	5.07	1.59	1.52
7	Z	1	NAG	C1-C2	5.03	1.59	1.52
7	W	2	NAG	C1-C2	4.92	1.59	1.52
7	f	2	NAG	C1-C2	4.78	1.58	1.52
7	d	2	NAG	C1-C2	4.76	1.58	1.52
7	g	2	NAG	C1-C2	4.74	1.58	1.52
7	X	2	NAG	C1-C2	4.71	1.58	1.52
8	Y	2	NAG	C1-C2	4.66	1.58	1.52
7	V	2	NAG	C1-C2	4.65	1.58	1.52
8	Q	2	NAG	C1-C2	4.62	1.58	1.52
7	G	2	NAG	C1-C2	4.61	1.58	1.52
7	I	2	NAG	C1-C2	4.60	1.58	1.52
7	Z	2	NAG	C1-C2	4.48	1.58	1.52
7	c	2	NAG	C1-C2	4.37	1.58	1.52
8	e	2	NAG	C1-C2	4.32	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	1	NAG	O5-C5	3.40	1.50	1.43
8	e	4	MAN	O5-C5	3.31	1.49	1.43
11	T	2	FUC	C2-C3	3.27	1.57	1.52
8	Y	4	MAN	O5-C5	3.24	1.49	1.43
7	g	1	NAG	O5-C5	3.24	1.49	1.43
7	g	2	NAG	O5-C5	3.21	1.49	1.43
7	Z	2	NAG	O5-C5	3.19	1.49	1.43
7	c	2	NAG	O5-C5	3.18	1.49	1.43
7	W	2	NAG	O5-C5	3.17	1.49	1.43
8	Q	4	MAN	O5-C5	3.17	1.49	1.43
7	f	2	NAG	O5-C5	3.17	1.49	1.43
7	G	2	NAG	O5-C5	3.17	1.49	1.43
7	X	2	NAG	O5-C5	3.16	1.49	1.43
8	Q	4	MAN	C2-C3	3.16	1.57	1.52
7	I	2	NAG	O5-C5	3.13	1.49	1.43
7	d	2	NAG	O5-C5	3.10	1.49	1.43
8	e	2	NAG	O5-C5	3.08	1.49	1.43
7	W	1	NAG	O5-C5	3.07	1.49	1.43
8	Y	4	MAN	C2-C3	3.07	1.57	1.52
8	e	4	MAN	C2-C3	3.07	1.57	1.52
7	V	2	NAG	O5-C5	3.05	1.49	1.43
11	T	2	FUC	O5-C5	3.03	1.49	1.43
7	G	1	NAG	O5-C5	3.00	1.49	1.43
7	f	1	NAG	O5-C5	2.99	1.49	1.43
7	Z	1	NAG	O5-C5	2.96	1.49	1.43
7	c	1	NAG	O5-C5	2.95	1.49	1.43
8	Y	2	NAG	O5-C5	2.93	1.49	1.43
8	Q	2	NAG	O5-C5	2.89	1.49	1.43
7	I	1	NAG	O5-C5	2.77	1.48	1.43
7	X	1	NAG	O5-C5	2.73	1.48	1.43
7	d	1	NAG	O5-C5	2.71	1.48	1.43
11	T	2	FUC	C1-C2	2.65	1.58	1.52
7	V	1	NAG	O5-C5	2.64	1.48	1.43
8	e	4	MAN	C1-C2	2.56	1.58	1.52
8	Y	4	MAN	C1-C2	2.55	1.58	1.52
8	Y	1	NAG	O5-C5	2.54	1.48	1.43
8	Q	1	NAG	O5-C5	2.54	1.48	1.43
8	e	1	NAG	O5-C5	2.53	1.48	1.43
8	e	2	NAG	C3-C2	2.49	1.57	1.52
7	W	1	NAG	C4-C5	2.49	1.58	1.53
7	g	1	NAG	O5-C1	2.49	1.47	1.43
7	f	2	NAG	C3-C2	2.48	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	4	MAN	C4-C5	2.47	1.58	1.53
7	d	2	NAG	C3-C2	2.47	1.57	1.52
8	e	2	NAG	C4-C5	2.46	1.58	1.53
7	G	2	NAG	C4-C5	2.45	1.58	1.53
7	I	2	NAG	C3-C2	2.45	1.57	1.52
8	Y	2	NAG	C3-C2	2.43	1.57	1.52
7	Z	1	NAG	O5-C1	2.43	1.47	1.43
7	V	2	NAG	C3-C2	2.43	1.57	1.52
8	Q	4	MAN	C1-C2	2.42	1.58	1.52
7	c	2	NAG	C4-C5	2.41	1.58	1.53
7	g	2	NAG	C3-C2	2.41	1.57	1.52
11	T	2	FUC	C4-C5	2.40	1.58	1.52
8	e	1	NAG	C3-C2	2.38	1.57	1.52
7	I	1	NAG	C3-C2	2.38	1.57	1.52
7	X	2	NAG	C3-C2	2.37	1.57	1.52
7	f	1	NAG	C3-C2	2.36	1.57	1.52
7	W	2	NAG	C3-C2	2.36	1.57	1.52
8	e	4	MAN	C4-C5	2.35	1.58	1.53
8	Q	4	MAN	C4-C5	2.35	1.58	1.53
7	Z	2	NAG	C3-C2	2.35	1.57	1.52
7	G	2	NAG	C3-C2	2.33	1.57	1.52
8	Q	2	NAG	C3-C2	2.33	1.57	1.52
7	g	2	NAG	C4-C5	2.33	1.58	1.53
7	X	1	NAG	C4-C3	2.32	1.58	1.52
7	g	1	NAG	C4-C5	2.29	1.57	1.53
7	d	2	NAG	C4-C5	2.29	1.57	1.53
7	f	1	NAG	O5-C1	2.27	1.47	1.43
7	G	1	NAG	C3-C2	2.26	1.57	1.52
7	d	1	NAG	C4-C5	2.26	1.57	1.53
7	I	2	NAG	C4-C5	2.26	1.57	1.53
7	Z	2	NAG	C4-C5	2.25	1.57	1.53
7	V	2	NAG	C4-C5	2.24	1.57	1.53
7	W	2	NAG	C4-C5	2.24	1.57	1.53
7	Z	1	NAG	C4-C5	2.24	1.57	1.53
7	f	2	NAG	C4-C5	2.24	1.57	1.53
7	V	1	NAG	C4-C5	2.23	1.57	1.53
8	Y	1	NAG	C3-C2	2.23	1.57	1.52
7	X	2	NAG	C4-C5	2.23	1.57	1.53
8	Y	2	NAG	C4-C5	2.21	1.57	1.53
7	c	1	NAG	O5-C1	2.21	1.47	1.43
7	I	1	NAG	C4-C3	2.21	1.58	1.52
7	f	1	NAG	C4-C5	2.21	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	1	NAG	C3-C2	2.21	1.57	1.52
7	G	2	NAG	C2-N2	2.21	1.49	1.46
7	d	1	NAG	O5-C1	2.21	1.47	1.43
7	d	1	NAG	C3-C2	2.19	1.57	1.52
7	X	1	NAG	C4-C5	2.19	1.57	1.53
7	X	1	NAG	C3-C2	2.19	1.57	1.52
8	Q	1	NAG	C3-C2	2.19	1.57	1.52
7	c	2	NAG	C3-C2	2.19	1.57	1.52
7	G	1	NAG	O5-C1	2.18	1.47	1.43
7	I	1	NAG	C4-C5	2.18	1.57	1.53
8	Q	2	NAG	C4-C5	2.17	1.57	1.53
7	V	1	NAG	C3-C2	2.16	1.57	1.52
8	e	4	MAN	O5-C1	2.15	1.47	1.43
7	V	1	NAG	O5-C1	2.15	1.47	1.43
7	X	2	NAG	C2-N2	2.14	1.49	1.46
7	c	2	NAG	C2-N2	2.13	1.49	1.46
8	Y	2	NAG	C4-C3	2.12	1.57	1.52
8	Q	4	MAN	O5-C1	2.12	1.47	1.43
7	X	1	NAG	C2-N2	2.12	1.49	1.46
7	c	2	NAG	C4-C3	2.12	1.57	1.52
8	Y	4	MAN	O5-C1	2.11	1.47	1.43
7	G	1	NAG	C4-C5	2.11	1.57	1.53
7	f	1	NAG	C4-C3	2.11	1.57	1.52
11	T	1	NAG	O5-C1	2.08	1.47	1.43
8	e	1	NAG	O5-C1	2.08	1.47	1.43
7	G	2	NAG	C4-C3	2.08	1.57	1.52
8	Q	1	NAG	O5-C1	2.08	1.47	1.43
8	e	2	NAG	C4-C3	2.08	1.57	1.52
7	c	1	NAG	C3-C2	2.07	1.56	1.52
7	d	2	NAG	C2-N2	2.07	1.49	1.46
7	d	1	NAG	C4-C3	2.07	1.57	1.52
8	Q	4	MAN	C4-C3	2.06	1.57	1.52
7	d	2	NAG	C4-C3	2.06	1.57	1.52
7	W	2	NAG	C2-N2	2.05	1.49	1.46
7	g	2	NAG	C2-N2	2.04	1.49	1.46
7	V	1	NAG	C4-C3	2.04	1.57	1.52
8	Y	4	MAN	C4-C3	2.03	1.57	1.52
7	X	2	NAG	C4-C3	2.03	1.57	1.52
7	W	1	NAG	C3-C2	2.02	1.56	1.52
11	T	1	NAG	C4-C5	2.01	1.57	1.53
7	I	2	NAG	C4-C3	2.01	1.57	1.52
8	Y	1	NAG	O5-C1	2.01	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	2	NAG	C4-C3	2.01	1.57	1.52
7	Z	2	NAG	C4-C3	2.01	1.57	1.52
8	e	4	MAN	C4-C3	2.00	1.57	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	1	NAG	C2-N2-C7	29.61	162.58	122.90
7	I	1	NAG	C2-N2-C7	28.72	161.38	122.90
7	X	1	NAG	C2-N2-C7	28.35	160.89	122.90
7	d	1	NAG	C8-C7-N2	5.62	125.44	116.12
7	I	1	NAG	C8-C7-N2	5.20	124.74	116.12
7	X	1	NAG	C8-C7-N2	4.96	124.34	116.12
7	d	1	NAG	O7-C7-N2	-3.83	115.22	121.98
11	i	1	NAG	C1-O5-C5	3.32	116.64	112.19
12	j	2	NAG	C2-N2-C7	3.32	127.35	122.90
7	I	1	NAG	O7-C7-N2	-3.23	116.27	121.98
7	f	1	NAG	C1-C2-N2	-2.80	106.02	110.43
12	U	2	NAG	C2-N2-C7	2.78	126.62	122.90
7	X	1	NAG	O7-C7-N2	-2.76	117.11	121.98
12	b	1	NAG	O6-C6-C5	-2.71	102.11	111.33
7	W	1	NAG	O4-C4-C3	-2.66	104.11	110.38
8	Y	1	NAG	C8-C7-N2	2.66	120.52	116.12
12	U	1	NAG	C4-C3-C2	-2.63	107.17	111.02
11	T	1	NAG	C8-C7-N2	2.60	120.44	116.12
9	h	1	NAG	O3-C3-C2	-2.56	104.08	109.40
12	U	1	NAG	O6-C6-C5	-2.56	102.61	111.33
9	h	2	NAG	C4-C3-C2	-2.49	107.36	111.02
8	Q	1	NAG	C8-C7-N2	2.46	120.20	116.12
8	e	1	NAG	C1-C2-N2	-2.45	106.57	110.43
8	e	1	NAG	C8-C7-N2	2.41	120.11	116.12
10	S	2	NAG	C2-N2-C7	-2.36	119.74	122.90
7	c	2	NAG	C8-C7-N2	2.31	119.95	116.12
7	g	1	NAG	C8-C7-N2	2.28	119.90	116.12
7	V	1	NAG	C1-C2-N2	-2.25	106.88	110.43
8	Y	1	NAG	O7-C7-C8	-2.25	118.04	122.05
8	e	2	NAG	C8-C7-N2	2.23	119.81	116.12
8	Y	2	NAG	C8-C7-N2	2.21	119.78	116.12
8	e	3	BMA	C2-C3-C4	-2.21	106.98	110.86
7	W	1	NAG	C1-C2-N2	-2.20	106.96	110.43
7	G	2	NAG	C8-C7-N2	2.20	119.76	116.12
12	j	3	FUC	C3-C4-C5	-2.18	106.50	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	2	NAG	C8-C7-N2	2.17	119.72	116.12
7	V	1	NAG	C1-O5-C5	2.16	115.08	112.19
8	Q	3	BMA	C2-C3-C4	-2.16	107.07	110.86
8	Q	1	NAG	O7-C7-C8	-2.15	118.23	122.05
7	d	2	NAG	C8-C7-N2	2.14	119.67	116.12
11	a	1	NAG	O6-C6-C5	-2.14	104.06	111.33
11	T	1	NAG	O7-C7-C8	-2.13	118.26	122.05
8	Q	2	NAG	C8-C7-N2	2.13	119.65	116.12
7	X	2	NAG	C8-C7-N2	2.13	119.65	116.12
8	Y	1	NAG	C1-O5-C5	2.11	115.01	112.19
7	I	2	NAG	C8-C7-N2	2.10	119.60	116.12
10	S	3	BMA	C6-C5-C4	-2.09	107.90	113.02
8	Y	3	BMA	C2-C3-C4	-2.08	107.20	110.86
9	h	1	NAG	O4-C4-C5	-2.06	104.24	109.32
7	V	1	NAG	C8-C7-N2	2.06	119.53	116.12
11	i	2	FUC	O5-C5-C4	2.05	113.24	109.55
8	e	1	NAG	O7-C7-C8	-2.04	118.43	122.05
11	i	2	FUC	C3-C4-C5	2.03	112.91	109.81
12	j	1	NAG	O6-C6-C5	-2.02	104.45	111.33
7	V	2	NAG	C8-C7-N2	2.01	119.46	116.12
7	g	1	NAG	O7-C7-C8	-2.01	118.47	122.05
7	G	2	NAG	O7-C7-C8	-2.01	118.48	122.05
7	g	2	NAG	C8-C7-N2	2.00	119.44	116.12

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	NAG	C1-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7
7	d	1	NAG	C1-C2-N2-C7
9	R	1	NAG	C8-C7-N2-C2
9	R	1	NAG	O7-C7-N2-C2
10	S	2	NAG	C8-C7-N2-C2
10	S	2	NAG	O7-C7-N2-C2
12	U	2	NAG	C1-C2-N2-C7
12	U	2	NAG	O7-C7-N2-C2
12	j	2	NAG	C1-C2-N2-C7
12	j	2	NAG	C8-C7-N2-C2
12	j	2	NAG	O7-C7-N2-C2
12	U	2	NAG	C8-C7-N2-C2
12	j	1	NAG	O5-C5-C6-O6

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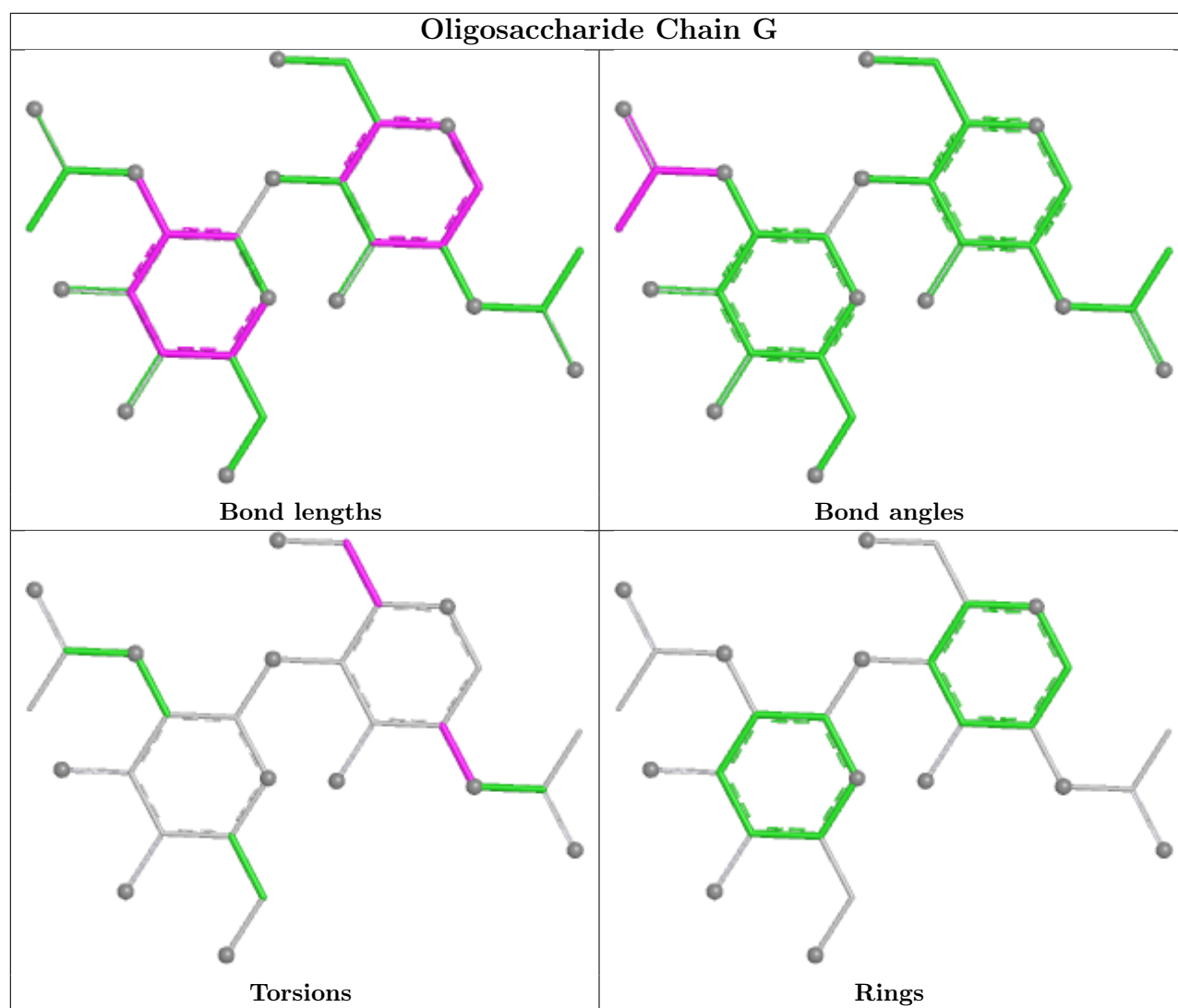
Mol	Chain	Res	Type	Atoms
10	S	4	MAN	O5-C5-C6-O6
12	U	1	NAG	C8-C7-N2-C2
12	b	1	NAG	C8-C7-N2-C2
12	j	1	NAG	C4-C5-C6-O6
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	d	1	NAG	C8-C7-N2-C2
7	d	1	NAG	O7-C7-N2-C2
12	U	1	NAG	O7-C7-N2-C2
12	b	1	NAG	O7-C7-N2-C2
10	S	3	BMA	O5-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6
8	Y	4	MAN	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
9	h	2	NAG	C8-C7-N2-C2
8	Y	3	BMA	O5-C5-C6-O6
12	b	2	NAG	C8-C7-N2-C2
7	c	1	NAG	C4-C5-C6-O6
10	S	3	BMA	C4-C5-C6-O6
10	S	4	MAN	C4-C5-C6-O6
9	h	2	NAG	O7-C7-N2-C2
12	j	1	NAG	C8-C7-N2-C2
12	b	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C1-C2-N2-C7
11	a	1	NAG	C1-C2-N2-C7
7	G	1	NAG	C4-C5-C6-O6
12	j	1	NAG	O7-C7-N2-C2

