



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 03:58 PM EDT

PDB ID : 8DP1
EMDB ID : EMD-27628
Title : Cryo-EM structure of HIV-1 Env(BG505.T332N SOSIP) in complex with DH1030.1 Fab
Authors : Gobeil, S.; Acharya, P.
Deposited on : 2022-07-14
Resolution : 3.46 Å(reported)
Based on initial models : 8DKF, 6MTJ

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

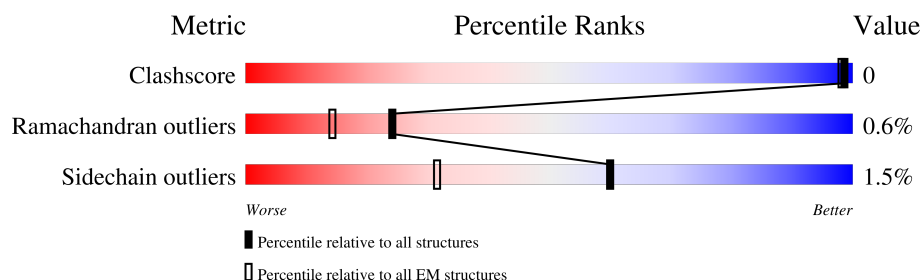
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	219	<div> <div>16%</div> <div>93%</div> <div>6%</div> </div>
1	M	219	<div> <div>14%</div> <div>93%</div> <div>5%</div> </div>
1	O	219	<div> <div>13%</div> <div>94%</div> <div>5%</div> </div>
2	E	230	<div> <div>11%</div> <div>93%</div> <div>• •</div> </div>
2	N	230	<div> <div>11%</div> <div>93%</div> <div>• •</div> </div>
2	R	230	<div> <div>12%</div> <div>91%</div> <div>6%</div> </div>
3	H	153	<div> <div>5%</div> <div>82%</div> <div>• • 13%</div> </div>
3	Q	153	<div> <div>5%</div> <div>84%</div> <div>• • 13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	S	153	
4	B	481	
4	J	481	
4	W	481	
5	A	10	
5	K	10	
5	V	10	
6	C	3	
6	D	3	
6	L	3	
6	U	3	
6	X	3	
7	G	2	
7	I	2	
7	P	2	
7	T	2	
7	Y	2	
7	Z	2	
8	a	5	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25000 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 DH1030.1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		
1	F	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		
1	O	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		

- Molecule 2 is a protein called DH1030.1 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		
2	E	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		
2	N	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		

- Molecule 3 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	133	Total	C	N	O	S	0	0
			1056	673	182	195	6		
3	H	133	Total	C	N	O	S	0	0
			1056	673	182	195	6		
3	Q	133	Total	C	N	O	S	0	0
			1056	673	182	195	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	559	PRO	ILE	conflict	UNP Q2N0S6
S	605	CYS	THR	conflict	UNP Q2N0S6
H	559	PRO	ILE	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	605	CYS	THR	conflict	UNP Q2N0S6
Q	559	PRO	ILE	conflict	UNP Q2N0S6
Q	605	CYS	THR	conflict	UNP Q2N0S6

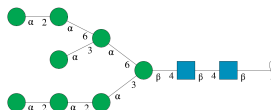
- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	440	Total	C	N	O	S	0	0
			3465	2177	614	646	28		
4	B	440	Total	C	N	O	S	0	0
			3465	2177	614	646	28		
4	J	440	Total	C	N	O	S	0	0
			3465	2177	614	646	28		

There are 24 discrepancies between the modelled and reference sequences:

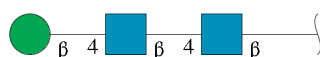
Chain	Residue	Modelled	Actual	Comment	Reference
W	137	ALA	ASN	engineered mutation	UNP Q2N0S6
W	332	ASN	THR	engineered mutation	UNP Q2N0S6
W	501	CYS	ALA	conflict	UNP Q2N0S6
W	509	ARG	-	expression tag	UNP Q2N0S6
W	510	ARG	-	expression tag	UNP Q2N0S6
W	511	ARG	-	expression tag	UNP Q2N0S6
W	512	ARG	-	expression tag	UNP Q2N0S6
W	513	ARG	-	expression tag	UNP Q2N0S6
B	137	ALA	ASN	engineered mutation	UNP Q2N0S6
B	332	ASN	THR	engineered mutation	UNP Q2N0S6
B	501	CYS	ALA	conflict	UNP Q2N0S6
B	509	ARG	-	expression tag	UNP Q2N0S6
B	510	ARG	-	expression tag	UNP Q2N0S6
B	511	ARG	-	expression tag	UNP Q2N0S6
B	512	ARG	-	expression tag	UNP Q2N0S6
B	513	ARG	-	expression tag	UNP Q2N0S6
J	137	ALA	ASN	engineered mutation	UNP Q2N0S6
J	332	ASN	THR	engineered mutation	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6
J	509	ARG	-	expression tag	UNP Q2N0S6
J	510	ARG	-	expression tag	UNP Q2N0S6
J	511	ARG	-	expression tag	UNP Q2N0S6
J	512	ARG	-	expression tag	UNP Q2N0S6
J	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	10	Total	C	N	O	0	0
			116	64	2	50		
5	K	10	Total	C	N	O	0	0
			116	64	2	50		
5	V	10	Total	C	N	O	0	0
			116	64	2	50		

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



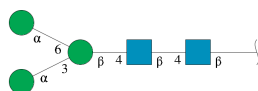
Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	3	Total	C	N	O	0	0
			39	22	2	15		
6	D	3	Total	C	N	O	0	0
			39	22	2	15		
6	L	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		

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



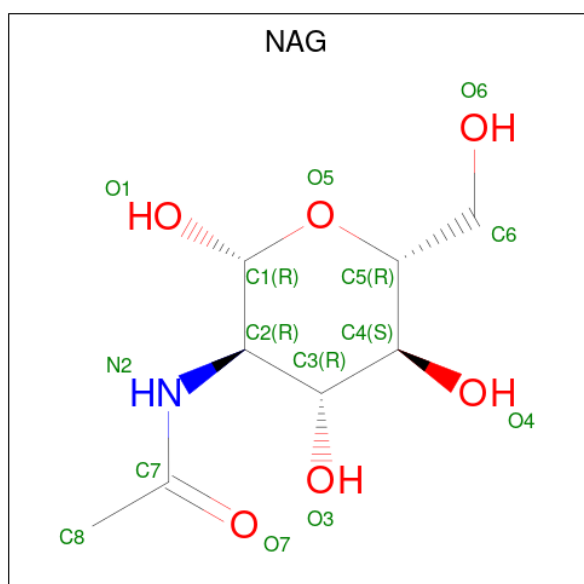
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
9	S	1	Total	C	N	O	0
			14	8	1	5	
9	S	1	Total	C	N	O	0
			14	8	1	5	
9	S	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	W	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	
9	H	1	Total	C	N	O	0
			14	8	1	5	

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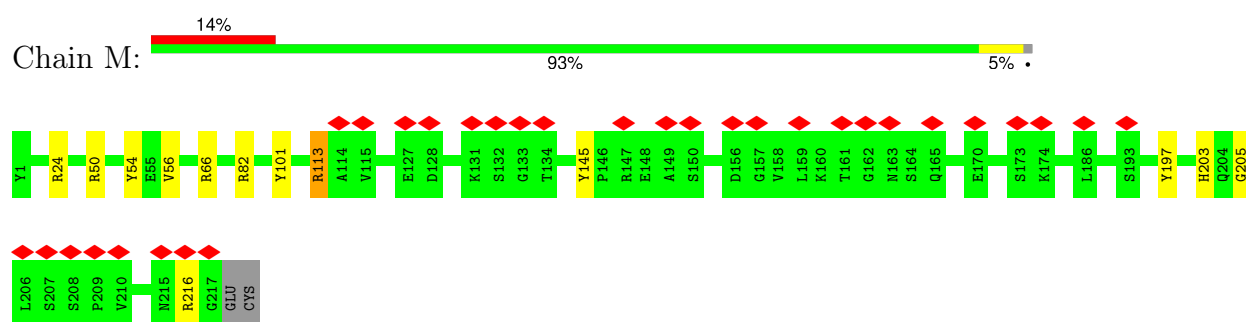
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Mol	Chain	Residues	Atoms				AltConf
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	J	1	Total	C	N	O	0
			14	8	1	5	
9	Q	1	Total	C	N	O	0
			14	8	1	5	
9	Q	1	Total	C	N	O	0
			14	8	1	5	
9	Q	1	Total	C	N	O	0
			14	8	1	5	

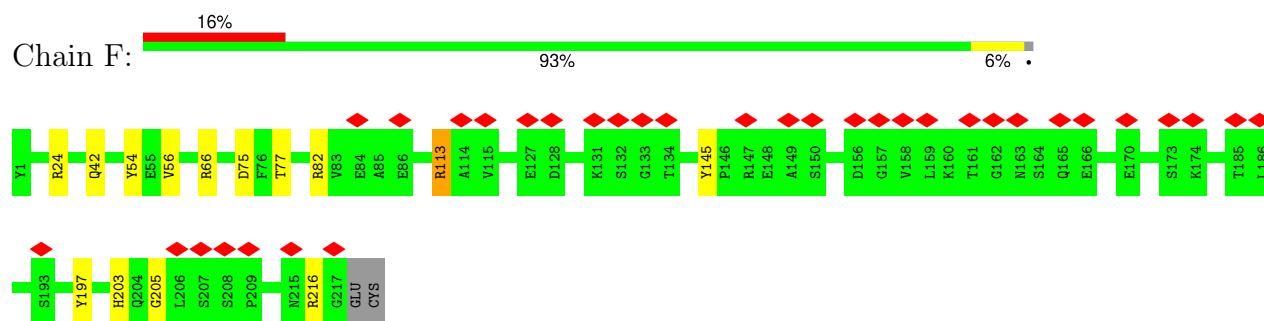
3 Residue-property plots [i](#)

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.

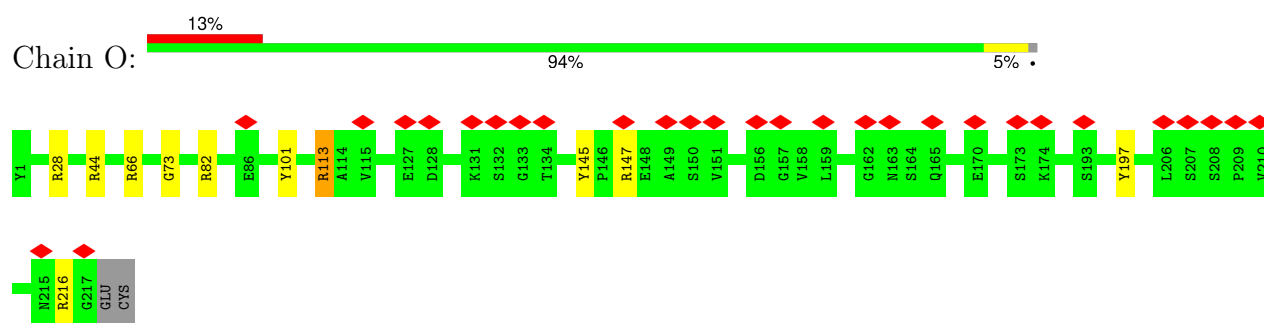
- Molecule 1: DH1030.1 Fab light chain



- Molecule 1: DH1030.1 Fab light chain

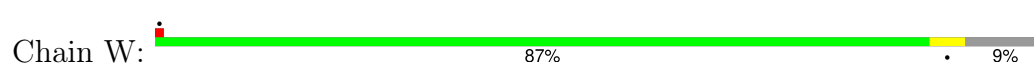


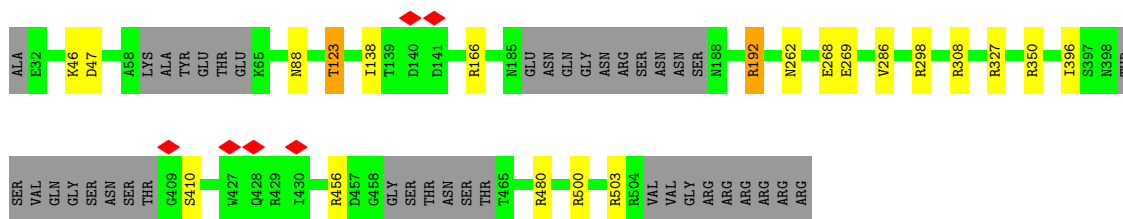
- Molecule 1: DH1030.1 Fab light chain



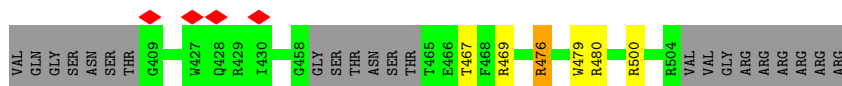
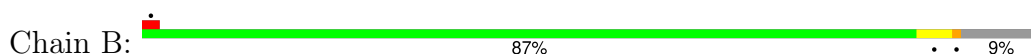
- Molecule 2: DH1030.1 Fab Heavy chain



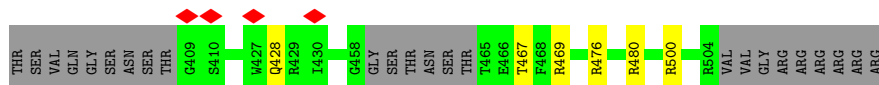
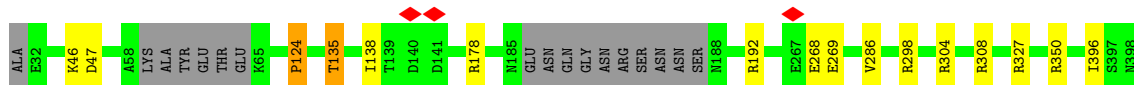
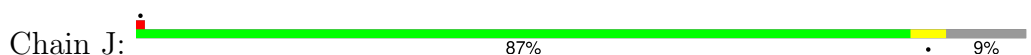




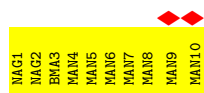
• Molecule 4: Envelope glycoprotein gp120



• Molecule 4: Envelope glycoprotein gp120



• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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



• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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





- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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



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



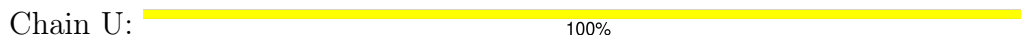
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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




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



MAG1
MAG2

- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

MAG1
MAG2
BMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	441080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.111	Depositor
Minimum map value	-1.266	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.9	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	F	0.67	0/1715	0.99	5/2334 (0.2%)
1	M	0.66	0/1715	0.99	7/2334 (0.3%)
1	O	0.67	0/1715	1.02	8/2334 (0.3%)
2	E	0.66	0/1769	1.06	7/2410 (0.3%)
2	N	0.66	0/1769	1.05	6/2410 (0.2%)
2	R	0.66	0/1769	1.05	10/2410 (0.4%)
3	H	0.59	0/1075	1.01	4/1458 (0.3%)
3	Q	0.59	0/1075	1.02	4/1458 (0.3%)
3	S	0.59	0/1075	1.02	3/1458 (0.2%)
4	B	0.61	0/3536	0.99	12/4797 (0.3%)
4	J	0.61	0/3536	0.99	11/4797 (0.2%)
4	W	0.61	0/3536	0.98	10/4797 (0.2%)
All	All	0.63	0/24285	1.01	87/32997 (0.3%)

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	F	0	3
1	M	0	3
1	O	0	2
2	E	0	2
2	N	0	1
2	R	0	2
3	H	0	1
3	Q	0	2
All	All	0	16

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	298	ARG	NE-CZ-NH1	9.05	124.82	120.30
4	B	298	ARG	NE-CZ-NH1	8.37	124.48	120.30
4	W	123	THR	CA-CB-OG1	8.36	126.55	109.00
3	Q	617	ARG	NE-CZ-NH1	8.11	124.35	120.30
3	S	617	ARG	NE-CZ-NH1	7.87	124.23	120.30
4	W	500	ARG	NE-CZ-NH1	7.85	124.22	120.30
3	H	617	ARG	NE-CZ-NH1	7.80	124.20	120.30
4	B	500	ARG	NE-CZ-NH1	7.77	124.19	120.30
4	W	298	ARG	NE-CZ-NH1	7.76	124.18	120.30
4	J	480	ARG	NE-CZ-NH1	7.73	124.17	120.30
4	J	124	PRO	CA-N-CD	-7.64	100.80	111.50
4	B	327	ARG	NE-CZ-NH1	7.55	124.08	120.30
4	W	350	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	N	65	ARG	NE-CZ-NH1	7.38	123.99	120.30
4	J	500	ARG	NE-CZ-NH1	7.32	123.96	120.30
4	B	480	ARG	NE-CZ-NH1	7.08	123.84	120.30
4	J	350	ARG	NE-CZ-NH1	7.06	123.83	120.30
4	W	456	ARG	NE-CZ-NH1	7.01	123.81	120.30
2	E	100	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	R	56	ARG	NE-CZ-NH1	6.92	123.76	120.30
4	J	308	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	N	100	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	E	65	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	E	56	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	N	33	TYR	CB-CG-CD2	-6.74	116.95	121.00
3	Q	542	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	S	542	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	O	66	ARG	NE-CZ-NH1	6.67	123.64	120.30
4	B	476	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	M	216	ARG	NE-CZ-NH1	6.43	123.52	120.30
4	J	327	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	M	113	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	F	216	ARG	NE-CZ-NH1	6.41	123.51	120.30
4	B	350	ARG	NE-CZ-NH1	6.39	123.50	120.30
4	W	480	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	M	82	ARG	NE-CZ-NH1	6.35	123.47	120.30
2	N	56	ARG	NE-CZ-NH1	6.34	123.47	120.30
4	B	308	ARG	NE-CZ-NH1	6.32	123.46	120.30
4	J	178	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	R	65	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	Q	588	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	O	147	ARG	NE-CZ-NH1	6.29	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	33	TYR	CB-CG-CD2	-6.29	117.23	121.00
3	H	542	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	O	113	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	R	100	ARG	NE-CZ-NH1	6.21	123.41	120.30
4	W	308	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	F	82	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	M	66	ARG	NE-CZ-NH1	6.14	123.37	120.30
4	B	469	ARG	NE-CZ-NH1	6.02	123.31	120.30
4	B	178	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	H	588	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	O	216	ARG	NE-CZ-NH1	5.97	123.28	120.30
3	H	643	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	E	38	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	113	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	O	101	TYR	CB-CG-CD2	-5.86	117.48	121.00
2	N	38	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	M	24	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	R	67	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	O	28	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	R	50	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	F	24	ARG	NE-CZ-NH1	5.63	123.12	120.30
4	J	476	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	E	72	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	Q	643	TYR	CB-CG-CD2	-5.60	117.64	121.00
4	W	503	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	O	82	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	E	141	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	F	66	ARG	NE-CZ-NH1	5.47	123.03	120.30
4	J	469	ARG	NE-CZ-NH1	5.40	123.00	120.30
4	J	304	ARG	NE-CZ-NH1	5.39	122.99	120.30
4	W	327	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	S	585	ARG	NE-CZ-NH1	5.32	122.96	120.30
4	B	304	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	O	44	ARG	NE-CZ-NH1	5.29	122.95	120.30
4	B	124	PRO	N-CA-C	5.27	125.80	112.10
2	R	98	ARG	NE-CZ-NH1	5.24	122.92	120.30
4	W	192	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	R	38	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	M	50	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	N	50	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	R	72	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	M	101	TYR	CB-CG-CD2	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	19	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	R	104	ARG	NE-CZ-NH1	5.08	122.84	120.30
4	B	192	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	100	ARG	Sidechain
2	E	206	TYR	Sidechain
1	F	145	TYR	Sidechain
1	F	197	TYR	Sidechain
1	F	54	TYR	Sidechain
3	H	617	ARG	Sidechain
1	M	145	TYR	Sidechain
1	M	197	TYR	Sidechain
1	M	54	TYR	Sidechain
2	N	206	TYR	Sidechain
1	O	145	TYR	Sidechain
1	O	197	TYR	Sidechain
3	Q	588	ARG	Sidechain
3	Q	617	ARG	Sidechain
2	R	206	TYR	Sidechain
2	R	94	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1676	0	1628	1	0
1	M	1676	0	1628	1	0
1	O	1676	0	1628	0	0
2	E	1725	0	1668	0	0
2	N	1725	0	1668	0	0
2	R	1725	0	1668	0	0
3	H	1056	0	1049	0	0
3	Q	1056	0	1049	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	1056	0	1049	0	0
4	B	3465	0	3408	1	0
4	J	3465	0	3407	0	0
4	W	3465	0	3407	1	0
5	A	116	0	97	0	0
5	K	116	0	97	0	0
5	V	116	0	97	0	0
6	C	39	0	34	0	0
6	D	39	0	34	0	0
6	L	39	0	34	0	0
6	U	39	0	34	0	0
6	X	39	0	34	0	0
7	G	28	0	25	0	0
7	I	28	0	25	0	0
7	P	28	0	25	0	0
7	T	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
8	a	61	0	52	0	0
9	B	112	0	104	0	0
9	H	42	0	39	0	0
9	J	112	0	104	0	0
9	Q	42	0	39	0	0
9	S	42	0	39	0	0
9	W	112	0	104	0	0
All	All	25000	0	24349	4	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 0.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:HIS:CE1	1:F:205:GLY:H	2.37	0.43
4:B:476:ARG:HA	4:B:479:TRP:CD1	2.54	0.43
4:W:396:ILE:HD12	4:W:396:ILE:H	1.82	0.42
1:M:203:HIS:CE1	1:M:205:GLY:H	2.39	0.41

