



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:16 AM UTC

PDB ID : 9B8F / pdb_00009b8f
EMDB ID : EMD-44344
Title : SARS CoV-2 full-length spike protein with Lys1269Ala and His1271Ala substitutions in the coatomer binding motif, 2RBD-up conformation (SPIKE-AXA)
Authors : Singh, S.; Hasan, S.S.
Deposited on : 2024-03-29
Resolution : 4.15 Å(reported)
Based on initial model : 7KRQ

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

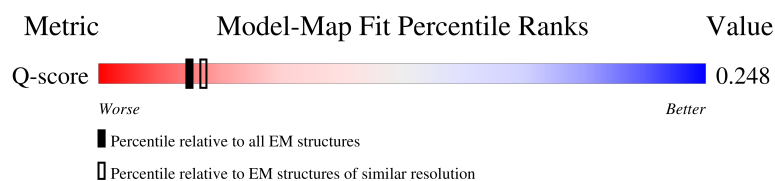
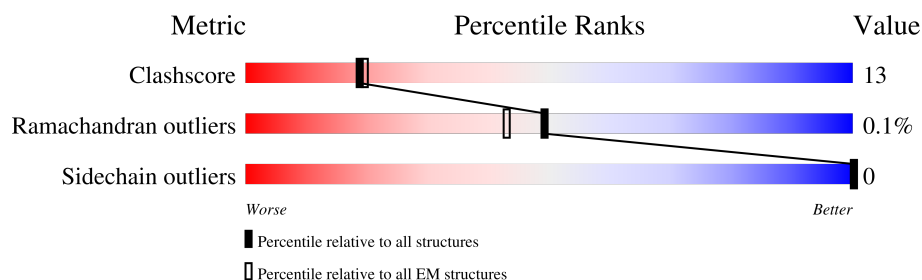
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.15 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.



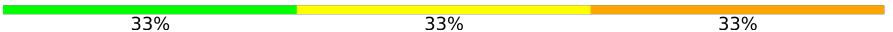
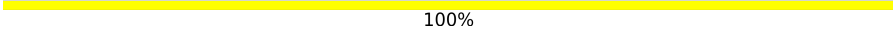
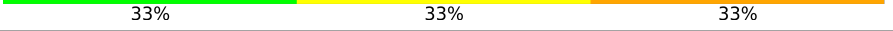
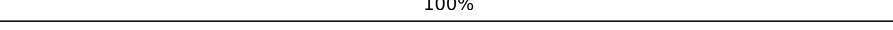
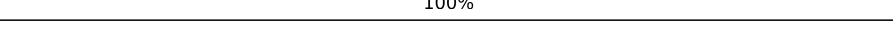
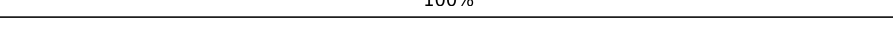
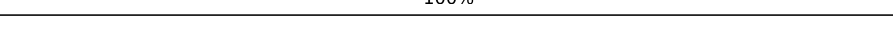
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5475 (3.66 - 4.65)

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	1312	
1	B	1312	
1	C	1312	
2	D	3	

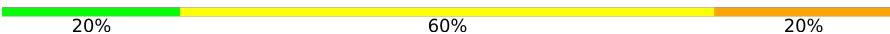
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Mol	Chain	Length	Quality of chain
2	L	3	 33% 67%
2	M	3	 33% 33% 33%
2	N	3	 33% 67%
2	P	3	 100%
2	R	3	 33% 67%
2	S	3	 33% 67%
2	U	3	 33% 67%
2	V	3	 33% 33% 33%
2	W	3	 67% 33%
2	X	3	 33% 67%
2	b	3	 33% 67%
3	E	4	 25% 75%
3	F	4	 25% 75%
4	G	2	 100%
4	I	2	 100%
4	K	2	 50% 50%
4	O	2	 100%
4	Q	2	 100%
4	T	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 100%
5	H	4	 50% 50%
6	J	4	 100%
6	Z	4	 25% 75%
7	Y	3	 33% 67%

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Mol	Chain	Length	Quality of chain
8	a	5	 20% 80%
8	d	5	 20% 60% 20%
9	c	4	 25% 25% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	-	-	X	-
2	BMA	D	3	-	-	X	-
3	NAG	E	1	-	-	X	-
3	BMA	E	3	-	-	X	-
3	MAN	E	4	-	-	X	-
3	NAG	F	1	-	-	X	-
3	NAG	F	2	-	-	X	-
3	MAN	F	4	-	-	X	-
9	NAG	c	1	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 51495 atoms, of which 25203 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1044	Total	C	H	N	O	S	0	0
			16045	5197	7909	1356	1547	36		
1	B	1076	Total	C	H	N	O	S	0	0
			16504	5360	8106	1399	1601	38		
1	C	1073	Total	C	H	N	O	S	0	0
			16425	5333	8070	1392	1594	36		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	insertion	UNP P0DTC2
A	-19	ALA	-	insertion	UNP P0DTC2
A	-18	TRP	-	insertion	UNP P0DTC2
A	-17	SER	-	insertion	UNP P0DTC2
A	-16	HIS	-	insertion	UNP P0DTC2
A	-15	PRO	-	insertion	UNP P0DTC2
A	-14	GLN	-	insertion	UNP P0DTC2
A	-13	PHE	-	insertion	UNP P0DTC2
A	-12	GLU	-	insertion	UNP P0DTC2
A	-11	LYS	-	insertion	UNP P0DTC2
A	-10	GLY	-	insertion	UNP P0DTC2
A	-9	GLY	-	insertion	UNP P0DTC2
A	-8	GLY	-	insertion	UNP P0DTC2
A	-7	SER	-	insertion	UNP P0DTC2
A	-6	GLY	-	insertion	UNP P0DTC2
A	-5	GLY	-	insertion	UNP P0DTC2
A	-4	GLY	-	insertion	UNP P0DTC2
A	-3	SER	-	insertion	UNP P0DTC2
A	-2	GLY	-	insertion	UNP P0DTC2
A	-1	GLY	-	insertion	UNP P0DTC2
A	0	SER	-	insertion	UNP P0DTC2
A	1	SER	-	insertion	UNP P0DTC2
A	2	ALA	-	insertion	UNP P0DTC2
A	3	TRP	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	insertion	UNP P0DTC2
A	5	HIS	-	insertion	UNP P0DTC2
A	6	PRO	-	insertion	UNP P0DTC2
A	7	GLN	-	insertion	UNP P0DTC2
A	8	PHE	-	insertion	UNP P0DTC2
A	9	GLU	-	insertion	UNP P0DTC2
A	10	LYS	-	insertion	UNP P0DTC2
A	11	SER	-	insertion	UNP P0DTC2
A	12	ALA	-	insertion	UNP P0DTC2
A	13	LEU	-	insertion	UNP P0DTC2
A	14	VAL	-	insertion	UNP P0DTC2
A	15	PRO	-	insertion	UNP P0DTC2
A	16	ARG	-	insertion	UNP P0DTC2
A	17	GLY	-	insertion	UNP P0DTC2
A	18	SER	-	insertion	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1269	ALA	LYS	engineered mutation	UNP P0DTC2
A	1271	ALA	HIS	engineered mutation	UNP P0DTC2
B	-20	SER	-	insertion	UNP P0DTC2
B	-19	ALA	-	insertion	UNP P0DTC2
B	-18	TRP	-	insertion	UNP P0DTC2
B	-17	SER	-	insertion	UNP P0DTC2
B	-16	HIS	-	insertion	UNP P0DTC2
B	-15	PRO	-	insertion	UNP P0DTC2
B	-14	GLN	-	insertion	UNP P0DTC2
B	-13	PHE	-	insertion	UNP P0DTC2
B	-12	GLU	-	insertion	UNP P0DTC2
B	-11	LYS	-	insertion	UNP P0DTC2
B	-10	GLY	-	insertion	UNP P0DTC2
B	-9	GLY	-	insertion	UNP P0DTC2
B	-8	GLY	-	insertion	UNP P0DTC2
B	-7	SER	-	insertion	UNP P0DTC2
B	-6	GLY	-	insertion	UNP P0DTC2
B	-5	GLY	-	insertion	UNP P0DTC2
B	-4	GLY	-	insertion	UNP P0DTC2
B	-3	SER	-	insertion	UNP P0DTC2
B	-2	GLY	-	insertion	UNP P0DTC2

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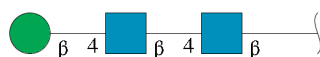
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	insertion	UNP P0DTC2
B	0	SER	-	insertion	UNP P0DTC2
B	1	SER	-	insertion	UNP P0DTC2
B	2	ALA	-	insertion	UNP P0DTC2
B	3	TRP	-	insertion	UNP P0DTC2
B	4	SER	-	insertion	UNP P0DTC2
B	5	HIS	-	insertion	UNP P0DTC2
B	6	PRO	-	insertion	UNP P0DTC2
B	7	GLN	-	insertion	UNP P0DTC2
B	8	PHE	-	insertion	UNP P0DTC2
B	9	GLU	-	insertion	UNP P0DTC2
B	10	LYS	-	insertion	UNP P0DTC2
B	11	SER	-	insertion	UNP P0DTC2
B	12	ALA	-	insertion	UNP P0DTC2
B	13	LEU	-	insertion	UNP P0DTC2
B	14	VAL	-	insertion	UNP P0DTC2
B	15	PRO	-	insertion	UNP P0DTC2
B	16	ARG	-	insertion	UNP P0DTC2
B	17	GLY	-	insertion	UNP P0DTC2
B	18	SER	-	insertion	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1269	ALA	LYS	engineered mutation	UNP P0DTC2
B	1271	ALA	HIS	engineered mutation	UNP P0DTC2
C	-20	SER	-	insertion	UNP P0DTC2
C	-19	ALA	-	insertion	UNP P0DTC2
C	-18	TRP	-	insertion	UNP P0DTC2
C	-17	SER	-	insertion	UNP P0DTC2
C	-16	HIS	-	insertion	UNP P0DTC2
C	-15	PRO	-	insertion	UNP P0DTC2
C	-14	GLN	-	insertion	UNP P0DTC2
C	-13	PHE	-	insertion	UNP P0DTC2
C	-12	GLU	-	insertion	UNP P0DTC2
C	-11	LYS	-	insertion	UNP P0DTC2
C	-10	GLY	-	insertion	UNP P0DTC2
C	-9	GLY	-	insertion	UNP P0DTC2
C	-8	GLY	-	insertion	UNP P0DTC2
C	-7	SER	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	insertion	UNP P0DTC2
C	-5	GLY	-	insertion	UNP P0DTC2
C	-4	GLY	-	insertion	UNP P0DTC2
C	-3	SER	-	insertion	UNP P0DTC2
C	-2	GLY	-	insertion	UNP P0DTC2
C	-1	GLY	-	insertion	UNP P0DTC2
C	0	SER	-	insertion	UNP P0DTC2
C	1	SER	-	insertion	UNP P0DTC2
C	2	ALA	-	insertion	UNP P0DTC2
C	3	TRP	-	insertion	UNP P0DTC2
C	4	SER	-	insertion	UNP P0DTC2
C	5	HIS	-	insertion	UNP P0DTC2
C	6	PRO	-	insertion	UNP P0DTC2
C	7	GLN	-	insertion	UNP P0DTC2
C	8	PHE	-	insertion	UNP P0DTC2
C	9	GLU	-	insertion	UNP P0DTC2
C	10	LYS	-	insertion	UNP P0DTC2
C	11	SER	-	insertion	UNP P0DTC2
C	12	ALA	-	insertion	UNP P0DTC2
C	13	LEU	-	insertion	UNP P0DTC2
C	14	VAL	-	insertion	UNP P0DTC2
C	15	PRO	-	insertion	UNP P0DTC2
C	16	ARG	-	insertion	UNP P0DTC2
C	17	GLY	-	insertion	UNP P0DTC2
C	18	SER	-	insertion	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1269	ALA	LYS	engineered mutation	UNP P0DTC2
C	1271	ALA	HIS	engineered mutation	UNP P0DTC2

- Molecule 2 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.



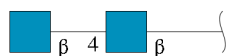
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	H	N	0	0
			73	22	34	2		
2	M	3	Total	C	H	N	0	0
			73	22	34	2		
2	N	3	Total	C	H	N	0	0
			73	22	34	2		
2	P	3	Total	C	H	N	0	0
			73	22	34	2		
2	R	3	Total	C	H	N	0	0
			73	22	34	2		
2	S	3	Total	C	H	N	0	0
			73	22	34	2		
2	U	3	Total	C	H	N	0	0
			73	22	34	2		
2	V	3	Total	C	H	N	0	0
			73	22	34	2		
2	W	3	Total	C	H	N	0	0
			73	22	34	2		
2	X	3	Total	C	H	N	0	0
			73	22	34	2		
2	b	3	Total	C	H	N	0	0
			73	22	34	2		

- Molecule 3 is an oligosaccharide called 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.



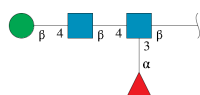
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		
3	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 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
4	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	e	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	f	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



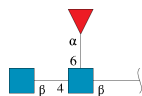
Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	4	Total	C	H	N	O	0	0
			92	28	43	2	19		

- Molecule 6 is an oligosaccharide called 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.



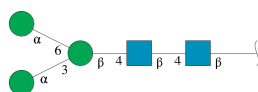
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	4	Total	C	H	N	O	0	0
			93	28	43	2	20		
6	Z	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	3	Total	C	H	N	O	0	0
			72	22	34	2	14		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



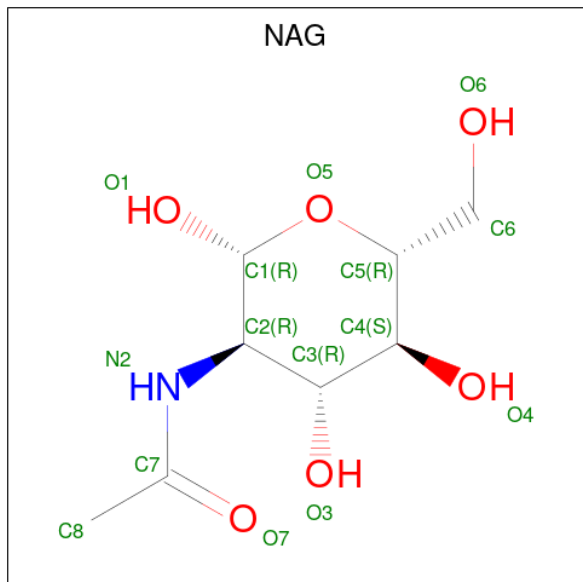
Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	5	Total	C	H	N	O	0	0
			113	34	52	2	25		
8	d	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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



[illegible]

- Molecule 1: Spike glycoprotein



MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	PRO	VAL	SER	SER	GLN	CYS	GLN	ASN	VAL	VAL	LEU	SER	TRP	SER	HIS	PRO	PRO	GLN	PHE	GLU	GLY	LYS	GLY	GLY	GLY	SER	SER	SER	SER	ALA	ALA	TRP	SER	HIS	PRO	PRO	GLN	PHE	GLU	LYS	SER	SER	ALA	ALA	VAL	VAL	PRO	ARG	GLY	SER	THR	THR	ARG
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THR	GLN	LEU	PRO	PRO	A27	S31	R34	D40	K41	V42	F43	S46	D53	L54	F59	S60	N61	F65	H66	A67	I68	H69	VAL	SER	GLY	THR	THR	ASN	GLY	K77	D80	E96	I101	G107	I108	I109	L110	D111	S112	L117	L118	I119	V120	N125	G126
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F135	C136	M137	D138	P139	M149	K150	S151	M152	M153	Y160	S161	V171	F175	L176	M177	D178	L179	E180	G181	K187	V193	F194	K195	Y204	L210	L216	P217	E224	P225	L226	V227	D228	L229	P230	L231	G232	G233	M234	L235	L236	R237	F238	Q239	T240	L241	L242	A243	L244
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ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	S254	Y265	R273	Y279	N280	T284	D287	A288	V289	D290	C291	S314	T315	S316	T323	T326	V327	R328	N331	N334	P337	F338	G339	E340	N343	A348	A352	W353	N354	R355	L358	S359	N360	Y365	S366
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L368	L369	L370	L371	L375	L376	L377	L378	L379	L382	L383	L384	L385	L388	L393	L394	L395	L398	L403	L404	L405	L406	L409	L415	L416	L422	L423	L432	L433	L436	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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GLY	PHE	ASN	TYR	THR	PHE	Y491	L492	Q493	S494	Y495	Q498	N501	G504	V512	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T531	V539	F543	L546	T547	G548	N556	K557	K558	G563	K564	F565	D568	T572	V576	R577	N603	T604	G605
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A609	6510	1611	7612	6613	6614	7615	6616	7625	A626	6627	Q628	1629	T630	6631	T632	Q633	R634	Q644	A647	Q648	C649	E661	1666	A672	T676	GLN	THR	ASN	ASX	PRO	GLY	ALA	ALA	ALA	SER	SER	VAL	ALA	6697	1692	6697	6698	6698	N703	S704	1712	1720
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E725	M731	D737	C738	T739	T742	G744	G749	S750	L753	L763	A766	T770	Q774	D775	K776	E780	D796	F817	L821	D830	Q836	T837	C838	L840	L841	L849	L850	L865	T866	M869	L870	A871
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T874	L878	A893	L894	Q901	R905	T912	Q913	L914	V915	L916	V917	R918	N919	Q920	K921	L922	L923	A924	N925	Q926		S929	K933	P986	E990	L996	1997	T1006	V1007	V1008	T1009	L1012	A1015	T1018	K1028	F1042	L1049	V1060	V1061	H1064	1065
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[illegible]

GLY	ILE	ASN	ALA	SER	VAL	VAL	ASN	ASN	LYS	ILE	ASP	ARG	LEU	ASN	GLU	VAL	ALA	ASN	LYS	ASN	LEU	ASP	LEU	GLN	GLU	GLY	LYS	TYR	GLU	GLN	TYR	GLN	ILE	LYS	TRP	TRP	PRO	TRP	TYR	ILE	ILE	ILE	ALA	GLY	GLY	LEU	ILE	ALA	ILE	ILE	VAL	VAL	MET	HA
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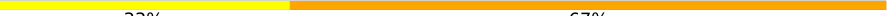
THR	ILE	MET	LEU	CYS	CYS	MET	THR	SER	SER	CYS	CYS	SER	CYS	CYS	LEU	LYS	GLY	CYS	CYS	SER	SER	CYS	CYS	LYS	PHE	ASP	ASP	GLU	ASP	ASP	SER	SER	GLU	PRO	VAL	LEU	LYS	GLY	VAL	ALA	ALA	LEU	ALA	TYR	THR
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- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2
BMA3

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

Chain L:  33% 67%

MAG1
MAG2
BMA3

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

Chain M:  33% 33% 33%

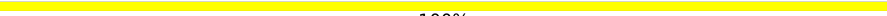
MAG1
MAG2
BMA3

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

Chain N:  33% 67%

MAG1
MAG2
BMA3

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

Chain P:  100%

MAG1
MAG2
BMA3

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

Chain R:  33% 67%

MAG1
MAG2
BMA3

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

Chain S:  33% 67%

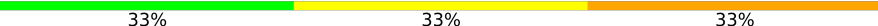
MAG1
MAG2
BMA3

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

Chain U:  33% 67%

MAG1
MAG2
BMA3

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

Chain V:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain W:  67% 33%

MAG1
MAG2
BMA3

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

Chain X:  33% 67%

MAG1
MAG2
BMA3

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

Chain b:  33% 67%

MAG1
MAG2
BMA3

- Molecule 3: 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 E:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 3: 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 F:  25% 75%



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

Chain G:  100%



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

Chain I:  100%



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

Chain K:  50% 50%



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

Chain O:  100%



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

Chain Q:  100%



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

Chain T:  50% 50%

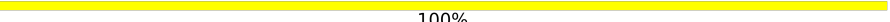


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

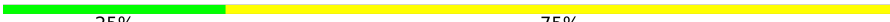
MAG1
MAG2
BMA3
FUC4

- Molecule 6: 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

Chain J:  100%

MAG1
MAG2
BMA3
MAN4

- Molecule 6: 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

Chain Z:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  33% 67%

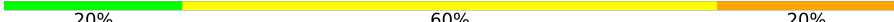
MAG1
MAG2
FUC3

- Molecule 8: alpha-D-mannopyranose-(1-3)-[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 a:  20% 80%

MAG1
MAG2
BGA3
MAN4
MAN5

- Molecule 8: alpha-D-mannopyranose-(1-3)-[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 d:  20% 60% 20%

MAG1
MAG2
BGA3
MAN4
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  25% 25% 50%

MAG1
MAG2
BGA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59137	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.19	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0607	Depositor
Map size ($\text{\AA}$)	332.112, 332.112, 332.112	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.221, 1.221, 1.221	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/8318	0.32	1/11312 (0.0%)
1	B	0.13	0/8594	0.33	2/11694 (0.0%)
1	C	0.13	0/8549	0.32	0/11638
All	All	0.13	0/25461	0.32	3/34644 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASN	CB-CA-C	-5.75	101.18	114.41
1	B	165	ASN	N-CA-CB	5.46	120.63	110.86
1	A	1134	ASN	N-CA-CB	-5.36	102.05	110.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1133	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	165	ASN	Peptide
1	C	233	ILE	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	8136	7909	7934	200	0
1	B	8398	8106	8135	221	0
1	C	8355	8070	8099	192	0
2	D	39	0	34	12	0
2	L	39	34	34	2	0
2	M	39	34	34	3	0
2	N	39	34	34	6	0
2	P	39	34	34	0	0
2	R	39	34	34	4	0
2	S	39	34	34	1	0
2	U	39	34	34	2	0
2	V	39	34	34	1	0
2	W	39	34	34	1	0
2	X	39	34	34	0	0
2	b	39	34	34	3	0
3	E	50	0	43	13	0
3	F	50	0	43	30	0
4	G	28	25	25	3	0
4	I	28	25	25	2	0
4	K	28	25	25	3	0
4	O	28	25	25	1	0
4	Q	28	25	25	0	0
4	T	28	25	25	1	0
4	e	28	25	25	1	0
4	f	28	25	25	0	0
5	H	49	43	43	3	0
6	J	50	43	43	6	0
6	Z	50	43	43	0	0
7	Y	38	34	34	4	0
8	a	61	52	52	3	0
8	d	61	52	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	c	50	43	43	12	0
10	A	84	78	78	6	0
10	B	98	91	91	9	0
10	C	70	65	65	3	0
All	All	26292	25203	25406	669	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 13.