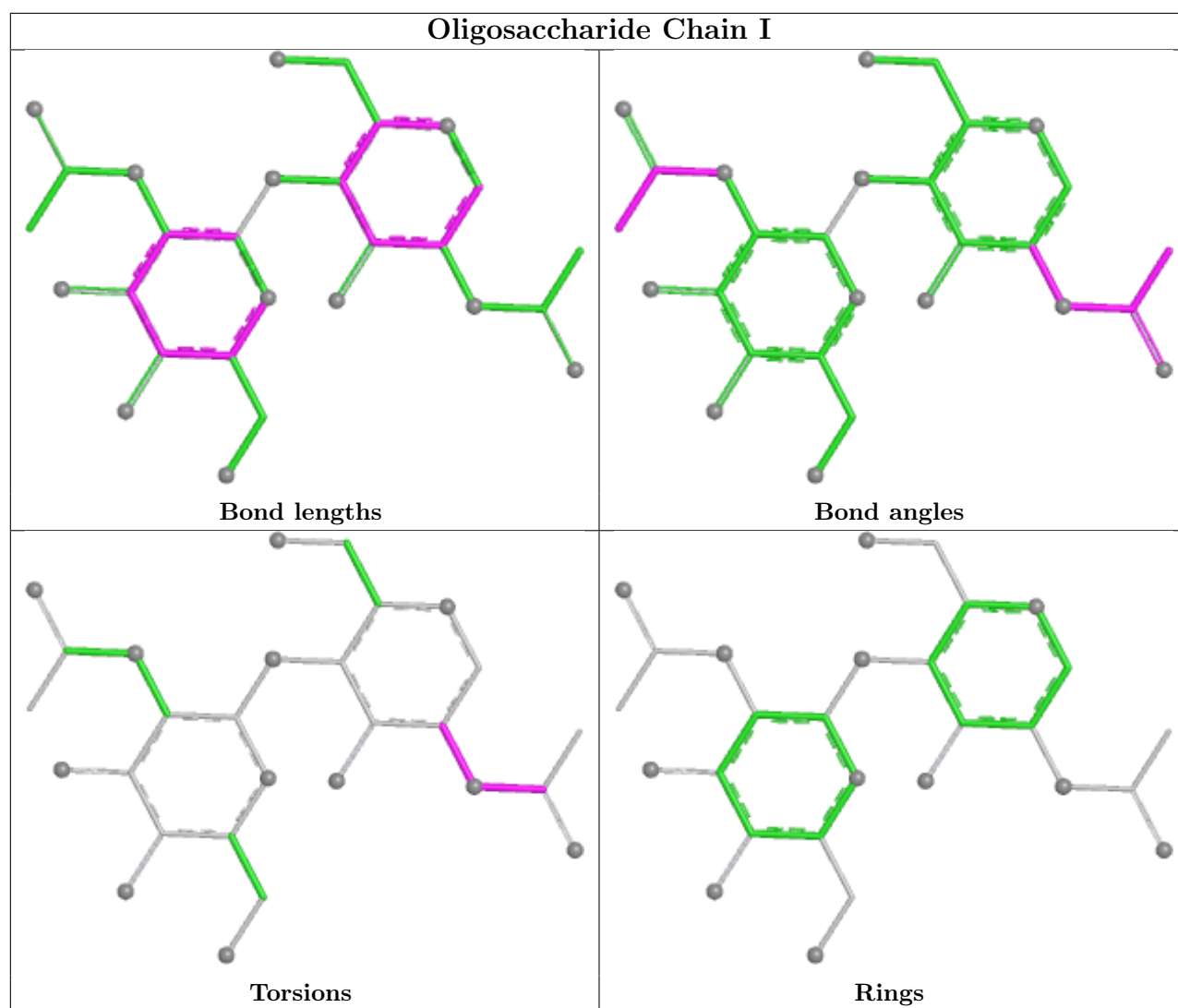
There are no ring outliers.

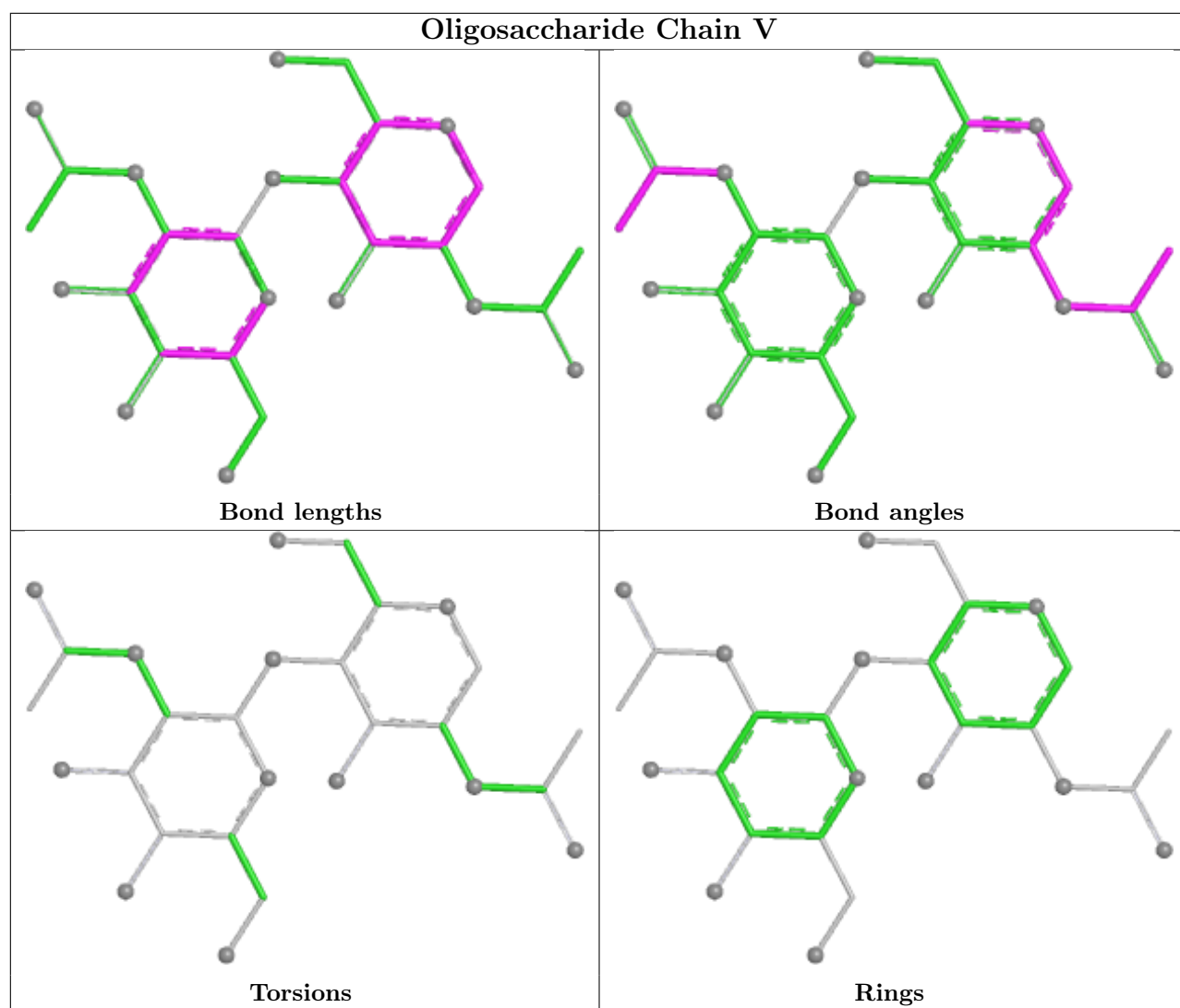
2 monomers are involved in 2 short contacts:

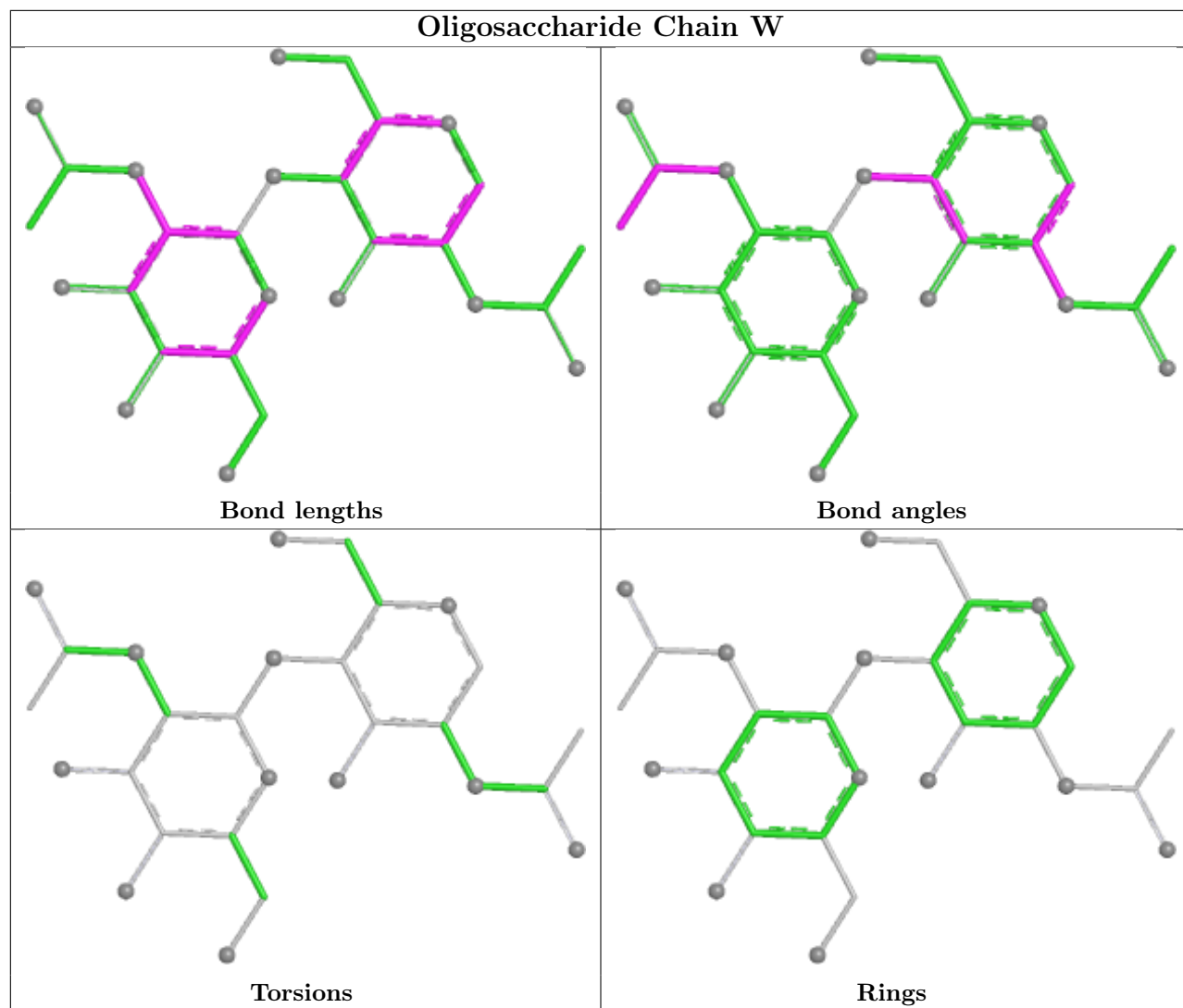
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Z	1	NAG	1	0
7	g	1	NAG	1	0

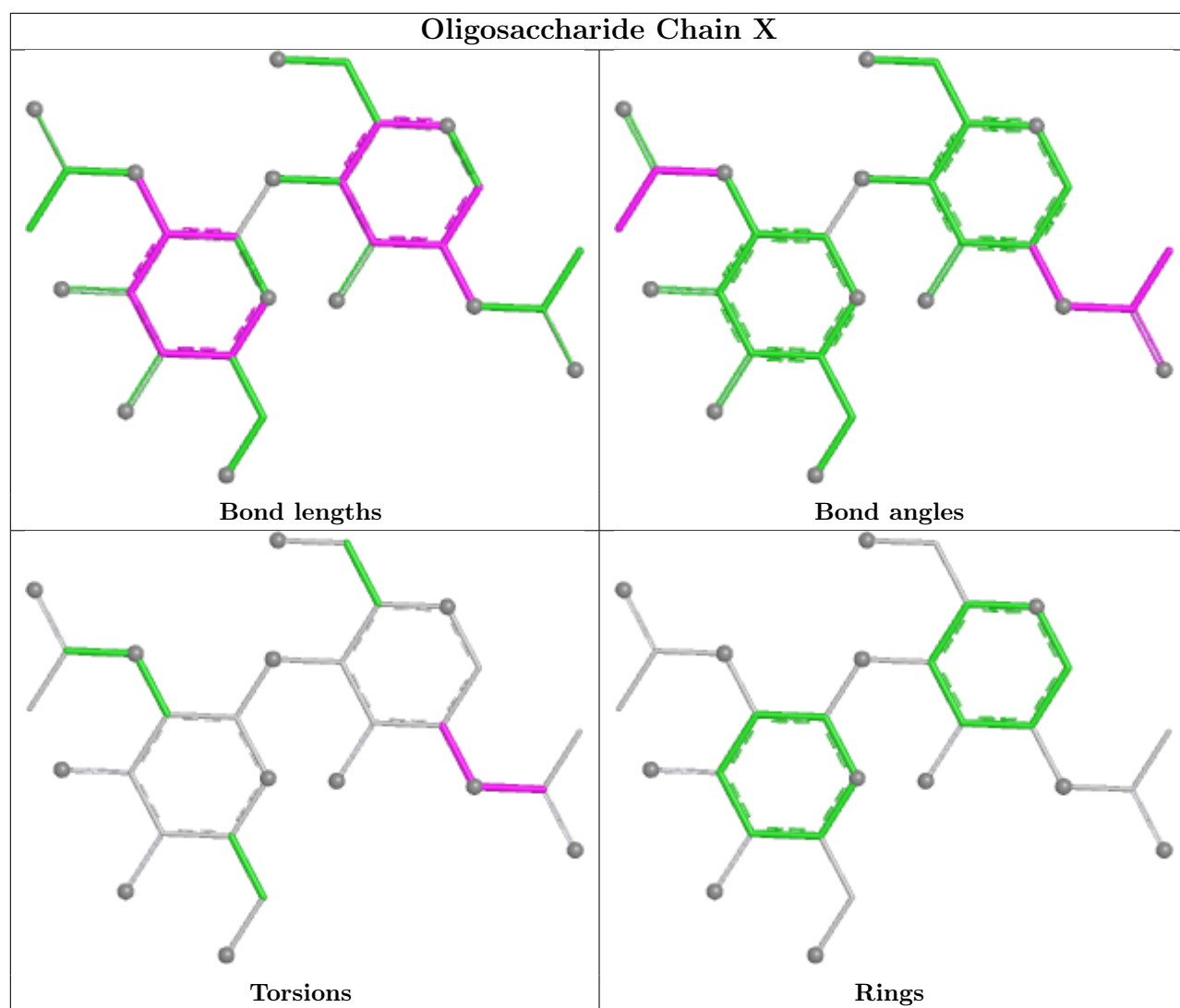
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

