



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 02:43 PM EDT

PDB ID : 9OM5 / pdb_00009om5
EMDB ID : EMD-70607
Title : Composite map of six VRC35 Fabs and three MEDI8852 Fabs bound to influenza H3N2 Victoria 2011 hemagglutinin
Authors : Cheng, J.; Cale, E.M.; Longo, N.; Sutton, M.S.; Lei, H.; Huang, R.; Morton, A.J.; Lang, Z.C.; Morano, N.C.; Roark, R.S.; Becker, J.E.; Tsybovsky, Y.; Li, N.; Zhang, B.; Du, H.; Rubin, S.; Shapiro, L.; Pierson, T.C.; Doria-Rose, N.A.; Kwong, P.D.; Zhou, T.
Deposited on : 2025-05-13
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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)

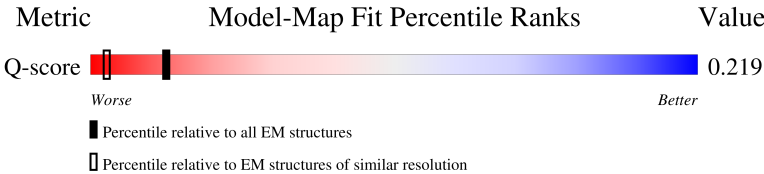
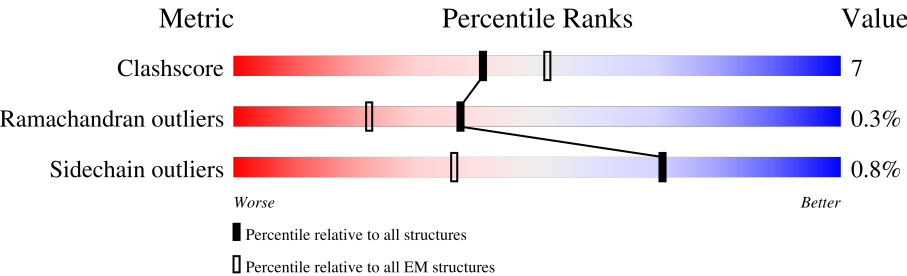
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)







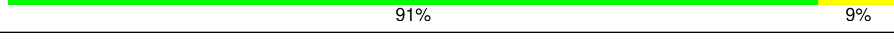
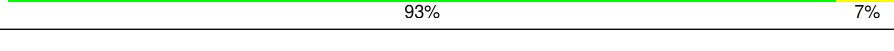
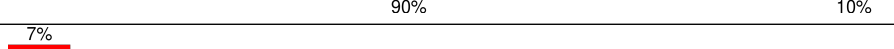
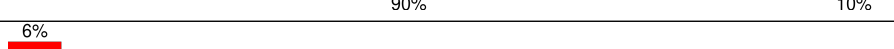
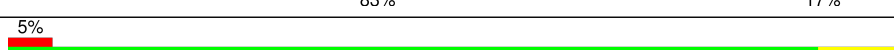
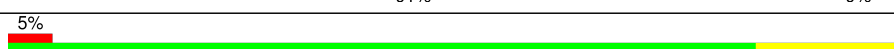
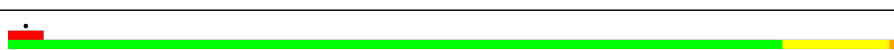

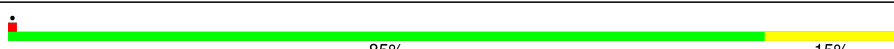





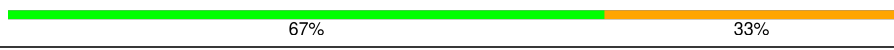
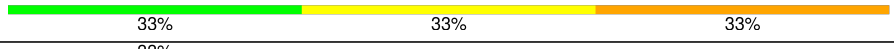

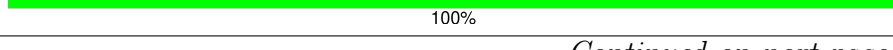

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	348	
1	C	348	
1	E	348	

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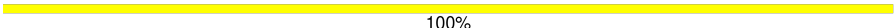

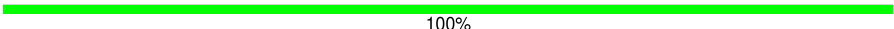

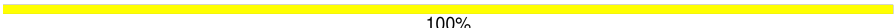

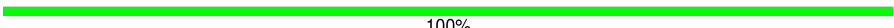

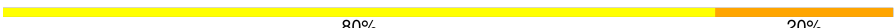
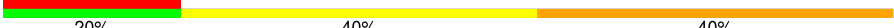
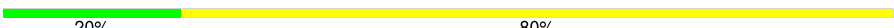
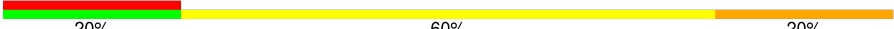
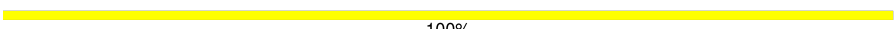


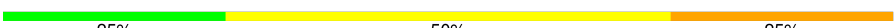
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	223	
2	D	223	
2	F	223	
3	G	227	
3	I	227	
3	K	227	
4	H	206	
4	J	206	
4	L	206	
5	a	222	
5	c	222	
5	e	222	
5	g	222	
5	i	222	
5	k	222	
6	b	219	
6	d	219	
6	f	219	
6	h	219	
6	j	219	
6	l	219	
7	M	3	
7	N	3	
7	P	3	
7	R	3	

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Mol	Chain	Length	Quality of chain
7	T	3	
7	U	3	
7	W	3	
7	Y	3	
7	m	3	
7	n	3	
7	p	3	
7	r	3	
8	O	5	
8	Q	5	
8	S	5	
8	X	5	
8	Z	5	
8	q	5	
8	s	5	
9	V	4	
9	o	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 42837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2537	1586	453	485	13		
1	C	325	Total	C	N	O	S	0	0
			2537	1586	453	485	13		
1	E	325	Total	C	N	O	S	0	0
			2537	1586	453	485	13		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	TYR	conflict	UNP A0A5P1MU07
A	30	CYS	THR	conflict	UNP A0A5P1MU07
A	328	ARG	-	expression tag	UNP A0A5P1MU07
A	329	ARG	-	expression tag	UNP A0A5P1MU07
A	330	ARG	-	expression tag	UNP A0A5P1MU07
A	331	ARG	-	expression tag	UNP A0A5P1MU07
A	332	ARG	-	expression tag	UNP A0A5P1MU07
C	-7	HIS	TYR	conflict	UNP A0A5P1MU07
C	30	CYS	THR	conflict	UNP A0A5P1MU07
C	328	ARG	-	expression tag	UNP A0A5P1MU07
C	329	ARG	-	expression tag	UNP A0A5P1MU07
C	330	ARG	-	expression tag	UNP A0A5P1MU07
C	331	ARG	-	expression tag	UNP A0A5P1MU07
C	332	ARG	-	expression tag	UNP A0A5P1MU07
E	-7	HIS	TYR	conflict	UNP A0A5P1MU07
E	30	CYS	THR	conflict	UNP A0A5P1MU07
E	328	ARG	-	expression tag	UNP A0A5P1MU07
E	329	ARG	-	expression tag	UNP A0A5P1MU07
E	330	ARG	-	expression tag	UNP A0A5P1MU07
E	331	ARG	-	expression tag	UNP A0A5P1MU07
E	332	ARG	-	expression tag	UNP A0A5P1MU07

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total 1393	C 867	N 245	O 274	S 7	0	0
2	D	173	Total 1393	C 867	N 245	O 274	S 7	0	0
2	F	173	Total 1393	C 867	N 245	O 274	S 7	0	0

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	CYS	GLN	conflict	UNP A0A2P1E3C0
B	177	SER	-	expression tag	UNP A0A2P1E3C0
B	178	GLY	-	expression tag	UNP A0A2P1E3C0
B	179	LEU	-	expression tag	UNP A0A2P1E3C0
B	180	GLU	-	expression tag	UNP A0A2P1E3C0
B	181	VAL	-	expression tag	UNP A0A2P1E3C0
B	182	LEU	-	expression tag	UNP A0A2P1E3C0
B	183	PHE	-	expression tag	UNP A0A2P1E3C0
B	184	GLN	-	expression tag	UNP A0A2P1E3C0
B	185	GLY	-	expression tag	UNP A0A2P1E3C0
B	186	PRO	-	expression tag	UNP A0A2P1E3C0
B	187	GLY	-	expression tag	UNP A0A2P1E3C0
B	188	SER	-	expression tag	UNP A0A2P1E3C0
B	189	GLY	-	expression tag	UNP A0A2P1E3C0
B	190	TYR	-	expression tag	UNP A0A2P1E3C0
B	191	ILE	-	expression tag	UNP A0A2P1E3C0
B	192	PRO	-	expression tag	UNP A0A2P1E3C0
B	193	GLU	-	expression tag	UNP A0A2P1E3C0
B	194	ALA	-	expression tag	UNP A0A2P1E3C0
B	195	PRO	-	expression tag	UNP A0A2P1E3C0
B	196	ARG	-	expression tag	UNP A0A2P1E3C0
B	197	ASP	-	expression tag	UNP A0A2P1E3C0
B	198	GLY	-	expression tag	UNP A0A2P1E3C0
B	199	GLN	-	expression tag	UNP A0A2P1E3C0
B	200	ALA	-	expression tag	UNP A0A2P1E3C0
B	201	TYR	-	expression tag	UNP A0A2P1E3C0
B	202	VAL	-	expression tag	UNP A0A2P1E3C0
B	203	ARG	-	expression tag	UNP A0A2P1E3C0
B	204	LYS	-	expression tag	UNP A0A2P1E3C0
B	205	ASP	-	expression tag	UNP A0A2P1E3C0
B	206	GLY	-	expression tag	UNP A0A2P1E3C0
B	207	GLU	-	expression tag	UNP A0A2P1E3C0
B	208	TRP	-	expression tag	UNP A0A2P1E3C0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	209	VAL	-	expression tag	UNP A0A2P1E3C0
B	210	LEU	-	expression tag	UNP A0A2P1E3C0
B	211	LEU	-	expression tag	UNP A0A2P1E3C0
B	212	SER	-	expression tag	UNP A0A2P1E3C0
B	213	THR	-	expression tag	UNP A0A2P1E3C0
B	214	PHE	-	expression tag	UNP A0A2P1E3C0
B	215	LEU	-	expression tag	UNP A0A2P1E3C0
B	216	GLY	-	expression tag	UNP A0A2P1E3C0
B	217	HIS	-	expression tag	UNP A0A2P1E3C0
B	218	HIS	-	expression tag	UNP A0A2P1E3C0
B	219	HIS	-	expression tag	UNP A0A2P1E3C0
B	220	HIS	-	expression tag	UNP A0A2P1E3C0
B	221	HIS	-	expression tag	UNP A0A2P1E3C0
B	222	HIS	-	expression tag	UNP A0A2P1E3C0
D	47	CYS	GLN	conflict	UNP A0A2P1E3C0
D	177	SER	-	expression tag	UNP A0A2P1E3C0
D	178	GLY	-	expression tag	UNP A0A2P1E3C0
D	179	LEU	-	expression tag	UNP A0A2P1E3C0
D	180	GLU	-	expression tag	UNP A0A2P1E3C0
D	181	VAL	-	expression tag	UNP A0A2P1E3C0
D	182	LEU	-	expression tag	UNP A0A2P1E3C0
D	183	PHE	-	expression tag	UNP A0A2P1E3C0
D	184	GLN	-	expression tag	UNP A0A2P1E3C0
D	185	GLY	-	expression tag	UNP A0A2P1E3C0
D	186	PRO	-	expression tag	UNP A0A2P1E3C0
D	187	GLY	-	expression tag	UNP A0A2P1E3C0
D	188	SER	-	expression tag	UNP A0A2P1E3C0
D	189	GLY	-	expression tag	UNP A0A2P1E3C0
D	190	TYR	-	expression tag	UNP A0A2P1E3C0
D	191	ILE	-	expression tag	UNP A0A2P1E3C0
D	192	PRO	-	expression tag	UNP A0A2P1E3C0
D	193	GLU	-	expression tag	UNP A0A2P1E3C0
D	194	ALA	-	expression tag	UNP A0A2P1E3C0
D	195	PRO	-	expression tag	UNP A0A2P1E3C0
D	196	ARG	-	expression tag	UNP A0A2P1E3C0
D	197	ASP	-	expression tag	UNP A0A2P1E3C0
D	198	GLY	-	expression tag	UNP A0A2P1E3C0
D	199	GLN	-	expression tag	UNP A0A2P1E3C0
D	200	ALA	-	expression tag	UNP A0A2P1E3C0
D	201	TYR	-	expression tag	UNP A0A2P1E3C0
D	202	VAL	-	expression tag	UNP A0A2P1E3C0
D	203	ARG	-	expression tag	UNP A0A2P1E3C0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	204	LYS	-	expression tag	UNP A0A2P1E3C0
D	205	ASP	-	expression tag	UNP A0A2P1E3C0
D	206	GLY	-	expression tag	UNP A0A2P1E3C0
D	207	GLU	-	expression tag	UNP A0A2P1E3C0
D	208	TRP	-	expression tag	UNP A0A2P1E3C0
D	209	VAL	-	expression tag	UNP A0A2P1E3C0
D	210	LEU	-	expression tag	UNP A0A2P1E3C0
D	211	LEU	-	expression tag	UNP A0A2P1E3C0
D	212	SER	-	expression tag	UNP A0A2P1E3C0
D	213	THR	-	expression tag	UNP A0A2P1E3C0
D	214	PHE	-	expression tag	UNP A0A2P1E3C0
D	215	LEU	-	expression tag	UNP A0A2P1E3C0
D	216	GLY	-	expression tag	UNP A0A2P1E3C0
D	217	HIS	-	expression tag	UNP A0A2P1E3C0
D	218	HIS	-	expression tag	UNP A0A2P1E3C0
D	219	HIS	-	expression tag	UNP A0A2P1E3C0
D	220	HIS	-	expression tag	UNP A0A2P1E3C0
D	221	HIS	-	expression tag	UNP A0A2P1E3C0
D	222	HIS	-	expression tag	UNP A0A2P1E3C0
F	47	CYS	GLN	conflict	UNP A0A2P1E3C0
F	177	SER	-	expression tag	UNP A0A2P1E3C0
F	178	GLY	-	expression tag	UNP A0A2P1E3C0
F	179	LEU	-	expression tag	UNP A0A2P1E3C0
F	180	GLU	-	expression tag	UNP A0A2P1E3C0
F	181	VAL	-	expression tag	UNP A0A2P1E3C0
F	182	LEU	-	expression tag	UNP A0A2P1E3C0
F	183	PHE	-	expression tag	UNP A0A2P1E3C0
F	184	GLN	-	expression tag	UNP A0A2P1E3C0
F	185	GLY	-	expression tag	UNP A0A2P1E3C0
F	186	PRO	-	expression tag	UNP A0A2P1E3C0
F	187	GLY	-	expression tag	UNP A0A2P1E3C0
F	188	SER	-	expression tag	UNP A0A2P1E3C0
F	189	GLY	-	expression tag	UNP A0A2P1E3C0
F	190	TYR	-	expression tag	UNP A0A2P1E3C0
F	191	ILE	-	expression tag	UNP A0A2P1E3C0
F	192	PRO	-	expression tag	UNP A0A2P1E3C0
F	193	GLU	-	expression tag	UNP A0A2P1E3C0
F	194	ALA	-	expression tag	UNP A0A2P1E3C0
F	195	PRO	-	expression tag	UNP A0A2P1E3C0
F	196	ARG	-	expression tag	UNP A0A2P1E3C0
F	197	ASP	-	expression tag	UNP A0A2P1E3C0
F	198	GLY	-	expression tag	UNP A0A2P1E3C0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	GLN	-	expression tag	UNP A0A2P1E3C0
F	200	ALA	-	expression tag	UNP A0A2P1E3C0
F	201	TYR	-	expression tag	UNP A0A2P1E3C0
F	202	VAL	-	expression tag	UNP A0A2P1E3C0
F	203	ARG	-	expression tag	UNP A0A2P1E3C0
F	204	LYS	-	expression tag	UNP A0A2P1E3C0
F	205	ASP	-	expression tag	UNP A0A2P1E3C0
F	206	GLY	-	expression tag	UNP A0A2P1E3C0
F	207	GLU	-	expression tag	UNP A0A2P1E3C0
F	208	TRP	-	expression tag	UNP A0A2P1E3C0
F	209	VAL	-	expression tag	UNP A0A2P1E3C0
F	210	LEU	-	expression tag	UNP A0A2P1E3C0
F	211	LEU	-	expression tag	UNP A0A2P1E3C0
F	212	SER	-	expression tag	UNP A0A2P1E3C0
F	213	THR	-	expression tag	UNP A0A2P1E3C0
F	214	PHE	-	expression tag	UNP A0A2P1E3C0
F	215	LEU	-	expression tag	UNP A0A2P1E3C0
F	216	GLY	-	expression tag	UNP A0A2P1E3C0
F	217	HIS	-	expression tag	UNP A0A2P1E3C0
F	218	HIS	-	expression tag	UNP A0A2P1E3C0
F	219	HIS	-	expression tag	UNP A0A2P1E3C0
F	220	HIS	-	expression tag	UNP A0A2P1E3C0
F	221	HIS	-	expression tag	UNP A0A2P1E3C0
F	222	HIS	-	expression tag	UNP A0A2P1E3C0

- Molecule 3 is a protein called MEDI8852 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	222	Total	C	N	O	S	0	0
			1680	1061	282	331	6		
3	I	222	Total	C	N	O	S	0	0
			1680	1061	282	331	6		
3	K	222	Total	C	N	O	S	0	0
			1680	1061	282	331	6		

- Molecule 4 is a protein called MEDI8852 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	206	Total	C	N	O	S	0	0
			1574	978	270	322	4		
4	J	206	Total	C	N	O	S	0	0
			1574	978	270	322	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	206	Total	C	N	O	S	0	0
			1574	978	270	322	4		

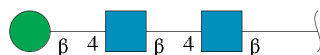
- Molecule 5 is a protein called VRC35 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		
5	c	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		
5	e	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		
5	g	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		
5	i	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		
5	k	222	Total	C	N	O	S	0	0
			1682	1072	280	323	7		

- Molecule 6 is a protein called VRC35 Fab light chain.

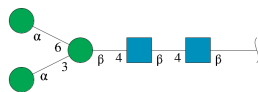
Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		
6	d	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		
6	f	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		
6	h	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		
6	j	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		
6	l	219	Total	C	N	O	S	0	0
			1689	1055	296	332	6		

- Molecule 7 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
7	M	3	Total	C	N	O	0	0
			39	22	2	15		
7	N	3	Total	C	N	O	0	0
			39	22	2	15		
7	P	3	Total	C	N	O	0	0
			39	22	2	15		
7	R	3	Total	C	N	O	0	0
			39	22	2	15		
7	T	3	Total	C	N	O	0	0
			39	22	2	15		
7	U	3	Total	C	N	O	0	0
			39	22	2	15		
7	W	3	Total	C	N	O	0	0
			39	22	2	15		
7	Y	3	Total	C	N	O	0	0
			39	22	2	15		
7	m	3	Total	C	N	O	0	0
			39	22	2	15		
7	n	3	Total	C	N	O	0	0
			39	22	2	15		
7	p	3	Total	C	N	O	0	0
			39	22	2	15		
7	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	5	Total	C	N	O	0	0
			61	34	2	25		
8	Q	5	Total	C	N	O	0	0
			61	34	2	25		
8	S	5	Total	C	N	O	0	0
			61	34	2	25		
8	X	5	Total	C	N	O	0	0
			61	34	2	25		
8	Z	5	Total	C	N	O	0	0
			61	34	2	25		

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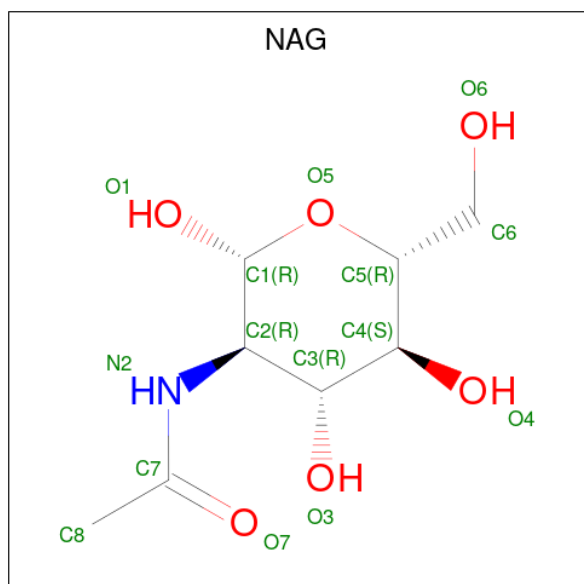
Mol	Chain	Residues	Atoms				AltConf	Trace
8	q	5	Total	C	N	O	0	0
			61	34	2	25		
8	s	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 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
9	V	4	Total	C	N	O	0	0
			50	28	2	20		
9	o	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



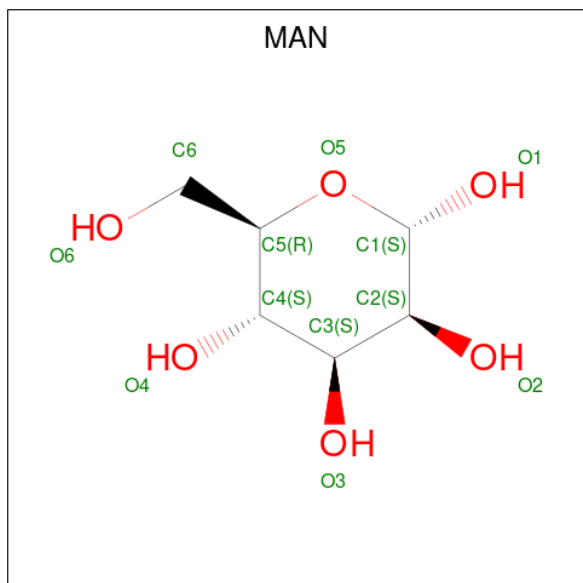
Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
10	D	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).

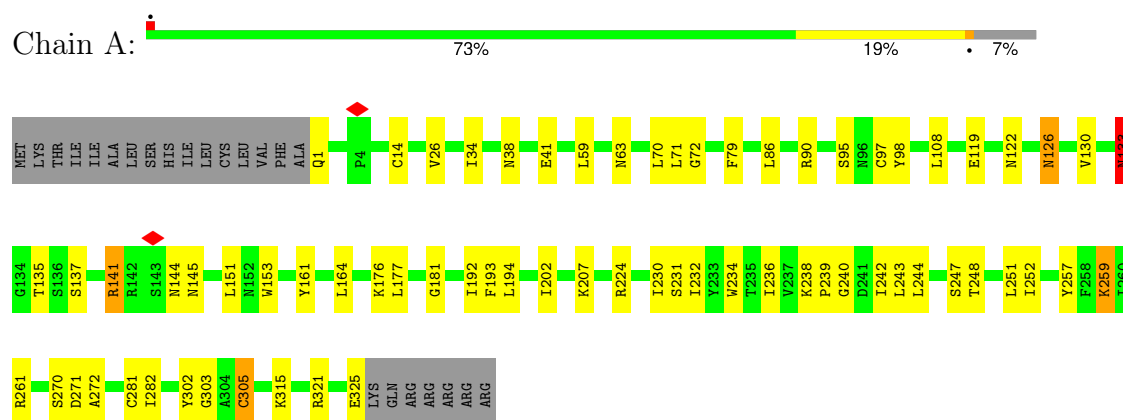


Mol	Chain	Residues	Atoms			AltConf
11	e	1	Total	C	O	0
			11	6	5	
11	i	1	Total	C	O	0
			11	6	5	

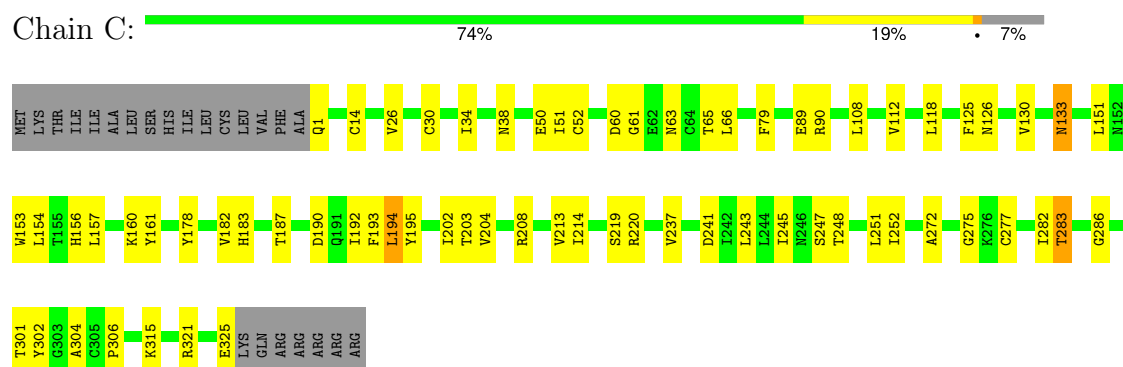
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

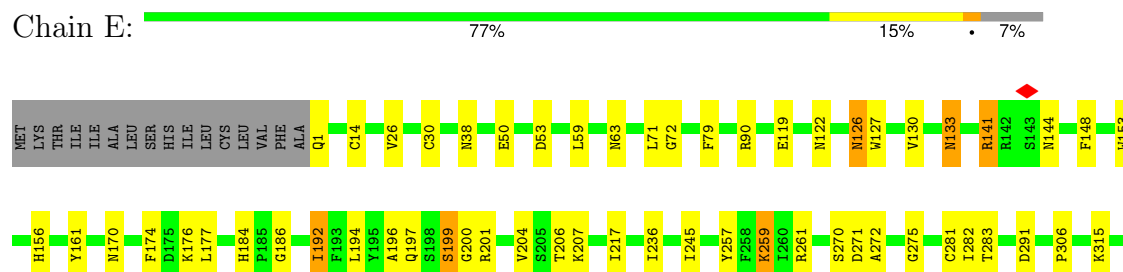
• Molecule 1: Hemagglutinin

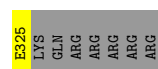


• Molecule 1: Hemagglutinin

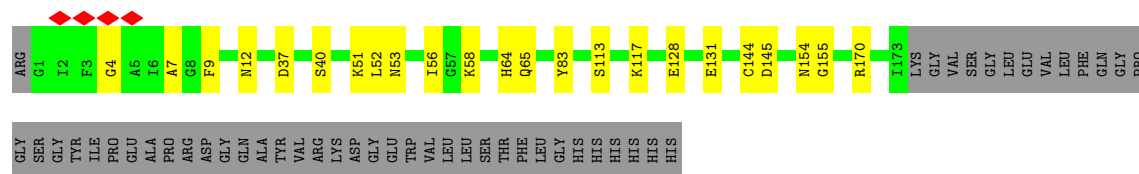


• Molecule 1: Hemagglutinin

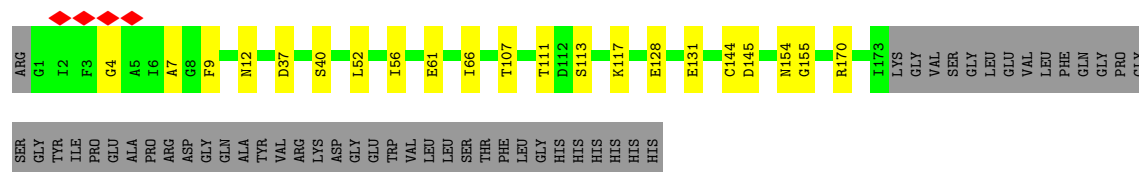




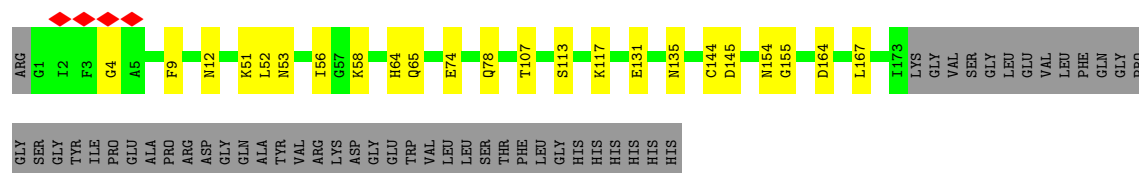
• Molecule 2: Hemagglutinin



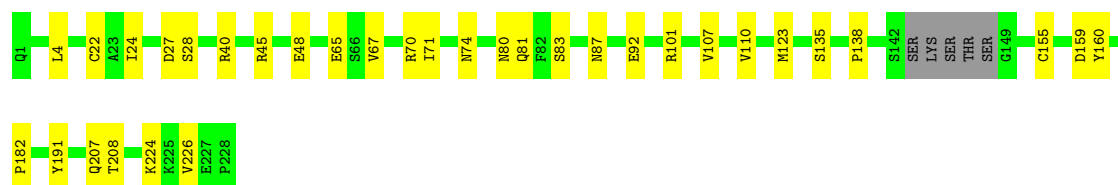
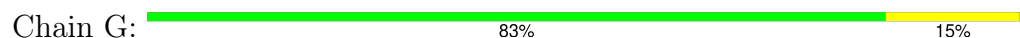
• Molecule 2: Hemagglutinin



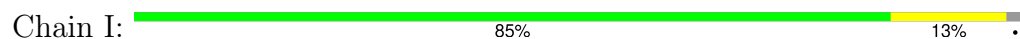
• Molecule 2: Hemagglutinin

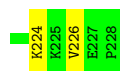


• Molecule 3: MEDI8852 Fab heavy chain



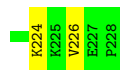
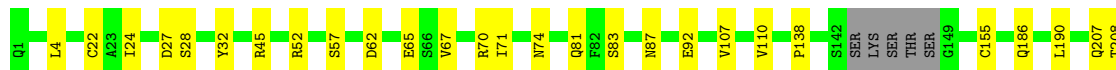
• Molecule 3: MEDI8852 Fab heavy chain