All (669) 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:3:BMA:H4	3:F:4:MAN:H5	1.27	1.14
3:E:3:BMA:H4	3:E:4:MAN:H5	1.39	1.02
1:B:1075:PHE:HD1	1:B:1098:ASN:HB3	1.25	1.01
3:F:1:NAG:H4	3:F:2:NAG:C7	1.99	0.92
1:A:142:GLY:O	1:A:155:SER:OG	1.89	0.89
6:J:3:BMA:O2	6:J:4:MAN:O5	1.89	0.89
1:C:314:GLN:NE2	1:C:315:THR:O	2.07	0.88
1:C:117:LEU:HD11	1:C:233:ILE:HD11	1.54	0.87
1:A:67:ALA:O	1:A:262:ALA:N	2.07	0.86
1:A:731:MET:SD	1:A:774:GLN:NE2	2.50	0.84
1:B:142:GLY:O	1:B:155:SER:OG	1.95	0.84
3:F:3:BMA:C4	3:F:4:MAN:H5	2.07	0.84
1:A:578:ASP:OD2	1:A:581:THR:N	2.12	0.83
7:Y:1:NAG:O3	7:Y:2:NAG:N2	2.11	0.83
1:B:155:SER:OG	1:B:156:GLU:OE1	1.97	0.82
1:B:1075:PHE:CD1	1:B:1098:ASN:HB3	2.11	0.81
1:C:1091:ARG:NH1	1:C:1120:THR:O	2.13	0.81
2:b:1:NAG:O6	2:b:2:NAG:O5	1.97	0.81
1:B:493:GLN:NE2	1:B:494:SER:O	2.14	0.81
1:B:746:SER:OG	1:B:748:GLU:OE1	1.98	0.81
1:C:1098:ASN:H	9:c:1:NAG:H82	1.44	0.81
1:A:645:THR:OG1	1:A:648:GLY:O	1.99	0.81
1:C:403:ARG:NH1	1:C:494:SER:OG	2.14	0.81
1:B:516:GLU:N	1:B:516:GLU:OE1	2.14	0.80
1:B:178:ASP:OD1	1:B:190:ARG:NH2	2.15	0.80
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.14	0.80
1:A:99:ASN:O	1:A:102:ARG:NH1	2.15	0.80
2:D:1:NAG:H61	2:D:2:NAG:H2	1.64	0.80
1:A:314:GLN:NE2	1:A:315:THR:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:OE1	1:B:274:THR:OG1	2.00	0.80
1:B:563:GLN:O	1:B:577:ARG:NH1	2.14	0.80
3:E:3:BMA:C4	3:E:4:MAN:H5	2.11	0.80
1:A:66:HIS:ND1	1:A:263:ALA:O	2.15	0.79
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.16	0.78
1:A:819:GLU:OE2	1:A:1055:SER:N	2.16	0.77
1:B:457:ARG:NH1	1:B:460:ASN:O	2.17	0.77
1:C:334:ASN:ND2	1:C:360:ASN:O	2.18	0.77
1:C:721:SER:OG	1:C:1066:THR:OG1	2.02	0.76
1:B:353:TRP:O	1:B:466:ARG:NE	2.19	0.76
1:B:619:GLU:OE2	2:R:1:NAG:O6	2.03	0.76
1:C:913:GLN:OE1	1:C:913:GLN:N	2.17	0.76
1:B:145:TYR:O	1:B:146:HIS:ND1	2.19	0.76
1:B:1006:THR:O	1:B:1009:THR:OG1	2.04	0.75
1:C:331:ASN:OD1	2:V:1:NAG:N2	2.19	0.75
3:F:1:NAG:C6	3:F:4:MAN:HO2	1.99	0.75
1:C:731:MET:N	1:C:774:GLN:OE1	2.20	0.75
1:A:224:GLU:N	1:A:224:GLU:OE1	2.19	0.75
1:A:1091:ARG:NH2	1:A:1117:THR:O	2.19	0.75
1:B:218:GLN:N	1:B:218:GLN:OE1	2.19	0.75
1:C:563:GLN:O	1:C:577:ARG:NH1	2.19	0.75
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.20	0.75
2:U:2:NAG:O3	2:U:3:BMA:O2	2.04	0.75
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.19	0.75
1:C:368:LEU:O	1:C:371:SER:OG	2.04	0.75
1:A:33:THR:OG1	1:A:219:GLY:O	2.06	0.74
3:F:1:NAG:H2	3:F:2:NAG:H82	1.70	0.74
8:a:1:NAG:O3	8:a:2:NAG:N2	2.19	0.74
1:A:563:GLN:NE2	1:B:42:VAL:O	2.20	0.74
1:B:328:ARG:NH1	1:B:542:ASN:O	2.21	0.73
1:B:408:ARG:NH1	1:B:414:GLN:OE1	2.21	0.73
1:C:409:GLN:OE1	1:C:422:ASN:ND2	2.20	0.73
1:A:803:SER:HB3	2:N:1:NAG:H81	1.70	0.73
1:A:1098:ASN:OD1	2:L:1:NAG:N2	2.21	0.73
1:C:1075:PHE:CD1	1:C:1098:ASN:HB3	2.24	0.73
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.22	0.73
1:A:913:GLN:N	1:A:913:GLN:OE1	2.22	0.72
1:B:895:GLN:N	1:B:895:GLN:OE1	2.22	0.72
1:C:422:ASN:OD1	1:C:423:TYR:N	2.21	0.71
1:B:143:VAL:N	1:B:243:ALA:O	2.23	0.71
1:C:224:GLU:N	1:C:224:GLU:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:N	1:C:504:GLY:O	2.23	0.71
1:B:1100:THR:HG22	1:B:1101:HIS:CE1	2.25	0.71
1:C:1100:THR:N	9:c:1:NAG:O7	2.23	0.71
1:C:609:ALA:HB2	1:C:692:ILE:HD12	1.73	0.70
1:A:1116:THR:N	1:A:1119:ASN:OD1	2.25	0.70
1:B:48:LEU:HD21	1:B:276:LEU:HD21	1.71	0.70
1:B:33:THR:OG1	1:B:219:GLY:O	2.08	0.70
1:C:712:ILE:CG1	1:C:1077:THR:HG21	2.20	0.70
1:A:1158:ASN:OD1	1:A:1159:HIS:N	2.24	0.70
1:B:1075:PHE:CE1	3:F:1:NAG:H82	2.26	0.70
1:A:436:TRP:NE1	1:A:509:ARG:O	2.24	0.70
2:N:2:NAG:HO3	2:N:3:BMA:HO2	0.71	0.70
1:B:761:THR:O	1:B:765:ARG:NH1	2.25	0.70
1:A:703:ASN:OD1	1:A:704:SER:N	2.25	0.69
1:A:118:LEU:HD23	1:A:118:LEU:O	1.93	0.69
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.24	0.69
1:C:547:THR:HG22	1:C:548:GLY:H	1.58	0.69
9:c:1:NAG:O6	9:c:2:NAG:O7	2.10	0.69
1:A:1139:ASP:OD2	1:A:1142:GLN:N	2.26	0.69
1:C:703:ASN:OD1	1:C:704:SER:N	2.26	0.69
8:a:4:MAN:O4	8:a:5:MAN:O4	2.11	0.68
1:A:309:GLU:O	1:A:313:TYR:OH	2.11	0.68
1:B:1116:THR:N	1:B:1119:ASN:OD1	2.25	0.68
1:A:985:ASP:N	1:A:988:GLU:OE2	2.26	0.68
1:C:1101:HIS:O	9:c:1:NAG:H83	1.94	0.68
1:B:751:ASN:OD1	1:B:752:LEU:N	2.27	0.68
1:B:315:THR:OG1	1:B:595:VAL:O	2.10	0.68
1:B:801:ASN:OD1	3:E:1:NAG:N2	2.27	0.68
3:F:1:NAG:H4	3:F:2:NAG:N2	2.06	0.67
1:B:1098:ASN:OD1	3:F:1:NAG:H2	1.94	0.67
1:A:34:ARG:NH1	1:A:221:SER:OG	2.26	0.67
1:C:117:LEU:HD11	1:C:233:ILE:CD1	2.25	0.67
1:A:68:ILE:O	1:A:77:LYS:N	2.28	0.67
1:B:721:SER:OG	1:B:1066:THR:OG1	2.13	0.67
1:B:354:ASN:OD1	1:B:355:ARG:N	2.29	0.66
1:C:568:ASP:OD2	1:C:572:THR:OG1	2.11	0.66
4:e:1:NAG:O4	4:e:1:NAG:O7	2.14	0.66
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.28	0.66
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.29	0.66
1:A:328:ARG:NH1	1:A:531:THR:O	2.29	0.66
1:B:1003:SER:O	1:B:1006:THR:OG1	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:NAG:H5	2:D:3:BMA:C2	2.25	0.66
1:B:166:CYS:SG	1:B:167:THR:N	2.69	0.65
3:F:2:NAG:H2	3:F:4:MAN:O3	1.96	0.65
1:B:1075:PHE:CD1	3:F:1:NAG:H82	2.31	0.65
1:B:761:THR:HG22	1:B:765:ARG:HH12	1.62	0.65
1:B:709:ASN:ND2	1:C:796:ASP:OD2	2.29	0.65
1:C:737:ASP:OD1	1:C:738:CYS:N	2.30	0.65
1:C:273:ARG:NH2	1:C:290:ASP:OD2	2.30	0.64
2:D:2:NAG:H5	2:D:3:BMA:O2	1.96	0.64
1:A:331:ASN:OD1	1:A:332:ILE:N	2.27	0.64
1:A:926:GLN:HE21	6:J:2:NAG:H81	1.63	0.64
1:C:1006:THR:O	1:C:1009:THR:OG1	2.14	0.64
1:C:1101:HIS:C	9:c:1:NAG:H83	2.22	0.64
1:A:134:GLN:NE2	1:A:164:ASN:OD1	2.28	0.64
1:B:455:LEU:N	1:B:491:PRO:O	2.31	0.64
1:C:919:ASN:O	1:C:923:ILE:HD12	1.99	0.63
1:B:1100:THR:HG22	1:B:1101:HIS:ND1	2.13	0.63
1:C:603:ASN:OD1	1:C:604:THR:N	2.31	0.63
1:C:634:ARG:HD2	1:C:634:ARG:O	1.99	0.63
1:A:822:LEU:HD22	1:A:938:LEU:HD21	1.81	0.63
1:C:498:GLN:OE1	1:C:501:ASN:ND2	2.32	0.63
1:A:334:ASN:OD1	1:A:335:LEU:N	2.32	0.62
1:A:344:ALA:O	1:A:509:ARG:NH1	2.32	0.62
1:B:909:ILE:HG22	1:B:909:ILE:O	1.98	0.62
1:C:403:ARG:NE	1:C:405:ASP:OD1	2.32	0.62
1:A:1134:ASN:CG	2:M:1:NAG:N2	2.54	0.62
1:C:1116:THR:N	1:C:1119:ASN:OD1	2.32	0.62
1:C:239:GLN:NE2	1:C:240:THR:O	2.33	0.61
1:B:314:GLN:OE1	1:B:315:THR:N	2.32	0.61
1:C:326:ILE:O	1:C:327:VAL:HG12	2.01	0.61
1:C:339:GLY:O	1:C:343:ASN:ND2	2.33	0.61
1:B:960:ASN:OD1	1:B:964:LYS:NZ	2.27	0.61
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.32	0.61
1:B:1009:THR:O	1:B:1013:ILE:HD12	2.01	0.61
1:A:1074:ASN:OD1	4:K:1:NAG:H2	1.99	0.61
1:B:1006:THR:O	1:B:1010:GLN:OE1	2.19	0.61
1:A:1134:ASN:OD1	2:M:1:NAG:C7	2.49	0.61
1:C:229:LEU:HB3	1:C:231:ILE:HD11	1.83	0.61
1:A:1074:ASN:OD1	4:K:1:NAG:H83	2.01	0.61
1:B:1036:GLN:O	1:B:1038:LYS:NZ	2.34	0.61
1:C:31:SER:O	1:C:59:PHE:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:O	1:A:531:THR:OG1	2.11	0.61
1:A:866:THR:OG1	1:A:869:MET:HE3	2.01	0.61
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.34	0.61
1:C:874:THR:O	1:C:878:LEU:HD23	2.01	0.61
3:E:3:BMA:H61	3:E:4:MAN:C5	2.29	0.60
1:A:884:SER:OG	1:A:887:THR:OG1	2.19	0.60
1:C:1075:PHE:HD1	1:C:1098:ASN:HB3	1.63	0.60
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.33	0.60
1:C:46:SER:N	1:C:279:TYR:O	2.35	0.60
2:D:2:NAG:O7	2:D:2:NAG:H3	2.00	0.60
1:C:149:ASN:ND2	10:C:1404:NAG:O6	2.34	0.60
1:B:994:ASP:OD1	1:B:995:ARG:N	2.35	0.59
1:A:603:ASN:ND2	10:A:1302:NAG:O6	2.27	0.59
1:B:1075:PHE:CZ	3:F:1:NAG:H82	2.36	0.59
1:B:731:MET:N	1:B:774:GLN:OE1	2.31	0.59
3:E:1:NAG:H4	3:E:2:NAG:C7	2.32	0.59
1:A:341:VAL:HG21	1:A:397:ALA:HB1	1.84	0.59
1:B:280:ASN:OD1	1:B:284:THR:N	2.32	0.59
1:B:393:THR:O	1:B:523:THR:HG22	2.02	0.59
1:A:326:ILE:HG23	1:A:541:PHE:HA	1.84	0.59
1:B:1096:VAL:HG22	3:F:1:NAG:H81	1.85	0.59
1:C:365:TYR:OH	1:C:385:THR:O	2.13	0.59
1:B:119:ILE:HG22	1:B:119:ILE:O	2.03	0.59
1:B:827:THR:O	1:B:949:GLN:NE2	2.35	0.59
1:B:1101:HIS:HB2	3:F:2:NAG:H83	1.85	0.58
4:G:1:NAG:H83	4:G:2:NAG:H61	1.83	0.58
3:E:1:NAG:H62	3:E:2:NAG:H2	1.84	0.58
1:A:717:ASN:ND2	6:J:1:NAG:O3	2.35	0.58
1:A:909:ILE:O	1:A:909:ILE:HG22	2.03	0.58
1:A:644:GLN:NE2	4:I:1:NAG:O7	2.37	0.58
2:S:1:NAG:O4	2:S:2:NAG:O7	2.22	0.58
1:A:281:GLU:OE1	1:A:281:GLU:N	2.32	0.58
1:C:119:ILE:HG22	1:C:119:ILE:O	2.02	0.58
1:C:512:VAL:HG12	1:C:512:VAL:O	2.04	0.58
1:A:1083:HIS:ND1	1:A:1136:THR:HA	2.19	0.58
3:F:1:NAG:O3	3:F:2:NAG:N2	2.37	0.58
1:B:884:SER:OG	1:B:887:THR:OG1	2.21	0.58
3:F:3:BMA:H61	3:F:4:MAN:C5	2.32	0.58
1:A:52:GLN:OE1	1:A:53:ASP:N	2.37	0.57
1:A:801:ASN:HB2	2:N:1:NAG:C7	2.34	0.57
1:C:616:ASN:HD22	7:Y:3:FUC:H61	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:N	1:B:484:GLU:OE2	2.34	0.57
1:B:776:LYS:O	1:B:780:GLU:OE1	2.22	0.57
1:C:1076:THR:N	1:C:1097:SER:O	2.37	0.57
1:A:782:PHE:HE2	1:A:870:ILE:HG23	1.69	0.57
1:B:124:THR:O	1:B:175:PHE:N	2.37	0.57
1:C:31:SER:HA	1:C:216:LEU:HD13	1.87	0.57
2:R:2:NAG:O3	2:R:3:BMA:O2	1.91	0.57
1:A:661:GLU:N	1:A:661:GLU:OE1	2.37	0.57
1:C:187:LYS:NZ	1:C:210:ILE:O	2.38	0.57
1:B:532:ASN:OD1	1:B:533:LEU:N	2.37	0.56
1:B:738:CYS:SG	1:B:739:THR:N	2.78	0.56
1:C:111:ASP:O	1:C:112:SER:OG	2.24	0.56
3:F:1:NAG:H4	3:F:2:NAG:O7	2.05	0.56
1:B:884:SER:OG	1:B:894:LEU:N	2.32	0.56
1:C:616:ASN:ND2	7:Y:3:FUC:H61	2.19	0.56
3:F:2:NAG:H4	3:F:4:MAN:H3	1.87	0.56
1:A:776:LYS:O	1:A:780:GLU:OE1	2.23	0.56
1:B:1101:HIS:ND1	3:F:2:NAG:O3	2.38	0.56
2:D:1:NAG:H61	2:D:2:NAG:C2	2.35	0.56
1:B:1008:VAL:O	1:B:1012:LEU:HD23	2.04	0.56
1:B:424:LYS:HG2	1:B:461:LEU:HD13	1.88	0.56
1:A:439:ASN:O	1:A:443:SER:OG	2.13	0.56
1:B:1153:ASP:OD1	1:C:1153:ASP:N	2.39	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.72	0.55
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.40	0.55
3:E:3:BMA:H61	3:E:4:MAN:H5	1.88	0.55
1:B:657:ASN:ND2	10:B:1404:NAG:O7	2.40	0.55
1:C:661:GLU:OE1	1:C:661:GLU:N	2.37	0.55
1:B:141:LEU:HD11	1:B:154:GLU:OE2	2.07	0.55
1:C:61:ASN:HB2	10:C:1401:NAG:N2	2.22	0.55
1:C:353:TRP:NE1	1:C:465:GLU:OE2	2.38	0.55
1:B:405:ASP:N	1:B:504:GLY:O	2.40	0.55
1:A:916:LEU:HD12	1:A:923:ILE:HD13	1.89	0.55
1:B:328:ARG:NH2	1:B:544:ASN:OD1	2.40	0.55
1:B:867:ASP:OD1	1:B:868:GLU:N	2.40	0.55
1:A:742:ILE:HG23	1:A:743:CYS:N	2.22	0.55
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.39	0.55
1:C:1075:PHE:CE1	1:C:1098:ASN:HB3	2.42	0.55
2:D:2:NAG:H3	2:D:3:BMA:O2	2.07	0.54
1:A:31:SER:OG	1:A:60:SER:OG	2.09	0.54
1:C:134:GLN:O	1:C:161:SER:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ASP:OD1	1:C:179:LEU:N	2.40	0.54
1:B:866:THR:O	1:B:870:ILE:HD12	2.07	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.36	0.54
1:B:1098:ASN:OD1	3:F:1:NAG:C2	2.56	0.54
1:C:118:LEU:HD11	1:C:120:VAL:HB	1.89	0.54
1:C:871:ALA:O	1:C:874:THR:OG1	2.22	0.54
1:B:568:ASP:OD1	1:B:569:ILE:N	2.39	0.54
1:C:546:LEU:HD23	1:C:565:PHE:CZ	2.43	0.54
1:C:776:LYS:NZ	1:C:780:GLU:OE2	2.34	0.54
1:A:287:ASP:OD1	1:A:288:ALA:N	2.39	0.54
5:H:1:NAG:N2	5:H:2:NAG:O7	2.37	0.54
1:A:113:LYS:HD2	1:A:114:THR:HG23	1.88	0.53
1:A:643:PHE:HD2	1:A:650:LEU:HD11	1.74	0.53
1:C:1098:ASN:OD1	9:c:1:NAG:N2	2.41	0.53
4:G:1:NAG:H83	4:G:2:NAG:C6	2.38	0.53
1:A:327:VAL:O	1:A:531:THR:N	2.41	0.53
1:A:409:GLN:N	1:A:409:GLN:OE1	2.40	0.53
1:A:445:VAL:O	1:A:498:GLN:NE2	2.39	0.53
1:B:866:THR:O	1:B:869:MET:N	2.42	0.53
1:C:375:SER:HG	1:C:436:TRP:CG	2.27	0.53
1:A:609:ALA:HB2	1:A:692:ILE:HD12	1.92	0.52
1:A:818:ILE:O	1:A:822:LEU:HD23	2.10	0.52
1:C:395:VAL:HG22	1:C:515:PHE:HA	1.90	0.52
1:C:543:PHE:O	1:C:546:LEU:HG	2.09	0.52
1:B:130:VAL:O	1:B:130:VAL:HG13	2.09	0.52
1:A:999:GLY:O	1:A:1002:GLN:NE2	2.36	0.52
1:C:1097:SER:HA	9:c:1:NAG:H82	1.92	0.52
3:F:2:NAG:H61	3:F:3:BMA:O5	2.09	0.52
1:A:1154:LYS:O	1:A:1158:ASN:ND2	2.42	0.52
10:A:1305:NAG:H83	10:A:1305:NAG:H3	1.91	0.52
1:B:403:ARG:NH1	1:B:505:TYR:O	2.43	0.52
6:J:3:BMA:HO2	6:J:4:MAN:C1	2.16	0.52
1:A:906:PHE:CE2	1:A:916:LEU:HD13	2.45	0.52
1:B:439:ASN:OD1	1:B:443:SER:OG	2.12	0.52
1:C:556:ASN:O	1:C:558:LYS:NZ	2.38	0.52
1:A:105:ILE:HG21	1:A:110:LEU:HD21	1.91	0.52
1:C:368:LEU:HD21	1:C:377:PHE:HB2	1.92	0.52
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.91	0.51
1:C:107:GLY:H	1:C:235:ILE:HG23	1.74	0.51
1:C:615:VAL:O	1:C:649:CYS:N	2.43	0.51
1:A:298:GLU:O	1:A:302:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1098:ASN:H	9:c:1:NAG:C8	2.21	0.51
1:B:616:ASN:ND2	2:R:1:NAG:O7	2.43	0.51
1:A:1088:HIS:ND1	1:A:1122:VAL:HG22	2.25	0.51
1:B:389:ASP:C	1:B:390:LEU:HD22	2.35	0.51
1:A:118:LEU:HD22	1:A:129:LYS:HD2	1.91	0.51
1:A:1148:PHE:O	1:A:1152:LEU:HD23	2.09	0.51
1:B:378:LYS:HD3	1:B:379:CYS:N	2.24	0.51
1:B:515:PHE:HE2	1:B:517:LEU:HD11	1.76	0.51
1:C:96:GLU:OE2	1:C:101:ILE:N	2.42	0.51
1:C:1091:ARG:NH1	1:C:1117:THR:O	2.39	0.51
1:B:165:ASN:OD1	1:B:166:CYS:O	2.28	0.51
1:B:815:ARG:NE	1:B:820:ASP:OD1	2.42	0.51
1:C:697:MET:SD	1:C:698:SER:N	2.84	0.51
1:C:287:ASP:OD1	1:C:288:ALA:N	2.43	0.51
1:A:650:LEU:HD13	1:A:653:ALA:HB3	1.91	0.50
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.46	0.50
1:C:40:ASP:OD1	1:C:41:LYS:N	2.39	0.50
1:C:720:ILE:HG22	1:C:926:GLN:HB3	1.92	0.50
1:A:762:GLN:OE1	1:A:765:ARG:NH2	2.44	0.50
1:B:143:VAL:HG23	1:B:143:VAL:O	2.11	0.50
1:A:1014:ARG:HA	1:A:1017:GLU:OE1	2.11	0.50
1:B:1098:ASN:OD1	3:F:2:NAG:H82	2.12	0.50
1:B:149:ASN:HA	10:B:1406:NAG:C1	2.42	0.50
1:C:125:ASN:OD1	1:C:171:VAL:HG13	2.12	0.50
1:B:515:PHE:CE2	1:B:517:LEU:HD11	2.47	0.50
1:B:582:LEU:HG	1:B:582:LEU:O	2.12	0.50
1:C:110:LEU:O	1:C:110:LEU:HD12	2.11	0.50
1:B:334:ASN:ND2	1:B:360:ASN:O	2.41	0.50
1:B:389:ASP:O	1:B:390:LEU:HD22	2.11	0.50
1:A:616:ASN:OD1	1:A:617:CYS:N	2.46	0.49
1:B:308:VAL:N	1:B:602:THR:OG1	2.39	0.49
1:A:776:LYS:O	1:A:779:GLN:N	2.45	0.49
1:B:380:TYR:CE2	1:B:412:PRO:HD2	2.47	0.49
1:A:560:LEU:HD11	1:B:282:ASN:O	2.12	0.49
1:C:1081:ILE:C	1:C:1132:ILE:HD11	2.38	0.49
1:C:177:MET:SD	1:C:177:MET:N	2.86	0.49
1:A:115:GLN:OE1	1:A:131:CYS:N	2.45	0.49
1:C:153:MET:N	1:C:179:LEU:O	2.45	0.49
1:A:86:PHE:CE2	1:A:90:VAL:HG22	2.48	0.49
1:A:817:PHE:CE2	1:A:821:LEU:HD11	2.48	0.49
1:B:530:SER:O	1:B:531:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ASN:OD1	1:B:659:SER:N	2.46	0.49
1:B:983:ARG:O	1:B:983:ARG:NH1	2.38	0.49
9:c:1:NAG:O3	9:c:2:NAG:N2	2.46	0.49
1:C:337:PRO:HD2	1:C:358:ILE:HG23	1.95	0.49
1:C:738:CYS:O	1:C:742:ILE:HG22	2.13	0.49
1:C:893:ALA:C	1:C:894:LEU:HD22	2.38	0.49
1:A:986:PRO:N	1:A:987:PRO:HD2	2.27	0.49
1:C:1008:VAL:O	1:C:1012:LEU:HD23	2.13	0.49
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.94	0.48
1:A:535:LYS:NZ	1:A:554:GLU:OE2	2.42	0.48
1:A:650:LEU:C	1:A:650:LEU:HD12	2.38	0.48
1:B:151:SER:O	1:B:152:TRP:HB2	2.13	0.48
1:A:111:ASP:OD2	1:A:113:LYS:HE3	2.13	0.48
1:B:239:GLN:OE1	1:B:240:THR:N	2.41	0.48
1:A:273:ARG:NH2	1:A:290:ASP:OD2	2.42	0.48
1:C:327:VAL:CG1	1:C:531:THR:HG23	2.44	0.48
1:B:365:TYR:N	1:B:388:ASN:OD1	2.47	0.48
1:A:28:TYR:O	1:A:29:THR:OG1	2.26	0.48
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.95	0.48
1:B:609:ALA:HB2	1:B:692:ILE:HD12	1.96	0.48
1:C:31:SER:O	1:C:59:PHE:CA	2.62	0.48
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.96	0.48
1:B:95:THR:HG22	1:B:189:LEU:HD13	1.96	0.48
1:B:663:ASP:N	1:B:671:CYS:SG	2.87	0.48
1:B:705:VAL:HG22	1:B:706:ALA:N	2.29	0.48
6:J:1:NAG:O4	6:J:1:NAG:N2	2.47	0.48
1:B:1001:LEU:CD1	1:B:1005:GLN:HE22	2.25	0.48
3:F:3:BMA:H61	3:F:4:MAN:H5	1.96	0.48
1:A:1095:PHE:O	1:A:1096:VAL:HG13	2.13	0.48
1:C:226:LEU:HD12	1:C:227:VAL:HG12	1.96	0.48
2:D:2:NAG:H3	2:D:3:BMA:O5	2.13	0.48
1:A:61:ASN:OD1	1:A:61:ASN:O	2.32	0.47
1:A:144:TYR:H	10:A:1305:NAG:H82	1.78	0.47
1:A:580:GLN:HB3	5:H:2:NAG:H81	1.95	0.47
1:B:345:THR:O	1:B:509:ARG:NH2	2.48	0.47
1:C:1134:ASN:OD1	8:d:1:NAG:C1	2.63	0.47
2:D:1:NAG:H4	2:D:2:NAG:H2	1.40	0.47
1:A:782:PHE:CE2	1:A:870:ILE:HG23	2.50	0.47
1:B:282:ASN:HB3	2:D:1:NAG:HN2	1.78	0.47
1:C:1098:ASN:N	9:c:1:NAG:H82	2.22	0.47
1:A:410:ILE:HG21	1:A:510:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:THR:O	1:C:744:GLY:N	2.47	0.47
1:C:1081:ILE:CD1	1:C:1133:VAL:HG23	2.44	0.47
1:B:29:THR:HG22	1:B:30:ASN:N	2.29	0.47
1:B:699:LEU:HD11	1:C:869:MET:HB2	1.96	0.47
1:C:753:LEU:C	1:C:753:LEU:HD12	2.39	0.47
1:A:365:TYR:HB3	1:A:387:LEU:HD23	1.97	0.47
1:A:926:GLN:NE2	6:J:2:NAG:H81	2.27	0.47
1:B:228:ASP:OD1	1:B:229:LEU:N	2.47	0.47
1:C:66:HIS:HB3	1:C:68:ILE:HD11	1.97	0.47
1:A:760:CYS:O	1:A:764:ASN:ND2	2.42	0.47
1:A:818:ILE:HD12	1:A:818:ILE:H	1.78	0.47
3:F:1:NAG:C4	3:F:2:NAG:N2	2.76	0.47
1:B:31:SER:O	1:B:59:PHE:HA	2.14	0.47
1:B:1129:VAL:HG22	1:B:1130:ILE:N	2.30	0.47
1:A:620:VAL:N	1:A:621:PRO:CD	2.77	0.46
1:B:461:LEU:HD12	1:B:461:LEU:C	2.41	0.46
1:C:1074:ASN:OD1	1:C:1075:PHE:N	2.48	0.46
1:B:152:TRP:O	1:B:153:MET:HB3	2.16	0.46
1:B:803:SER:O	1:B:806:LEU:N	2.48	0.46
1:C:611:LEU:HD23	1:C:612:TYR:N	2.30	0.46
1:A:817:PHE:O	1:A:821:LEU:HD13	2.15	0.46
1:C:34:ARG:HG3	1:C:216:LEU:HD11	1.96	0.46
1:C:409:GLN:HB2	1:C:422:ASN:HD21	1.81	0.46
3:E:1:NAG:H4	3:E:2:NAG:H2	1.47	0.46
1:A:871:ALA:HA	1:A:874:THR:HG22	1.98	0.46
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.97	0.46
1:B:752:LEU:HD11	1:B:990:GLU:OE1	2.15	0.46
1:B:1001:LEU:O	1:B:1005:GLN:OE1	2.33	0.46
1:B:945:LEU:HD12	1:B:945:LEU:N	2.31	0.46
1:B:985:ASP:HB2	1:B:986:PRO:HD2	1.96	0.46
1:C:327:VAL:HG13	1:C:328:ARG:H	1.80	0.46
1:B:1001:LEU:HD12	1:B:1005:GLN:HE22	1.80	0.46
1:B:1075:PHE:CG	3:F:1:NAG:H82	2.50	0.46
1:C:152:TRP:NE1	1:C:181:GLY:O	2.48	0.46
1:C:375:SER:HB2	1:C:436:TRP:CB	2.46	0.46
1:A:411:ALA:CB	1:A:433:VAL:HG11	2.46	0.46
1:B:906:PHE:O	1:B:911:VAL:N	2.44	0.46
1:C:382:VAL:HG23	1:C:383:SER:N	2.31	0.46
1:C:712:ILE:HG13	1:C:1077:THR:HG21	1.96	0.46
1:C:1081:ILE:HD12	1:C:1133:VAL:HG23	1.98	0.46
1:B:36:VAL:HG13	1:B:36:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:O	1:C:150:LYS:CB	2.64	0.46
1:C:379:CYS:HB2	1:C:432:CYS:HA	1.96	0.46
1:A:1015:ALA:HA	1:A:1018:ILE:HG22	1.97	0.46
1:B:733:LYS:NZ	1:B:862:PRO:O	2.45	0.46
1:C:712:ILE:HB	1:C:1077:THR:HG21	1.98	0.46
1:C:742:ILE:HG23	1:C:743:CYS:N	2.30	0.46
1:A:1141:LEU:HG	1:A:1145:LEU:HD23	1.97	0.46
4:O:1:NAG:O3	4:O:2:NAG:C1	2.63	0.46
1:A:149:ASN:ND2	1:A:151:SER:O	2.49	0.45
1:B:717:ASN:HB2	1:B:1071:GLN:HB2	1.97	0.45
1:C:830:ASP:HA	1:C:850:ILE:HG12	1.97	0.45
1:A:822:LEU:CD2	1:A:938:LEU:HD21	2.45	0.45
1:B:131:CYS:HB3	1:B:166:CYS:HA	1.98	0.45
1:B:468:ILE:O	1:B:468:ILE:HG22	2.17	0.45
1:B:569:ILE:HD11	1:C:849:LEU:HA	1.97	0.45
1:A:125:ASN:HD21	1:A:171:VAL:HG12	1.82	0.45
1:A:392:PHE:N	1:A:524:VAL:O	2.50	0.45
1:B:273:ARG:NE	1:B:290:ASP:OD2	2.45	0.45
1:B:660:TYR:O	1:B:698:SER:N	2.40	0.45
1:C:118:LEU:HG	1:C:120:VAL:HG12	1.99	0.45
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.99	0.45
1:C:766:ALA:O	1:C:770:ILE:HG12	2.16	0.45
1:A:338:PHE:O	1:A:341:VAL:HG12	2.16	0.45
1:A:619:GLU:O	1:A:622:VAL:HG23	2.17	0.45
1:C:231:ILE:HG22	1:C:233:ILE:HG12	1.97	0.45
1:C:348:ALA:HB1	1:C:352:ALA:O	2.17	0.45
1:A:391:CYS:HA	1:A:525:CYS:HA	1.99	0.45
1:A:776:LYS:O	1:A:777:ASN:C	2.58	0.45
1:A:1045:LYS:NZ	1:B:889:GLY:O	2.50	0.45
1:C:817:PHE:O	1:C:821:LEU:HD13	2.17	0.45
1:A:44:ARG:O	1:A:283:GLY:HA2	2.16	0.45
1:A:346:ARG:HH21	1:A:401:VAL:HG21	1.82	0.45
1:A:954:GLN:O	1:A:957:GLN:NE2	2.49	0.45
1:A:1075:PHE:HD1	1:A:1098:ASN:HA	1.81	0.45
1:B:34:ARG:HG3	1:B:216:LEU:HD11	1.98	0.45
1:C:323:THR:O	1:C:539:VAL:HA	2.17	0.45
3:F:2:NAG:H4	3:F:4:MAN:C3	2.46	0.45
1:B:146:HIS:HA	1:B:150:LYS:HB2	1.99	0.45
1:C:315:THR:OG1	1:C:316:SER:N	2.50	0.45
1:C:996:LEU:HD12	1:C:997:ILE:N	2.32	0.45
1:A:177:MET:HE1	1:A:207:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:LEU:HD12	1:A:1002:GLN:N	2.32	0.45
1:B:763:LEU:HD13	1:B:1004:LEU:CD2	2.46	0.45
1:C:242:LEU:HD23	1:C:242:LEU:H	1.82	0.45
1:C:743:CYS:SG	1:C:753:LEU:HD23	2.56	0.45
1:C:865:LEU:HA	1:C:869:MET:HE3	1.99	0.45
1:C:1099:GLY:C	9:c:1:NAG:O7	2.58	0.45
1:B:440:ASN:OD1	1:B:441:LEU:N	2.49	0.45
1:B:1075:PHE:CE2	3:F:1:NAG:H82	2.51	0.45
1:B:609:ALA:HB2	1:B:692:ILE:CD1	2.47	0.45
1:A:323:THR:N	1:A:538:CYS:O	2.33	0.44
1:B:150:LYS:HB3	10:B:1406:NAG:H81	1.99	0.44
1:B:689:SER:OG	1:B:690:GLN:N	2.49	0.44
1:B:984:LEU:HD22	1:B:988:GLU:HG3	1.98	0.44
1:B:998:THR:HG23	1:B:1002:GLN:HE22	1.81	0.44
1:A:27:ALA:N	1:A:64:TRP:O	2.51	0.44
1:B:818:ILE:HD12	1:B:818:ILE:H	1.83	0.44
1:C:327:VAL:HG13	1:C:328:ARG:N	2.32	0.44
1:B:134:GLN:N	1:B:162:SER:O	2.47	0.44
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.17	0.44
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.43	0.44
1:A:712:ILE:O	1:A:1074:ASN:HA	2.16	0.44
1:C:1088:HIS:CD2	1:C:1122:VAL:HG22	2.52	0.44
1:B:720:ILE:HG22	1:B:926:GLN:HB3	1.99	0.44
3:F:1:NAG:H2	3:F:2:NAG:C8	2.44	0.44
1:A:290:ASP:O	1:A:297:SER:HB3	2.18	0.44
1:B:534:VAL:HG12	1:B:535:LYS:N	2.33	0.44
1:B:576:VAL:HG22	1:B:577:ARG:N	2.32	0.44
1:C:1076:THR:O	1:C:1097:SER:N	2.46	0.44
2:D:2:NAG:H5	2:D:3:BMA:H2	1.99	0.44
1:A:737:ASP:OD1	1:A:739:THR:N	2.51	0.44
1:B:165:ASN:HB2	10:B:1407:NAG:C7	2.48	0.44
1:B:380:TYR:CZ	1:B:412:PRO:HD2	2.52	0.44
1:B:801:ASN:CG	3:E:1:NAG:N2	2.76	0.44
1:C:327:VAL:HG22	1:C:328:ARG:H	1.82	0.44
1:C:576:VAL:HG22	1:C:577:ARG:N	2.33	0.44
1:B:127:VAL:O	1:B:128:ILE:C	2.61	0.44
1:B:474:GLN:OE1	1:B:480:CYS:HB3	2.18	0.44
1:C:112:SER:HB3	1:C:134:GLN:HA	2.00	0.44
1:B:475:ALA:HB3	1:B:489:TYR:OH	2.17	0.43
1:A:43:PHE:HE1	1:A:282:ASN:O	2.01	0.43
1:A:176:LEU:O	1:A:177:MET:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HD11	1:A:533:LEU:HA	2.00	0.43
1:C:331:ASN:OD1	1:C:331:ASN:O	2.36	0.43
3:E:1:NAG:H4	3:E:2:NAG:N2	2.16	0.43
1:B:1091:ARG:NE	1:B:1118:ASP:O	2.35	0.43
1:C:750:SER:O	1:C:753:LEU:HG	2.17	0.43
3:F:1:NAG:O4	3:F:1:NAG:O6	2.29	0.43
9:c:1:NAG:H2	9:c:2:NAG:H82	2.00	0.43
1:A:115:GLN:NE2	1:A:167:THR:OG1	2.52	0.43
1:A:801:ASN:CB	2:N:1:NAG:N2	2.81	0.43
1:A:1074:ASN:OD1	4:K:1:NAG:C2	2.65	0.43
1:A:1141:LEU:HD21	1:A:1145:LEU:HG	2.01	0.43
1:A:48:LEU:HB3	1:A:276:LEU:HD11	2.01	0.43
1:A:912:THR:O	1:A:915:VAL:HG22	2.18	0.43
1:B:985:ASP:O	1:B:986:PRO:C	2.60	0.43
1:B:1074:ASN:OD1	4:T:1:NAG:N2	2.51	0.43
1:A:34:ARG:HG3	1:A:216:LEU:HD12	2.00	0.43
1:A:282:ASN:HB2	4:G:1:NAG:O5	2.18	0.43
1:A:777:ASN:O	1:A:781:VAL:HG22	2.18	0.43
1:C:912:THR:O	1:C:915:VAL:HG22	2.19	0.43
3:E:1:NAG:H4	3:E:2:NAG:O7	2.18	0.43
1:A:411:ALA:HB2	1:A:433:VAL:HG11	2.00	0.43
1:B:105:ILE:CG1	1:B:241:LEU:HD21	2.49	0.43
1:B:287:ASP:OD1	1:B:288:ALA:N	2.52	0.43
1:B:448:ASN:ND2	1:B:451:TYR:OH	2.51	0.43
1:B:870:ILE:HD12	1:B:870:ILE:H	1.83	0.43
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.52	0.43
2:W:2:NAG:O3	2:W:3:BMA:C1	2.67	0.43
1:B:438:SER:OG	1:B:507:PRO:O	2.36	0.43
1:C:65:PHE:HB3	1:C:265:TYR:CZ	2.54	0.43
1:C:512:VAL:O	1:C:513:LEU:C	2.61	0.43
1:C:1076:THR:HB	1:C:1097:SER:HB2	2.01	0.43
1:A:87:ASN:O	1:A:88:ASP:OD1	2.36	0.43
1:A:776:LYS:C	1:A:780:GLU:OE1	2.62	0.43
1:C:850:ILE:HD12	1:C:850:ILE:H	1.84	0.43
1:A:30:ASN:HD22	10:A:1304:NAG:H81	1.83	0.43
1:A:534:VAL:HG22	1:A:535:LYS:H	1.83	0.43
1:A:117:LEU:HD11	1:A:233:ILE:HD11	2.01	0.42
1:A:149:ASN:HB2	10:A:1305:NAG:O5	2.19	0.42
1:B:149:ASN:HA	10:B:1406:NAG:C7	2.48	0.42
1:C:61:ASN:HB2	10:C:1401:NAG:C7	2.49	0.42
1:C:986:PRO:O	1:C:990:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.54	0.42
1:B:1081:ILE:C	1:B:1132:ILE:HD11	2.44	0.42
1:B:1110:TYR:CE1	3:F:1:NAG:H83	2.54	0.42
1:C:108:THR:O	1:C:237:ARG:NE	2.52	0.42
1:C:340:GLU:HA	1:C:343:ASN:HD22	1.84	0.42
1:A:1003:SER:O	1:A:1006:THR:OG1	2.30	0.42
1:B:428:ASP:OD1	1:B:428:ASP:N	2.47	0.42
1:B:676:THR:HA	1:B:690:GLN:HA	2.01	0.42
1:B:1129:VAL:HG22	1:B:1130:ILE:H	1.83	0.42
1:C:901:GLN:O	1:C:905:ARG:HG2	2.19	0.42
1:A:766:ALA:O	1:A:770:ILE:HG12	2.20	0.42
1:A:901:GLN:O	1:A:905:ARG:HG2	2.19	0.42
1:B:960:ASN:O	1:B:964:LYS:HG2	2.19	0.42
1:C:929:SER:OG	1:C:933:LYS:NZ	2.52	0.42
1:A:615:VAL:HG12	1:A:616:ASN:N	2.34	0.42
1:B:676:THR:N	1:B:690:GLN:OE1	2.53	0.42
1:B:1129:VAL:HG23	1:C:917:TYR:HB3	2.00	0.42
1:C:290:ASP:OD1	1:C:291:CYS:N	2.46	0.42
1:C:625:HIS:HB2	1:C:634:ARG:HE	1.84	0.42
1:C:1142:GLN:NE2	1:C:1146:ASP:OD1	2.47	0.42
2:D:2:NAG:C3	2:D:3:BMA:O5	2.67	0.42
1:B:392:PHE:CE1	1:B:515:PHE:CE2	3.08	0.42
1:B:578:ASP:OD1	1:B:580:GLN:N	2.53	0.42
1:C:666:ILE:HD11	1:C:672:ALA:HB2	2.01	0.42
2:D:1:NAG:H4	2:D:2:NAG:N2	2.21	0.42
1:A:713:ALA:HA	1:A:1074:ASN:HB3	2.02	0.42
1:C:919:ASN:O	1:C:920:GLN:C	2.62	0.42
1:A:712:ILE:HD11	1:B:897:PRO:HD3	2.01	0.42
1:A:817:PHE:O	1:A:821:LEU:CD1	2.68	0.42
1:A:1013:ILE:O	1:A:1017:GLU:OE1	2.38	0.42
1:A:1015:ALA:O	1:A:1018:ILE:HG22	2.19	0.42
1:B:427:ASP:OD1	1:B:427:ASP:N	2.51	0.42
1:B:616:ASN:OD1	1:B:616:ASN:C	2.63	0.42
1:B:1110:TYR:HE1	3:F:1:NAG:H83	1.85	0.42
1:C:175:PHE:HB3	1:C:177:MET:HE1	2.02	0.42
1:C:382:VAL:HG23	1:C:383:SER:H	1.85	0.42
7:Y:1:NAG:O3	7:Y:2:NAG:C1	2.67	0.42
1:A:731:MET:HE1	1:A:1018:ILE:HG21	2.02	0.42
1:A:895:GLN:OE1	1:A:895:GLN:N	2.44	0.42
1:A:1010:GLN:O	1:A:1013:ILE:HG22	2.20	0.42
1:B:141:LEU:HD11	1:B:154:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:GLY:O	1:B:498:GLN:NE2	2.52	0.42
1:B:517:LEU:O	1:B:519:HIS:NE2	2.53	0.42
1:C:712:ILE:HG12	1:C:1077:THR:HG21	1.97	0.42
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.41	0.42
1:A:118:LEU:HB3	1:A:129:LYS:HB2	2.02	0.42
1:B:280:ASN:OD1	1:B:283:GLY:N	2.53	0.42
1:B:776:LYS:O	1:B:779:GLN:HB3	2.19	0.42
1:C:53:ASP:OD2	1:C:195:LYS:NZ	2.53	0.42
1:C:921:LYS:O	1:C:925:ASN:ND2	2.52	0.42
1:A:119:ILE:HG23	1:A:128:ILE:CD1	2.49	0.41
1:A:225:PRO:C	1:A:226:LEU:HD12	2.45	0.41
1:A:605:SER:OG	1:A:606:ASN:N	2.53	0.41
1:A:928:ASN:HA	1:A:931:ILE:HG12	2.02	0.41
1:A:1050:MET:SD	1:A:1051:SER:N	2.93	0.41
1:B:874:THR:O	1:B:878:LEU:HD23	2.19	0.41
1:B:1076:THR:HB	1:B:1097:SER:O	2.20	0.41
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.55	0.41
1:C:216:LEU:HD23	1:C:217:PRO:O	2.19	0.41
1:C:614:GLY:N	1:C:647:ALA:O	2.49	0.41
1:A:801:ASN:HB2	2:N:1:NAG:N2	2.35	0.41
1:B:713:ALA:HA	1:B:1074:ASN:HA	2.01	0.41
1:A:66:HIS:CG	1:A:263:ALA:O	2.73	0.41
1:A:149:ASN:CB	10:A:1305:NAG:O5	2.68	0.41
1:A:1134:ASN:OD1	2:M:1:NAG:N2	2.52	0.41
1:B:726:ILE:C	1:B:727:LEU:HD12	2.45	0.41
1:B:417:LYS:HG2	1:B:421:TYR:CZ	2.55	0.41
1:B:761:THR:O	1:B:765:ARG:CZ	2.69	0.41
1:C:605:SER:OG	1:C:606:ASN:N	2.53	0.41
1:C:644:GLN:NE2	1:C:648:GLY:O	2.54	0.41
1:C:763:LEU:HD22	1:C:1008:VAL:HG11	2.01	0.41
1:B:165:ASN:CB	10:B:1407:NAG:N2	2.84	0.41
1:B:375:SER:N	1:B:435:ALA:O	2.54	0.41
1:B:616:ASN:ND2	2:R:1:NAG:C7	2.84	0.41
1:B:1152:LEU:HB2	1:C:1152:LEU:HD11	2.03	0.41
1:C:712:ILE:CB	1:C:1077:THR:HG21	2.51	0.41
2:b:1:NAG:HO6	2:b:2:NAG:C1	2.24	0.41
1:A:86:PHE:N	1:A:236:THR:O	2.46	0.41
1:A:617:CYS:HA	1:A:620:VAL:HG13	2.02	0.41
1:A:738:CYS:O	1:A:742:ILE:HG22	2.21	0.41
1:A:931:ILE:HA	1:A:934:ILE:HG12	2.03	0.41
1:B:860:VAL:O	1:B:860:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:VAL:HG21	1:C:229:LEU:HD21	2.02	0.41
1:C:743:CYS:HB3	1:C:749:CYS:HB3	2.00	0.41
1:C:1060:VAL:HG22	1:C:1061:VAL:N	2.36	0.41
1:A:737:ASP:OD1	1:A:737:ASP:C	2.63	0.41
1:A:1009:THR:O	1:A:1012:LEU:HG	2.21	0.41
1:B:339:GLY:O	1:B:343:ASN:OD1	2.39	0.41
1:B:416:GLY:O	1:B:417:LYS:C	2.63	0.41
1:C:406:GLU:O	1:C:409:GLN:HG3	2.21	0.41
1:A:541:PHE:CD2	1:A:552:LEU:HD21	2.56	0.41
1:C:866:THR:OG1	1:C:869:MET:HE2	2.21	0.41
1:C:919:ASN:HB2	1:C:923:ILE:CD1	2.51	0.41
1:C:1082:CYS:SG	1:C:1132:ILE:HD13	2.61	0.41
1:C:1097:SER:OG	1:C:1102:TRP:CE2	2.74	0.41
2:N:1:NAG:O7	2:N:2:NAG:H83	2.21	0.41
1:A:90:VAL:HG23	1:A:194:PHE:HD2	1.86	0.41
1:A:119:ILE:HG12	1:A:128:ILE:HD12	2.02	0.41
1:A:331:ASN:HB2	5:H:1:NAG:C2	2.51	0.41
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.02	0.41
1:A:996:LEU:HD11	1:A:1000:ARG:HE	1.86	0.41
1:A:1002:GLN:HA	1:A:1005:GLN:HG3	2.03	0.41
1:A:1101:HIS:CD2	2:L:2:NAG:H81	2.56	0.41
1:A:1138:TYR:OH	1:A:1143:PRO:HG3	2.20	0.41
1:B:165:ASN:CB	10:B:1407:NAG:C7	2.98	0.41
1:B:165:ASN:CG	10:B:1407:NAG:N2	2.78	0.41
1:B:215:ASP:OD1	1:B:266:TYR:OH	2.31	0.41
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.41	0.41
1:B:557:LYS:HZ1	1:C:43:PHE:HZ	1.67	0.41
1:B:620:VAL:N	1:B:621:PRO:CD	2.83	0.41
1:B:1103:PHE:C	1:B:1115:ILE:HD11	2.46	0.41
1:B:599:THR:OG1	1:B:608:VAL:HG12	2.20	0.41
1:B:1029:MET:SD	1:B:1033:VAL:HG21	2.61	0.41
1:C:327:VAL:HG22	1:C:328:ARG:N	2.37	0.41
3:E:3:BMA:C6	3:E:4:MAN:H5	2.51	0.41
1:A:444:LYS:HD2	1:A:446:GLY:H	1.86	0.40
1:A:1129:VAL:HG22	1:A:1130:ILE:N	2.35	0.40
1:C:433:VAL:HG13	1:C:433:VAL:O	2.21	0.40
1:A:335:LEU:HD22	1:A:367:VAL:HG11	2.02	0.40
1:A:445:VAL:HG23	1:A:446:GLY:N	2.36	0.40
1:A:820:ASP:O	1:A:824:ASN:ND2	2.54	0.40
1:B:196:ASN:ND2	1:B:233:ILE:O	2.54	0.40
1:B:928:ASN:O	1:B:931:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:ILE:HA	1:B:934:ILE:HG12	2.03	0.40
2:U:1:NAG:H83	2:U:1:NAG:H3	2.03	0.40
8:a:2:NAG:H3	8:a:3:BMA:O5	2.22	0.40
1:A:569:ILE:HD12	1:A:569:ILE:H	1.87	0.40
1:A:885:GLY:N	1:A:896:ILE:HD11	2.36	0.40
1:B:148:ASN:O	10:B:1406:NAG:N2	2.54	0.40
1:C:80:ASP:OD1	1:C:80:ASP:N	2.54	0.40
1:C:193:VAL:HB	1:C:204:TYR:HB2	2.04	0.40
1:C:1129:VAL:HG22	1:C:1130:ILE:N	2.35	0.40
1:C:1148:PHE:O	1:C:1152:LEU:HB2	2.21	0.40
3:E:3:BMA:H4	3:E:4:MAN:C5	2.29	0.40
4:I:1:NAG:H4	4:I:2:NAG:H2	1.97	0.40
1:A:350:VAL:HG13	1:A:351:TYR:N	2.37	0.40
1:A:742:ILE:CG2	1:A:743:CYS:N	2.85	0.40
1:A:790:LYS:NZ	1:A:791:THR:O	2.50	0.40
1:B:129:LYS:HG2	1:B:131:CYS:SG	2.61	0.40
1:C:135:PHE:HA	1:C:160:TYR:HA	2.03	0.40
1:C:354:ASN:OD1	1:C:355:ARG:N	2.55	0.40
2:b:2:NAG:N2	2:b:2:NAG:O4	2.54	0.40
1:A:336:CYS:O	1:A:338:PHE:N	2.48	0.40
1:B:885:GLY:N	1:B:896:ILE:HD11	2.37	0.40
1:B:901:GLN:O	1:B:905:ARG:HG2	2.22	0.40
1:C:393:THR:OG1	1:C:394:ASN:N	2.54	0.40
1:C:1015:ALA:HA	1:C:1018:ILE:HG22	2.04	0.40
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.55	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	1028/1312 (78%)	950 (92%)	78 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1064/1312 (81%)	968 (91%)	95 (9%)	1 (0%)	48	82
1	C	1061/1312 (81%)	941 (89%)	117 (11%)	3 (0%)	36	70
All	All	3153/3936 (80%)	2859 (91%)	290 (9%)	4 (0%)	49	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	LYS
1	C	327	VAL
1	C	234	ASN
1	B	332	ILE