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	F	215/219 (98%)	208 (97%)	6 (3%)	1 (0%)	25	59
1	M	215/219 (98%)	210 (98%)	4 (2%)	1 (0%)	25	59
1	O	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	25	59
2	E	223/230 (97%)	212 (95%)	11 (5%)	0	100	100
2	N	223/230 (97%)	212 (95%)	11 (5%)	0	100	100
2	R	223/230 (97%)	213 (96%)	10 (4%)	0	100	100
3	H	129/153 (84%)	122 (95%)	6 (5%)	1 (1%)	16	50
3	Q	129/153 (84%)	121 (94%)	8 (6%)	0	100	100
3	S	129/153 (84%)	122 (95%)	7 (5%)	0	100	100
4	B	430/481 (89%)	406 (94%)	19 (4%)	5 (1%)	11	43
4	J	430/481 (89%)	404 (94%)	22 (5%)	4 (1%)	14	48
4	W	430/481 (89%)	406 (94%)	19 (4%)	5 (1%)	11	43
All	All	2991/3249 (92%)	2842 (95%)	131 (4%)	18 (1%)	24	55

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	124	PRO
4	W	88	ASN
4	W	138	ILE
4	W	262	ASN
4	W	410	SER
4	B	88	ASN
3	H	519	PHE
4	J	269	GLU
4	W	269	GLU
4	B	269	GLU
4	B	141	ASP
4	J	135	THR

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Mol	Chain	Res	Type
4	B	135	THR
4	B	138	ILE
1	F	56	VAL
1	O	73	GLY
4	J	138	ILE
1	M	56	VAL

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	F	192/194 (99%)	188 (98%)	4 (2%)	48	72
1	M	192/194 (99%)	191 (100%)	1 (0%)	86	92
1	O	192/194 (99%)	191 (100%)	1 (0%)	86	92
2	E	192/195 (98%)	190 (99%)	2 (1%)	73	84
2	N	192/195 (98%)	189 (98%)	3 (2%)	58	76
2	R	192/195 (98%)	188 (98%)	4 (2%)	48	72
3	H	114/129 (88%)	112 (98%)	2 (2%)	54	75
3	Q	114/129 (88%)	113 (99%)	1 (1%)	75	86
3	S	114/129 (88%)	113 (99%)	1 (1%)	75	86
4	B	392/427 (92%)	386 (98%)	6 (2%)	60	78
4	J	392/427 (92%)	383 (98%)	9 (2%)	45	71
4	W	392/427 (92%)	385 (98%)	7 (2%)	54	75
All	All	2670/2835 (94%)	2629 (98%)	41 (2%)	60	78

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	113	ARG
2	R	35	ASP
2	R	56	ARG
2	R	117	GLN

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Mol	Chain	Res	Type
2	R	119	VAL
3	S	618	ASN
4	W	46	LYS
4	W	47	ASP
4	W	123	THR
4	W	166	ARG
4	W	192	ARG
4	W	268	GLU
4	W	286	VAL
4	B	46	LYS
4	B	192	ARG
4	B	268	GLU
4	B	286	VAL
4	B	327	ARG
4	B	467	THR
2	E	117	GLN
2	E	119	VAL
1	F	42	GLN
1	F	75	ASP
1	F	77	THR
1	F	113	ARG
3	H	618	ASN
3	H	651	ASN
4	J	46	LYS
4	J	47	ASP
4	J	135	THR
4	J	192	ARG
4	J	268	GLU
4	J	286	VAL
4	J	396	ILE
4	J	428	GLN
4	J	467	THR
2	N	117	GLN
2	N	119	VAL
2	N	150	LEU
1	O	113	ARG
3	Q	658	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

62 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1	5,4	14,14,15	0.92	0	17,19,21	0.86	1 (5%)
5	MAN	A	10	5	11,11,12	1.46	2 (18%)	15,15,17	1.31	3 (20%)
5	NAG	A	2	5	14,14,15	0.91	1 (7%)	17,19,21	0.91	0
5	BMA	A	3	5	11,11,12	0.76	0	15,15,17	1.07	1 (6%)
5	MAN	A	4	5	11,11,12	1.10	1 (9%)	15,15,17	1.28	1 (6%)
5	MAN	A	5	5	11,11,12	0.92	0	15,15,17	1.56	2 (13%)
5	MAN	A	6	5	11,11,12	0.76	1 (9%)	15,15,17	1.11	2 (13%)
5	MAN	A	7	5	11,11,12	1.32	2 (18%)	15,15,17	1.15	2 (13%)
5	MAN	A	8	5	11,11,12	1.59	3 (27%)	15,15,17	1.38	2 (13%)
5	MAN	A	9	5	11,11,12	1.46	2 (18%)	15,15,17	1.45	1 (6%)
6	NAG	C	1	6,4	14,14,15	1.09	1 (7%)	17,19,21	0.80	0
6	NAG	C	2	6	14,14,15	1.40	4 (28%)	17,19,21	1.49	4 (23%)
6	BMA	C	3	6	11,11,12	1.20	1 (9%)	15,15,17	0.69	0
6	NAG	D	1	6,4	14,14,15	1.04	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	D	2	6	14,14,15	1.41	2 (14%)	17,19,21	0.95	0
6	BMA	D	3	6	11,11,12	1.29	0	15,15,17	1.54	2 (13%)
7	NAG	G	1	7,4	14,14,15	1.17	1 (7%)	17,19,21	0.73	0
7	NAG	G	2	7	14,14,15	1.25	3 (21%)	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	1	7,4	14,14,15	1.07	2 (14%)	17,19,21	1.05	2 (11%)
7	NAG	I	2	7	14,14,15	1.23	2 (14%)	17,19,21	0.82	0
5	NAG	K	1	5	14,14,15	0.86	0	17,19,21	1.19	2 (11%)
5	MAN	K	10	5	11,11,12	1.58	2 (18%)	15,15,17	1.35	3 (20%)
5	NAG	K	2	5	14,14,15	0.80	0	17,19,21	0.93	0
5	BMA	K	3	5	11,11,12	0.68	0	15,15,17	1.21	1 (6%)
5	MAN	K	4	5	11,11,12	1.08	1 (9%)	15,15,17	0.99	1 (6%)
5	MAN	K	5	5	11,11,12	0.93	1 (9%)	15,15,17	1.63	3 (20%)
5	MAN	K	6	5	11,11,12	0.76	1 (9%)	15,15,17	0.95	0
5	MAN	K	7	5	11,11,12	1.39	2 (18%)	15,15,17	1.20	2 (13%)
5	MAN	K	8	5	11,11,12	1.65	3 (27%)	15,15,17	1.19	2 (13%)
5	MAN	K	9	5	11,11,12	1.44	2 (18%)	15,15,17	1.38	1 (6%)
6	NAG	L	1	6,4	14,14,15	1.10	1 (7%)	17,19,21	0.79	0
6	NAG	L	2	6	14,14,15	1.32	2 (14%)	17,19,21	1.01	0
6	BMA	L	3	6	11,11,12	1.27	2 (18%)	15,15,17	0.75	0
7	NAG	P	1	7,4	14,14,15	1.02	1 (7%)	17,19,21	0.68	0
7	NAG	P	2	7	14,14,15	1.28	2 (14%)	17,19,21	1.13	2 (11%)
7	NAG	T	1	7,4	14,14,15	1.19	1 (7%)	17,19,21	0.87	0
7	NAG	T	2	7	14,14,15	1.16	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	U	1	6,4	14,14,15	1.09	1 (7%)	17,19,21	1.02	2 (11%)
6	NAG	U	2	6	14,14,15	1.32	3 (21%)	17,19,21	1.39	3 (17%)
6	BMA	U	3	6	11,11,12	1.22	2 (18%)	15,15,17	1.07	2 (13%)
5	NAG	V	1	5,4	14,14,15	0.96	0	17,19,21	0.80	0
5	MAN	V	10	5	11,11,12	1.46	2 (18%)	15,15,17	1.50	3 (20%)
5	NAG	V	2	5	14,14,15	0.87	0	17,19,21	0.96	0
5	BMA	V	3	5	11,11,12	0.79	0	15,15,17	1.10	1 (6%)
5	MAN	V	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	V	5	5	11,11,12	0.93	0	15,15,17	1.56	2 (13%)
5	MAN	V	6	5	11,11,12	0.85	1 (9%)	15,15,17	1.26	1 (6%)
5	MAN	V	7	5	11,11,12	1.40	1 (9%)	15,15,17	1.25	2 (13%)
5	MAN	V	8	5	11,11,12	1.63	3 (27%)	15,15,17	1.18	0
5	MAN	V	9	5	11,11,12	1.38	2 (18%)	15,15,17	1.13	1 (6%)
6	NAG	X	1	6,4	14,14,15	1.07	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	X	2	6	14,14,15	1.28	2 (14%)	17,19,21	0.85	0
6	BMA	X	3	6	11,11,12	1.28	2 (18%)	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Y	1	7,4	14,14,15	1.21	2 (14%)	17,19,21	0.93	1 (5%)
7	NAG	Y	2	7	14,14,15	1.28	2 (14%)	17,19,21	0.94	1 (5%)
7	NAG	Z	1	7,4	14,14,15	1.16	1 (7%)	17,19,21	0.95	1 (5%)
7	NAG	Z	2	7	14,14,15	1.25	1 (7%)	17,19,21	1.16	1 (5%)
8	NAG	a	1	8,4	14,14,15	0.99	0	17,19,21	0.83	0
8	NAG	a	2	8	14,14,15	1.12	1 (7%)	17,19,21	1.26	2 (11%)
8	BMA	a	3	8	11,11,12	1.33	2 (18%)	15,15,17	1.67	3 (20%)
8	MAN	a	4	8	11,11,12	1.37	2 (18%)	15,15,17	0.74	0
8	MAN	a	5	8	11,11,12	1.36	2 (18%)	15,15,17	0.95	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	10	5	-	1/2/19/22	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
5	BMA	A	3	5	-	1/2/19/22	0/1/1/1
5	MAN	A	4	5	-	0/2/19/22	0/1/1/1
5	MAN	A	5	5	-	0/2/19/22	0/1/1/1
5	MAN	A	6	5	-	0/2/19/22	0/1/1/1
5	MAN	A	7	5	-	2/2/19/22	0/1/1/1
5	MAN	A	8	5	-	0/2/19/22	0/1/1/1
5	MAN	A	9	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	3/6/23/26	0/1/1/1
6	BMA	C	3	6	-	0/2/19/22	0/1/1/1
6	NAG	D	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	1/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
7	NAG	I	1	7,4	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5	-	0/6/23/26	0/1/1/1
5	MAN	K	10	5	-	0/2/19/22	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
5	MAN	K	7	5	-	2/2/19/22	0/1/1/1
5	MAN	K	8	5	-	0/2/19/22	0/1/1/1
5	MAN	K	9	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
7	NAG	P	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	3/6/23/26	0/1/1/1
7	NAG	T	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
6	NAG	U	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
5	NAG	V	1	5,4	-	0/6/23/26	0/1/1/1
5	MAN	V	10	5	-	1/2/19/22	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	BMA	V	3	5	-	2/2/19/22	0/1/1/1
5	MAN	V	4	5	-	0/2/19/22	0/1/1/1
5	MAN	V	5	5	-	0/2/19/22	0/1/1/1
5	MAN	V	6	5	-	0/2/19/22	0/1/1/1
5	MAN	V	7	5	-	2/2/19/22	0/1/1/1
5	MAN	V	8	5	-	0/2/19/22	0/1/1/1
5	MAN	V	9	5	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
6	BMA	X	3	6	-	1/2/19/22	0/1/1/1
7	NAG	Y	1	7,4	-	1/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	NAG	Z	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
8	NAG	a	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	3/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	0/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2	NAG	O4-C4	3.21	1.50	1.43
5	K	10	MAN	O5-C5	3.20	1.49	1.43
5	K	8	MAN	O5-C5	3.17	1.49	1.43
5	V	10	MAN	O5-C5	3.16	1.49	1.43
5	V	8	MAN	O5-C5	3.10	1.49	1.43
8	a	5	MAN	O5-C5	3.06	1.49	1.43
8	a	4	MAN	O5-C5	3.01	1.49	1.43
5	A	10	MAN	O5-C5	2.98	1.49	1.43
5	A	9	MAN	O5-C5	2.90	1.49	1.43
7	Z	2	NAG	O5-C5	2.86	1.49	1.43
5	A	8	MAN	O5-C5	2.86	1.49	1.43
7	Y	2	NAG	O5-C5	2.85	1.49	1.43
7	P	2	NAG	O5-C5	2.77	1.48	1.43
5	K	9	MAN	O5-C5	2.71	1.48	1.43
6	C	3	BMA	O5-C5	2.70	1.48	1.43
5	A	9	MAN	O5-C1	2.69	1.48	1.43
5	V	9	MAN	O5-C5	2.63	1.48	1.43
5	K	9	MAN	O5-C1	2.61	1.48	1.43
5	A	4	MAN	O5-C5	2.60	1.48	1.43
5	K	8	MAN	C2-C3	2.60	1.56	1.52
6	C	2	NAG	O5-C5	2.59	1.48	1.43
6	L	2	NAG	O5-C5	2.58	1.48	1.43
6	U	2	NAG	O5-C5	2.56	1.48	1.43
5	V	8	MAN	O2-C2	2.54	1.48	1.43
5	K	7	MAN	O5-C5	2.53	1.48	1.43
7	T	2	NAG	O5-C5	2.53	1.48	1.43
6	X	2	NAG	O5-C5	2.52	1.48	1.43
5	V	7	MAN	O5-C5	2.52	1.48	1.43
5	K	4	MAN	O5-C5	2.51	1.48	1.43
7	Y	1	NAG	O4-C4	2.50	1.49	1.43
7	Y	1	NAG	O5-C5	2.50	1.48	1.43
7	I	2	NAG	O5-C5	2.47	1.48	1.43
6	U	3	BMA	O5-C5	2.46	1.48	1.43
5	A	8	MAN	O2-C2	2.46	1.48	1.43
6	L	3	BMA	O5-C5	2.46	1.48	1.43
5	A	7	MAN	O5-C5	2.45	1.48	1.43
5	V	4	MAN	O5-C5	2.45	1.48	1.43
8	a	3	BMA	O5-C5	2.44	1.48	1.43
6	C	1	NAG	O5-C5	2.41	1.48	1.43
5	A	8	MAN	C2-C3	2.41	1.56	1.52
8	a	3	BMA	O3-C3	2.41	1.48	1.43
7	Z	1	NAG	O5-C5	2.39	1.48	1.43
5	V	8	MAN	C2-C3	2.39	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	2	NAG	O5-C5	2.37	1.48	1.43
6	U	2	NAG	O5-C1	2.36	1.47	1.43
5	V	9	MAN	O5-C1	2.35	1.47	1.43
5	K	7	MAN	O5-C1	2.35	1.47	1.43
6	C	2	NAG	O4-C4	2.35	1.48	1.43
7	G	2	NAG	O5-C5	2.34	1.48	1.43
5	K	8	MAN	O2-C2	2.33	1.48	1.43
5	K	10	MAN	C2-C3	2.33	1.56	1.52
6	U	1	NAG	O5-C5	2.31	1.47	1.43
6	C	2	NAG	C1-C2	2.28	1.55	1.52
7	I	1	NAG	O5-C5	2.27	1.47	1.43
6	C	2	NAG	O5-C1	2.26	1.47	1.43
6	D	2	NAG	O5-C5	2.25	1.47	1.43
5	V	6	MAN	O5-C5	2.25	1.47	1.43
6	D	1	NAG	O5-C5	2.24	1.47	1.43
6	L	1	NAG	O5-C5	2.23	1.47	1.43
7	P	2	NAG	O5-C1	2.20	1.47	1.43
7	I	1	NAG	O4-C4	2.20	1.48	1.43
5	A	2	NAG	O5-C5	2.17	1.47	1.43
6	U	3	BMA	O5-C1	2.17	1.47	1.43
6	L	3	BMA	O5-C1	2.16	1.47	1.43
7	G	2	NAG	C1-C2	2.15	1.55	1.52
8	a	4	MAN	O5-C1	2.15	1.47	1.43
5	K	5	MAN	O5-C1	2.14	1.47	1.43
6	X	3	BMA	O5-C5	2.14	1.47	1.43
7	I	2	NAG	C1-C2	2.12	1.55	1.52
5	A	10	MAN	C2-C3	2.11	1.55	1.52
6	X	2	NAG	O4-C4	2.10	1.48	1.43
6	L	2	NAG	C1-C2	2.09	1.55	1.52
7	T	1	NAG	O5-C5	2.08	1.47	1.43
7	G	1	NAG	O4-C4	2.08	1.48	1.43
7	P	1	NAG	O5-C5	2.07	1.47	1.43
6	X	3	BMA	O5-C1	2.07	1.47	1.43
5	A	6	MAN	O5-C5	2.07	1.47	1.43
5	K	6	MAN	O5-C5	2.06	1.47	1.43
8	a	5	MAN	O5-C1	2.06	1.47	1.43
7	G	2	NAG	O5-C1	2.05	1.47	1.43
6	U	2	NAG	C1-C2	2.02	1.55	1.52
7	Y	2	NAG	C1-C2	2.02	1.55	1.52
5	A	7	MAN	O5-C1	2.01	1.47	1.43
5	V	10	MAN	O5-C1	2.01	1.47	1.43
6	X	1	NAG	O5-C5	2.01	1.47	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3	BMA	O5-C1-C2	4.67	121.92	110.79
8	a	3	BMA	O5-C1-C2	4.55	121.64	110.79
5	A	9	MAN	C1-O5-C5	4.45	118.14	112.19
5	K	5	MAN	C1-C2-C3	4.33	115.95	109.64
5	K	9	MAN	C1-O5-C5	4.22	117.84	112.19
5	A	4	MAN	C1-O5-C5	4.19	117.81	112.19
5	A	5	MAN	C1-C2-C3	4.16	115.71	109.64
5	V	5	MAN	C1-C2-C3	4.06	115.55	109.64
5	K	3	BMA	C3-C4-C5	-3.87	103.21	110.23
6	U	2	NAG	C4-C3-C2	-3.73	105.55	111.02
6	C	2	NAG	C4-C3-C2	-3.56	105.80	111.02
5	V	4	MAN	C1-O5-C5	3.51	116.89	112.19
7	Z	2	NAG	C1-O5-C5	3.31	116.63	112.19
5	V	6	MAN	C1-O5-C5	3.21	116.49	112.19
5	K	4	MAN	C1-O5-C5	3.16	116.42	112.19
5	V	3	BMA	C3-C4-C5	-3.13	104.56	110.23
5	V	5	MAN	C1-O5-C5	3.00	116.21	112.19
5	V	9	MAN	C1-O5-C5	2.95	116.14	112.19
5	K	5	MAN	C1-O5-C5	2.92	116.09	112.19
5	A	7	MAN	C1-O5-C5	2.89	116.06	112.19
8	a	2	NAG	C1-C2-N2	2.85	114.93	110.43
6	D	1	NAG	O4-C4-C3	-2.84	103.67	110.38
5	K	10	MAN	C1-O5-C5	2.84	115.99	112.19
8	a	3	BMA	O2-C2-C1	2.83	115.69	109.22
8	a	2	NAG	O5-C1-C2	-2.80	106.96	111.29
5	K	7	MAN	C1-O5-C5	2.78	115.91	112.19
5	K	7	MAN	C6-C5-C4	2.62	119.45	113.02
5	V	7	MAN	C6-C5-C4	2.61	119.42	113.02
5	A	3	BMA	C3-C4-C5	-2.58	105.56	110.23
5	V	10	MAN	O5-C1-C2	2.57	116.92	110.79
8	a	3	BMA	C1-C2-C3	-2.56	105.91	109.64
5	V	10	MAN	C1-O5-C5	2.56	115.62	112.19
5	A	8	MAN	C1-O5-C5	2.55	115.61	112.19
6	U	3	BMA	C1-O5-C5	2.55	115.60	112.19
7	P	2	NAG	C1-O5-C5	2.54	115.59	112.19
5	V	7	MAN	C1-O5-C5	2.52	115.56	112.19
5	K	1	NAG	C3-C4-C5	2.44	114.65	110.23
6	C	2	NAG	O4-C4-C3	2.42	116.08	110.38
5	A	10	MAN	C1-C2-C3	2.41	113.15	109.64
5	A	8	MAN	C1-C2-C3	2.40	113.14	109.64
5	A	5	MAN	C1-O5-C5	2.40	115.40	112.19
5	K	1	NAG	O5-C1-C2	-2.39	107.59	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	10	MAN	C1-C2-C3	2.37	113.10	109.64
5	A	10	MAN	C6-C5-C4	2.34	118.77	113.02
6	U	1	NAG	C1-O5-C5	2.33	115.31	112.19
7	T	2	NAG	C1-O5-C5	2.31	115.29	112.19
5	K	10	MAN	C1-C2-C3	2.28	112.97	109.64
6	U	2	NAG	O4-C4-C3	2.27	115.72	110.38
6	U	2	NAG	O5-C5-C4	-2.26	105.34	110.83
7	Y	1	NAG	C4-C3-C2	2.23	114.29	111.02
7	Z	1	NAG	O5-C1-C2	-2.22	107.86	111.29
7	P	2	NAG	O5-C1-C2	-2.21	107.87	111.29
6	X	1	NAG	O4-C4-C3	-2.21	105.18	110.38
8	a	5	MAN	C1-O5-C5	2.19	115.12	112.19
6	D	3	BMA	O2-C2-C1	2.18	114.21	109.22
7	I	1	NAG	C4-C3-C2	2.18	114.21	111.02
7	Y	2	NAG	C1-O5-C5	2.16	115.08	112.19
5	K	8	MAN	C1-C2-C3	2.15	112.78	109.64
6	U	1	NAG	O4-C4-C3	-2.12	105.37	110.38
5	A	7	MAN	C6-C5-C4	2.12	118.22	113.02
6	C	2	NAG	O5-C5-C4	-2.11	105.70	110.83
5	K	10	MAN	O5-C1-C2	2.09	115.77	110.79
5	K	5	MAN	O5-C5-C4	-2.08	105.77	110.83
6	U	3	BMA	C1-C2-C3	2.06	112.65	109.64
5	A	6	MAN	C2-C3-C4	-2.05	107.26	110.86
7	I	1	NAG	O4-C4-C3	-2.05	105.55	110.38
7	G	2	NAG	C1-C2-N2	2.05	113.66	110.43
6	C	2	NAG	O4-C4-C5	2.03	114.32	109.32
5	A	10	MAN	C1-O5-C5	2.02	114.90	112.19
5	A	6	MAN	C1-O5-C5	2.02	114.89	112.19
5	A	1	NAG	C1-O5-C5	2.00	114.87	112.19
5	K	8	MAN	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	2	NAG	C1-C2-N2-C7
6	X	2	NAG	C1-C2-N2-C7
5	A	7	MAN	O5-C5-C6-O6
5	K	7	MAN	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
5	V	7	MAN	O5-C5-C6-O6
6	C	2	NAG	O5-C5-C6-O6