• Molecule 3: MEDI8852 Fab heavy chain

Chain K: 85% 13%



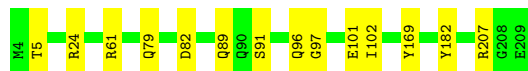
• Molecule 4: MEDI8852 Fab light chain

Chain H: 91% 9%



• Molecule 4: MEDI8852 Fab light chain

Chain J: 93% 7%



• Molecule 4: MEDI8852 Fab light chain

Chain L: 90% 10%



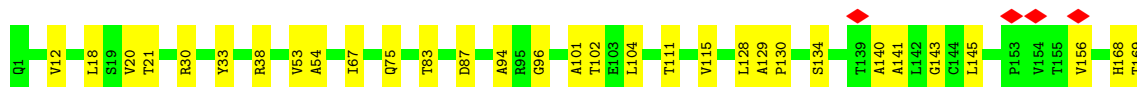
• Molecule 5: VRC35 Fab heavy chain

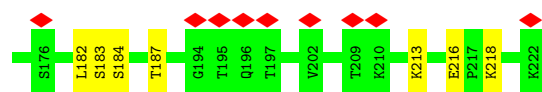
Chain a: 7% 90% 10%



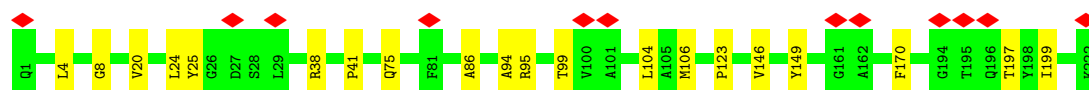
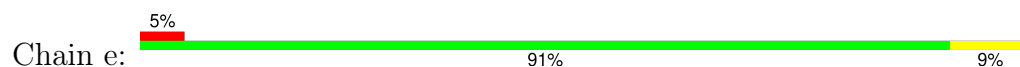
• Molecule 5: VRC35 Fab heavy chain

Chain c: 6% 83% 17%

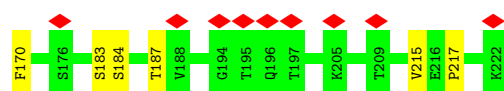
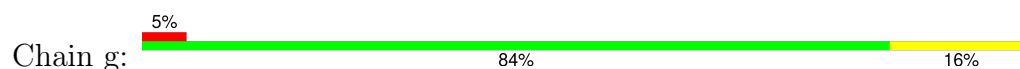




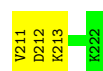
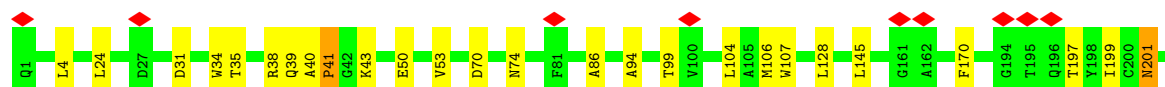
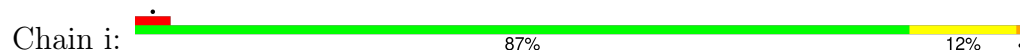
- Molecule 5: VRC35 Fab heavy chain



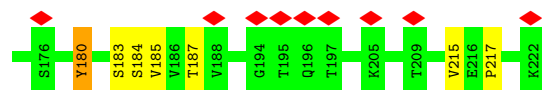
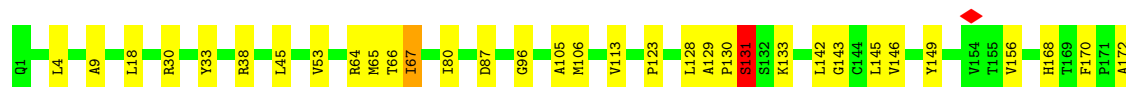
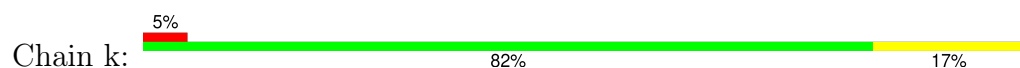
- Molecule 5: VRC35 Fab heavy chain



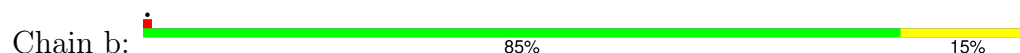
- Molecule 5: VRC35 Fab heavy chain

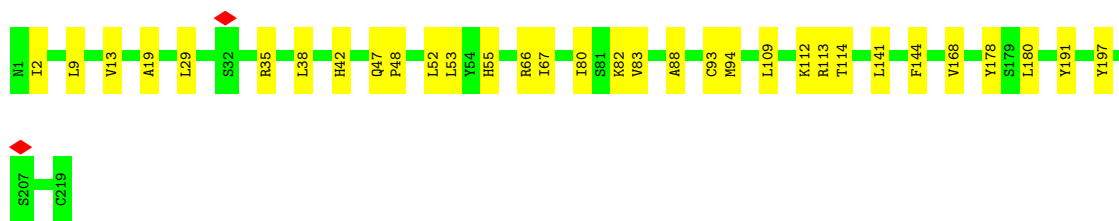


- Molecule 5: VRC35 Fab heavy chain

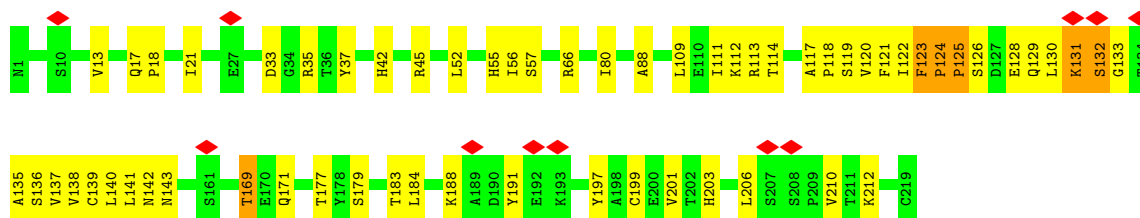


- Molecule 6: VRC35 Fab light chain

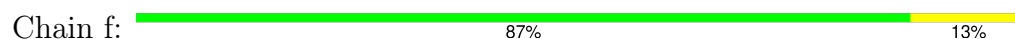




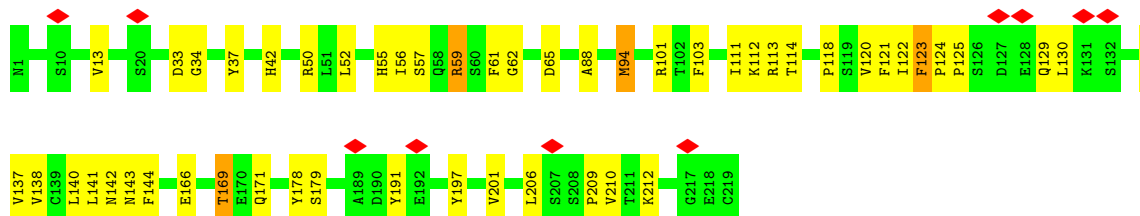
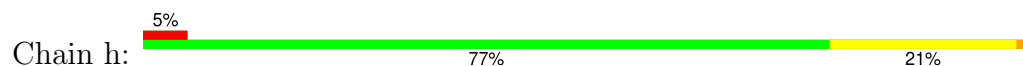
- Molecule 6: VRC35 Fab light chain



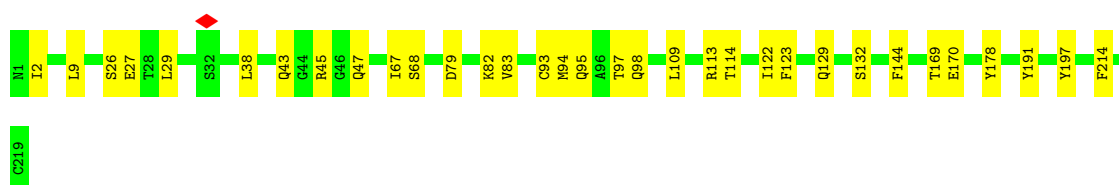
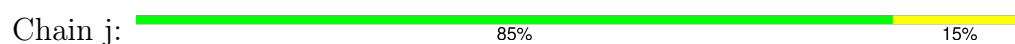
- Molecule 6: VRC35 Fab light chain




- Molecule 6: VRC35 Fab light chain

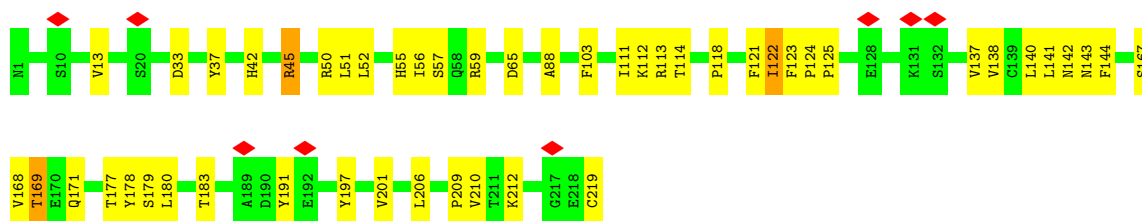


- Molecule 6: VRC35 Fab light chain



- Molecule 6: VRC35 Fab light chain

Chain L:  78% 21%



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

Chain M:  67% 33%



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

Chain N:  33% 33% 33%



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

Chain P:  33% 67% 33%



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

Chain R:  100%



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

Chain T:  67% 33%



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

Chain U:  100%



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

Chain W:  33% 67% 33%



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

Chain Y:  100%



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

Chain m:  67% 33%



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

Chain n:  100%



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

Chain p:  33% 67% 33%



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

Chain r:  100%


MAG1
MAG2
BMA3

- 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 O:  60% 40%


MAG1
MAG2
BMA3
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 Q:  80% 20%

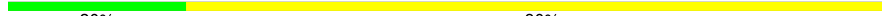
MAG1
MAG2
BMA3
MAN4
MAN5

- 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 S:  20% 20% 40% 40%

MAG1
MAG2
BMA3
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 X:  20% 80%

MAG1
MAG2
BMA3
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 Z:  20% 20% 60% 20%


MAG1
MAG2
BMA3
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 q:  100%


NAG1
NAG2
BMA3
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 s:  20% 20% 40% 40%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 9: 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 V:  75% 25%

NAG1
NAG2
BMA3
MAN4

- Molecule 9: 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 o:  25% 50% 25%

NAG1
NAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1780000	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 ($e^-/\text{\AA}^2$)	54.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	38.508	Depositor
Minimum map value	-21.400	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.376	Depositor
Recommended contour level	2	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/2594	0.50	0/3527
1	C	0.31	0/2594	0.68	2/3527 (0.1%)
1	E	0.22	0/2594	0.49	0/3527
2	B	0.18	0/1417	0.35	0/1902
2	D	0.20	0/1417	0.40	0/1902
2	F	0.18	0/1417	0.38	0/1902
3	G	0.18	0/1723	0.43	0/2357
3	I	0.17	0/1723	0.41	0/2357
3	K	0.17	0/1723	0.39	0/2357
4	H	0.15	0/1607	0.33	0/2179
4	J	0.15	0/1607	0.34	0/2179
4	L	0.15	0/1607	0.34	0/2179
5	a	0.18	0/1726	0.42	0/2359
5	c	0.33	0/1726	0.51	0/2359
5	e	0.36	2/1726 (0.1%)	0.58	3/2359 (0.1%)
5	g	0.30	0/1726	0.50	0/2359
5	i	0.21	0/1726	0.47	1/2359 (0.0%)
5	k	0.31	0/1726	0.56	0/2359
6	b	0.17	0/1726	0.37	0/2344
6	d	0.37	0/1726	0.64	5/2344 (0.2%)
6	f	0.19	0/1726	0.39	0/2344
6	h	0.62	2/1726 (0.1%)	0.71	5/2344 (0.2%)
6	j	0.20	0/1726	0.40	0/2344
6	l	0.35	0/1726	0.58	2/2344 (0.1%)
All	All	0.27	4/42735 (0.0%)	0.49	18/58113 (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
6	d	0	1
6	h	0	1
6	l	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	209	PRO	CG-CD	-20.25	0.81	1.50
5	e	41	PRO	CG-CD	-10.44	1.15	1.50
6	h	209	PRO	N-CD	10.39	1.62	1.47
5	e	41	PRO	N-CD	6.74	1.57	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	209	PRO	N-CD-CG	-21.29	71.27	103.20
6	l	209	PRO	CA-N-CD	-13.10	93.66	112.00
5	e	41	PRO	N-CD-CG	-12.13	85.00	103.20
6	h	209	PRO	CA-CB-CG	-11.41	82.82	104.50
5	e	41	PRO	CA-N-CD	-11.31	96.16	112.00
6	d	125	PRO	N-CA-C	-9.71	92.47	112.47
6	d	123	PHE	N-CA-CB	8.66	125.88	110.90
6	d	124	PRO	N-CA-C	-7.91	101.05	110.70
6	h	209	PRO	CA-N-CD	-7.86	101.00	112.00
1	C	193	PHE	CA-C-N	7.57	139.61	122.19
1	C	193	PHE	C-N-CA	7.57	139.61	122.19
5	e	41	PRO	CA-CB-CG	-7.41	90.43	104.50
6	d	123	PHE	CB-CA-C	-7.11	101.50	110.96
6	l	209	PRO	N-CD-CG	-6.71	93.14	103.20
5	i	41	PRO	CA-N-CD	-6.43	103.00	112.00
6	h	209	PRO	CB-CG-CD	5.97	125.22	106.10
6	d	123	PHE	CA-CB-CG	-5.90	107.90	113.80
6	h	209	PRO	N-CA-CB	-5.42	98.30	103.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLY	Peptide
6	d	169	THR	Peptide

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Mol	Chain	Res	Type	Group
6	h	169	THR	Peptide
6	l	169	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2537	0	2484	44	0
1	C	2537	0	2484	48	0
1	E	2537	0	2484	38	0
2	B	1393	0	1325	14	0
2	D	1393	0	1325	13	0
2	F	1393	0	1325	14	0
3	G	1680	0	1630	20	0
3	I	1680	0	1630	16	0
3	K	1680	0	1630	16	0
4	H	1574	0	1524	12	0
4	J	1574	0	1524	7	0
4	L	1574	0	1524	12	0
5	a	1682	0	1669	15	0
5	c	1682	0	1670	40	0
5	e	1682	0	1669	15	0
5	g	1682	0	1670	29	0
5	i	1682	0	1669	21	0
5	k	1682	0	1670	35	0
6	b	1689	0	1652	20	0
6	d	1689	0	1653	82	0
6	f	1689	0	1652	17	0
6	h	1689	0	1653	47	0
6	j	1689	0	1652	21	0
6	l	1689	0	1653	42	0
7	M	39	0	34	2	0
7	N	39	0	34	1	0
7	P	39	0	34	1	0
7	R	39	0	34	0	0
7	T	39	0	34	1	0
7	U	39	0	34	3	0
7	W	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Y	39	0	34	0	0
7	m	39	0	34	2	0
7	n	39	0	34	1	0
7	p	39	0	34	1	0
7	r	39	0	34	0	0
8	O	61	0	52	3	0
8	Q	61	0	52	1	0
8	S	61	0	52	2	0
8	X	61	0	52	0	0
8	Z	61	0	52	1	0
8	q	61	0	52	0	0
8	s	61	0	52	2	0
9	V	50	0	43	2	0
9	o	50	0	43	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
10	F	14	0	13	0	0
11	e	11	0	10	1	0
11	i	11	0	10	1	0
All	All	42837	0	41738	580	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 7.