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	905/1135 (80%)	905 (100%)	0	100	100
1	B	931/1135 (82%)	931 (100%)	0	100	100
1	C	925/1135 (82%)	925 (100%)	0	100	100
All	All	2761/3405 (81%)	2761 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	644	GLN
1	A	925	ASN
1	A	928	ASN
1	A	1010	GLN
1	A	1011	GLN
1	A	1058	HIS

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Mol	Chain	Res	Type
1	A	1106	GLN
1	B	928	ASN
1	B	1048	HIS
1	C	115	GLN
1	C	448	ASN
1	C	544	ASN
1	C	925	ASN
1	C	928	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

89 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	1.99	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	D	2	2	14,14,15	2.05	4 (28%)	17,19,21	1.43	2 (11%)
2	BMA	D	3	2	11,11,12	0.90	1 (9%)	15,15,17	0.92	1 (6%)
3	NAG	E	1	1,3	14,14,15	2.05	5 (35%)	17,19,21	1.03	2 (11%)
3	NAG	E	2	3	14,14,15	2.01	3 (21%)	17,19,21	1.14	2 (11%)
3	BMA	E	3	3	11,11,12	0.46	0	15,15,17	0.71	0
3	MAN	E	4	3	11,11,12	0.86	0	15,15,17	1.49	2 (13%)
3	NAG	F	1	1,3	14,14,15	2.30	4 (28%)	17,19,21	1.96	4 (23%)
3	NAG	F	2	3	14,14,15	2.14	4 (28%)	17,19,21	1.45	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	0.66	0	15,15,17	0.84	0
3	MAN	F	4	3	11,11,12	0.89	1 (9%)	15,15,17	1.57	2 (13%)
4	NAG	G	1	1,4	14,14,15	2.42	5 (35%)	17,19,21	2.58	8 (47%)
4	NAG	G	2	4	14,14,15	2.02	4 (28%)	17,19,21	1.25	1 (5%)
5	NAG	H	1	1,5	14,14,15	2.14	4 (28%)	17,19,21	1.56	3 (17%)
5	NAG	H	2	5	14,14,15	1.95	3 (21%)	17,19,21	1.97	5 (29%)
5	BMA	H	3	5	11,11,12	0.54	0	15,15,17	0.66	0
5	FUC	H	4	5	10,10,11	0.76	0	14,14,16	0.65	0
4	NAG	I	1	1,4	14,14,15	2.09	5 (35%)	17,19,21	1.32	1 (5%)
4	NAG	I	2	4	14,14,15	2.09	4 (28%)	17,19,21	1.12	1 (5%)
6	NAG	J	1	1,6	14,14,15	2.07	5 (35%)	17,19,21	1.28	2 (11%)
6	NAG	J	2	6	14,14,15	2.03	5 (35%)	17,19,21	1.18	2 (11%)
6	BMA	J	3	6	11,11,12	1.12	1 (9%)	15,15,17	0.87	0
6	MAN	J	4	6	11,11,12	1.28	3 (27%)	15,15,17	2.39	3 (20%)
4	NAG	K	1	1,4	14,14,15	2.07	4 (28%)	17,19,21	1.71	4 (23%)
4	NAG	K	2	4	14,14,15	1.94	4 (28%)	17,19,21	1.11	2 (11%)
2	NAG	L	1	1,2	14,14,15	2.16	4 (28%)	17,19,21	1.48	2 (11%)
2	NAG	L	2	2	14,14,15	1.95	4 (28%)	17,19,21	1.30	1 (5%)
2	BMA	L	3	2	11,11,12	0.95	1 (9%)	15,15,17	0.84	0
2	NAG	M	1	1,2	14,14,15	2.28	6 (42%)	17,19,21	2.38	8 (47%)
2	NAG	M	2	2	14,14,15	1.96	4 (28%)	17,19,21	1.57	3 (17%)
2	BMA	M	3	2	11,11,12	0.46	0	15,15,17	0.74	0
2	NAG	N	1	1,2	14,14,15	2.05	4 (28%)	17,19,21	1.55	3 (17%)
2	NAG	N	2	2	14,14,15	1.92	4 (28%)	17,19,21	1.23	1 (5%)
2	BMA	N	3	2	11,11,12	0.68	0	15,15,17	0.72	0
4	NAG	O	1	4	14,14,15	1.95	5 (35%)	17,19,21	1.33	2 (11%)
4	NAG	O	2	4	14,14,15	1.99	4 (28%)	17,19,21	1.09	2 (11%)
2	NAG	P	1	1,2	14,14,15	2.03	4 (28%)	17,19,21	1.39	3 (17%)
2	NAG	P	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.41	3 (17%)
2	BMA	P	3	2	11,11,12	0.64	0	15,15,17	0.86	1 (6%)
4	NAG	Q	1	1,4	14,14,15	2.05	4 (28%)	17,19,21	1.21	2 (11%)
4	NAG	Q	2	4	14,14,15	2.07	4 (28%)	17,19,21	1.44	3 (17%)
2	NAG	R	1	1,2	14,14,15	2.07	4 (28%)	17,19,21	1.28	2 (11%)
2	NAG	R	2	2	14,14,15	2.26	5 (35%)	17,19,21	2.22	5 (29%)
2	BMA	R	3	2	11,11,12	0.62	0	15,15,17	0.77	0
2	NAG	S	1	1,2	14,14,15	2.09	4 (28%)	17,19,21	2.04	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	S	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.31	2 (11%)
2	BMA	S	3	2	11,11,12	0.55	0	15,15,17	0.75	0
4	NAG	T	1	1,4	14,14,15	1.98	3 (21%)	17,19,21	1.28	1 (5%)
4	NAG	T	2	4	14,14,15	1.97	4 (28%)	17,19,21	1.29	2 (11%)
2	NAG	U	1	1,2	14,14,15	2.05	4 (28%)	17,19,21	1.60	4 (23%)
2	NAG	U	2	2	14,14,15	2.05	4 (28%)	17,19,21	1.26	2 (11%)
2	BMA	U	3	2	11,11,12	0.65	0	15,15,17	0.69	0
2	NAG	V	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	2.14	4 (23%)
2	NAG	V	2	2	14,14,15	1.94	3 (21%)	17,19,21	1.22	2 (11%)
2	BMA	V	3	2	11,11,12	0.72	0	15,15,17	0.69	0
2	NAG	W	1	1,2	14,14,15	1.88	3 (21%)	17,19,21	2.13	7 (41%)
2	NAG	W	2	2	14,14,15	1.92	3 (21%)	17,19,21	1.36	3 (17%)
2	BMA	W	3	2	11,11,12	0.57	0	15,15,17	0.68	0
2	NAG	X	1	1,2	14,14,15	2.00	4 (28%)	17,19,21	1.35	2 (11%)
2	NAG	X	2	2	14,14,15	1.98	4 (28%)	17,19,21	1.47	2 (11%)
2	BMA	X	3	2	11,11,12	0.59	0	15,15,17	0.68	0
7	NAG	Y	1	7	14,14,15	1.97	5 (35%)	17,19,21	1.31	2 (11%)
7	NAG	Y	2	7	14,14,15	2.06	3 (21%)	17,19,21	1.42	3 (17%)
7	FUC	Y	3	7	10,10,11	0.60	0	14,14,16	0.73	0
6	NAG	Z	1	1,6	14,14,15	1.94	5 (35%)	17,19,21	1.26	2 (11%)
6	NAG	Z	2	6	14,14,15	1.95	3 (21%)	17,19,21	1.00	1 (5%)
6	BMA	Z	3	6	11,11,12	0.53	0	15,15,17	0.86	0
6	MAN	Z	4	6	11,11,12	0.59	0	15,15,17	0.99	2 (13%)
8	NAG	a	1	8,1	14,14,15	2.04	5 (35%)	17,19,21	1.16	2 (11%)
8	NAG	a	2	8	14,14,15	2.15	4 (28%)	17,19,21	1.62	4 (23%)
8	BMA	a	3	8	11,11,12	0.58	0	15,15,17	0.71	0
8	MAN	a	4	8	11,11,12	0.76	0	15,15,17	1.41	3 (20%)
8	MAN	a	5	8	11,11,12	0.64	0	15,15,17	1.32	1 (6%)
2	NAG	b	1	2	14,14,15	2.04	5 (35%)	17,19,21	1.40	3 (17%)
2	NAG	b	2	2	14,14,15	2.08	4 (28%)	17,19,21	1.20	2 (11%)
2	BMA	b	3	2	11,11,12	0.63	0	15,15,17	0.68	0
9	NAG	c	1	1,9	14,14,15	1.83	5 (35%)	17,19,21	2.29	6 (35%)
9	NAG	c	2	9	14,14,15	1.90	3 (21%)	17,19,21	2.06	4 (23%)
9	BMA	c	3	9	11,11,12	0.82	0	15,15,17	0.81	0
9	MAN	c	4	9	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
8	NAG	d	1	8	14,14,15	2.02	4 (28%)	17,19,21	1.46	2 (11%)
8	NAG	d	2	8	14,14,15	1.94	3 (21%)	17,19,21	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	d	3	8	11,11,12	0.81	0	15,15,17	0.79	0
8	MAN	d	4	8	11,11,12	0.75	0	15,15,17	1.18	2 (13%)
8	MAN	d	5	8	11,11,12	0.67	0	15,15,17	0.84	1 (6%)
4	NAG	e	1	1,4	14,14,15	1.94	4 (28%)	17,19,21	1.29	2 (11%)
4	NAG	e	2	4	14,14,15	2.00	4 (28%)	17,19,21	1.08	1 (5%)
4	NAG	f	1	1,4	14,14,15	2.08	5 (35%)	17,19,21	1.25	2 (11%)
4	NAG	f	2	4	14,14,15	2.06	4 (28%)	17,19,21	1.32	2 (11%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	Y	3	7	-	-	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	6/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	1/1/1/1
8	MAN	a	4	8	-	0/2/19/22	0/1/1/1
8	MAN	a	5	8	-	1/2/19/22	1/1/1/1
2	NAG	b	1	2	-	1/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	BMA	b	3	2	-	2/2/19/22	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	1/6/23/26	0/1/1/1
9	BMA	c	3	9	-	2/2/19/22	0/1/1/1
9	MAN	c	4	9	-	0/2/19/22	0/1/1/1
8	NAG	d	1	8	-	5/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	BMA	d	3	8	-	2/2/19/22	0/1/1/1
8	MAN	d	4	8	-	1/2/19/22	0/1/1/1
8	MAN	d	5	8	-	0/2/19/22	0/1/1/1
4	NAG	e	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	5.60	1.53	1.43
2	R	2	NAG	O5-C1	5.34	1.52	1.43
3	F	2	NAG	O5-C1	4.86	1.51	1.43
2	S	1	NAG	O5-C1	4.73	1.51	1.43
3	F	1	NAG	C7-N2	4.71	1.49	1.34
8	a	2	NAG	O5-C1	4.65	1.51	1.43
2	b	2	NAG	O5-C1	4.65	1.51	1.43
5	H	1	NAG	O5-C1	4.64	1.51	1.43
4	Q	1	NAG	O5-C1	4.59	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	O5-C1	4.57	1.51	1.43
4	Q	2	NAG	O5-C1	4.56	1.51	1.43
7	Y	2	NAG	O5-C1	4.54	1.51	1.43
4	I	1	NAG	O5-C1	4.51	1.51	1.43
4	f	2	NAG	O5-C1	4.51	1.51	1.43
2	N	1	NAG	O5-C1	4.50	1.51	1.43
2	P	1	NAG	O5-C1	4.48	1.51	1.43
2	P	2	NAG	O5-C1	4.43	1.51	1.43
8	a	1	NAG	O5-C1	4.43	1.51	1.43
2	R	1	NAG	O5-C1	4.41	1.51	1.43
2	L	1	NAG	O5-C1	4.38	1.51	1.43
3	E	1	NAG	O5-C1	4.36	1.51	1.43
3	F	1	NAG	O5-C1	4.34	1.51	1.43
4	K	1	NAG	C7-N2	4.34	1.48	1.34
6	J	1	NAG	O5-C1	4.33	1.51	1.43
2	U	2	NAG	O5-C1	4.31	1.50	1.43
4	e	2	NAG	O5-C1	4.30	1.50	1.43
4	O	2	NAG	O5-C1	4.30	1.50	1.43
2	U	1	NAG	O5-C1	4.29	1.50	1.43
6	J	2	NAG	O5-C1	4.28	1.50	1.43
2	D	2	NAG	O5-C1	4.26	1.50	1.43
5	H	2	NAG	O5-C1	4.25	1.50	1.43
4	T	2	NAG	O5-C1	4.24	1.50	1.43
3	E	2	NAG	O5-C1	4.23	1.50	1.43
2	b	1	NAG	O5-C1	4.20	1.50	1.43
4	G	1	NAG	C7-N2	4.19	1.47	1.34
4	f	1	NAG	O5-C1	4.19	1.50	1.43
2	D	1	NAG	O5-C1	4.18	1.50	1.43
8	d	1	NAG	O5-C1	4.16	1.50	1.43
4	G	2	NAG	O5-C1	4.15	1.50	1.43
2	V	1	NAG	C7-N2	4.14	1.47	1.34
4	T	1	NAG	O5-C1	4.14	1.50	1.43
2	X	1	NAG	O5-C1	4.13	1.50	1.43
2	V	2	NAG	O5-C1	4.13	1.50	1.43
2	S	2	NAG	O5-C1	4.11	1.50	1.43
2	L	2	NAG	O5-C1	4.09	1.50	1.43
4	K	2	NAG	O5-C1	4.09	1.50	1.43
2	L	1	NAG	C7-N2	4.06	1.47	1.34
2	N	2	NAG	O5-C1	4.05	1.50	1.43
2	U	1	NAG	C7-N2	4.03	1.47	1.34
6	Z	2	NAG	O5-C1	4.02	1.50	1.43
4	e	1	NAG	O5-C1	4.02	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	2	NAG	C7-N2	4.02	1.47	1.34
2	M	2	NAG	C7-N2	4.02	1.47	1.34
5	H	1	NAG	C7-N2	4.02	1.47	1.34
7	Y	1	NAG	O5-C1	3.99	1.50	1.43
2	U	2	NAG	C7-N2	3.99	1.47	1.34
8	d	2	NAG	O5-C1	3.99	1.50	1.43
4	I	1	NAG	C7-N2	3.98	1.47	1.34
2	W	2	NAG	O5-C1	3.98	1.50	1.43
4	T	1	NAG	C7-N2	3.98	1.47	1.34
2	M	1	NAG	C7-N2	3.97	1.47	1.34
2	X	1	NAG	C7-N2	3.97	1.47	1.34
6	Z	2	NAG	C7-N2	3.97	1.47	1.34
2	D	2	NAG	C7-N2	3.97	1.47	1.34
4	G	2	NAG	C7-N2	3.96	1.47	1.34
2	X	2	NAG	O5-C1	3.96	1.50	1.43
2	R	2	NAG	C7-N2	3.96	1.47	1.34
2	X	2	NAG	C7-N2	3.95	1.47	1.34
4	Q	2	NAG	C7-N2	3.95	1.47	1.34
3	E	2	NAG	C7-N2	3.95	1.47	1.34
2	R	1	NAG	C7-N2	3.95	1.47	1.34
8	d	2	NAG	C7-N2	3.95	1.47	1.34
4	I	2	NAG	C7-N2	3.93	1.47	1.34
4	O	1	NAG	O5-C1	3.91	1.50	1.43
4	T	2	NAG	C7-N2	3.90	1.46	1.34
9	c	2	NAG	C7-N2	3.90	1.46	1.34
3	F	2	NAG	C7-N2	3.89	1.46	1.34
4	O	1	NAG	C7-N2	3.89	1.46	1.34
2	V	2	NAG	C7-N2	3.89	1.46	1.34
2	S	2	NAG	C7-N2	3.88	1.46	1.34
6	J	1	NAG	C7-N2	3.88	1.46	1.34
2	W	1	NAG	C7-N2	3.87	1.46	1.34
2	W	2	NAG	C7-N2	3.87	1.46	1.34
4	e	1	NAG	C7-N2	3.87	1.46	1.34
4	f	2	NAG	C7-N2	3.87	1.46	1.34
4	e	2	NAG	C7-N2	3.87	1.46	1.34
8	d	1	NAG	C7-N2	3.87	1.46	1.34
4	O	2	NAG	C7-N2	3.87	1.46	1.34
6	Z	1	NAG	C7-N2	3.87	1.46	1.34
2	b	2	NAG	C7-N2	3.86	1.46	1.34
4	Q	1	NAG	C7-N2	3.86	1.46	1.34
7	Y	2	NAG	C7-N2	3.86	1.46	1.34
2	P	2	NAG	C7-N2	3.86	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	1	NAG	C7-N2	3.85	1.46	1.34
5	H	2	NAG	C7-N2	3.85	1.46	1.34
2	P	1	NAG	C7-N2	3.85	1.46	1.34
2	N	1	NAG	C7-N2	3.84	1.46	1.34
6	Z	1	NAG	O5-C1	3.84	1.50	1.43
6	J	2	NAG	C7-N2	3.84	1.46	1.34
4	K	2	NAG	C7-N2	3.83	1.46	1.34
3	E	1	NAG	C7-N2	3.83	1.46	1.34
2	D	1	NAG	C7-N2	3.83	1.46	1.34
2	L	2	NAG	C7-N2	3.82	1.46	1.34
8	a	1	NAG	C7-N2	3.82	1.46	1.34
2	N	2	NAG	C7-N2	3.80	1.46	1.34
2	S	1	NAG	C7-N2	3.78	1.46	1.34
7	Y	1	NAG	C7-N2	3.77	1.46	1.34
4	G	1	NAG	O5-C5	3.76	1.50	1.43
2	M	2	NAG	O5-C1	3.75	1.50	1.43
4	f	1	NAG	C7-N2	3.69	1.46	1.34
4	K	1	NAG	O5-C1	3.61	1.49	1.43
9	c	2	NAG	O5-C1	3.57	1.49	1.43
9	c	1	NAG	C7-N2	3.55	1.45	1.34
2	W	1	NAG	O5-C1	3.53	1.49	1.43
2	M	1	NAG	O5-C1	3.46	1.49	1.43
2	V	1	NAG	O5-C1	3.46	1.49	1.43
9	c	1	NAG	O5-C1	3.25	1.49	1.43
2	M	1	NAG	C2-N2	3.10	1.51	1.46
2	M	1	NAG	C1-C2	3.07	1.56	1.52
2	M	1	NAG	O5-C5	3.02	1.49	1.43
2	V	1	NAG	C2-N2	2.98	1.51	1.46
3	F	1	NAG	C2-N2	2.96	1.51	1.46
4	G	2	NAG	C2-N2	2.93	1.51	1.46
8	a	2	NAG	C2-N2	2.88	1.51	1.46
2	S	1	NAG	O5-C5	2.83	1.49	1.43
2	U	1	NAG	C2-N2	2.83	1.50	1.46
4	K	1	NAG	C2-N2	2.77	1.50	1.46
2	L	1	NAG	O5-C5	2.77	1.48	1.43
2	R	1	NAG	C2-N2	2.75	1.50	1.46
9	c	2	NAG	C2-N2	2.75	1.50	1.46
2	M	2	NAG	C2-N2	2.70	1.50	1.46
3	E	2	NAG	C2-N2	2.70	1.50	1.46
2	D	2	NAG	C2-N2	2.69	1.50	1.46
2	L	3	BMA	C1-C2	2.68	1.58	1.52
5	H	1	NAG	C2-N2	2.67	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	2	NAG	C2-N2	2.67	1.50	1.46
3	F	2	NAG	C2-N2	2.66	1.50	1.46
4	f	1	NAG	O5-C5	2.65	1.48	1.43
5	H	2	NAG	C2-N2	2.64	1.50	1.46
8	d	2	NAG	C2-N2	2.63	1.50	1.46
2	R	2	NAG	O5-C5	2.62	1.48	1.43
6	J	4	MAN	C1-C2	2.62	1.58	1.52
6	J	1	NAG	O5-C5	2.62	1.48	1.43
4	e	1	NAG	C2-N2	2.62	1.50	1.46
6	Z	2	NAG	C2-N2	2.61	1.50	1.46
4	I	2	NAG	C2-N2	2.60	1.50	1.46
2	L	1	NAG	C2-N2	2.60	1.50	1.46
3	F	1	NAG	O5-C5	2.60	1.48	1.43
4	G	1	NAG	C2-N2	2.59	1.50	1.46
7	Y	2	NAG	C2-N2	2.57	1.50	1.46
4	Q	2	NAG	C2-N2	2.57	1.50	1.46
4	T	1	NAG	C2-N2	2.55	1.50	1.46
9	c	1	NAG	C2-N2	2.54	1.50	1.46
2	X	1	NAG	C2-N2	2.53	1.50	1.46
2	S	2	NAG	C2-N2	2.52	1.50	1.46
4	I	1	NAG	C2-N2	2.51	1.50	1.46
2	b	1	NAG	O5-C5	2.51	1.48	1.43
2	W	2	NAG	C2-N2	2.50	1.50	1.46
6	J	2	NAG	C2-N2	2.50	1.50	1.46
2	W	1	NAG	C2-N2	2.50	1.50	1.46
4	O	1	NAG	C2-N2	2.49	1.50	1.46
2	X	2	NAG	C2-N2	2.48	1.50	1.46
4	e	2	NAG	C2-N2	2.48	1.50	1.46
4	Q	1	NAG	C2-N2	2.45	1.50	1.46
2	V	2	NAG	C2-N2	2.44	1.50	1.46
2	P	2	NAG	C2-N2	2.44	1.50	1.46
8	d	1	NAG	C2-N2	2.43	1.50	1.46
4	T	2	NAG	C2-N2	2.42	1.50	1.46
2	R	1	NAG	O5-C5	2.42	1.48	1.43
6	J	1	NAG	C2-N2	2.41	1.50	1.46
2	D	1	NAG	C2-N2	2.41	1.50	1.46
2	R	2	NAG	C2-N2	2.41	1.50	1.46
3	E	1	NAG	C2-N2	2.40	1.50	1.46
4	f	2	NAG	C2-N2	2.40	1.50	1.46
2	b	1	NAG	C2-N2	2.40	1.50	1.46
4	O	2	NAG	C2-N2	2.40	1.50	1.46
2	P	1	NAG	C2-N2	2.39	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2	NAG	O5-C5	2.39	1.48	1.43
2	N	1	NAG	C2-N2	2.39	1.50	1.46
2	M	1	NAG	C3-C2	-2.38	1.47	1.52
2	b	2	NAG	C2-N2	2.37	1.50	1.46
4	f	2	NAG	O5-C5	2.37	1.48	1.43
4	f	1	NAG	C2-N2	2.37	1.50	1.46
6	Z	1	NAG	C2-N2	2.36	1.50	1.46
4	K	2	NAG	C2-N2	2.35	1.50	1.46
2	L	2	NAG	C2-N2	2.35	1.50	1.46
8	a	1	NAG	O5-C5	2.33	1.48	1.43
5	H	1	NAG	O5-C5	2.33	1.48	1.43
3	E	1	NAG	O5-C5	2.32	1.48	1.43
2	S	2	NAG	O5-C5	2.32	1.47	1.43
7	Y	1	NAG	O5-C5	2.31	1.47	1.43
8	a	1	NAG	C2-N2	2.31	1.50	1.46
6	J	4	MAN	O5-C1	2.31	1.47	1.43
2	X	2	NAG	O5-C5	2.30	1.47	1.43
4	I	1	NAG	O5-C5	2.30	1.47	1.43
2	N	2	NAG	O5-C5	2.29	1.47	1.43
7	Y	1	NAG	C2-N2	2.28	1.50	1.46
2	L	2	NAG	O5-C5	2.28	1.47	1.43
4	K	1	NAG	C3-C2	-2.28	1.47	1.52
8	a	1	NAG	C3-C2	-2.27	1.47	1.52
2	N	2	NAG	C2-N2	2.27	1.50	1.46
2	X	1	NAG	O5-C5	2.26	1.47	1.43
4	f	1	NAG	C3-C2	-2.25	1.47	1.52
2	b	2	NAG	O5-C5	2.25	1.47	1.43
3	F	2	NAG	O5-C5	2.25	1.47	1.43
2	D	2	NAG	O5-C5	2.25	1.47	1.43
2	b	1	NAG	C3-C2	-2.24	1.47	1.52
4	Q	1	NAG	O5-C5	2.24	1.47	1.43
4	I	2	NAG	O5-C5	2.21	1.47	1.43
8	a	2	NAG	O5-C5	2.21	1.47	1.43
2	U	2	NAG	O5-C5	2.20	1.47	1.43
3	E	1	NAG	C3-C2	-2.20	1.47	1.52
2	D	1	NAG	O5-C5	2.19	1.47	1.43
2	R	2	NAG	C3-C2	-2.19	1.47	1.52
7	Y	1	NAG	C3-C2	-2.19	1.47	1.52
6	J	1	NAG	C3-C2	-2.18	1.47	1.52
4	K	2	NAG	O5-C5	2.18	1.47	1.43
2	D	3	BMA	C1-C2	2.17	1.57	1.52
4	O	2	NAG	O5-C5	2.17	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	NAG	C2-N2	2.15	1.49	1.46
6	J	4	MAN	O5-C5	2.14	1.47	1.43
4	Q	2	NAG	O5-C5	2.14	1.47	1.43
6	Z	1	NAG	O5-C5	2.14	1.47	1.43
6	J	3	BMA	C4-C3	2.12	1.57	1.52
8	d	1	NAG	O5-C5	2.12	1.47	1.43
4	T	2	NAG	O5-C5	2.12	1.47	1.43
2	P	1	NAG	O5-C5	2.11	1.47	1.43
4	e	2	NAG	O5-C5	2.10	1.47	1.43
4	O	1	NAG	O5-C5	2.10	1.47	1.43
6	Z	1	NAG	C3-C2	-2.10	1.48	1.52
6	J	2	NAG	C3-C2	-2.09	1.48	1.52
2	N	1	NAG	O5-C5	2.09	1.47	1.43
4	G	2	NAG	O5-C5	2.08	1.47	1.43
9	c	1	NAG	O7-C7	-2.08	1.18	1.23
2	M	2	NAG	C3-C2	-2.07	1.48	1.52
2	U	1	NAG	O5-C5	2.07	1.47	1.43
4	G	1	NAG	C3-C2	-2.03	1.48	1.52
4	I	1	NAG	C3-C2	-2.03	1.48	1.52
4	e	1	NAG	O5-C5	2.03	1.47	1.43
9	c	1	NAG	C3-C2	-2.03	1.48	1.52
2	P	2	NAG	O5-C5	2.02	1.47	1.43
3	F	4	MAN	C1-C2	2.01	1.57	1.52
4	O	1	NAG	C3-C2	-2.00	1.48	1.52

