



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 10:54 AM EST

PDB ID : 7T73  
EMDB ID : EMD-25732  
Title : HIV-1 Envelope ApexGT2.2MUT in complex with PCT64.LMCA Fab  
Authors : Berndsen, Z.T.  
Deposited on : 2021-12-14  
Resolution : 4.00 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](mailto:validation@mail.wwpdb.org)

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<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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

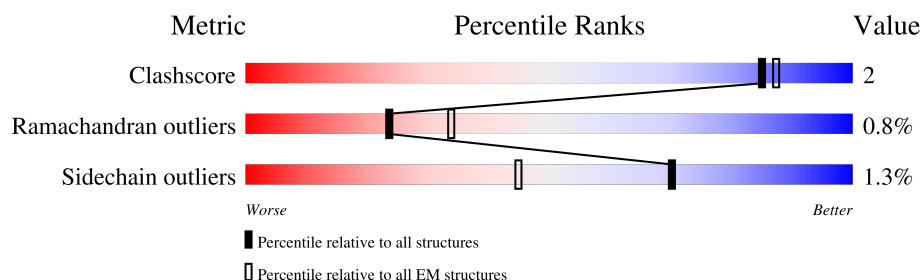
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	H	238	<div> <div>29%</div> <div>52%</div> <div>45%</div> </div>
2	L	214	<div> <div>26%</div> <div>44%</div> <div>5%</div> <div>50%</div> </div>
3	A	504	<div> <div>82%</div> <div>5%</div> <div>12%</div> </div>
3	C	504	<div> <div>81%</div> <div>14%</div> </div>
3	E	504	<div> <div>81%</div> <div>6%</div> <div>12%</div> </div>
4	B	162	<div> <div>64%</div> <div>8%</div> <div>27%</div> </div>
4	D	162	<div> <div>63%</div> <div>7%</div> <div>27%</div> </div>
4	F	162	<div> <div>60%</div> <div>12%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
5	G	2	 100%
5	I	2	 100%
5	K	2	 100%
5	M	2	 50% 100%
5	O	2	 100%
5	Q	2	 100%
5	T	2	 50% 100%
5	U	2	 100%
6	J	4	 100%
6	P	4	 100%
6	S	4	 100%
7	N	3	 100%
7	R	3	 33% 67% 33%
8	V	7	 14% 29% 71%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	F	701	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16010 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 PCT64.LMCA Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	132	Total	C	N	O	S	0	0
			1046	660	171	209	6		

- Molecule 2 is a protein called PCT64.LMCA Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	106	Total	C	N	O	S	0	0
			801	504	134	161	2		

- Molecule 3 is a protein called HIV Envelope ApexGT2.2MUT gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	441	Total	C	N	O	S	0	0
			3458	2171	606	654	27		
3	C	433	Total	C	N	O	S	0	0
			3392	2129	592	644	27		
3	E	441	Total	C	N	O	S	0	0
			3458	2171	606	654	27		

- Molecule 4 is a protein called HIV Envelope ApexGT2.2MUT gp41.

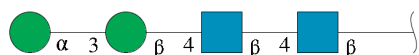
Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	118	Total	C	N	O	S	0	0
			934	587	162	179	6		
4	D	118	Total	C	N	O	S	0	0
			934	587	162	179	6		
4	F	118	Total	C	N	O	S	0	0
			934	587	162	179	6		

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



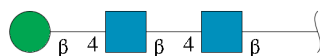
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		

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



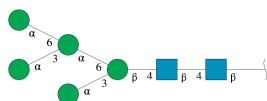
Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	4	Total	C	N	O	0	0
			50	28	2	20		
6	P	4	Total	C	N	O	0	0
			50	28	2	20		
6	S	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