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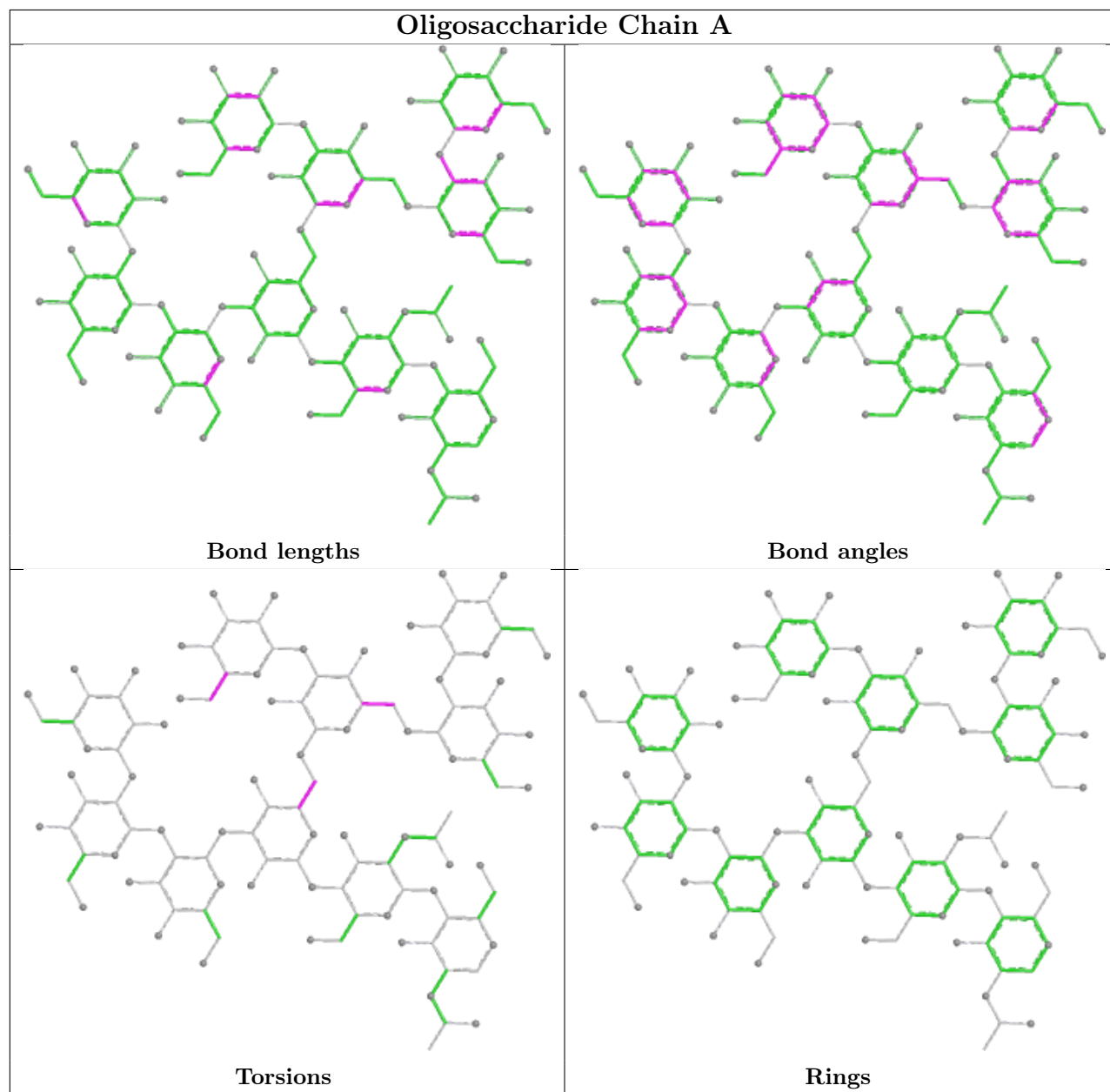
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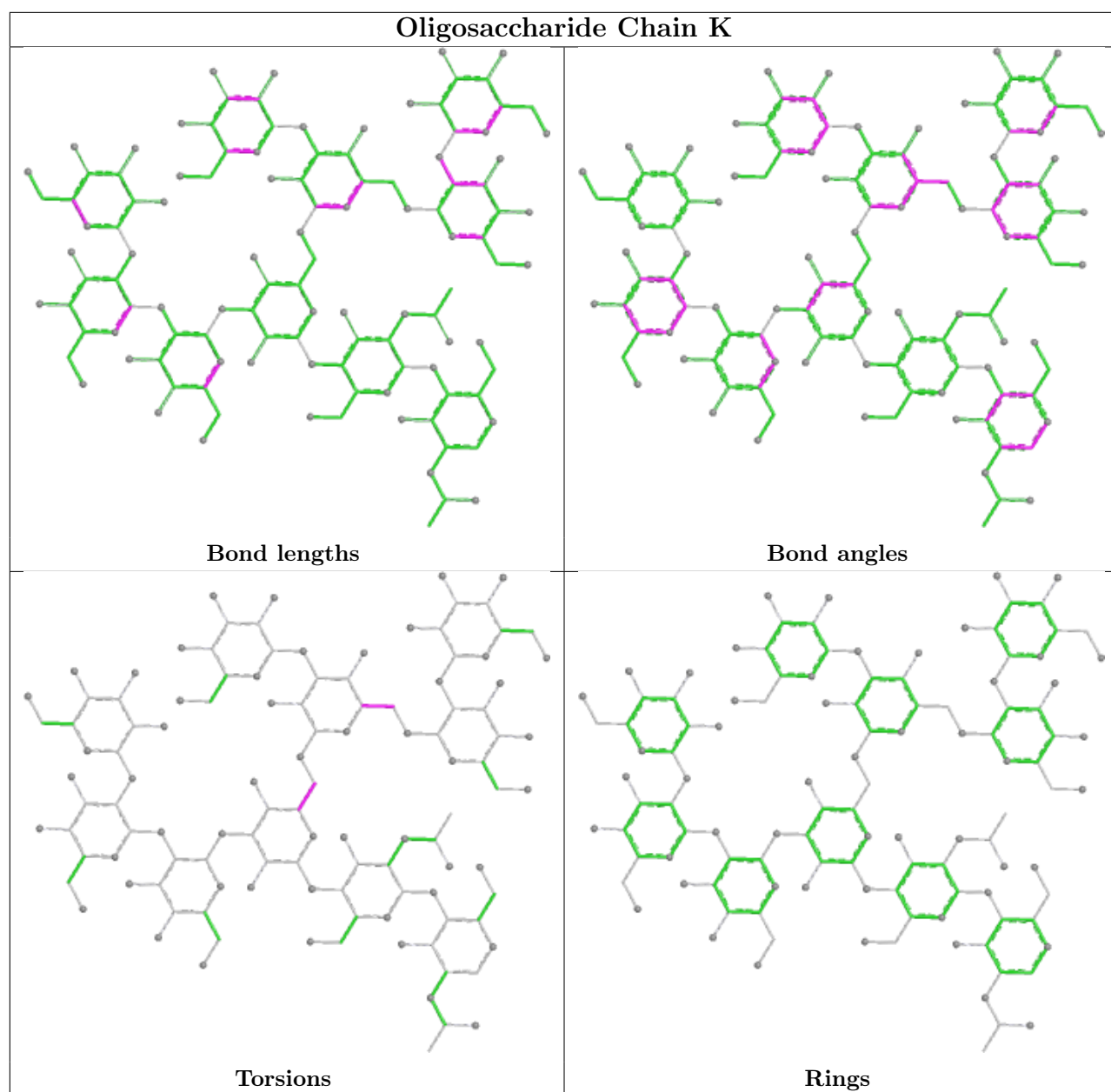
Mol	Chain	Res	Type	Atoms
8	a	3	BMA	O5-C5-C6-O6
6	C	2	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
5	A	7	MAN	C4-C5-C6-O6
5	K	7	MAN	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
5	V	10	MAN	O5-C5-C6-O6
5	A	10	MAN	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
5	A	3	BMA	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	V	7	MAN	C4-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
6	L	2	NAG	C1-C2-N2-C7
7	G	2	NAG	C1-C2-N2-C7
7	T	1	NAG	C1-C2-N2-C7
7	Z	1	NAG	C1-C2-N2-C7
7	G	2	NAG	C3-C2-N2-C7
7	P	2	NAG	C3-C2-N2-C7
7	Z	1	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7
5	V	3	BMA	C4-C5-C6-O6
6	U	2	NAG	C1-C2-N2-C7
7	P	2	NAG	C1-C2-N2-C7
7	Z	2	NAG	C1-C2-N2-C7
8	a	2	NAG	C1-C2-N2-C7
7	Y	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C3-C2-N2-C7
6	U	2	NAG	C3-C2-N2-C7
7	T	1	NAG	C3-C2-N2-C7
8	a	2	NAG	C3-C2-N2-C7
7	I	1	NAG	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6

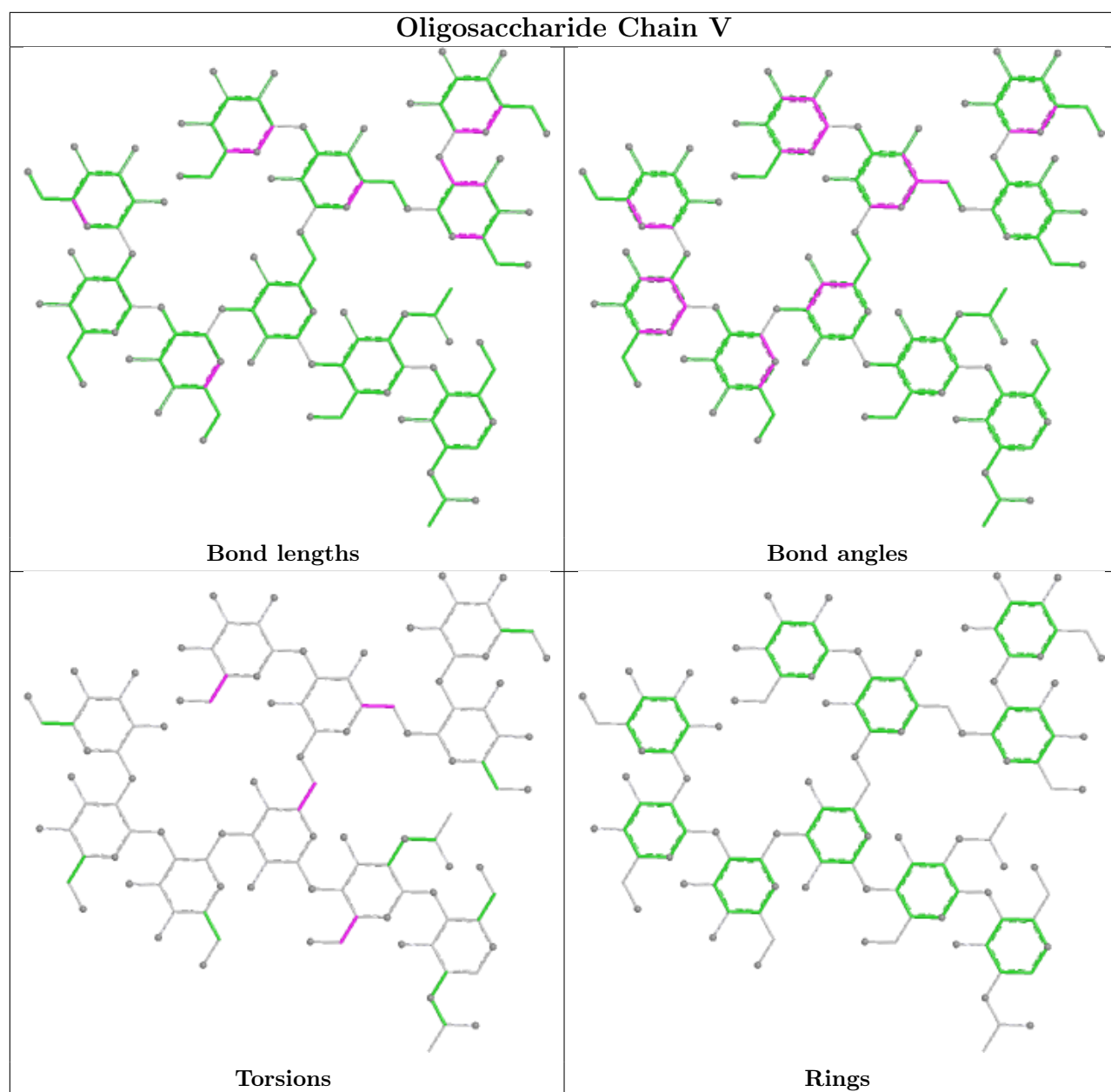
There are no ring outliers.