All (580) 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)
6:h:123:PHE:CE2	6:h:136:SER:O	1.88	1.24
6:d:122:ILE:HG22	6:d:139:CYS:HA	1.46	0.94
5:c:145:LEU:HD13	6:d:183:THR:HG22	1.52	0.92
6:d:121:PHE:HB2	6:d:140:LEU:HD23	1.53	0.89
5:k:128:LEU:HD13	6:l:140:LEU:HB2	1.56	0.86
5:c:129:ALA:HB2	6:d:123:PHE:HB2	1.55	0.86
6:h:123:PHE:CD2	6:h:136:SER:O	2.30	0.84
6:d:124:PRO:HB3	6:d:137:VAL:HA	1.61	0.82
6:d:124:PRO:HB3	6:d:138:VAL:HG23	1.63	0.80
6:h:123:PHE:HE2	6:h:136:SER:O	1.63	0.79
5:g:128:LEU:HD13	6:h:140:LEU:HB2	1.64	0.79
2:F:52:LEU:O	2:F:56:ILE:N	2.19	0.75
6:d:124:PRO:O	6:d:126:SER:N	2.20	0.75
6:h:141:LEU:HD11	6:h:201:VAL:HG21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:218:LYS:HB2	6:d:123:PHE:HD2	1.52	0.74
6:l:141:LEU:HD11	6:l:201:VAL:HG21	1.69	0.74
5:c:128:LEU:HD13	6:d:140:LEU:HB2	1.69	0.74
2:B:52:LEU:O	2:B:56:ILE:N	2.20	0.74
2:B:51:LYS:NZ	1:E:30:CYS:SG	2.60	0.73
6:d:124:PRO:HA	6:d:138:VAL:CG2	2.17	0.73
5:k:128:LEU:HD12	5:k:143:GLY:HA3	1.69	0.73
5:a:38:ARG:NH2	5:a:86:ALA:O	2.22	0.72
6:f:200:GLU:OE1	6:f:211:THR:OG1	2.05	0.72
5:e:38:ARG:NH2	5:e:86:ALA:O	2.23	0.72
6:d:124:PRO:HG3	6:d:137:VAL:HG13	1.70	0.71
5:i:38:ARG:NH2	5:i:86:ALA:O	2.24	0.71
6:d:33:ASP:OD2	6:d:37:TYR:OH	2.07	0.71
2:D:52:LEU:O	2:D:56:ILE:N	2.23	0.71
6:h:33:ASP:OD2	6:h:37:TYR:OH	2.08	0.71
5:k:30:ARG:NH2	9:o:4:MAN:O4	2.23	0.70
6:f:45:ARG:NH1	6:f:170:GLU:OE1	2.24	0.70
6:d:120:VAL:HA	6:d:140:LEU:O	1.91	0.70
5:a:218:LYS:NZ	5:a:220:CYS:SG	2.65	0.70
6:l:125:PRO:HG3	6:l:219:CYS:HB3	1.74	0.70
1:A:141:ARG:O	1:A:144:ASN:ND2	2.25	0.70
5:c:30:ARG:NH2	8:O:4:MAN:O4	2.25	0.69
4:J:96:GLN:NE2	4:J:97:GLY:O	2.26	0.69
5:k:130:PRO:HA	6:l:121:PHE:CE2	2.28	0.69
1:E:141:ARG:O	1:E:144:ASN:ND2	2.25	0.69
6:j:45:ARG:NH1	6:j:170:GLU:OE1	2.25	0.69
4:L:96:GLN:NE2	4:L:97:GLY:O	2.26	0.69
6:d:13:VAL:O	6:d:112:LYS:N	2.26	0.69
1:A:95:SER:O	1:A:224:ARG:NH1	2.25	0.68
4:H:96:GLN:NE2	4:H:97:GLY:O	2.26	0.68
6:l:168:VAL:HG22	6:l:180:LEU:HD13	1.76	0.68
5:i:99:THR:O	11:i:301:MAN:O2	2.12	0.68
5:g:30:ARG:NH2	9:V:4:MAN:O4	2.27	0.67
2:F:74:GLU:O	2:F:78:GLN:NE2	2.27	0.67
1:C:30:CYS:SG	2:F:51:LYS:NZ	2.66	0.67
5:c:128:LEU:HD12	5:c:143:GLY:HA3	1.75	0.67
6:d:118:PRO:HG2	6:d:203:HIS:CB	2.24	0.67
6:l:33:ASP:OD2	6:l:37:TYR:OH	2.12	0.66
5:k:142:LEU:HD13	5:k:215:VAL:HG11	1.78	0.66
3:G:135:SER:OG	3:G:159:ASP:OD1	2.08	0.66
6:b:113:ARG:NH2	6:b:114:THR:OG1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:118:PRO:HG2	6:d:203:HIS:HB3	1.76	0.66
7:m:2:NAG:O4	7:m:2:NAG:O7	2.13	0.66
7:M:2:NAG:O4	7:M:2:NAG:O7	2.13	0.66
5:c:134:SER:HB2	6:d:119:SER:HB2	1.77	0.66
2:D:131:GLU:N	2:D:131:GLU:OE1	2.30	0.65
5:a:99:THR:OG1	8:O:3:BMA:O3	2.14	0.65
7:T:2:NAG:O4	7:T:2:NAG:O7	2.14	0.65
2:F:131:GLU:OE1	2:F:131:GLU:N	2.29	0.65
6:d:124:PRO:HA	6:d:138:VAL:HG23	1.78	0.65
6:l:13:VAL:O	6:l:112:LYS:N	2.28	0.65
4:L:5:THR:OG1	4:L:24:ARG:NH2	2.29	0.65
6:h:13:VAL:O	6:h:112:LYS:N	2.28	0.65
5:g:33:TYR:O	5:g:96:GLY:N	2.30	0.65
5:g:130:PRO:HA	6:h:121:PHE:CD2	2.32	0.65
6:l:121:PHE:HB2	6:l:140:LEU:HB3	1.78	0.65
6:d:124:PRO:CB	6:d:138:VAL:HG23	2.27	0.64
5:e:99:THR:O	11:e:301:MAN:O2	2.14	0.64
5:k:18:LEU:HD22	5:k:80:ILE:HD13	1.77	0.64
6:j:113:ARG:NH2	6:j:114:THR:OG1	2.29	0.64
1:A:119:GLU:O	1:A:259:LYS:NZ	2.31	0.64
2:B:131:GLU:N	2:B:131:GLU:OE1	2.31	0.64
8:s:3:BMA:O4	8:s:4:MAN:O5	2.16	0.64
6:d:124:PRO:O	6:d:125:PRO:C	2.40	0.64
3:G:74:ASN:OD1	3:G:83:SER:OG	2.15	0.63
1:A:257:TYR:O	1:A:259:LYS:NZ	2.31	0.63
5:g:63:VAL:HG13	5:g:65:MET:HE3	1.79	0.63
4:L:101:GLU:OE2	4:L:169:TYR:OH	2.16	0.63
6:d:124:PRO:CB	6:d:137:VAL:HA	2.29	0.63
6:l:206:LEU:HD13	6:l:210:VAL:HG23	1.79	0.63
6:d:206:LEU:HD13	6:d:210:VAL:HG23	1.81	0.63
6:f:113:ARG:NH2	6:f:114:THR:OG1	2.31	0.62
5:c:218:LYS:HB2	6:d:123:PHE:CD2	2.34	0.62
6:h:42:HIS:HB2	6:h:52:LEU:HD11	1.81	0.62
1:E:119:GLU:OE1	1:E:261:ARG:NH1	2.32	0.62
6:d:111:ILE:N	6:d:171:GLN:OE1	2.32	0.62
6:j:191:TYR:O	6:j:197:TYR:OH	2.18	0.62
5:i:201:ASN:ND2	5:i:212:ASP:OD1	2.33	0.61
6:l:42:HIS:HB2	6:l:52:LEU:HD11	1.81	0.61
1:A:238:LYS:NZ	1:A:239:PRO:O	2.33	0.61
1:C:251:LEU:O	1:C:252:ILE:HD13	1.99	0.61
6:j:45:ARG:N	6:j:47:GLN:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:O	1:E:259:LYS:NZ	2.33	0.61
4:H:182:TYR:O	4:H:207:ARG:NH2	2.33	0.61
6:d:184:LEU:HD23	6:d:197:TYR:OH	2.01	0.61
2:D:113:SER:OG	2:D:117:LYS:NZ	2.33	0.61
1:C:283:THR:OG1	1:C:286:GLY:O	2.18	0.61
6:d:125:PRO:HB2	6:d:129:GLN:HG3	1.83	0.61
1:E:257:TYR:O	1:E:259:LYS:NZ	2.29	0.60
4:L:89:GLN:NE2	4:L:91:SER:O	2.34	0.60
6:f:191:TYR:O	6:f:197:TYR:OH	2.18	0.60
1:C:50:GLU:OE1	1:C:275:GLY:N	2.34	0.60
5:a:99:THR:O	8:O:5:MAN:O2	2.19	0.60
6:b:47:GLN:NE2	6:b:48:PRO:O	2.35	0.60
2:B:53:ASN:O	2:B:58:LYS:NZ	2.29	0.60
6:d:120:VAL:HB	6:d:212:LYS:HG3	1.82	0.60
2:F:113:SER:OG	2:F:117:LYS:NZ	2.35	0.60
5:c:20:VAL:HG21	5:c:111:THR:HG21	1.84	0.60
6:d:118:PRO:HD2	6:d:206:LEU:HG	1.82	0.59
3:I:74:ASN:OD1	3:I:83:SER:OG	2.15	0.59
4:J:89:GLN:NE2	4:J:91:SER:O	2.35	0.59
5:g:38:ARG:NH1	5:g:87:ASP:OD1	2.35	0.59
6:d:17:GLN:NE2	6:d:18:PRO:O	2.36	0.59
6:b:42:HIS:HB2	6:b:52:LEU:HD11	1.85	0.59
3:G:45:ARG:NH1	3:G:92:GLU:OE2	2.36	0.59
6:d:111:ILE:O	6:d:171:GLN:NE2	2.36	0.59
6:h:206:LEU:HD13	6:h:210:VAL:HG23	1.85	0.58
3:K:74:ASN:OD1	3:K:83:SER:OG	2.17	0.58
4:L:182:TYR:O	4:L:207:ARG:NH2	2.35	0.58
1:A:325:GLU:OE1	2:B:12:ASN:ND2	2.36	0.58
3:G:65:GLU:N	3:G:65:GLU:OE1	2.36	0.58
2:B:128:GLU:O	2:B:170:ARG:NH2	2.36	0.58
5:a:4:LEU:HD21	5:a:106:MET:HE3	1.85	0.58
6:d:42:HIS:HB2	6:d:52:LEU:HD11	1.86	0.58
2:B:113:SER:OG	2:B:117:LYS:NZ	2.37	0.58
5:c:18:LEU:HB2	5:c:83:THR:HG21	1.85	0.58
6:d:113:ARG:NH2	6:d:114:THR:OG1	2.37	0.58
3:I:138:PRO:HB3	3:I:226:VAL:HG22	1.86	0.58
5:c:38:ARG:NH1	5:c:87:ASP:OD1	2.37	0.58
5:k:38:ARG:NH1	5:k:87:ASP:OD1	2.37	0.58
1:E:192:ILE:HD12	1:E:194:LEU:HD11	1.85	0.57
6:l:113:ARG:NH2	6:l:114:THR:OG1	2.37	0.57
4:H:89:GLN:NE2	4:H:91:SER:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:130:PRO:HD2	5:k:217:PRO:HA	1.85	0.57
3:K:138:PRO:HB3	3:K:226:VAL:HG22	1.85	0.57
5:i:35:THR:OG1	5:i:50:GLU:OE2	2.22	0.57
6:d:124:PRO:CA	6:d:138:VAL:HG23	2.35	0.57
6:d:142:ASN:OD1	6:d:179:SER:OG	2.21	0.57
4:J:182:TYR:O	4:J:207:ARG:NH2	2.36	0.57
1:C:204:VAL:HG22	1:C:245:ILE:HG12	1.87	0.57
6:l:111:ILE:O	6:l:171:GLN:NE2	2.38	0.57
1:E:170:ASN:ND2	1:E:174:PHE:O	2.38	0.57
5:e:75:GLN:N	5:e:75:GLN:OE1	2.38	0.57
5:i:99:THR:OG1	9:o:3:BMA:O3	2.23	0.57
6:h:123:PHE:HD2	6:h:137:VAL:HA	1.69	0.56
6:d:42:HIS:NE2	6:d:88:ALA:O	2.38	0.56
1:C:26:VAL:HG12	1:C:315:LYS:HB3	1.85	0.56
3:G:138:PRO:HB3	3:G:226:VAL:HG22	1.87	0.56
5:k:130:PRO:HA	6:l:121:PHE:CD2	2.39	0.56
3:G:4:LEU:HD22	3:G:22:CYS:SG	2.46	0.56
5:k:66:THR:OG1	5:k:67:ILE:N	2.38	0.56
6:b:38:LEU:HD12	6:b:94:MET:O	2.06	0.56
6:l:122:ILE:HD13	6:l:122:ILE:H	1.70	0.56
6:h:121:PHE:HB2	6:h:140:LEU:HB3	1.86	0.56
5:k:33:TYR:O	5:k:96:GLY:N	2.39	0.56
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.88	0.56
6:l:42:HIS:O	6:l:50:ARG:N	2.39	0.56
5:k:4:LEU:HD21	5:k:106:MET:HE1	1.87	0.56
1:A:59:LEU:HD23	1:A:79:PHE:CZ	2.41	0.55
6:d:124:PRO:HA	6:d:138:VAL:HG21	1.87	0.55
6:l:59:ARG:NH2	6:l:65:ASP:OD1	2.40	0.55
6:h:113:ARG:NH2	6:h:114:THR:OG1	2.39	0.55
1:C:325:GLU:OE1	2:D:12:ASN:ND2	2.39	0.55
6:h:142:ASN:OD1	6:h:179:SER:OG	2.24	0.55
1:C:237:VAL:HG21	1:C:243:LEU:HB3	1.87	0.55
3:G:107:VAL:O	3:G:110:VAL:HG12	2.06	0.55
5:k:45:LEU:HD13	6:l:103:PHE:CD2	2.41	0.55
5:c:130:PRO:HA	6:d:121:PHE:CD2	2.42	0.55
3:K:65:GLU:N	3:K:65:GLU:OE1	2.40	0.55
1:E:270:SER:OG	1:E:271:ASP:N	2.40	0.55
3:K:70:ARG:NH1	3:K:87:ASN:O	2.40	0.55
6:d:33:ASP:O	6:d:35:ARG:NE	2.39	0.54
6:h:144:PHE:O	6:h:178:TYR:N	2.41	0.54
6:j:26:SER:OG	6:j:27:GLU:OE2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:65:GLU:N	3:I:65:GLU:OE1	2.39	0.54
1:A:181:GLY:O	1:A:252:ILE:N	2.38	0.54
1:A:248:THR:N	7:N:1:NAG:H81	2.23	0.54
6:f:21:ILE:HD11	6:f:109:LEU:HD12	1.89	0.54
6:f:38:LEU:HD12	6:f:94:MET:O	2.07	0.54
1:A:26:VAL:HG12	1:A:315:LYS:HB3	1.88	0.54
1:A:207:LYS:NZ	1:A:240:GLY:O	2.37	0.54
1:C:182:VAL:HG21	1:C:213:VAL:HG21	1.89	0.54
1:C:194:LEU:HD13	1:C:195:TYR:CD2	2.42	0.54
3:K:107:VAL:O	3:K:110:VAL:HG12	2.06	0.54
5:g:45:LEU:HD13	6:h:103:PHE:CD2	2.42	0.54
7:p:1:NAG:H3	7:p:1:NAG:H83	1.90	0.54
6:f:2:ILE:HG21	6:f:29:LEU:HD21	1.90	0.54
3:G:70:ARG:NH1	3:G:87:ASN:O	2.40	0.54
5:a:127:PRO:HB3	5:a:215:VAL:HG22	1.90	0.54
6:f:12:PRO:O	6:f:112:LYS:NZ	2.40	0.54
3:I:155:CYS:SG	3:I:224:LYS:NZ	2.80	0.54
4:J:5:THR:OG1	4:J:24:ARG:NH2	2.41	0.54
3:K:207:GLN:NE2	3:K:208:THR:O	2.41	0.54
1:A:130:VAL:HG11	1:A:161:TYR:CE1	2.42	0.53
1:C:192:ILE:HD12	1:C:192:ILE:O	2.09	0.53
3:I:107:VAL:O	3:I:110:VAL:HG12	2.07	0.53
6:j:38:LEU:HD12	6:j:94:MET:O	2.08	0.53
5:c:128:LEU:HD21	6:d:138:VAL:HG12	1.91	0.53
6:h:111:ILE:O	6:h:171:GLN:NE2	2.42	0.53
3:I:70:ARG:NH1	3:I:87:ASN:O	2.40	0.53
3:I:207:GLN:NE2	3:I:208:THR:O	2.40	0.53
1:C:51:ILE:HG13	1:C:272:ALA:HB3	1.91	0.53
3:G:207:GLN:NE2	3:G:208:THR:O	2.42	0.53
6:d:120:VAL:HG11	6:d:199:CYS:SG	2.49	0.53
1:A:321:ARG:NH1	2:B:7:ALA:HB2	2.24	0.53
1:E:281:CYS:SG	1:E:283:THR:OG1	2.66	0.53
6:j:68:SER:O	6:j:79:ASP:N	2.40	0.53
6:h:59:ARG:NH2	6:h:65:ASP:OD2	2.42	0.53
1:C:321:ARG:NH1	2:D:7:ALA:HB2	2.24	0.53
2:F:64:HIS:O	2:F:65:GLN:NE2	2.42	0.53
5:c:168:HIS:HE2	6:d:177:THR:HG1	1.54	0.53
2:F:4:GLY:O	2:F:9:PHE:N	2.42	0.53
5:a:40:ALA:HB3	5:a:43:LYS:CD	2.39	0.53
1:E:325:GLU:OE1	2:F:12:ASN:ND2	2.41	0.52
6:j:38:LEU:HD11	6:j:93:CYS:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:NH2	1:A:272:ALA:O	2.42	0.52
6:d:120:VAL:HB	6:d:212:LYS:CG	2.39	0.52
6:d:137:VAL:HG23	6:d:191:TYR:OH	2.10	0.52
6:j:9:LEU:HD12	6:j:109:LEU:HA	1.92	0.52
1:E:1:GLN:NE2	2:F:135:ASN:O	2.42	0.52
5:c:141:ALA:HB1	6:d:142:ASN:HD22	1.75	0.52
1:A:135:THR:O	1:A:145:ASN:ND2	2.42	0.52
6:l:167:SER:O	6:l:180:LEU:HD12	2.09	0.52
1:E:59:LEU:HD23	1:E:79:PHE:CZ	2.45	0.52
5:c:128:LEU:HD12	5:c:143:GLY:CA	2.40	0.52
1:C:213:VAL:O	1:C:214:ILE:HD13	2.10	0.51
1:E:194:LEU:O	1:E:194:LEU:HD12	2.10	0.51
6:b:38:LEU:HD11	6:b:93:CYS:HB2	1.91	0.51
5:c:33:TYR:O	5:c:96:GLY:N	2.43	0.51
7:W:1:NAG:H83	7:W:1:NAG:H3	1.92	0.51
6:d:131:LYS:O	6:d:133:GLY:N	2.44	0.51
6:j:27:GLU:OE2	6:j:27:GLU:N	2.43	0.51
1:C:154:LEU:O	1:C:161:TYR:OH	2.24	0.51
1:C:304:ALA:HB2	2:D:61:GLU:HA	1.93	0.51
5:c:130:PRO:HA	6:d:121:PHE:HD2	1.75	0.51
7:P:1:NAG:H83	7:P:1:NAG:H3	1.91	0.51
1:E:126:ASN:OD1	8:s:1:NAG:N2	2.43	0.51
3:I:186:GLN:N	3:I:190:LEU:O	2.42	0.51
3:K:155:CYS:SG	3:K:224:LYS:NZ	2.80	0.51
3:I:135:SER:OG	3:I:159:ASP:OD1	2.29	0.51
5:k:187:THR:HG23	6:l:142:ASN:ND2	2.25	0.51
5:k:145:LEU:HD11	6:l:183:THR:CG2	2.40	0.51
1:E:90:ARG:NH2	1:E:272:ALA:O	2.44	0.50
5:c:145:LEU:HD12	6:d:138:VAL:HG13	1.92	0.50
5:a:65:MET:SD	5:a:66:THR:N	2.84	0.50
6:l:144:PHE:O	6:l:178:TYR:N	2.43	0.50
2:B:83:TYR:CD2	2:D:66:ILE:HD13	2.46	0.50
1:C:157:LEU:N	1:C:160:LYS:O	2.44	0.50
1:C:247:SER:C	7:U:1:NAG:H81	2.36	0.50
6:h:129:GLN:OE1	6:h:136:SER:N	2.45	0.50
1:E:206:THR:OG1	1:E:207:LYS:N	2.45	0.50
2:D:107:THR:O	2:D:111:THR:HG23	2.11	0.50
6:h:123:PHE:HB3	6:h:138:VAL:H	1.77	0.50
6:l:140:LEU:HD12	6:l:141:LEU:N	2.27	0.50
1:C:213:VAL:C	1:C:214:ILE:HD13	2.36	0.50
2:D:4:GLY:O	2:D:9:PHE:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:GLN:N	1:E:14:CYS:SG	2.85	0.50
1:E:50:GLU:OE2	1:E:275:GLY:N	2.45	0.50
1:E:291:ASP:N	1:E:291:ASP:OD1	2.45	0.50
2:B:64:HIS:O	2:B:65:GLN:NE2	2.44	0.50
3:K:4:LEU:HD22	3:K:22:CYS:SG	2.52	0.50
4:L:138:ARG:HD2	4:L:159:VAL:HG11	1.92	0.50
1:C:65:THR:HG1	1:C:89:GLU:CD	2.18	0.49
4:H:5:THR:OG1	4:H:24:ARG:NH2	2.45	0.49
6:f:24:ARG:NH1	6:f:76:PHE:O	2.45	0.49
1:A:108:LEU:HD13	1:A:234:TRP:CD1	2.48	0.49
3:I:4:LEU:HD22	3:I:22:CYS:SG	2.51	0.49
1:E:26:VAL:HG12	1:E:315:LYS:HB3	1.94	0.49
6:b:19:ALA:HB3	6:b:80:ILE:CG2	2.42	0.49
6:d:131:LYS:O	6:d:132:SER:C	2.55	0.49
5:i:40:ALA:HB1	5:i:41:PRO:HD3	1.93	0.49
6:d:141:LEU:HD21	6:d:201:VAL:HG13	1.94	0.49
5:i:39:GLN:OE1	6:j:43:GLN:NE2	2.44	0.49
1:A:122:ASN:HB3	7:M:2:NAG:H81	1.93	0.49
1:A:126:ASN:OD1	8:S:1:NAG:N2	2.46	0.49
5:g:12:VAL:HG21	5:g:18:LEU:HG	1.95	0.49
5:k:131:SER:CB	6:l:212:LYS:HZ2	2.24	0.49
1:A:137:SER:OG	6:h:34:GLY:N	2.45	0.49
2:B:144:CYS:SG	2:B:145:ASP:N	2.86	0.49
5:g:102:THR:HG21	6:h:37:TYR:CD2	2.48	0.49
5:g:187:THR:HG23	6:h:142:ASN:ND2	2.27	0.49
6:h:111:ILE:N	6:h:171:GLN:OE1	2.43	0.49
1:C:52:CYS:H	1:C:282:ILE:HD11	1.78	0.49
3:I:160:TYR:OH	3:I:163:GLU:OE2	2.20	0.49
6:b:9:LEU:HD12	6:b:109:LEU:HA	1.95	0.49
2:D:128:GLU:O	2:D:170:ARG:NH1	2.44	0.48
5:g:74:ASN:O	5:g:74:ASN:ND2	2.46	0.48
6:l:123:PHE:HB3	6:l:138:VAL:HB	1.95	0.48
1:C:51:ILE:CD1	1:C:272:ALA:HB3	2.43	0.48
6:d:123:PHE:O	6:d:124:PRO:C	2.55	0.48
4:J:101:GLU:OE2	4:J:169:TYR:OH	2.31	0.48
5:e:4:LEU:HD21	5:e:106:MET:HE3	1.94	0.48
6:f:38:LEU:HD11	6:f:93:CYS:HB2	1.96	0.48
5:c:12:VAL:HG21	5:c:18:LEU:HG	1.96	0.48
5:i:4:LEU:HD21	5:i:106:MET:HE3	1.94	0.48
6:j:129:GLN:O	6:j:132:SER:OG	2.26	0.48
1:C:51:ILE:HD12	1:C:272:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:206:LEU:HD13	6:d:210:VAL:CG2	2.44	0.48
6:f:68:SER:N	6:f:79:ASP:O	2.46	0.48
8:Z:3:BMA:O4	8:Z:4:MAN:O5	2.16	0.48
1:A:97:CYS:SG	1:A:98:TYR:N	2.84	0.48
1:C:1:GLN:N	1:C:14:CYS:SG	2.87	0.48
1:A:86:LEU:HD22	1:A:302:TYR:CG	2.48	0.47
5:g:142:LEU:HD13	5:g:215:VAL:HG11	1.96	0.47
5:i:4:LEU:HB3	5:i:24:LEU:HD23	1.94	0.47
1:E:282:ILE:HG22	1:E:282:ILE:O	2.15	0.47
6:d:118:PRO:HG3	6:d:203:HIS:CD2	2.49	0.47
5:k:185:VAL:HG11	6:l:140:LEU:HD13	1.96	0.47
1:A:119:GLU:OE1	1:A:261:ARG:NH1	2.47	0.47
1:C:79:PHE:O	1:C:118:LEU:HD13	2.14	0.47
6:f:200:GLU:OE2	6:f:201:VAL:N	2.48	0.47
5:g:183:SER:OG	5:g:184:SER:N	2.46	0.47
4:L:139:GLU:OE1	4:L:139:GLU:N	2.47	0.47
5:g:4:LEU:HD13	5:g:109:PRO:HD3	1.96	0.47
5:g:130:PRO:HD2	5:g:217:PRO:HA	1.97	0.47
8:S:3:BMA:O4	8:S:4:MAN:O5	2.16	0.47
1:A:242:ILE:HG22	1:A:244:LEU:HD11	1.97	0.47
1:A:282:ILE:O	1:A:282:ILE:HG22	2.15	0.47
1:C:187:THR:OG1	1:C:219:SER:N	2.48	0.47
1:C:190:ASP:O	1:C:194:LEU:HD12	2.15	0.47
1:C:203:THR:O	1:C:203:THR:OG1	2.31	0.47
1:C:208:ARG:NH2	1:C:241:ASP:OD2	2.47	0.47
6:b:52:LEU:HD13	6:b:67:ILE:HD13	1.97	0.47
5:g:187:THR:HG21	6:h:143:ASN:CG	2.40	0.47
6:h:94:MET:HE1	6:h:101:ARG:HB3	1.96	0.47
5:k:187:THR:HG21	6:l:143:ASN:CG	2.40	0.47
6:b:168:VAL:HG22	6:b:180:LEU:HD13	1.95	0.47
6:b:144:PHE:O	6:b:178:TYR:N	2.44	0.47
2:F:53:ASN:O	2:F:58:LYS:NZ	2.27	0.47
5:c:33:TYR:HB3	5:c:101:ALA:HB2	1.97	0.47
5:e:24:LEU:HD21	5:e:95:ARG:HH11	1.79	0.47
6:l:118:PRO:HG2	6:l:206:LEU:HD11	1.96	0.47
1:A:1:GLN:N	1:A:14:CYS:SG	2.88	0.46
1:C:51:ILE:CG1	1:C:272:ALA:HB3	2.45	0.46
1:E:156:HIS:CE1	1:E:196:ALA:HB3	2.50	0.46
6:l:141:LEU:HD11	6:l:201:VAL:CG2	2.42	0.46
2:B:4:GLY:O	2:B:9:PHE:N	2.46	0.46
1:C:151:LEU:HG	1:C:252:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:66:ARG:HG3	6:d:80:ILE:HG23	1.97	0.46
5:e:4:LEU:HB3	5:e:24:LEU:HD23	1.97	0.46
5:k:128:LEU:HD21	6:l:138:VAL:HG12	1.98	0.46
5:e:197:THR:HG22	5:e:199:ILE:HD13	1.98	0.46
6:f:19:ALA:HB3	6:f:80:ILE:CG2	2.45	0.46
5:i:128:LEU:HD23	6:j:123:PHE:CB	2.45	0.46
1:C:301:THR:OG1	1:C:302:TYR:N	2.48	0.46
6:h:42:HIS:O	6:h:50:ARG:N	2.44	0.46
5:k:170:PHE:O	6:l:45:ARG:NH2	2.48	0.46
1:E:204:VAL:HG13	1:E:245:ILE:HG12	1.98	0.46
5:c:53:VAL:HG12	5:c:54:ALA:H	1.79	0.46
6:h:125:PRO:CB	6:h:130:LEU:HD11	2.46	0.46
5:i:94:ALA:CB	5:i:104:LEU:HD11	2.45	0.46
6:l:111:ILE:N	6:l:171:GLN:OE1	2.44	0.46
3:G:160:TYR:O	3:G:191:TYR:N	2.47	0.46
5:c:94:ALA:HB3	5:c:104:LEU:HD12	1.97	0.46
5:c:102:THR:HG21	6:d:37:TYR:CD2	2.50	0.46
6:d:131:LYS:C	6:d:133:GLY:N	2.73	0.46
1:A:98:TYR:CD1	1:A:230:ILE:HD11	2.50	0.46
3:I:32:TYR:OH	3:I:57:SER:OG	2.32	0.46
5:c:129:ALA:CB	6:d:123:PHE:HB2	2.38	0.46
1:C:108:LEU:O	1:C:112:VAL:HG22	2.15	0.46
1:E:133:ASN:N	1:E:153:TRP:O	2.49	0.46
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.49	0.46
6:d:129:GLN:O	6:d:130:LEU:C	2.58	0.46
1:E:200:GLY:H	1:E:201:ARG:HH22	1.63	0.46
3:G:40:ARG:O	3:G:48:GLU:N	2.48	0.46
5:c:128:LEU:HD13	6:d:140:LEU:HD22	1.97	0.46
1:C:153:TRP:HA	1:C:252:ILE:HG23	1.98	0.46
1:A:192:ILE:HD13	1:A:194:LEU:HD11	1.98	0.45
2:B:37:ASP:OD2	2:B:40:SER:OG	2.29	0.45
6:d:130:LEU:HD23	6:d:135:ALA:HB2	1.98	0.45
6:b:191:TYR:O	6:b:197:TYR:OH	2.34	0.45
5:c:140:ALA:HA	6:d:121:PHE:CZ	2.52	0.45
5:c:140:ALA:HA	6:d:121:PHE:HZ	1.81	0.45
6:f:129:GLN:O	6:f:132:SER:OG	2.22	0.45
5:g:128:LEU:HD12	5:g:143:GLY:HA3	1.99	0.45
1:C:248:THR:N	7:U:1:NAG:H81	2.31	0.45
2:F:51:LYS:HE2	2:F:107:THR:HG23	1.98	0.45
6:d:130:LEU:HB3	6:d:188:LYS:HE3	1.99	0.45
6:f:68:SER:O	6:f:79:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:130:PRO:HA	6:h:121:PHE:CE2	2.51	0.45
6:h:123:PHE:CE1	6:h:124:PRO:O	2.69	0.45
6:h:125:PRO:HB3	6:h:130:LEU:HD11	1.97	0.45
5:k:53:VAL:HG21	7:n:3:BMA:H4	1.97	0.45
2:D:144:CYS:SG	2:D:145:ASP:N	2.87	0.45
5:g:106:MET:SD	5:g:107:TRP:N	2.90	0.45
1:A:41:GLU:OE1	1:A:315:LYS:NZ	2.44	0.45
1:C:156:HIS:ND1	1:C:157:LEU:O	2.50	0.45
5:c:128:LEU:HD22	6:d:121:PHE:O	2.16	0.45
5:e:25:TYR:OH	6:h:62:GLY:O	2.33	0.45
5:e:99:THR:OG1	9:V:3:BMA:O3	2.33	0.45
6:j:2:ILE:HG21	6:j:29:LEU:HD21	1.99	0.45
5:k:105:ALA:HB1	6:l:51:LEU:HD13	1.97	0.45
5:c:128:LEU:HA	6:d:123:PHE:H	1.80	0.45
6:h:141:LEU:HD11	6:h:201:VAL:CG2	2.41	0.45
1:E:156:HIS:HD1	1:E:161:TYR:HD2	1.64	0.45
1:E:184:HIS:HB3	1:E:217:ILE:HD13	1.99	0.45
3:G:155:CYS:SG	3:G:224:LYS:NZ	2.84	0.45
4:L:29:LEU:O	4:L:33:THR:OG1	2.30	0.45
5:c:187:THR:HG23	6:d:142:ASN:ND2	2.32	0.45
5:e:170:PHE:CE1	6:f:169:THR:HG23	2.52	0.45
5:i:197:THR:HG22	5:i:199:ILE:HD13	1.99	0.45
6:l:42:HIS:NE2	6:l:88:ALA:O	2.48	0.45
1:E:122:ASN:HB3	7:m:2:NAG:H81	1.99	0.45
4:J:61:ARG:NH2	4:J:82:ASP:OD1	2.50	0.45
4:J:79:GLN:O	4:J:102:ILE:HD11	2.17	0.45
1:E:71:LEU:HD23	1:E:148:PHE:CE2	2.52	0.44
5:a:36:TRP:O	5:a:48:VAL:N	2.47	0.44
5:c:21:THR:HG21	5:c:75:GLN:OE1	2.17	0.44
5:c:33:TYR:CB	5:c:101:ALA:HB2	2.48	0.44
1:A:270:SER:OG	1:A:271:ASP:N	2.48	0.44
5:a:4:LEU:HB3	5:a:24:LEU:HD23	1.98	0.44
6:d:120:VAL:HG22	6:d:201:VAL:HG21	1.99	0.44
1:E:72:GLY:O	1:E:141:ARG:NH2	2.36	0.44
1:E:133:ASN:N	1:E:133:ASN:OD1	2.51	0.44
5:g:60:ASN:CG	5:g:63:VAL:HG21	2.42	0.44
2:B:154:ASN:OD1	2:B:155:GLY:N	2.50	0.44
5:c:156:VAL:HG11	5:c:184:SER:HB3	1.99	0.44
5:c:187:THR:HG21	6:d:143:ASN:CG	2.42	0.44
5:i:104:LEU:HD23	5:i:107:TRP:CZ2	2.52	0.44
6:j:95:GLN:NE2	6:j:98:GLN:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:OD1	1:C:90:ARG:NE	2.49	0.44
1:E:186:GLY:HA2	1:E:217:ILE:HG23	2.00	0.44
3:I:24:ILE:O	3:I:80:ASN:ND2	2.50	0.44
5:i:170:PHE:CE1	6:j:169:THR:HG23	2.52	0.44
3:G:182:PRO:O	4:H:158:SER:OG	2.25	0.44
4:H:61:ARG:NH2	4:H:82:ASP:OD1	2.49	0.44
6:h:191:TYR:O	6:h:197:TYR:OH	2.35	0.44
5:k:129:ALA:N	6:l:124:PRO:HD3	2.33	0.44
5:k:168:HIS:HE2	6:l:177:THR:HG1	1.57	0.44
5:c:182:LEU:HD12	5:c:183:SER:N	2.33	0.44
1:A:70:LEU:HD23	1:A:71:LEU:HD12	1.99	0.43
1:A:243:LEU:C	1:A:244:LEU:HD12	2.43	0.43
1:C:66:LEU:HD21	1:C:112:VAL:HG23	1.99	0.43
2:F:154:ASN:OD1	2:F:155:GLY:N	2.51	0.43
4:H:138:ARG:CD	4:H:159:VAL:HG11	2.47	0.43
3:K:32:TYR:OH	3:K:57:SER:OG	2.31	0.43
5:i:70:ASP:O	5:i:74:ASN:N	2.51	0.43
6:b:82:LYS:NZ	6:b:83:VAL:O	2.43	0.43
5:k:131:SER:HB2	6:l:212:LYS:HZ2	1.83	0.43
6:b:2:ILE:HG21	6:b:29:LEU:HD21	1.99	0.43
5:i:34:TRP:CH2	5:i:53:VAL:HG13	2.54	0.43
3:G:24:ILE:O	3:G:80:ASN:ND2	2.51	0.43
4:H:138:ARG:HD2	4:H:159:VAL:HG11	2.00	0.43
5:k:123:PRO:HB2	5:k:146:VAL:CG1	2.47	0.43
5:k:128:LEU:HD12	5:k:143:GLY:CA	2.43	0.43
1:E:184:HIS:HB3	1:E:217:ILE:HG21	1.99	0.43
5:a:4:LEU:HD21	5:a:106:MET:CE	2.47	0.43
6:h:118:PRO:HG2	6:h:206:LEU:HD11	2.00	0.43
1:A:86:LEU:HD22	1:A:302:TYR:CD1	2.54	0.43
1:E:200:GLY:H	1:E:201:ARG:NH2	2.16	0.43
5:k:133:LYS:N	6:l:212:LYS:HZ1	2.17	0.43
3:K:186:GLN:N	3:K:190:LEU:O	2.47	0.43
6:d:129:GLN:OE1	6:d:136:SER:HB2	2.18	0.43
5:e:4:LEU:HD21	5:e:106:MET:CE	2.48	0.43
6:h:55:HIS:O	6:h:57:SER:N	2.52	0.43
5:i:40:ALA:HB3	5:i:43:LYS:HD2	2.00	0.43
1:A:34:ILE:HD11	1:A:321:ARG:HD3	2.00	0.43
1:C:182:VAL:HG22	1:C:202:ILE:HD13	2.00	0.43
2:F:164:ASP:O	2:F:167:LEU:HD12	2.19	0.43
6:b:13:VAL:O	6:b:112:LYS:N	2.52	0.43
6:b:88:ALA:HA	6:b:109:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:o:3:BMA:O4	9:o:3:BMA:O6	2.35	0.43
2:D:154:ASN:OD1	2:D:155:GLY:N	2.51	0.43
5:c:169:THR:O	6:d:169:THR:HG22	2.19	0.43
6:d:55:HIS:O	6:d:57:SER:N	2.51	0.43
6:h:123:PHE:CZ	6:h:124:PRO:O	2.72	0.43
3:G:4:LEU:HD23	3:G:24:ILE:HA	2.01	0.43
4:H:79:GLN:O	4:H:102:ILE:HD11	2.19	0.43
4:L:79:GLN:O	4:L:102:ILE:HD11	2.18	0.43
6:b:53:LEU:HD11	6:b:67:ILE:HG22	2.00	0.43
5:e:146:VAL:HG22	5:e:149:TYR:CD1	2.53	0.43
6:j:144:PHE:O	6:j:178:TYR:N	2.48	0.43
6:b:19:ALA:HB3	6:b:80:ILE:HG22	2.00	0.42
6:h:166:GLU:OE1	6:h:166:GLU:N	2.47	0.42
6:j:29:LEU:O	6:j:97:THR:OG1	2.28	0.42
6:d:21:ILE:HD11	6:d:109:LEU:HD12	2.01	0.42
5:g:131:SER:CB	6:h:212:LYS:HZ2	2.31	0.42
4:H:161:GLU:OE1	4:H:161:GLU:N	2.52	0.42
1:A:133:ASN:N	1:A:153:TRP:O	2.52	0.42
3:I:183:ALA:HB1	3:I:191:TYR:HD2	1.85	0.42
3:K:27:ASP:OD1	3:K:28:SER:N	2.52	0.42
6:d:137:VAL:HG21	6:d:197:TYR:CE1	2.55	0.42
5:k:9:ALA:O	5:k:113:VAL:HG22	2.20	0.42
1:A:72:GLY:O	1:A:141:ARG:NH2	2.37	0.42
3:G:27:ASP:OD1	3:G:28:SER:N	2.52	0.42
5:g:156:VAL:HG11	5:g:184:SER:HB3	2.01	0.42
6:h:120:VAL:HA	6:h:140:LEU:O	2.20	0.42
5:i:4:LEU:HD21	5:i:106:MET:CE	2.50	0.42
5:i:211:VAL:HG22	5:i:213:LYS:HZ1	1.85	0.42
6:j:68:SER:N	6:j:79:ASP:O	2.52	0.42
1:A:281:CYS:HB2	1:A:305:CYS:HB3	1.82	0.42
1:C:133:ASN:OD1	1:C:133:ASN:N	2.53	0.42
1:C:219:SER:O	1:C:220:ARG:NE	2.53	0.42
6:h:42:HIS:NE2	6:h:88:ALA:O	2.48	0.42
2:D:37:ASP:OD2	2:D:40:SER:OG	2.32	0.42
5:g:53:VAL:HG21	7:U:3:BMA:C4	2.50	0.42
5:g:170:PHE:HA	6:h:169:THR:HA	2.01	0.42
5:k:183:SER:OG	5:k:184:SER:N	2.52	0.42
1:A:151:LEU:HD12	1:A:252:ILE:HG22	2.02	0.42
1:C:60:ASP:OD1	1:C:61:GLY:N	2.52	0.42
6:d:122:ILE:O	6:d:122:ILE:HG13	2.20	0.42
6:d:129:GLN:CD	6:d:136:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:64:ARG:O	5:k:65:MET:HE2	2.20	0.42
6:l:123:PHE:CE1	6:l:137:VAL:HA	2.55	0.42
6:l:191:TYR:O	6:l:197:TYR:OH	2.38	0.42
1:E:127:TRP:O	1:E:130:VAL:HG22	2.20	0.42
3:K:67:VAL:O	3:K:71:ILE:HG22	2.20	0.42
6:d:118:PRO:HD2	6:d:206:LEU:CD2	2.50	0.42
5:k:123:PRO:HB3	5:k:149:TYR:HB3	2.02	0.42
5:k:172:ALA:HB3	5:k:180:TYR:CE1	2.55	0.42
6:l:142:ASN:OD1	6:l:179:SER:OG	2.37	0.42
1:C:34:ILE:HD11	1:C:321:ARG:HD3	2.02	0.42
6:d:125:PRO:HB3	6:d:128:GLU:HB3	2.02	0.42
1:A:202:ILE:HD12	1:A:202:ILE:H	1.85	0.41
1:C:130:VAL:CG2	1:C:154:LEU:HD12	2.50	0.41
6:h:123:PHE:CD2	6:h:137:VAL:HA	2.54	0.41
5:i:145:LEU:HD12	5:i:145:LEU:O	2.19	0.41
1:A:133:ASN:N	1:A:133:ASN:OD1	2.52	0.41
3:K:45:ARG:NH1	3:K:92:GLU:OE2	2.53	0.41
5:a:30:ARG:HA	5:a:53:VAL:HG21	2.02	0.41
5:e:94:ALA:HB1	5:e:104:LEU:HD22	2.01	0.41
6:l:55:HIS:O	6:l:57:SER:N	2.52	0.41
2:F:144:CYS:SG	2:F:145:ASP:N	2.91	0.41
3:K:4:LEU:HD23	3:K:24:ILE:HA	2.01	0.41
5:k:156:VAL:HG11	5:k:184:SER:HB3	2.03	0.41
5:a:48:VAL:HG11	5:a:78:LEU:HD11	2.02	0.41
5:c:87:ASP:HB2	5:c:115:VAL:HG21	2.02	0.41
5:c:216:GLU:OE1	5:c:216:GLU:N	2.49	0.41
5:g:130:PRO:HA	6:h:121:PHE:HD2	1.80	0.41
5:i:31:ASP:OD1	5:i:99:THR:HG22	2.20	0.41
6:j:82:LYS:NZ	6:j:83:VAL:O	2.48	0.41
1:E:177:LEU:HD12	1:E:236:ILE:HG22	2.02	0.41
3:K:81:GLN:OE1	3:K:81:GLN:N	2.54	0.41
5:a:40:ALA:HB1	5:a:41:PRO:CD	2.51	0.41
5:g:38:ARG:NH2	5:g:46:GLN:OE1	2.53	0.41
6:h:122:ILE:HG13	6:h:123:PHE:H	1.85	0.41
5:k:170:PHE:HA	6:l:169:THR:HA	2.02	0.41
1:A:177:LEU:HD12	1:A:236:ILE:HG22	2.03	0.41
1:A:231:SER:O	1:A:232:ILE:HD12	2.21	0.41
1:A:251:LEU:HD12	1:A:252:ILE:N	2.36	0.41
6:b:35:ARG:NH2	6:b:55:HIS:O	2.54	0.41
6:b:141:LEU:HD22	6:b:180:LEU:HD23	2.03	0.41
6:d:117:ALA:HA	6:d:118:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:122:ILE:CG2	6:d:139:CYS:HA	2.33	0.41
1:A:164:LEU:N	1:A:247:SER:O	2.54	0.41
1:C:51:ILE:HG23	1:C:282:ILE:HG21	2.03	0.41
1:C:182:VAL:HG21	1:C:213:VAL:CG2	2.51	0.41
1:E:199:SER:CB	1:E:201:ARG:HH22	2.33	0.41
3:G:101:ARG:NH2	8:Q:4:MAN:O4	2.54	0.41
4:H:17:ASP:N	4:H:17:ASP:OD1	2.53	0.41
3:I:67:VAL:O	3:I:71:ILE:HG22	2.20	0.41
4:L:148:ASN:N	4:L:148:ASN:OD1	2.54	0.41
5:c:213:LYS:NZ	6:d:128:GLU:OE1	2.53	0.41
6:d:129:GLN:NE2	6:d:136:SER:H	2.18	0.41
5:g:37:VAL:HG11	6:h:103:PHE:CZ	2.56	0.41
5:g:87:ASP:HB2	5:g:115:VAL:HG21	2.03	0.41
6:h:123:PHE:CD2	6:h:138:VAL:HG23	2.56	0.41
3:G:67:VAL:O	3:G:71:ILE:HG22	2.20	0.41
3:K:52:ARG:NE	3:K:62:ASP:OD2	2.53	0.41
6:f:9:LEU:HD12	6:f:109:LEU:HA	2.02	0.41
6:j:122:ILE:HG21	6:j:214:PHE:CE1	2.55	0.41
4:H:116:PRO:HG3	4:H:126:ALA:HB1	2.01	0.40
1:C:51:ILE:O	1:C:51:ILE:HG22	2.21	0.40
1:E:53:ASP:OD1	1:E:53:ASP:N	2.53	0.40
3:G:123:MET:HE2	3:G:123:MET:HA	2.02	0.40
3:I:81:GLN:OE1	3:I:81:GLN:N	2.54	0.40
6:d:121:PHE:H	6:d:140:LEU:HB3	1.86	0.40
6:b:66:ARG:NH1	6:b:80:ILE:HD11	2.36	0.40
5:e:123:PRO:HB2	5:e:146:VAL:HG23	2.03	0.40
5:g:9:ALA:O	5:g:113:VAL:HG22	2.22	0.40
1:A:192:ILE:HG22	1:A:193:PHE:N	2.37	0.40
6:d:130:LEU:O	6:d:131:LYS:C	2.64	0.40
5:e:8:GLY:HA3	5:e:20:VAL:HG12	2.03	0.40
3:G:81:GLN:N	3:G:81:GLN:OE1	2.54	0.40
4:L:17:ASP:OD1	4:L:17:ASP:N	2.54	0.40
5:a:46:GLN:OE1	5:a:47:TRP:N	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	323/348 (93%)	279 (86%)	42 (13%)	2 (1%)	21	50
1	C	323/348 (93%)	268 (83%)	53 (16%)	2 (1%)	21	50
1	E	323/348 (93%)	276 (85%)	43 (13%)	4 (1%)	10	35
2	B	171/223 (77%)	161 (94%)	10 (6%)	0	100	100
2	D	171/223 (77%)	158 (92%)	13 (8%)	0	100	100
2	F	171/223 (77%)	160 (94%)	11 (6%)	0	100	100
3	G	218/227 (96%)	209 (96%)	9 (4%)	0	100	100
3	I	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
3	K	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
4	H	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
4	J	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
4	L	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
5	a	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
5	c	220/222 (99%)	199 (90%)	21 (10%)	0	100	100
5	e	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
5	g	220/222 (99%)	195 (89%)	24 (11%)	1 (0%)	24	54
5	i	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
5	k	220/222 (99%)	198 (90%)	21 (10%)	1 (0%)	24	54
6	b	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
6	d	217/219 (99%)	208 (96%)	6 (3%)	3 (1%)	9	31
6	f	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
6	h	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	24	54
6	j	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
6	l	217/219 (99%)	213 (98%)	3 (1%)	1 (0%)	24	54
All	All	5370/5658 (95%)	5023 (94%)	332 (6%)	15 (0%)	37	65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	CYS
1	C	306	PRO
6	d	131	LYS
6	d	132	SER
1	E	197	GLN
1	E	199	SER
6	h	56	ILE
6	l	56	ILE
1	E	192	ILE
6	d	56	ILE
5	g	131	SER
1	A	133	ASN
5	k	131	SER
1	C	283	THR
1	E	306	PRO