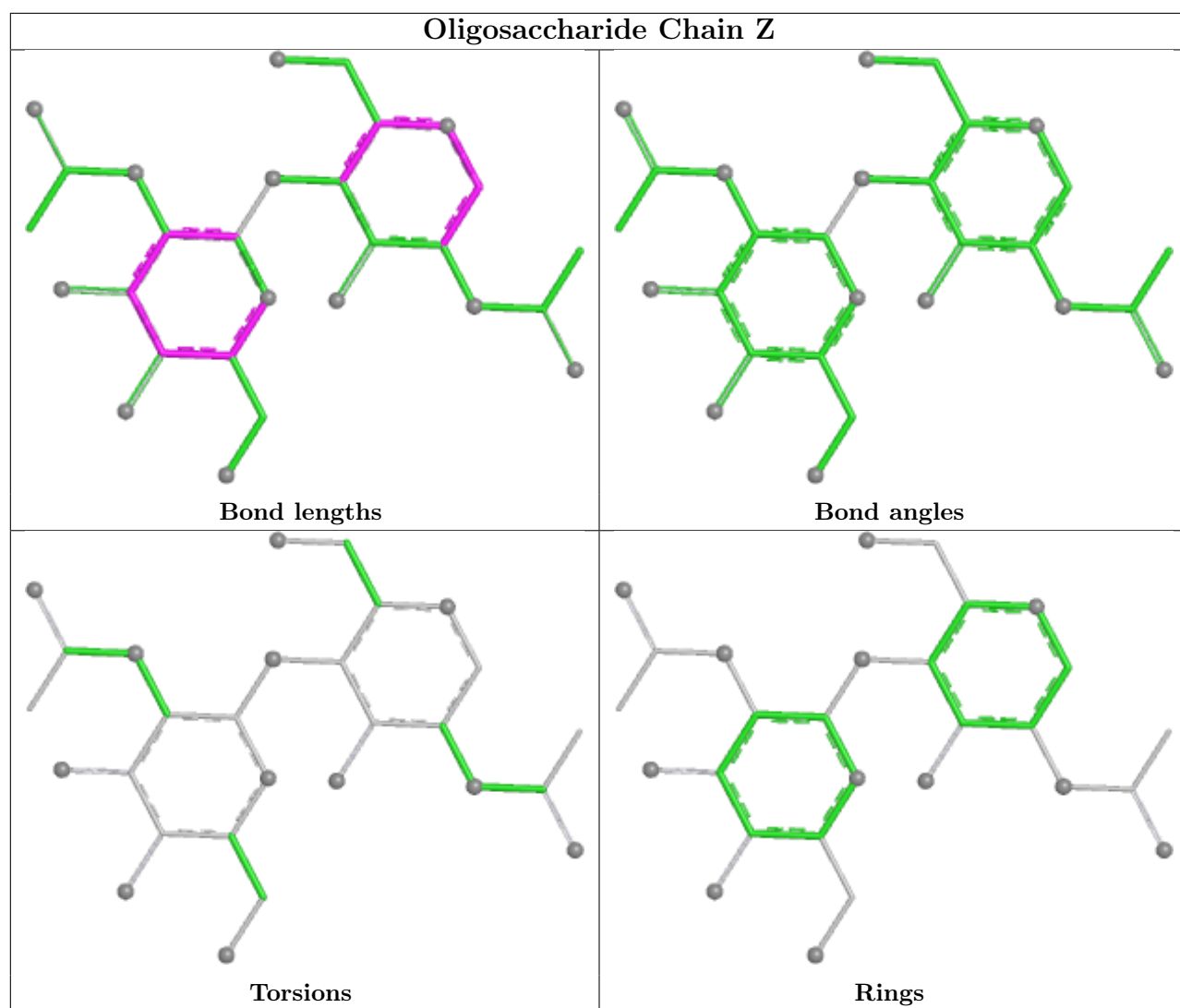


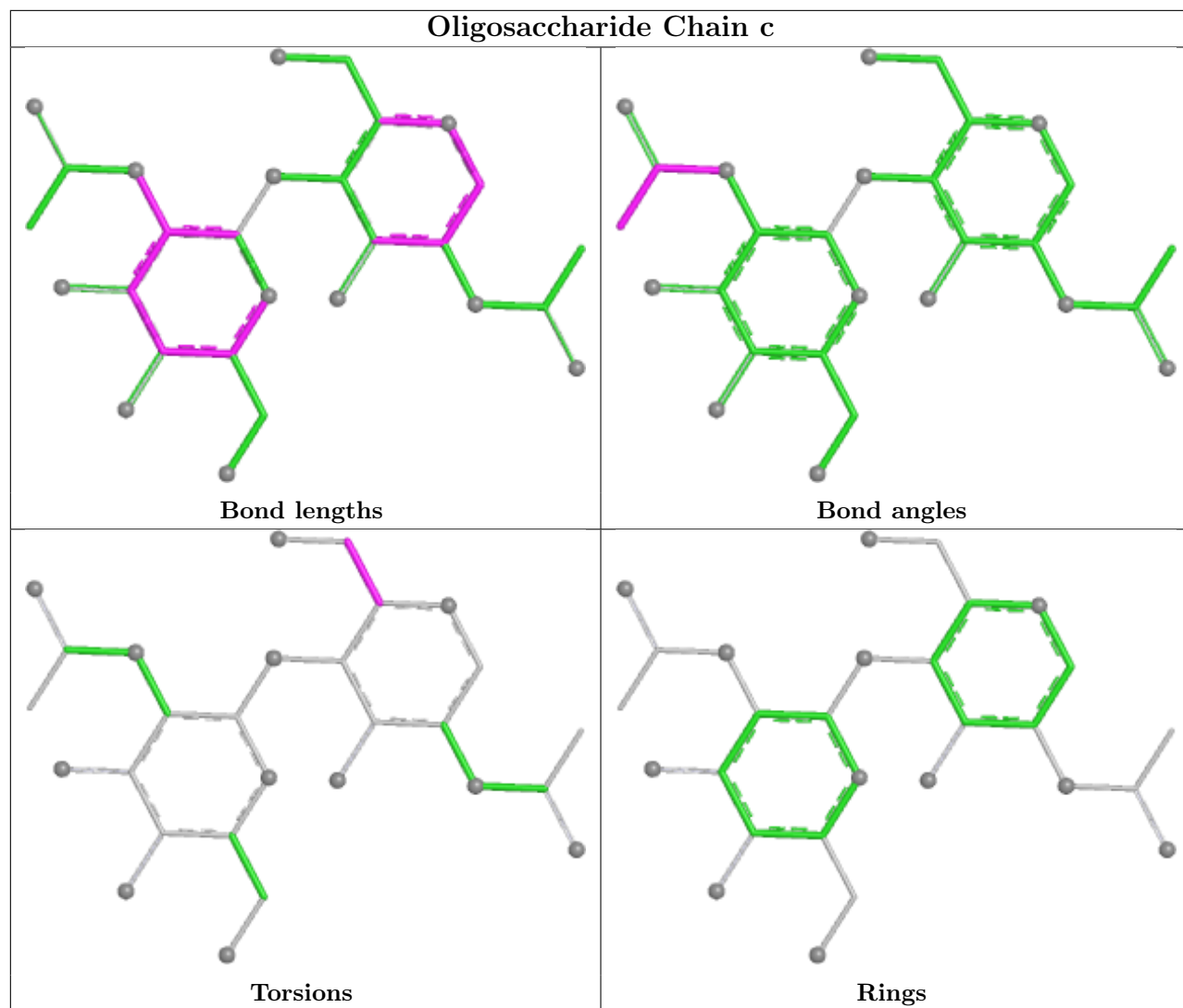


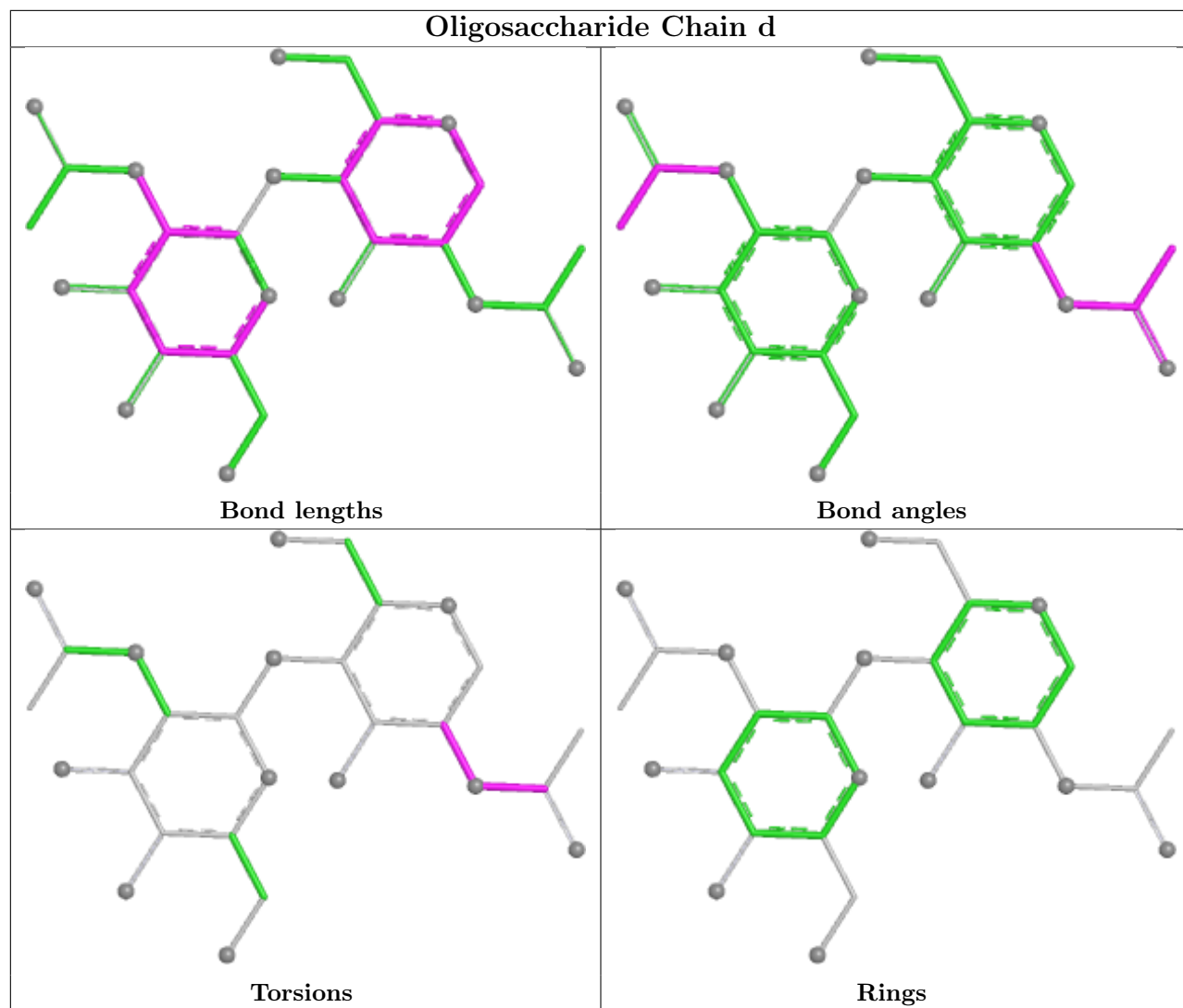


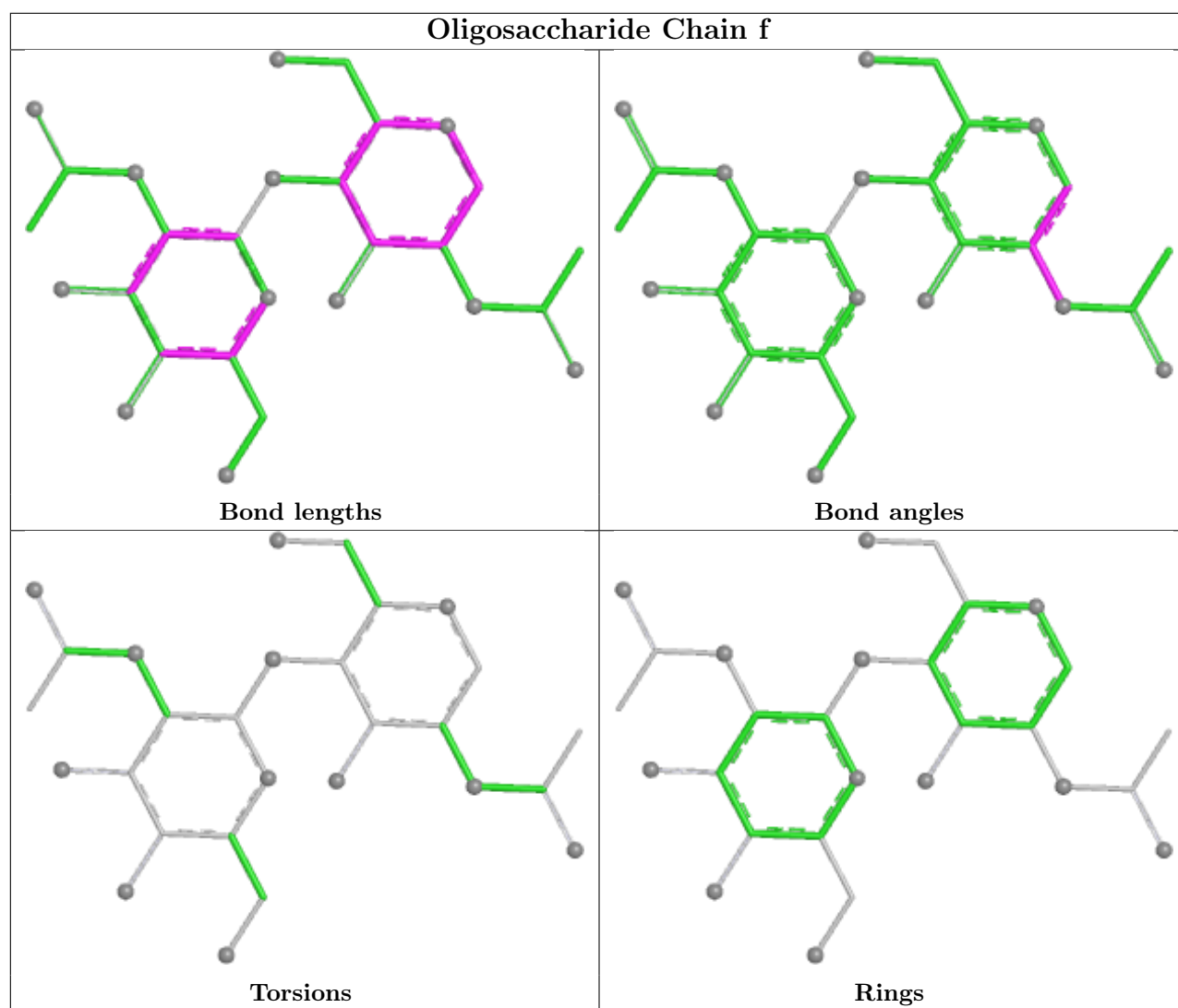


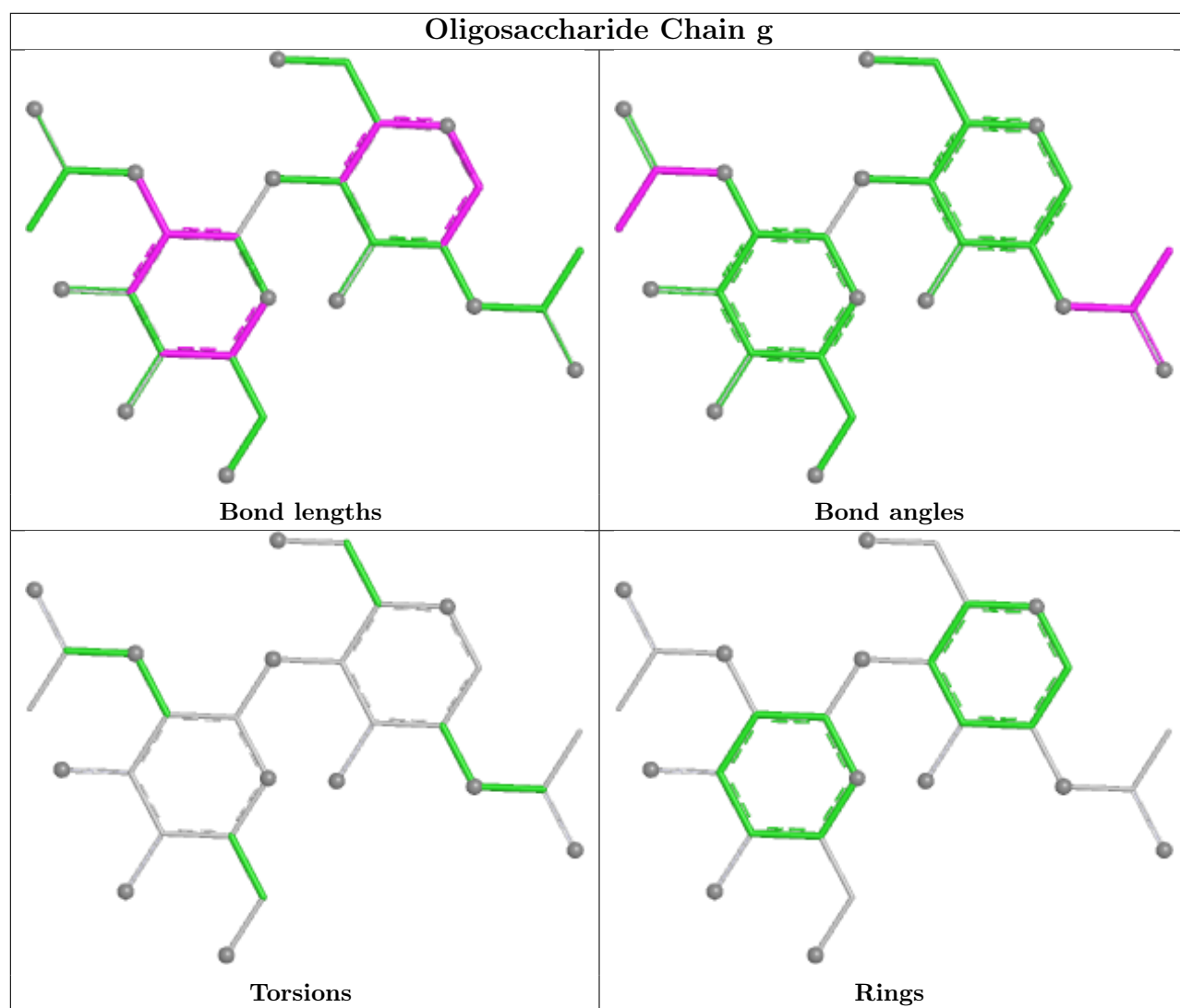


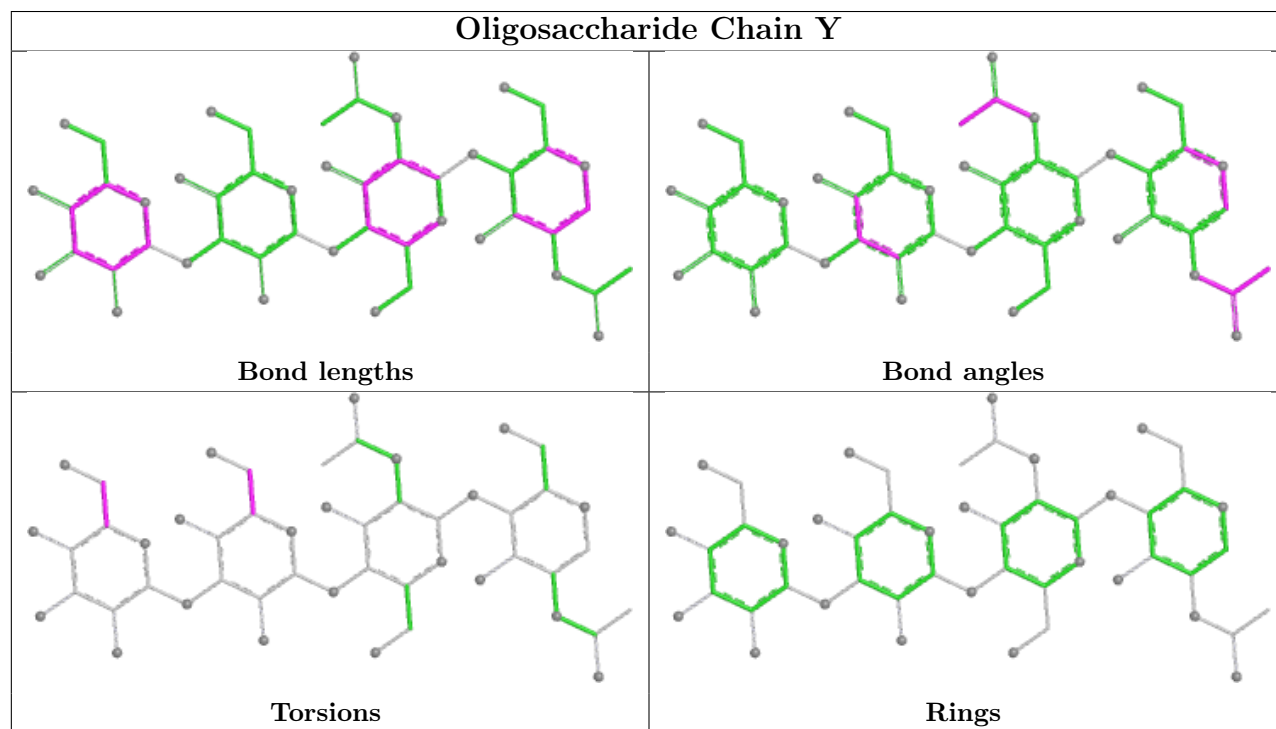
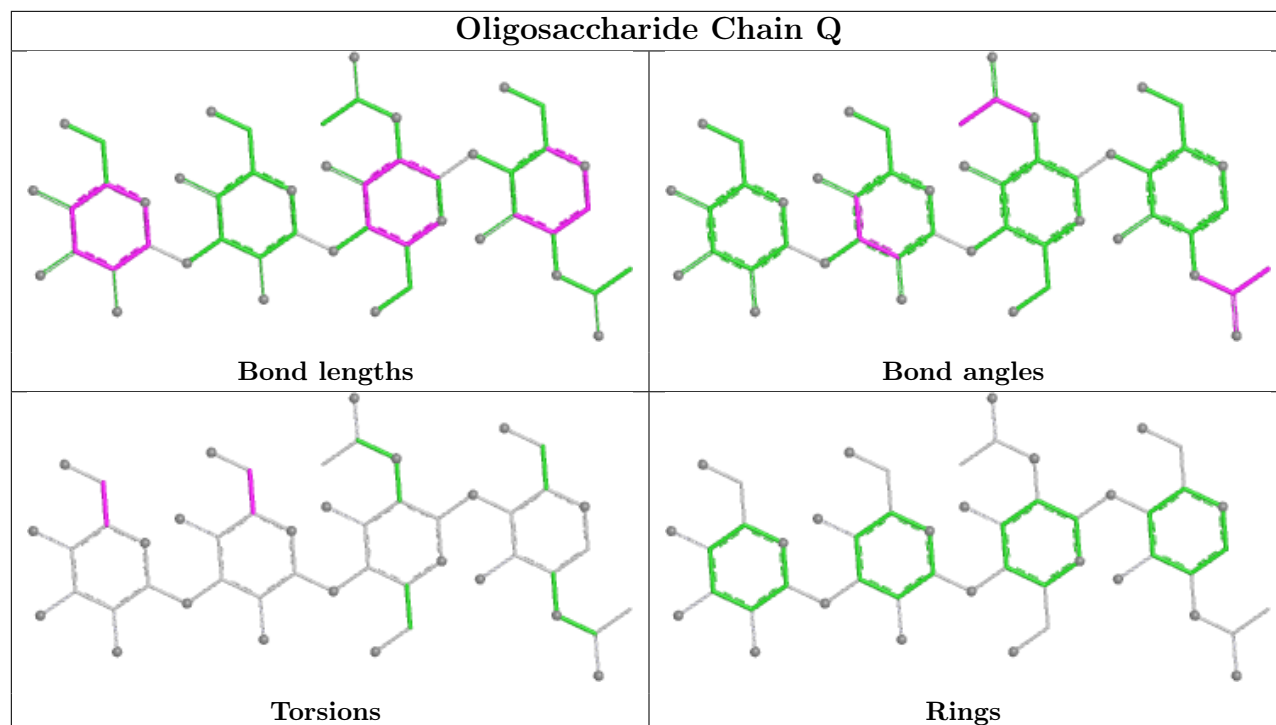