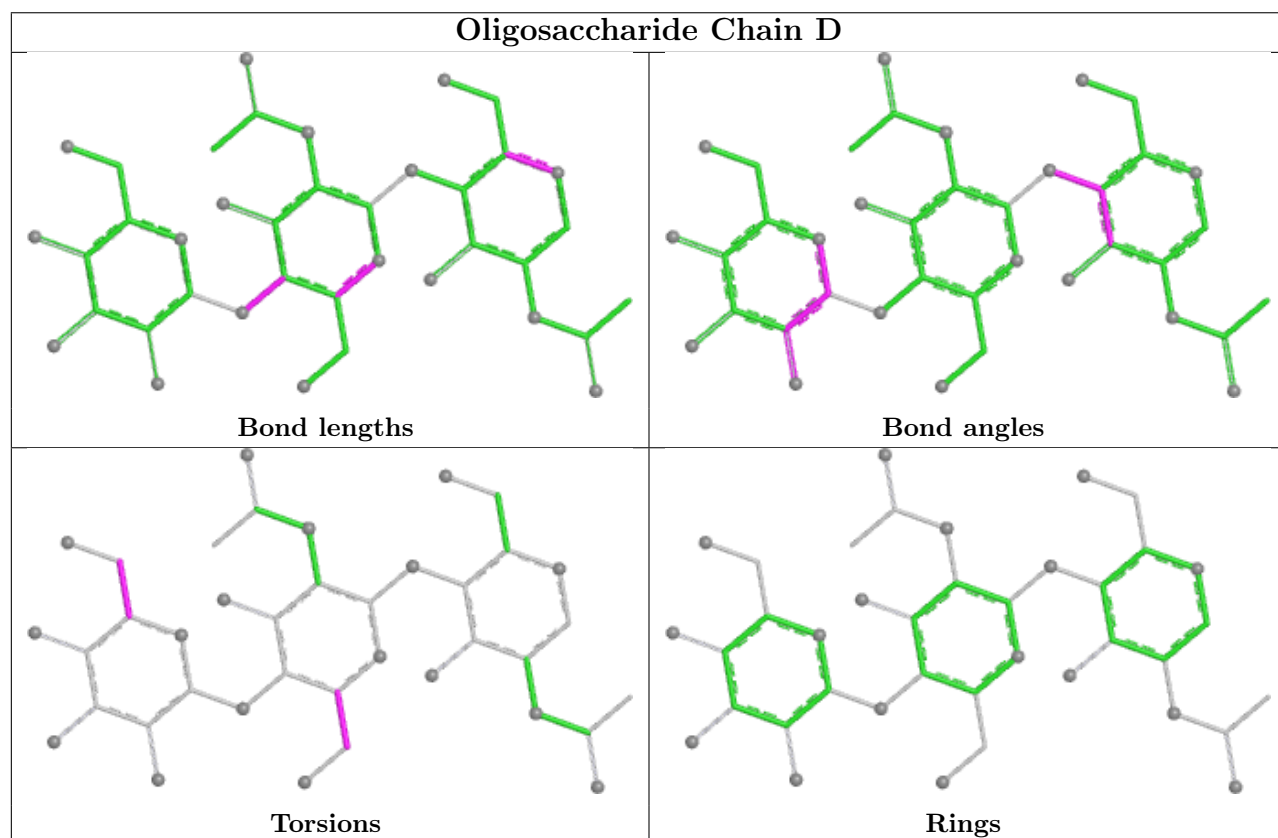
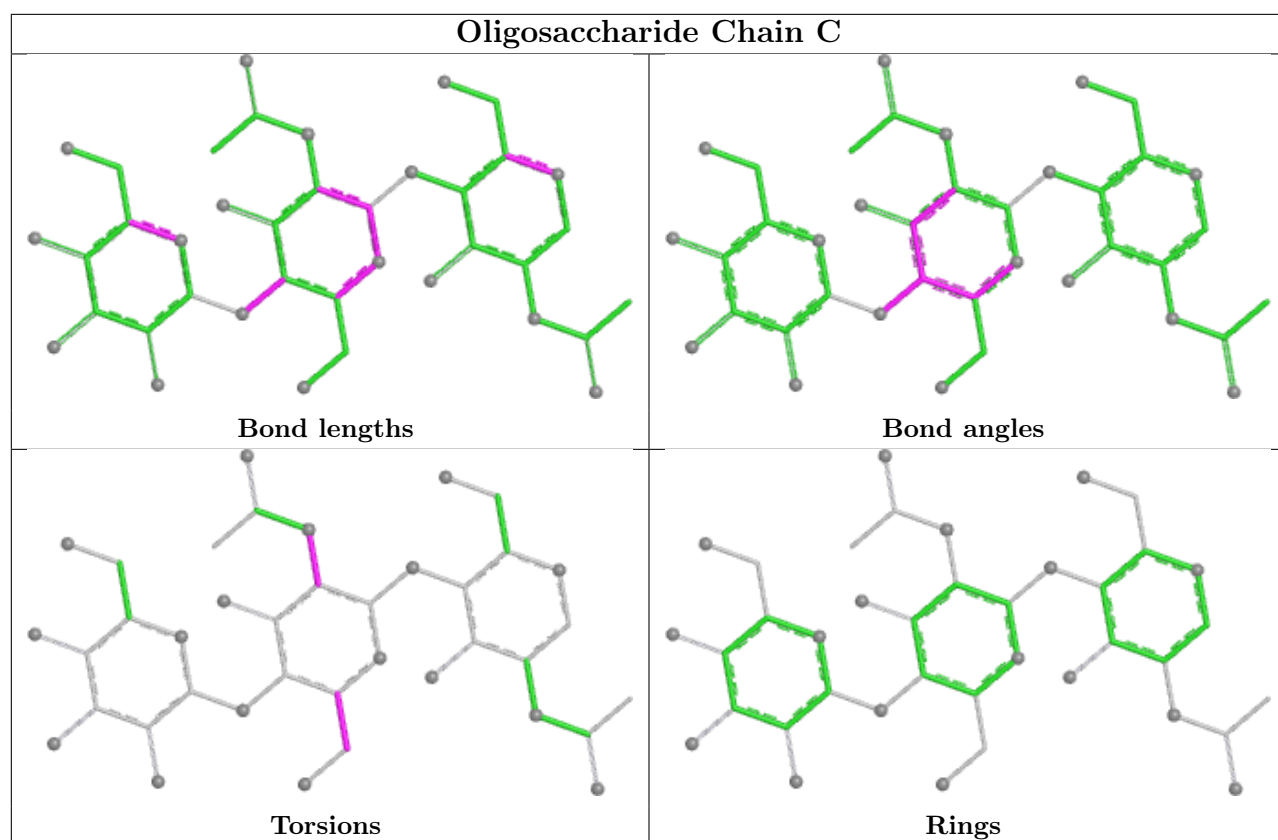
No monomer is involved in short contacts.

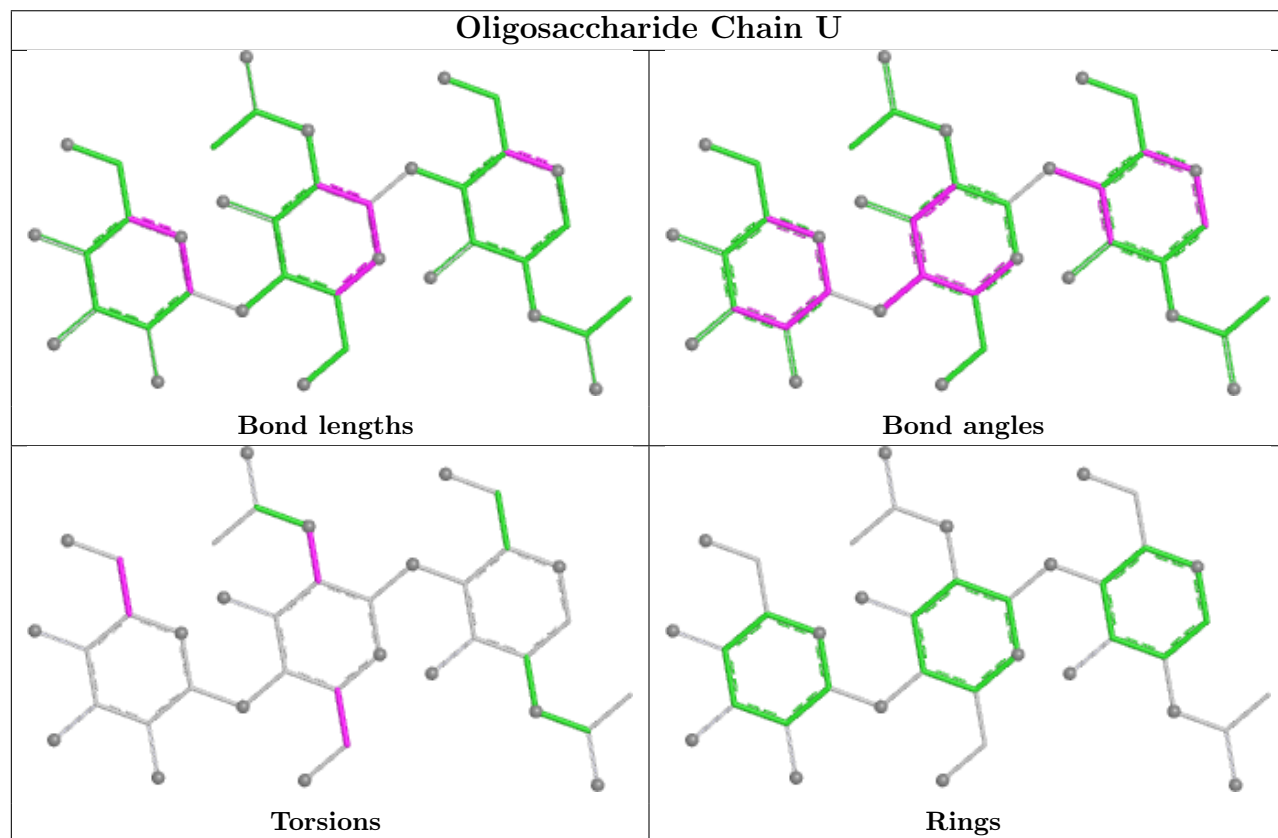
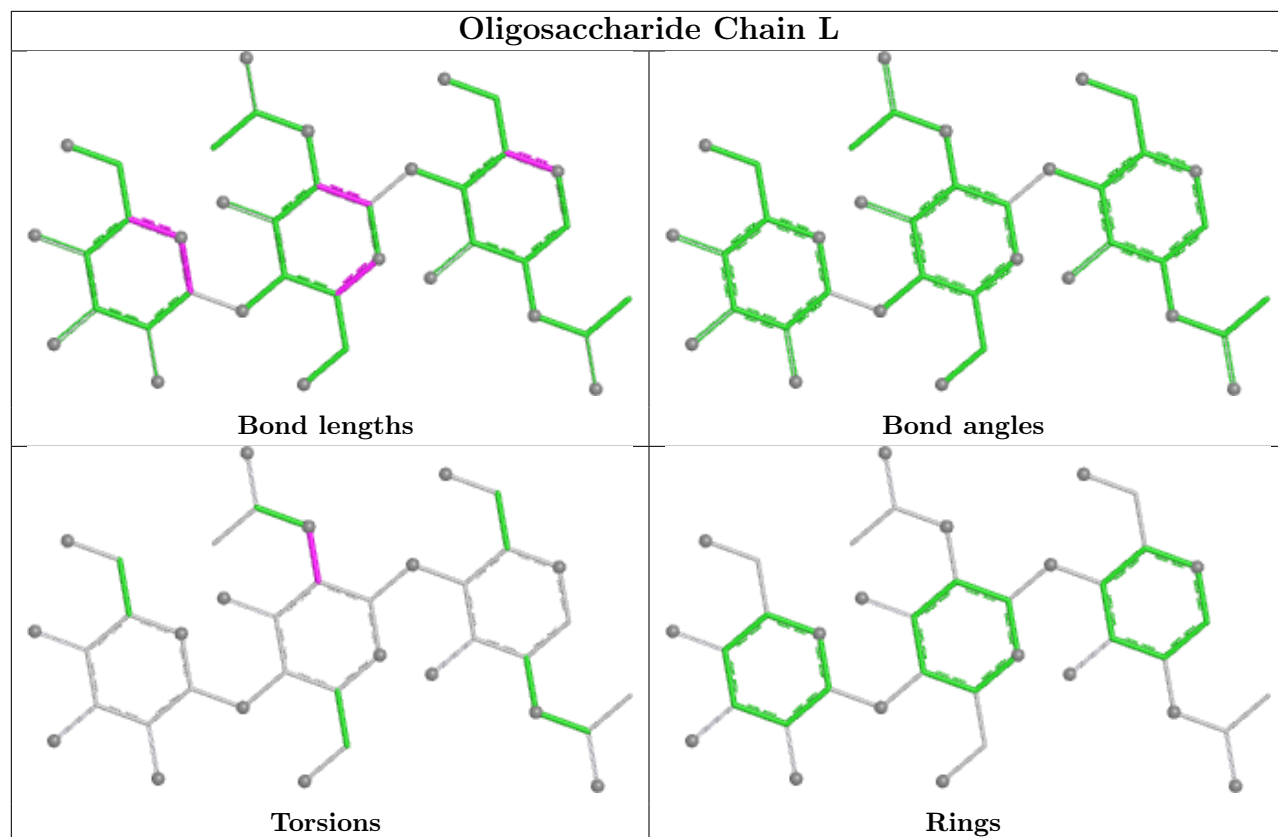
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