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	288/309 (93%)	281 (98%)	7 (2%)	43	62
1	C	288/309 (93%)	280 (97%)	8 (3%)	38	60
1	E	288/309 (93%)	281 (98%)	7 (2%)	43	62
2	B	146/186 (78%)	146 (100%)	0	100	100
2	D	146/186 (78%)	146 (100%)	0	100	100
2	F	146/186 (78%)	146 (100%)	0	100	100
3	G	192/198 (97%)	192 (100%)	0	100	100
3	I	192/198 (97%)	192 (100%)	0	100	100
3	K	192/198 (97%)	192 (100%)	0	100	100
4	H	180/181 (99%)	180 (100%)	0	100	100
4	J	180/181 (99%)	180 (100%)	0	100	100
4	L	180/181 (99%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	a	189/189 (100%)	189 (100%)	0	100	100
5	c	189/189 (100%)	188 (100%)	1 (0%)	81	81
5	e	189/189 (100%)	189 (100%)	0	100	100
5	g	189/189 (100%)	187 (99%)	2 (1%)	65	74
5	i	189/189 (100%)	188 (100%)	1 (0%)	81	81
5	k	189/189 (100%)	186 (98%)	3 (2%)	55	68
6	b	191/191 (100%)	191 (100%)	0	100	100
6	d	191/191 (100%)	190 (100%)	1 (0%)	81	81
6	f	191/191 (100%)	191 (100%)	0	100	100
6	h	191/191 (100%)	187 (98%)	4 (2%)	47	64
6	j	191/191 (100%)	190 (100%)	1 (0%)	81	81
6	l	191/191 (100%)	189 (99%)	2 (1%)	68	75
All	All	4698/4902 (96%)	4661 (99%)	37 (1%)	70	77

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	63	ASN
1	A	126	ASN
1	A	133	ASN
1	A	141	ARG
1	A	176	LYS
1	A	259	LYS
1	C	38	ASN
1	C	63	ASN
1	C	125	PHE
1	C	126	ASN
1	C	133	ASN
1	C	178	TYR
1	C	194	LEU
1	C	277	CYS
1	E	38	ASN
1	E	63	ASN
1	E	126	ASN
1	E	133	ASN
1	E	141	ARG
1	E	176	LYS

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Mol	Chain	Res	Type
1	E	259	LYS
5	c	67	ILE
6	d	45	ARG
5	g	67	ILE
5	g	131	SER
6	h	59	ARG
6	h	61	PHE
6	h	94	MET
6	h	123	PHE
5	i	201	ASN
6	j	67	ILE
5	k	67	ILE
5	k	131	SER
5	k	180	TYR
6	l	45	ARG
6	l	122	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	144	ASN
1	A	211	GLN
2	B	12	ASN
2	B	26	HIS
1	C	6	ASN
1	C	17	HIS
1	C	81	ASN
2	D	12	ASN
2	D	129	ASN
1	E	6	ASN
1	E	132	GLN
1	E	144	ASN
2	F	12	ASN
3	G	41	GLN
3	I	41	GLN
3	I	120	GLN
4	J	156	GLN
3	K	41	GLN
3	K	120	GLN
4	L	156	GLN
6	f	1	ASN

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Mol	Chain	Res	Type
6	j	165	GLN
5	k	3	GLN
6	l	143	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 ⓘ

79 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	M	1	7,1	14,14,15	0.56	0	17,19,21	0.62	0
7	NAG	M	2	7	14,14,15	0.60	1 (7%)	17,19,21	0.63	0
7	BMA	M	3	7	11,11,12	0.54	0	15,15,17	0.70	0
7	NAG	N	1	7,1	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
7	NAG	N	2	7	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
7	BMA	N	3	7	11,11,12	0.69	0	15,15,17	0.68	0
8	NAG	O	1	8,1	14,14,15	0.33	0	17,19,21	0.70	1 (5%)
8	NAG	O	2	8	14,14,15	0.68	1 (7%)	17,19,21	0.78	1 (5%)
8	BMA	O	3	8	11,11,12	0.63	0	15,15,17	0.82	0
8	MAN	O	4	8	11,11,12	0.91	0	15,15,17	1.10	2 (13%)
8	MAN	O	5	8	11,11,12	0.83	0	15,15,17	1.13	1 (6%)
7	NAG	P	1	7,1	14,14,15	0.35	0	17,19,21	1.44	2 (11%)
7	NAG	P	2	7	14,14,15	0.29	0	17,19,21	0.43	0
7	BMA	P	3	7	11,11,12	0.63	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	Q	1	8,1	14,14,15	0.82	1 (7%)	17,19,21	1.11	2 (11%)
8	NAG	Q	2	8	14,14,15	0.25	0	17,19,21	0.90	1 (5%)
8	BMA	Q	3	8	11,11,12	0.64	0	15,15,17	1.03	1 (6%)
8	MAN	Q	4	8	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
8	MAN	Q	5	8	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
7	NAG	R	1	7	14,14,15	0.20	0	17,19,21	0.45	0
7	NAG	R	2	7	14,14,15	0.21	0	17,19,21	0.44	0
7	BMA	R	3	7	11,11,12	0.86	0	15,15,17	0.84	0
8	NAG	S	1	8,1	14,14,15	0.22	0	17,19,21	0.65	1 (5%)
8	NAG	S	2	8	14,14,15	0.25	0	17,19,21	0.50	0
8	BMA	S	3	8	11,11,12	0.59	0	15,15,17	0.74	0
8	MAN	S	4	8	11,11,12	0.93	0	15,15,17	1.24	2 (13%)
8	MAN	S	5	8	11,11,12	0.78	0	15,15,17	1.35	2 (13%)
7	NAG	T	1	7,1	14,14,15	0.47	0	17,19,21	0.59	0
7	NAG	T	2	7	14,14,15	0.57	0	17,19,21	0.64	0
7	BMA	T	3	7	11,11,12	0.55	0	15,15,17	0.72	0
7	NAG	U	1	7,1	14,14,15	0.32	0	17,19,21	0.77	0
7	NAG	U	2	7	14,14,15	0.38	0	17,19,21	1.07	1 (5%)
7	BMA	U	3	7	11,11,12	0.70	0	15,15,17	0.79	0
9	NAG	V	1	9,1	14,14,15	0.74	0	17,19,21	1.02	1 (5%)
9	NAG	V	2	9	14,14,15	0.68	1 (7%)	17,19,21	0.80	1 (5%)
9	BMA	V	3	9	11,11,12	0.50	0	15,15,17	0.73	0
9	MAN	V	4	9	11,11,12	0.87	0	15,15,17	1.06	2 (13%)
7	NAG	W	1	7,1	14,14,15	0.56	0	17,19,21	1.49	3 (17%)
7	NAG	W	2	7	14,14,15	0.37	0	17,19,21	0.46	0
7	BMA	W	3	7	11,11,12	0.65	0	15,15,17	0.72	0
8	NAG	X	1	8,1	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
8	NAG	X	2	8	14,14,15	0.37	0	17,19,21	0.70	0
8	BMA	X	3	8	11,11,12	0.67	0	15,15,17	1.33	3 (20%)
8	MAN	X	4	8	11,11,12	0.62	0	15,15,17	1.09	2 (13%)
8	MAN	X	5	8	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
7	NAG	Y	1	7	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	Y	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	BMA	Y	3	7	11,11,12	0.79	0	15,15,17	0.78	0
8	NAG	Z	1	8,1	14,14,15	0.23	0	17,19,21	0.71	1 (5%)
8	NAG	Z	2	8	14,14,15	0.21	0	17,19,21	0.47	0
8	BMA	Z	3	8	11,11,12	0.60	0	15,15,17	0.79	0
8	MAN	Z	4	8	11,11,12	0.95	0	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	Z	5	8	11,11,12	0.85	0	15,15,17	1.33	1 (6%)
7	NAG	m	1	7,1	14,14,15	0.54	0	17,19,21	0.62	0
7	NAG	m	2	7	14,14,15	0.60	1 (7%)	17,19,21	0.64	0
7	BMA	m	3	7	11,11,12	0.54	0	15,15,17	0.70	0
7	NAG	n	1	7,1	14,14,15	0.33	0	17,19,21	0.94	1 (5%)
7	NAG	n	2	7	14,14,15	0.37	0	17,19,21	1.08	1 (5%)
7	BMA	n	3	7	11,11,12	0.67	0	15,15,17	0.72	0
9	NAG	o	1	9,1	14,14,15	0.28	0	17,19,21	0.61	0
9	NAG	o	2	9	14,14,15	0.72	1 (7%)	17,19,21	0.78	1 (5%)
9	BMA	o	3	9	11,11,12	0.60	0	15,15,17	0.82	0
9	MAN	o	4	9	11,11,12	1.12	1 (9%)	15,15,17	1.30	3 (20%)
7	NAG	p	1	7,1	14,14,15	0.38	0	17,19,21	1.45	3 (17%)
7	NAG	p	2	7	14,14,15	0.27	0	17,19,21	0.43	0
7	BMA	p	3	7	11,11,12	0.63	0	15,15,17	0.71	0
8	NAG	q	1	8,1	14,14,15	0.81	1 (7%)	17,19,21	1.12	2 (11%)
8	NAG	q	2	8	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
8	BMA	q	3	8	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
8	MAN	q	4	8	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
8	MAN	q	5	8	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
7	NAG	r	1	7	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	r	2	7	14,14,15	0.22	0	17,19,21	0.43	0
7	BMA	r	3	7	11,11,12	0.86	0	15,15,17	0.84	0
8	NAG	s	1	8,1	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
8	NAG	s	2	8	14,14,15	0.21	0	17,19,21	0.49	0
8	BMA	s	3	8	11,11,12	0.62	0	15,15,17	0.77	0
8	MAN	s	4	8	11,11,12	0.92	0	15,15,17	1.21	2 (13%)
8	MAN	s	5	8	11,11,12	0.77	0	15,15,17	1.41	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
8	NAG	O	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	O	2	8	-	3/6/23/26	0/1/1/1
8	BMA	O	3	8	-	2/2/19/22	0/1/1/1
8	MAN	O	4	8	-	2/2/19/22	0/1/1/1
8	MAN	O	5	8	-	1/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	P	2	7	-	4/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	1/2/19/22	0/1/1/1
7	NAG	R	1	7	-	1/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
8	NAG	S	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	BMA	S	3	8	-	2/2/19/22	0/1/1/1
8	MAN	S	4	8	-	1/2/19/22	0/1/1/1
8	MAN	S	5	8	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	NAG	U	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	4/6/23/26	0/1/1/1
7	BMA	U	3	7	-	0/2/19/22	0/1/1/1
9	NAG	V	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	V	2	9	-	3/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	2/2/19/22	0/1/1/1
7	NAG	W	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	W	2	7	-	4/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
8	NAG	X	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	X	2	8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	0/2/19/22	0/1/1/1
8	MAN	X	5	8	-	1/2/19/22	0/1/1/1
7	NAG	Y	1	7	-	1/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Y	3	7	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Z	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Z	5	8	-	0/2/19/22	0/1/1/1
7	NAG	m	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	m	2	7	-	2/6/23/26	0/1/1/1
7	BMA	m	3	7	-	0/2/19/22	0/1/1/1
7	NAG	n	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	4/6/23/26	0/1/1/1
7	BMA	n	3	7	-	0/2/19/22	0/1/1/1
9	NAG	o	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	o	2	9	-	3/6/23/26	0/1/1/1
9	BMA	o	3	9	-	2/2/19/22	0/1/1/1
9	MAN	o	4	9	-	2/2/19/22	0/1/1/1
7	NAG	p	1	7,1	-	6/6/23/26	0/1/1/1
7	NAG	p	2	7	-	4/6/23/26	0/1/1/1
7	BMA	p	3	7	-	0/2/19/22	0/1/1/1
8	NAG	q	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	q	5	8	-	2/2/19/22	0/1/1/1
7	NAG	r	1	7	-	1/6/23/26	0/1/1/1
7	NAG	r	2	7	-	1/6/23/26	0/1/1/1
7	BMA	r	3	7	-	0/2/19/22	0/1/1/1
8	NAG	s	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	s	2	8	-	2/6/23/26	0/1/1/1
8	BMA	s	3	8	-	2/2/19/22	0/1/1/1
8	MAN	s	4	8	-	1/2/19/22	0/1/1/1
8	MAN	s	5	8	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	1	NAG	O5-C1	-2.79	1.39	1.43
8	q	1	NAG	O5-C1	-2.79	1.39	1.43
9	o	2	NAG	C1-C2	2.38	1.55	1.52
9	V	2	NAG	C1-C2	2.31	1.55	1.52
8	O	2	NAG	C1-C2	2.26	1.55	1.52
9	o	4	MAN	C4-C3	2.18	1.58	1.52
7	m	2	NAG	O5-C1	-2.10	1.40	1.43
7	M	2	NAG	O5-C1	-2.09	1.40	1.43

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	1	NAG	C2-N2-C7	4.75	129.26	122.90
7	p	1	NAG	C2-N2-C7	4.66	129.15	122.90
7	P	1	NAG	C2-N2-C7	4.63	129.10	122.90
8	s	5	MAN	C1-O5-C5	4.24	117.87	112.19
8	Z	5	MAN	C1-O5-C5	4.01	117.56	112.19
8	S	5	MAN	C1-O5-C5	3.95	117.48	112.19
7	N	1	NAG	C1-O5-C5	3.68	117.11	112.19
9	V	1	NAG	C1-O5-C5	3.44	116.80	112.19
8	S	4	MAN	C1-O5-C5	3.07	116.30	112.19
8	X	4	MAN	C1-O5-C5	3.06	116.29	112.19
8	X	3	BMA	C1-C2-C3	3.04	114.07	109.64
8	s	4	MAN	C1-O5-C5	2.98	116.18	112.19
8	Z	4	MAN	C1-O5-C5	2.97	116.17	112.19
8	O	5	MAN	C1-O5-C5	2.95	116.14	112.19
7	n	1	NAG	C1-O5-C5	2.71	115.82	112.19
9	o	4	MAN	C3-C4-C5	2.67	115.07	110.23
7	N	2	NAG	C2-N2-C7	2.60	126.39	122.90
7	n	2	NAG	C2-N2-C7	2.60	126.38	122.90
7	U	2	NAG	C2-N2-C7	2.59	126.37	122.90
8	Q	4	MAN	C1-O5-C5	2.58	115.64	112.19
9	o	4	MAN	C2-C3-C4	2.57	115.38	110.86
8	q	4	MAN	C1-O5-C5	2.55	115.61	112.19
8	O	2	NAG	C2-N2-C7	2.53	126.29	122.90
9	V	2	NAG	C2-N2-C7	2.49	126.24	122.90
9	o	2	NAG	C2-N2-C7	2.44	126.17	122.90
8	q	3	BMA	C1-C2-C3	2.43	113.19	109.64
8	Q	5	MAN	C1-O5-C5	2.40	115.41	112.19
8	Q	3	BMA	C1-C2-C3	2.39	113.13	109.64
8	X	3	BMA	C1-O5-C5	2.39	115.38	112.19
8	O	4	MAN	C1-O5-C5	2.36	115.35	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	1	NAG	C1-C2-N2	2.35	114.14	110.43
8	q	1	NAG	C2-N2-C7	2.35	126.05	122.90
8	X	5	MAN	C1-O5-C5	2.35	115.33	112.19
8	X	1	NAG	C2-N2-C7	2.34	126.04	122.90
9	o	4	MAN	O2-C2-C3	-2.31	105.36	110.15
8	s	5	MAN	O2-C2-C3	-2.31	105.37	110.15
8	Q	1	NAG	C3-C4-C5	2.30	114.40	110.23
8	q	5	MAN	C1-O5-C5	2.30	115.27	112.19
8	S	4	MAN	O2-C2-C3	-2.30	105.40	110.15
8	q	1	NAG	C3-C4-C5	2.29	114.39	110.23
8	S	5	MAN	O2-C2-C3	-2.27	105.46	110.15
8	Q	1	NAG	C2-N2-C7	2.26	125.93	122.90
8	Z	4	MAN	O2-C2-C3	-2.26	105.47	110.15
8	s	4	MAN	O2-C2-C3	-2.25	105.49	110.15
8	Z	1	NAG	C2-N2-C7	2.24	125.91	122.90
7	P	1	NAG	C1-C2-N2	2.20	113.90	110.43
9	V	4	MAN	C1-O5-C5	2.20	115.14	112.19
7	p	1	NAG	C1-C2-N2	2.20	113.90	110.43
8	O	1	NAG	C1-O5-C5	2.20	115.13	112.19
7	W	1	NAG	C1-O5-C5	2.19	115.12	112.19
8	X	5	MAN	O2-C2-C3	-2.18	105.64	110.15
8	O	4	MAN	O2-C2-C3	-2.17	105.66	110.15
8	Q	4	MAN	O2-C2-C3	-2.16	105.67	110.15
8	Q	5	MAN	O2-C2-C3	-2.14	105.71	110.15
8	q	5	MAN	O2-C2-C3	-2.14	105.71	110.15
8	X	4	MAN	O2-C2-C3	-2.14	105.73	110.15
8	q	4	MAN	O2-C2-C3	-2.13	105.74	110.15
8	Q	2	NAG	C3-C4-C5	2.13	114.09	110.23
8	q	2	NAG	C3-C4-C5	2.12	114.08	110.23
9	V	4	MAN	O2-C2-C3	-2.11	105.78	110.15
8	S	1	NAG	C2-N2-C7	2.07	125.67	122.90
8	X	3	BMA	O2-C2-C3	-2.05	105.91	110.15
8	s	1	NAG	C2-N2-C7	2.04	125.63	122.90
7	p	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
7	m	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
8	Q	3	BMA	O5-C5-C6-O6
8	q	3	BMA	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	O	3	BMA	C4-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
8	X	3	BMA	O5-C5-C6-O6
8	Z	3	BMA	O5-C5-C6-O6
8	s	3	BMA	O5-C5-C6-O6
9	o	4	MAN	O5-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
9	o	3	BMA	O5-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6
8	Q	3	BMA	C4-C5-C6-O6
8	q	3	BMA	C4-C5-C6-O6
8	O	3	BMA	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
8	X	3	BMA	C4-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
8	s	3	BMA	C4-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
8	Z	3	BMA	C4-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O7-C7-N2-C2
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
7	n	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	n	2	NAG	O7-C7-N2-C2
7	p	1	NAG	C8-C7-N2-C2
7	p	1	NAG	O7-C7-N2-C2
8	O	2	NAG	C8-C7-N2-C2
8	O	2	NAG	O7-C7-N2-C2
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
8	X	1	NAG	C8-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
8	Z	1	NAG	C8-C7-N2-C2
8	Z	1	NAG	O7-C7-N2-C2
8	q	1	NAG	C8-C7-N2-C2
8	q	1	NAG	O7-C7-N2-C2
8	s	1	NAG	C8-C7-N2-C2
8	s	1	NAG	O7-C7-N2-C2
9	V	2	NAG	C8-C7-N2-C2
9	V	2	NAG	O7-C7-N2-C2
9	o	2	NAG	C8-C7-N2-C2
9	o	2	NAG	O7-C7-N2-C2
7	W	1	NAG	O5-C5-C6-O6
8	O	4	MAN	O5-C5-C6-O6
9	V	4	MAN	O5-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
8	q	5	MAN	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	r	2	NAG	O5-C5-C6-O6
7	Y	2	NAG	O5-C5-C6-O6
8	Q	5	MAN	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
8	S	4	MAN	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
8	Z	4	MAN	O5-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
8	s	4	MAN	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	O	5	MAN	O5-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
7	n	2	NAG	C4-C5-C6-O6
8	X	1	NAG	O5-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	r	1	NAG	O5-C5-C6-O6
8	X	5	MAN	O5-C5-C6-O6
9	o	4	MAN	C4-C5-C6-O6
8	O	2	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	o	2	NAG	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
7	M	1	NAG	C1-C2-N2-C7
7	P	2	NAG	C1-C2-N2-C7
7	T	1	NAG	C1-C2-N2-C7
7	W	2	NAG	C1-C2-N2-C7
7	m	1	NAG	C1-C2-N2-C7
7	p	2	NAG	C1-C2-N2-C7
8	O	1	NAG	C1-C2-N2-C7
8	S	2	NAG	C1-C2-N2-C7
8	Z	2	NAG	C1-C2-N2-C7
8	s	2	NAG	C1-C2-N2-C7
9	o	1	NAG	C1-C2-N2-C7
9	o	3	BMA	C4-C5-C6-O6
7	P	2	NAG	C3-C2-N2-C7
7	T	1	NAG	C3-C2-N2-C7
7	p	2	NAG	C3-C2-N2-C7
8	S	2	NAG	C3-C2-N2-C7
8	X	2	NAG	C3-C2-N2-C7
8	Z	2	NAG	C3-C2-N2-C7
8	s	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C3-C2-N2-C7
9	V	3	BMA	C4-C5-C6-O6
8	s	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	W	1	NAG	C1-C2-N2-C7
7	p	1	NAG	C1-C2-N2-C7
8	X	1	NAG	C1-C2-N2-C7
7	M	1	NAG	C3-C2-N2-C7
7	P	1	NAG	C3-C2-N2-C7
7	W	1	NAG	C3-C2-N2-C7
7	W	2	NAG	C3-C2-N2-C7
7	m	1	NAG	C3-C2-N2-C7
7	p	1	NAG	C3-C2-N2-C7
8	O	1	NAG	C3-C2-N2-C7
9	o	1	NAG	C3-C2-N2-C7
8	q	5	MAN	C4-C5-C6-O6
9	V	4	MAN	C4-C5-C6-O6
8	s	1	NAG	O5-C5-C6-O6
8	O	4	MAN	C4-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6

There are no ring outliers.