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	4	MAN	C1-O5-C5	8.12	123.07	112.19
4	G	1	NAG	C1-O5-C5	6.81	121.31	112.19
2	V	1	NAG	C1-O5-C5	-6.64	103.28	112.19
3	F	1	NAG	C1-O5-C5	-6.36	103.67	112.19
2	R	2	NAG	C1-O5-C5	5.69	119.81	112.19
5	H	2	NAG	C4-C3-C2	5.27	118.74	111.02
2	S	1	NAG	C1-O5-C5	5.08	118.99	112.19
3	F	4	MAN	C1-O5-C5	4.96	118.83	112.19
3	E	4	MAN	C1-O5-C5	4.94	118.80	112.19
2	W	1	NAG	C3-C4-C5	4.86	119.05	110.23
9	c	2	NAG	C3-C4-C5	4.78	118.90	110.23
2	M	1	NAG	O4-C4-C3	-4.63	99.47	110.38
8	a	2	NAG	C8-C7-N2	4.57	123.69	116.12
2	U	1	NAG	C8-C7-N2	4.51	123.60	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NAG	C3-C4-C5	4.39	118.18	110.23
4	K	1	NAG	C8-C7-N2	4.37	123.37	116.12
9	c	1	NAG	C2-N2-C7	-4.35	117.08	122.90
8	a	5	MAN	C1-O5-C5	4.29	117.93	112.19
9	c	2	NAG	C4-C3-C2	4.24	117.23	111.02
2	M	1	NAG	O5-C5-C4	4.01	120.57	110.83
2	N	1	NAG	C1-C2-N2	3.93	116.62	110.43
2	W	1	NAG	C4-C3-C2	3.89	116.73	111.02
9	c	1	NAG	C8-C7-N2	3.86	122.52	116.12
9	c	1	NAG	C3-C4-C5	3.74	117.01	110.23
2	M	2	NAG	C8-C7-N2	3.60	122.08	116.12
8	a	4	MAN	C1-O5-C5	3.57	116.97	112.19
2	L	1	NAG	C8-C7-N2	3.50	121.92	116.12
5	H	1	NAG	C8-C7-N2	3.49	121.90	116.12
2	M	1	NAG	O5-C1-C2	-3.39	106.04	111.29
2	R	2	NAG	C2-N2-C7	-3.39	118.36	122.90
2	X	1	NAG	C8-C7-N2	3.37	121.71	116.12
4	T	1	NAG	C8-C7-N2	3.34	121.66	116.12
2	V	2	NAG	C1-O5-C5	-3.34	107.71	112.19
4	G	1	NAG	C8-C7-N2	3.32	121.62	116.12
2	D	2	NAG	C1-O5-C5	3.32	116.63	112.19
2	V	1	NAG	C4-C3-C2	3.31	115.87	111.02
4	Q	2	NAG	C8-C7-N2	3.29	121.57	116.12
9	c	1	NAG	C4-C3-C2	3.27	115.81	111.02
8	d	4	MAN	C1-O5-C5	3.26	116.56	112.19
4	I	1	NAG	C8-C7-N2	3.23	121.47	116.12
4	f	2	NAG	C1-O5-C5	3.22	116.50	112.19
2	R	2	NAG	O5-C1-C2	3.22	116.27	111.29
9	c	1	NAG	C1-O5-C5	-3.18	107.92	112.19
2	X	2	NAG	C8-C7-N2	3.16	121.35	116.12
8	d	1	NAG	C8-C7-N2	3.13	121.31	116.12
3	F	2	NAG	C2-N2-C7	-3.11	118.73	122.90
4	G	1	NAG	O5-C5-C4	3.10	118.37	110.83
4	G	2	NAG	C1-O5-C5	-3.08	108.06	112.19
4	e	1	NAG	C4-C3-C2	3.06	115.51	111.02
9	c	1	NAG	O7-C7-N2	-3.06	116.57	121.98
5	H	2	NAG	C3-C4-C5	3.04	115.74	110.23
2	R	2	NAG	C4-C3-C2	-3.02	106.58	111.02
2	b	2	NAG	C2-N2-C7	-3.01	118.87	122.90
3	F	2	NAG	C1-O5-C5	3.00	116.21	112.19
7	Y	2	NAG	O5-C1-C2	2.94	115.83	111.29
3	F	1	NAG	C8-C7-N2	2.89	120.91	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	2	NAG	C8-C7-N2	2.86	120.87	116.12
8	d	2	NAG	O5-C1-C2	2.84	115.68	111.29
8	d	1	NAG	O4-C4-C5	2.84	116.31	109.32
2	U	1	NAG	C4-C3-C2	-2.81	106.90	111.02
9	c	4	MAN	C1-O5-C5	2.77	115.90	112.19
2	S	2	NAG	C8-C7-N2	2.77	120.71	116.12
2	U	2	NAG	C1-O5-C5	2.75	115.88	112.19
2	S	1	NAG	C1-C2-N2	-2.75	106.10	110.43
2	P	2	NAG	C2-N2-C7	-2.74	119.23	122.90
4	K	1	NAG	C1-O5-C5	-2.74	108.52	112.19
4	G	1	NAG	C4-C3-C2	2.73	115.01	111.02
2	W	1	NAG	C1-O5-C5	-2.72	108.54	112.19
2	V	1	NAG	C3-C4-C5	2.71	115.15	110.23
7	Y	2	NAG	C1-O5-C5	2.71	115.82	112.19
3	F	2	NAG	C8-C7-N2	2.69	120.58	116.12
3	F	4	MAN	O2-C2-C3	-2.68	104.61	110.15
2	b	2	NAG	C8-C7-N2	2.67	120.55	116.12
4	f	1	NAG	O4-C4-C5	2.66	115.88	109.32
4	G	1	NAG	C2-N2-C7	-2.66	119.33	122.90
2	R	1	NAG	C8-C7-N2	2.66	120.53	116.12
2	M	2	NAG	C1-O5-C5	-2.66	108.63	112.19
2	P	1	NAG	C2-N2-C7	-2.59	119.43	122.90
2	N	1	NAG	O5-C1-C2	-2.59	107.29	111.29
2	P	2	NAG	C8-C7-N2	2.57	120.38	116.12
4	O	1	NAG	C8-C7-N2	2.55	120.35	116.12
2	D	1	NAG	C2-N2-C7	-2.54	119.49	122.90
8	a	4	MAN	O2-C2-C3	-2.54	104.89	110.15
4	O	1	NAG	C2-N2-C7	-2.54	119.50	122.90
8	a	1	NAG	C2-N2-C7	-2.54	119.50	122.90
2	W	2	NAG	C1-O5-C5	-2.53	108.79	112.19
2	D	3	BMA	O2-C2-C3	-2.52	104.93	110.15
6	J	4	MAN	O5-C1-C2	2.51	116.78	110.79
7	Y	1	NAG	C2-N2-C7	-2.49	119.56	122.90
4	T	2	NAG	C8-C7-N2	2.49	120.25	116.12
6	J	1	NAG	C1-O5-C5	2.48	115.51	112.19
2	P	1	NAG	C8-C7-N2	2.48	120.23	116.12
4	Q	2	NAG	C1-O5-C5	2.48	115.51	112.19
2	M	1	NAG	C6-C5-C4	-2.48	106.93	113.02
3	E	2	NAG	C8-C7-N2	2.46	120.20	116.12
6	Z	4	MAN	C1-O5-C5	2.46	115.48	112.19
4	K	2	NAG	C2-N2-C7	-2.45	119.62	122.90
5	H	1	NAG	C1-O5-C5	2.43	115.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	2	NAG	O5-C1-C2	-2.42	107.54	111.29
8	d	4	MAN	O2-C2-C3	-2.42	105.14	110.15
4	Q	1	NAG	C8-C7-N2	2.42	120.13	116.12
3	E	2	NAG	C2-N2-C7	-2.41	119.67	122.90
2	b	1	NAG	C8-C7-N2	2.41	120.11	116.12
2	W	2	NAG	C8-C7-N2	2.41	120.11	116.12
2	M	2	NAG	C3-C4-C5	2.40	114.59	110.23
7	Y	2	NAG	C8-C7-N2	2.40	120.10	116.12
2	W	1	NAG	C8-C7-N2	2.40	120.10	116.12
2	S	2	NAG	C2-N2-C7	-2.39	119.70	122.90
4	I	2	NAG	C8-C7-N2	2.39	120.08	116.12
7	Y	1	NAG	C8-C7-N2	2.38	120.06	116.12
4	T	2	NAG	C2-N2-C7	-2.38	119.71	122.90
4	Q	1	NAG	C2-N2-C7	-2.38	119.72	122.90
8	a	1	NAG	C8-C7-N2	2.37	120.05	116.12
2	P	1	NAG	C1-O5-C5	2.36	115.35	112.19
4	G	1	NAG	C6-C5-C4	-2.36	107.23	113.02
2	X	2	NAG	C3-C4-C5	2.34	114.48	110.23
8	d	2	NAG	C8-C7-N2	2.33	119.99	116.12
8	a	2	NAG	C4-C3-C2	-2.33	107.60	111.02
4	f	2	NAG	C8-C7-N2	2.33	119.98	116.12
9	c	4	MAN	O2-C2-C3	-2.32	105.34	110.15
2	D	1	NAG	C8-C7-N2	2.32	119.97	116.12
4	O	2	NAG	C8-C7-N2	2.32	119.97	116.12
6	J	4	MAN	O2-C2-C3	-2.32	105.35	110.15
6	J	2	NAG	C1-C2-N2	2.32	114.08	110.43
2	S	1	NAG	C2-N2-C7	-2.31	119.80	122.90
6	J	1	NAG	C8-C7-N2	2.31	119.95	116.12
6	Z	1	NAG	C2-N2-C7	-2.31	119.81	122.90
2	S	1	NAG	C6-C5-C4	-2.30	107.37	113.02
4	K	2	NAG	C8-C7-N2	2.29	119.91	116.12
2	b	1	NAG	C2-N2-C7	-2.29	119.84	122.90
2	D	2	NAG	C3-C4-C5	2.28	114.36	110.23
4	O	2	NAG	C2-N2-C7	-2.27	119.86	122.90
2	W	1	NAG	O4-C4-C3	-2.26	105.05	110.38
2	U	2	NAG	C8-C7-N2	2.23	119.81	116.12
6	Z	1	NAG	O4-C4-C5	2.22	114.80	109.32
6	Z	2	NAG	C8-C7-N2	2.22	119.80	116.12
3	E	4	MAN	O2-C2-C3	-2.22	105.55	110.15
2	M	1	NAG	C4-C3-C2	2.22	114.27	111.02
5	H	2	NAG	C8-C7-N2	2.22	119.80	116.12
2	L	1	NAG	O5-C1-C2	-2.22	107.86	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	NAG	C2-N2-C7	2.21	125.86	122.90
4	f	1	NAG	C8-C7-N2	2.20	119.76	116.12
8	a	2	NAG	O7-C7-N2	-2.20	118.10	121.98
2	S	1	NAG	C4-C3-C2	2.19	114.23	111.02
3	F	1	NAG	C1-C2-N2	2.18	113.87	110.43
2	M	1	NAG	C1-O5-C5	2.18	115.11	112.19
2	V	1	NAG	C8-C7-N2	2.18	119.74	116.12
2	L	2	NAG	C8-C7-N2	2.17	119.72	116.12
2	S	1	NAG	C8-C7-N2	2.17	119.72	116.12
8	a	2	NAG	O7-C7-C8	-2.16	118.21	122.05
8	d	5	MAN	O2-C2-C3	-2.16	105.67	110.15
2	P	3	BMA	C1-O5-C5	2.16	115.08	112.19
2	U	1	NAG	O7-C7-N2	-2.16	118.17	121.98
9	c	2	NAG	C8-C7-N2	2.15	119.69	116.12
4	Q	2	NAG	O5-C1-C2	2.15	114.62	111.29
4	e	2	NAG	C8-C7-N2	2.15	119.68	116.12
2	U	1	NAG	O7-C7-C8	-2.15	118.23	122.05
2	N	1	NAG	O4-C4-C5	2.14	114.61	109.32
4	K	1	NAG	O7-C7-N2	-2.14	118.19	121.98
8	a	4	MAN	C1-C2-C3	2.14	112.76	109.64
2	W	2	NAG	C2-N2-C7	-2.13	120.04	122.90
6	Z	4	MAN	O2-C2-C3	-2.13	105.74	110.15
2	b	1	NAG	O4-C4-C3	-2.12	105.39	110.38
5	H	2	NAG	C1-C2-N2	-2.11	107.10	110.43
2	X	1	NAG	C1-O5-C5	-2.10	109.37	112.19
2	W	1	NAG	O5-C1-C2	-2.10	108.04	111.29
2	W	1	NAG	C2-N2-C7	-2.09	120.10	122.90
4	e	1	NAG	C8-C7-N2	2.09	119.58	116.12
4	G	1	NAG	O7-C7-C8	-2.09	118.33	122.05
5	H	1	NAG	C4-C3-C2	2.09	114.07	111.02
4	G	1	NAG	O4-C4-C3	2.08	115.28	110.38
5	H	2	NAG	C2-N2-C7	-2.07	120.12	122.90
2	R	1	NAG	C1-O5-C5	-2.06	109.42	112.19
3	E	1	NAG	C2-N2-C7	-2.06	120.14	122.90
6	J	2	NAG	C4-C3-C2	-2.06	108.00	111.02
2	V	2	NAG	C8-C7-N2	2.06	119.53	116.12
2	N	2	NAG	C2-N2-C7	-2.04	120.17	122.90
4	K	1	NAG	O7-C7-C8	-2.03	118.43	122.05
3	F	1	NAG	O7-C7-C8	-2.01	118.47	122.05
3	E	1	NAG	C8-C7-N2	2.01	119.45	116.12
2	P	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7
2	V	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C3-C2-N2-C7
4	e	1	NAG	C1-C2-N2-C7
4	f	1	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	J	2	NAG	C1-C2-N2-C7
8	d	2	NAG	C1-C2-N2-C7
9	c	2	NAG	C1-C2-N2-C7
4	O	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
8	d	3	BMA	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
9	c	3	BMA	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
8	d	3	BMA	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
6	Z	4	MAN	O5-C5-C6-O6
9	c	3	BMA	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C8-C7-N2-C2
2	X	1	NAG	O7-C7-N2-C2
2	X	2	NAG	C8-C7-N2-C2
2	X	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
8	a	2	NAG	C8-C7-N2-C2
8	a	2	NAG	O7-C7-N2-C2
8	d	1	NAG	C8-C7-N2-C2
8	d	1	NAG	O7-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	X	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
8	d	4	MAN	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
8	a	5	MAN	O5-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C1-C2-N2-C7
2	U	1	NAG	C1-C2-N2-C7
2	U	2	NAG	C1-C2-N2-C7
2	W	1	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
2	X	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7
2	U	2	NAG	C3-C2-N2-C7
2	W	1	NAG	C3-C2-N2-C7
6	Z	2	NAG	C3-C2-N2-C7
2	V	1	NAG	C4-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	b	3	BMA	C4-C5-C6-O6
2	M	2	NAG	C1-C2-N2-C7
2	S	1	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7
6	Z	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	d	1	NAG	C1-C2-N2-C7
6	Z	4	MAN	C4-C5-C6-O6
2	M	1	NAG	C3-C2-N2-C7
2	V	1	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
8	d	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	a	3	BMA	C1-C2-C3-C4-C5-O5
8	a	5	MAN	C1-C2-C3-C4-C5-O5

56 monomers are involved in 118 short contacts:

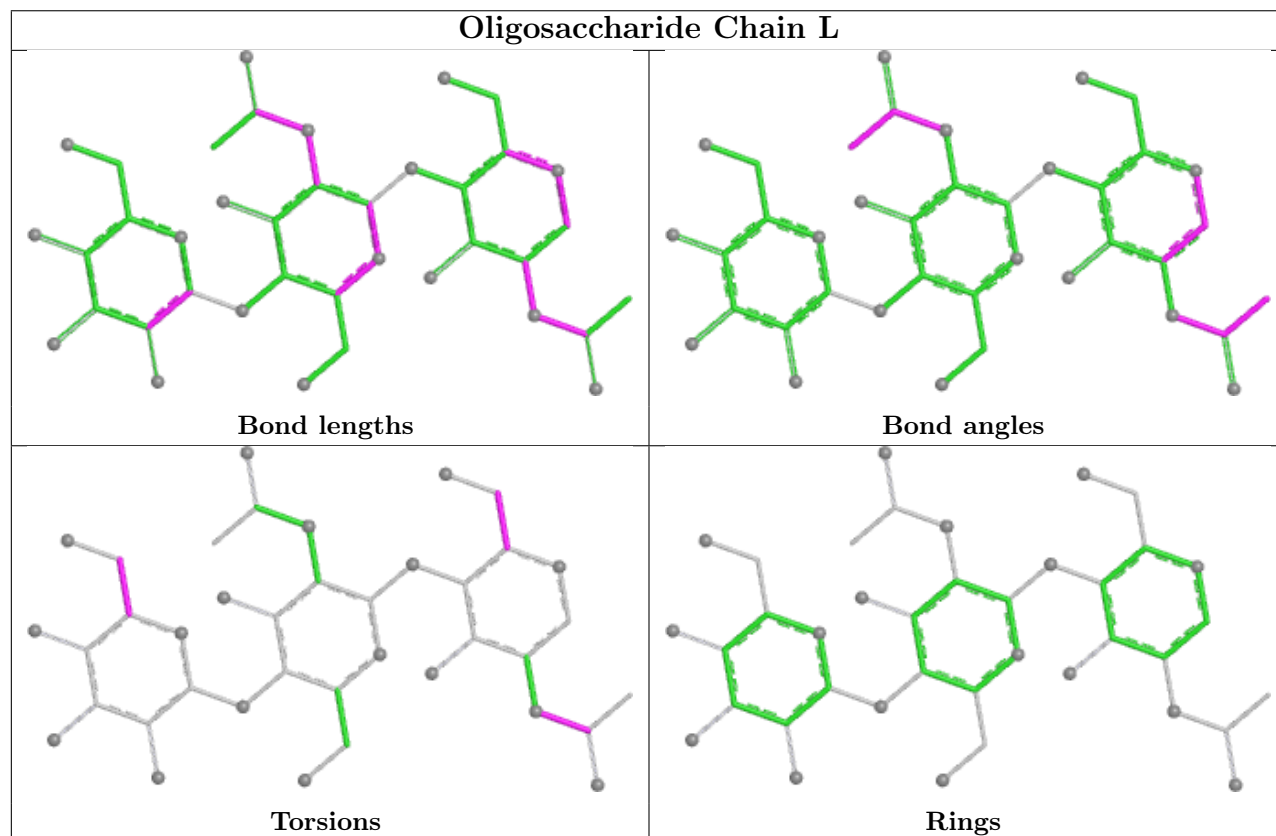
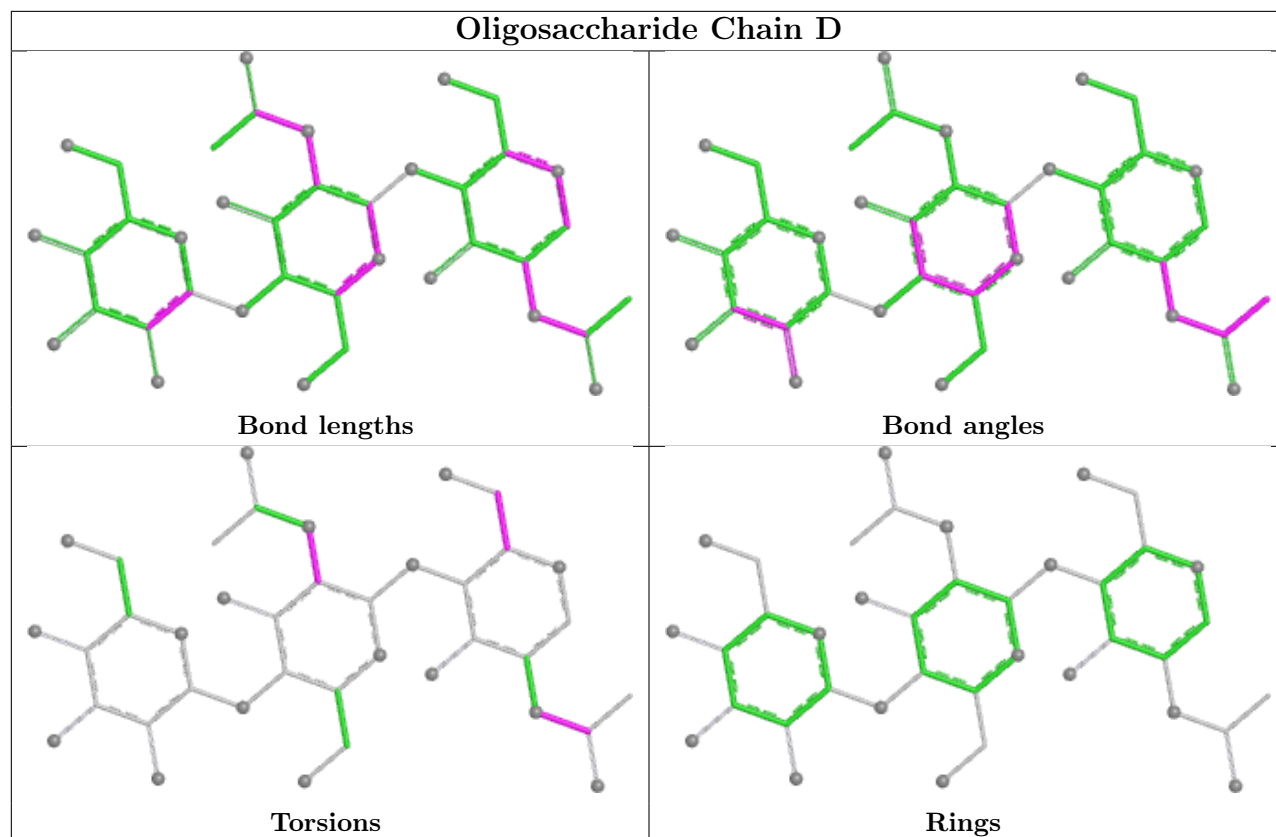
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	G	1	NAG	3	0
2	V	1	NAG	1	0
8	d	1	NAG	1	0
3	F	4	MAN	8	0
2	N	1	NAG	5	0
2	U	3	BMA	1	0
2	D	3	BMA	6	0
3	E	2	NAG	5	0
8	a	3	BMA	1	0
8	a	1	NAG	1	0
4	K	1	NAG	3	0
2	U	2	NAG	1	0
2	L	2	NAG	1	0
3	E	1	NAG	7	0
2	b	2	NAG	3	0
4	T	1	NAG	1	0
2	U	1	NAG	1	0
5	H	1	NAG	2	0
9	c	1	NAG	12	0
6	J	4	MAN	2	0
2	D	1	NAG	5	0

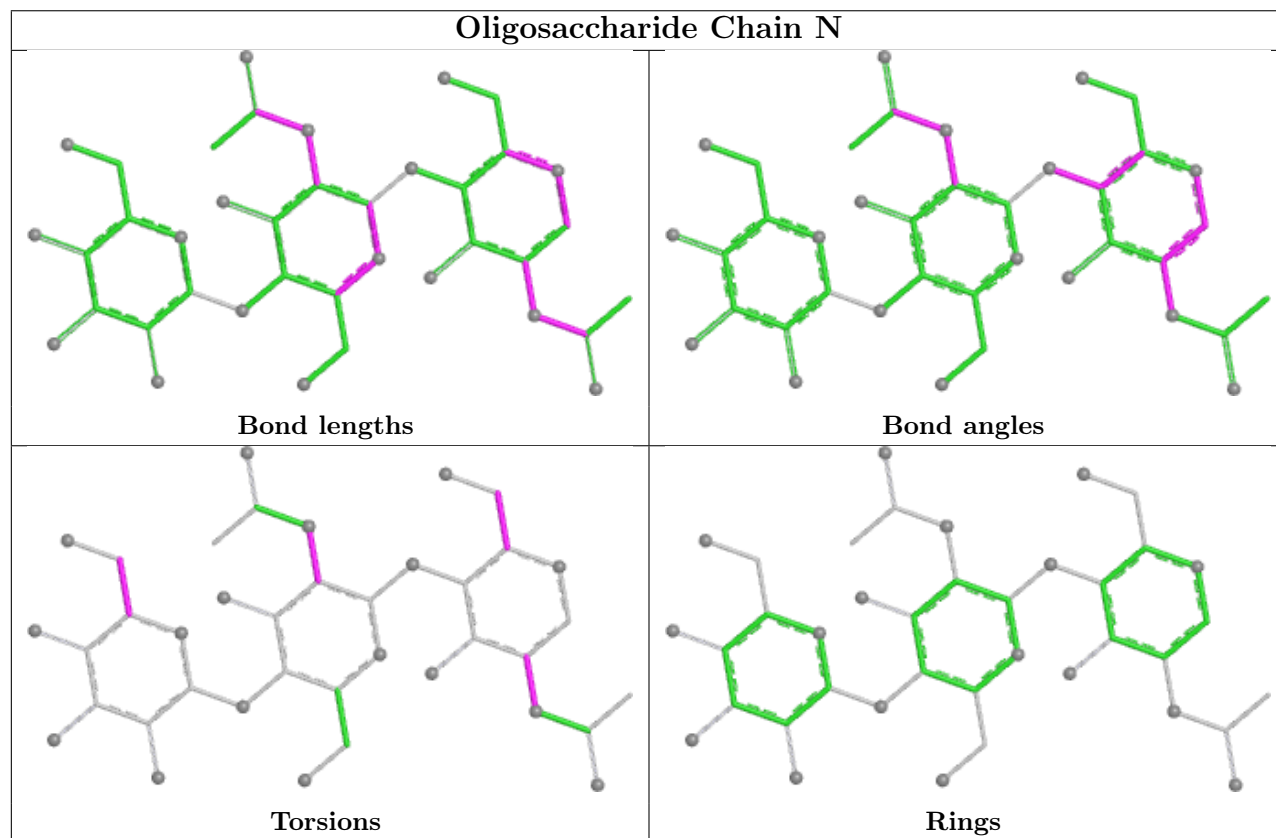
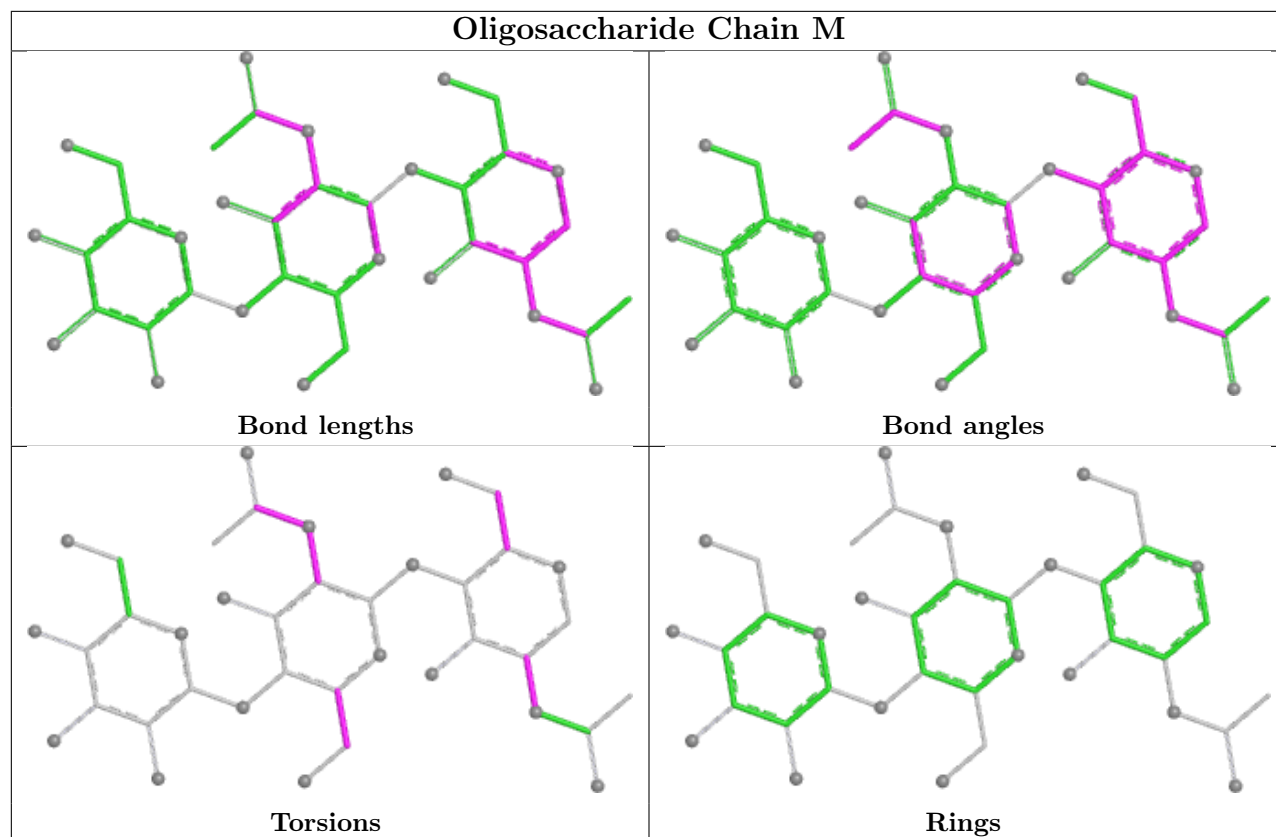
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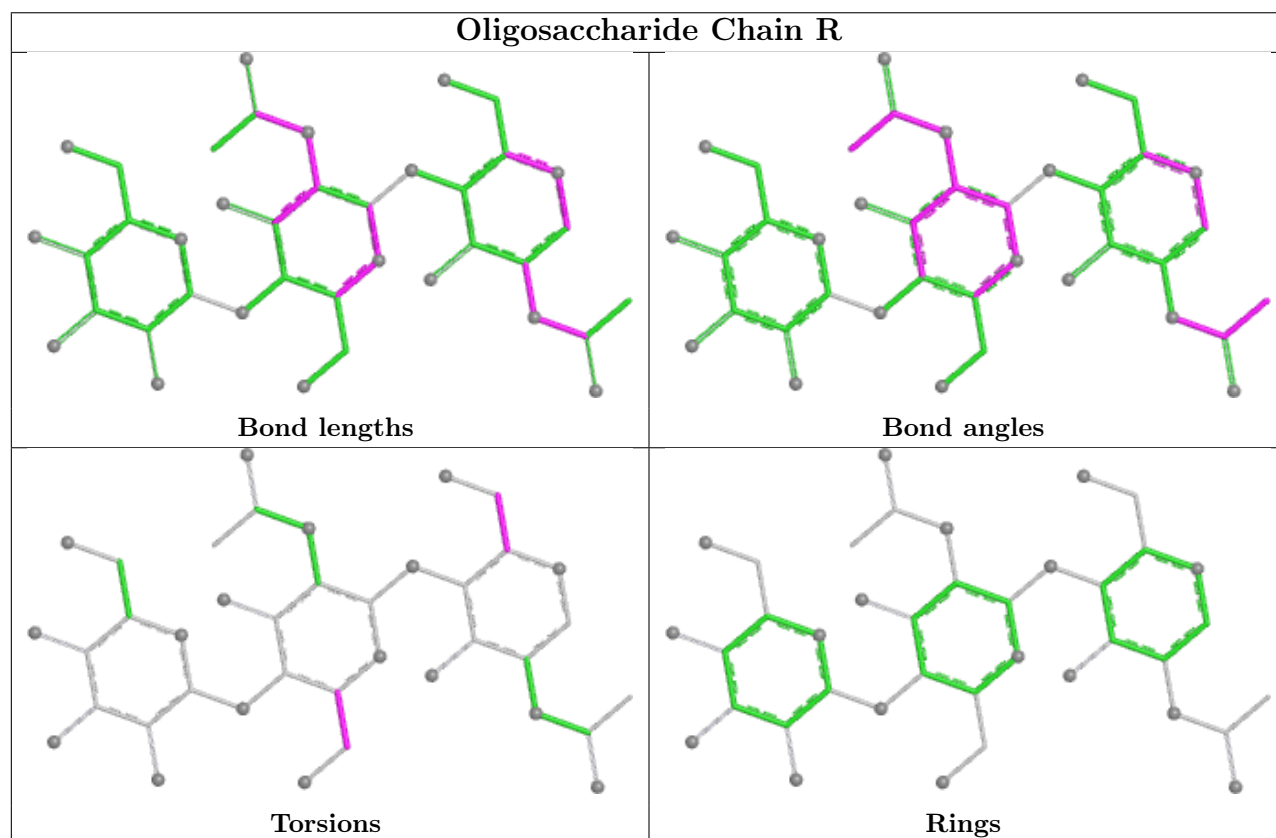
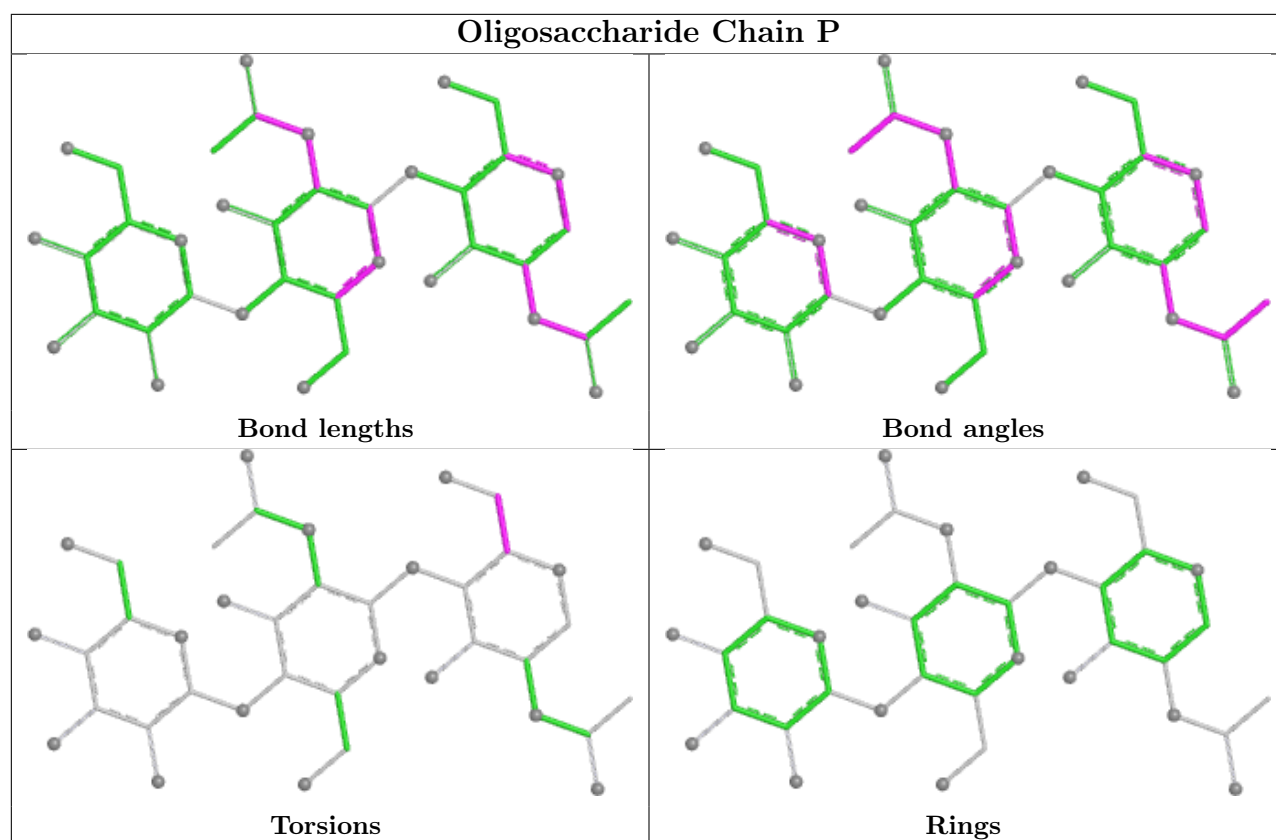
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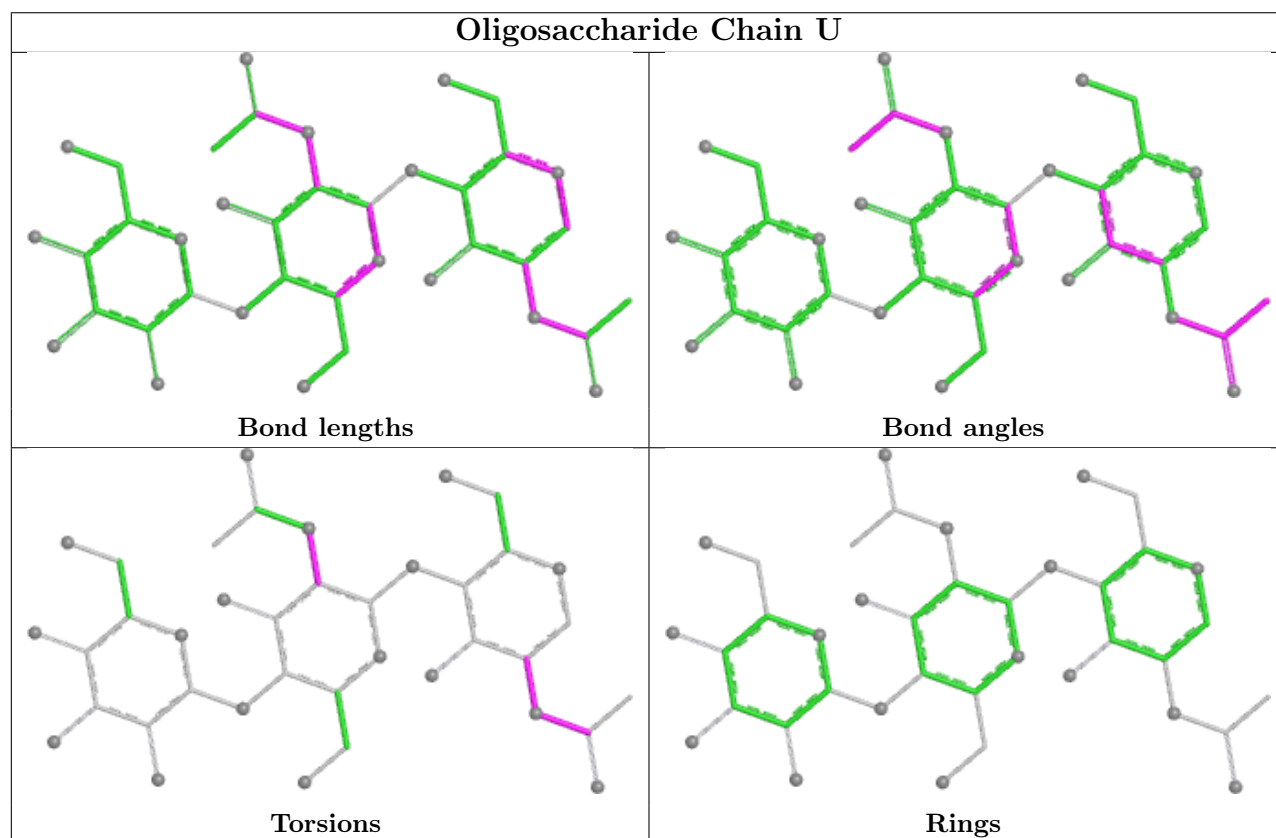
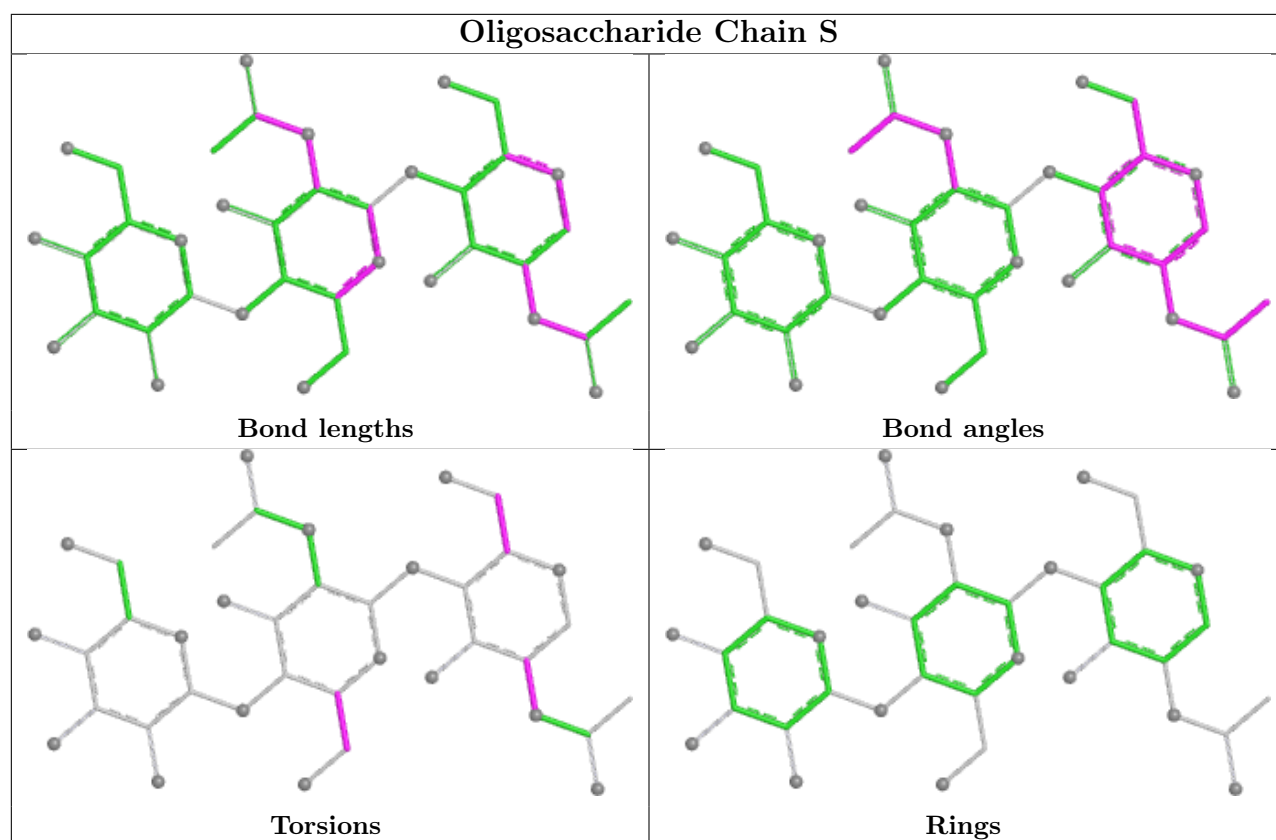
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	3	BMA	1	0
3	E	3	BMA	6	0
3	F	1	NAG	19	0
2	S	1	NAG	1	0
8	a	5	MAN	1	0
3	F	3	BMA	5	0
8	a	4	MAN	1	0
2	R	1	NAG	3	0
6	J	2	NAG	2	0
8	a	2	NAG	2	0
2	D	2	NAG	11	0
4	O	2	NAG	1	0
2	M	1	NAG	3	0
2	W	3	BMA	1	0
4	O	1	NAG	1	0
7	Y	1	NAG	2	0
4	G	2	NAG	2	0
7	Y	2	NAG	2	0
2	b	1	NAG	2	0
5	H	2	NAG	2	0
9	c	2	NAG	3	0
2	N	2	NAG	2	0
2	W	2	NAG	1	0
2	L	1	NAG	1	0
4	I	2	NAG	1	0
4	e	1	NAG	1	0
2	R	2	NAG	1	0
3	E	4	MAN	6	0
7	Y	3	FUC	2	0
3	F	2	NAG	14	0
2	R	3	BMA	1	0
6	J	3	BMA	2	0
6	J	1	NAG	2	0
2	S	2	NAG	1	0