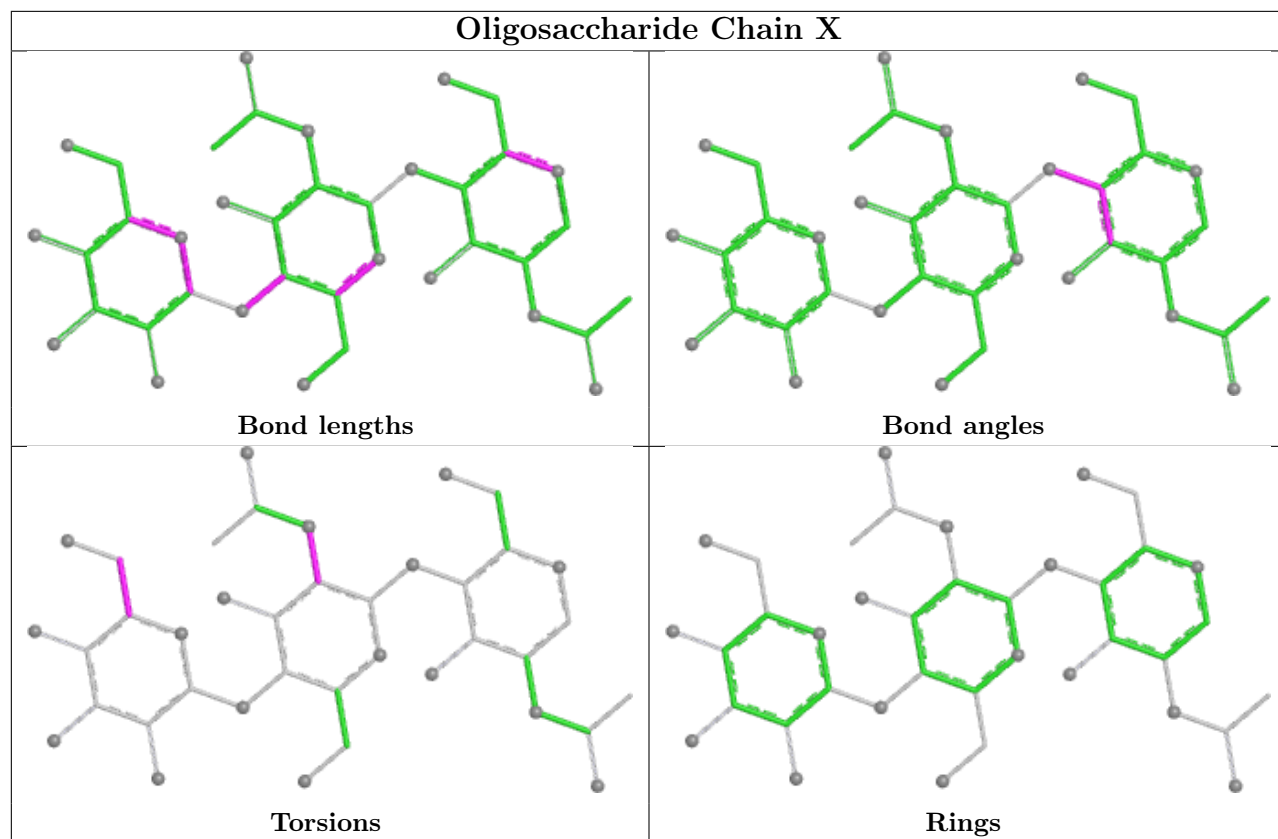


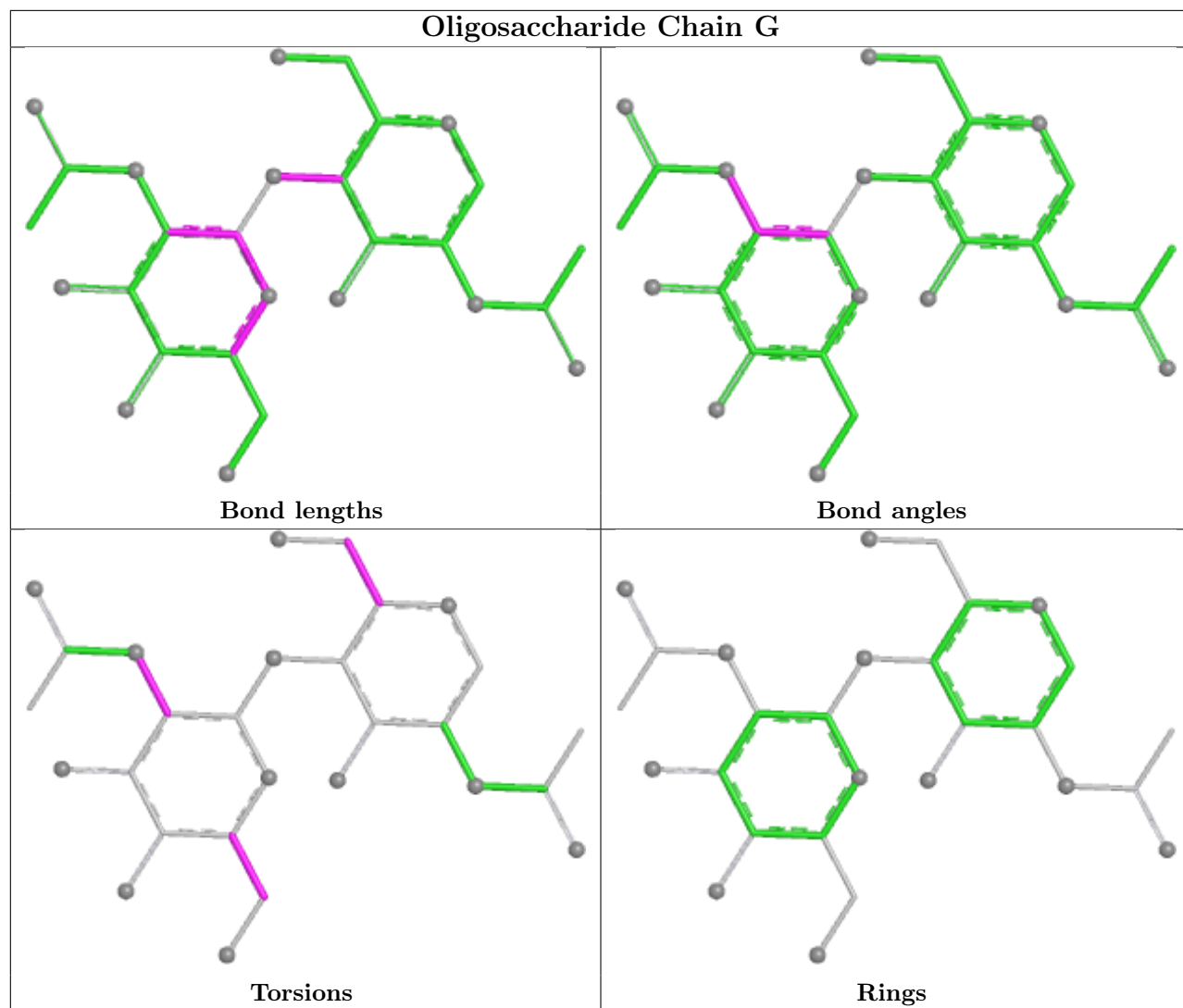


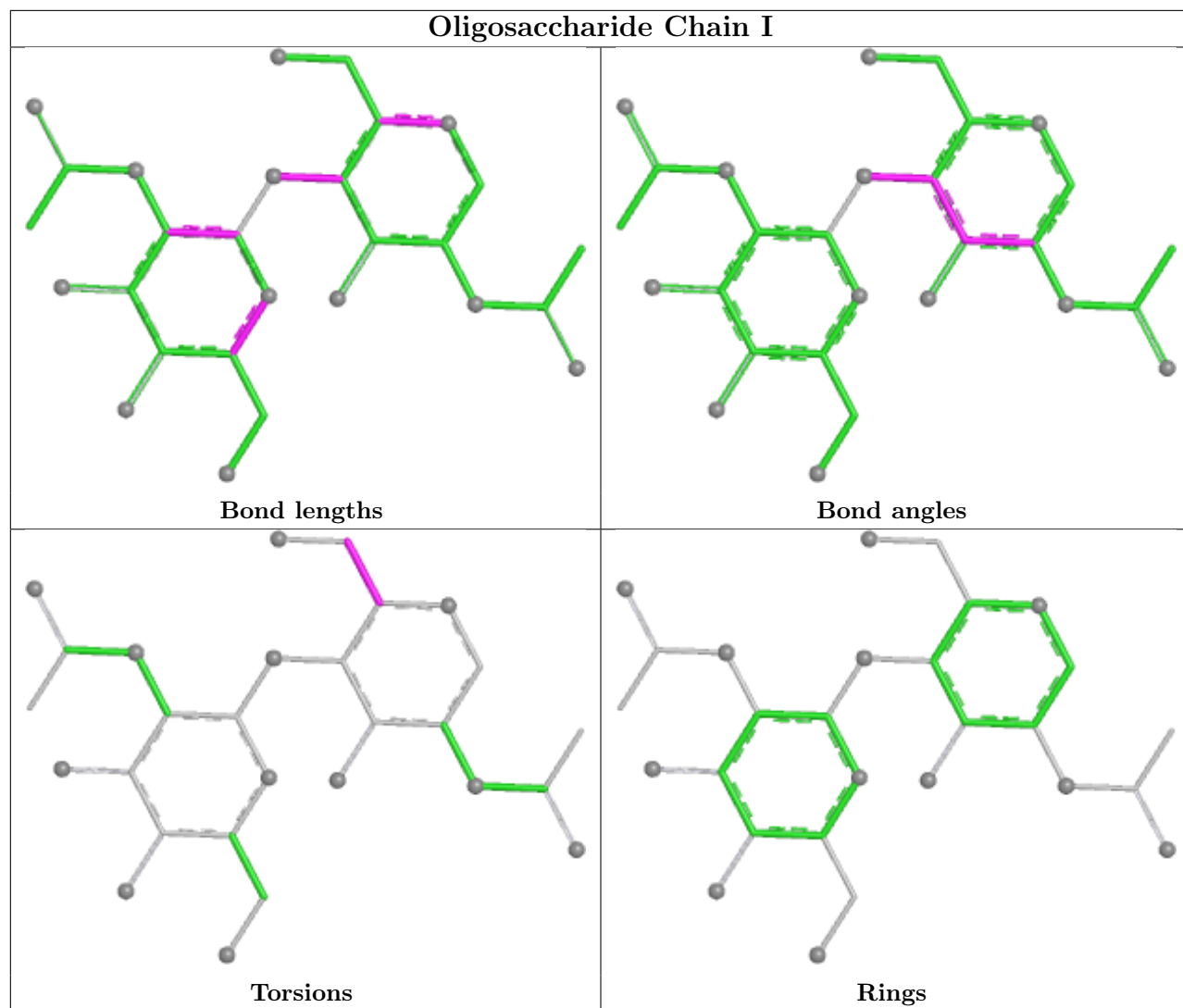


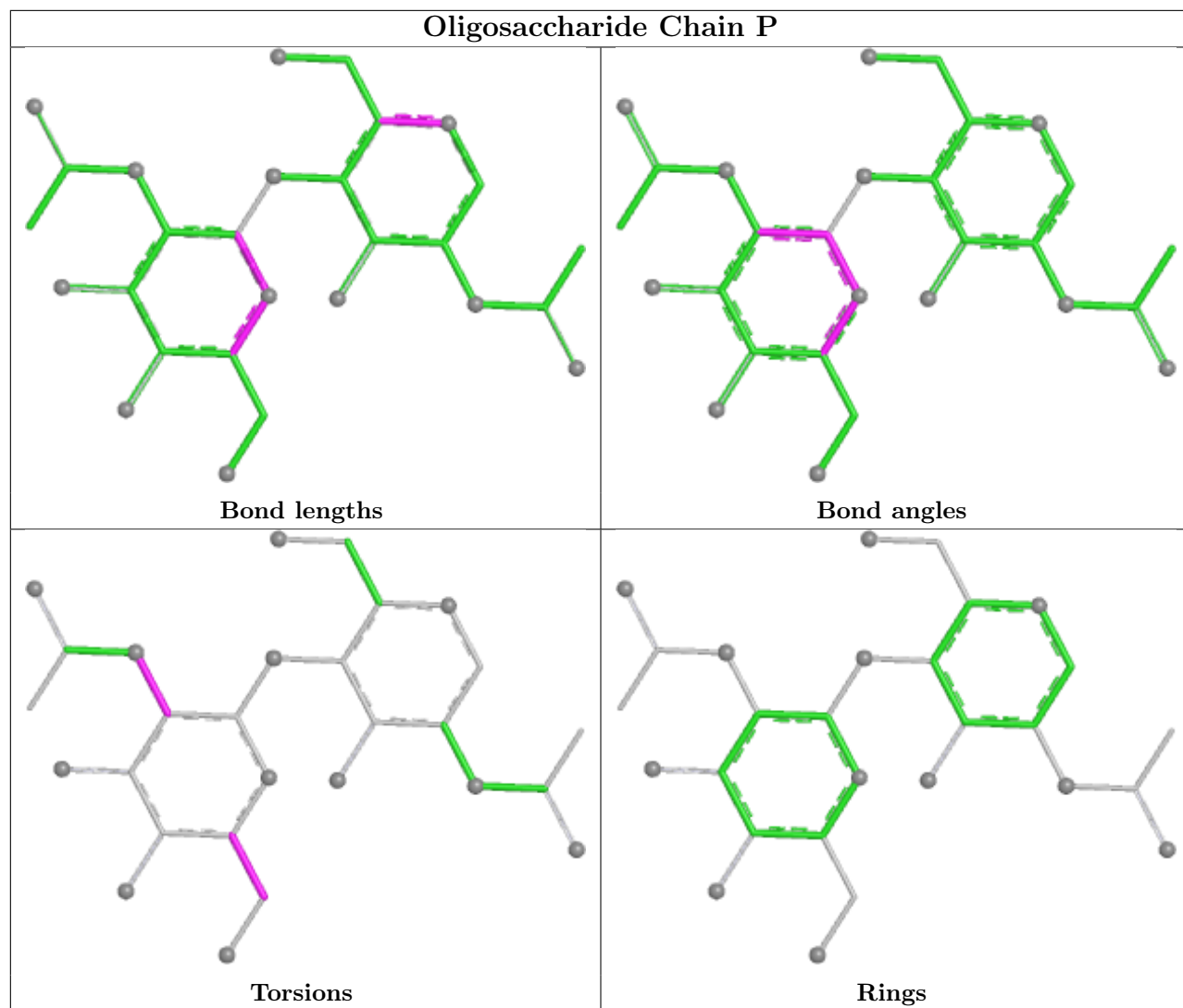


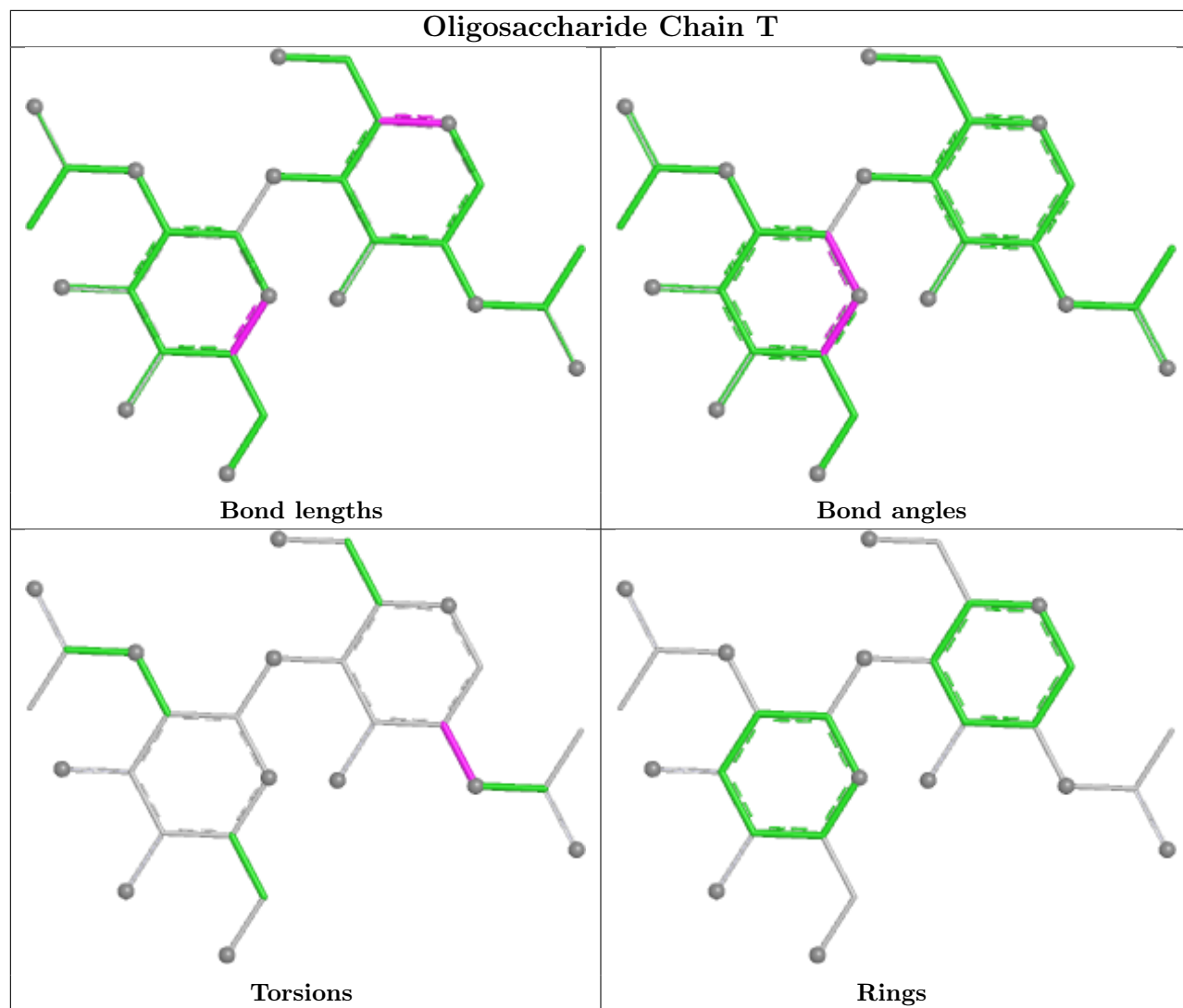


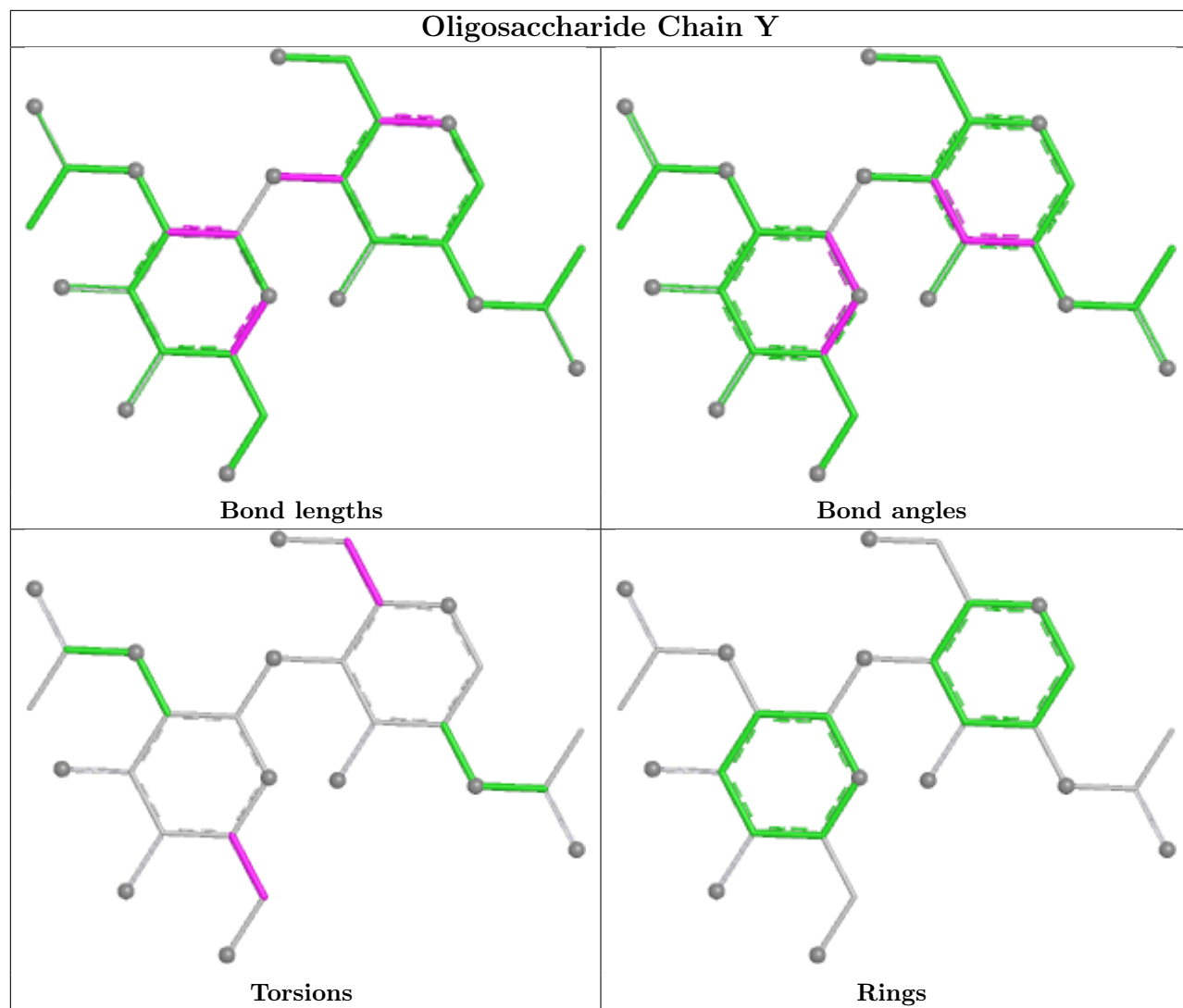


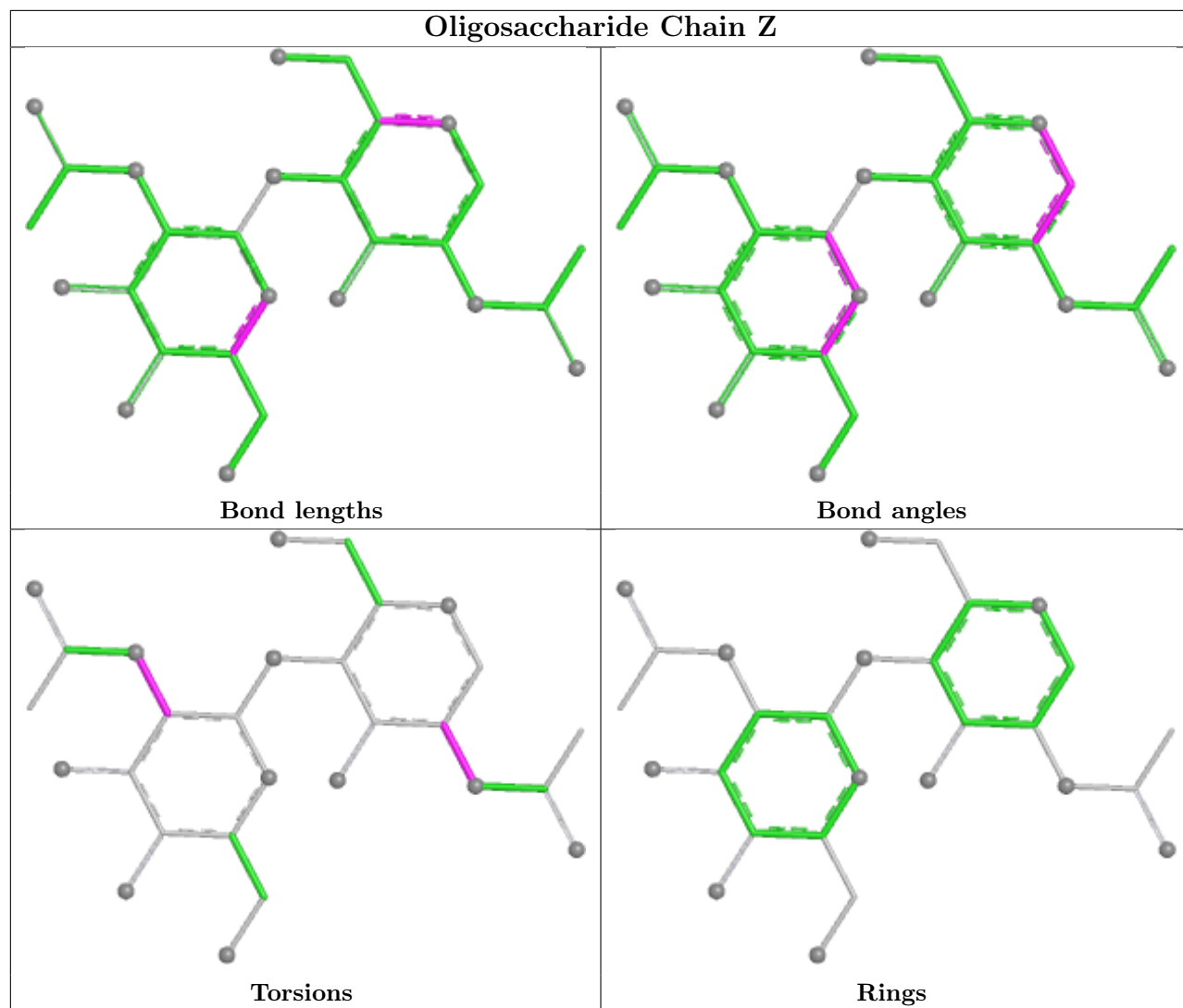


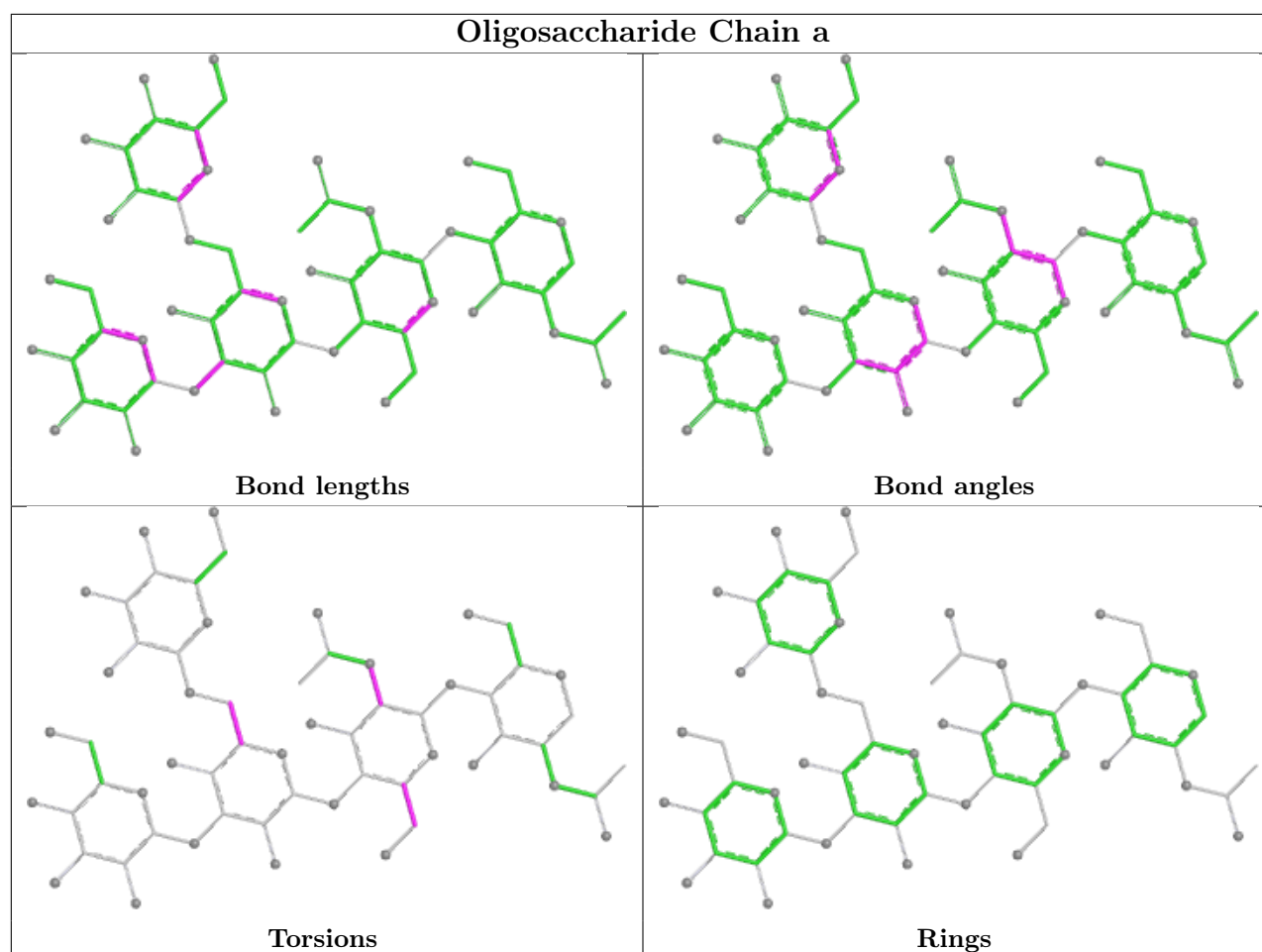












5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
9	NAG	W	605	4	14,14,15	1.28	3 (21%)	17,19,21	0.57	0
9	NAG	H	702	3	14,14,15	1.16	2 (14%)	17,19,21	1.45	1 (5%)
9	NAG	J	602	4	14,14,15	1.10	1 (7%)	17,19,21	0.74	0
9	NAG	B	601	4	14,14,15	1.10	1 (7%)	17,19,21	0.80	0
9	NAG	H	703	3	14,14,15	1.12	1 (7%)	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	W	601	4	14,14,15	1.05	1 (7%)	17,19,21	0.97	1 (5%)
9	NAG	W	603	4	14,14,15	1.10	1 (7%)	17,19,21	0.70	0
9	NAG	Q	701	3	14,14,15	1.17	1 (7%)	17,19,21	0.94	1 (5%)
9	NAG	J	608	4	14,14,15	0.96	1 (7%)	17,19,21	0.85	1 (5%)
9	NAG	B	602	4	14,14,15	1.14	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	S	702	3	14,14,15	1.12	2 (14%)	17,19,21	1.18	1 (5%)
9	NAG	B	603	4	14,14,15	1.23	1 (7%)	17,19,21	0.96	1 (5%)
9	NAG	B	607	4	14,14,15	1.12	1 (7%)	17,19,21	0.86	1 (5%)
9	NAG	J	606	4	14,14,15	1.34	3 (21%)	17,19,21	0.77	1 (5%)
9	NAG	H	701	3	14,14,15	1.16	1 (7%)	17,19,21	0.83	1 (5%)
9	NAG	B	606	4	14,14,15	1.35	3 (21%)	17,19,21	0.83	1 (5%)
9	NAG	W	608	4	14,14,15	0.98	1 (7%)	17,19,21	0.67	0
9	NAG	B	604	4	14,14,15	1.10	1 (7%)	17,19,21	0.76	0
9	NAG	W	606	4	14,14,15	1.29	2 (14%)	17,19,21	1.09	1 (5%)
9	NAG	J	607	4	14,14,15	1.10	1 (7%)	17,19,21	0.83	0
9	NAG	W	604	4	14,14,15	1.12	1 (7%)	17,19,21	0.79	0
9	NAG	Q	702	3	14,14,15	1.17	2 (14%)	17,19,21	1.45	1 (5%)
9	NAG	S	701	3	14,14,15	1.25	2 (14%)	17,19,21	1.03	1 (5%)
9	NAG	S	703	3	14,14,15	1.25	1 (7%)	17,19,21	0.77	1 (5%)
9	NAG	Q	703	3	14,14,15	1.15	1 (7%)	17,19,21	0.90	1 (5%)
9	NAG	J	604	4	14,14,15	1.18	2 (14%)	17,19,21	0.74	0
9	NAG	W	602	4	14,14,15	1.17	1 (7%)	17,19,21	0.93	1 (5%)
9	NAG	J	603	4	14,14,15	1.08	1 (7%)	17,19,21	1.12	1 (5%)
9	NAG	J	605	4	14,14,15	1.29	1 (7%)	17,19,21	0.69	0
9	NAG	W	607	4	14,14,15	1.09	1 (7%)	17,19,21	0.82	0
9	NAG	B	608	4	14,14,15	1.01	1 (7%)	17,19,21	0.63	0
9	NAG	B	605	4	14,14,15	1.33	3 (21%)	17,19,21	0.67	0
9	NAG	J	601	4	14,14,15	1.11	1 (7%)	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	W	605	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	H	702	3	-	1/6/23/26	0/1/1/1
9	NAG	J	602	4	-	0/6/23/26	0/1/1/1
9	NAG	B	601	4	-	0/6/23/26	0/1/1/1
9	NAG	H	703	3	-	1/6/23/26	0/1/1/1
9	NAG	W	601	4	-	0/6/23/26	0/1/1/1
9	NAG	W	603	4	-	2/6/23/26	0/1/1/1
9	NAG	Q	701	3	-	0/6/23/26	0/1/1/1
9	NAG	J	608	4	-	0/6/23/26	0/1/1/1
9	NAG	B	602	4	-	1/6/23/26	0/1/1/1
9	NAG	S	702	3	-	1/6/23/26	0/1/1/1
9	NAG	B	603	4	-	1/6/23/26	0/1/1/1
9	NAG	B	607	4	-	1/6/23/26	0/1/1/1
9	NAG	J	606	4	-	0/6/23/26	0/1/1/1
9	NAG	H	701	3	-	1/6/23/26	0/1/1/1
9	NAG	B	606	4	-	0/6/23/26	0/1/1/1
9	NAG	W	608	4	-	0/6/23/26	0/1/1/1
9	NAG	B	604	4	-	1/6/23/26	0/1/1/1
9	NAG	W	606	4	-	0/6/23/26	0/1/1/1
9	NAG	J	607	4	-	1/6/23/26	0/1/1/1
9	NAG	W	604	4	-	1/6/23/26	0/1/1/1
9	NAG	Q	702	3	-	1/6/23/26	0/1/1/1
9	NAG	S	701	3	-	0/6/23/26	0/1/1/1
9	NAG	S	703	3	-	1/6/23/26	0/1/1/1
9	NAG	Q	703	3	-	1/6/23/26	0/1/1/1
9	NAG	J	604	4	-	1/6/23/26	0/1/1/1
9	NAG	W	602	4	-	0/6/23/26	0/1/1/1
9	NAG	J	603	4	-	1/6/23/26	0/1/1/1
9	NAG	J	605	4	-	0/6/23/26	0/1/1/1
9	NAG	W	607	4	-	1/6/23/26	0/1/1/1
9	NAG	B	608	4	-	0/6/23/26	0/1/1/1
9	NAG	B	605	4	-	0/6/23/26	0/1/1/1
9	NAG	J	601	4	-	0/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	605	NAG	O5-C5	3.17	1.49	1.43