26 monomers are involved in 27 short contacts:

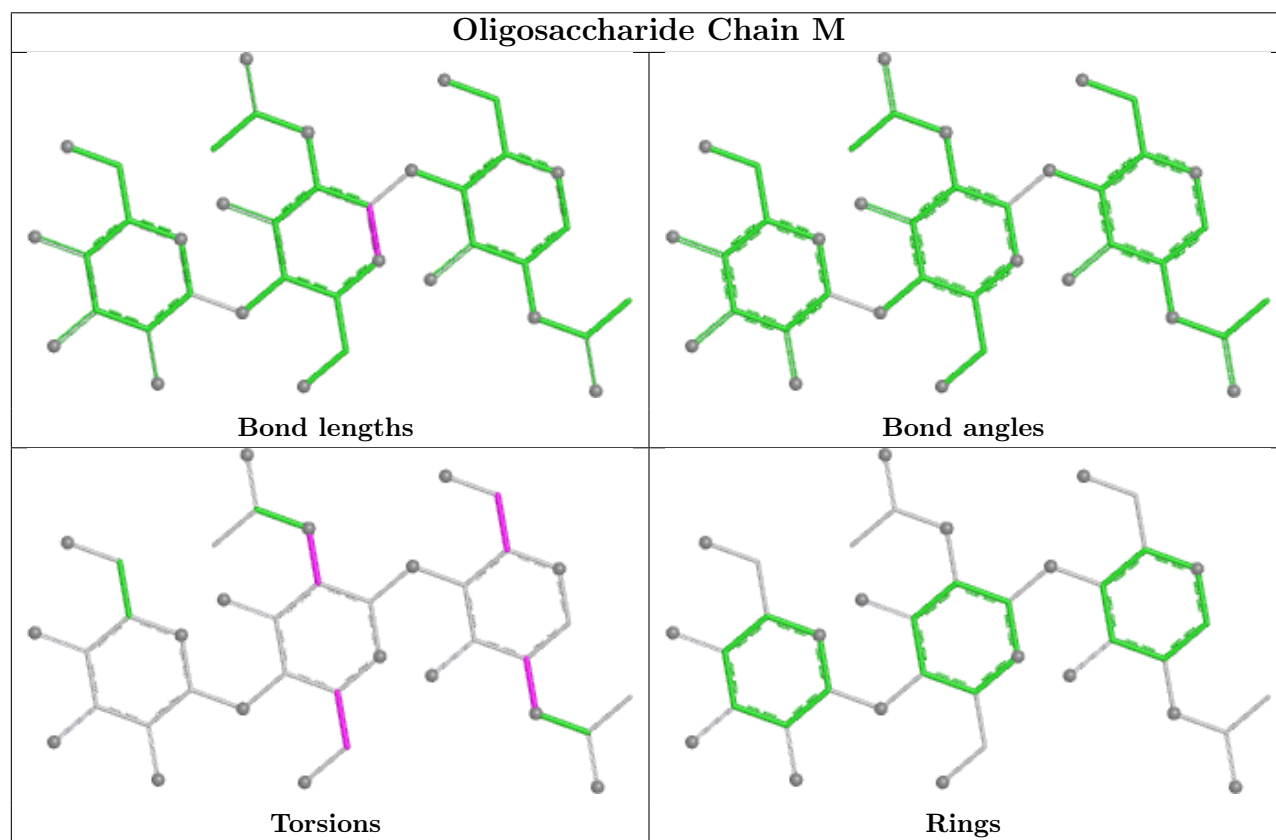
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	5	MAN	1	0
8	S	1	NAG	1	0
9	o	4	MAN	1	0
8	s	1	NAG	1	0
7	n	3	BMA	1	0
8	s	3	BMA	1	0
7	N	1	NAG	1	0
9	V	4	MAN	1	0
8	O	3	BMA	1	0
8	Z	4	MAN	1	0
9	V	3	BMA	1	0
8	O	4	MAN	1	0
7	p	1	NAG	1	0
7	U	1	NAG	2	0
7	P	1	NAG	1	0
8	S	4	MAN	1	0
8	s	4	MAN	1	0
7	U	3	BMA	1	0
7	m	2	NAG	2	0
7	W	1	NAG	1	0
7	T	2	NAG	1	0

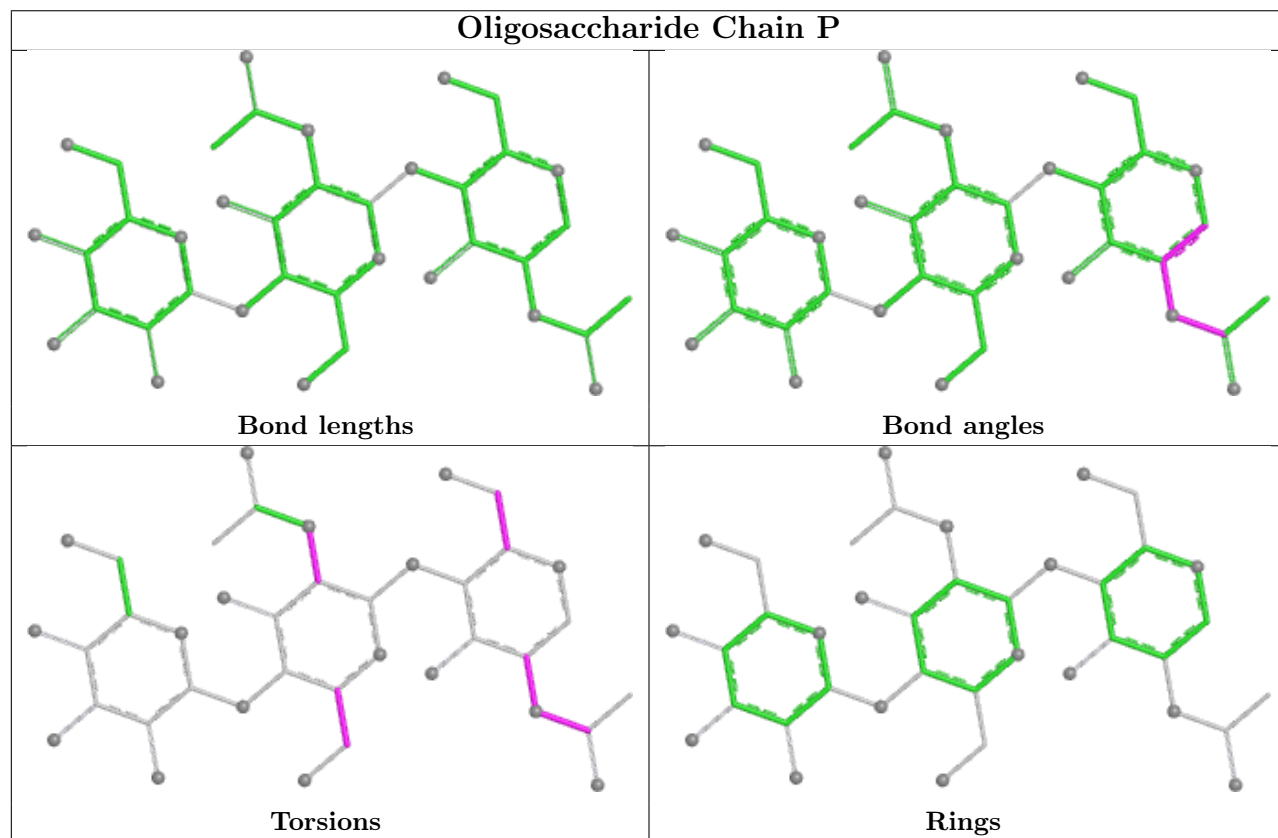
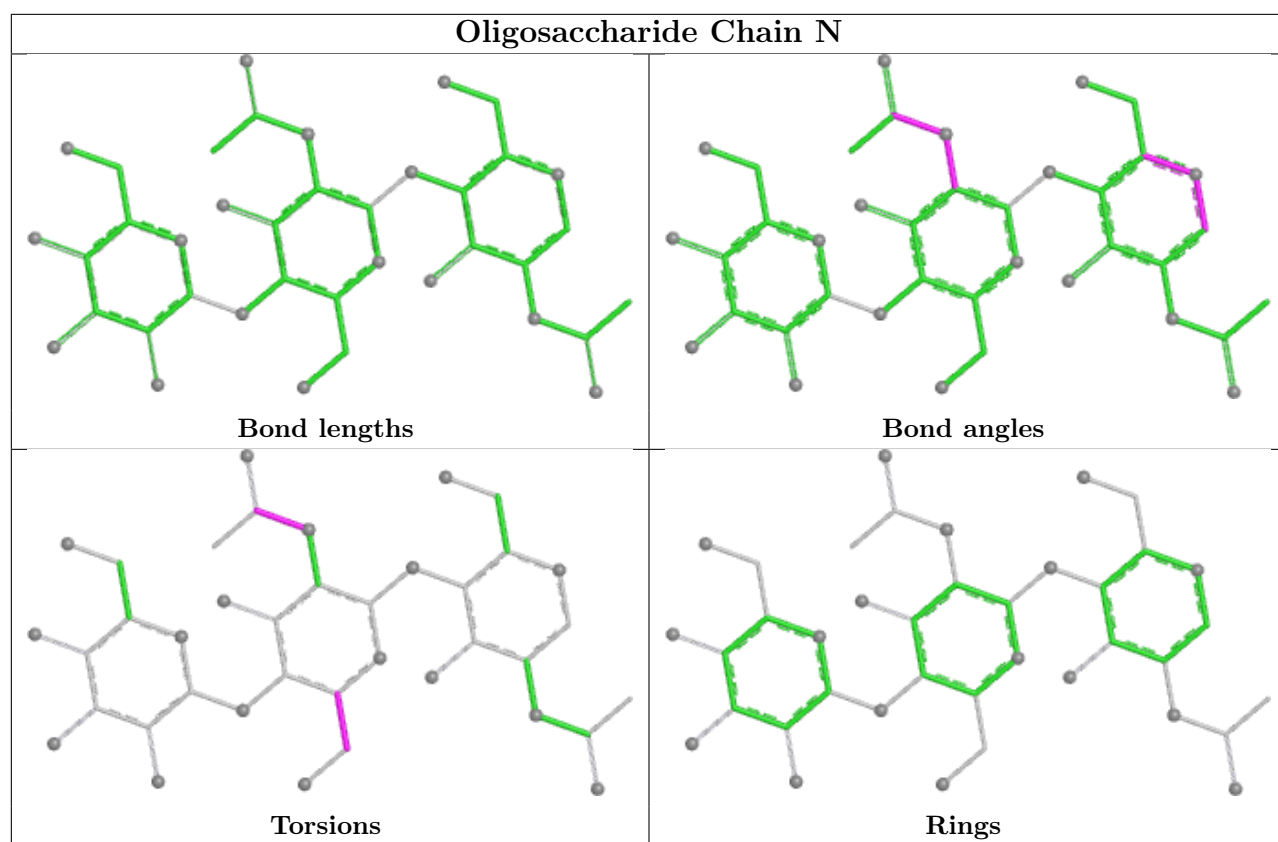
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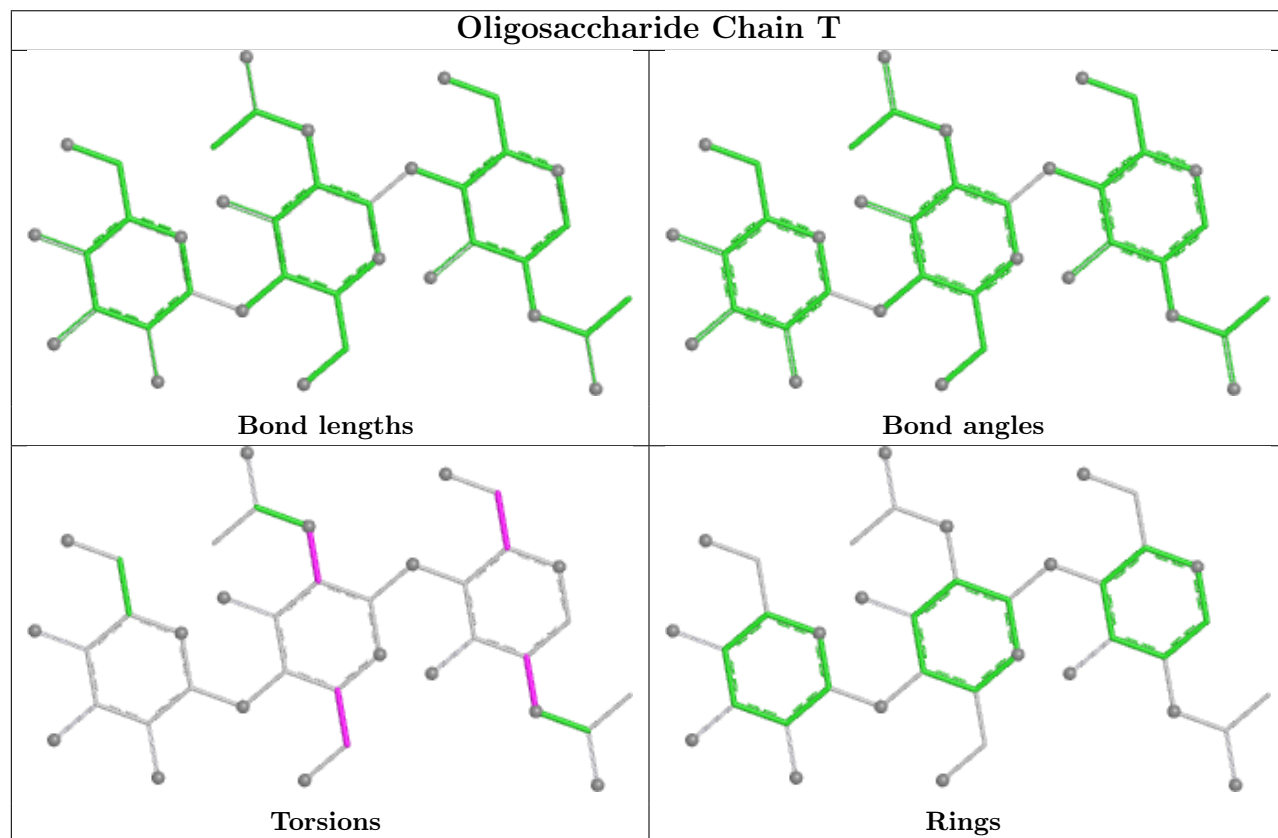
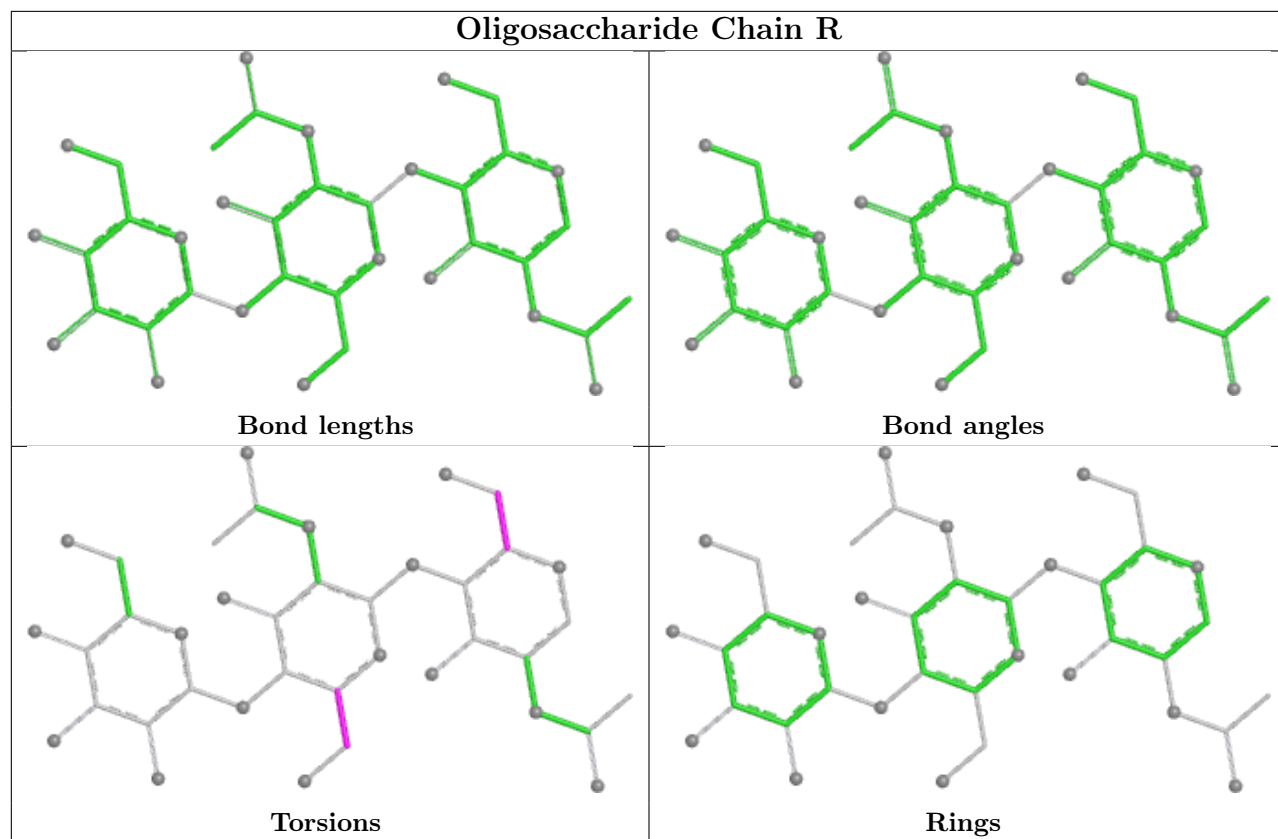
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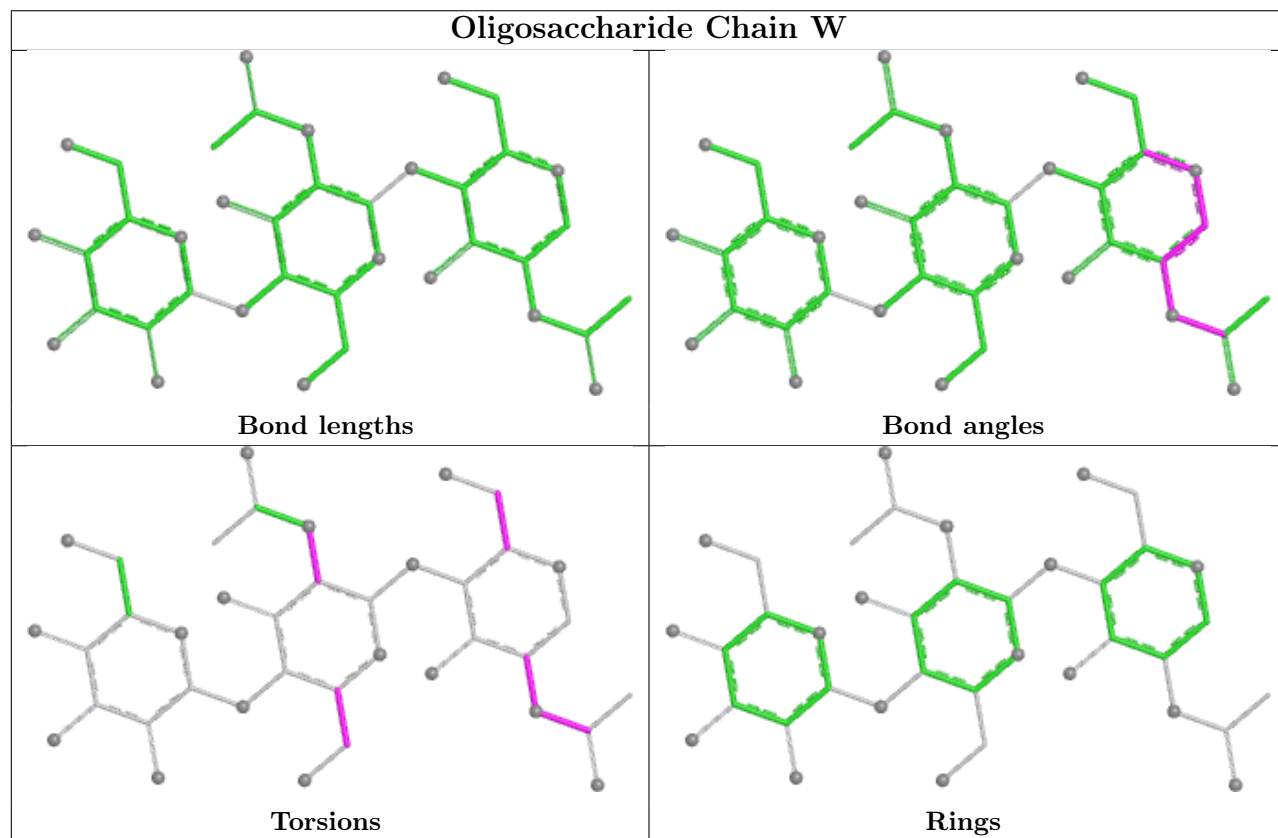
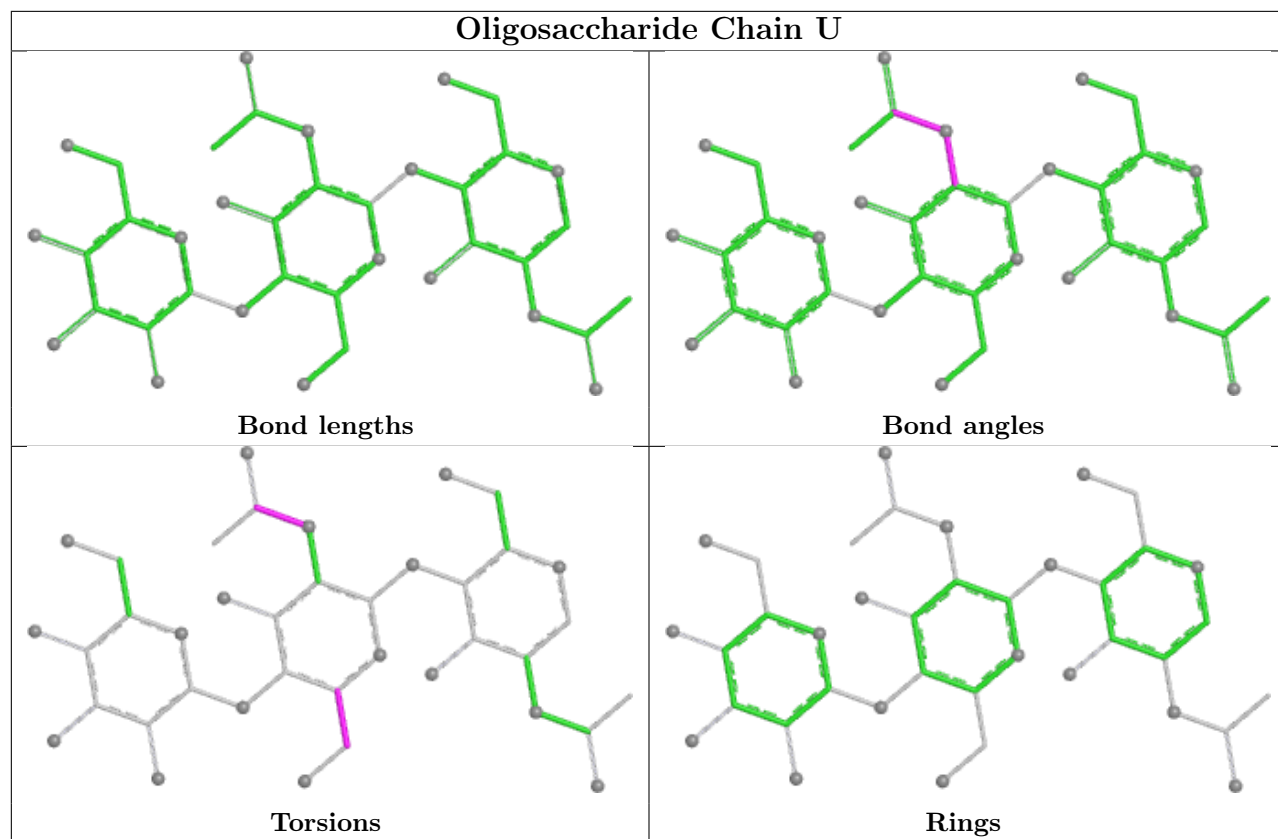
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	3	BMA	1	0
7	M	2	NAG	2	0
8	Z	3	BMA	1	0
9	o	3	BMA	2	0
8	Q	4	MAN	1	0

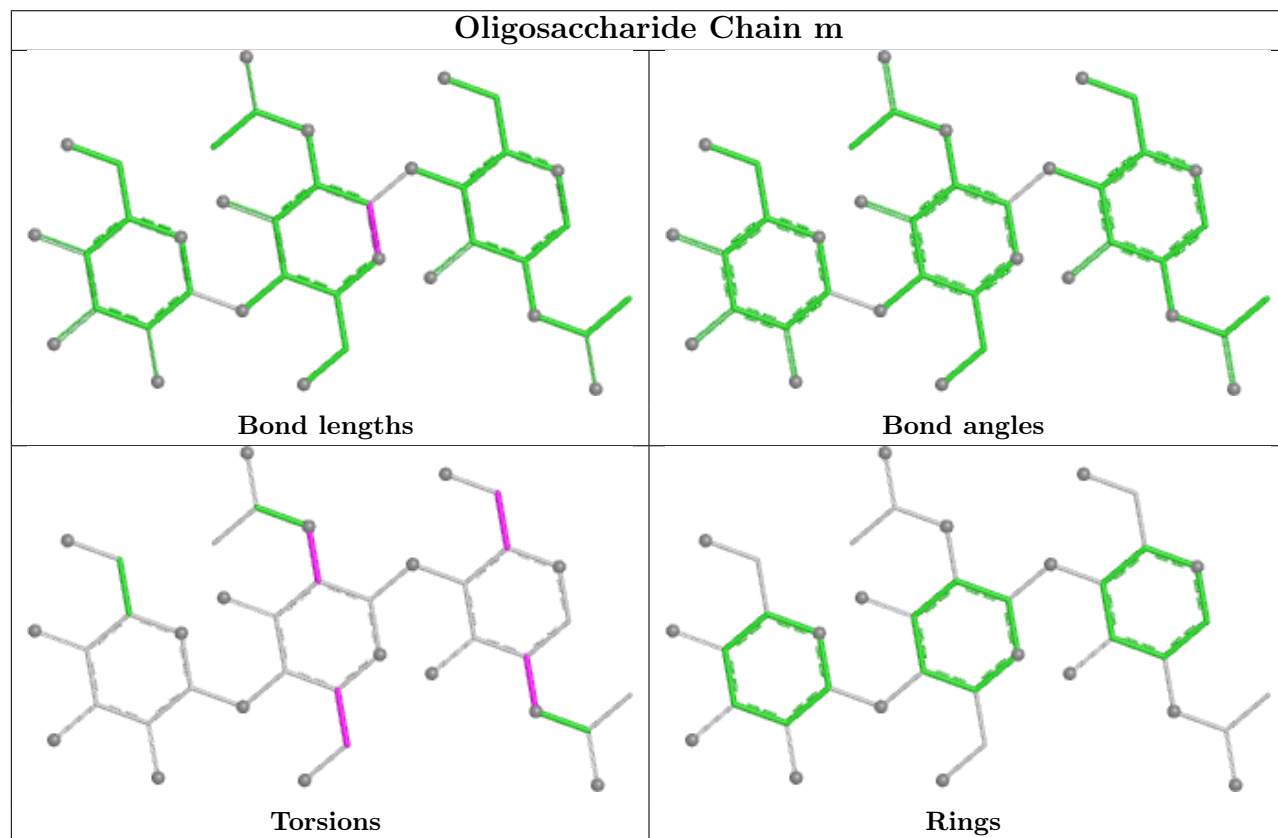
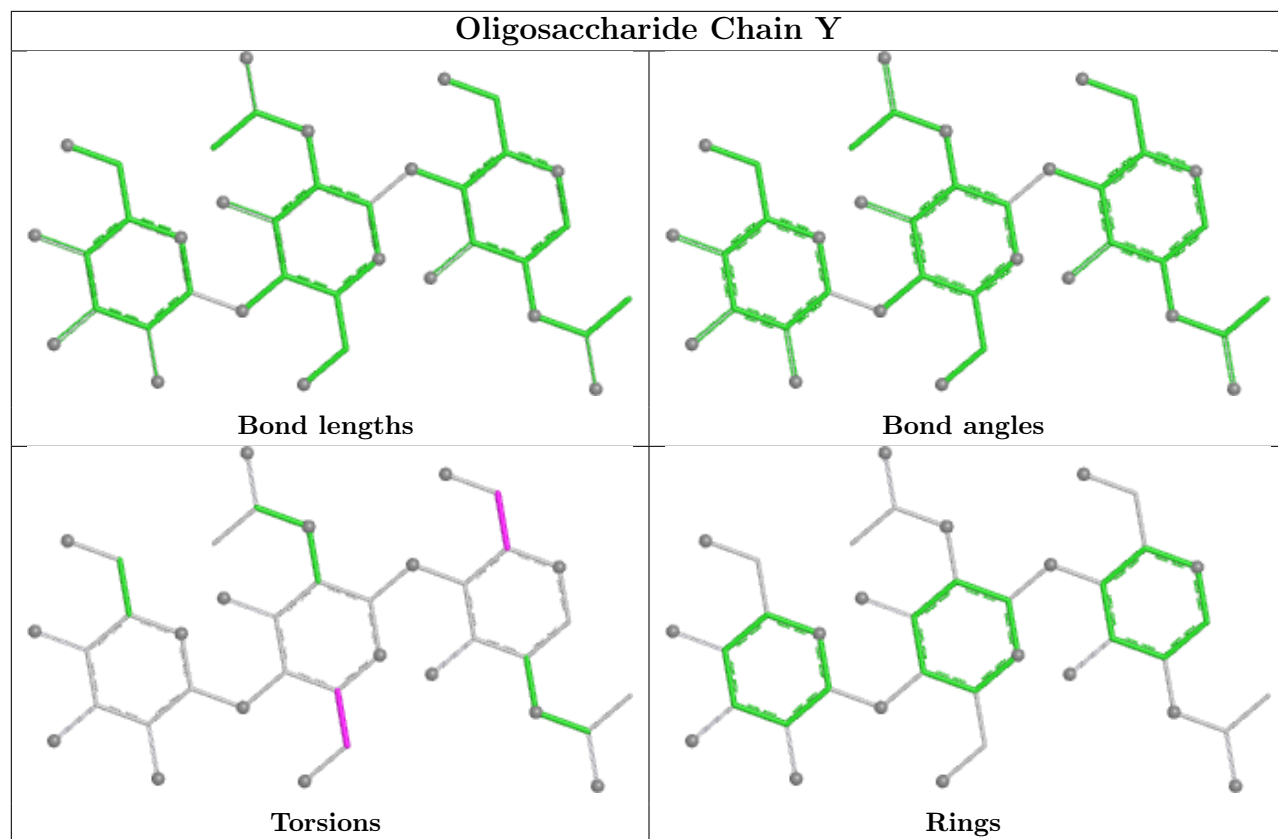
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