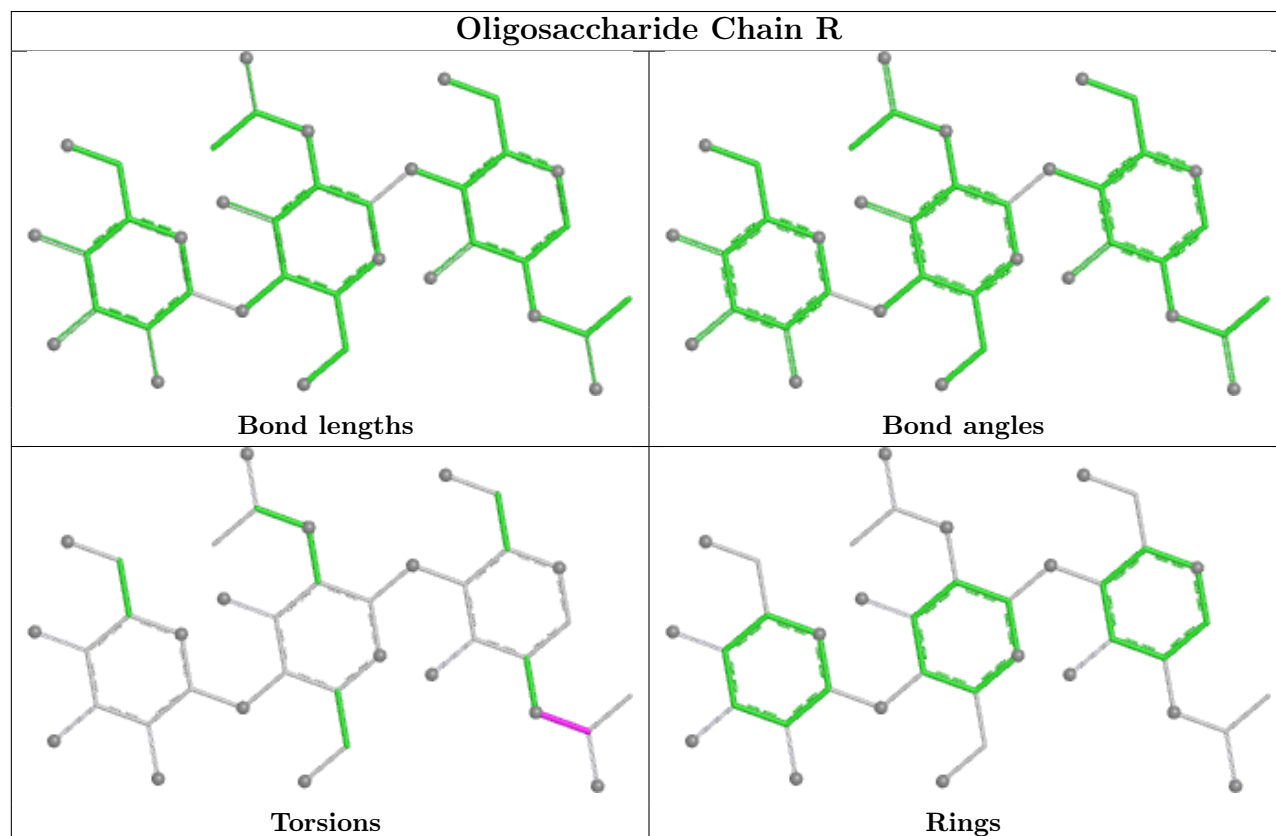
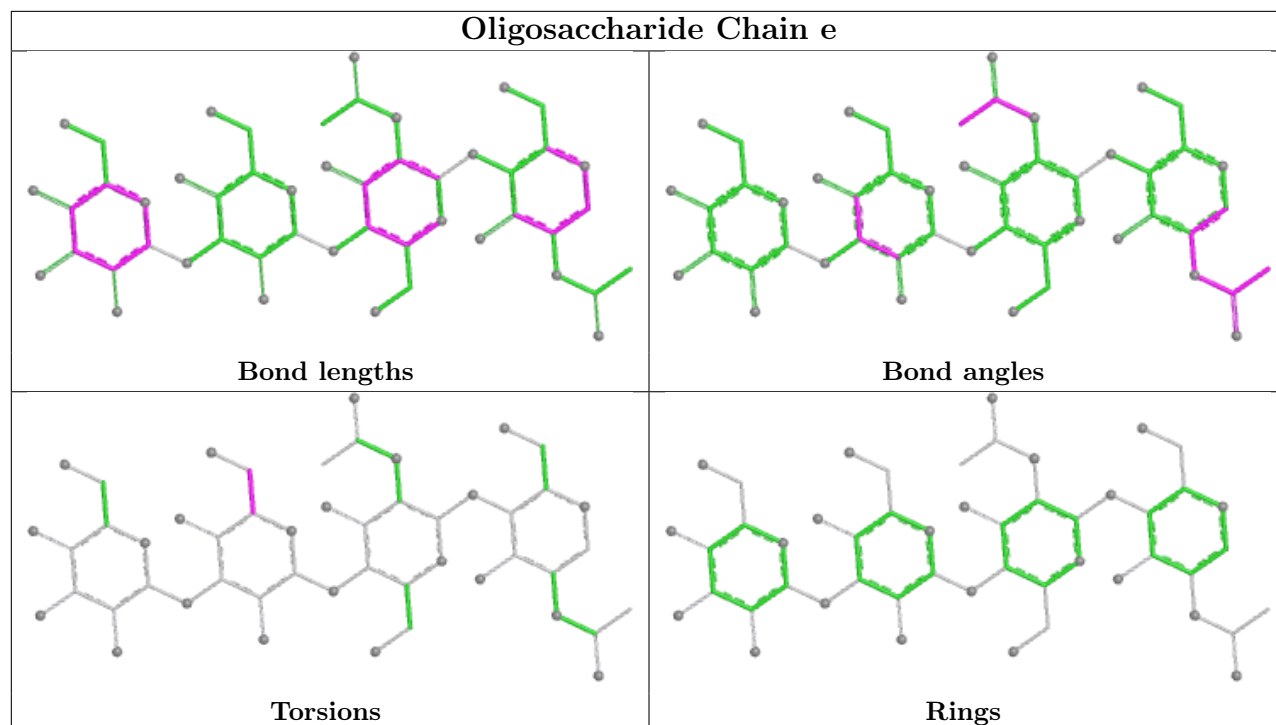