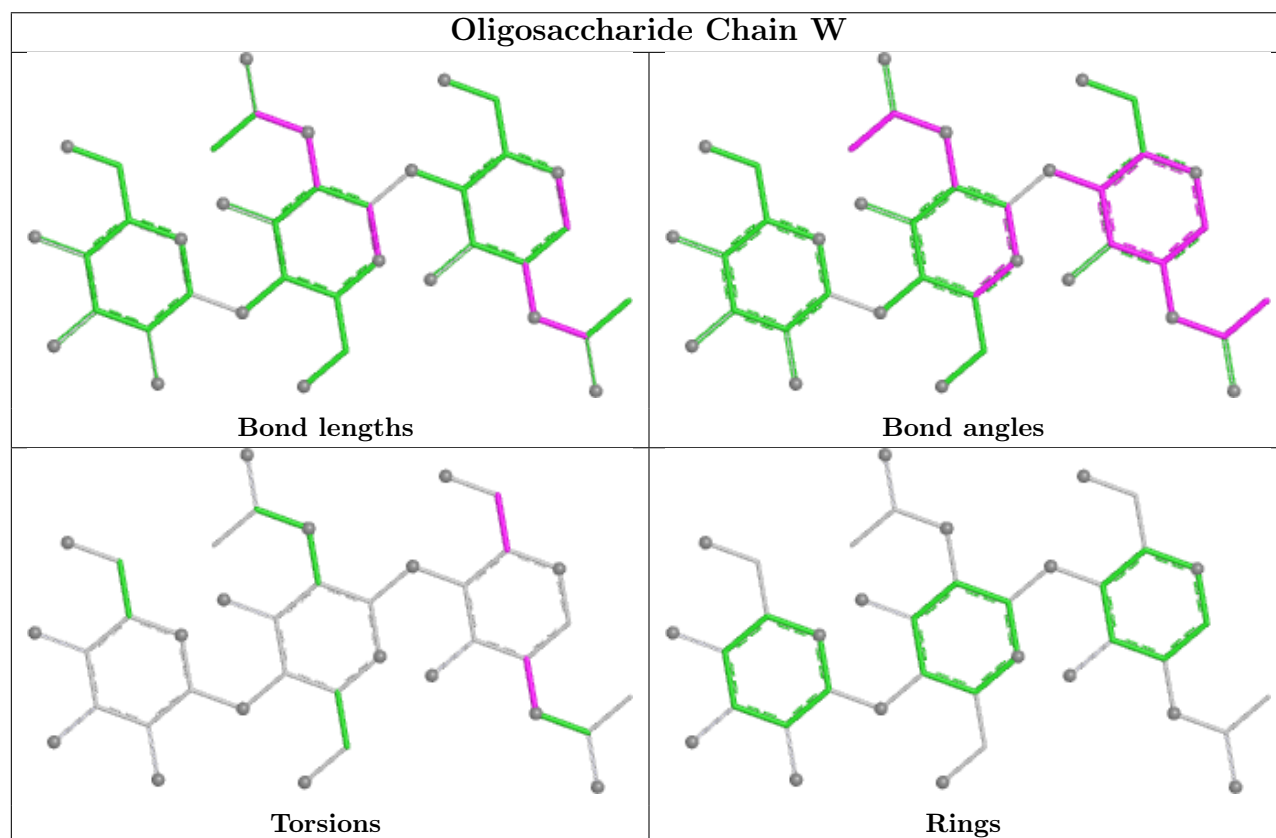
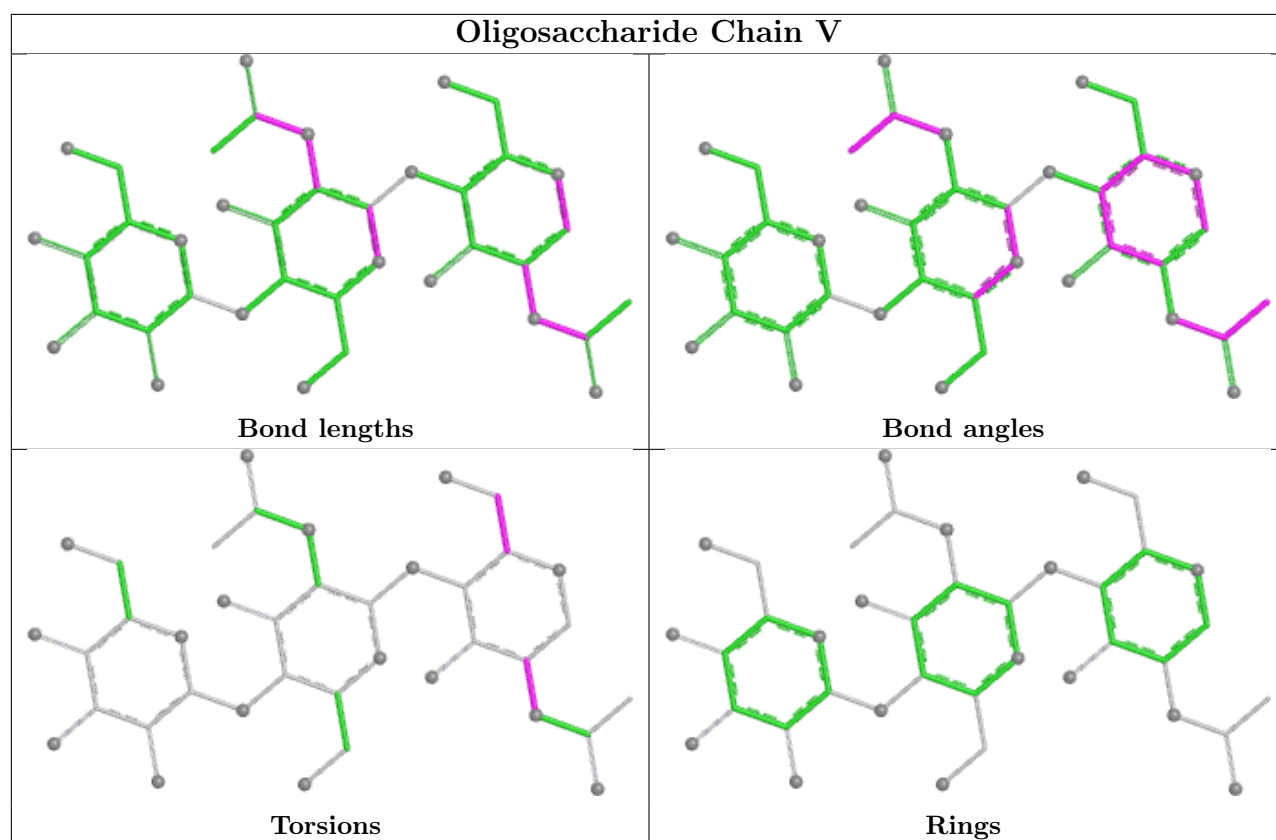
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

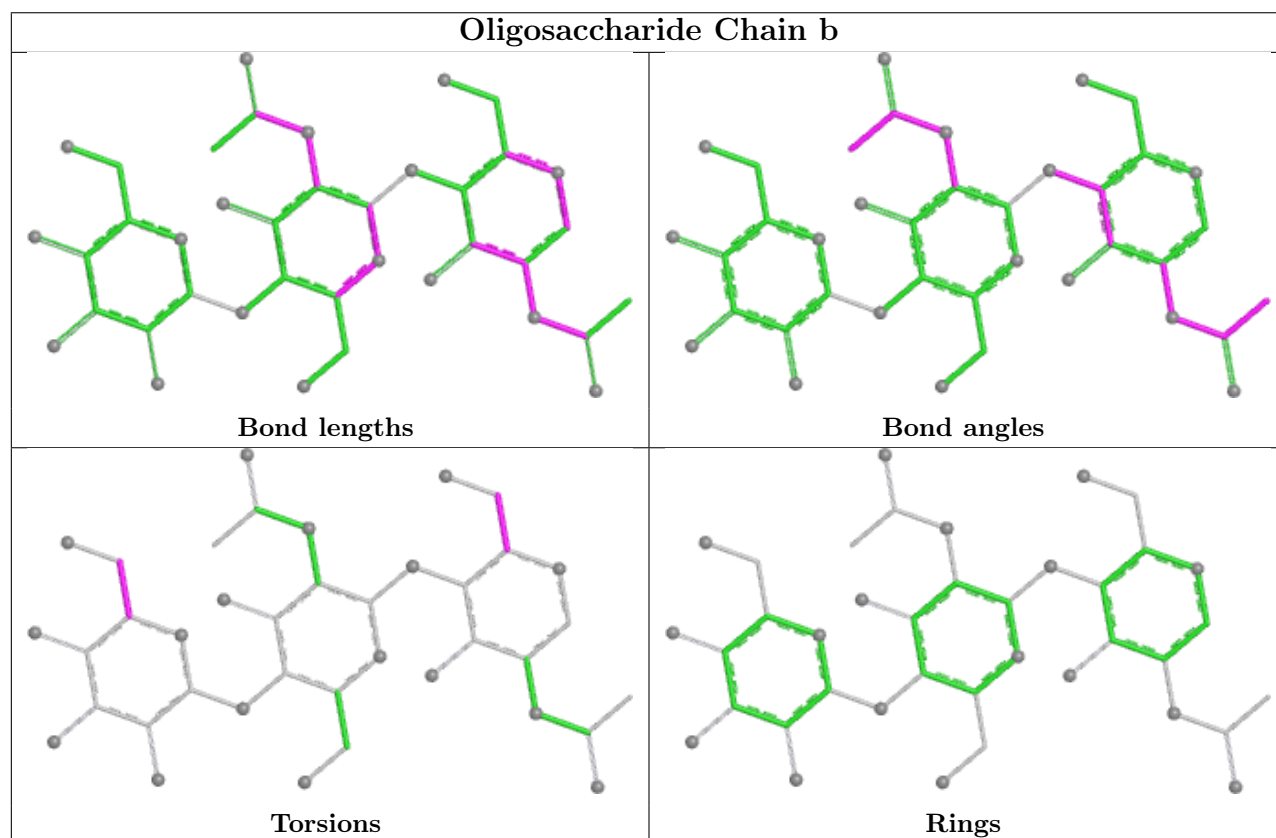
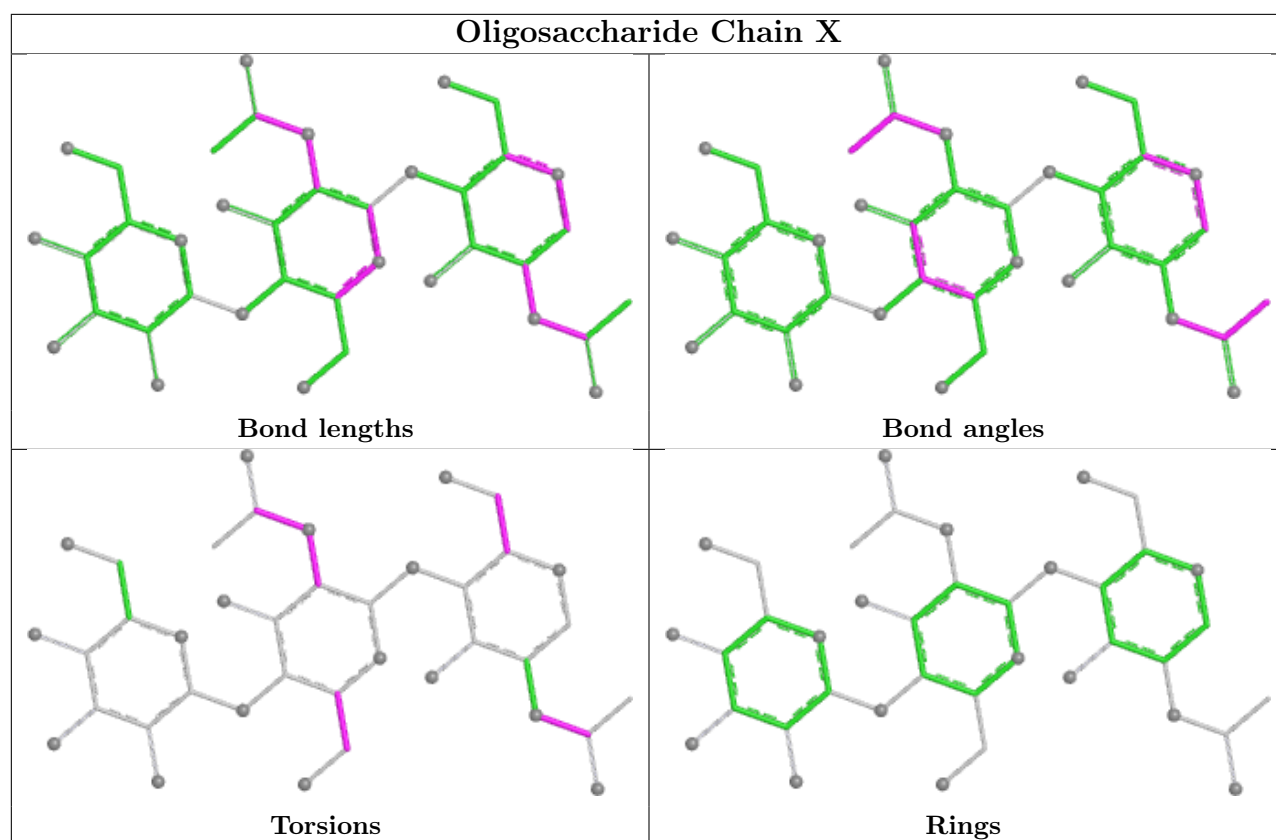


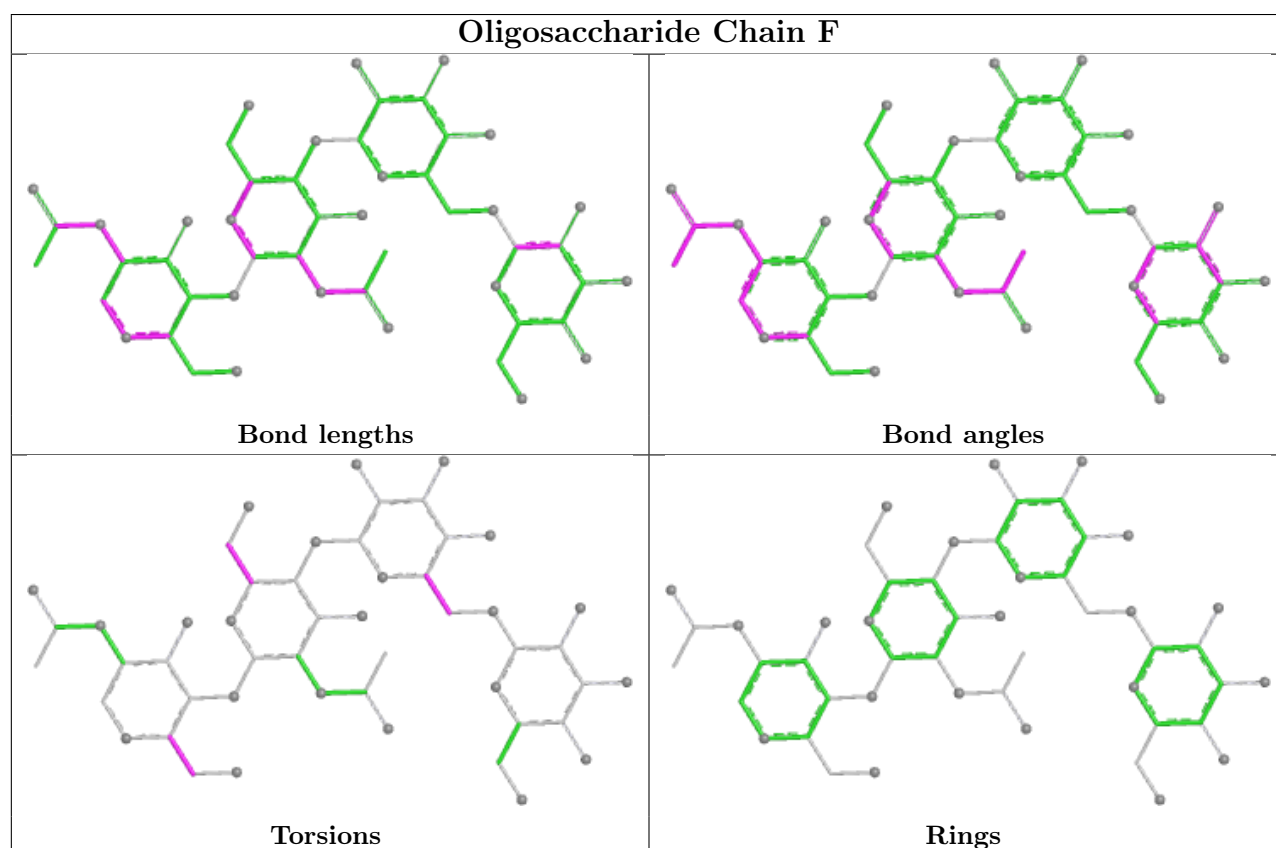
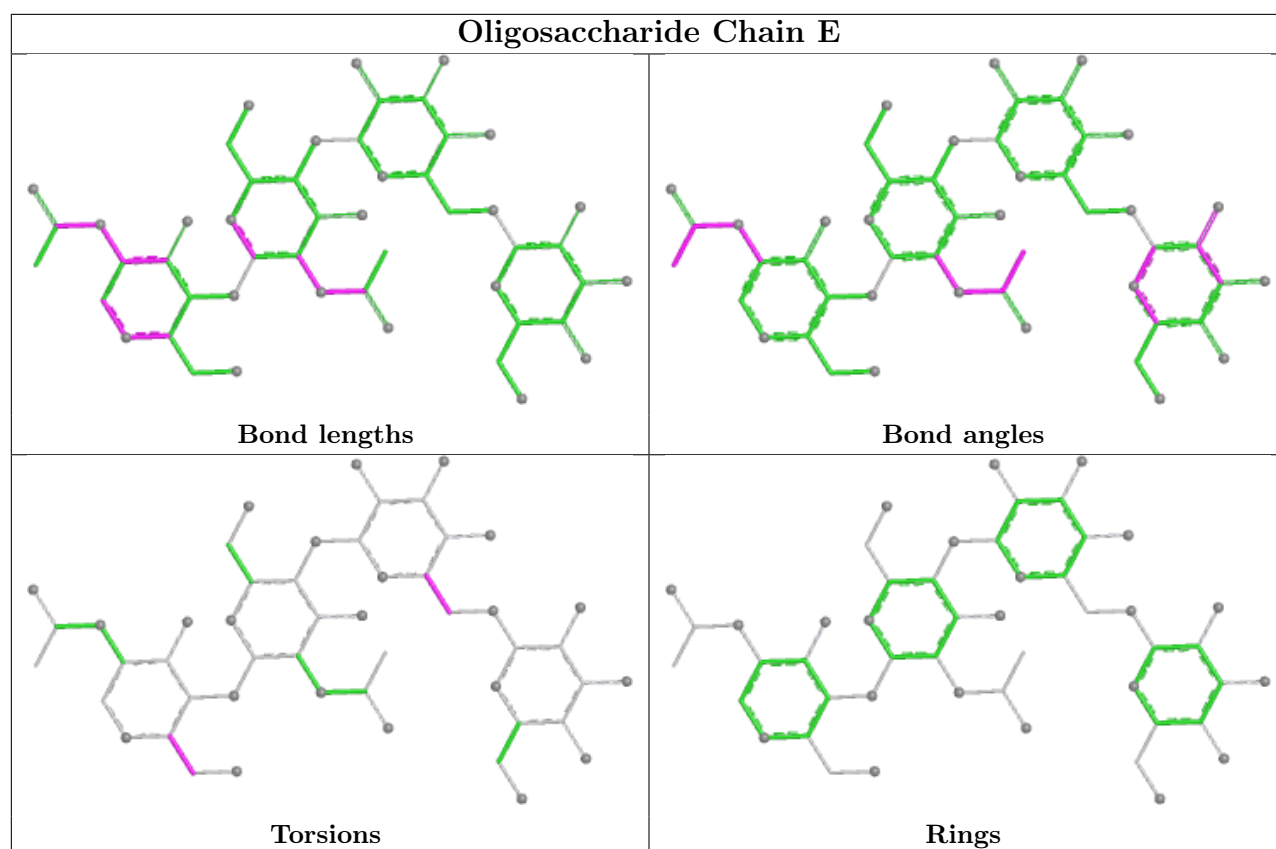