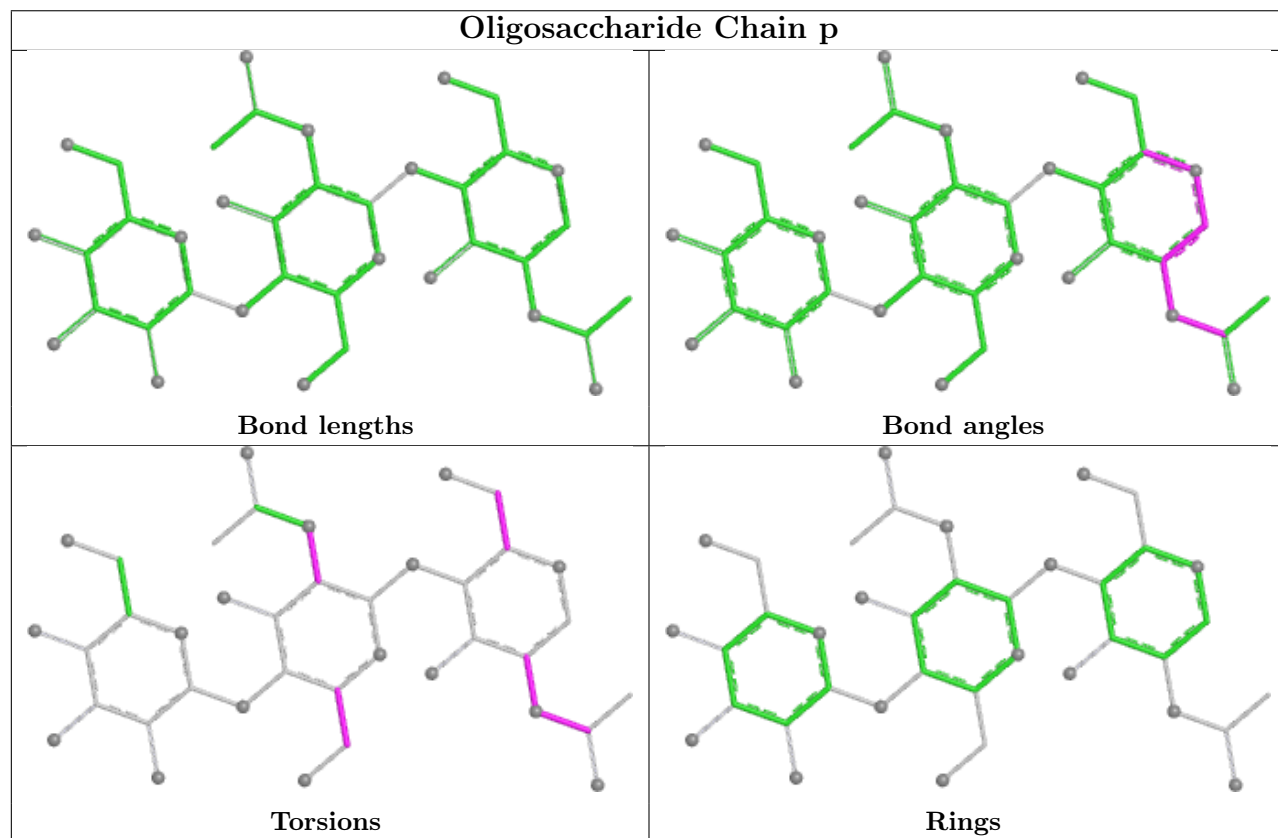
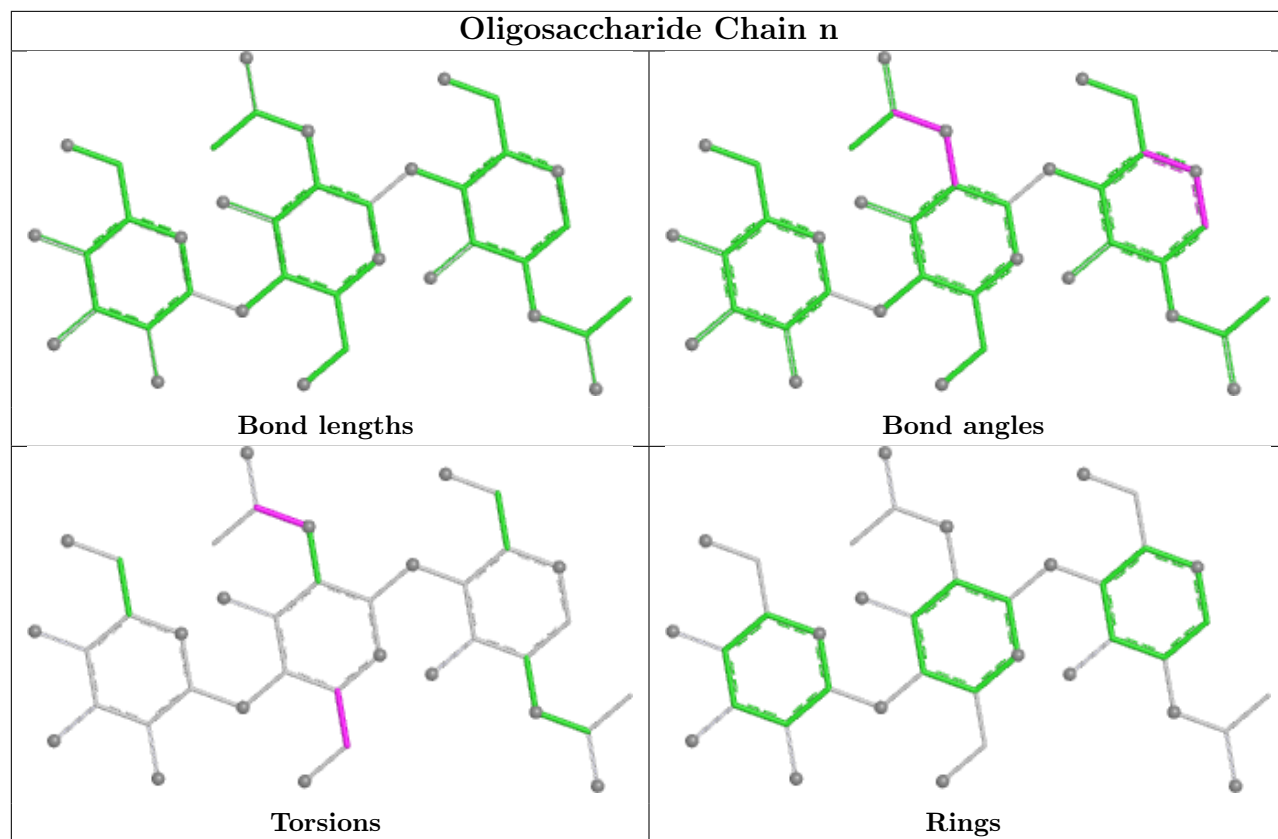


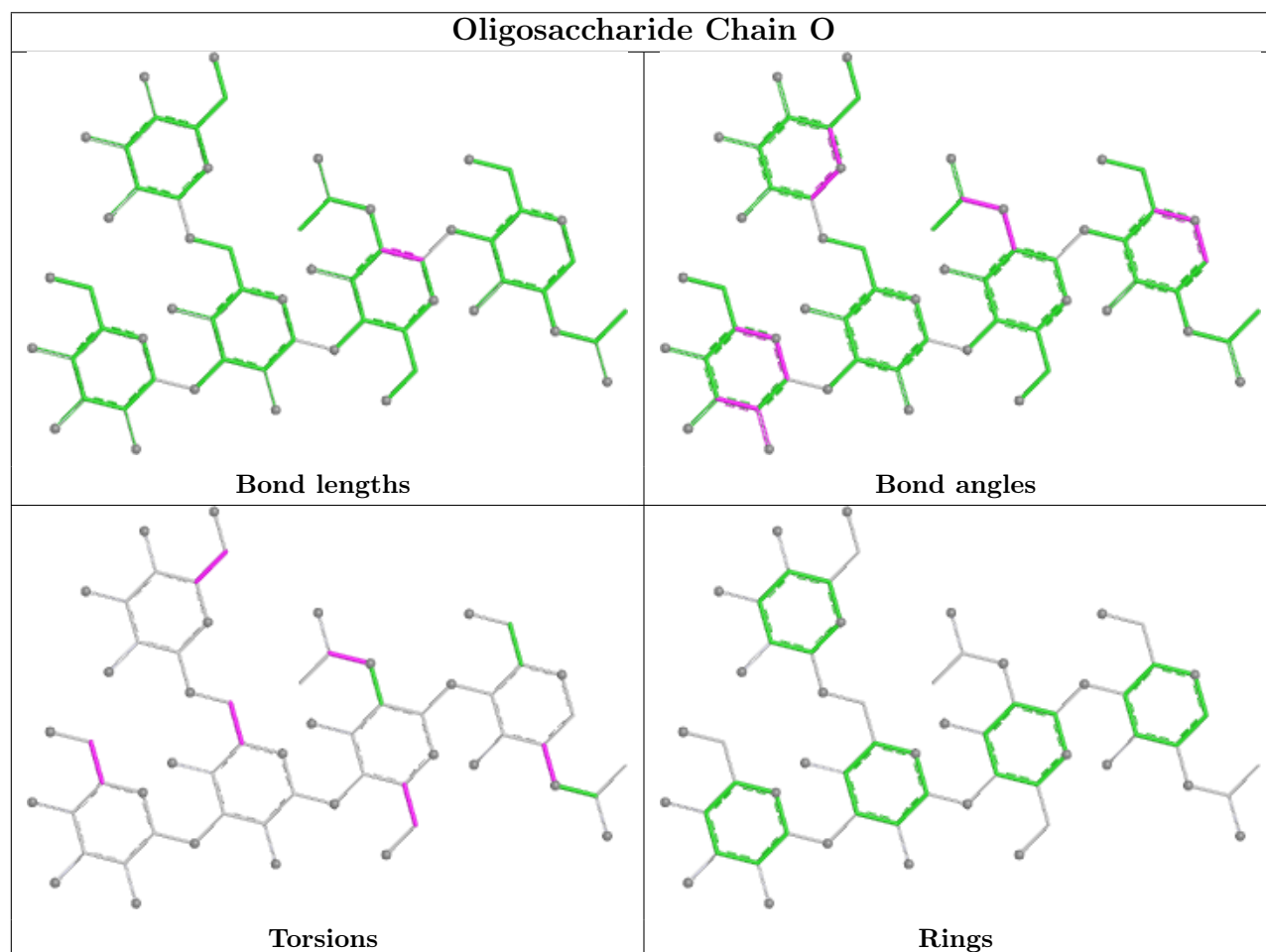
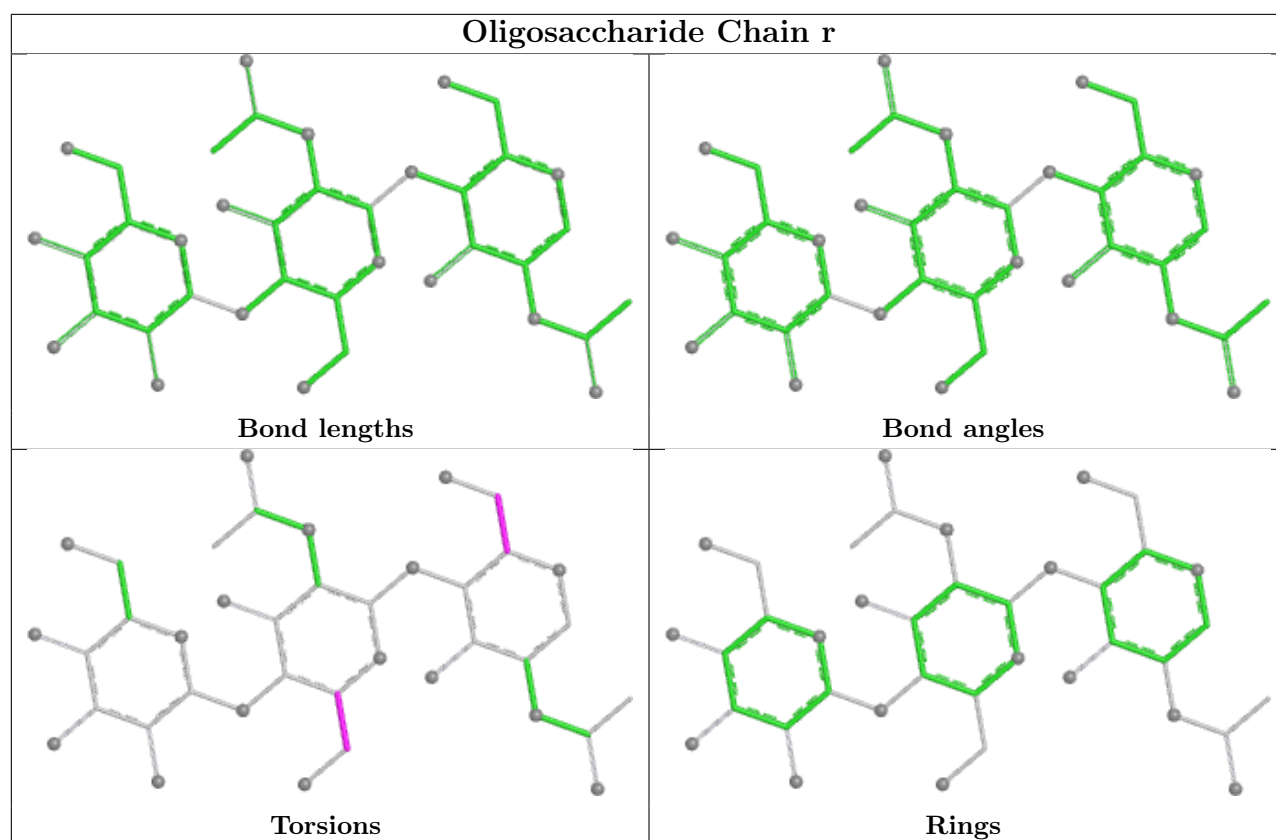