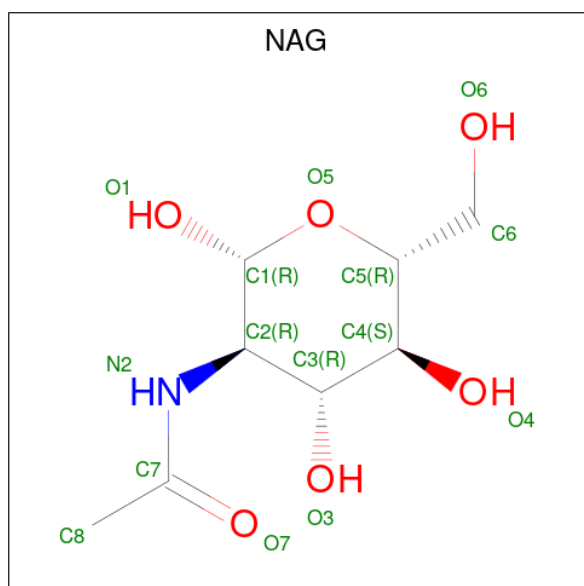
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	3	Total	C	N	O	0	0
			39	22	2	15		
7	R	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

- 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	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	A	1	Total	C	N	O	0
			154	88	11	55	
9	B	1	Total	C	N	O	0
			42	24	3	15	
9	B	1	Total	C	N	O	0
			42	24	3	15	
9	B	1	Total	C	N	O	0
			42	24	3	15	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	

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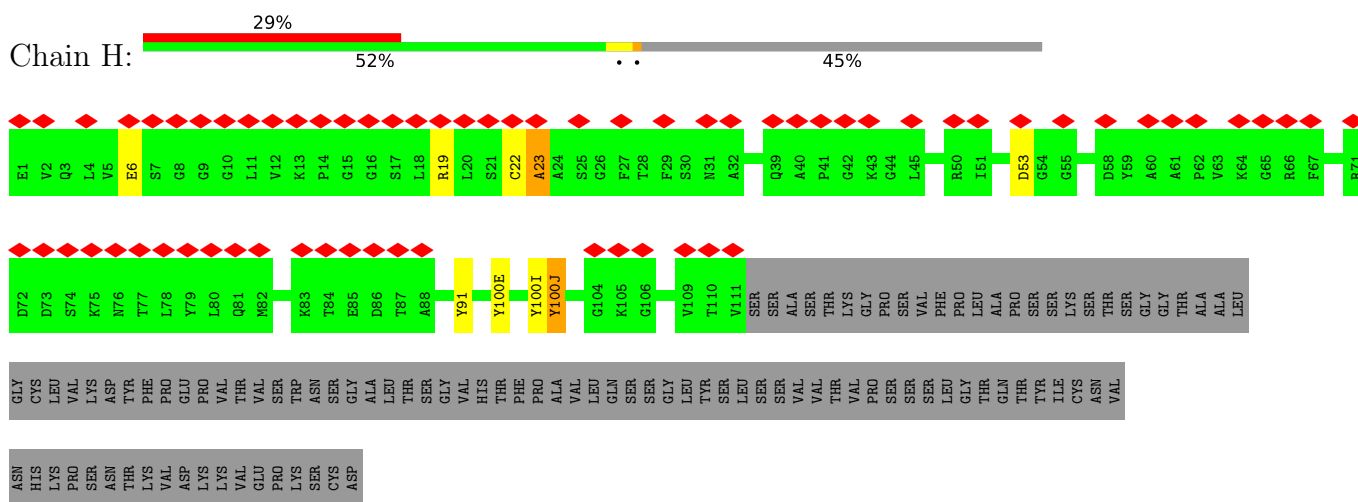
Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	C	1	Total	C	N	O	0
			140	80	10	50	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	E	1	Total	C	N	O	0
			98	56	7	35	
9	D	1	Total	C	N	O	0
			42	24	3	15	
9	D	1	Total	C	N	O	0
			42	24	3	15	
9	D	1	Total	C	N	O	0
			42	24	3	15	
9	F	1	Total	C	N	O	0
			42	24	3	15	
9	F	1	Total	C	N	O	0
			42	24	3	15	
9	F	1	Total	C	N	O	0
			42	24	3	15	