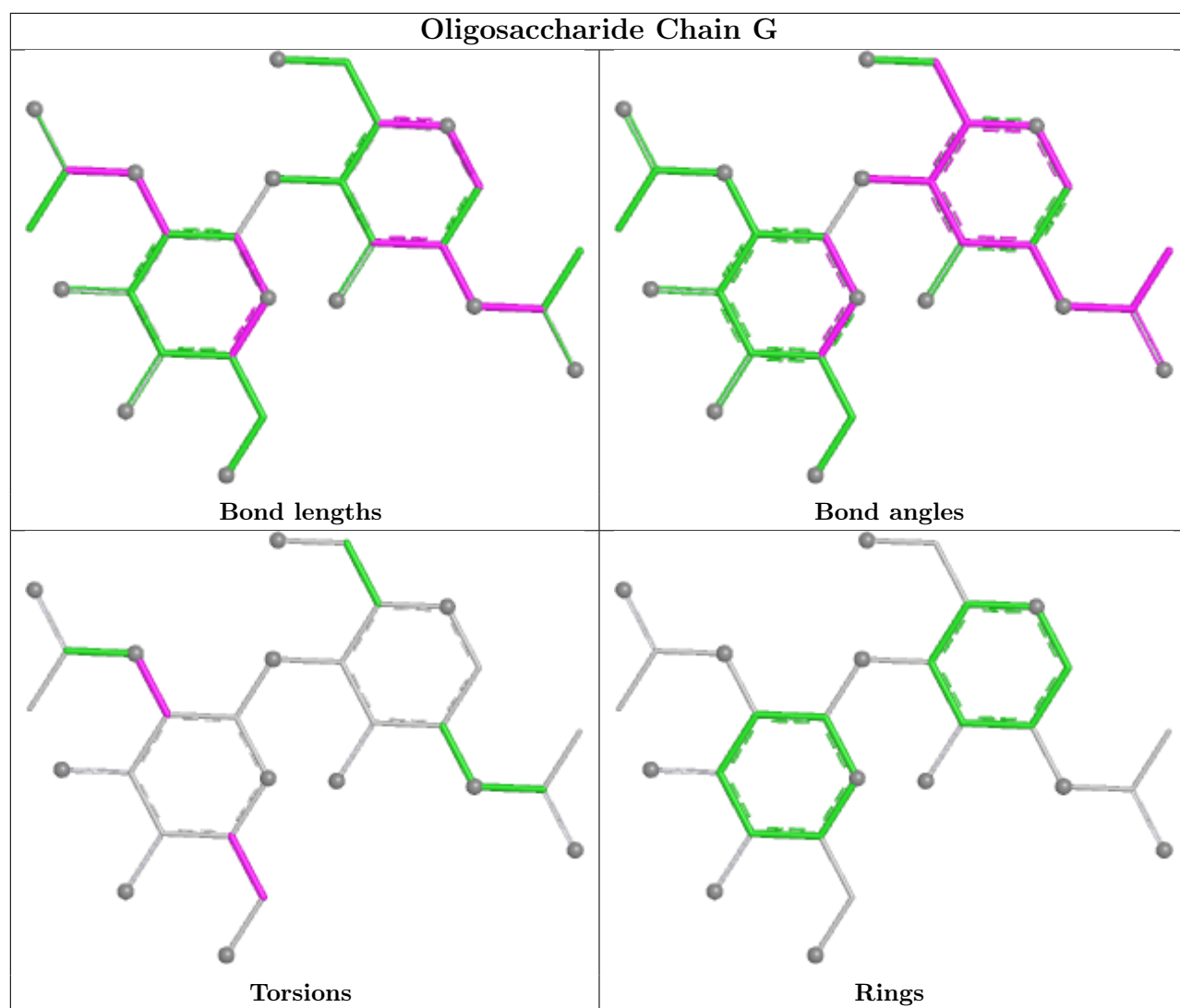


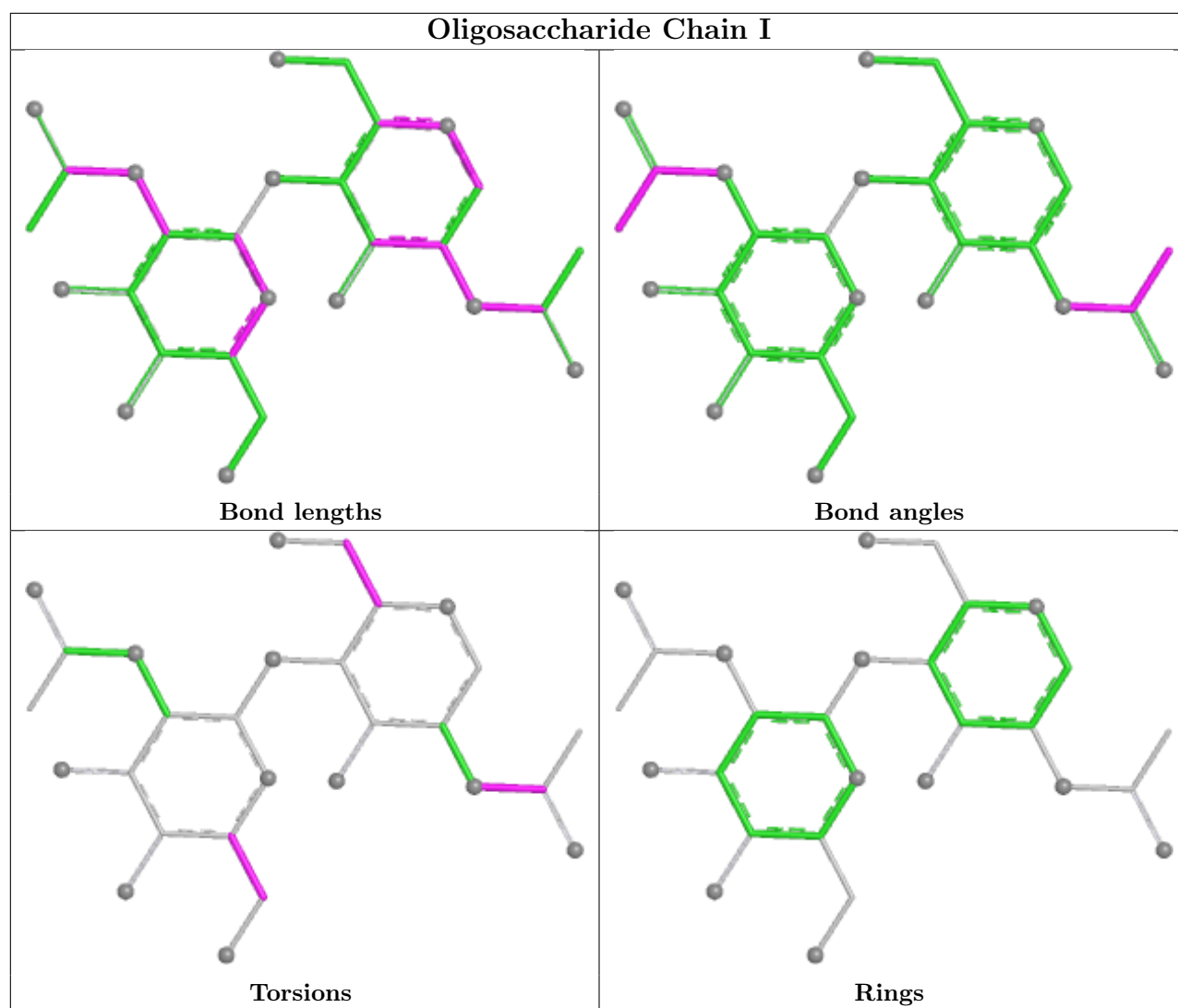


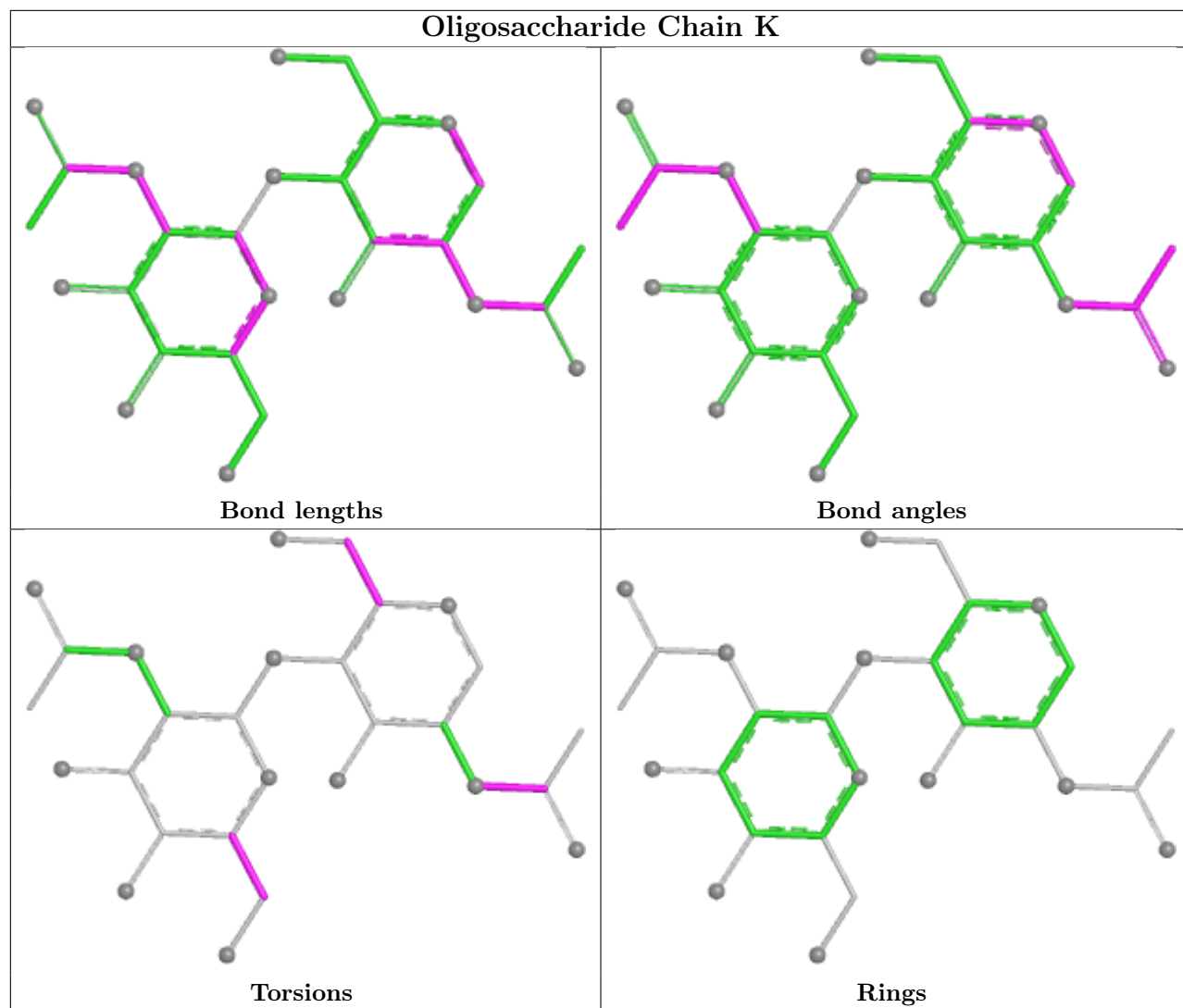


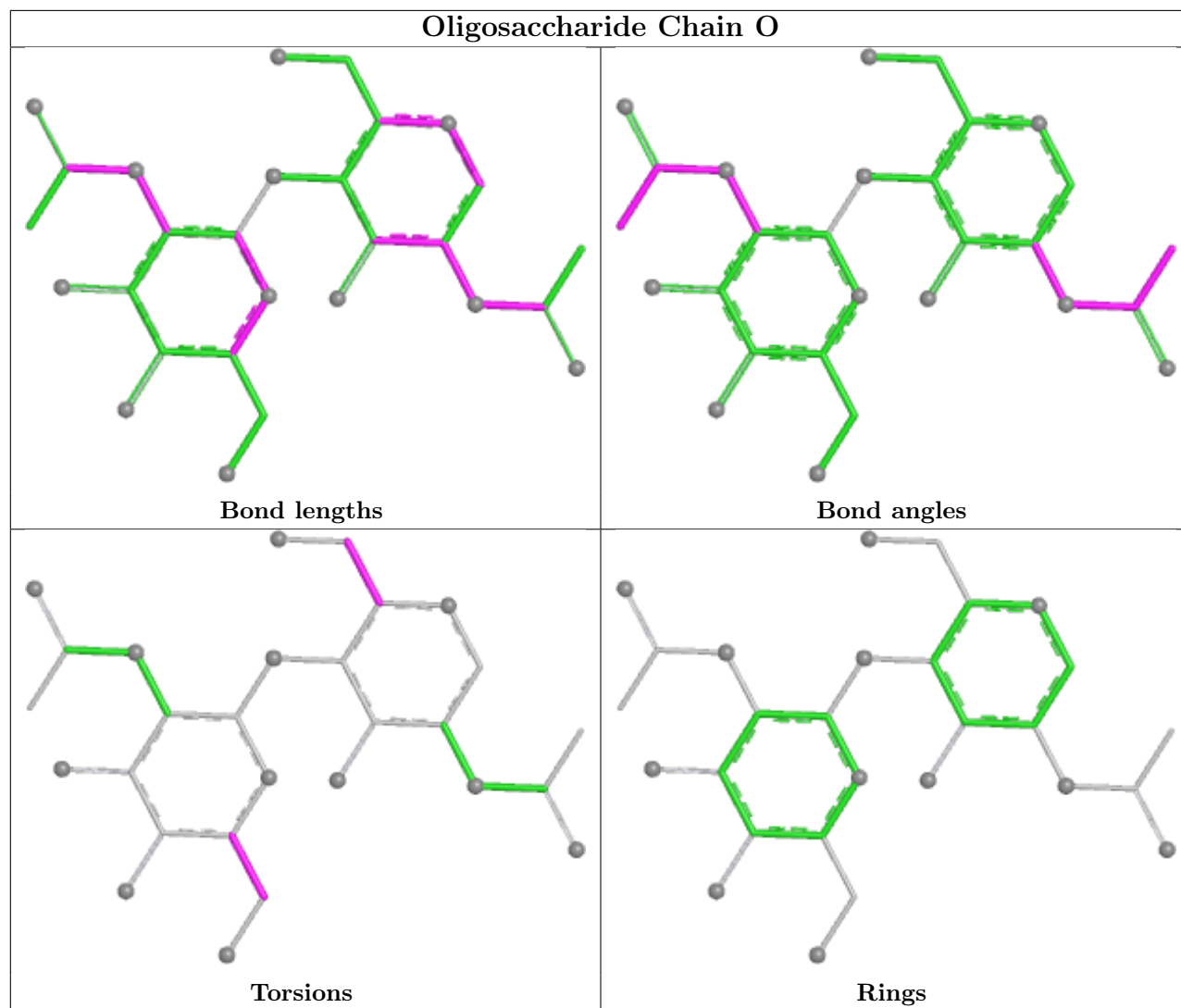


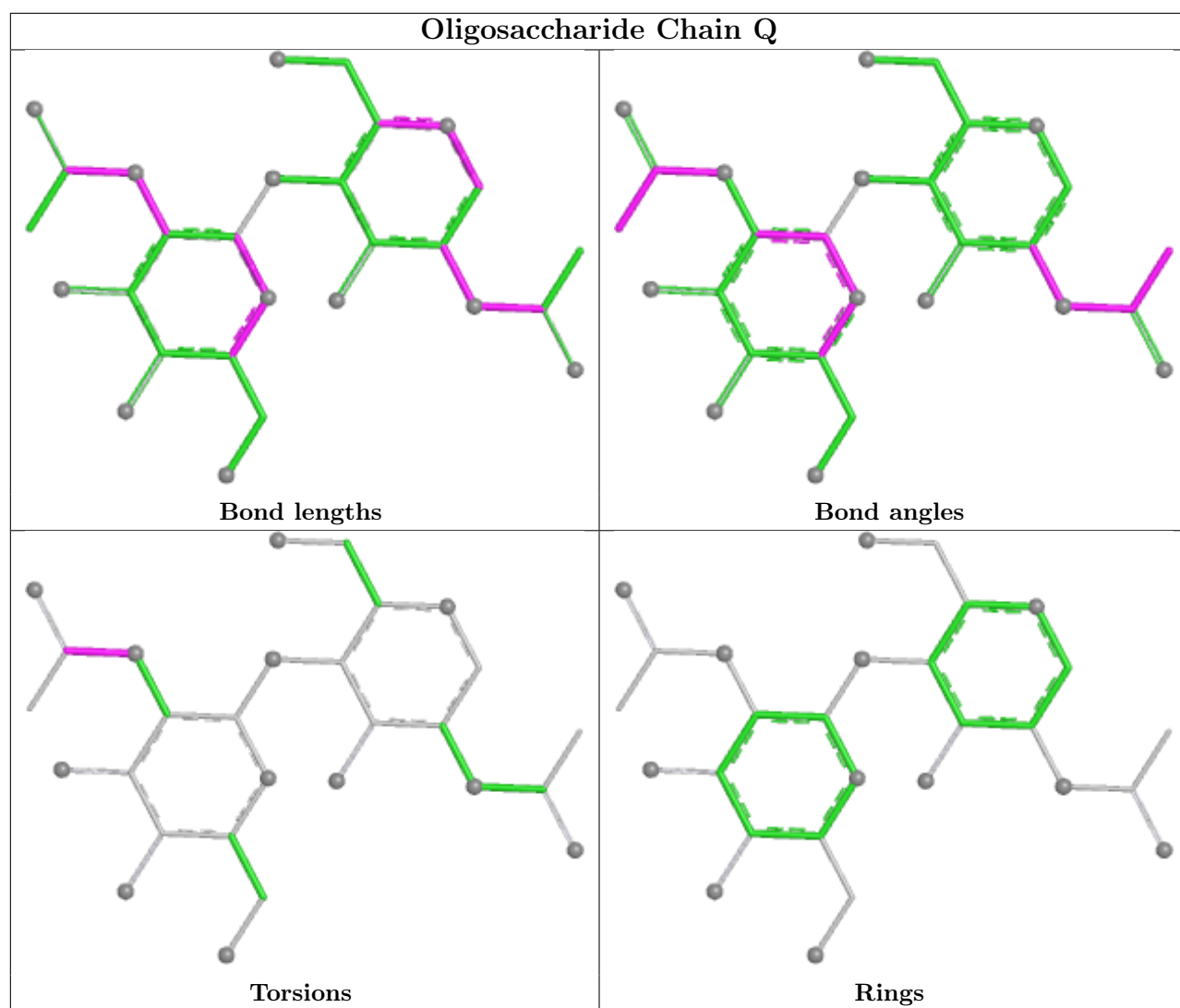


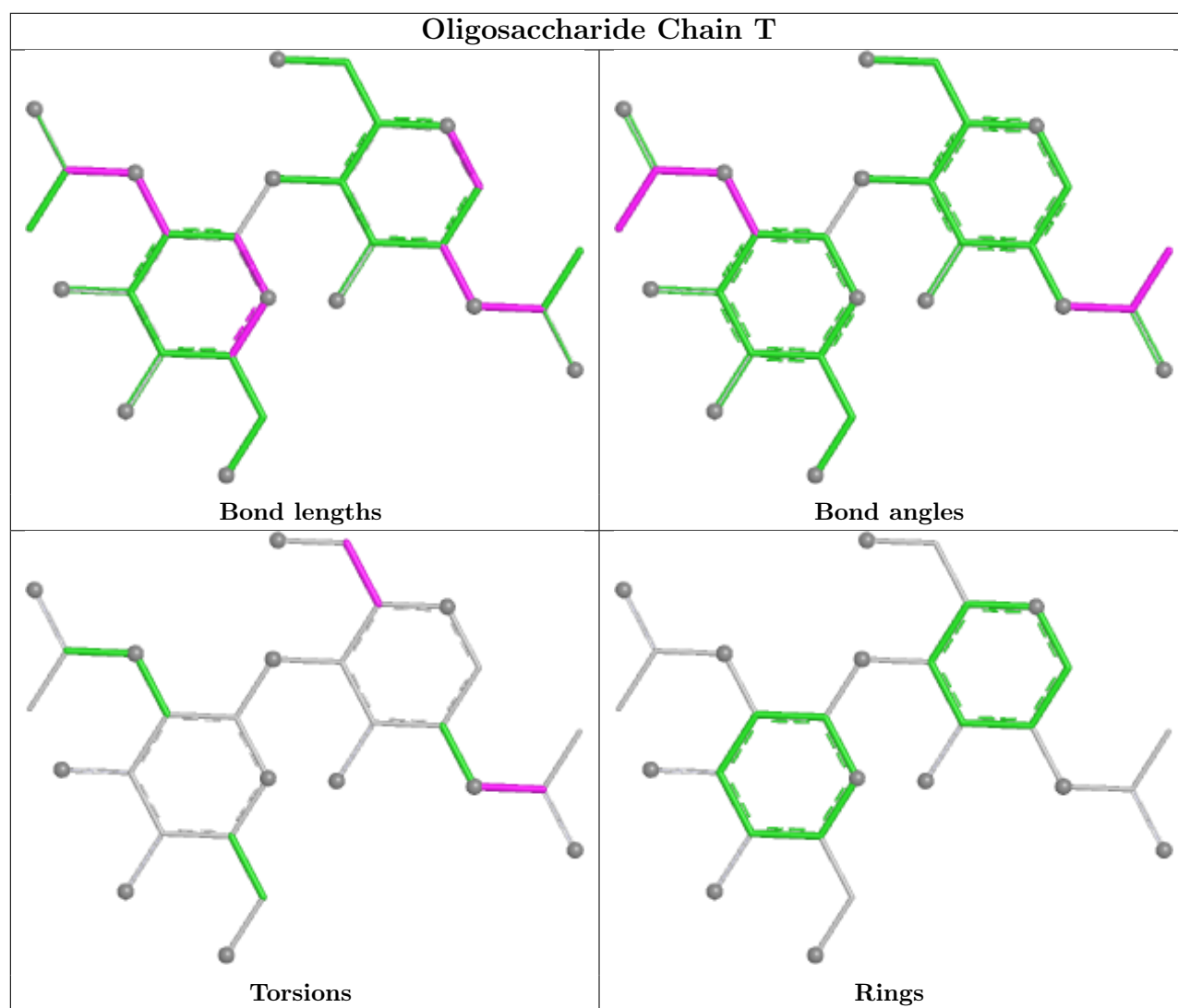


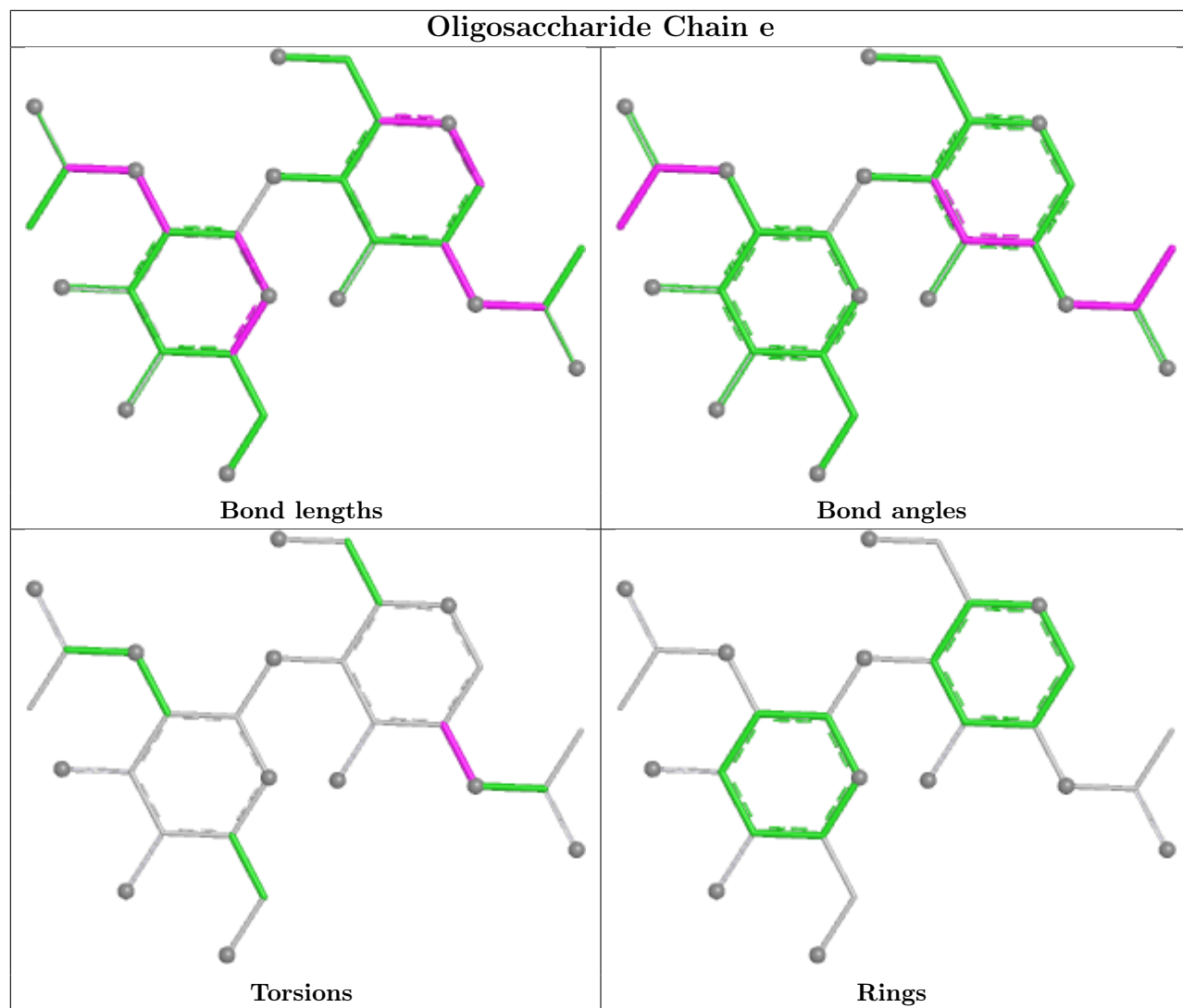


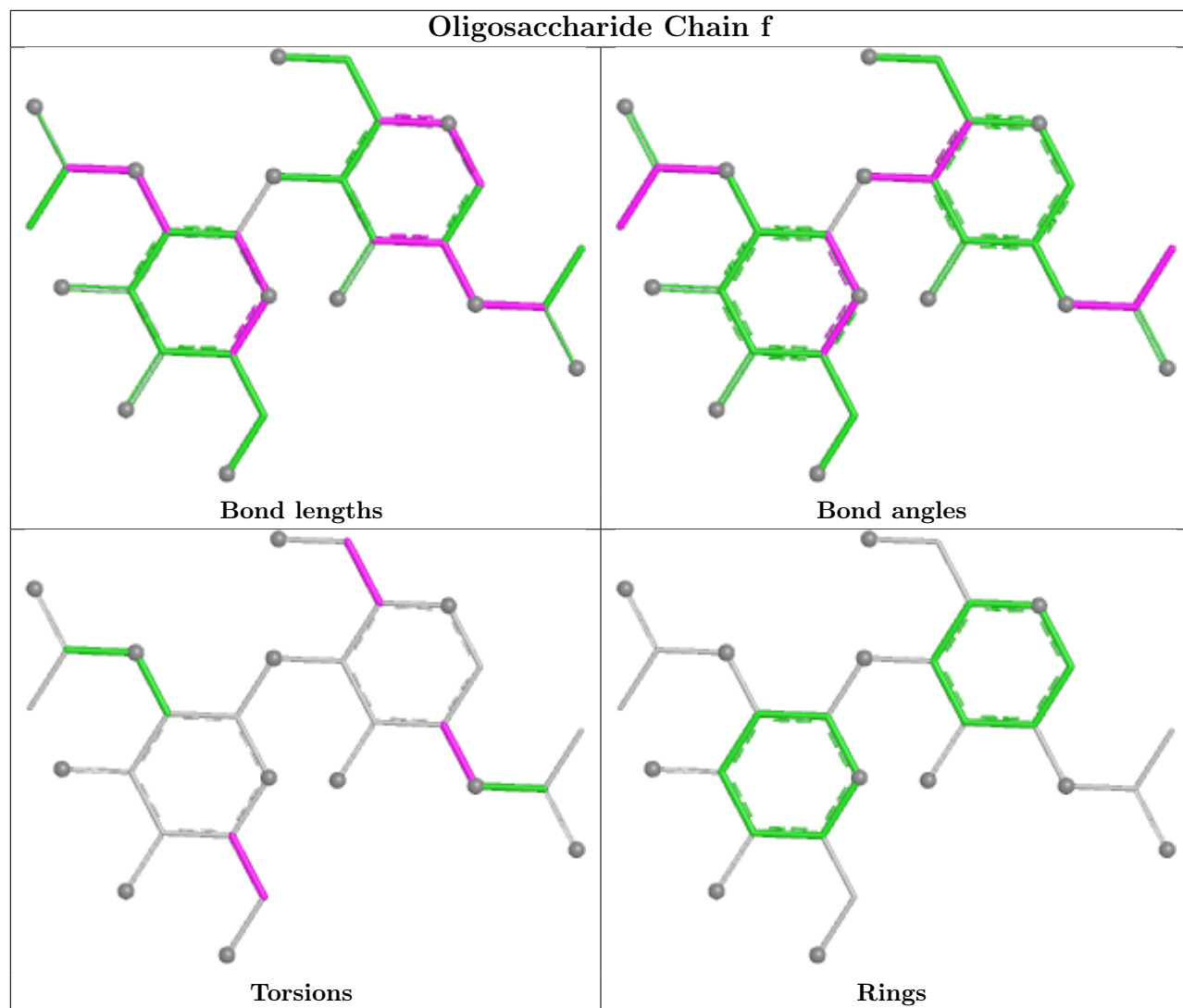




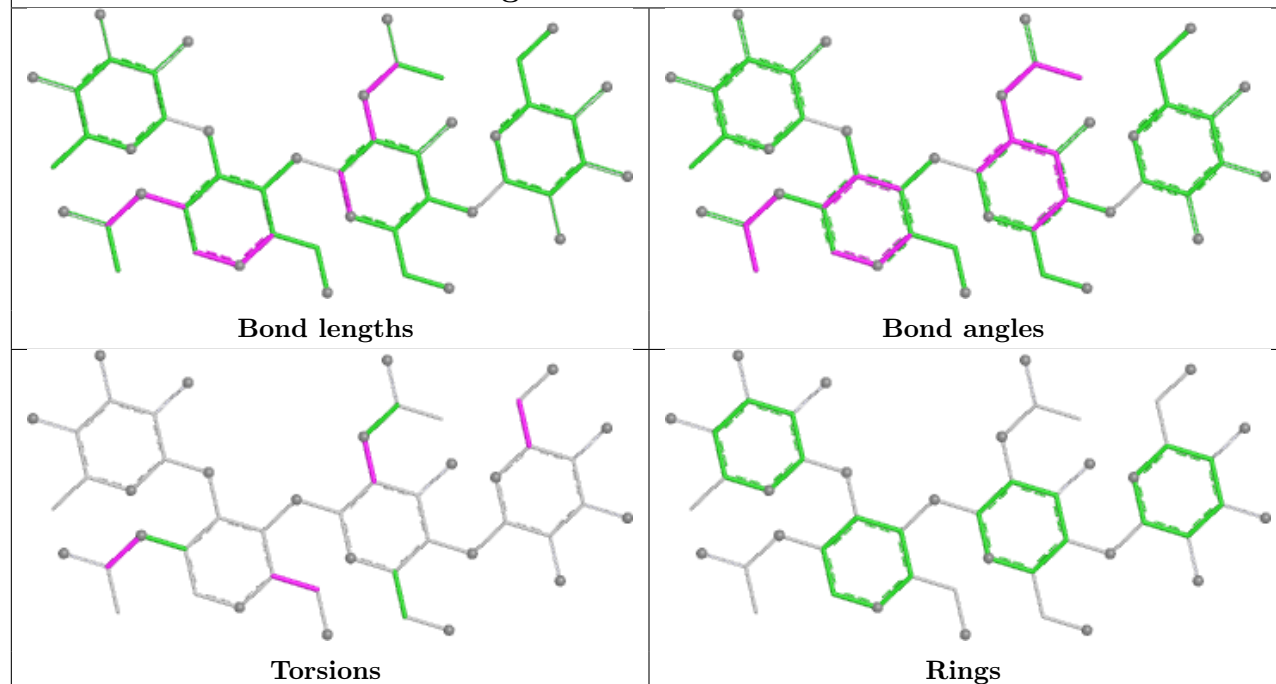




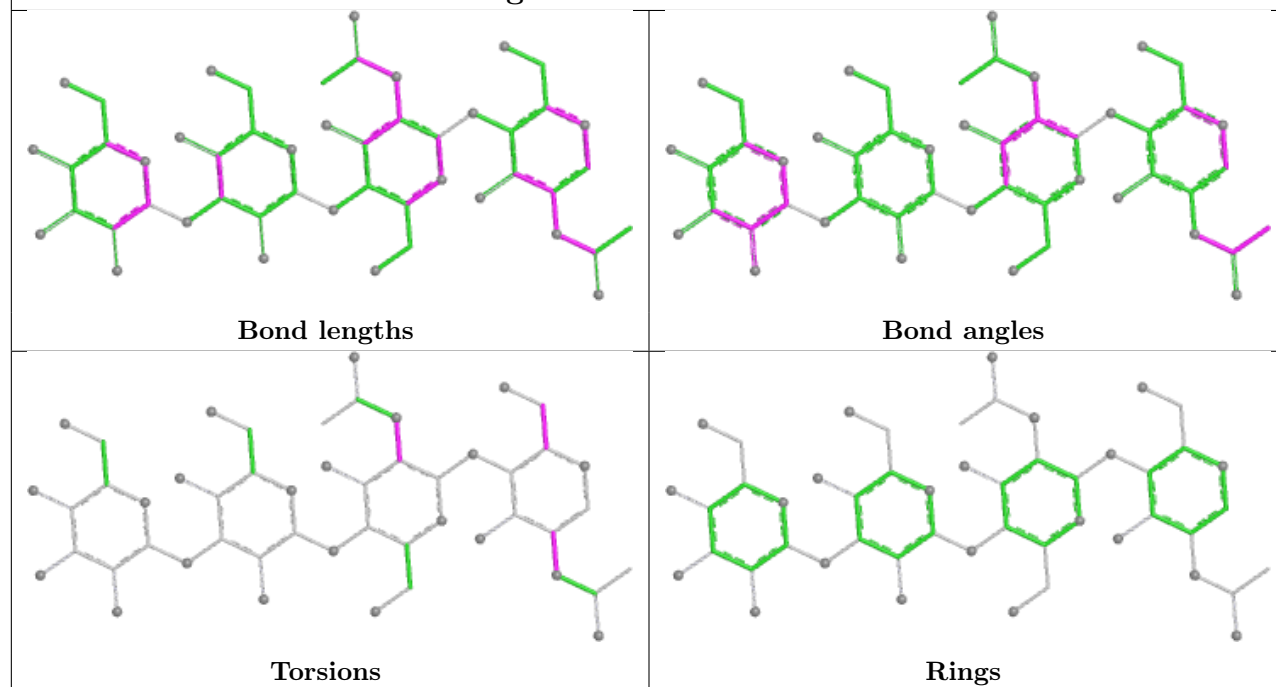


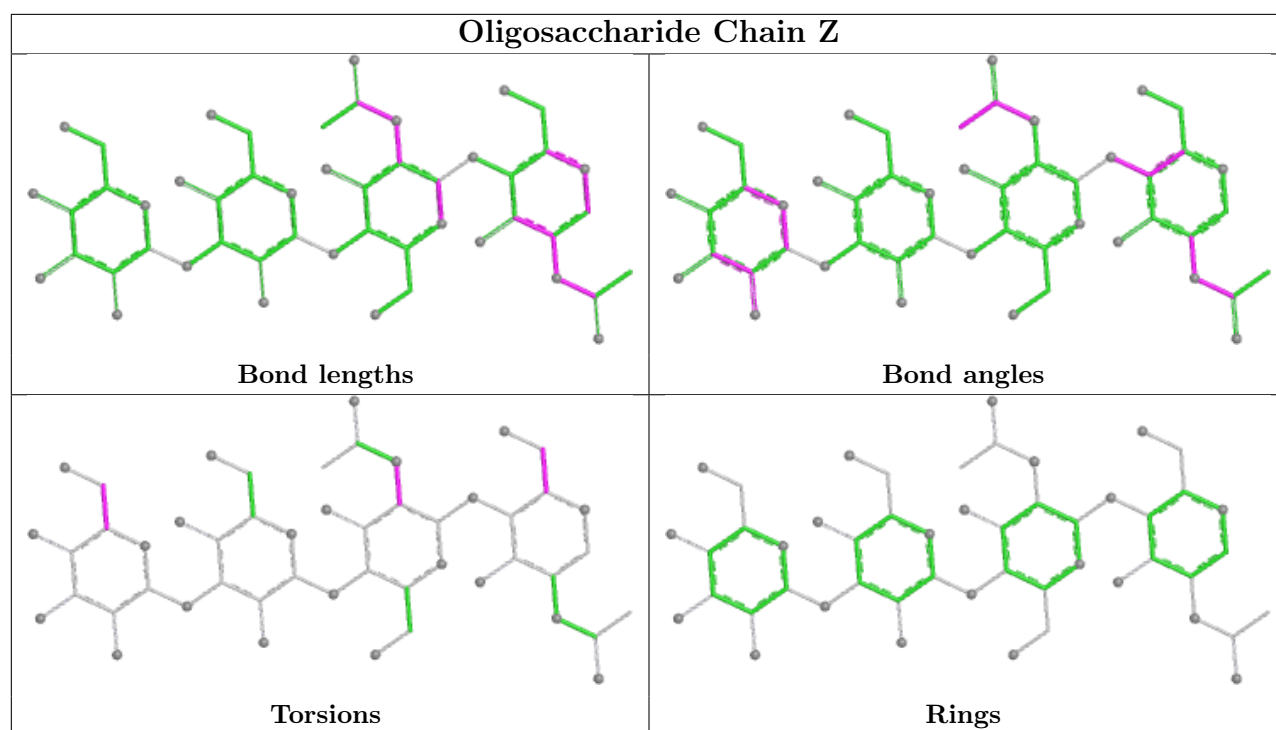


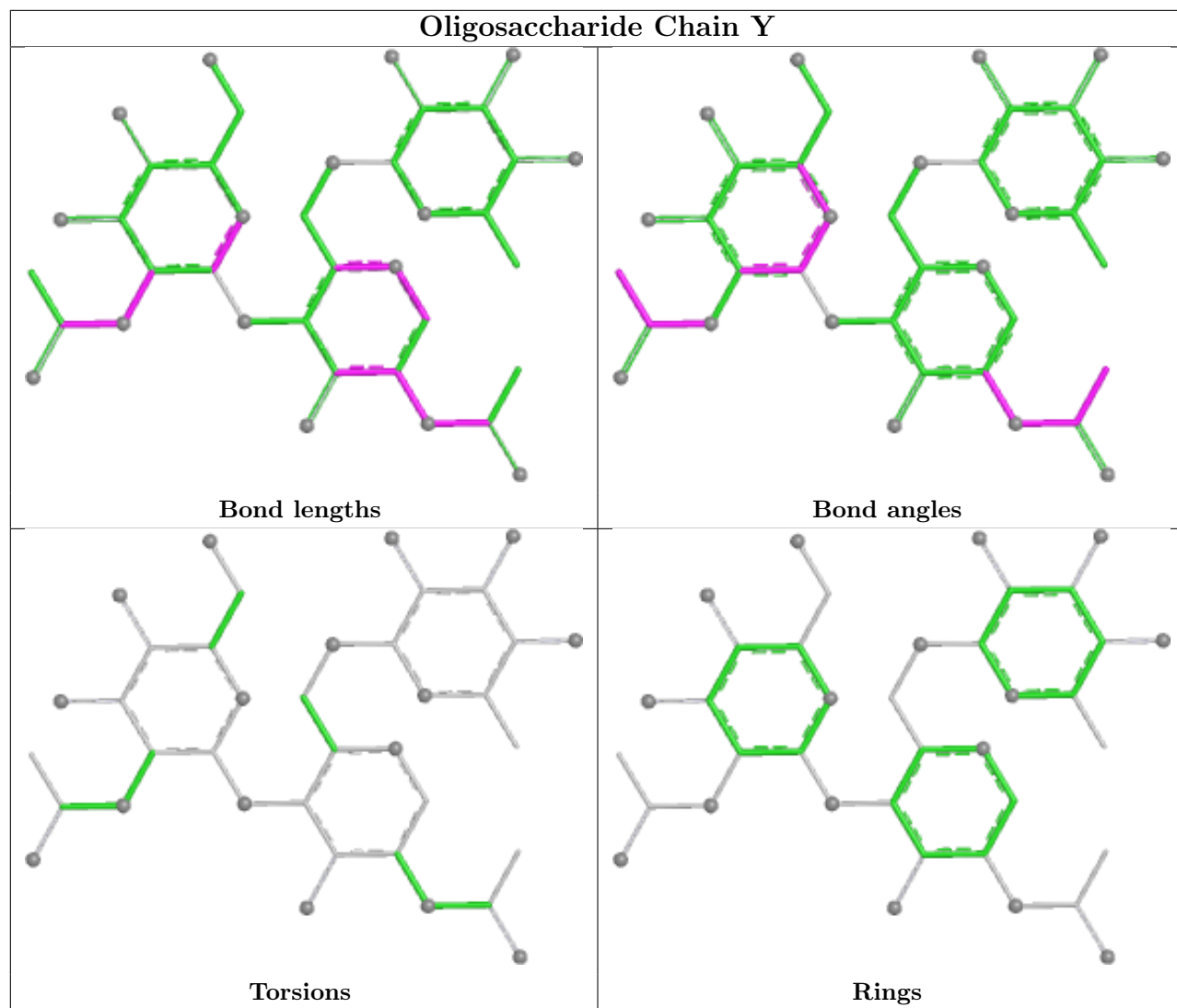
Oligosaccharide Chain H

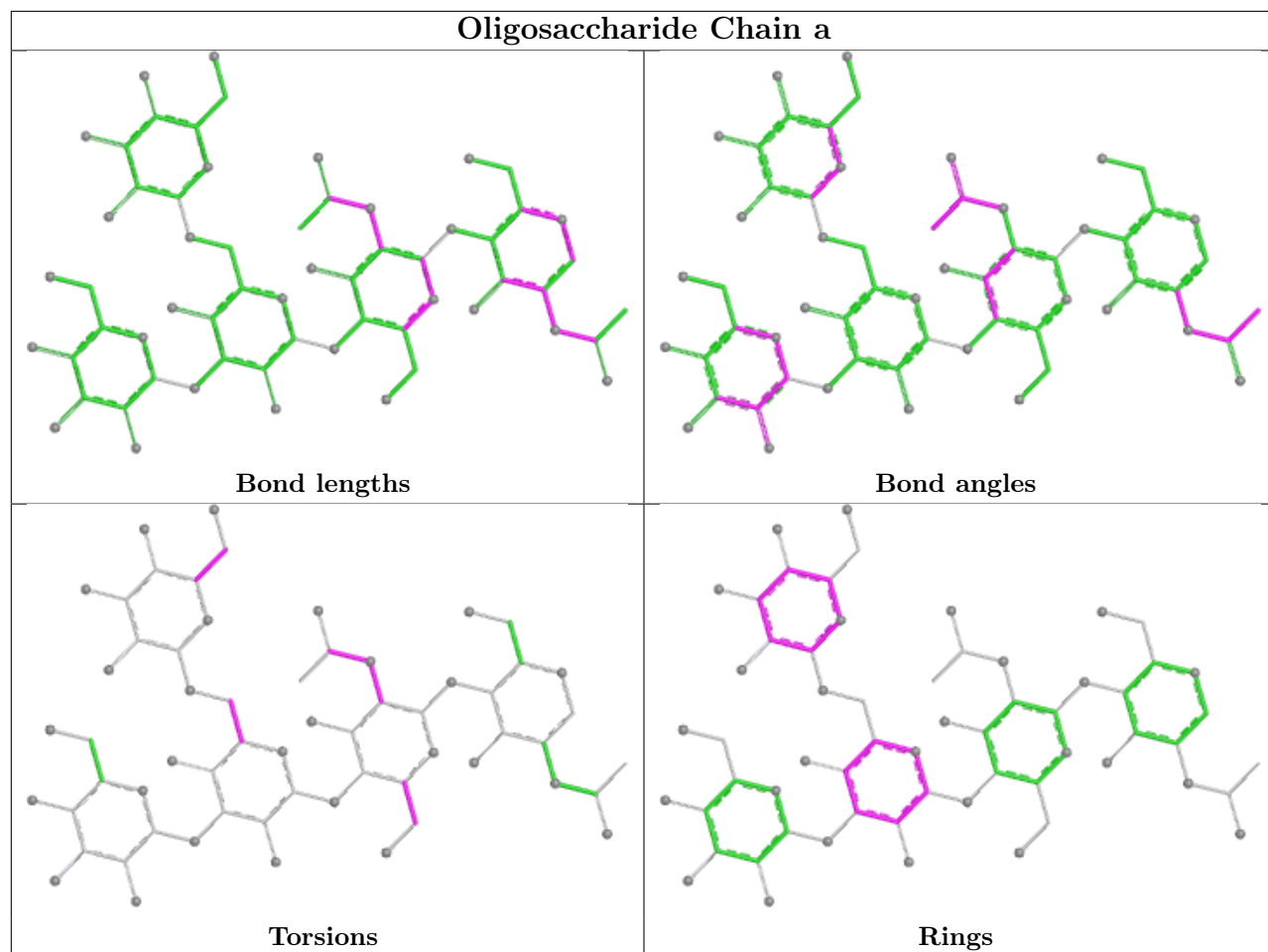


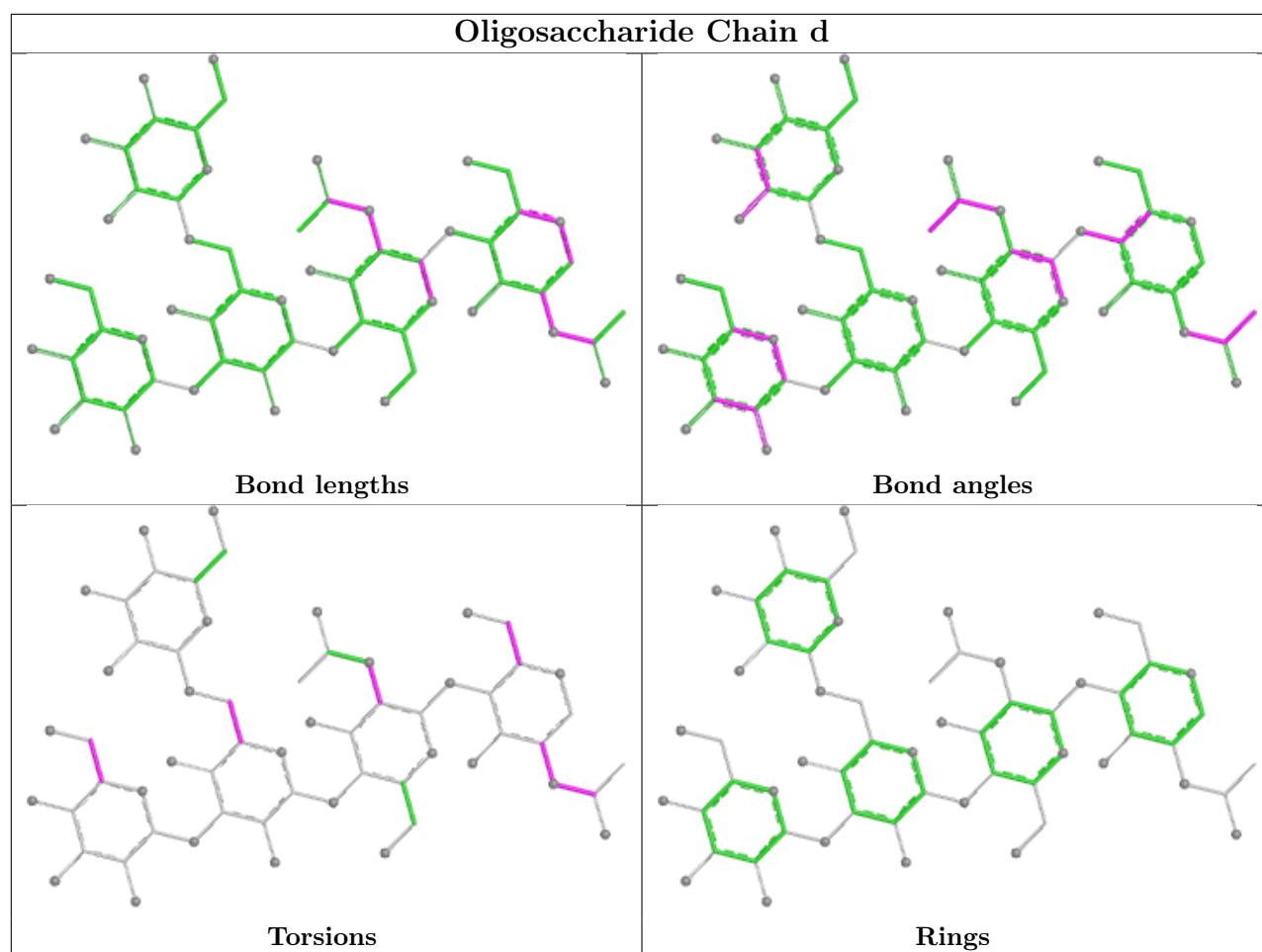
Oligosaccharide Chain J

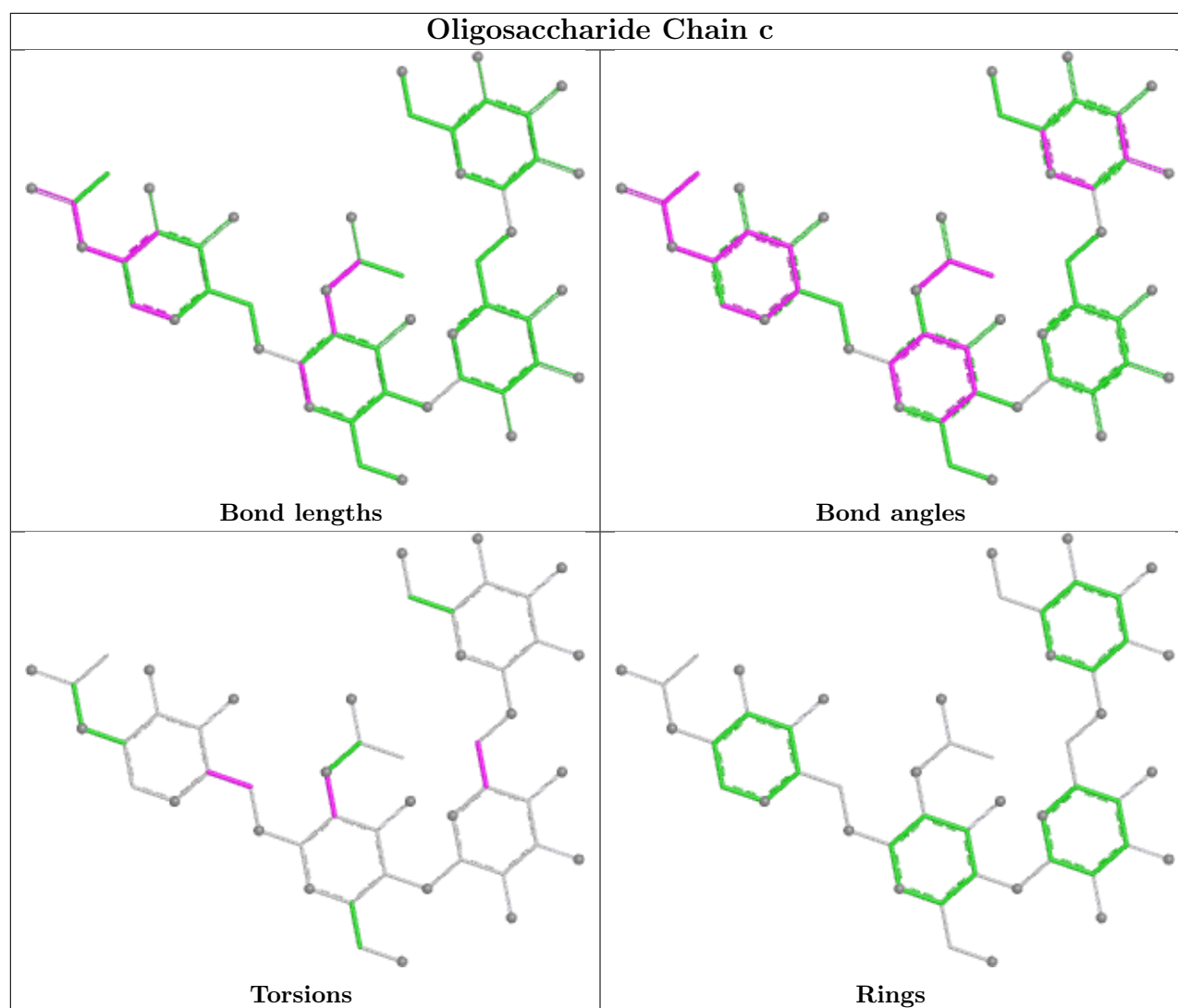












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
10	NAG	C	1403	1	14,14,15	1.93	3 (21%)	17,19,21	1.91	2 (11%)
10	NAG	B	1406	1	14,14,15	2.09	4 (28%)	17,19,21	2.62	7 (41%)
10	NAG	B	1407	1	14,14,15	2.36	5 (35%)	17,19,21	1.46	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	C	1405	1	14,14,15	2.02	4 (28%)	17,19,21	0.99	1 (5%)
10	NAG	B	1403	1	14,14,15	2.05	4 (28%)	17,19,21	1.37	4 (23%)
10	NAG	B	1402	1	14,14,15	2.05	4 (28%)	17,19,21	1.26	2 (11%)
10	NAG	C	1401	1	14,14,15	2.03	3 (21%)	17,19,21	1.50	2 (11%)
10	NAG	A	1305	1	14,14,15	2.21	4 (28%)	17,19,21	1.72	5 (29%)
10	NAG	B	1405	1	14,14,15	1.96	4 (28%)	17,19,21	1.18	2 (11%)
10	NAG	A	1303	1	14,14,15	1.99	4 (28%)	17,19,21	1.04	2 (11%)
10	NAG	A	1301	1	14,14,15	2.01	4 (28%)	17,19,21	1.08	2 (11%)
10	NAG	C	1404	1	14,14,15	2.01	4 (28%)	17,19,21	1.60	5 (29%)
10	NAG	A	1302	1	14,14,15	2.02	4 (28%)	17,19,21	1.19	2 (11%)
10	NAG	A	1306	1	14,14,15	2.04	3 (21%)	17,19,21	1.48	3 (17%)
10	NAG	C	1402	1	14,14,15	2.02	4 (28%)	17,19,21	1.21	1 (5%)
10	NAG	B	1404	1	14,14,15	1.99	4 (28%)	17,19,21	1.17	2 (11%)
10	NAG	B	1401	1	14,14,15	2.04	4 (28%)	17,19,21	1.20	1 (5%)
10	NAG	A	1304	1	14,14,15	2.16	4 (28%)	17,19,21	2.13	3 (17%)

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
10	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
10	NAG	B	1406	1	-	5/6/23/26	0/1/1/1
10	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1403	1	-	3/6/23/26	0/1/1/1
10	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
10	NAG	C	1401	1	-	4/6/23/26	0/1/1/1
10	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
10	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1402	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	1404	1	-	3/6/23/26	0/1/1/1
10	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1304	1	-	3/6/23/26	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1305	NAG	O5-C1	4.84	1.51	1.43
10	A	1304	NAG	O5-C1	4.80	1.51	1.43
10	B	1407	NAG	O5-C1	4.69	1.51	1.43
10	B	1403	NAG	O5-C1	4.53	1.51	1.43
10	B	1401	NAG	O5-C1	4.41	1.51	1.43
10	C	1405	NAG	O5-C1	4.39	1.51	1.43
10	B	1402	NAG	O5-C1	4.39	1.51	1.43
10	C	1401	NAG	O5-C1	4.34	1.51	1.43
10	A	1301	NAG	O5-C1	4.34	1.51	1.43
10	A	1303	NAG	O5-C1	4.33	1.51	1.43
10	A	1306	NAG	O5-C1	4.33	1.51	1.43
10	C	1402	NAG	O5-C1	4.31	1.50	1.43
10	C	1404	NAG	O5-C1	4.28	1.50	1.43
10	B	1406	NAG	O5-C1	4.24	1.50	1.43
10	B	1404	NAG	O5-C1	4.23	1.50	1.43
10	B	1405	NAG	O5-C1	4.20	1.50	1.43
10	A	1305	NAG	C7-N2	4.16	1.47	1.34
10	A	1302	NAG	O5-C1	4.14	1.50	1.43
10	B	1406	NAG	C7-N2	4.12	1.47	1.34
10	A	1306	NAG	C7-N2	4.10	1.47	1.34
10	C	1401	NAG	C7-N2	4.07	1.47	1.34
10	A	1304	NAG	C7-N2	4.04	1.47	1.34
10	C	1403	NAG	O5-C1	4.03	1.50	1.43
10	C	1402	NAG	C7-N2	3.94	1.47	1.34
10	B	1401	NAG	C7-N2	3.94	1.47	1.34
10	A	1302	NAG	C7-N2	3.93	1.47	1.34
10	B	1407	NAG	C7-N2	3.92	1.47	1.34
10	C	1404	NAG	C7-N2	3.92	1.47	1.34
10	C	1405	NAG	C7-N2	3.92	1.47	1.34
10	B	1404	NAG	C7-N2	3.90	1.46	1.34
10	B	1402	NAG	C7-N2	3.90	1.46	1.34
10	B	1403	NAG	C7-N2	3.87	1.46	1.34
10	A	1301	NAG	C7-N2	3.86	1.46	1.34
10	B	1405	NAG	C7-N2	3.85	1.46	1.34
10	A	1303	NAG	C7-N2	3.82	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1403	NAG	C7-N2	3.80	1.46	1.34
10	B	1407	NAG	C2-N2	3.50	1.52	1.46
10	B	1407	NAG	C1-C2	3.44	1.57	1.52
10	B	1406	NAG	C2-N2	3.07	1.51	1.46
10	A	1306	NAG	C2-N2	3.03	1.51	1.46
10	A	1305	NAG	C2-N2	2.99	1.51	1.46
10	A	1304	NAG	C2-N2	2.87	1.51	1.46
10	B	1404	NAG	C2-N2	2.58	1.50	1.46
10	C	1402	NAG	C2-N2	2.56	1.50	1.46
10	C	1401	NAG	C2-N2	2.54	1.50	1.46
10	B	1402	NAG	O5-C5	2.54	1.48	1.43
10	C	1404	NAG	C2-N2	2.53	1.50	1.46
10	A	1302	NAG	C2-N2	2.53	1.50	1.46
10	B	1401	NAG	C2-N2	2.52	1.50	1.46
10	C	1405	NAG	C2-N2	2.51	1.50	1.46
10	B	1402	NAG	C2-N2	2.48	1.50	1.46
10	A	1301	NAG	C2-N2	2.46	1.50	1.46
10	B	1403	NAG	C2-N2	2.46	1.50	1.46
10	B	1405	NAG	C2-N2	2.42	1.50	1.46
10	A	1303	NAG	C2-N2	2.38	1.50	1.46
10	B	1403	NAG	O5-C5	2.37	1.48	1.43
10	C	1404	NAG	O5-C5	2.36	1.48	1.43
10	C	1403	NAG	C2-N2	2.35	1.50	1.46
10	A	1302	NAG	O5-C5	2.33	1.48	1.43
10	A	1301	NAG	O5-C5	2.32	1.48	1.43
10	A	1305	NAG	O5-C5	2.29	1.47	1.43
10	B	1401	NAG	O5-C5	2.28	1.47	1.43
10	A	1304	NAG	O5-C5	2.22	1.47	1.43
10	B	1407	NAG	O5-C5	2.22	1.47	1.43
10	A	1303	NAG	O5-C5	2.21	1.47	1.43
10	C	1405	NAG	O5-C5	2.21	1.47	1.43
10	B	1404	NAG	O5-C5	2.20	1.47	1.43
10	C	1402	NAG	O5-C5	2.17	1.47	1.43
10	B	1405	NAG	O5-C5	2.13	1.47	1.43
10	B	1406	NAG	O5-C5	2.10	1.47	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1403	NAG	C1-O5-C5	6.13	120.40	112.19