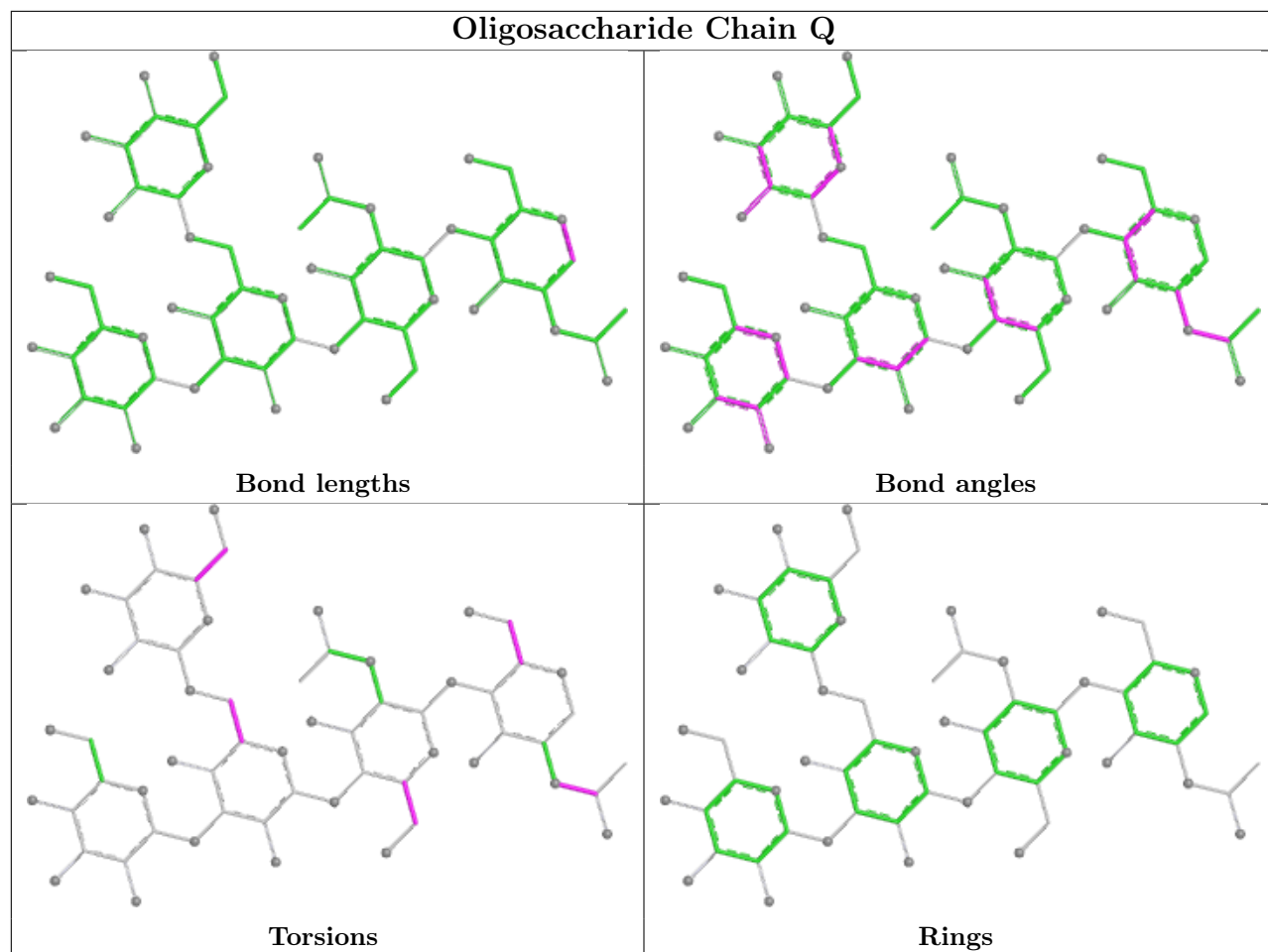


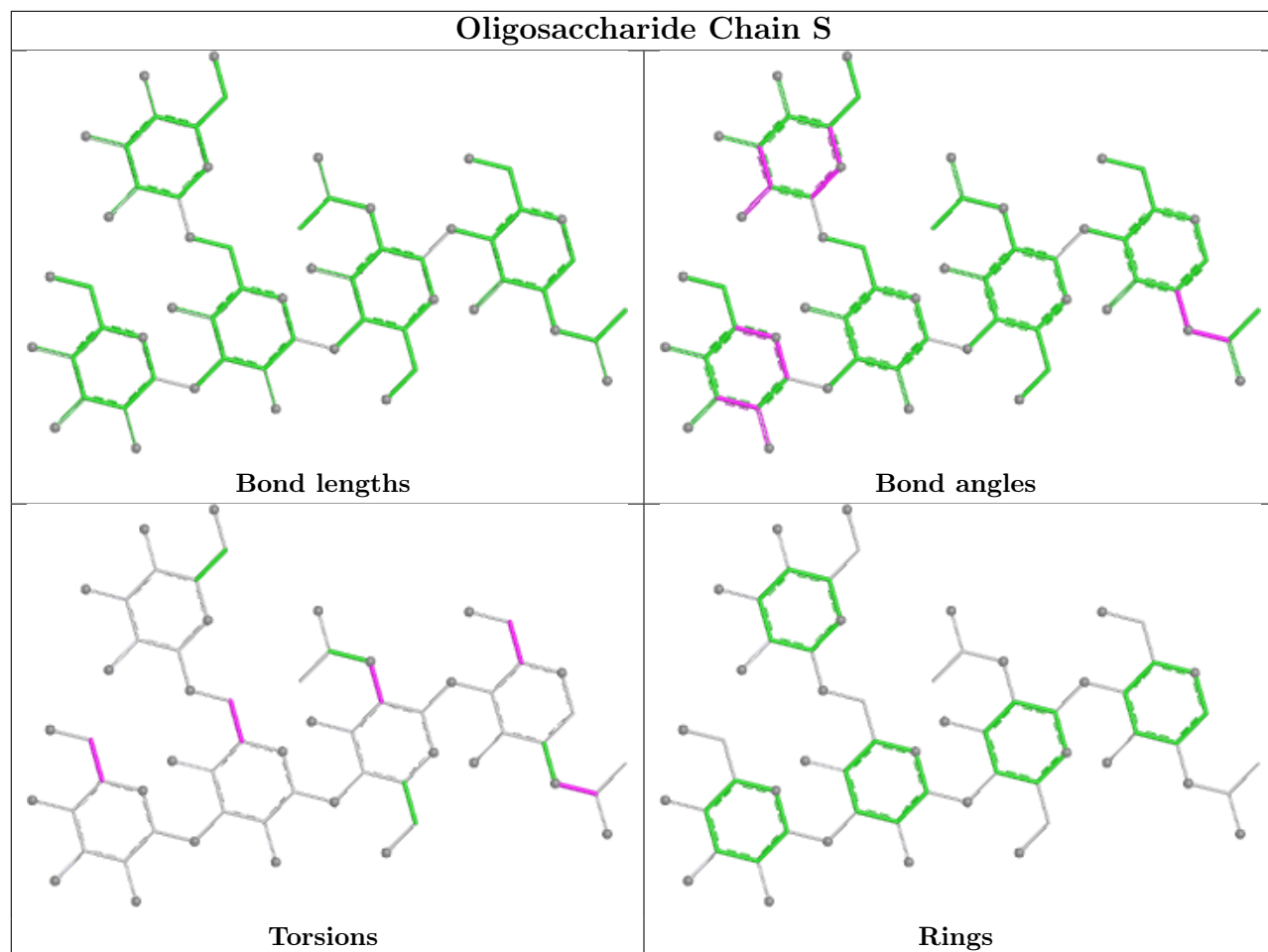


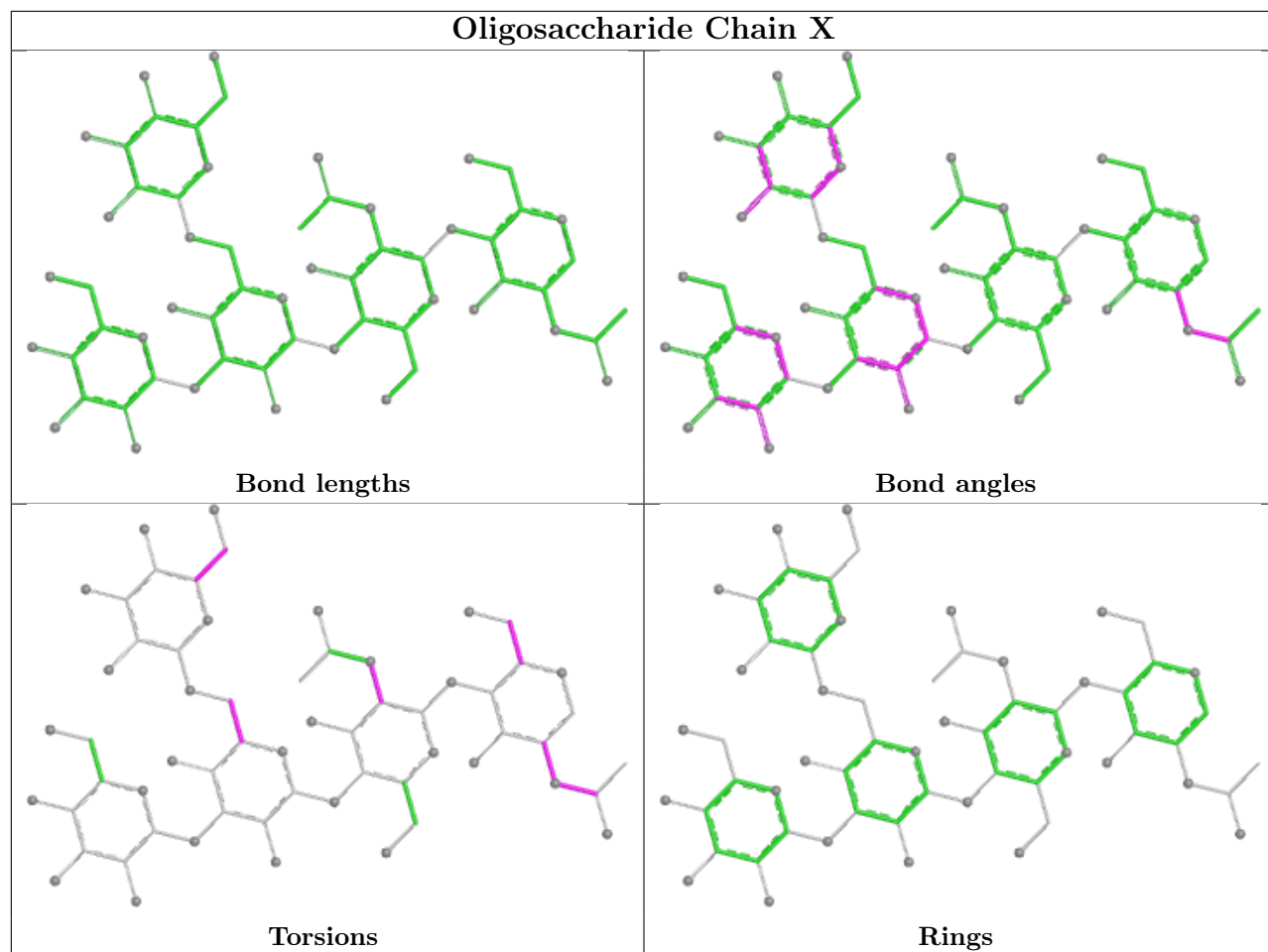


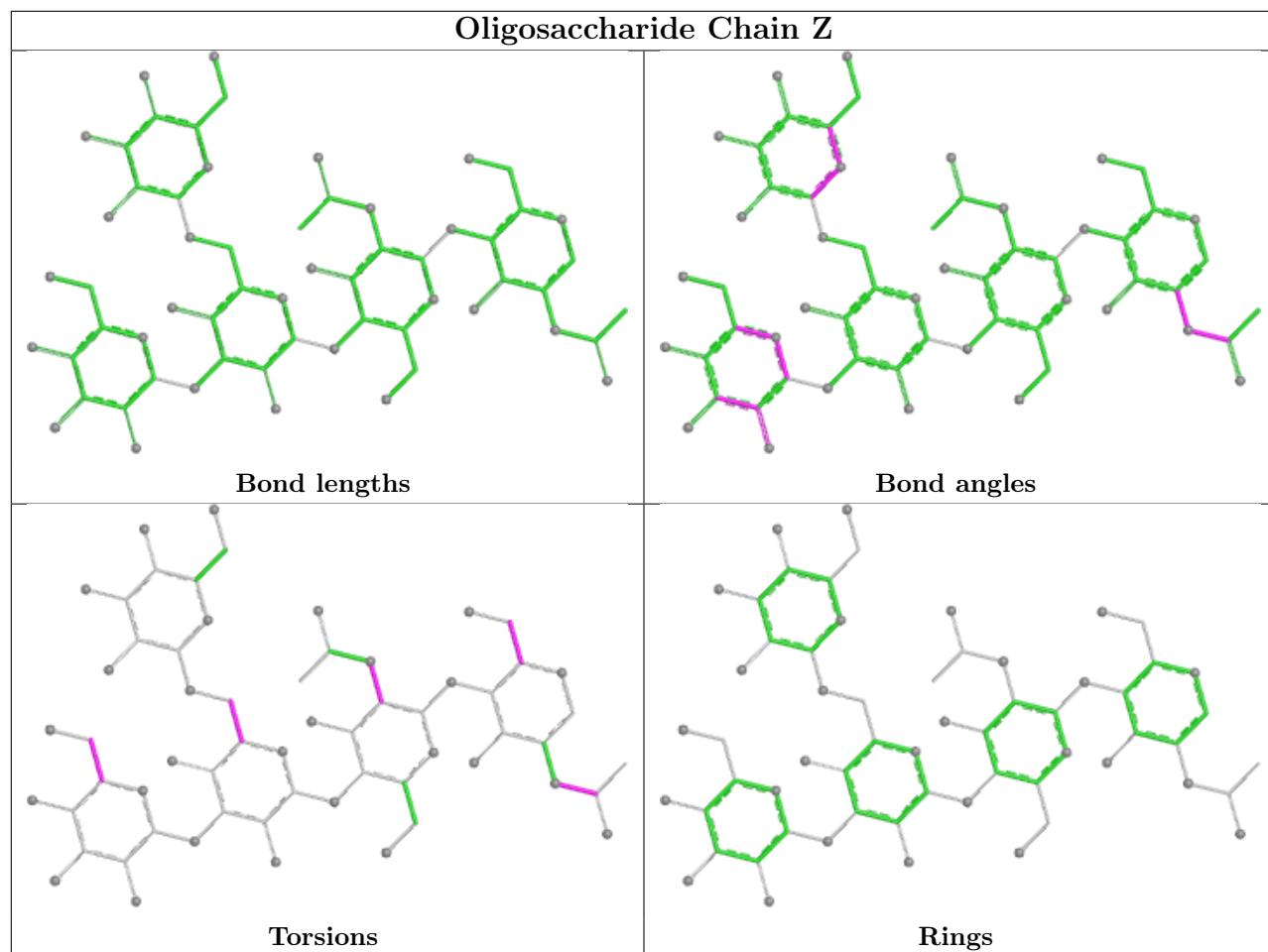


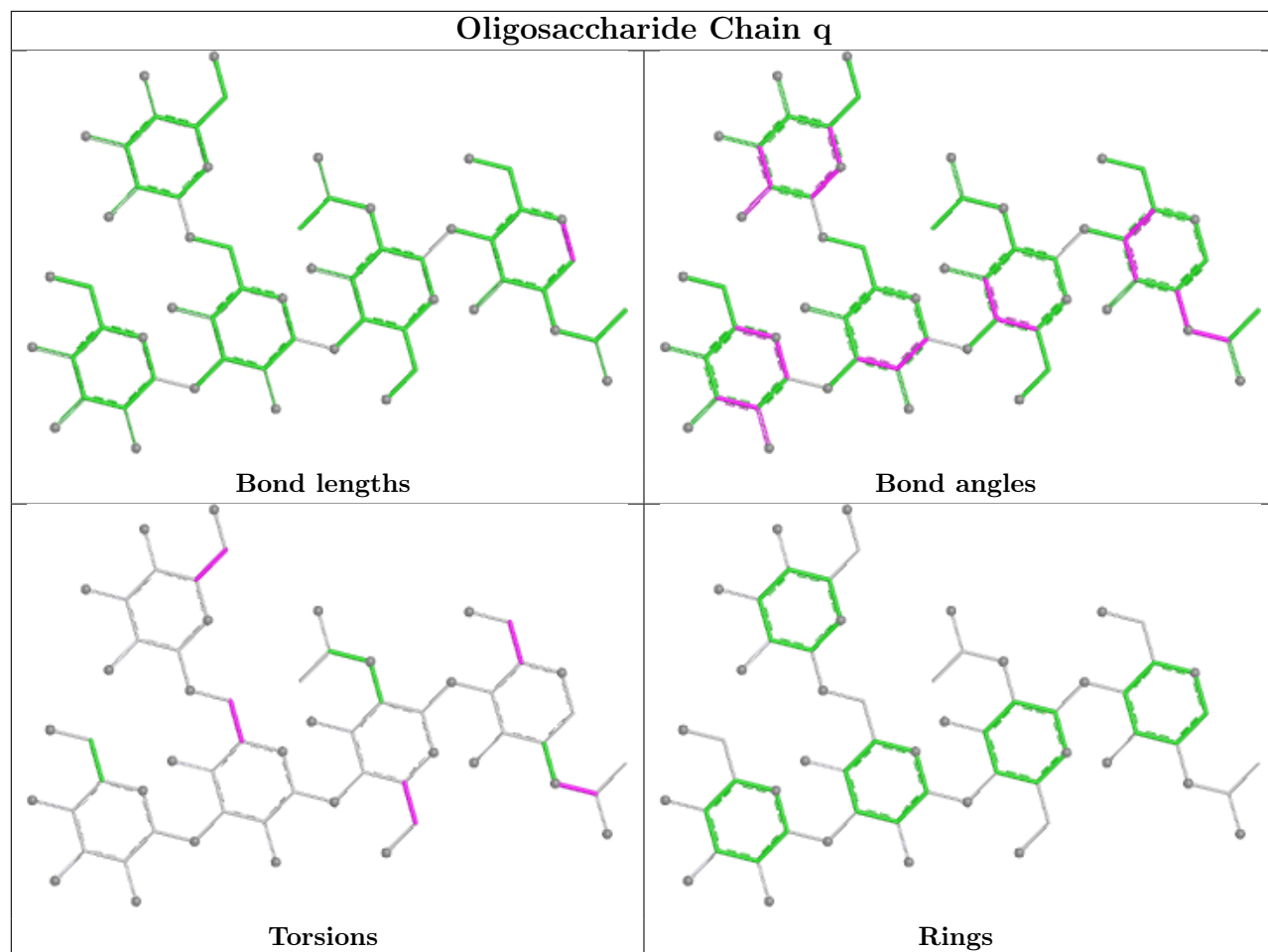


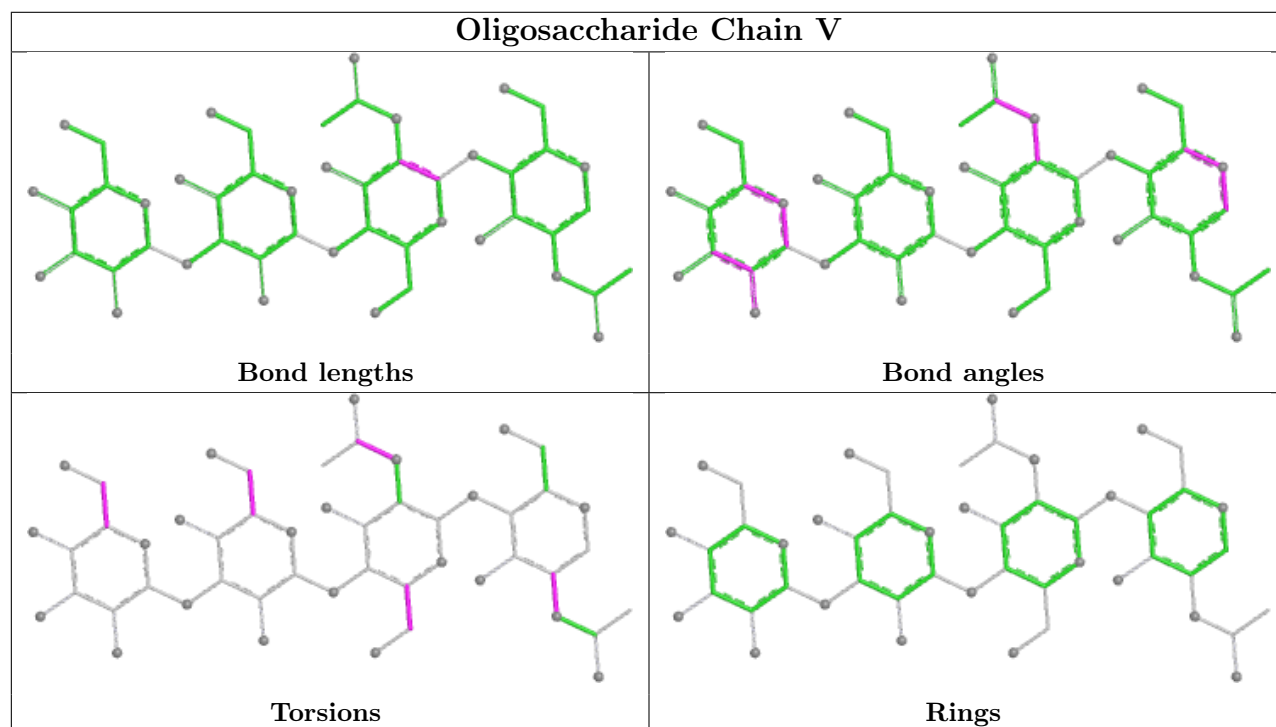
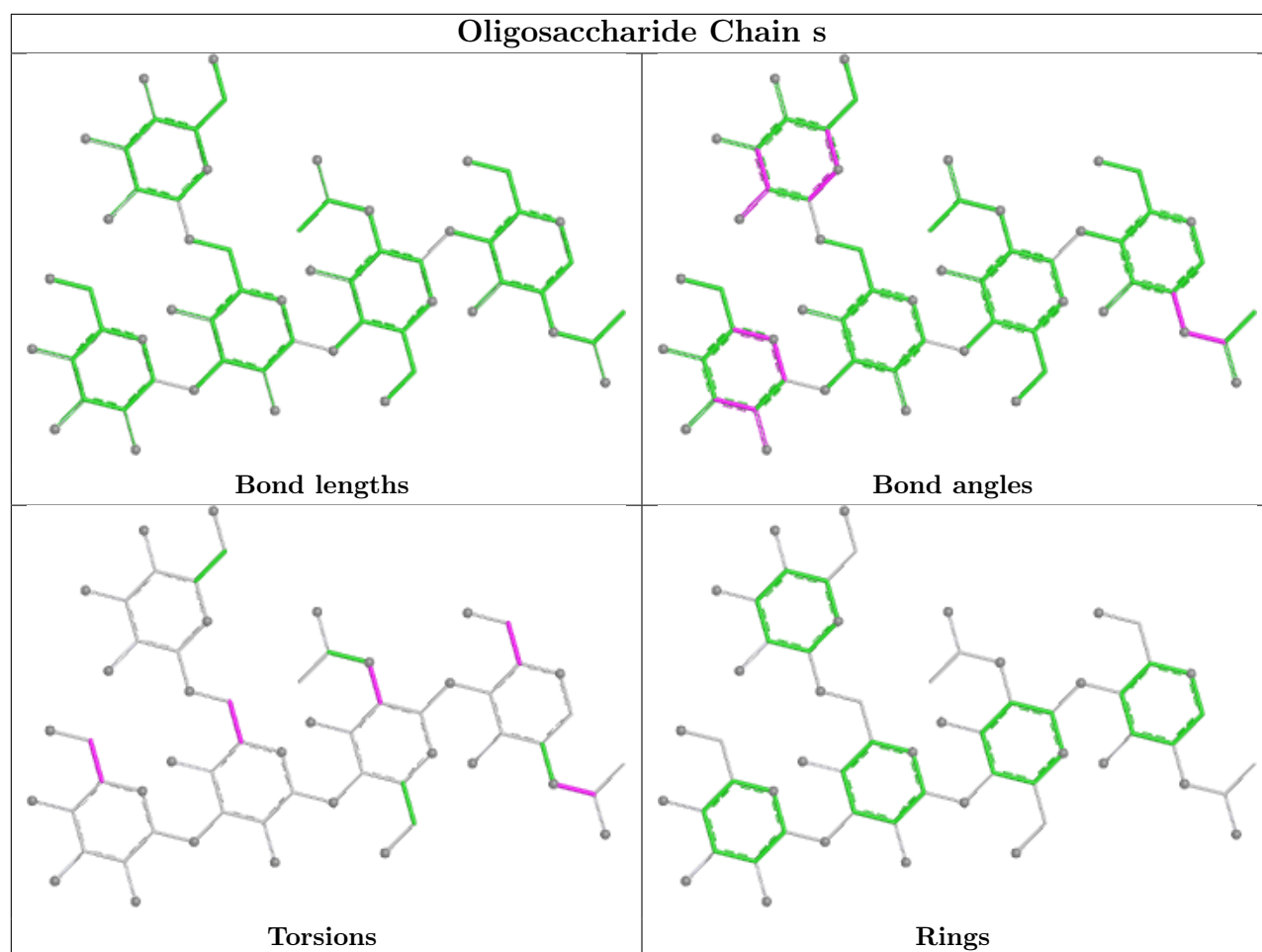


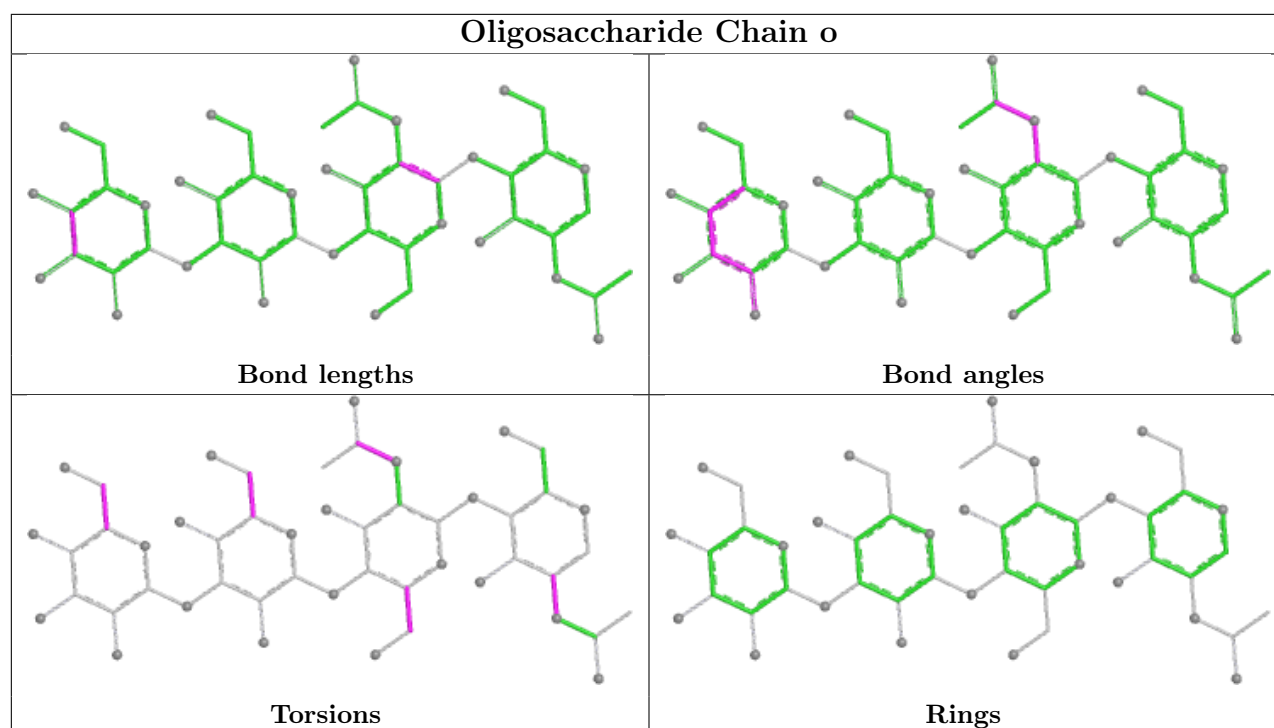












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
11	MAN	i	301	-	11,11,12	0.94	1 (9%)	15,15,17	1.23	2 (13%)
10	NAG	D	301	2	14,14,15	0.44	0	17,19,21	0.37	0
10	NAG	F	301	2	14,14,15	0.43	0	17,19,21	0.38	0
10	NAG	B	301	2	14,14,15	0.45	0	17,19,21	0.38	0
11	MAN	e	301	-	11,11,12	0.94	1 (9%)	15,15,17	1.22	2 (13%)

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
11	MAN	i	301	-	-	1/2/19/22	0/1/1/1
10	NAG	D	301	2	-	0/6/23/26	0/1/1/1
10	NAG	F	301	2	-	0/6/23/26	0/1/1/1
10	NAG	B	301	2	-	0/6/23/26	0/1/1/1
11	MAN	e	301	-	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	e	301	MAN	O5-C1	-2.08	1.40	1.43
11	i	301	MAN	O5-C1	-2.01	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	i	301	MAN	C1-O5-C5	3.49	116.86	112.19
11	e	301	MAN	C1-O5-C5	3.43	116.78	112.19
11	i	301	MAN	O2-C2-C3	-2.10	105.79	110.15
11	e	301	MAN	O2-C2-C3	-2.09	105.83	110.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	i	301	MAN	O5-C5-C6-O6
11	e	301	MAN	O5-C5-C6-O6

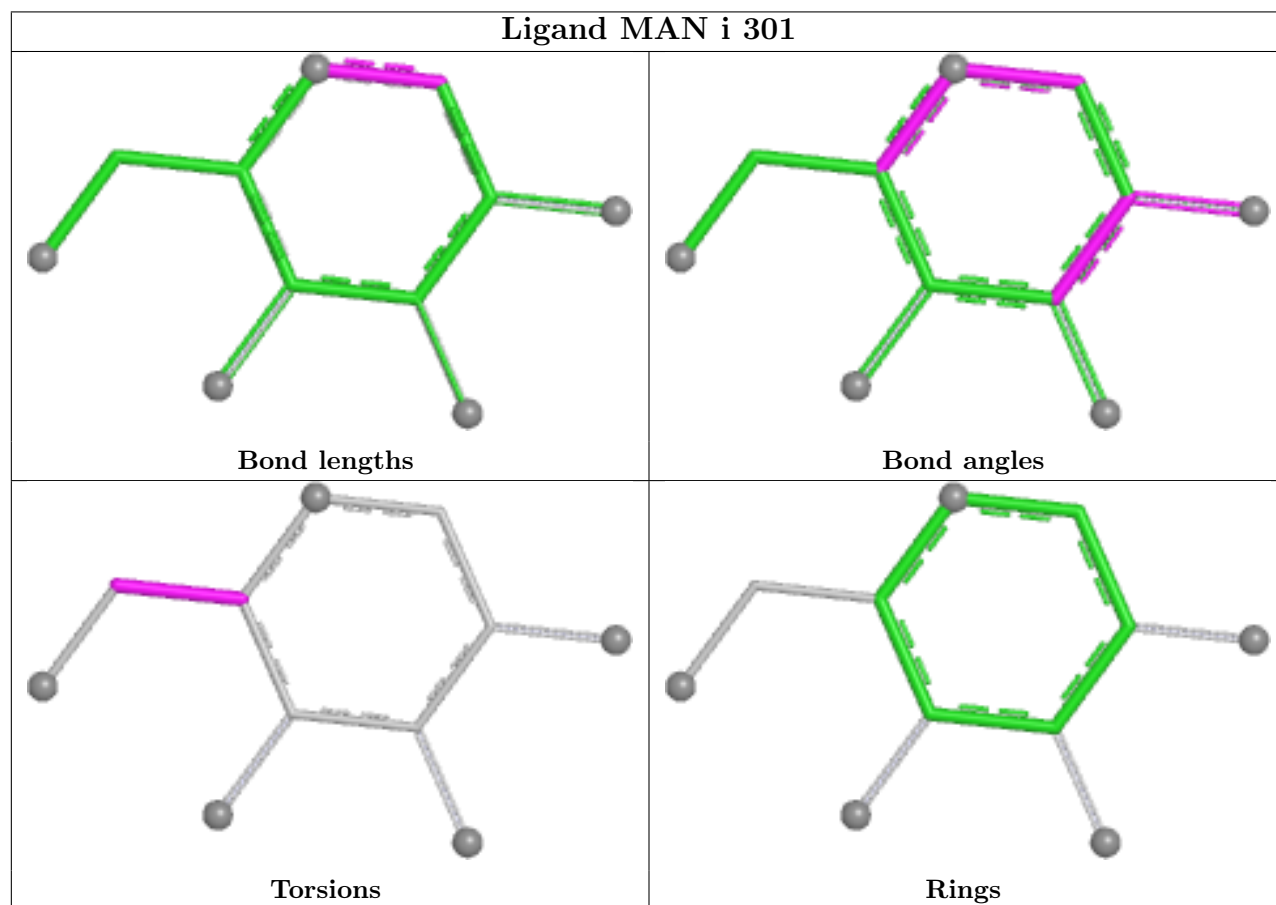
There are no ring outliers.

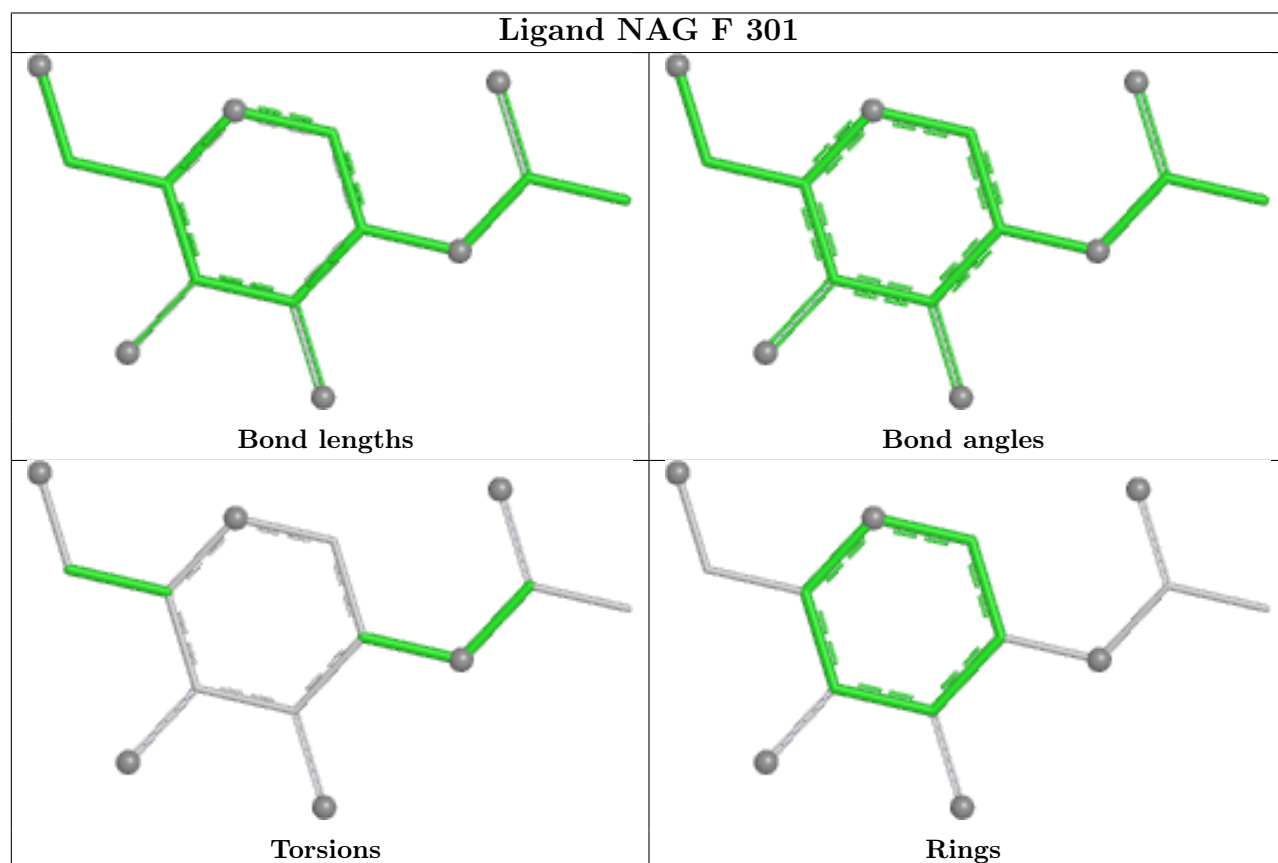
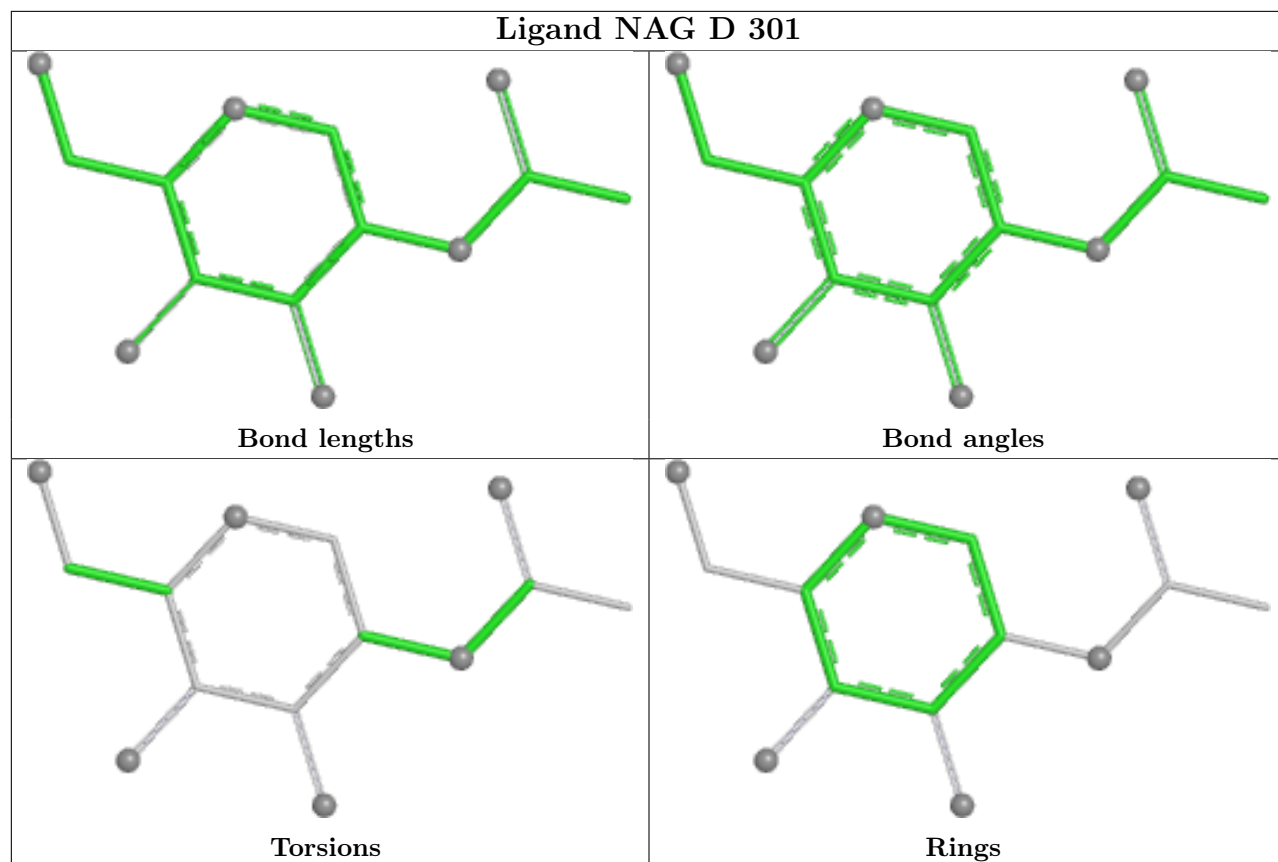
2 monomers are involved in 2 short contacts:

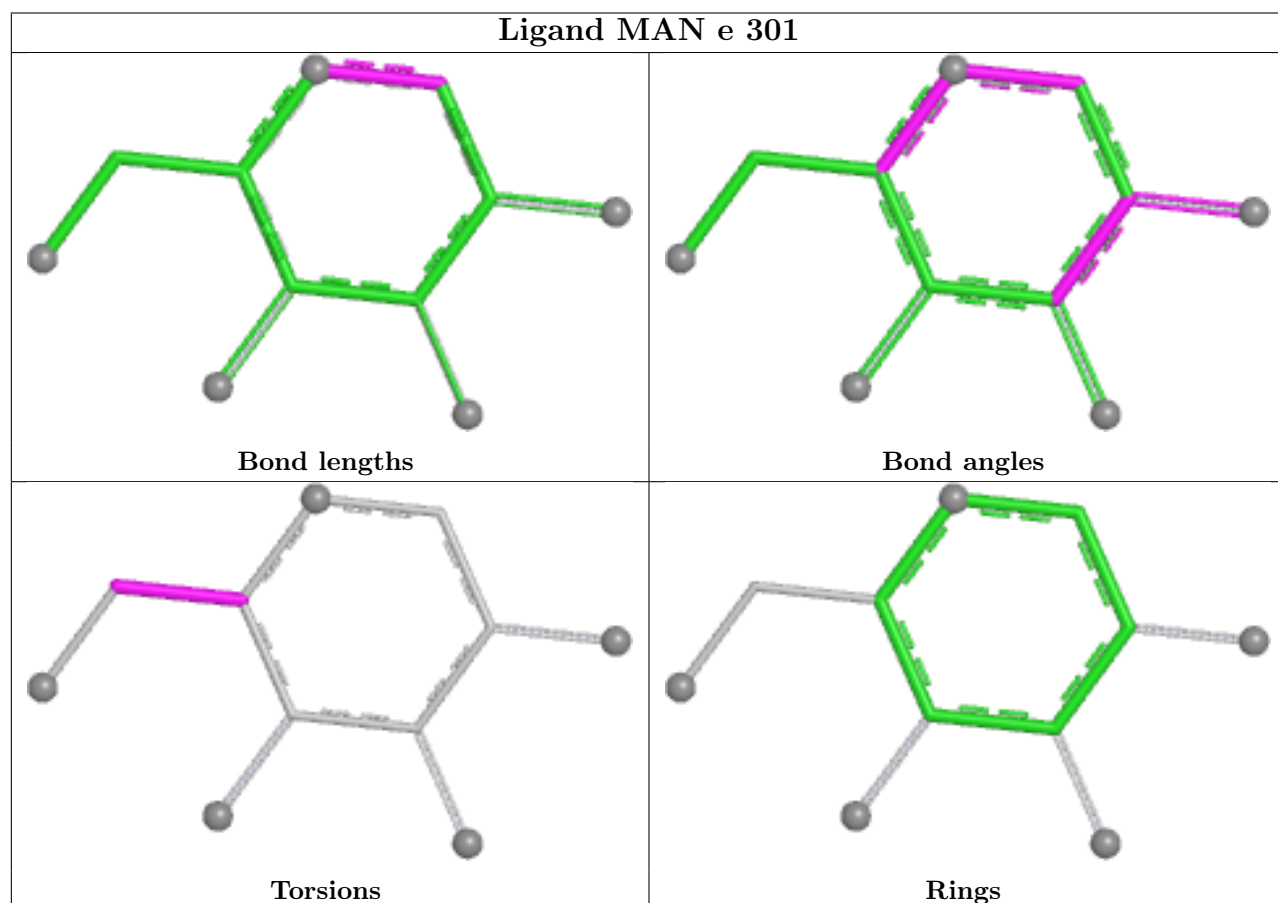
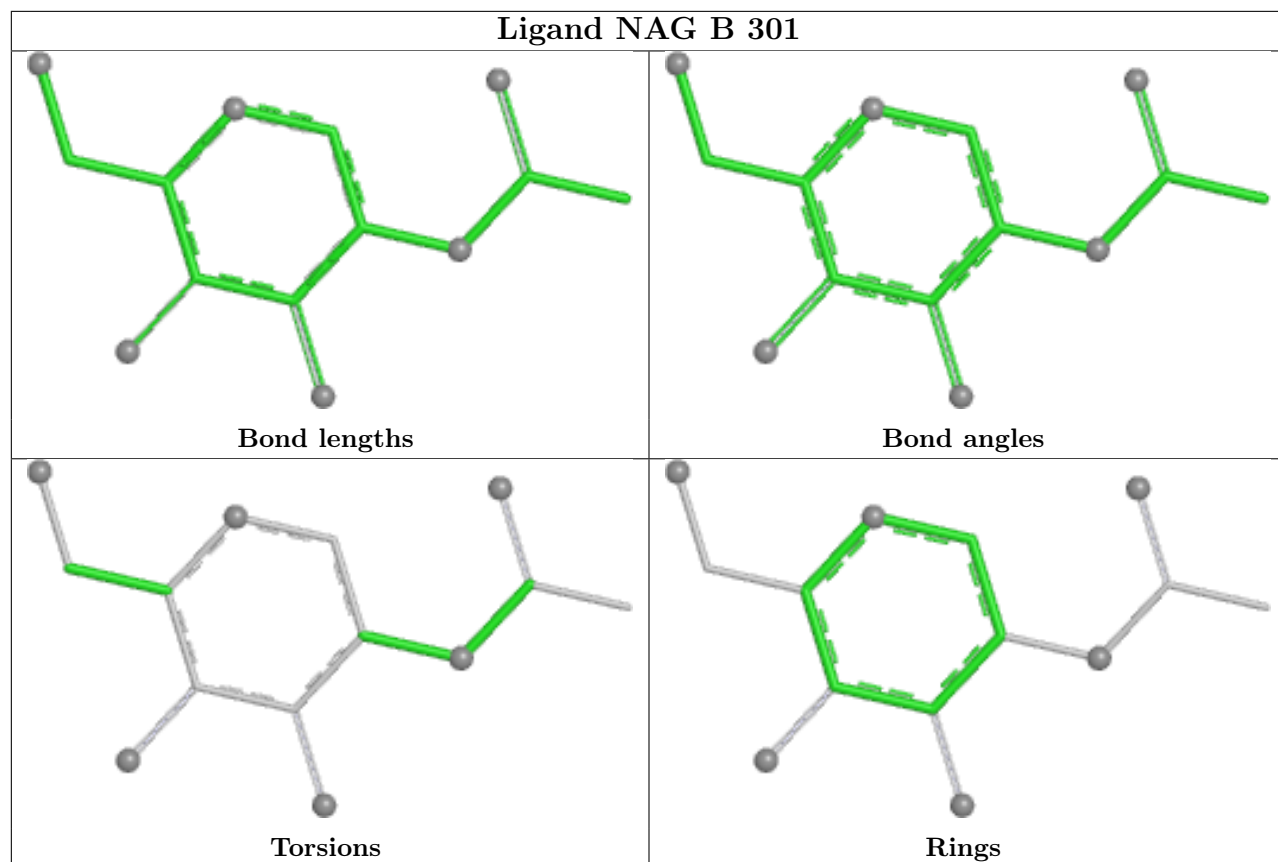
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	i	301	MAN	1	0
11	e	301	MAN	1	0

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

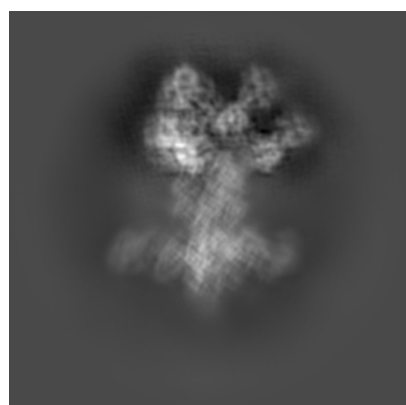
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70607. These allow visual inspection of the internal detail of the map and identification of artifacts.