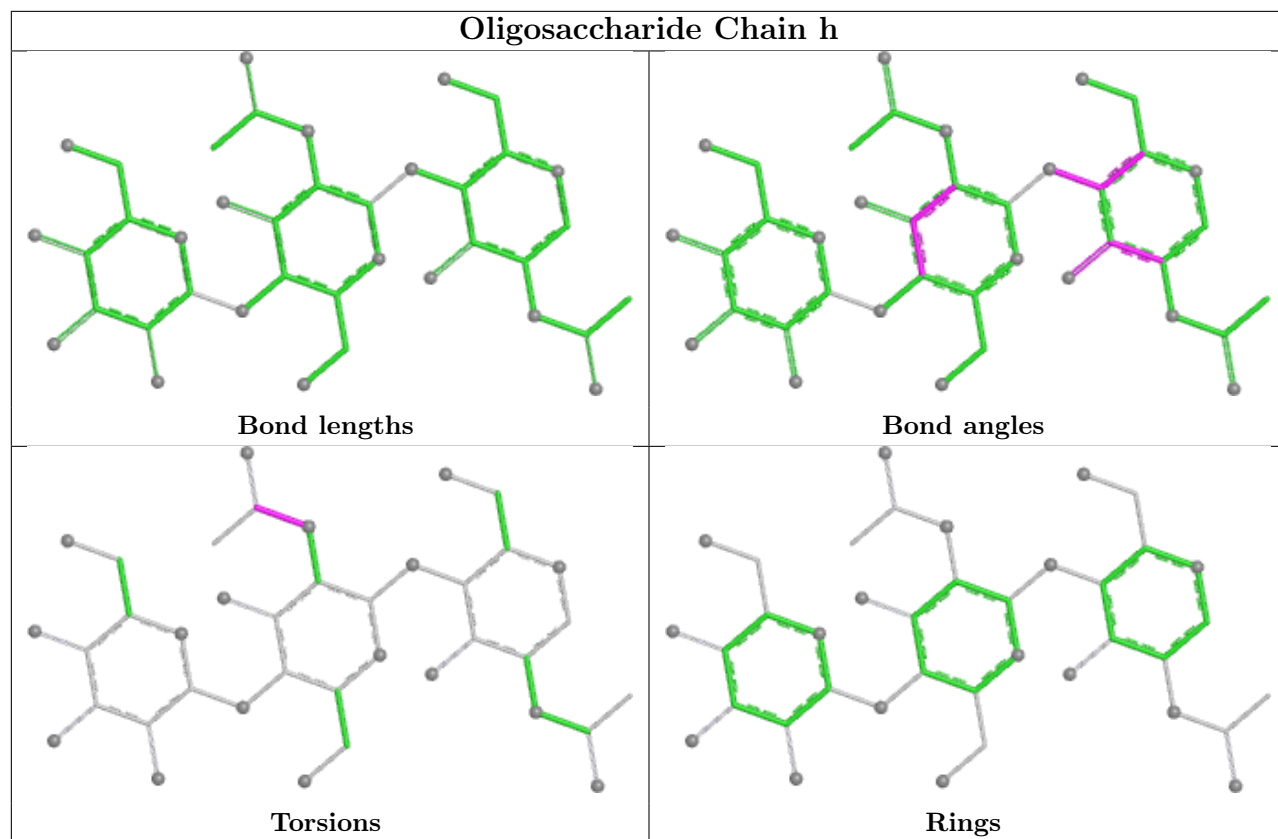


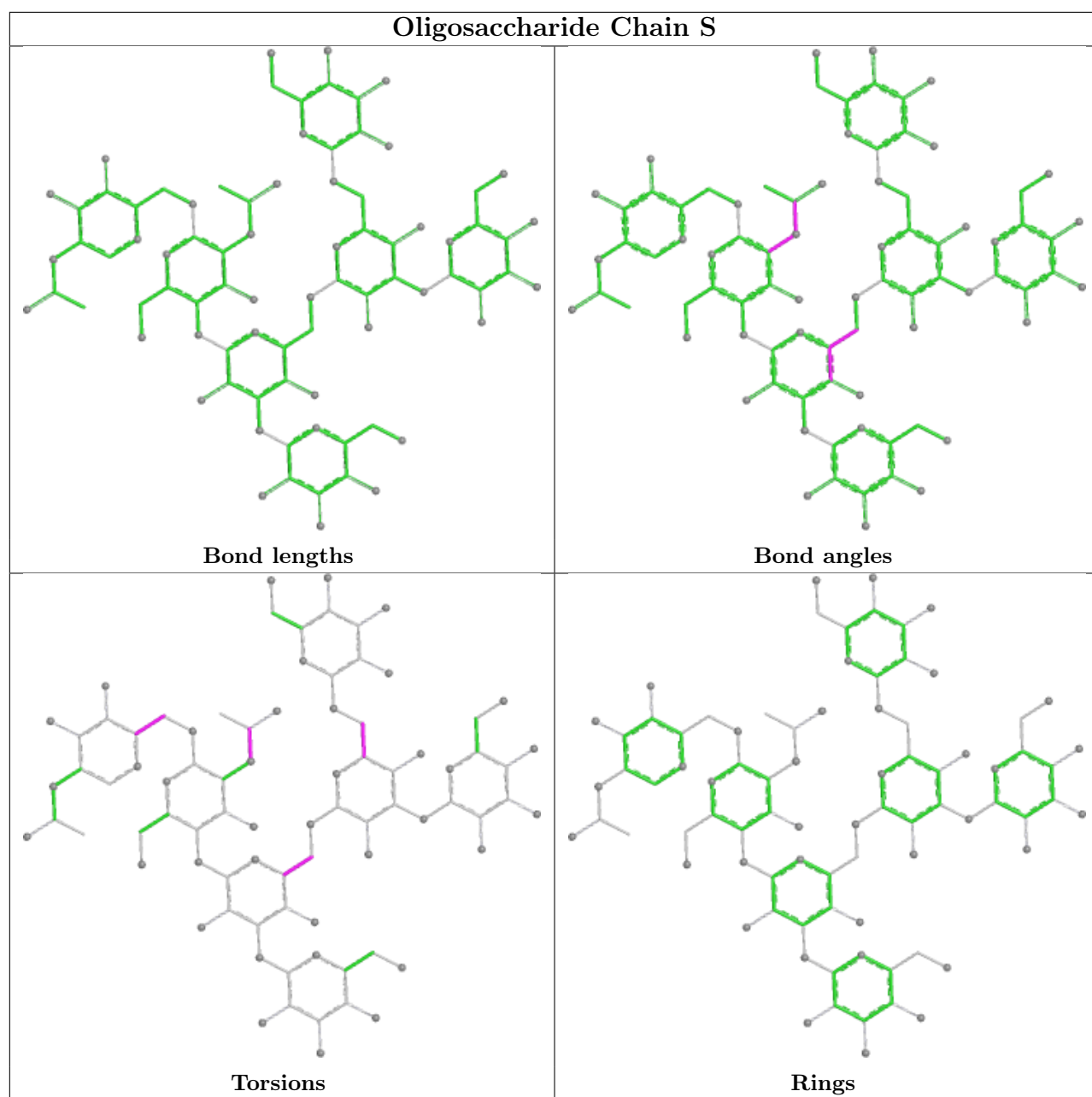


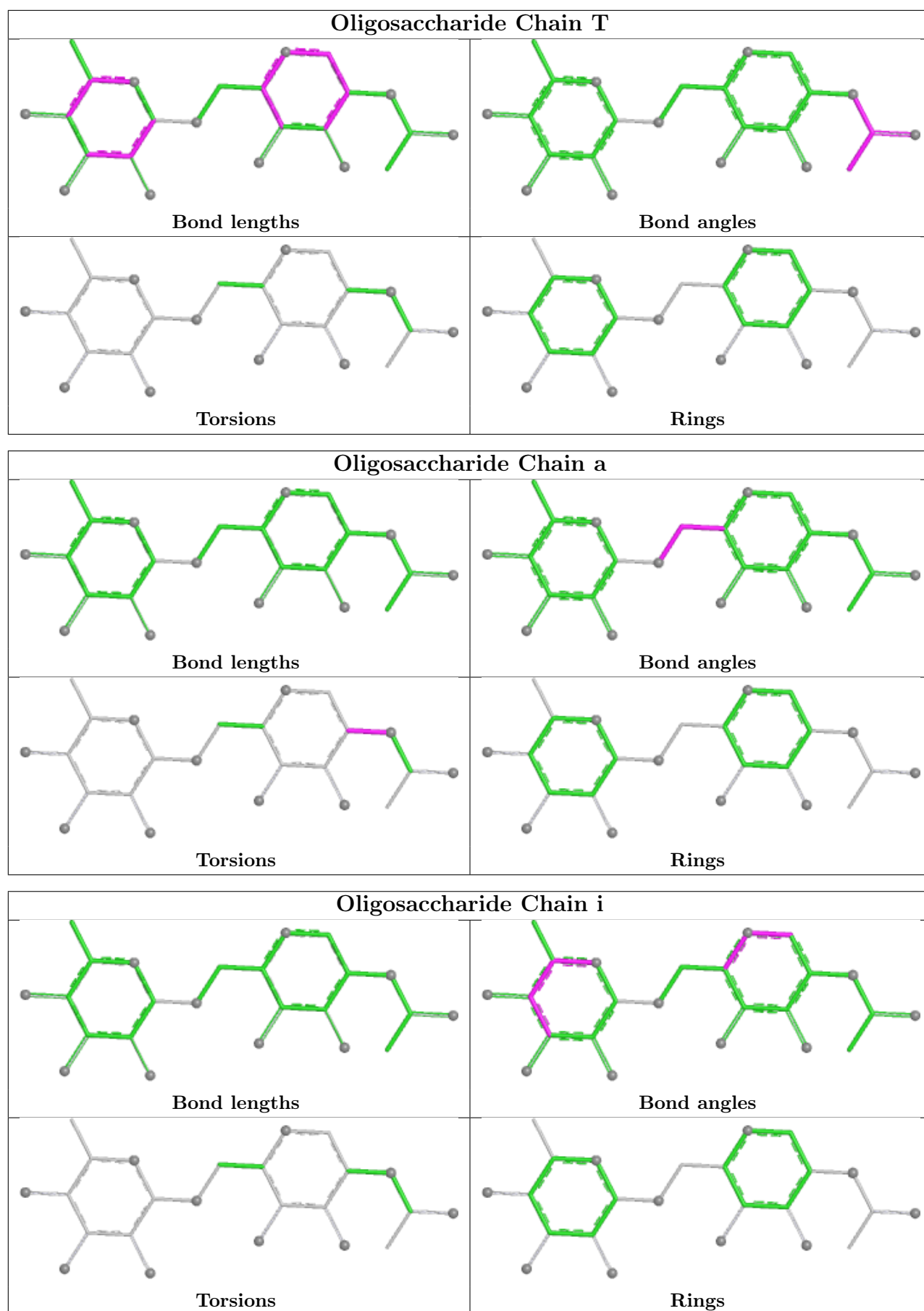


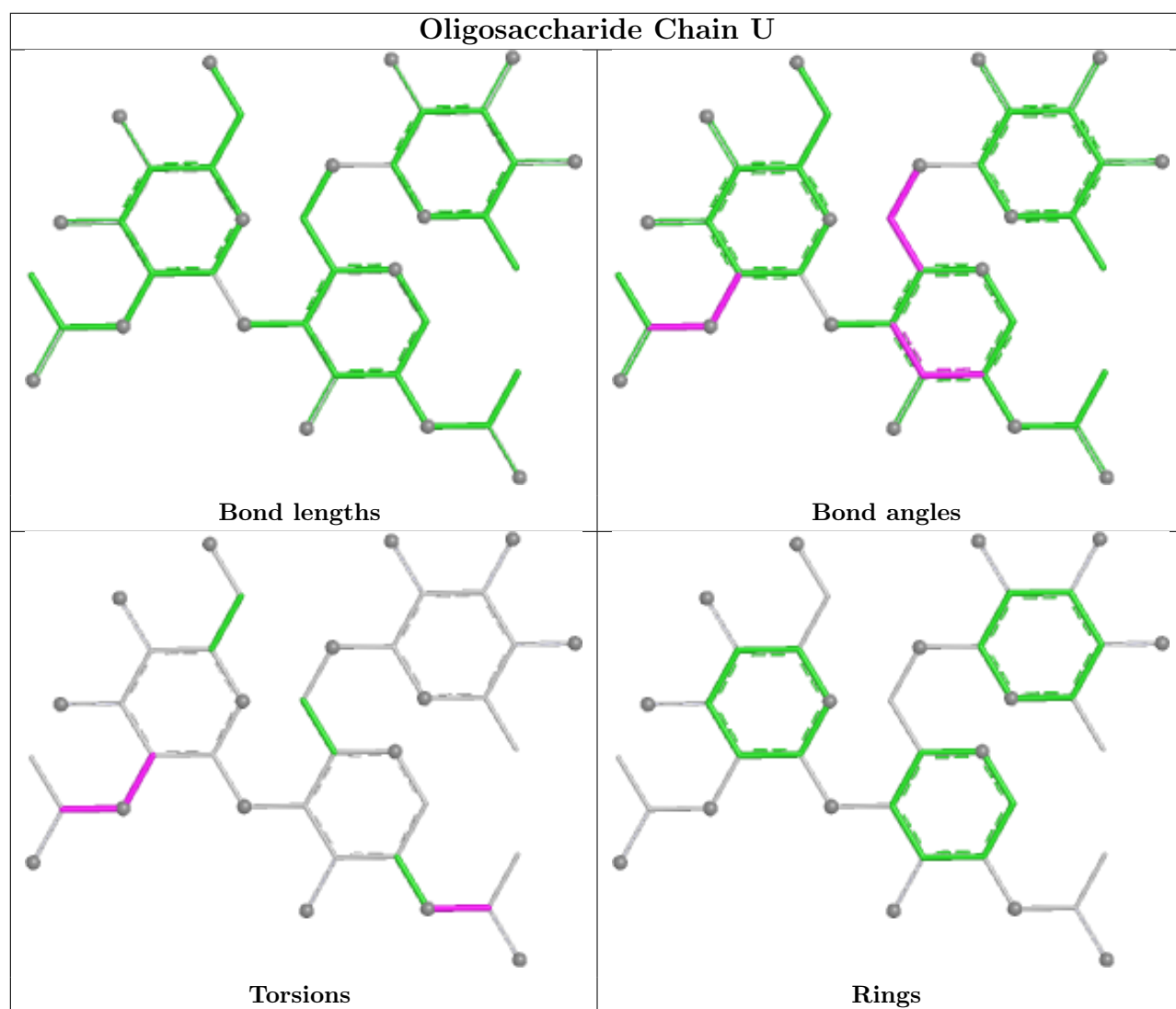


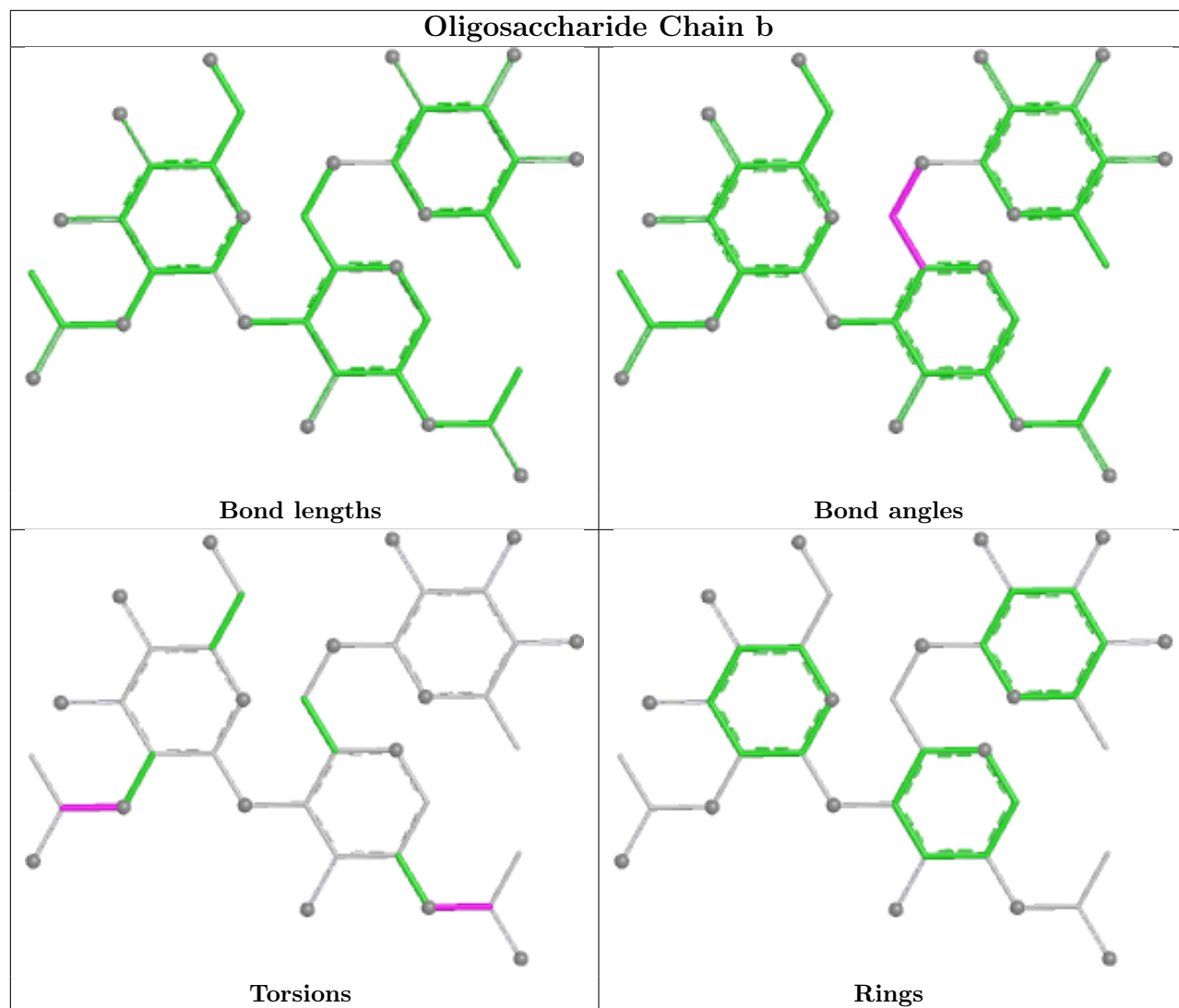


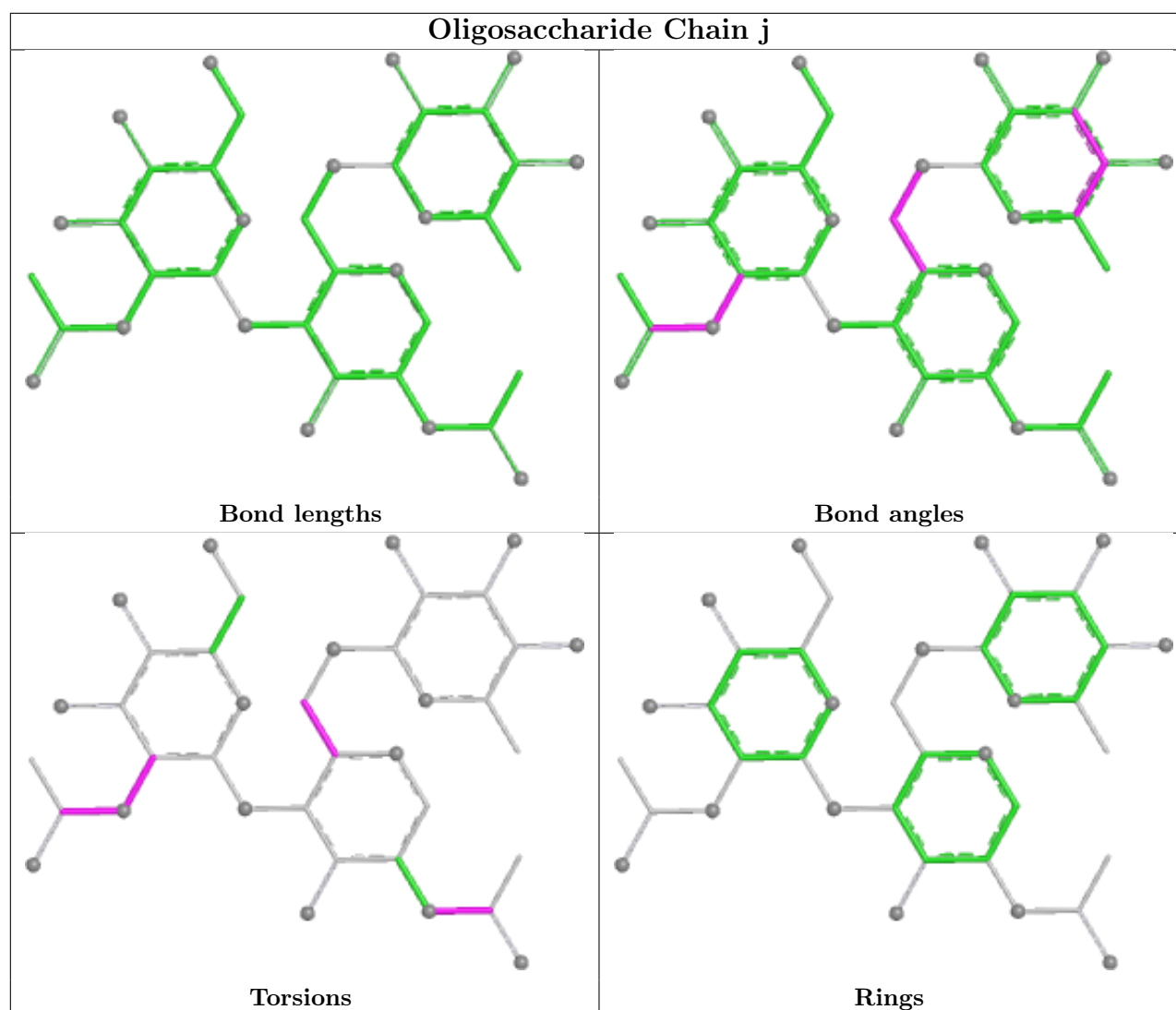












5.6 Ligand geometry [i](#)

41 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	$\# Z > 2$
13	NAG	A	606	1	14,14,15	2.23	6 (42%)	17,19,21	1.13	1 (5%)
13	NAG	D	701	2	14,14,15	0.36	0	17,19,21	0.62	0
13	NAG	A	609	1	14,14,15	2.11	5 (35%)	17,19,21	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	A	607	1	14,14,15	2.26	6 (42%)	17,19,21	0.99	2 (11%)
13	NAG	C	609	1	14,14,15	2.14	5 (35%)	17,19,21	1.01	0
13	NAG	E	611	1	14,14,15	2.15	5 (35%)	17,19,21	1.02	1 (5%)
13	NAG	E	604	1	14,14,15	2.22	6 (42%)	17,19,21	0.96	1 (5%)
13	NAG	A	601	1	14,14,15	1.94	5 (35%)	17,19,21	1.13	3 (17%)
13	NAG	B	702	2	14,14,15	0.28	0	17,19,21	0.59	0
13	NAG	E	602	1	14,14,15	2.13	6 (42%)	17,19,21	1.09	2 (11%)
13	NAG	A	603	1	14,14,15	2.21	6 (42%)	17,19,21	1.01	1 (5%)
13	NAG	E	603	1	14,14,15	2.18	7 (50%)	17,19,21	1.14	3 (17%)
13	NAG	A	611	1	14,14,15	2.05	5 (35%)	17,19,21	1.04	1 (5%)
13	NAG	E	605	1	14,14,15	2.10	5 (35%)	17,19,21	1.02	1 (5%)
13	NAG	E	607	1	14,14,15	2.23	7 (50%)	17,19,21	1.08	2 (11%)
13	NAG	C	607	1	14,14,15	2.24	6 (42%)	17,19,21	1.00	1 (5%)
13	NAG	C	612	1	14,14,15	2.20	6 (42%)	17,19,21	1.08	2 (11%)
13	NAG	B	701	2	14,14,15	0.32	0	17,19,21	0.61	0
13	NAG	E	610	1	14,14,15	2.17	5 (35%)	17,19,21	0.97	1 (5%)
13	NAG	F	701	2	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
13	NAG	C	610	1	14,14,15	2.22	5 (35%)	17,19,21	0.93	1 (5%)
13	NAG	C	601	1	14,14,15	2.01	6 (42%)	17,19,21	1.10	2 (11%)
13	NAG	C	605	1	14,14,15	2.09	5 (35%)	17,19,21	1.09	1 (5%)
13	NAG	E	601	1	14,14,15	2.05	7 (50%)	17,19,21	1.19	2 (11%)
13	NAG	A	605	1	14,14,15	2.11	5 (35%)	17,19,21	1.07	1 (5%)
13	NAG	E	608	1	14,14,15	2.15	5 (35%)	17,19,21	1.10	2 (11%)
13	NAG	A	608	1	14,14,15	2.18	5 (35%)	17,19,21	1.15	2 (11%)
13	NAG	C	604	1	14,14,15	2.23	6 (42%)	17,19,21	0.96	1 (5%)
13	NAG	C	608	1	14,14,15	2.16	5 (35%)	17,19,21	0.90	0
13	NAG	C	602	1	14,14,15	2.16	6 (42%)	17,19,21	1.20	2 (11%)
13	NAG	A	602	1	14,14,15	2.22	6 (42%)	17,19,21	1.17	2 (11%)
13	NAG	D	702	2	14,14,15	0.28	0	17,19,21	0.80	0
13	NAG	E	606	1	14,14,15	2.27	6 (42%)	17,19,21	1.06	1 (5%)
13	NAG	A	604	1	14,14,15	2.19	5 (35%)	17,19,21	0.97	1 (5%)
13	NAG	F	702	2	14,14,15	0.31	0	17,19,21	0.68	0
13	NAG	C	603	1	14,14,15	2.26	5 (35%)	17,19,21	0.99	1 (5%)
13	NAG	C	606	1	14,14,15	2.25	6 (42%)	17,19,21	1.07	1 (5%)
13	NAG	C	611	1	14,14,15	2.05	5 (35%)	17,19,21	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	E	609	1	14,14,15	2.14	4 (28%)	17,19,21	1.03	1 (5%)
13	NAG	A	610	1	14,14,15	2.16	5 (35%)	17,19,21	0.92	0
13	NAG	A	612	1	14,14,15	2.26	5 (35%)	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	606	1	-	1/6/23/26	0/1/1/1
13	NAG	D	701	2	-	3/6/23/26	0/1/1/1
13	NAG	A	609	1	-	1/6/23/26	0/1/1/1
13	NAG	A	607	1	-	2/6/23/26	0/1/1/1
13	NAG	C	609	1	-	1/6/23/26	0/1/1/1
13	NAG	E	611	1	-	0/6/23/26	0/1/1/1
13	NAG	E	604	1	-	0/6/23/26	0/1/1/1
13	NAG	A	601	1	-	0/6/23/26	0/1/1/1
13	NAG	B	702	2	-	1/6/23/26	0/1/1/1
13	NAG	E	602	1	-	1/6/23/26	0/1/1/1
13	NAG	A	603	1	-	0/6/23/26	0/1/1/1
13	NAG	E	603	1	-	0/6/23/26	0/1/1/1
13	NAG	A	611	1	-	1/6/23/26	0/1/1/1
13	NAG	E	605	1	-	1/6/23/26	0/1/1/1
13	NAG	E	607	1	-	2/6/23/26	0/1/1/1
13	NAG	C	607	1	-	2/6/23/26	0/1/1/1
13	NAG	C	612	1	-	0/6/23/26	0/1/1/1
13	NAG	B	701	2	-	3/6/23/26	0/1/1/1
13	NAG	E	610	1	-	1/6/23/26	0/1/1/1
13	NAG	F	701	2	-	2/6/23/26	0/1/1/1
13	NAG	C	610	1	-	1/6/23/26	0/1/1/1
13	NAG	C	601	1	-	0/6/23/26	0/1/1/1
13	NAG	C	605	1	-	1/6/23/26	0/1/1/1
13	NAG	E	601	1	-	0/6/23/26	0/1/1/1
13	NAG	A	605	1	-	1/6/23/26	0/1/1/1
13	NAG	E	608	1	-	0/6/23/26	0/1/1/1
13	NAG	A	608	1	-	0/6/23/26	0/1/1/1
13	NAG	C	604	1	-	0/6/23/26	0/1/1/1
13	NAG	C	608	1	-	2/6/23/26	0/1/1/1
13	NAG	C	602	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	602	1	-	1/6/23/26	0/1/1/1
13	NAG	D	702	2	-	0/6/23/26	0/1/1/1
13	NAG	E	606	1	-	1/6/23/26	0/1/1/1
13	NAG	A	604	1	-	0/6/23/26	0/1/1/1
13	NAG	F	702	2	-	2/6/23/26	0/1/1/1
13	NAG	C	603	1	-	0/6/23/26	0/1/1/1
13	NAG	C	606	1	-	0/6/23/26	0/1/1/1
13	NAG	C	611	1	-	0/6/23/26	0/1/1/1
13	NAG	E	609	1	-	1/6/23/26	0/1/1/1
13	NAG	A	610	1	-	1/6/23/26	0/1/1/1
13	NAG	A	612	1	-	0/6/23/26	0/1/1/1