9	B	606	NAG	O5-C5	3.03	1.49	1.43
9	W	605	NAG	O5-C5	2.97	1.49	1.43
9	J	606	NAG	O5-C5	2.88	1.49	1.43
9	W	606	NAG	O5-C5	2.87	1.49	1.43
9	B	605	NAG	O5-C5	2.86	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	NAG	O5-C5	2.68	1.48	1.43
9	W	602	NAG	O5-C5	2.68	1.48	1.43
9	H	701	NAG	O5-C5	2.67	1.48	1.43
9	S	701	NAG	O5-C5	2.66	1.48	1.43
9	B	603	NAG	O5-C5	2.64	1.48	1.43
9	S	703	NAG	O5-C5	2.62	1.48	1.43
9	J	601	NAG	O5-C5	2.56	1.48	1.43
9	B	607	NAG	O5-C5	2.50	1.48	1.43
9	J	603	NAG	O5-C5	2.48	1.48	1.43
9	H	703	NAG	O5-C5	2.45	1.48	1.43
9	J	602	NAG	O5-C5	2.45	1.48	1.43
9	W	604	NAG	O5-C5	2.44	1.48	1.43
9	B	605	NAG	C1-C2	2.43	1.55	1.52
9	Q	701	NAG	O5-C5	2.43	1.48	1.43
9	W	607	NAG	O5-C5	2.41	1.48	1.43
9	J	607	NAG	O5-C5	2.39	1.48	1.43
9	J	606	NAG	C1-C2	2.39	1.55	1.52
9	W	601	NAG	O5-C5	2.37	1.48	1.43
9	W	608	NAG	O5-C5	2.36	1.48	1.43
9	B	608	NAG	O5-C5	2.35	1.48	1.43
9	J	604	NAG	O5-C5	2.34	1.48	1.43
9	Q	703	NAG	O5-C5	2.34	1.48	1.43
9	H	702	NAG	C1-C2	2.33	1.55	1.52
9	B	602	NAG	O5-C5	2.30	1.47	1.43
9	B	606	NAG	O5-C1	2.28	1.47	1.43
9	W	603	NAG	O5-C5	2.28	1.47	1.43
9	B	606	NAG	C1-C2	2.28	1.55	1.52
9	Q	702	NAG	C1-C2	2.26	1.55	1.52
9	Q	702	NAG	O5-C5	2.20	1.47	1.43
9	W	606	NAG	C1-C2	2.20	1.55	1.52
9	J	608	NAG	O5-C5	2.19	1.47	1.43
9	S	701	NAG	C1-C2	2.15	1.55	1.52
9	B	602	NAG	C1-C2	2.15	1.55	1.52
9	J	606	NAG	O5-C1	2.13	1.47	1.43
9	S	702	NAG	C1-C2	2.11	1.55	1.52
9	J	604	NAG	C1-C2	2.09	1.55	1.52
9	H	702	NAG	O5-C5	2.08	1.47	1.43
9	B	605	NAG	O5-C1	2.05	1.47	1.43
9	B	604	NAG	O5-C5	2.05	1.47	1.43
9	W	605	NAG	O5-C1	2.02	1.47	1.43
9	S	702	NAG	O5-C5	2.02	1.47	1.43
9	W	605	NAG	C1-C2	2.01	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	702	NAG	C1-O5-C5	5.58	119.66	112.19
9	H	702	NAG	C1-O5-C5	5.40	119.42	112.19
9	S	702	NAG	C1-O5-C5	4.34	118.00	112.19
9	J	603	NAG	C1-O5-C5	3.75	117.22	112.19
9	J	601	NAG	C1-O5-C5	3.42	116.77	112.19
9	S	701	NAG	C1-O5-C5	3.32	116.63	112.19
9	W	606	NAG	C1-O5-C5	3.29	116.60	112.19
9	Q	701	NAG	C1-O5-C5	3.24	116.53	112.19
9	B	603	NAG	C1-O5-C5	3.23	116.51	112.19
9	W	601	NAG	C1-O5-C5	2.87	116.03	112.19
9	W	602	NAG	C1-O5-C5	2.65	115.74	112.19
9	Q	703	NAG	C1-O5-C5	2.54	115.59	112.19
9	J	608	NAG	C1-O5-C5	2.44	115.45	112.19
9	B	606	NAG	C1-O5-C5	2.44	115.45	112.19
9	H	701	NAG	C1-O5-C5	2.32	115.30	112.19
9	B	602	NAG	C1-O5-C5	2.13	115.04	112.19
9	J	606	NAG	C1-O5-C5	2.13	115.03	112.19
9	S	703	NAG	C1-O5-C5	2.04	114.92	112.19
9	B	607	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	702	NAG	O5-C5-C6-O6
9	H	703	NAG	O5-C5-C6-O6
9	J	607	NAG	O5-C5-C6-O6
9	W	604	NAG	O5-C5-C6-O6
9	Q	703	NAG	O5-C5-C6-O6
9	B	604	NAG	O5-C5-C6-O6
9	J	604	NAG	O5-C5-C6-O6
9	B	607	NAG	O5-C5-C6-O6
9	W	603	NAG	O5-C5-C6-O6
9	J	603	NAG	O5-C5-C6-O6
9	Q	702	NAG	O5-C5-C6-O6
9	S	702	NAG	O5-C5-C6-O6
9	W	607	NAG	O5-C5-C6-O6
9	S	703	NAG	O5-C5-C6-O6
9	B	603	NAG	O5-C5-C6-O6
9	W	603	NAG	C1-C2-N2-C7
9	H	701	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	B	602	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-27628. These allow visual inspection of the internal detail of the map and identification of artifacts.

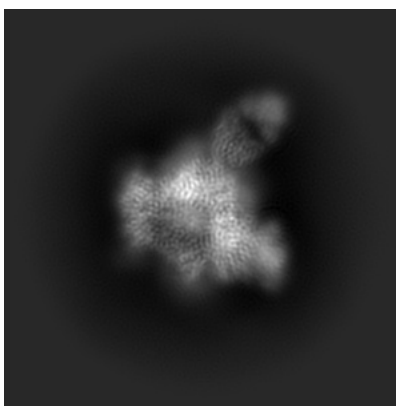
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

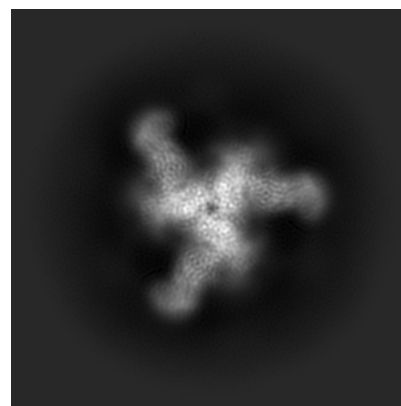
6.1.1 Primary map



X



Y

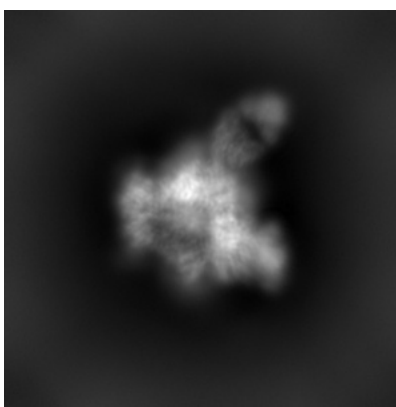


Z

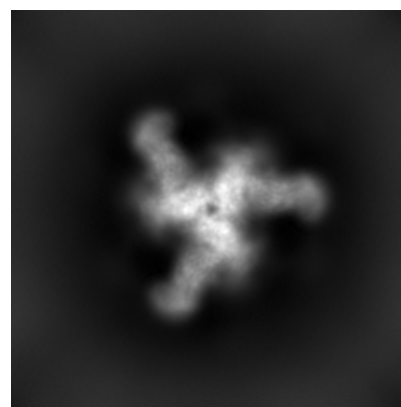
6.1.2 Raw map



X



Y

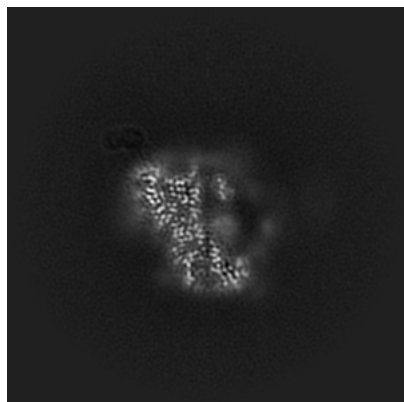


Z

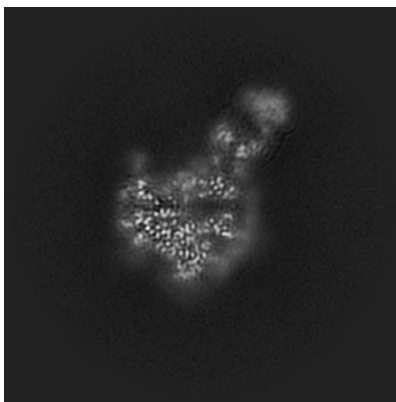
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