10	B	1406	NAG	C1-O5-C5	4.91	118.77	112.19
10	B	1406	NAG	C4-C3-C2	4.90	118.20	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1305	NAG	C8-C7-N2	4.75	124.00	116.12
10	A	1304	NAG	O5-C1-C2	4.72	118.60	111.29
10	A	1304	NAG	C1-O5-C5	4.35	118.02	112.19
10	B	1406	NAG	C8-C7-N2	4.15	123.00	116.12
10	A	1304	NAG	C8-C7-N2	4.01	122.77	116.12
10	C	1401	NAG	C8-C7-N2	3.77	122.38	116.12
10	C	1403	NAG	C4-C3-C2	3.68	116.41	111.02
10	B	1406	NAG	C3-C4-C5	3.53	116.64	110.23
10	B	1407	NAG	C6-C5-C4	-3.31	104.90	113.02
10	A	1306	NAG	C8-C7-N2	3.27	121.55	116.12
10	B	1401	NAG	C8-C7-N2	3.25	121.51	116.12
10	C	1402	NAG	C8-C7-N2	3.18	121.40	116.12
10	C	1404	NAG	C3-C4-C5	3.17	115.98	110.23
10	C	1401	NAG	C4-C3-C2	3.15	115.63	111.02
10	A	1306	NAG	C1-O5-C5	-3.03	108.12	112.19
10	B	1406	NAG	O5-C1-C2	2.99	115.92	111.29
10	B	1406	NAG	C6-C5-C4	-2.78	106.19	113.02
10	B	1404	NAG	C8-C7-N2	2.53	120.31	116.12
10	B	1402	NAG	C8-C7-N2	2.51	120.28	116.12
10	B	1402	NAG	C2-N2-C7	-2.51	119.54	122.90
10	C	1404	NAG	C2-N2-C7	-2.50	119.56	122.90
10	C	1404	NAG	C8-C7-N2	2.49	120.24	116.12
10	B	1403	NAG	C8-C7-N2	2.42	120.13	116.12
10	B	1403	NAG	C2-N2-C7	-2.38	119.71	122.90
10	C	1404	NAG	C4-C3-C2	2.36	114.48	111.02
10	B	1405	NAG	C8-C7-N2	2.33	119.97	116.12
10	A	1305	NAG	C1-O5-C5	2.30	115.28	112.19
10	B	1403	NAG	C1-O5-C5	2.30	115.27	112.19
10	A	1305	NAG	O7-C7-C8	-2.29	117.98	122.05
10	A	1301	NAG	C8-C7-N2	2.27	119.88	116.12
10	A	1303	NAG	C2-N2-C7	-2.26	119.87	122.90
10	B	1406	NAG	O5-C5-C4	2.25	116.29	110.83
10	A	1302	NAG	C1-C2-N2	-2.24	106.90	110.43
10	A	1305	NAG	O7-C7-N2	-2.24	118.02	121.98
10	A	1303	NAG	C8-C7-N2	2.23	119.82	116.12
10	B	1404	NAG	C2-N2-C7	-2.21	119.93	122.90
10	C	1405	NAG	C8-C7-N2	2.19	119.75	116.12
10	A	1305	NAG	O5-C1-C2	2.16	114.64	111.29
10	B	1405	NAG	C2-N2-C7	-2.15	120.01	122.90
10	C	1404	NAG	C1-O5-C5	2.08	114.98	112.19
10	A	1301	NAG	C2-N2-C7	-2.08	120.12	122.90
10	B	1403	NAG	C3-C4-C5	2.06	113.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1306	NAG	C4-C3-C2	2.06	114.04	111.02
10	B	1407	NAG	C8-C7-N2	2.06	119.53	116.12
10	A	1302	NAG	C8-C7-N2	2.05	119.51	116.12

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1304	NAG	C1-C2-N2-C7
10	B	1407	NAG	C3-C2-N2-C7
10	C	1405	NAG	C1-C2-N2-C7
10	B	1402	NAG	O5-C5-C6-O6
10	B	1404	NAG	O5-C5-C6-O6
10	C	1402	NAG	O5-C5-C6-O6
10	B	1405	NAG	O5-C5-C6-O6
10	B	1402	NAG	C4-C5-C6-O6
10	C	1401	NAG	O5-C5-C6-O6
10	B	1404	NAG	C4-C5-C6-O6
10	C	1402	NAG	C4-C5-C6-O6
10	C	1405	NAG	O5-C5-C6-O6
10	C	1401	NAG	C4-C5-C6-O6
10	B	1405	NAG	C4-C5-C6-O6
10	A	1304	NAG	C8-C7-N2-C2
10	A	1304	NAG	O7-C7-N2-C2
10	A	1305	NAG	C8-C7-N2-C2
10	A	1305	NAG	O7-C7-N2-C2
10	A	1306	NAG	C8-C7-N2-C2
10	A	1306	NAG	O7-C7-N2-C2
10	B	1401	NAG	C8-C7-N2-C2
10	B	1401	NAG	O7-C7-N2-C2
10	B	1406	NAG	C8-C7-N2-C2
10	B	1406	NAG	O7-C7-N2-C2
10	C	1401	NAG	C8-C7-N2-C2
10	C	1401	NAG	O7-C7-N2-C2
10	C	1402	NAG	C8-C7-N2-C2
10	C	1402	NAG	O7-C7-N2-C2
10	C	1405	NAG	C4-C5-C6-O6
10	B	1403	NAG	O5-C5-C6-O6
10	B	1406	NAG	O5-C5-C6-O6
10	B	1403	NAG	C3-C2-N2-C7
10	C	1403	NAG	O5-C5-C6-O6
10	A	1302	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
10	B	1403	NAG	C1-C2-N2-C7
10	B	1406	NAG	C1-C2-N2-C7
10	A	1302	NAG	C3-C2-N2-C7
10	A	1305	NAG	C1-C2-N2-C7
10	B	1402	NAG	C1-C2-N2-C7
10	B	1404	NAG	C1-C2-N2-C7
10	A	1305	NAG	C3-C2-N2-C7
10	B	1406	NAG	C3-C2-N2-C7
10	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1406	NAG	4	0
10	B	1407	NAG	4	0
10	C	1401	NAG	2	0
10	A	1305	NAG	4	0
10	C	1404	NAG	1	0
10	A	1302	NAG	1	0
10	B	1404	NAG	1	0
10	A	1304	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

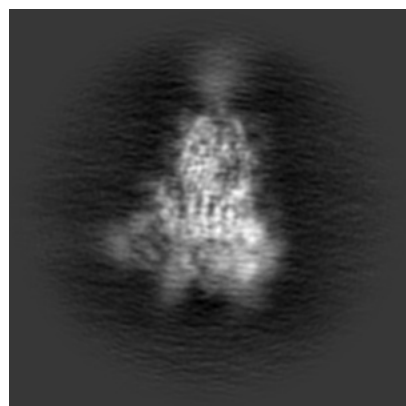
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44344. These allow visual inspection of the internal detail of the map and identification of artifacts.

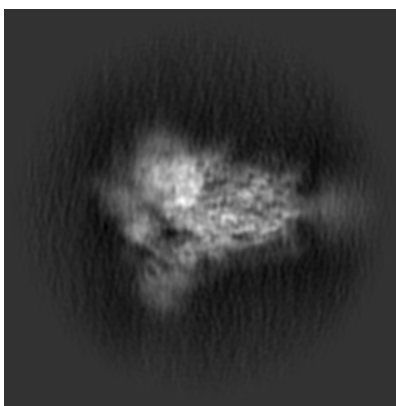
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

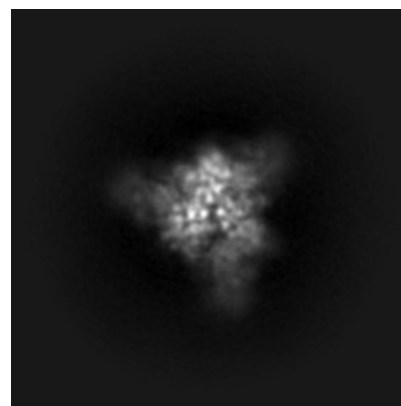
6.1.1 Primary map



X

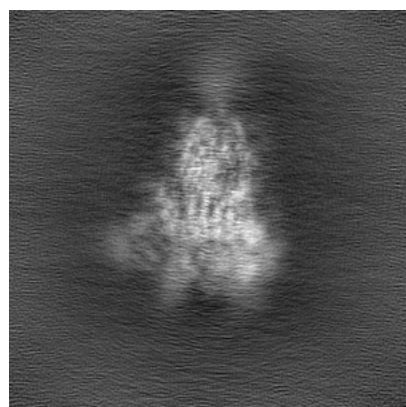


Y

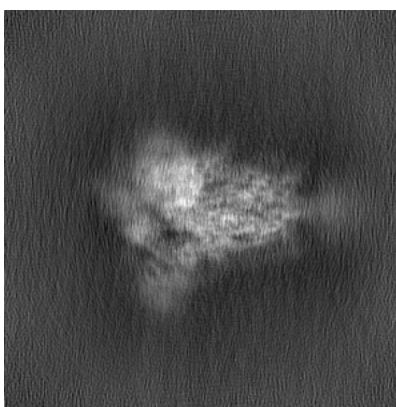


Z

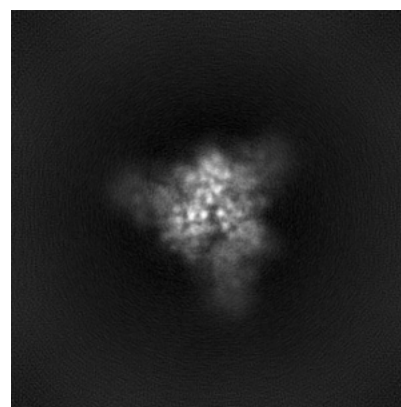
6.1.2 Raw map



X



Y

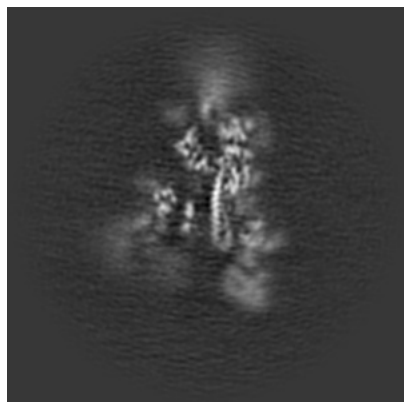


Z

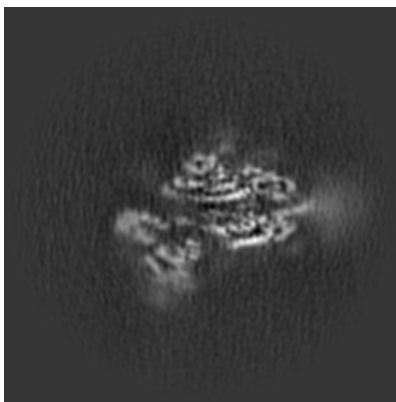
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

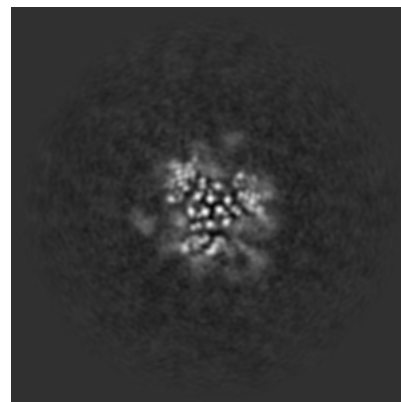
6.2.1 Primary map



X Index: 136

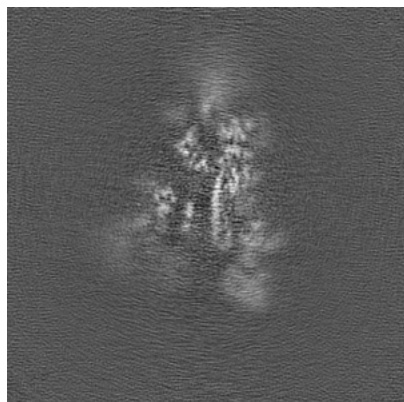


Y Index: 136

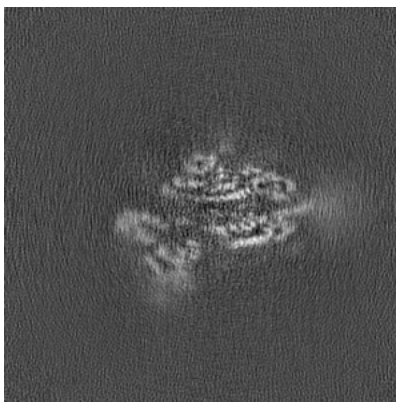


Z Index: 136

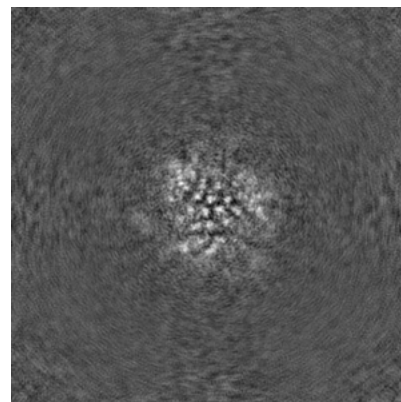
6.2.2 Raw map



X Index: 136



Y Index: 136

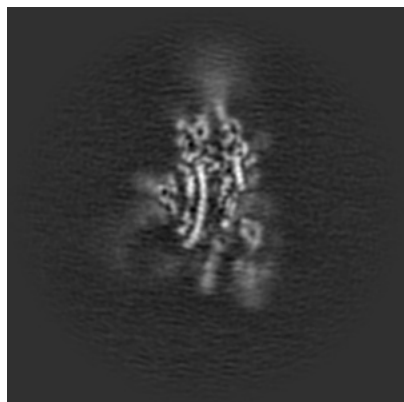


Z Index: 136

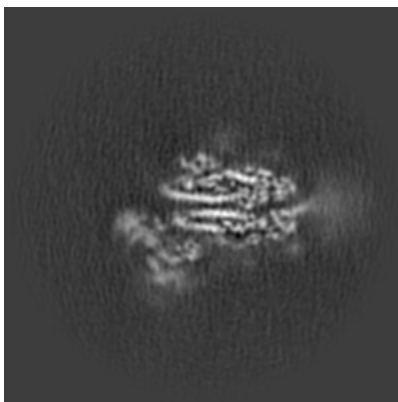
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

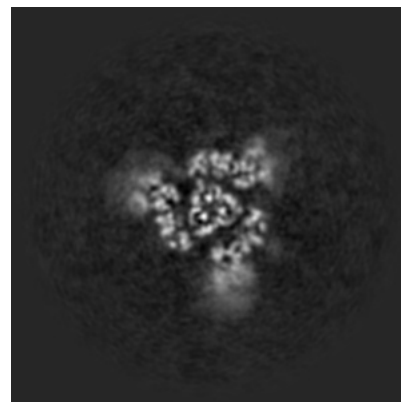
6.3.1 Primary map



X Index: 130

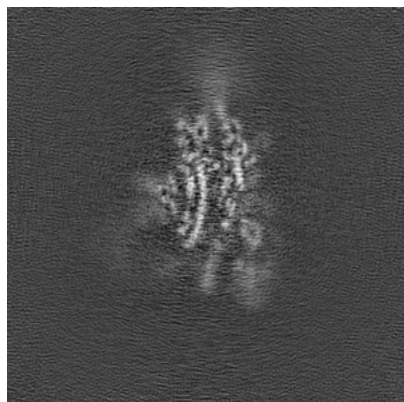


Y Index: 133

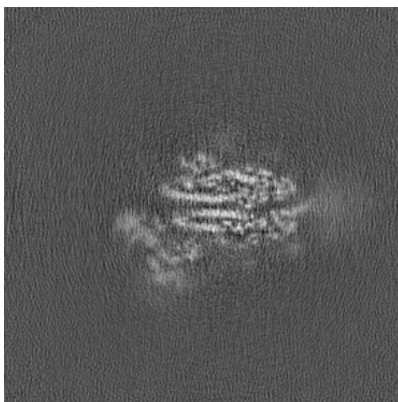


Z Index: 121

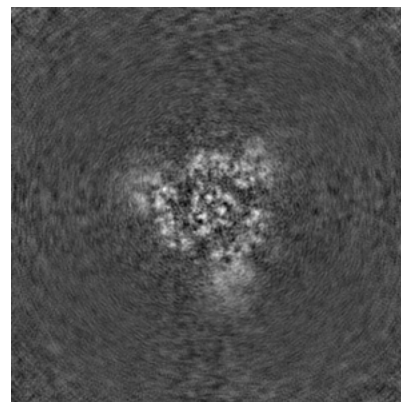
6.3.2 Raw map



X Index: 130



Y Index: 133

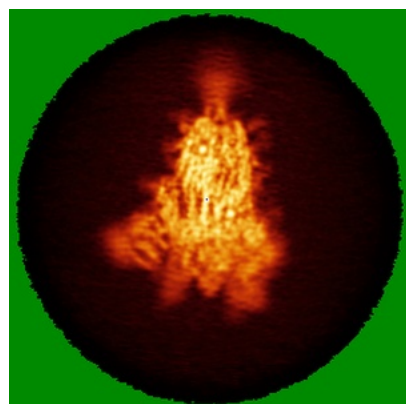


Z Index: 121

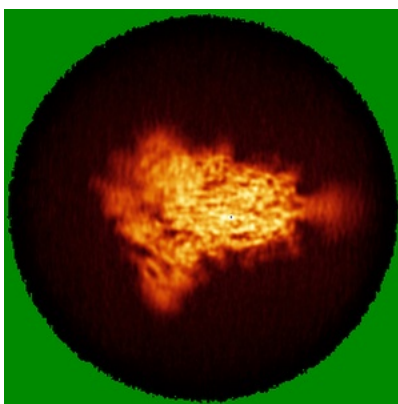
The images above show the largest variance slices of the map in three orthogonal directions.