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	612	NAG	C1-C2	5.85	1.60	1.52
13	C	603	NAG	C1-C2	5.84	1.60	1.52
13	C	606	NAG	C1-C2	5.78	1.60	1.52
13	C	610	NAG	C1-C2	5.76	1.60	1.52
13	A	602	NAG	C1-C2	5.75	1.60	1.52
13	E	606	NAG	C1-C2	5.73	1.60	1.52
13	A	606	NAG	C1-C2	5.69	1.60	1.52
13	A	607	NAG	C1-C2	5.66	1.60	1.52
13	E	610	NAG	C1-C2	5.64	1.60	1.52
13	E	608	NAG	C1-C2	5.63	1.60	1.52
13	A	610	NAG	C1-C2	5.62	1.60	1.52
13	A	608	NAG	C1-C2	5.61	1.60	1.52
13	C	602	NAG	C1-C2	5.60	1.60	1.52
13	A	603	NAG	C1-C2	5.59	1.60	1.52
13	C	612	NAG	C1-C2	5.57	1.59	1.52
13	E	609	NAG	C1-C2	5.51	1.59	1.52
13	C	604	NAG	C1-C2	5.49	1.59	1.52
13	C	609	NAG	C1-C2	5.47	1.59	1.52
13	E	603	NAG	C1-C2	5.47	1.59	1.52
13	E	604	NAG	C1-C2	5.46	1.59	1.52
13	A	605	NAG	C1-C2	5.43	1.59	1.52
13	E	605	NAG	C1-C2	5.43	1.59	1.52
13	C	607	NAG	C1-C2	5.40	1.59	1.52
13	C	608	NAG	C1-C2	5.38	1.59	1.52
13	A	604	NAG	C1-C2	5.34	1.59	1.52
13	E	611	NAG	C1-C2	5.32	1.59	1.52
13	E	602	NAG	C1-C2	5.29	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	607	NAG	C1-C2	5.28	1.59	1.52
13	A	609	NAG	C1-C2	5.25	1.59	1.52
13	C	605	NAG	C1-C2	5.21	1.59	1.52
13	C	611	NAG	C1-C2	4.95	1.59	1.52
13	E	601	NAG	C1-C2	4.90	1.59	1.52
13	A	611	NAG	C1-C2	4.81	1.58	1.52
13	A	601	NAG	C1-C2	4.62	1.58	1.52
13	C	601	NAG	C1-C2	4.55	1.58	1.52
13	C	607	NAG	O5-C5	3.63	1.50	1.43
13	C	608	NAG	O5-C5	3.56	1.50	1.43
13	A	604	NAG	O5-C5	3.55	1.50	1.43
13	E	607	NAG	O5-C5	3.48	1.50	1.43
13	E	604	NAG	O5-C5	3.47	1.50	1.43
13	A	607	NAG	O5-C5	3.47	1.50	1.43
13	C	604	NAG	O5-C5	3.46	1.50	1.43
13	E	611	NAG	O5-C5	3.42	1.50	1.43
13	C	601	NAG	O5-C5	3.40	1.50	1.43
13	C	610	NAG	O5-C5	3.40	1.50	1.43
13	A	612	NAG	O5-C5	3.40	1.50	1.43
13	A	611	NAG	O5-C5	3.36	1.50	1.43
13	C	606	NAG	O5-C5	3.36	1.50	1.43
13	A	608	NAG	O5-C5	3.34	1.49	1.43
13	C	609	NAG	O5-C5	3.33	1.49	1.43
13	E	606	NAG	O5-C5	3.31	1.49	1.43
13	E	609	NAG	O5-C5	3.30	1.49	1.43
13	A	609	NAG	O5-C5	3.29	1.49	1.43
13	C	612	NAG	O5-C5	3.27	1.49	1.43
13	E	610	NAG	O5-C5	3.26	1.49	1.43
13	C	603	NAG	O5-C5	3.25	1.49	1.43
13	A	610	NAG	O5-C5	3.25	1.49	1.43
13	E	608	NAG	O5-C5	3.24	1.49	1.43
13	E	602	NAG	O5-C5	3.23	1.49	1.43
13	A	603	NAG	O5-C5	3.23	1.49	1.43
13	C	611	NAG	O5-C5	3.21	1.49	1.43
13	A	606	NAG	O5-C5	3.21	1.49	1.43
13	C	605	NAG	O5-C5	3.19	1.49	1.43
13	E	601	NAG	O5-C5	3.19	1.49	1.43
13	A	601	NAG	O5-C5	3.14	1.49	1.43
13	E	603	NAG	O5-C5	3.13	1.49	1.43
13	E	605	NAG	O5-C5	3.07	1.49	1.43
13	A	602	NAG	O5-C5	3.06	1.49	1.43
13	A	605	NAG	O5-C5	3.00	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	602	NAG	O5-C5	2.97	1.49	1.43
13	C	604	NAG	O5-C1	2.85	1.48	1.43
13	C	607	NAG	O5-C1	2.84	1.48	1.43
13	A	607	NAG	O5-C1	2.83	1.48	1.43
13	E	604	NAG	O5-C1	2.82	1.48	1.43
13	A	604	NAG	O5-C1	2.80	1.48	1.43
13	E	606	NAG	O5-C1	2.72	1.48	1.43
13	E	607	NAG	O5-C1	2.72	1.48	1.43
13	A	611	NAG	O5-C1	2.71	1.48	1.43
13	A	609	NAG	O5-C1	2.68	1.48	1.43
13	C	605	NAG	O5-C1	2.67	1.48	1.43
13	C	603	NAG	O5-C1	2.67	1.48	1.43
13	A	606	NAG	O5-C1	2.65	1.48	1.43
13	C	606	NAG	O5-C1	2.64	1.48	1.43
13	C	601	NAG	O5-C1	2.63	1.48	1.43
13	C	609	NAG	O5-C1	2.63	1.48	1.43
13	A	612	NAG	O5-C1	2.62	1.48	1.43
13	E	603	NAG	O5-C1	2.61	1.48	1.43
13	C	610	NAG	O5-C1	2.61	1.48	1.43
13	E	609	NAG	O5-C1	2.60	1.48	1.43
13	C	608	NAG	O5-C1	2.60	1.48	1.43
13	C	612	NAG	O5-C1	2.59	1.48	1.43
13	A	608	NAG	O5-C1	2.57	1.48	1.43
13	A	605	NAG	O5-C1	2.56	1.48	1.43
13	C	611	NAG	O5-C1	2.56	1.48	1.43
13	A	610	NAG	O5-C1	2.55	1.48	1.43
13	A	603	NAG	O5-C1	2.53	1.47	1.43
13	E	608	NAG	O5-C1	2.53	1.47	1.43
13	E	610	NAG	O5-C1	2.52	1.47	1.43
13	C	603	NAG	C3-C2	2.51	1.57	1.52
13	E	601	NAG	O5-C1	2.51	1.47	1.43
13	E	602	NAG	O5-C1	2.50	1.47	1.43
13	A	602	NAG	O5-C1	2.50	1.47	1.43
13	E	605	NAG	O5-C1	2.48	1.47	1.43
13	E	611	NAG	O5-C1	2.47	1.47	1.43
13	C	602	NAG	O5-C1	2.45	1.47	1.43
13	C	612	NAG	C3-C2	2.41	1.57	1.52
13	A	612	NAG	C3-C2	2.40	1.57	1.52
13	E	607	NAG	C4-C5	2.38	1.58	1.53
13	C	607	NAG	C4-C5	2.38	1.58	1.53
13	A	601	NAG	O5-C1	2.38	1.47	1.43
13	C	602	NAG	C3-C2	2.36	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	610	NAG	C3-C2	2.36	1.57	1.52
13	E	611	NAG	C3-C2	2.34	1.57	1.52
13	A	603	NAG	C4-C5	2.34	1.58	1.53
13	E	606	NAG	C2-N2	2.34	1.50	1.46
13	E	602	NAG	C3-C2	2.33	1.57	1.52
13	A	603	NAG	C3-C2	2.33	1.57	1.52
13	E	610	NAG	C3-C2	2.33	1.57	1.52
13	A	607	NAG	C4-C5	2.32	1.58	1.53
13	A	602	NAG	C3-C2	2.31	1.57	1.52
13	C	604	NAG	C4-C5	2.31	1.58	1.53
13	A	610	NAG	C3-C2	2.31	1.57	1.52
13	E	606	NAG	C3-C2	2.30	1.57	1.52
13	A	602	NAG	C2-N2	2.30	1.50	1.46
13	E	607	NAG	C3-C2	2.30	1.57	1.52
13	E	604	NAG	C3-C2	2.28	1.57	1.52
13	E	604	NAG	C4-C5	2.27	1.57	1.53
13	C	604	NAG	C3-C2	2.27	1.57	1.52
13	E	602	NAG	C4-C5	2.27	1.57	1.53
13	E	603	NAG	C4-C5	2.27	1.57	1.53
13	A	607	NAG	C3-C2	2.26	1.57	1.52
13	E	607	NAG	C2-N2	2.26	1.50	1.46
13	A	608	NAG	C3-C2	2.25	1.57	1.52
13	C	606	NAG	C3-C2	2.25	1.57	1.52
13	A	604	NAG	C3-C2	2.24	1.57	1.52
13	A	606	NAG	C4-C5	2.24	1.57	1.53
13	A	604	NAG	C4-C5	2.24	1.57	1.53
13	E	608	NAG	C4-C5	2.23	1.57	1.53
13	E	606	NAG	C4-C5	2.23	1.57	1.53
13	E	609	NAG	C4-C5	2.23	1.57	1.53
13	A	609	NAG	C4-C5	2.22	1.57	1.53
13	A	611	NAG	C3-C2	2.22	1.57	1.52
13	A	606	NAG	C3-C2	2.21	1.57	1.52
13	C	601	NAG	C3-C2	2.21	1.57	1.52
13	A	605	NAG	C3-C2	2.20	1.57	1.52
13	C	608	NAG	C4-C5	2.20	1.57	1.53
13	E	605	NAG	C3-C2	2.19	1.57	1.52
13	C	603	NAG	C4-C5	2.19	1.57	1.53
13	A	601	NAG	C4-C5	2.19	1.57	1.53
13	A	606	NAG	C2-N2	2.18	1.49	1.46
13	C	606	NAG	C2-N2	2.17	1.49	1.46
13	A	612	NAG	C4-C5	2.17	1.57	1.53
13	C	611	NAG	C3-C2	2.16	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	605	NAG	C4-C5	2.16	1.57	1.53
13	E	601	NAG	C4-C5	2.16	1.57	1.53
13	A	608	NAG	C4-C5	2.16	1.57	1.53
13	C	607	NAG	C3-C2	2.16	1.57	1.52
13	A	602	NAG	C4-C5	2.15	1.57	1.53
13	E	603	NAG	C3-C2	2.15	1.57	1.52
13	C	610	NAG	C4-C5	2.15	1.57	1.53
13	E	603	NAG	C2-N2	2.14	1.49	1.46
13	A	611	NAG	C4-C5	2.13	1.57	1.53
13	A	610	NAG	C4-C5	2.13	1.57	1.53
13	C	609	NAG	C4-C5	2.13	1.57	1.53
13	C	602	NAG	C4-C5	2.13	1.57	1.53
13	C	608	NAG	C3-C2	2.12	1.57	1.52
13	C	607	NAG	C2-N2	2.12	1.49	1.46
13	C	605	NAG	C3-C2	2.12	1.57	1.52
13	C	609	NAG	C3-C2	2.12	1.57	1.52
13	E	607	NAG	C4-C3	2.12	1.57	1.52
13	C	602	NAG	C2-N2	2.12	1.49	1.46
13	A	609	NAG	C3-C2	2.11	1.56	1.52
13	A	605	NAG	C4-C5	2.11	1.57	1.53
13	C	612	NAG	C4-C5	2.10	1.57	1.53
13	C	611	NAG	C4-C5	2.09	1.57	1.53
13	E	610	NAG	C4-C5	2.09	1.57	1.53
13	E	601	NAG	C3-C2	2.08	1.56	1.52
13	C	606	NAG	C4-C5	2.08	1.57	1.53
13	E	608	NAG	C3-C2	2.07	1.56	1.52
13	C	601	NAG	C4-C5	2.07	1.57	1.53
13	E	601	NAG	C2-N2	2.07	1.49	1.46
13	E	611	NAG	C4-C5	2.06	1.57	1.53
13	E	605	NAG	C4-C5	2.05	1.57	1.53
13	E	603	NAG	C4-C3	2.04	1.57	1.52
13	C	601	NAG	C4-C3	2.03	1.57	1.52
13	A	601	NAG	C3-C2	2.03	1.56	1.52
13	E	601	NAG	C4-C3	2.03	1.57	1.52
13	E	602	NAG	C2-N2	2.03	1.49	1.46
13	A	603	NAG	C4-C3	2.02	1.57	1.52
13	A	607	NAG	C2-N2	2.01	1.49	1.46
13	C	612	NAG	C2-N2	2.01	1.49	1.46
13	E	604	NAG	C2-N2	2.01	1.49	1.46
13	C	604	NAG	C2-N2	2.00	1.49	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	602	NAG	C8-C7-N2	3.27	121.53	116.12
13	A	602	NAG	C8-C7-N2	3.17	121.37	116.12
13	E	601	NAG	C8-C7-N2	3.05	121.18	116.12
13	E	602	NAG	C8-C7-N2	2.95	121.01	116.12
13	F	701	NAG	C1-O5-C5	2.84	115.99	112.19
13	E	607	NAG	C8-C7-N2	2.78	120.74	116.12
13	C	612	NAG	C8-C7-N2	2.73	120.65	116.12
13	C	611	NAG	C8-C7-N2	2.72	120.62	116.12
13	C	601	NAG	C8-C7-N2	2.67	120.55	116.12
13	A	606	NAG	C8-C7-N2	2.63	120.48	116.12
13	A	602	NAG	O7-C7-C8	-2.60	117.43	122.05
13	C	606	NAG	C8-C7-N2	2.58	120.39	116.12
13	C	607	NAG	C8-C7-N2	2.52	120.30	116.12
13	E	601	NAG	O7-C7-C8	-2.52	117.58	122.05
13	E	606	NAG	C8-C7-N2	2.50	120.27	116.12
13	A	608	NAG	C1-C2-N2	-2.49	106.51	110.43
13	A	607	NAG	C8-C7-N2	2.48	120.23	116.12
13	A	601	NAG	C1-C2-N2	-2.47	106.55	110.43
13	A	608	NAG	C8-C7-N2	2.43	120.15	116.12
13	E	608	NAG	C1-C2-N2	-2.43	106.61	110.43
13	A	601	NAG	C8-C7-N2	2.41	120.12	116.12
13	C	602	NAG	O7-C7-C8	-2.40	117.78	122.05
13	E	603	NAG	C8-C7-N2	2.36	120.03	116.12
13	A	611	NAG	C1-C2-N2	-2.27	106.85	110.43
13	C	604	NAG	C8-C7-N2	2.23	119.82	116.12
13	E	603	NAG	O7-C7-C8	-2.23	118.09	122.05
13	A	603	NAG	C8-C7-N2	2.23	119.81	116.12
13	E	608	NAG	C8-C7-N2	2.21	119.78	116.12
13	A	605	NAG	C8-C7-N2	2.21	119.78	116.12
13	C	612	NAG	O7-C7-C8	-2.20	118.13	122.05
13	E	611	NAG	C8-C7-N2	2.20	119.76	116.12
13	A	604	NAG	C8-C7-N2	2.20	119.76	116.12
13	C	611	NAG	O7-C7-C8	-2.18	118.17	122.05
13	E	604	NAG	C8-C7-N2	2.16	119.70	116.12
13	E	603	NAG	C1-C2-N2	-2.15	107.04	110.43
13	C	603	NAG	C8-C7-N2	2.14	119.66	116.12
13	A	601	NAG	O7-C7-C8	-2.13	118.25	122.05
13	C	605	NAG	C8-C7-N2	2.13	119.66	116.12
13	E	609	NAG	C1-C2-N2	-2.12	107.09	110.43
13	E	607	NAG	O7-C7-C8	-2.11	118.29	122.05
13	A	612	NAG	C8-C7-N2	2.09	119.59	116.12
13	E	605	NAG	C8-C7-N2	2.07	119.55	116.12
13	C	601	NAG	O7-C7-C8	-2.05	118.40	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	602	NAG	O7-C7-C8	-2.05	118.41	122.05
13	E	610	NAG	C8-C7-N2	2.03	119.49	116.12
13	A	607	NAG	O7-C7-C8	-2.02	118.46	122.05
13	C	610	NAG	C8-C7-N2	2.02	119.46	116.12

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	701	NAG	C8-C7-N2-C2
13	B	701	NAG	O7-C7-N2-C2
13	F	701	NAG	C8-C7-N2-C2
13	F	701	NAG	O7-C7-N2-C2
13	E	607	NAG	O5-C5-C6-O6
13	A	607	NAG	O5-C5-C6-O6
13	C	608	NAG	O5-C5-C6-O6
13	C	607	NAG	O5-C5-C6-O6
13	D	701	NAG	C8-C7-N2-C2
13	A	602	NAG	O5-C5-C6-O6
13	C	610	NAG	O5-C5-C6-O6
13	C	609	NAG	O5-C5-C6-O6
13	E	609	NAG	O5-C5-C6-O6
13	E	610	NAG	O5-C5-C6-O6
13	F	702	NAG	C8-C7-N2-C2
13	A	610	NAG	O5-C5-C6-O6
13	A	605	NAG	O5-C5-C6-O6
13	E	605	NAG	O5-C5-C6-O6
13	A	609	NAG	O5-C5-C6-O6
13	A	611	NAG	O5-C5-C6-O6
13	C	602	NAG	O5-C5-C6-O6
13	E	606	NAG	O5-C5-C6-O6
13	E	602	NAG	O5-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	C	605	NAG	O5-C5-C6-O6
13	A	606	NAG	O5-C5-C6-O6
13	B	701	NAG	O5-C5-C6-O6
13	D	701	NAG	O7-C7-N2-C2
13	F	702	NAG	O7-C7-N2-C2
13	E	607	NAG	C4-C5-C6-O6
13	D	701	NAG	C1-C2-N2-C7
13	A	607	NAG	C4-C5-C6-O6
13	C	607	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	C	608	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	611	NAG	1	0
13	C	611	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	151:ARG	C	152:GLY	N	4.22

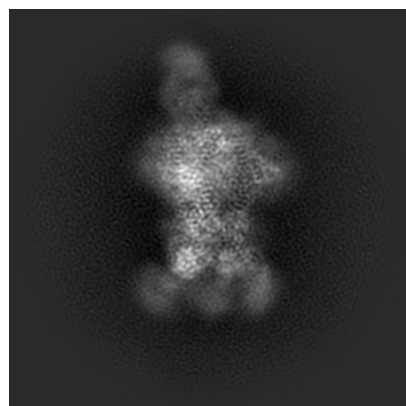
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25755. These allow visual inspection of the internal detail of the map and identification of artifacts.

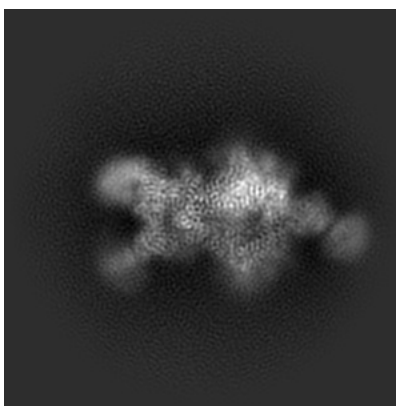
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

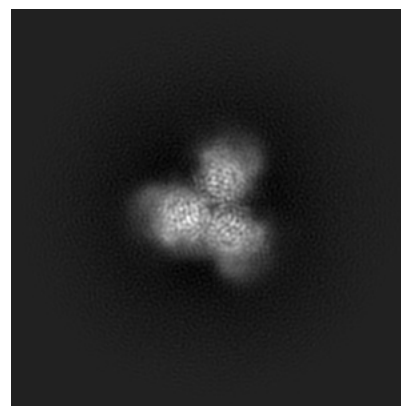
6.1.1 Primary map



X

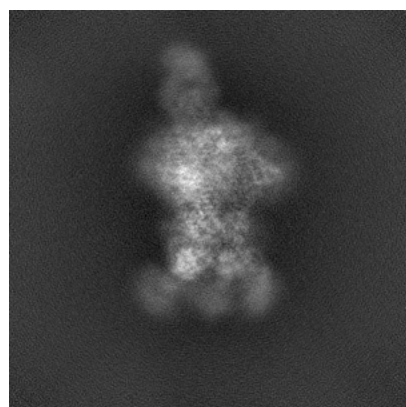


Y

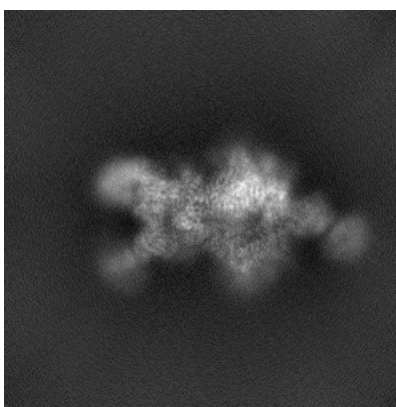


Z

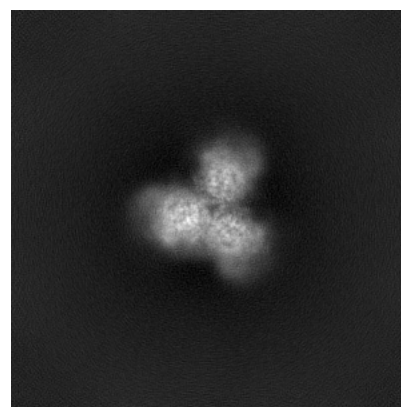
6.1.2 Raw map



X



Y

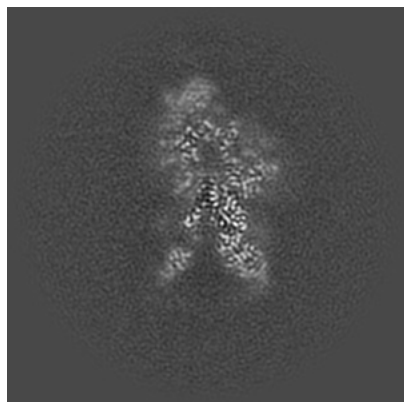


Z

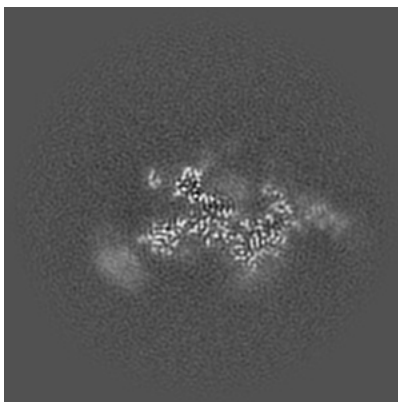
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