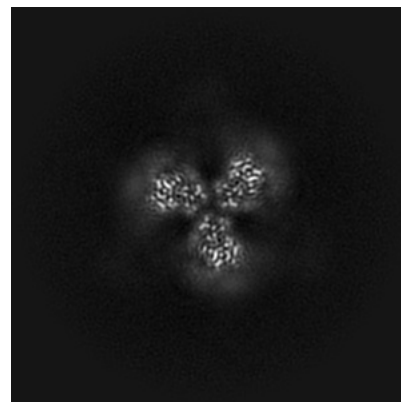
6.2.1 Primary map



X Index: 160

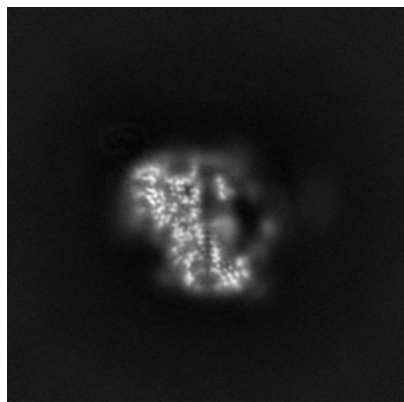


Y Index: 160

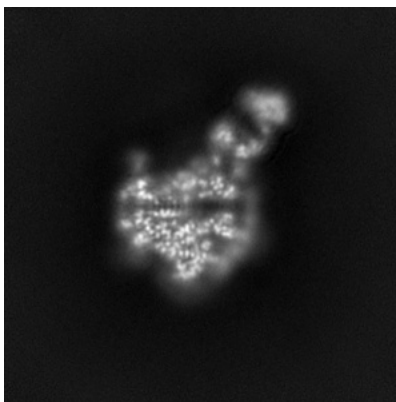


Z Index: 160

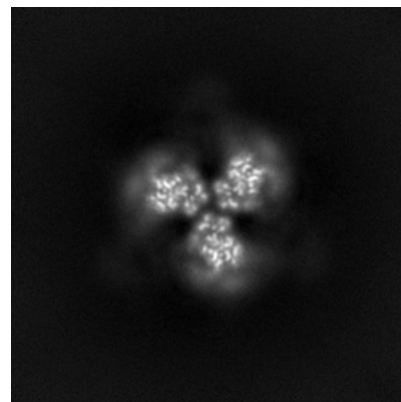
6.2.2 Raw map



X Index: 160



Y Index: 160

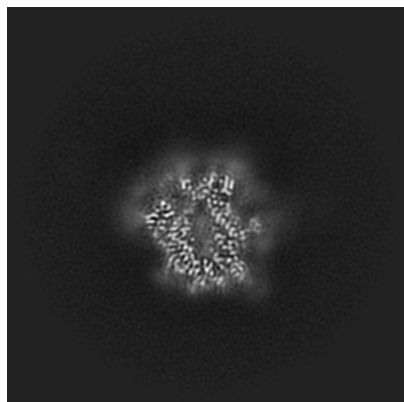


Z Index: 160

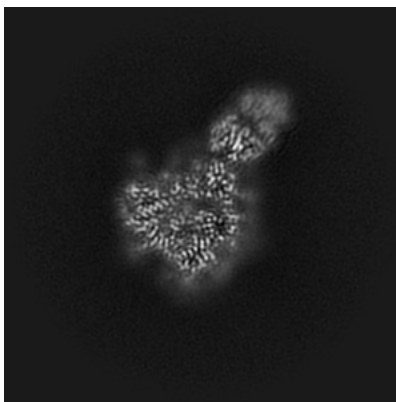
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

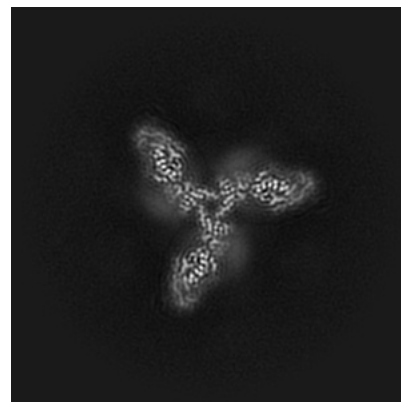
6.3.1 Primary map



X Index: 171

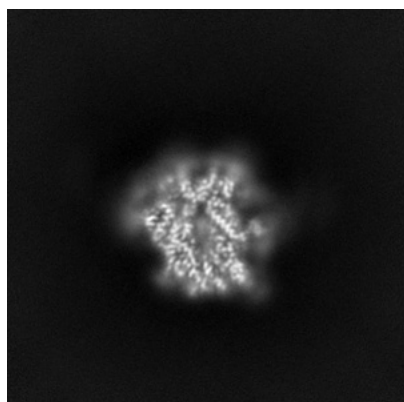


Y Index: 167

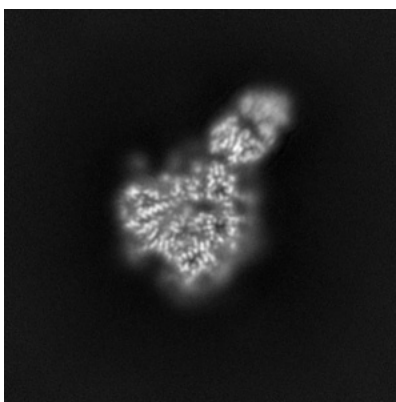


Z Index: 181

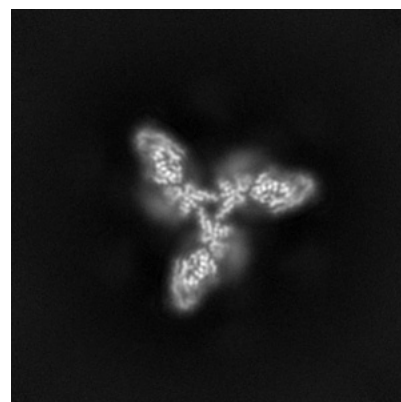
6.3.2 Raw map



X Index: 170



Y Index: 167

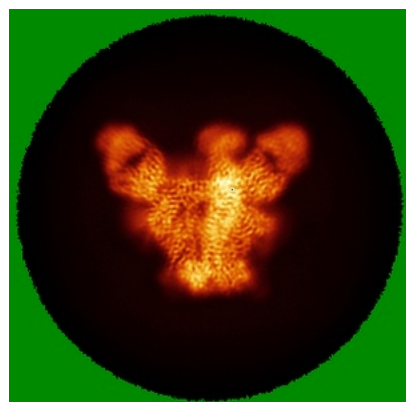


Z Index: 181

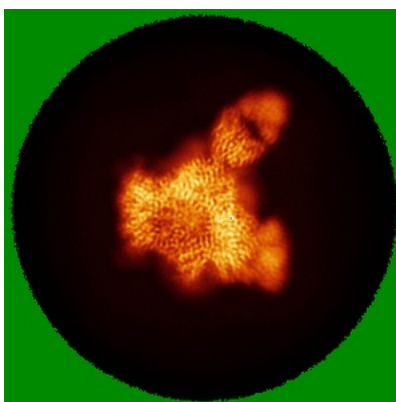
The images above show the largest variance slices of the map in three orthogonal directions.

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

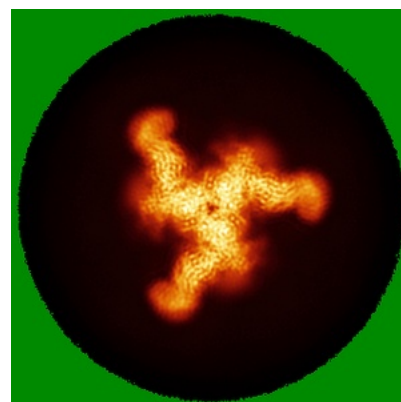
6.4.1 Primary map



X

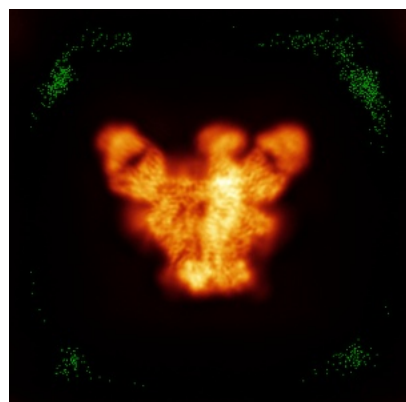


Y

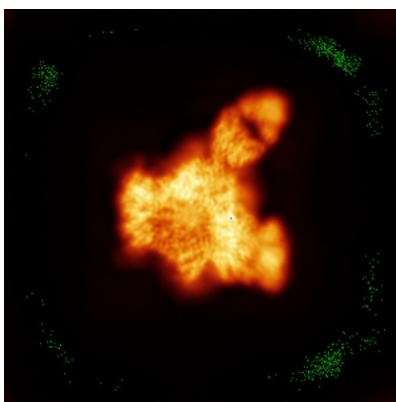


Z

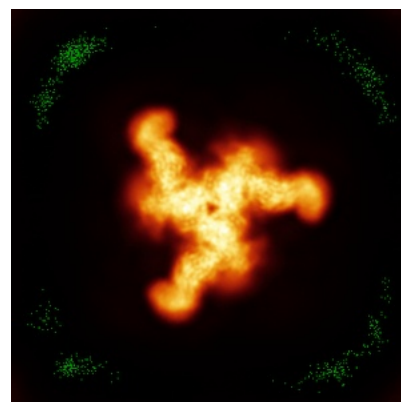
6.4.2 Raw map



X



Y

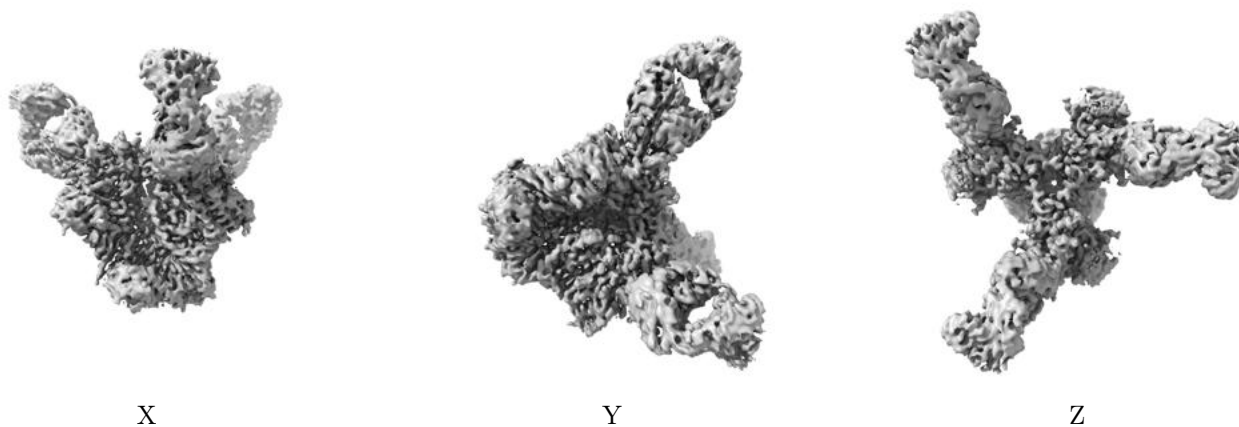


Z

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

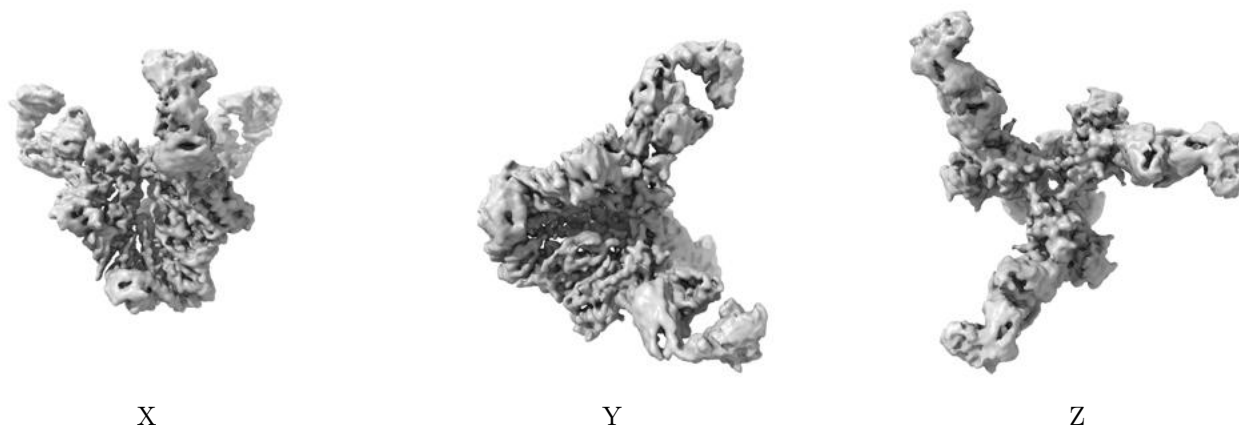
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

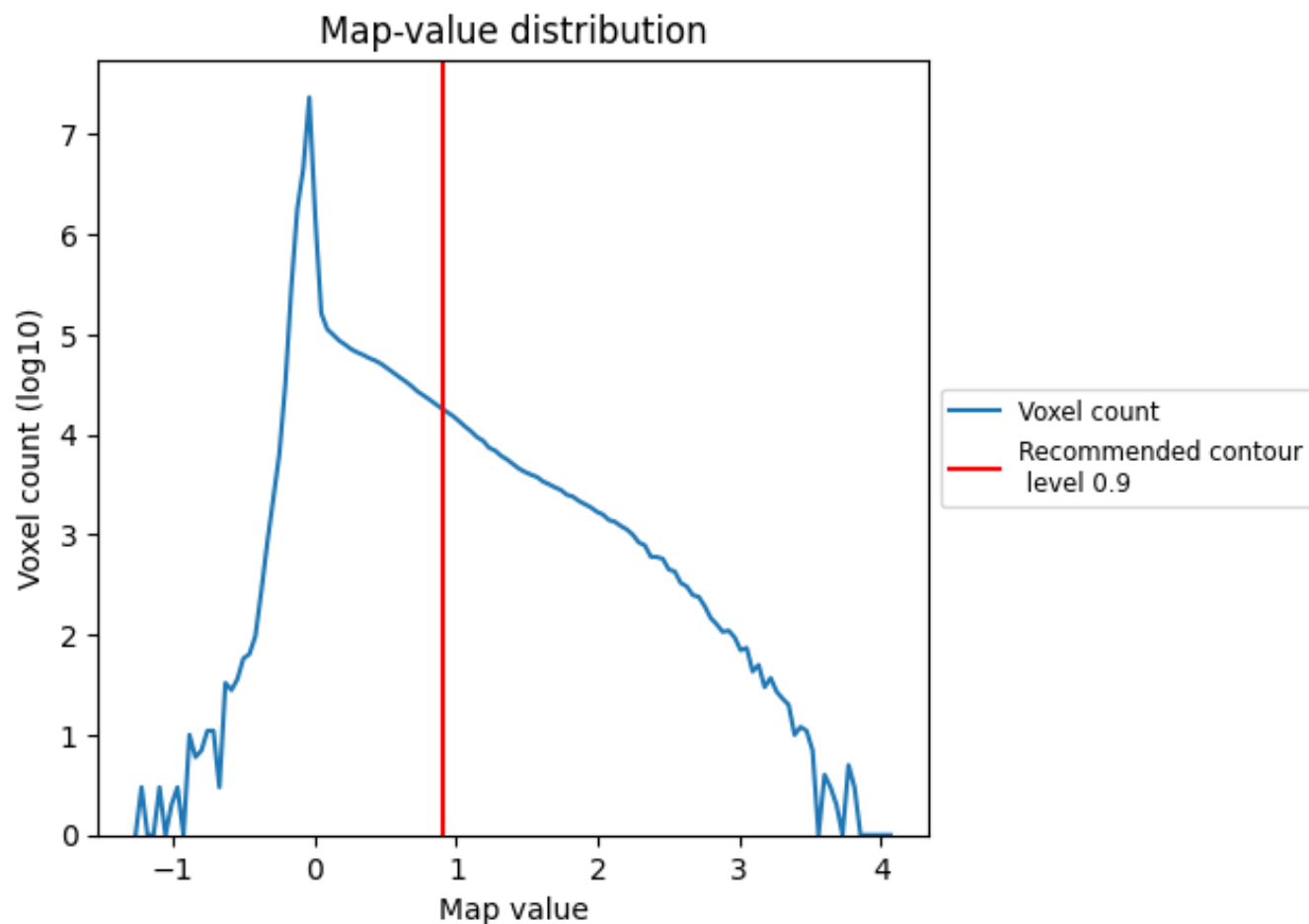
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

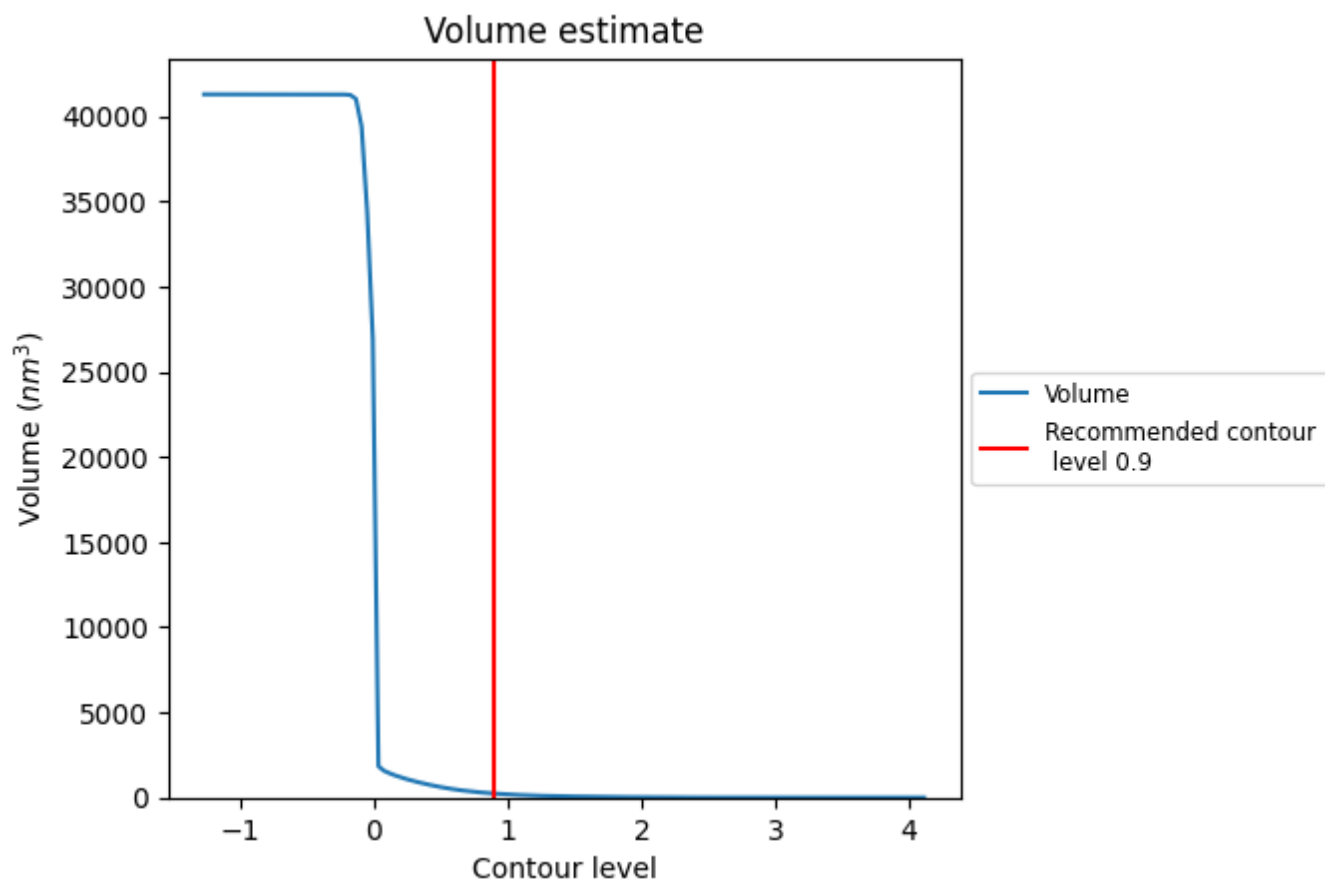
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