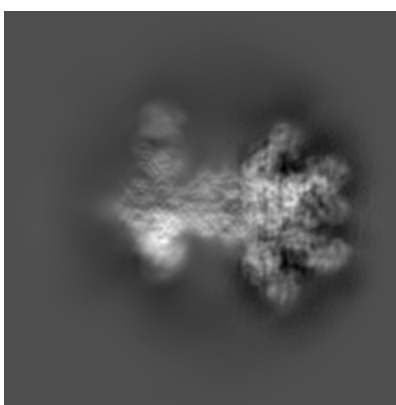
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

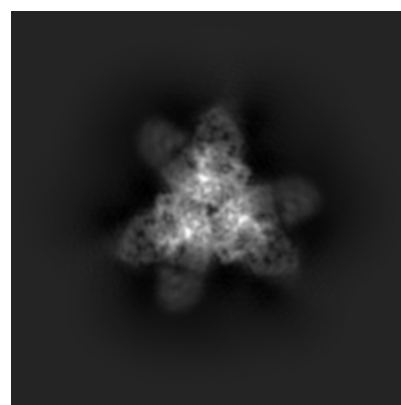
6.1.1 Primary map



X



Y

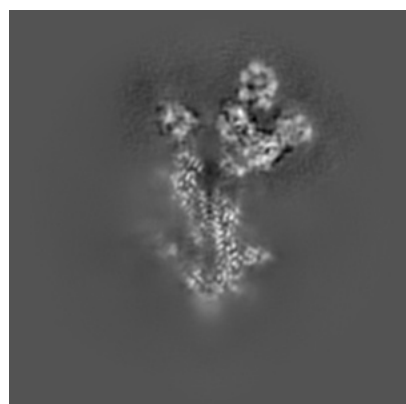


Z

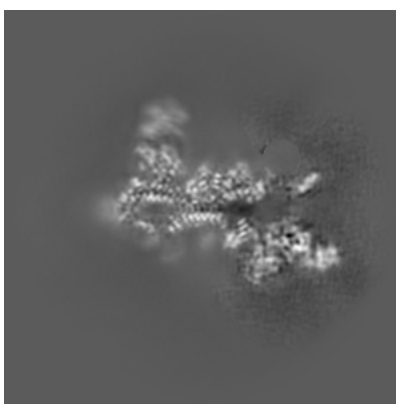
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

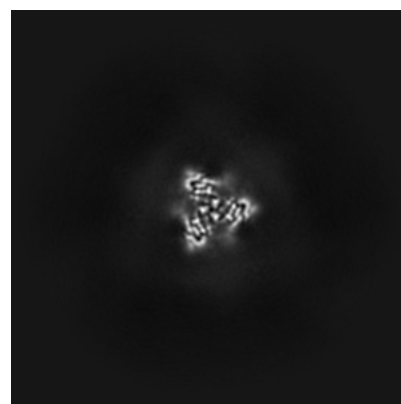
6.2.1 Primary map



X Index: 210



Y Index: 210

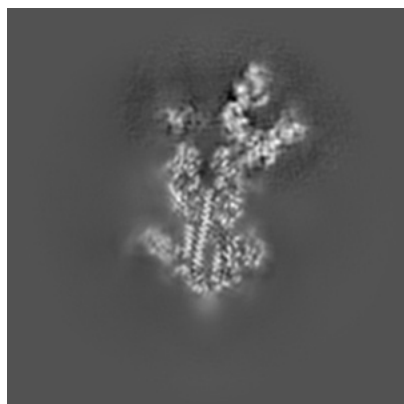


Z Index: 210

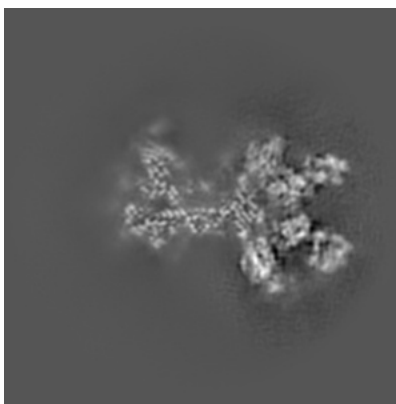
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

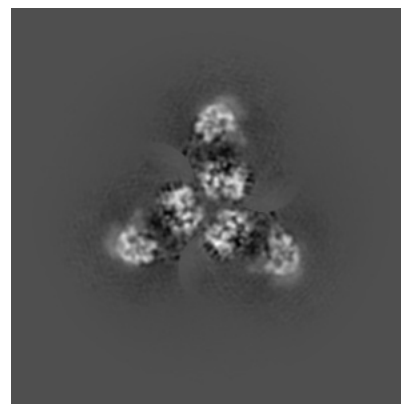
6.3.1 Primary map



X Index: 203



Y Index: 192

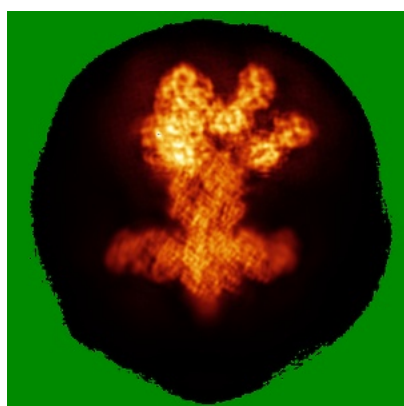


Z Index: 294

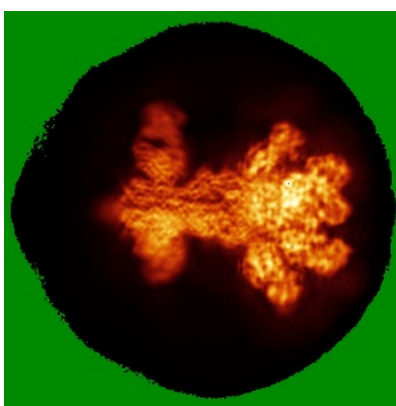
The images above show the largest variance slices of the map in three orthogonal directions.

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

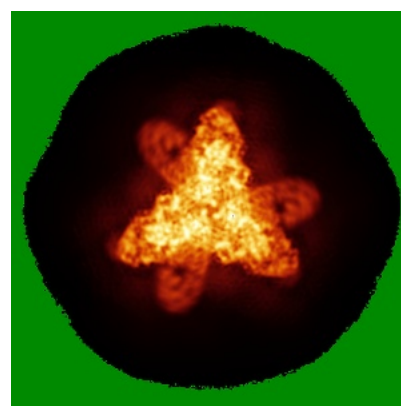
6.4.1 Primary map



X



Y



Z

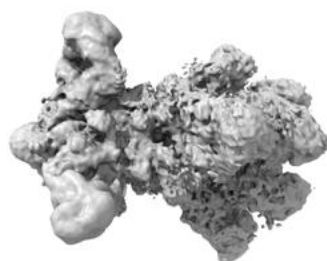
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

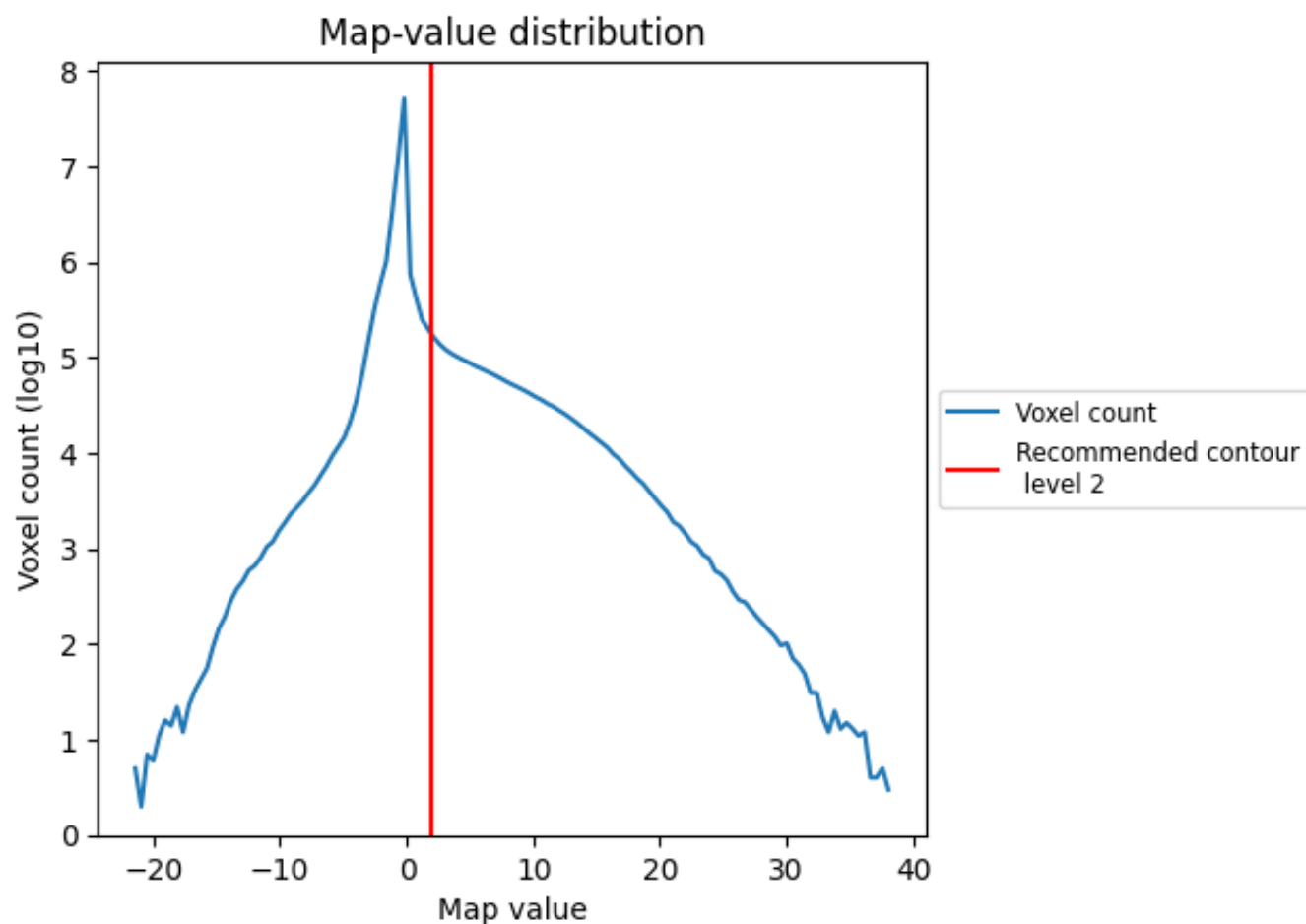
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

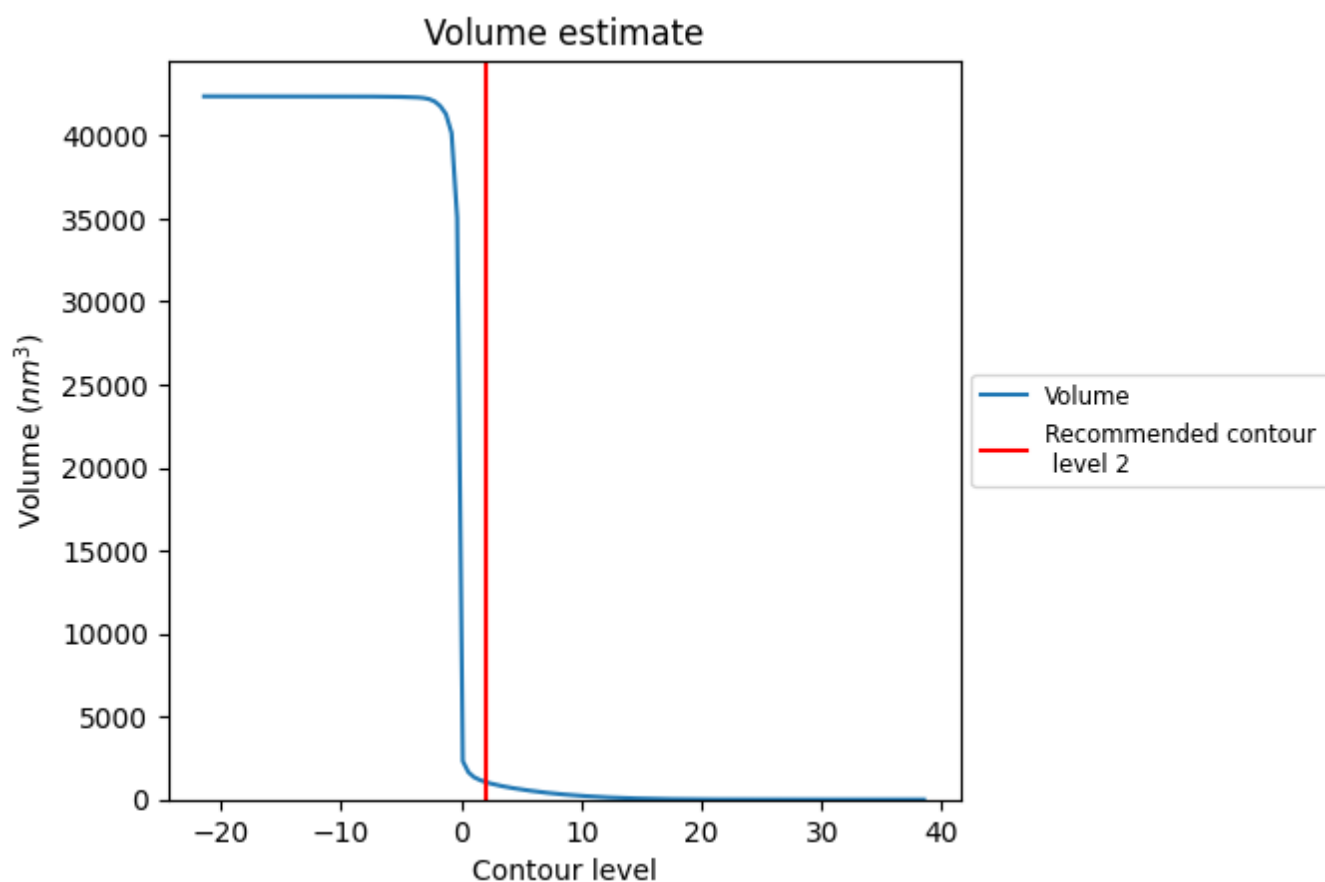
This section contains the results of statistical analysis of the map.

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.

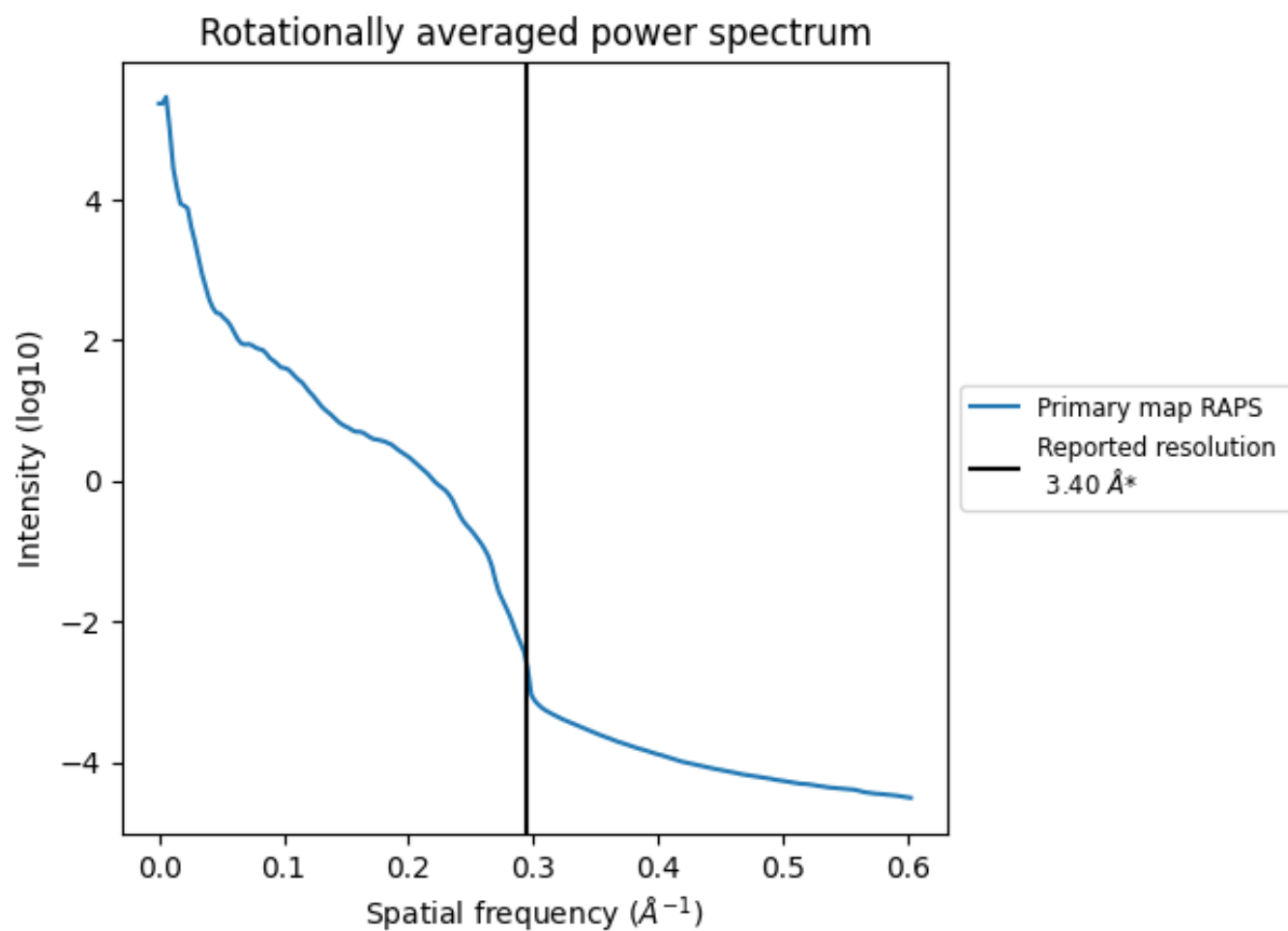
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1063 nm³; this corresponds to an approximate mass of 960 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 0.294 Å⁻¹

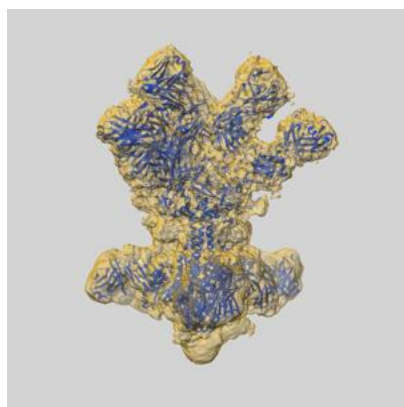
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

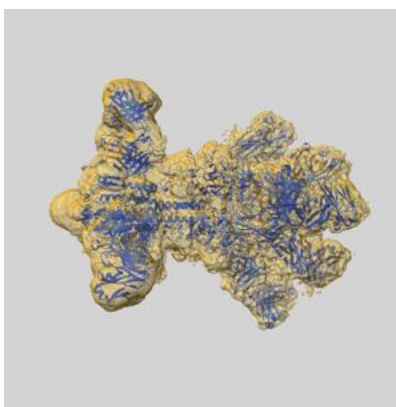
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70607 and PDB model 9OM5. Per-residue inclusion information can be found in section [3](#) on page [14](#).

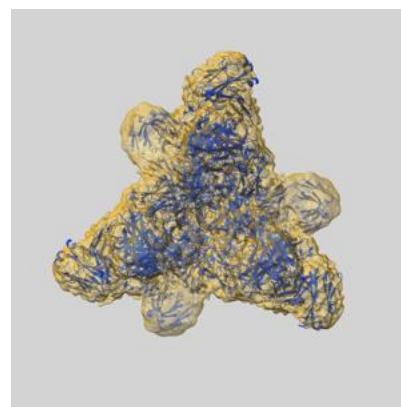
9.1 Map-model overlay [i](#)



X



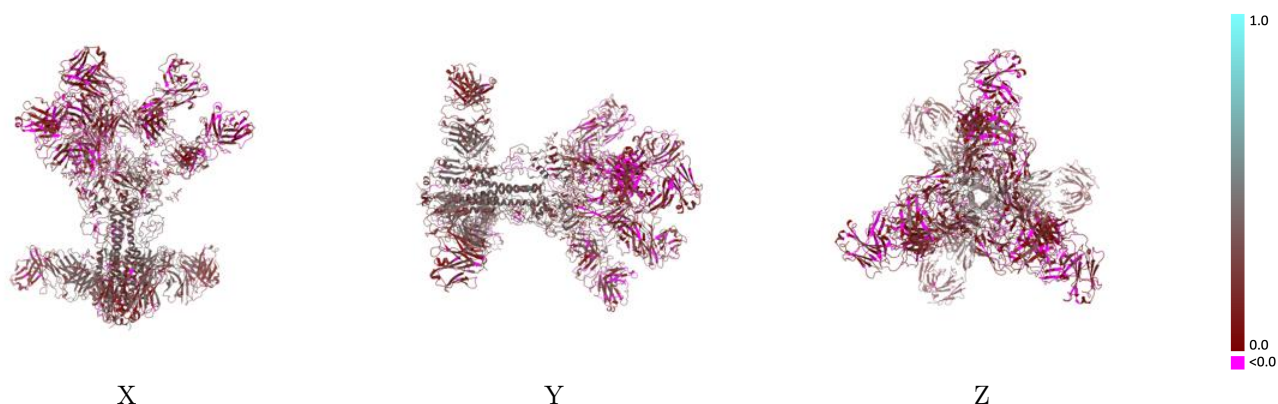
Y



Z

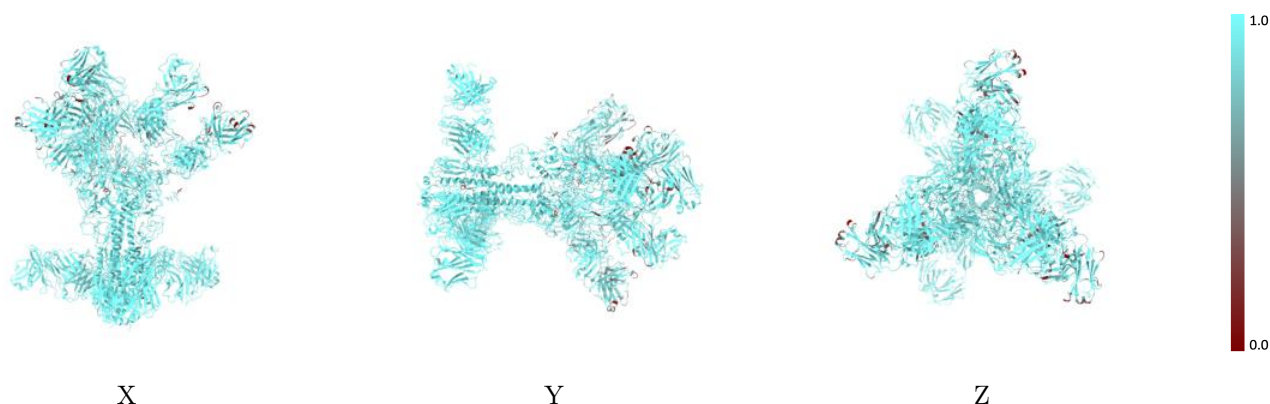
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



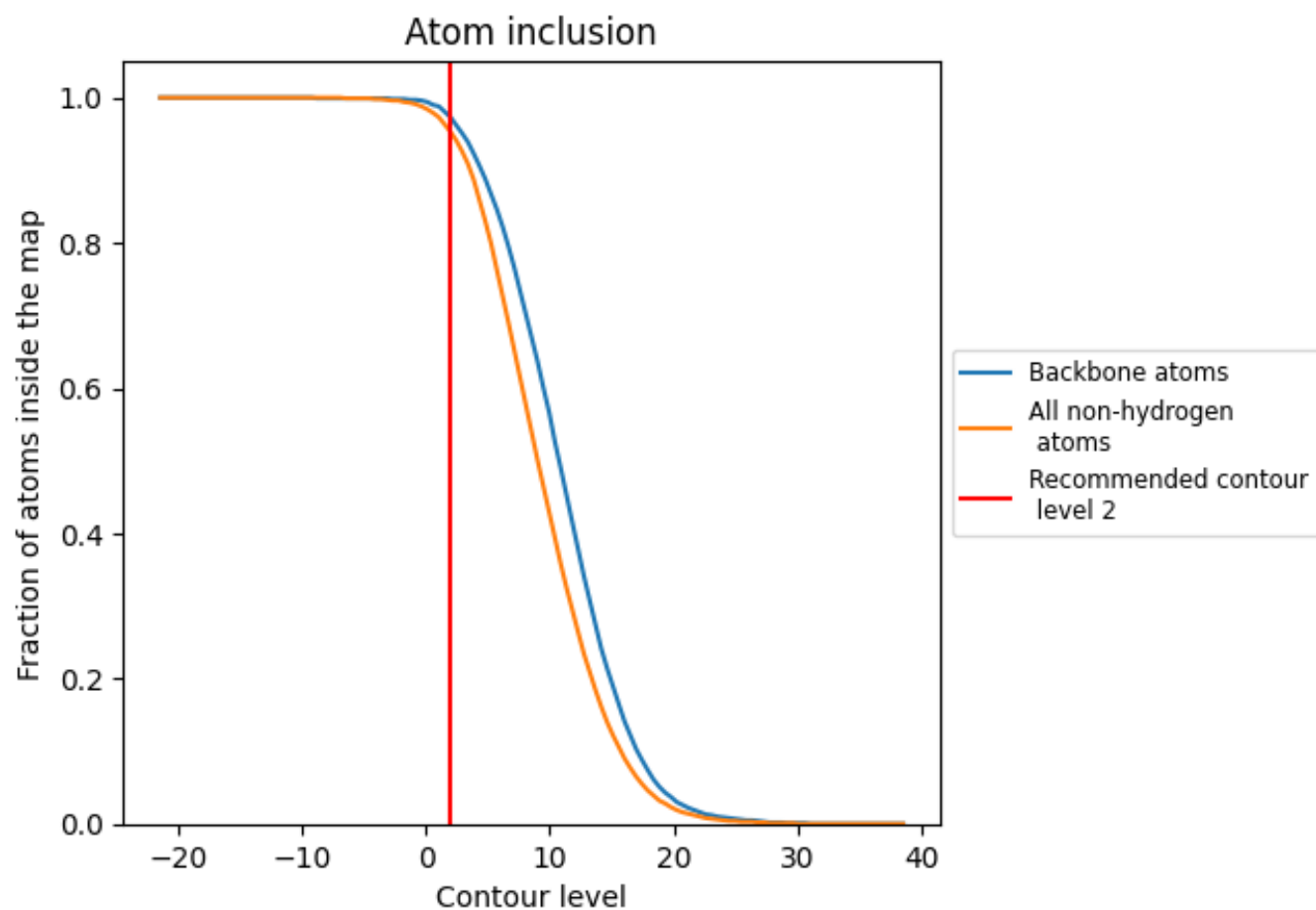
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.2190
A	 0.9800	 0.2670
B	 0.9740	 0.3270
C	 0.9900	 0.3550
D	 0.9750	 0.3460
E	 0.9810	 0.2690
F	 0.9750	 0.3320
G	 0.9940	 0.2760
H	 0.9960	 0.2640
I	 0.9980	 0.2810
J	 0.9940	 0.2700
K	 0.9980	 0.2840
L	 0.9940	 0.2720
M	 1.0000	 0.2540
N	 0.5900	 -0.0520
O	 0.9020	 0.0990
P	 0.6670	 0.1860
Q	 1.0000	 0.1420
R	 0.8970	 0.0630
S	 0.8030	 0.1480
T	 1.0000	 0.2600
U	 0.6920	 0.0090
V	 0.9000	 0.1240
W	 0.6670	 0.1730
X	 1.0000	 0.3170
Y	 0.8970	 0.0780
Z	 0.7540	 0.1400
a	 0.8780	 0.1400
b	 0.9550	 0.1540
c	 0.8940	 0.1440
d	 0.9170	 0.1270
e	 0.9010	 0.1430
f	 0.9670	 0.1550
g	 0.9080	 0.1400
h	 0.9320	 0.1390



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Chain	Atom inclusion	Q-score
i	 0.9030	 0.1450
j	 0.9630	 0.1570
k	 0.9050	 0.1400
l	 0.9310	 0.1360
m	 1.0000	 0.2580
n	 0.6920	 -0.0080
o	 0.9200	 0.1470
p	 0.6670	 0.1910
q	 1.0000	 0.1490
r	 0.8970	 0.1030
s	 0.7540	 0.1360