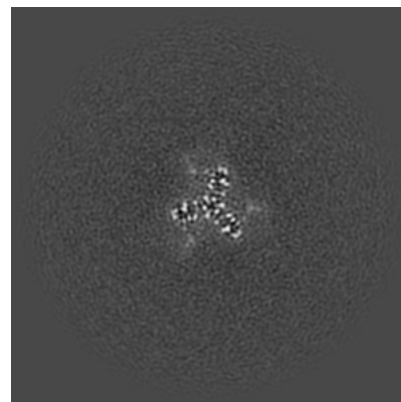
6.2.1 Primary map



X Index: 150

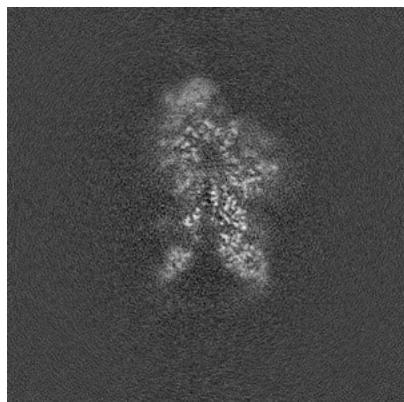


Y Index: 150

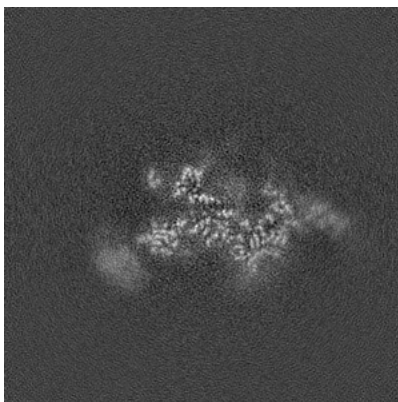


Z Index: 150

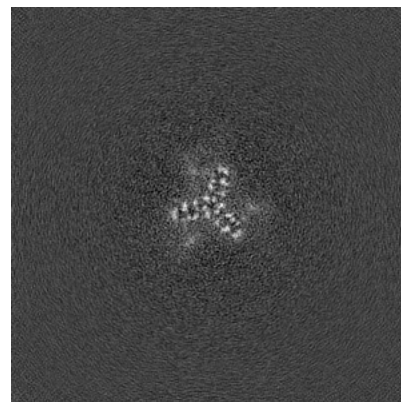
6.2.2 Raw map



X Index: 150



Y Index: 150

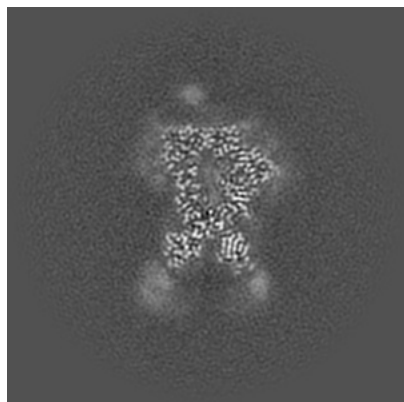


Z Index: 150

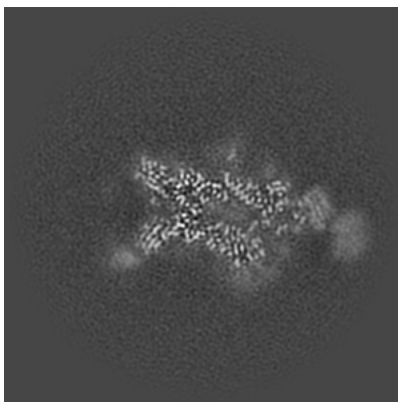
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

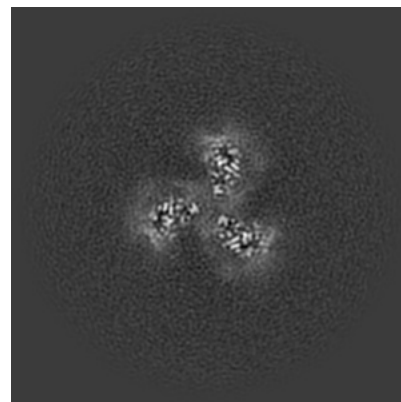
6.3.1 Primary map



X Index: 160

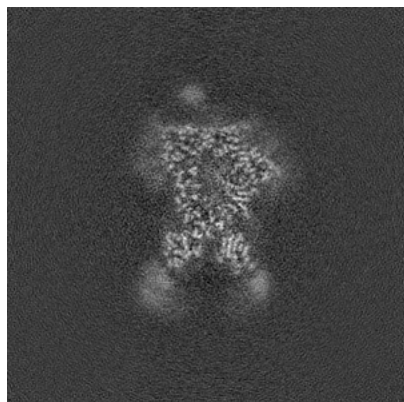


Y Index: 139

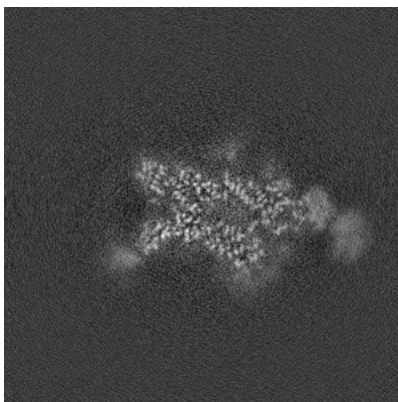


Z Index: 178

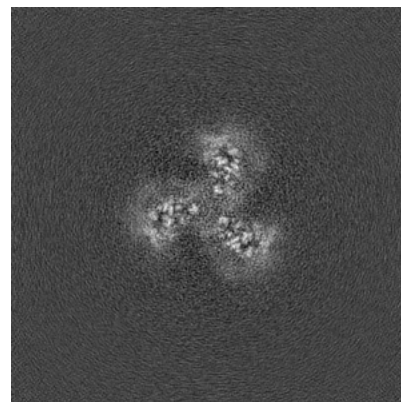
6.3.2 Raw map



X Index: 160



Y Index: 140

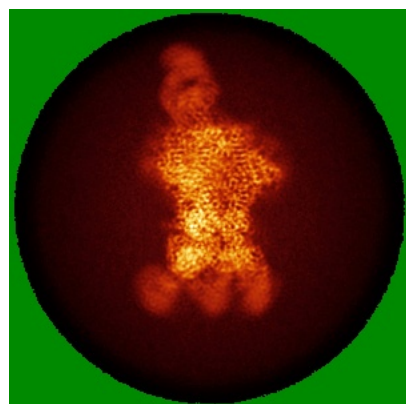


Z Index: 178

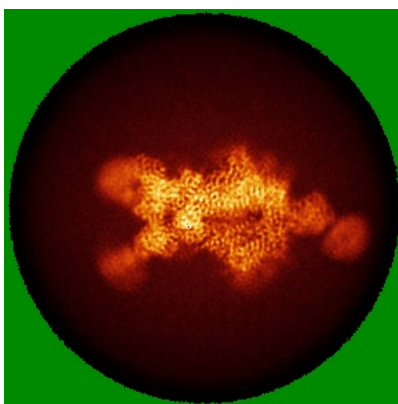
The images above show the largest variance slices of the map in three orthogonal directions.

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

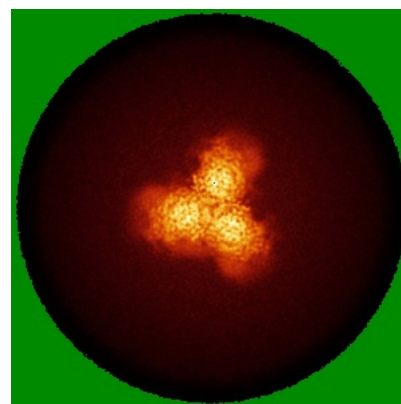
6.4.1 Primary map



X

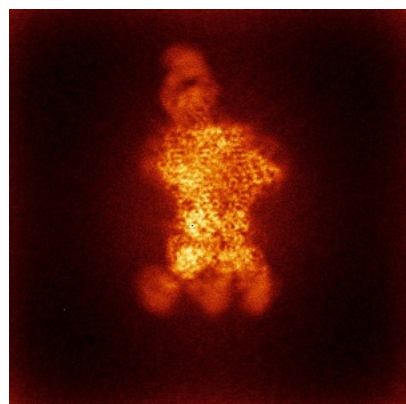


Y

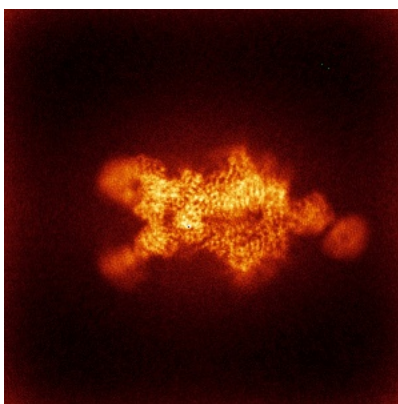


Z

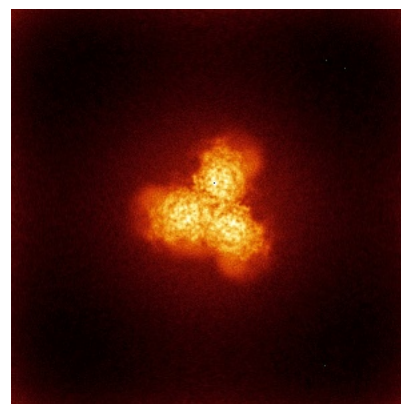
6.4.2 Raw map



X



Y

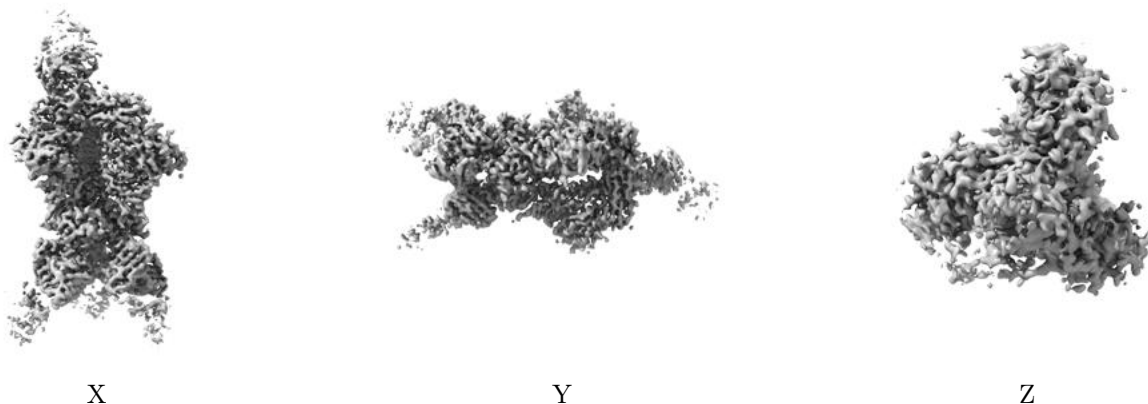


Z

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.

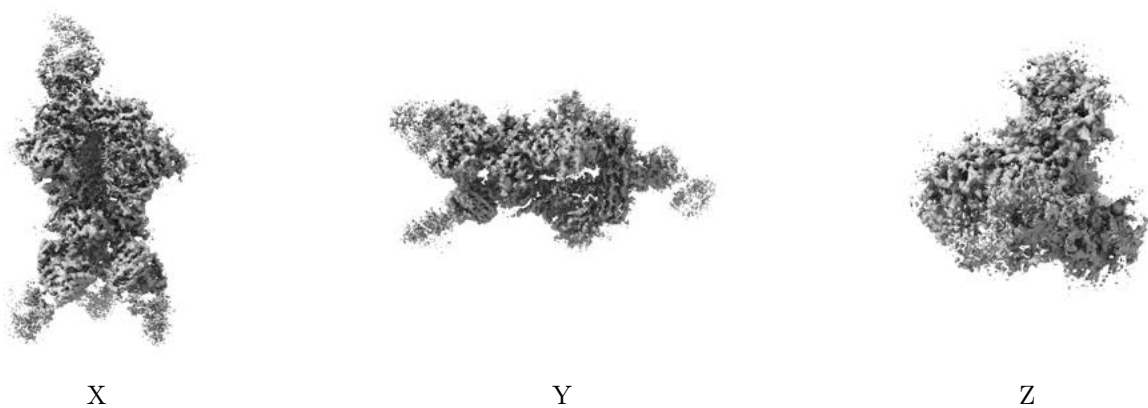
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.293. 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.

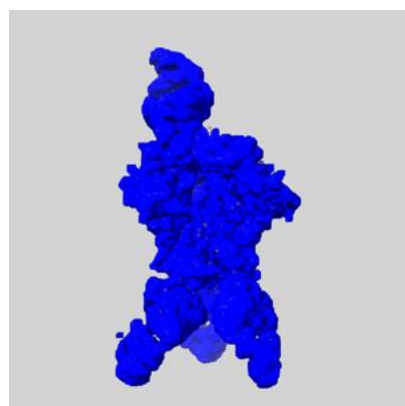
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

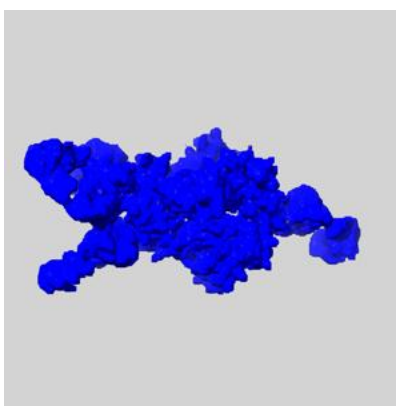
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

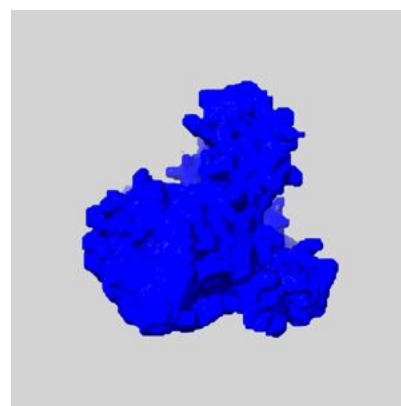
6.6.1 emd_25755_msk_1.map [i](#)



X



Y

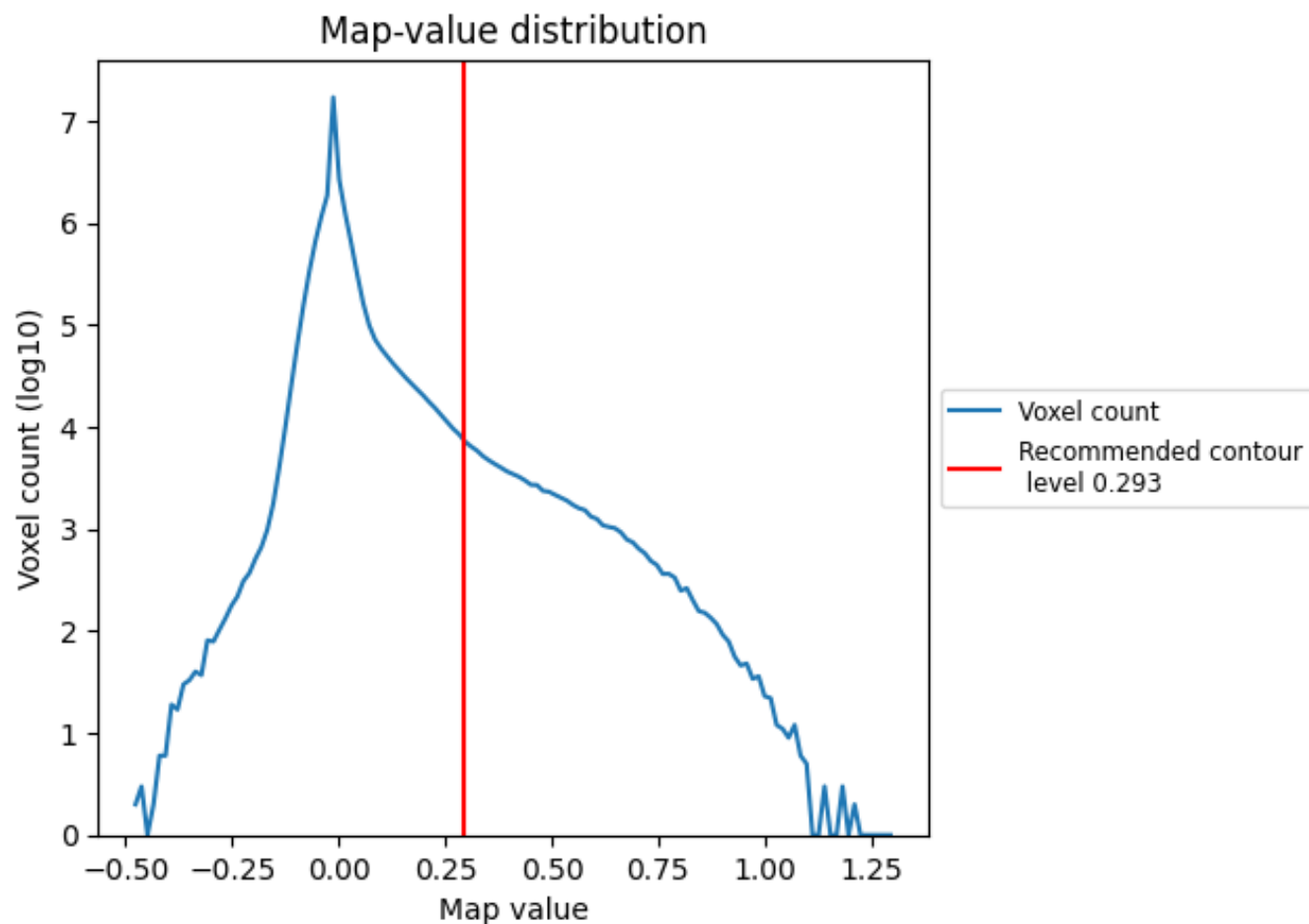


Z

7 Map analysis [i](#)

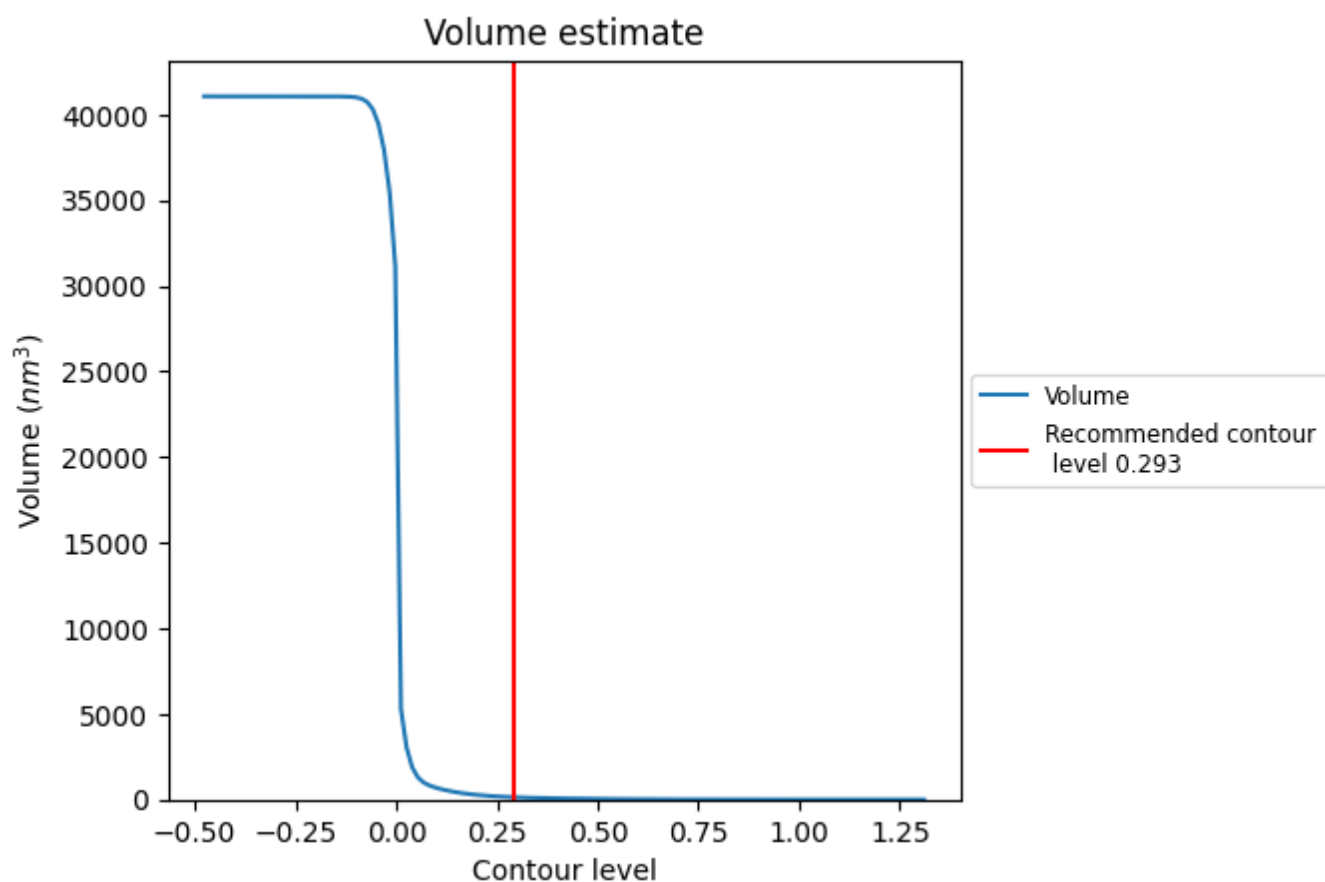
This section contains the results of statistical analysis of the map.