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

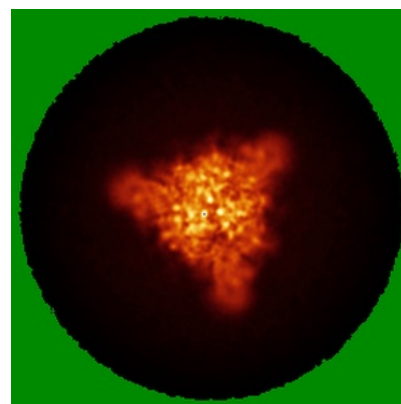
6.4.1 Primary map



X

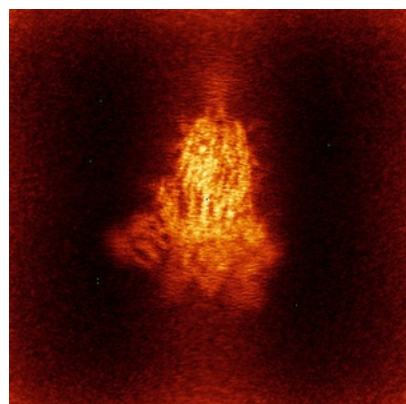


Y

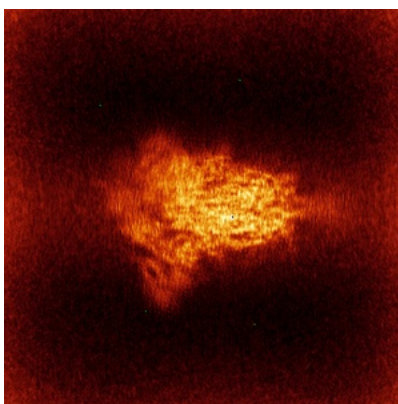


Z

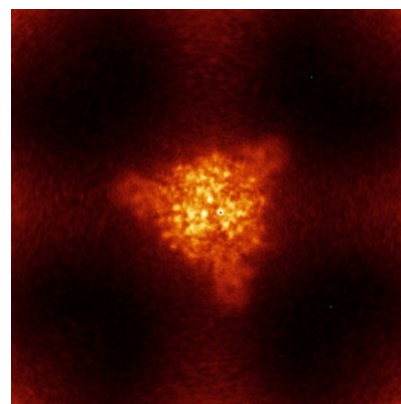
6.4.2 Raw map



X



Y

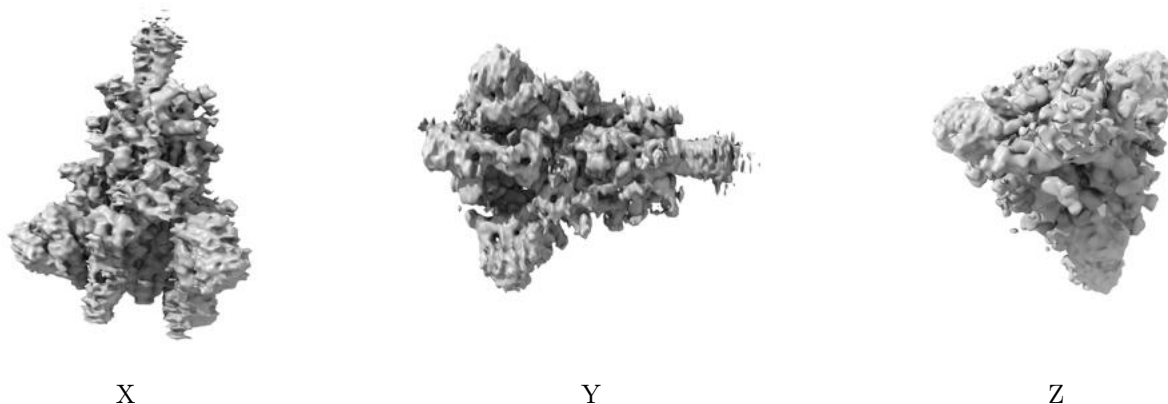


Z

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 0.0607. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

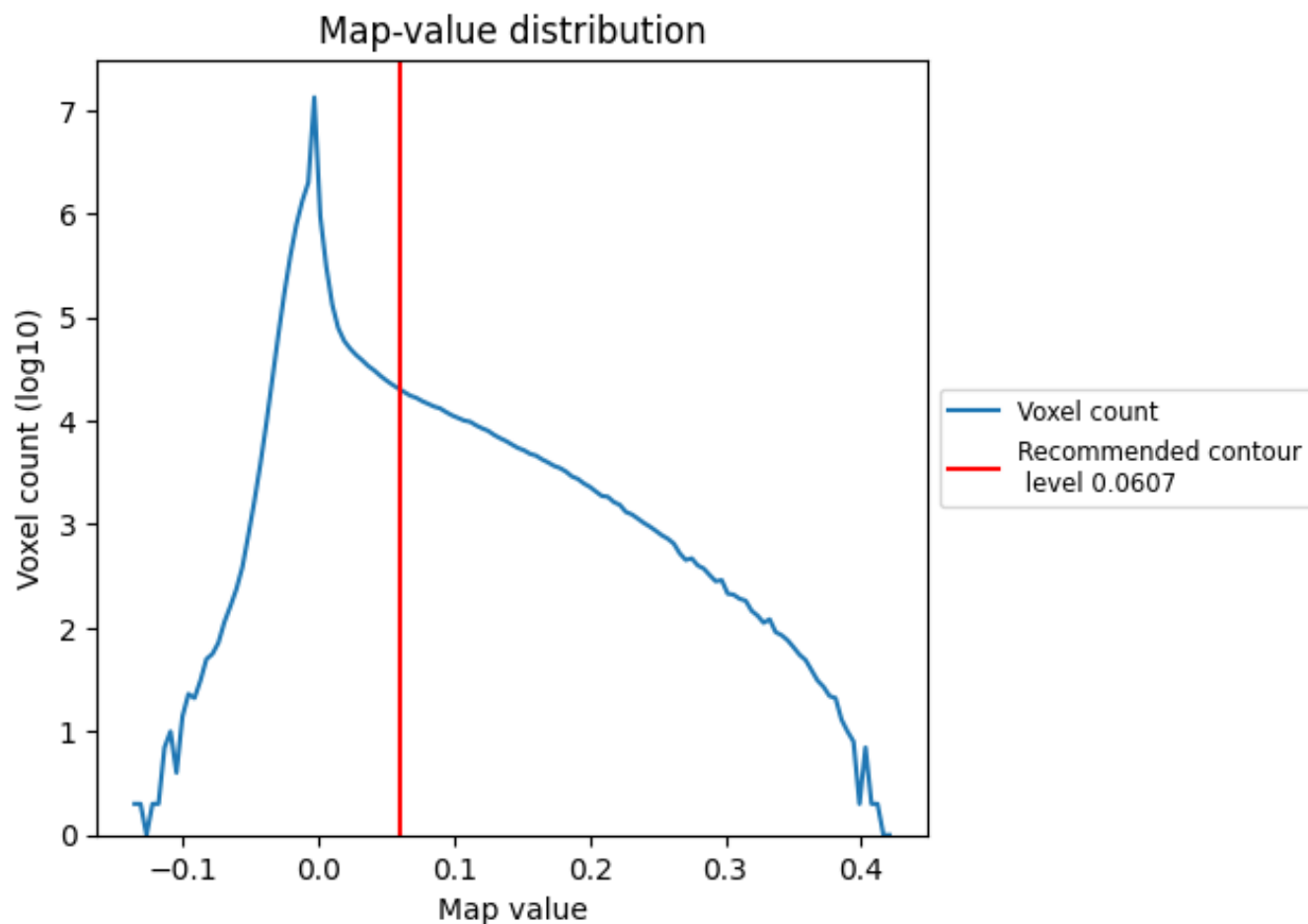
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

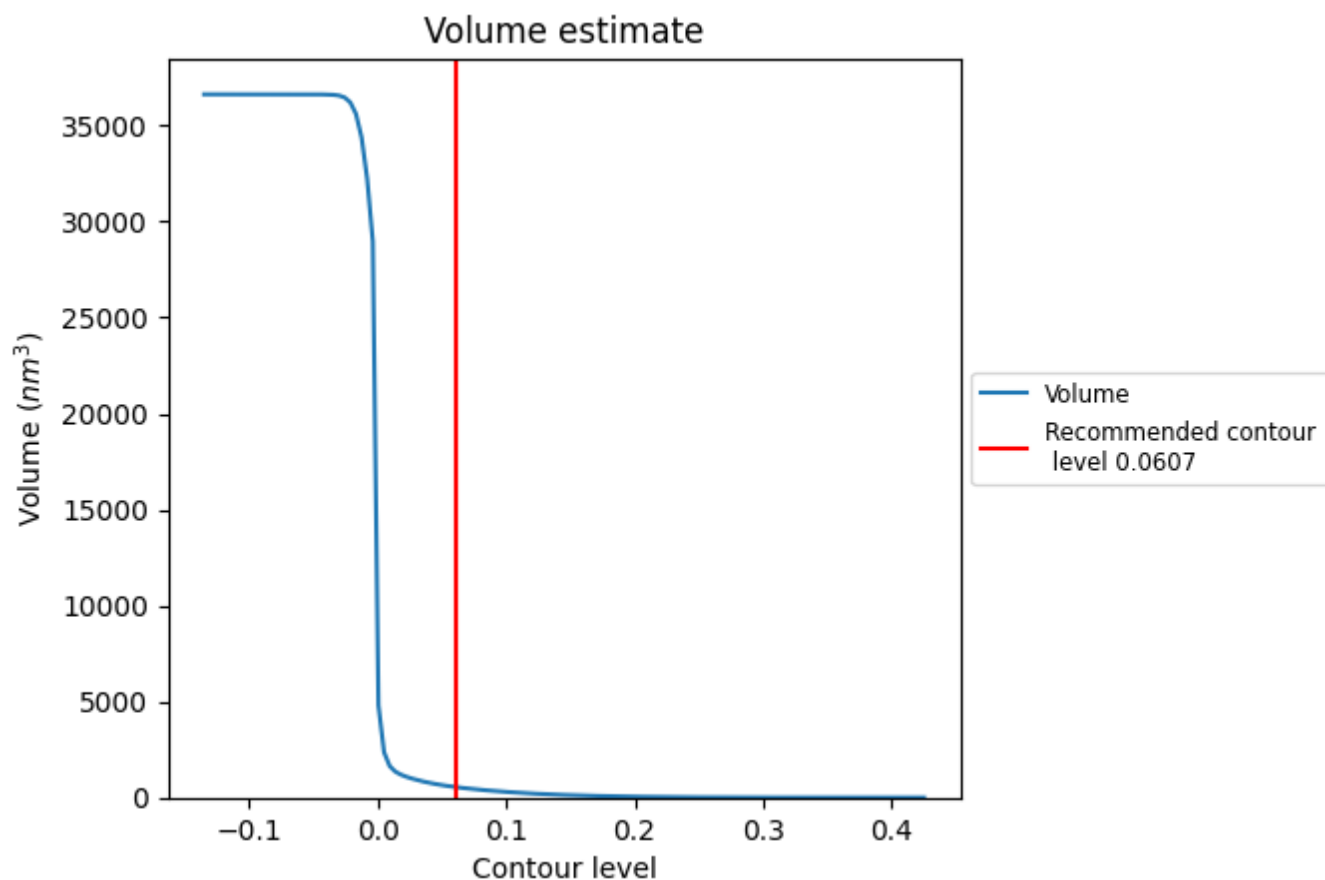
This section contains the results of statistical analysis of the map.

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.

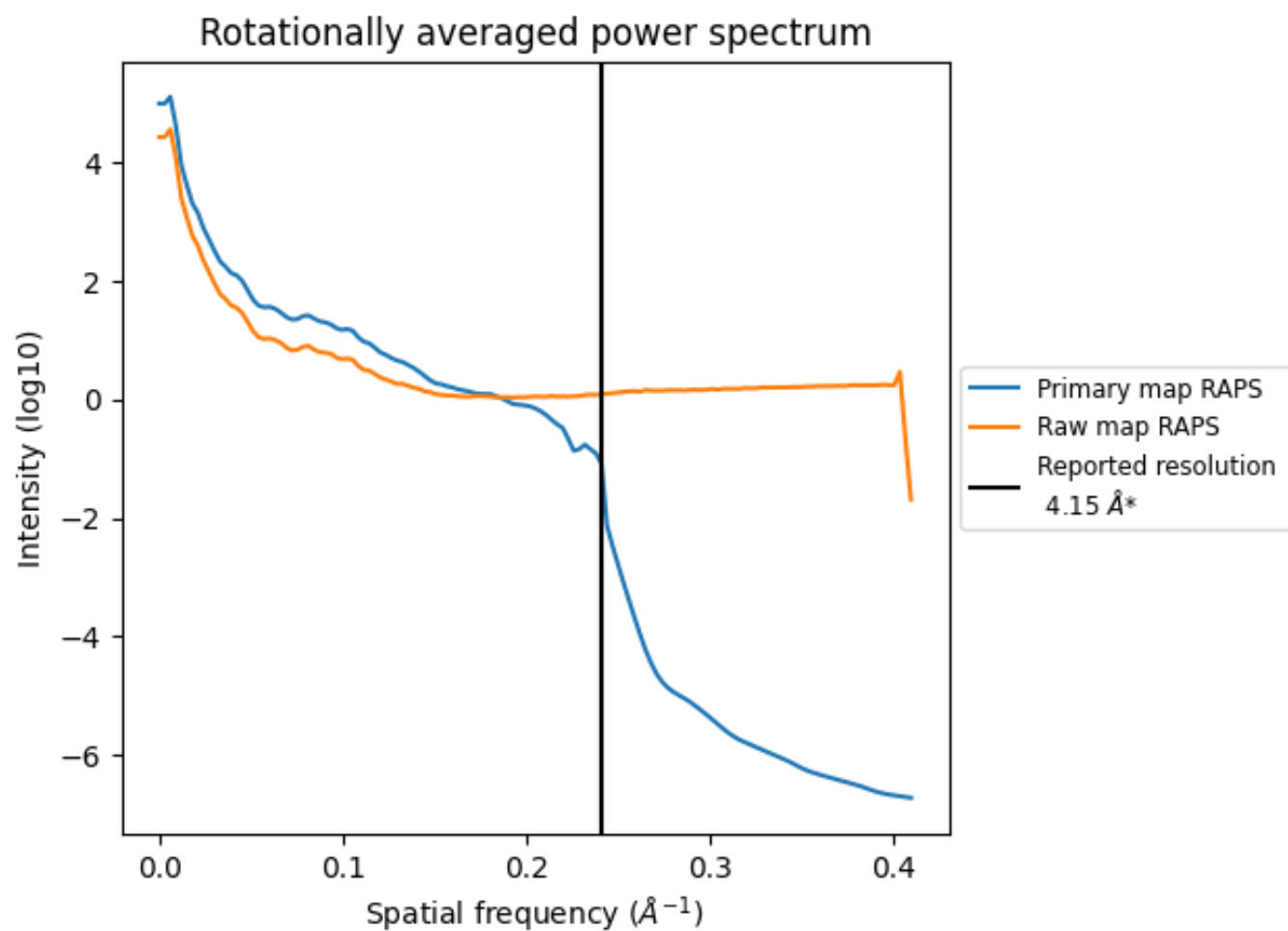
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 ⓘ

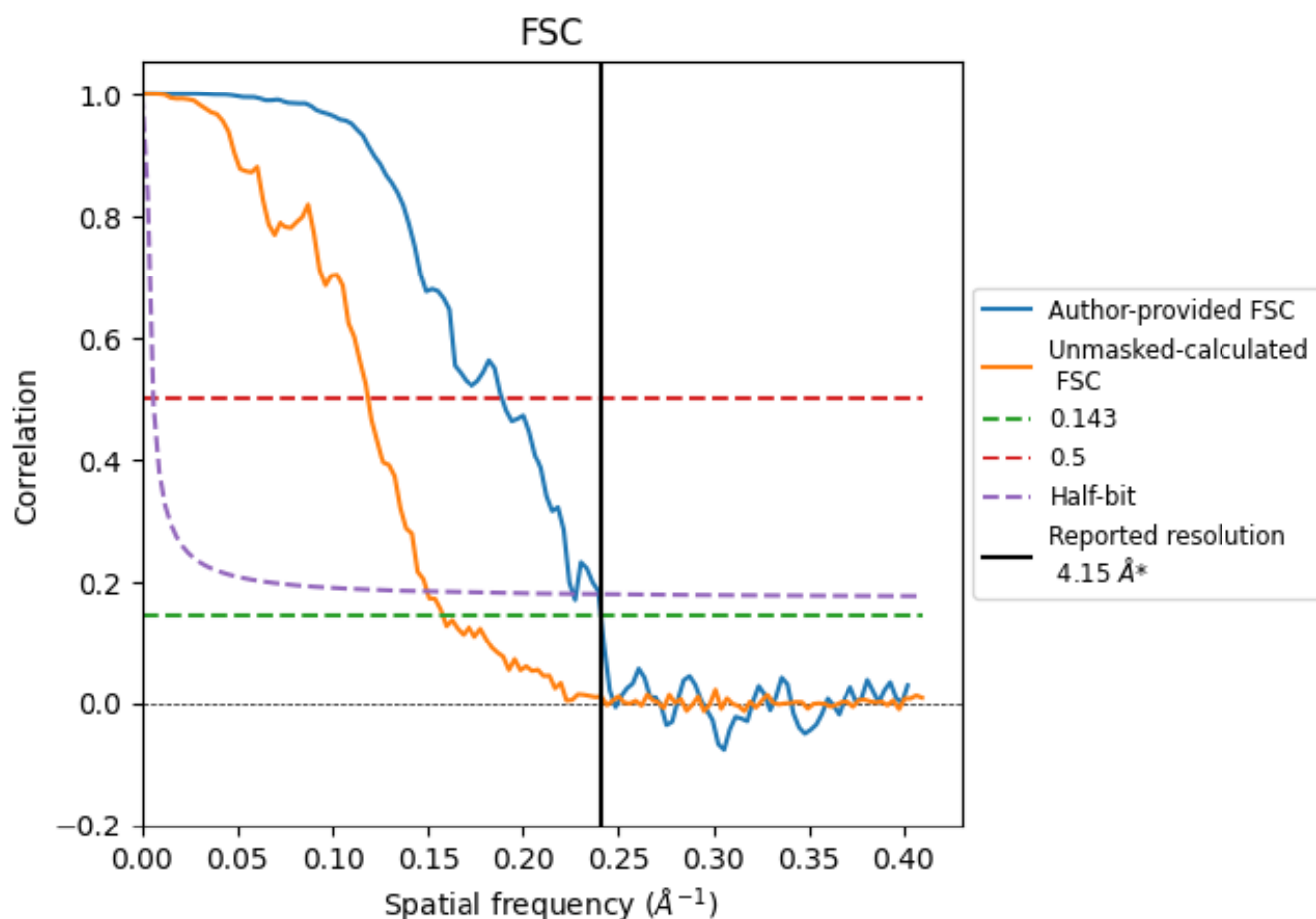


*Reported resolution corresponds to spatial frequency of 0.241 Å⁻¹

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 0.241 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

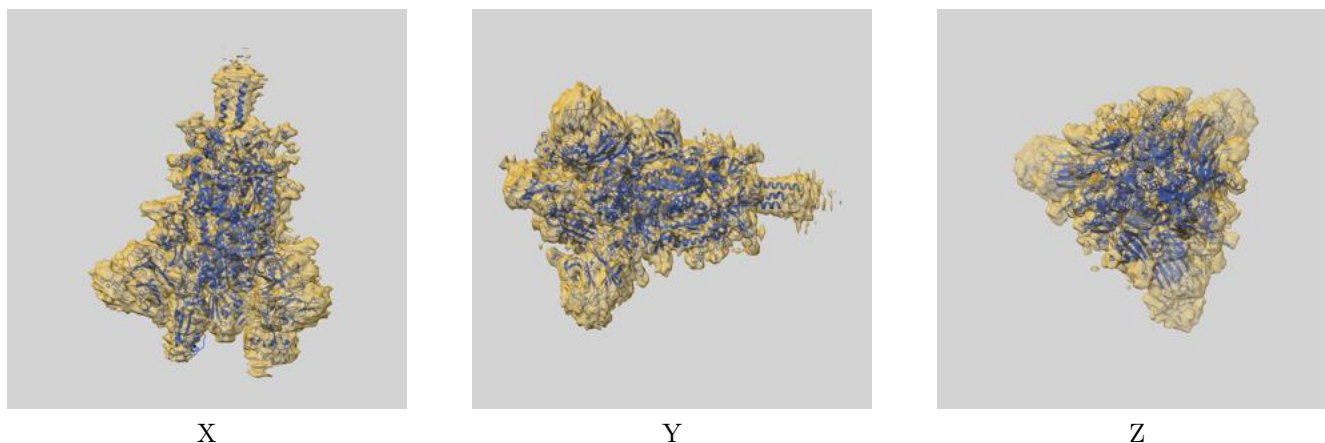
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.15	-	-
Author-provided FSC curve	4.15	5.29	4.42
Unmasked-calculated*	6.34	8.43	6.69

*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 6.34 differs from the reported value 4.15 by more than 10 %

9 Map-model fit [i](#)

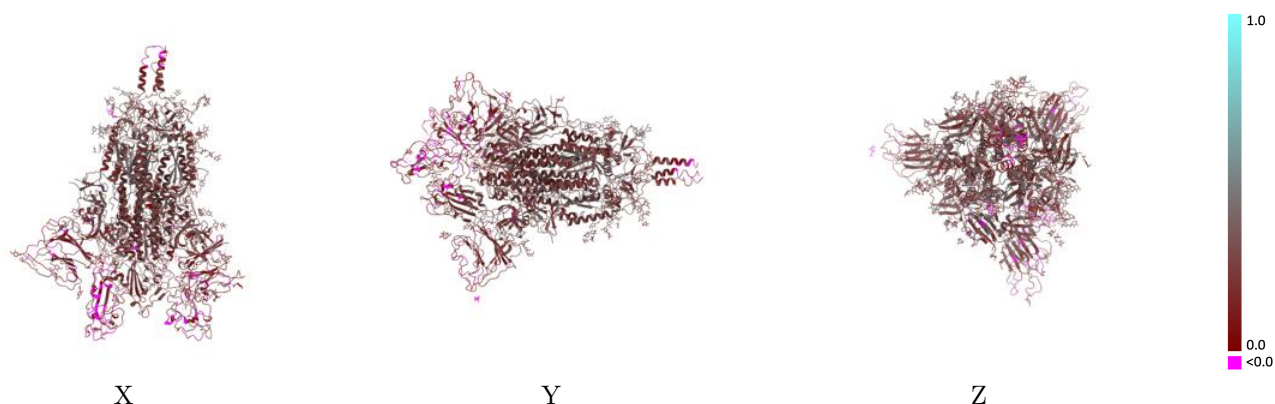
This section contains information regarding the fit between EMDB map EMD-44344 and PDB model 9B8F. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



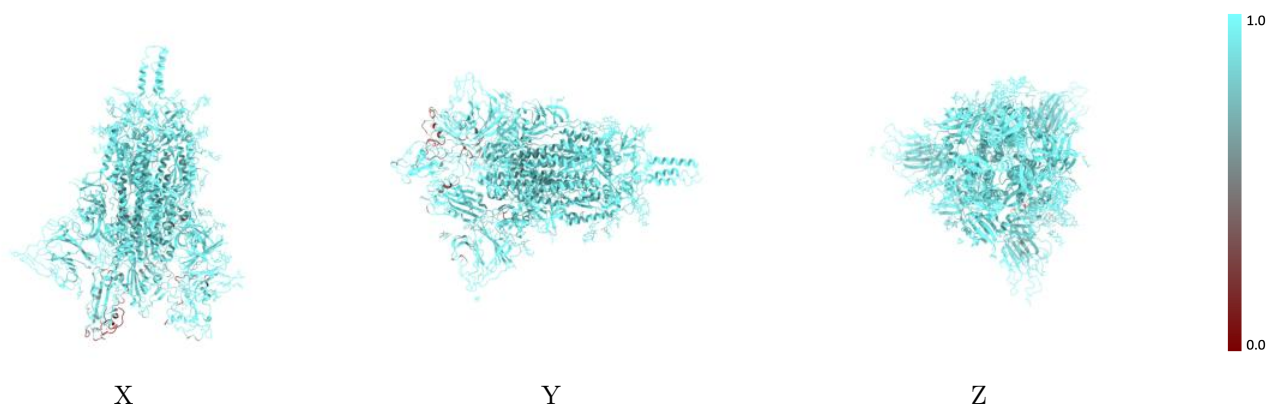
The images above show the 3D surface view of the map at the recommended contour level 0.0607 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



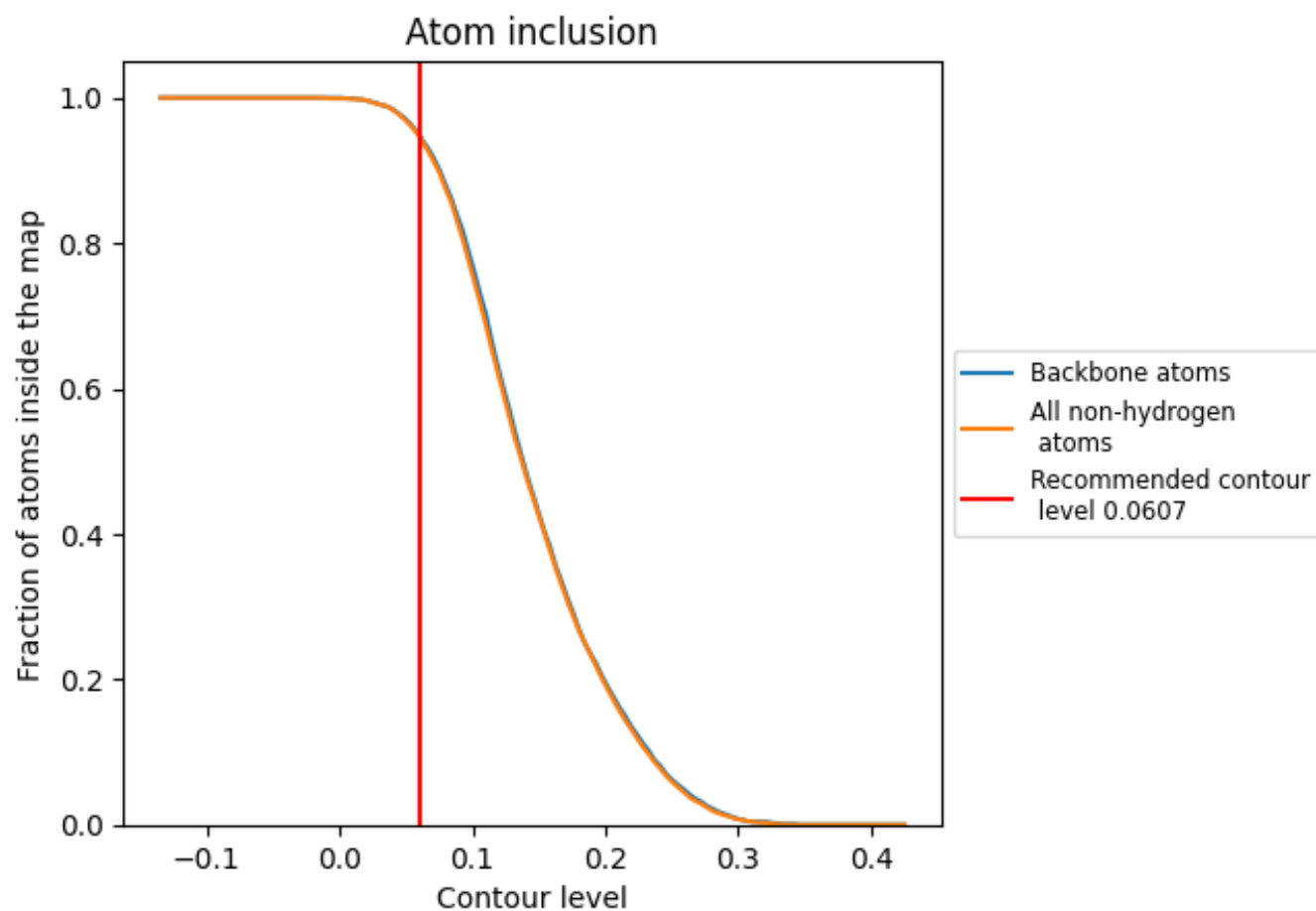
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0607).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0607) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.2480
A	 0.9190	 0.2350
B	 0.9670	 0.2570
C	 0.9520	 0.2460
D	 0.9490	 0.2530
E	 1.0000	 0.3320
F	 0.9400	 0.1930
G	 0.8570	 0.2910
H	 0.9390	 0.1380
I	 0.8930	 0.2210
J	 0.9600	 0.2600
K	 1.0000	 0.3920
L	 1.0000	 0.3700
M	 1.0000	 0.3540
N	 0.9740	 0.2790
O	 0.9640	 0.2820
P	 0.9490	 0.3520
Q	 0.9640	 0.3040
R	 0.8720	 0.2020
S	 0.9740	 0.3720
T	 1.0000	 0.2710
U	 1.0000	 0.3120
V	 1.0000	 0.2850
W	 0.9740	 0.2400
X	 0.9740	 0.2470
Y	 0.9740	 0.2210
Z	 0.9400	 0.3100
a	 0.9840	 0.2990
b	 0.9740	 0.2760
c	 0.9800	 0.3100
d	 1.0000	 0.2700
e	 1.0000	 0.3960
f	 0.7860	 0.1960