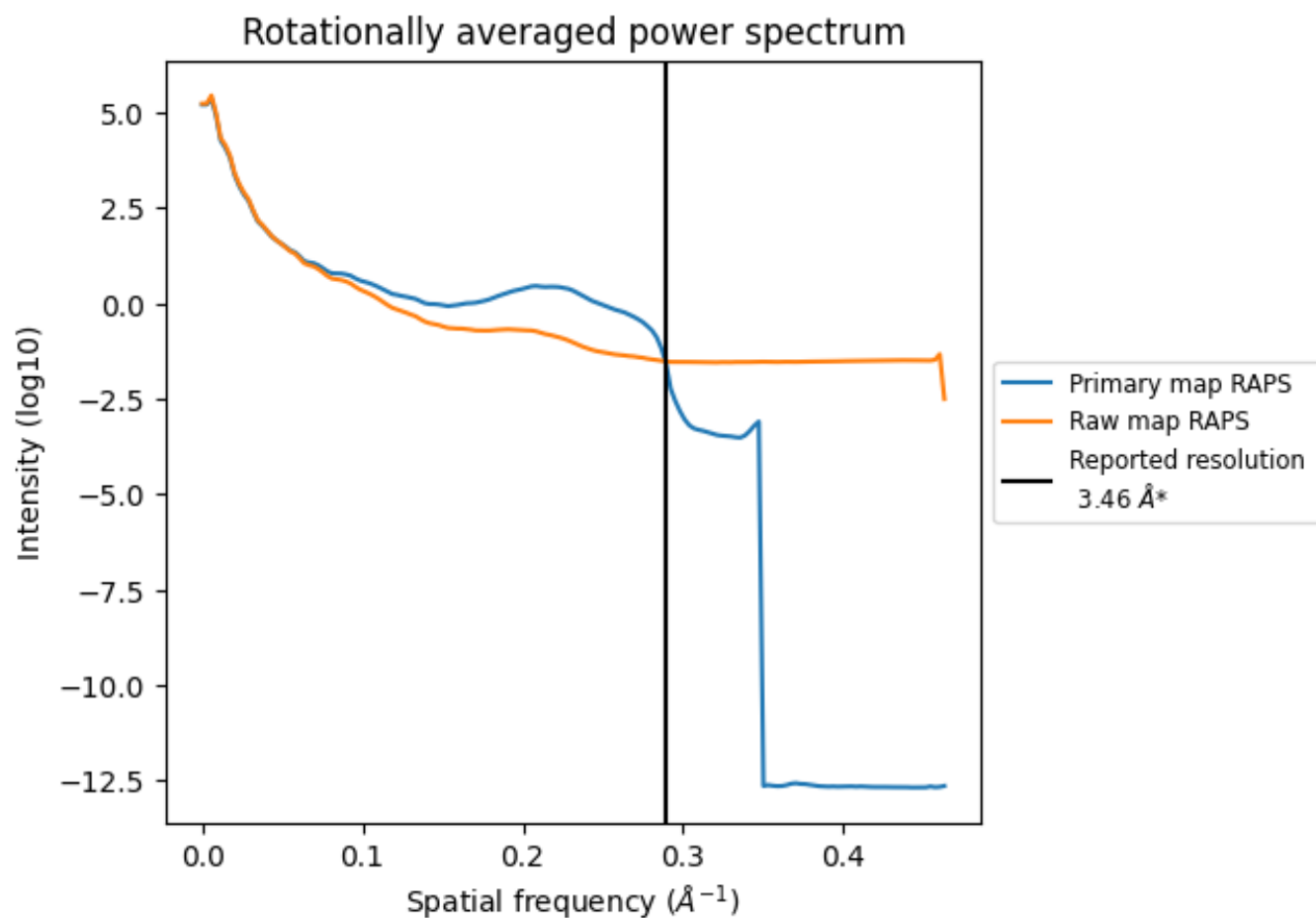
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm^3 ; this corresponds to an approximate mass of 215 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 ⓘ

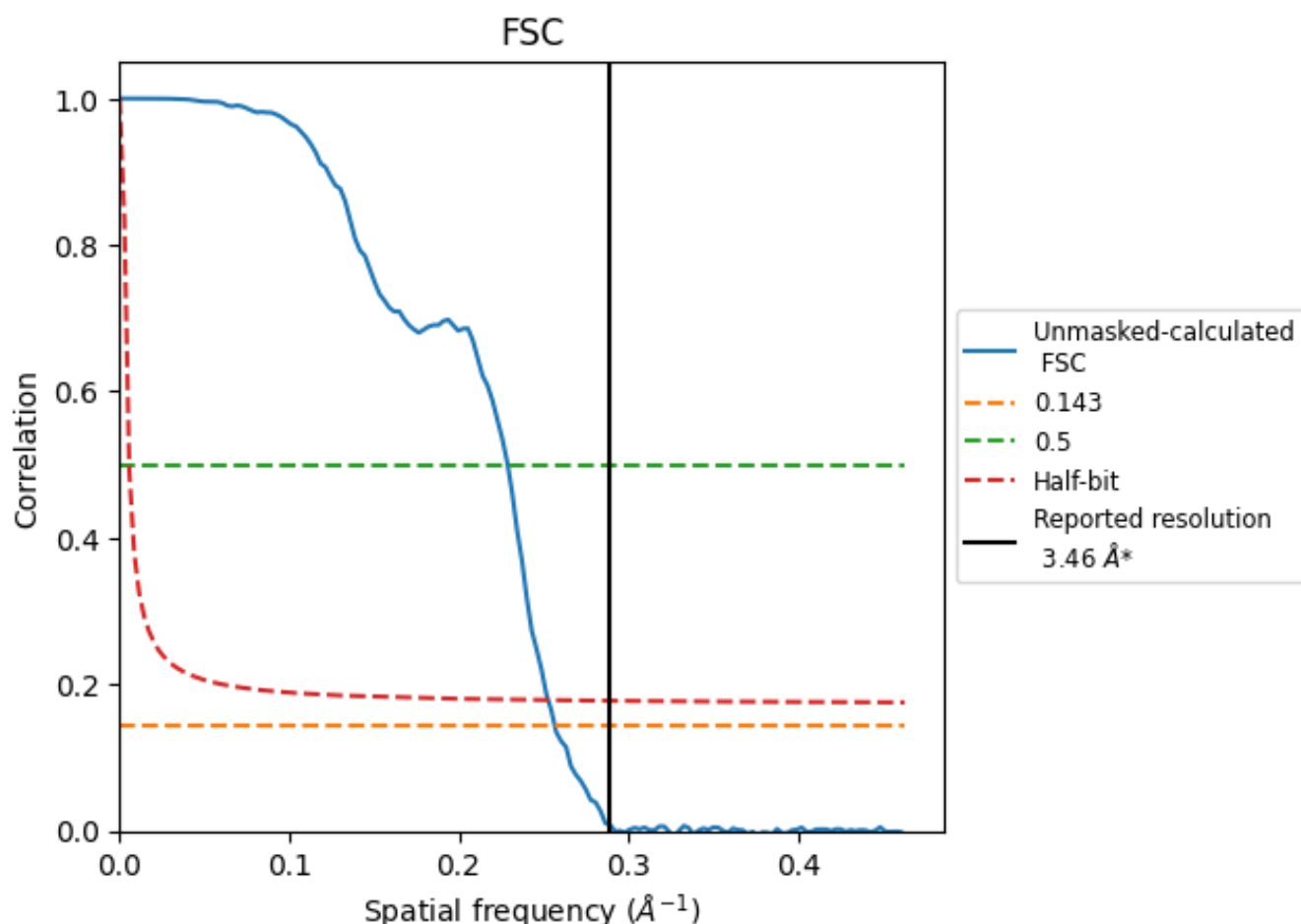


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.289 \AA^{-1}

8.2 Resolution estimates [i](#)

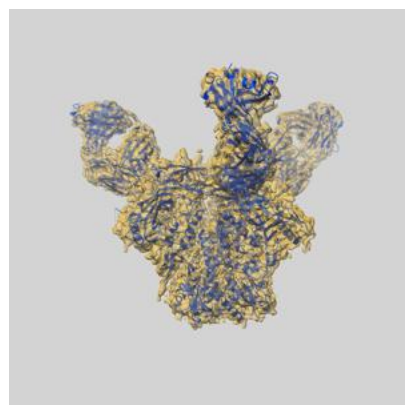
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	4.37	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.46 by more than 10 %

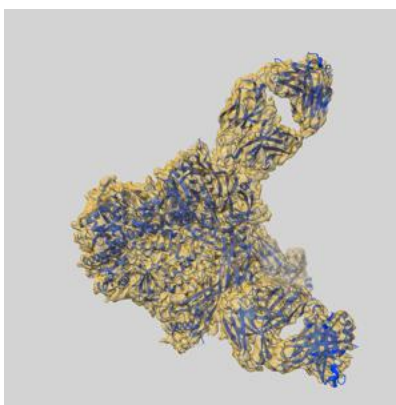
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27628 and PDB model 8DP1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

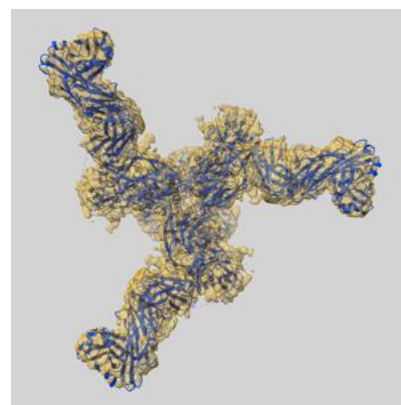
9.1 Map-model overlay [i](#)



X



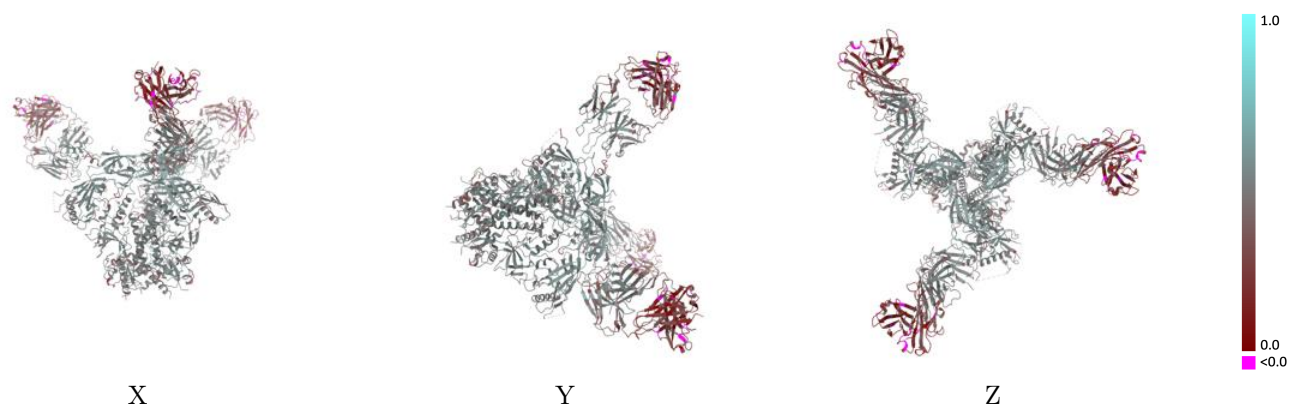
Y



Z

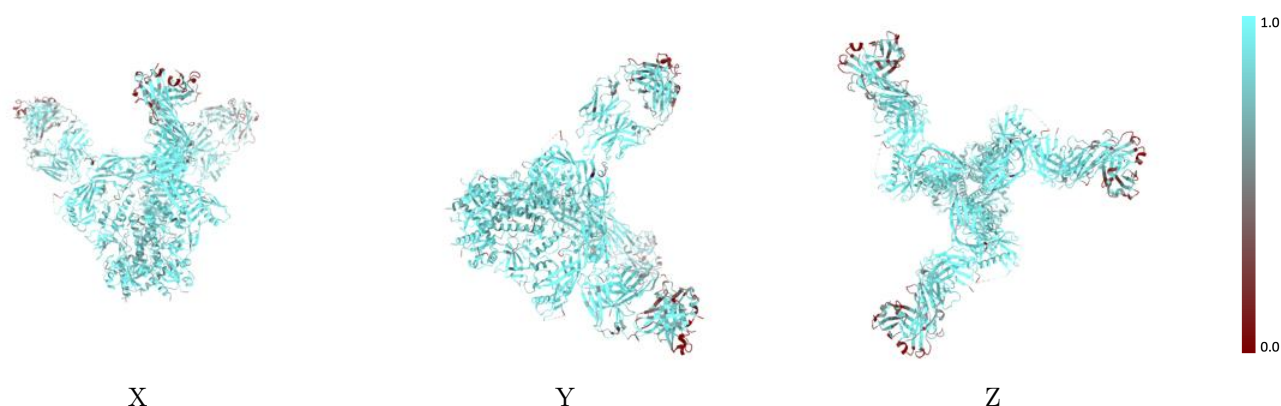
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



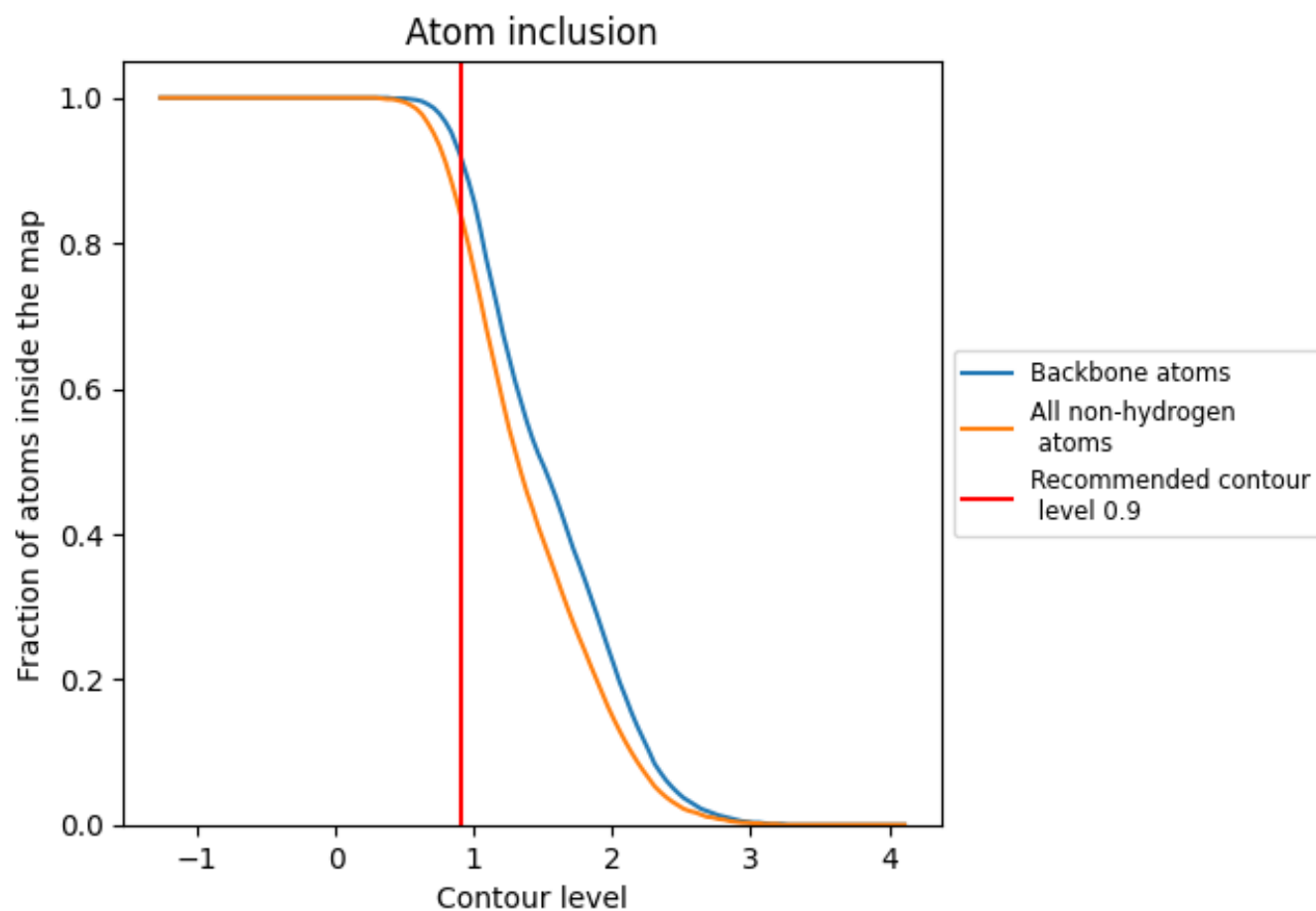
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.4330
A	 0.7070	 0.3630
B	 0.9110	 0.4960
C	 0.8210	 0.4400
D	 0.5130	 0.4310
E	 0.7950	 0.3810
F	 0.7570	 0.3380
G	 0.5710	 0.3960
H	 0.8490	 0.4580
I	 0.7140	 0.4780
J	 0.9050	 0.4980
K	 0.6900	 0.3520
L	 0.6150	 0.4960
M	 0.7670	 0.3390
N	 0.8040	 0.3740
O	 0.7710	 0.3380
P	 0.7140	 0.4860
Q	 0.8480	 0.4600
R	 0.7970	 0.3780
S	 0.8440	 0.4560
T	 0.7140	 0.4780
U	 0.7950	 0.4550
V	 0.7070	 0.3590
W	 0.9090	 0.4970
X	 0.6150	 0.4860
Y	 0.7140	 0.4670
Z	 0.7140	 0.4890
a	 0.6890	 0.4410