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.

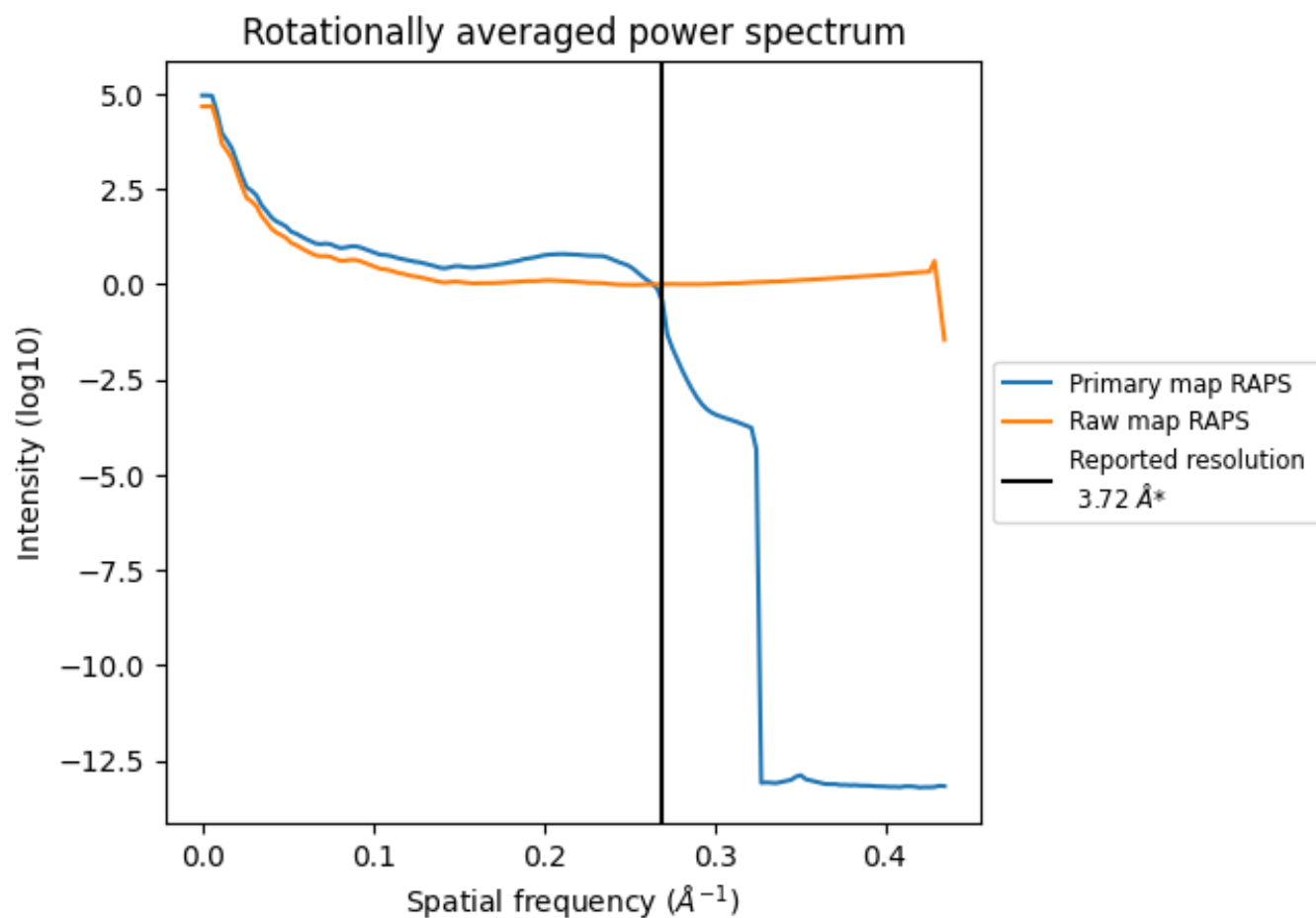
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm^3 ; this corresponds to an approximate mass of 121 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 ⓘ

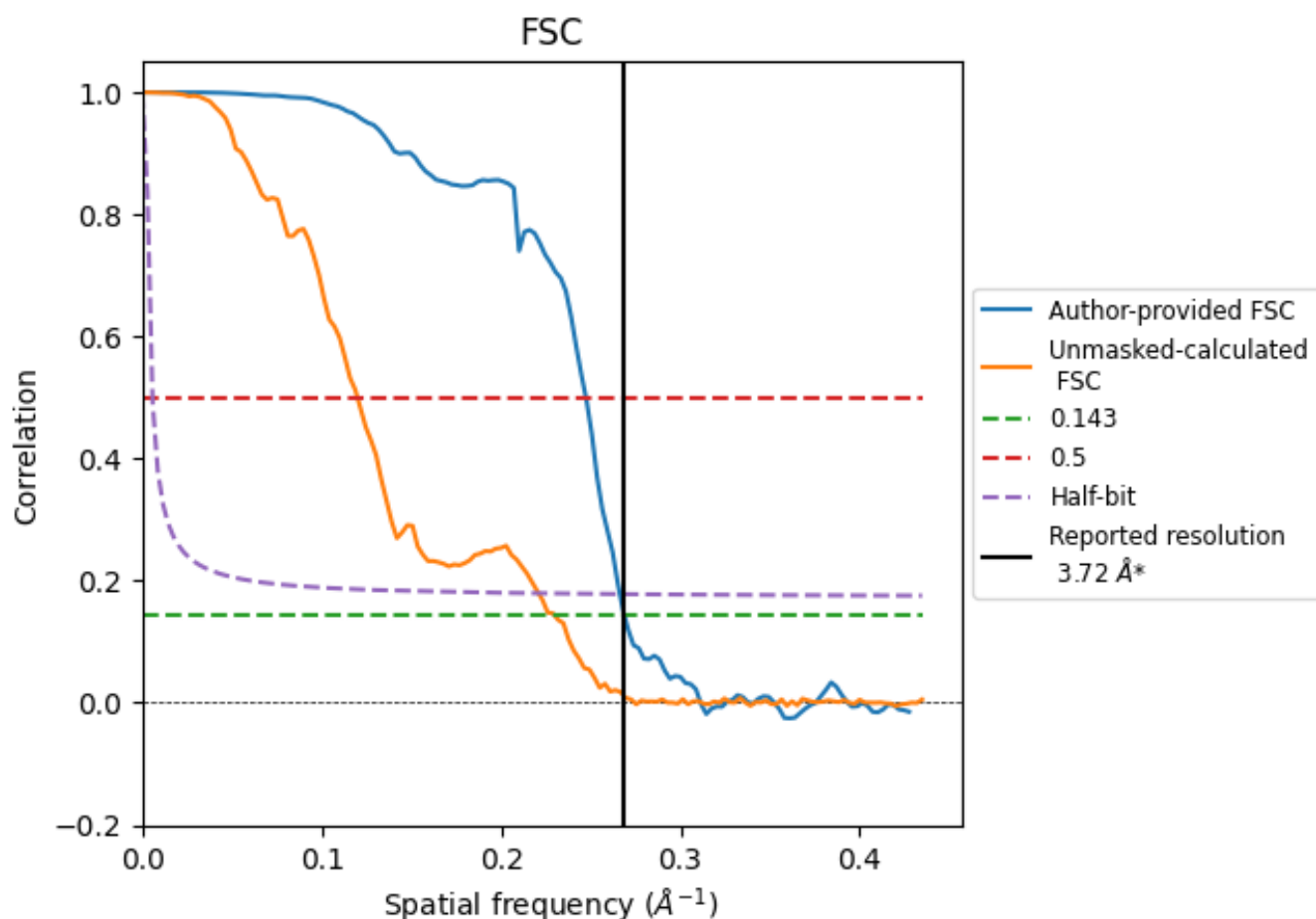


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

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 0.269 Å⁻¹

8.2 Resolution estimates [i](#)

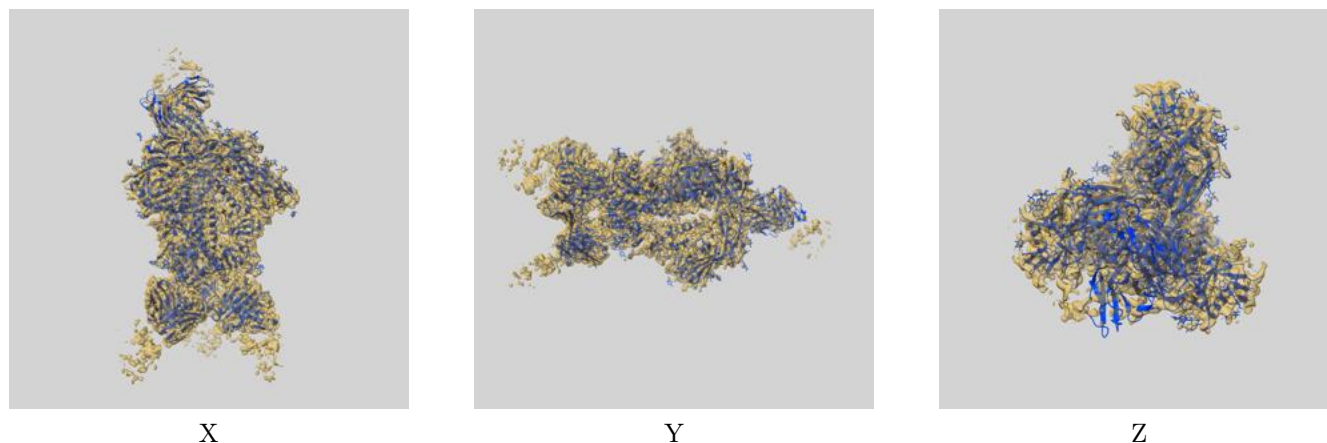
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.72	4.04	3.76
Unmasked-calculated*	4.35	8.33	4.52

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

9 Map-model fit [i](#)

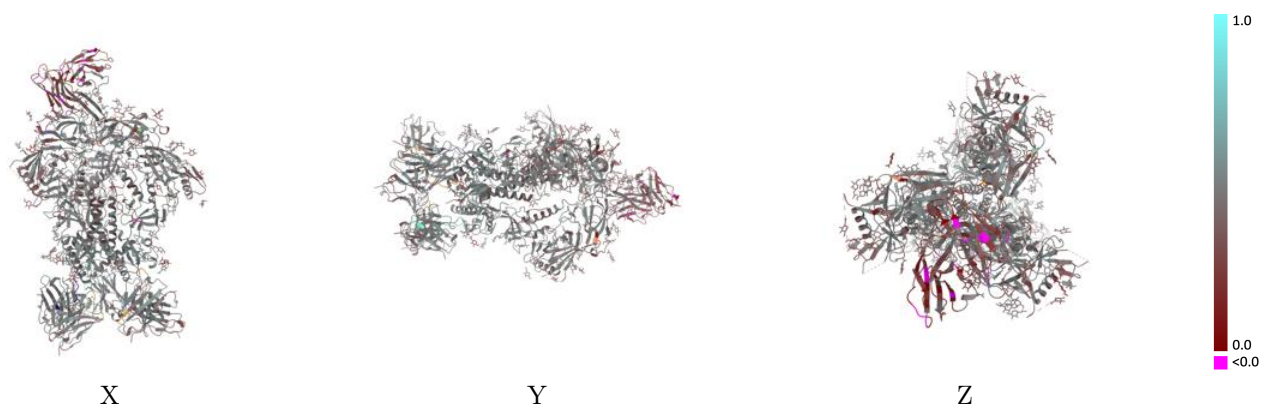
This section contains information regarding the fit between EMDB map EMD-25755 and PDB model 7T9B. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



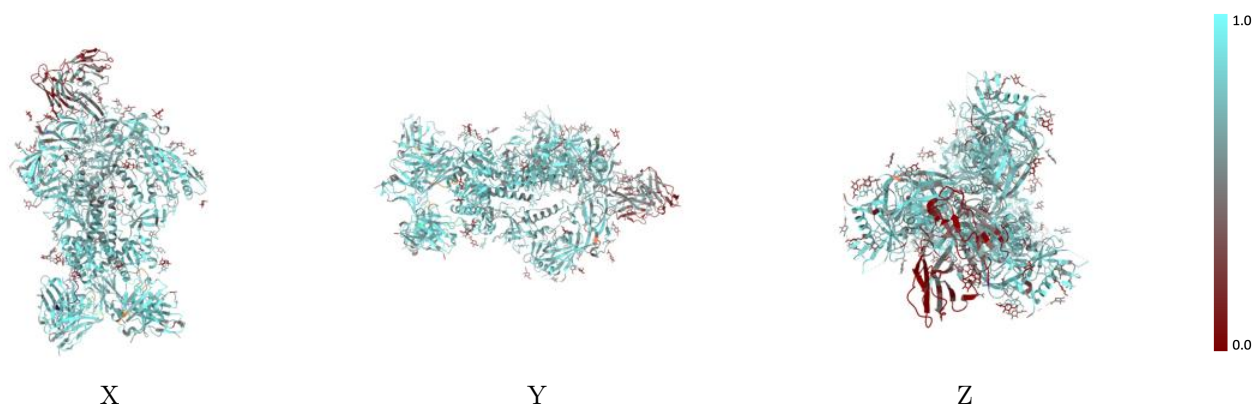
The images above show the 3D surface view of the map at the recommended contour level 0.293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



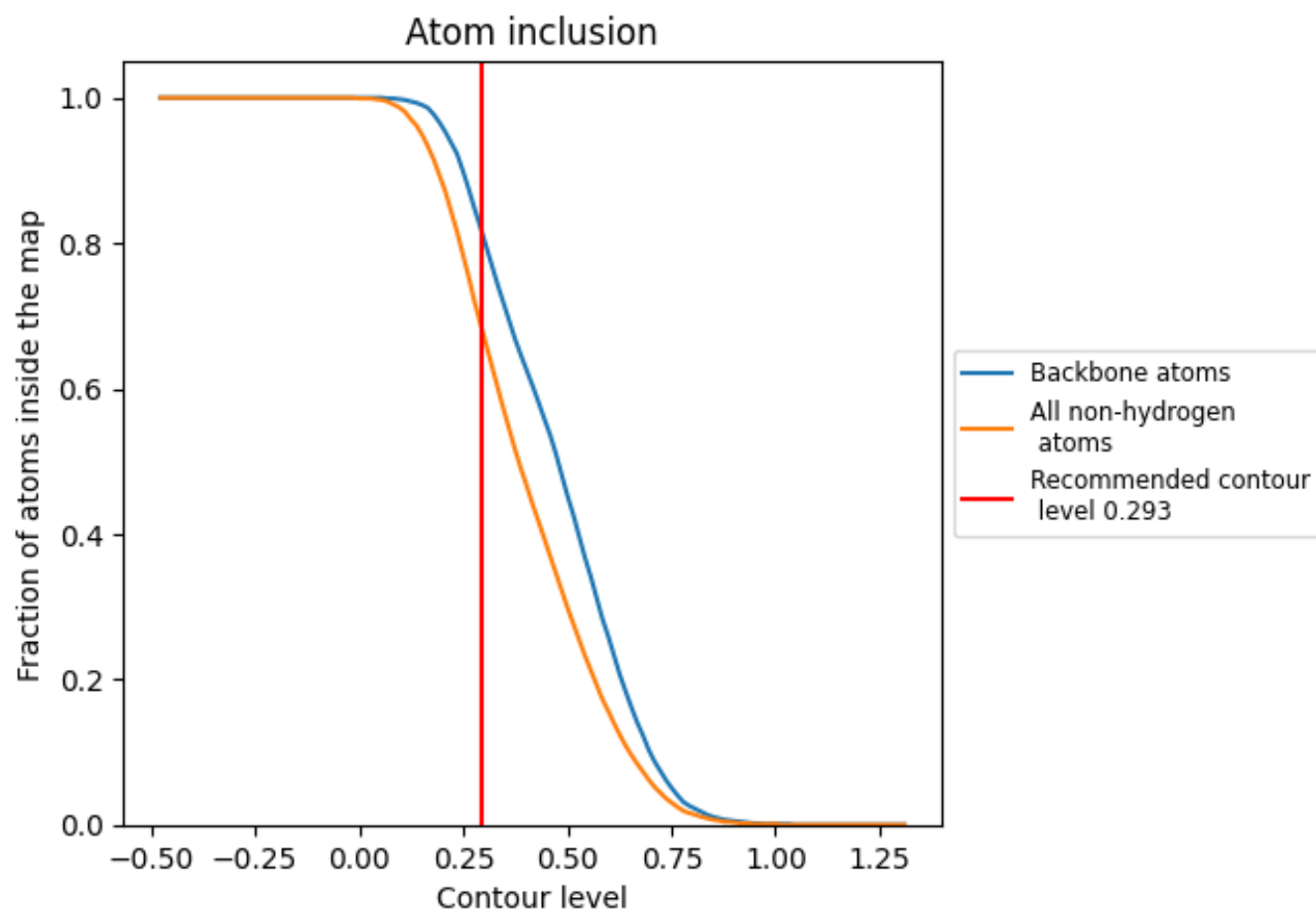
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.293).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.4380
A	 0.7030	 0.4520
B	 0.7550	 0.4760
C	 0.7040	 0.4400
D	 0.7720	 0.4750
E	 0.7050	 0.4500
F	 0.7610	 0.4760
G	 0.5360	 0.3290
H	 0.3390	 0.2830
I	 0.5360	 0.4580
J	 0.7620	 0.4650
K	 0.7730	 0.4580
L	 0.3380	 0.2880
M	 0.7680	 0.4620
N	 0.7710	 0.4540
O	 0.7560	 0.4590
P	 0.7620	 0.4500
Q	 0.5000	 0.3640
R	 0.2310	 0.3570
S	 0.4340	 0.3820
T	 0.2500	 0.3080
U	 0.2890	 0.4470
V	 0.5000	 0.3880
W	 0.4640	 0.3590
X	 0.5710	 0.4390
Y	 0.4400	 0.4110
Z	 0.4290	 0.3690
a	 0.3750	 0.3300
b	 0.2890	 0.4720
c	 0.4640	 0.3550
d	 0.4290	 0.4180
e	 0.5200	 0.4710
f	 0.5000	 0.4270
g	 0.5000	 0.4060
h	 0.5640	 0.4140



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Chain	Atom inclusion	Q-score
i	 0.2920	 0.3320
j	 0.3160	 0.3960