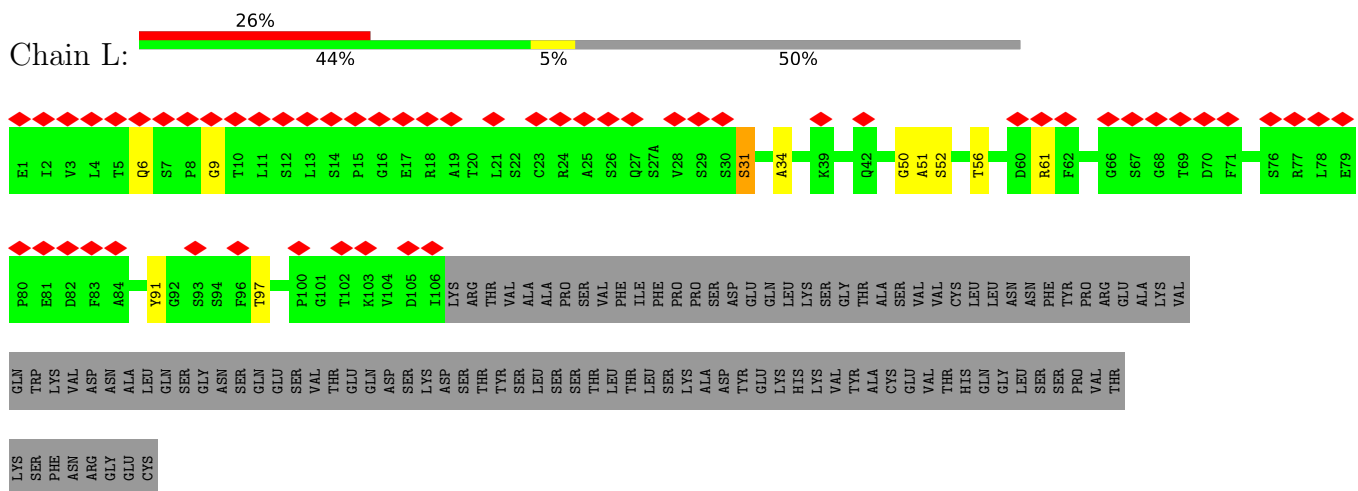
### 3 Residue-property plots

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.

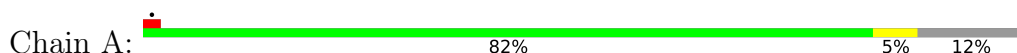
- Molecule 1: PCT64.LMCA Fab Heavy Chain




- Molecule 2: PCT64.LMCA Fab Light Chain

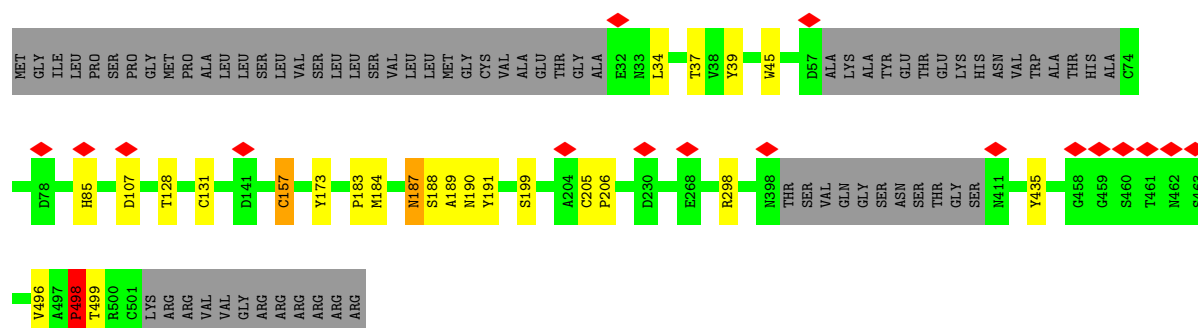


- Molecule 3: HIV Envelope ApexGT2.2MUT gp120




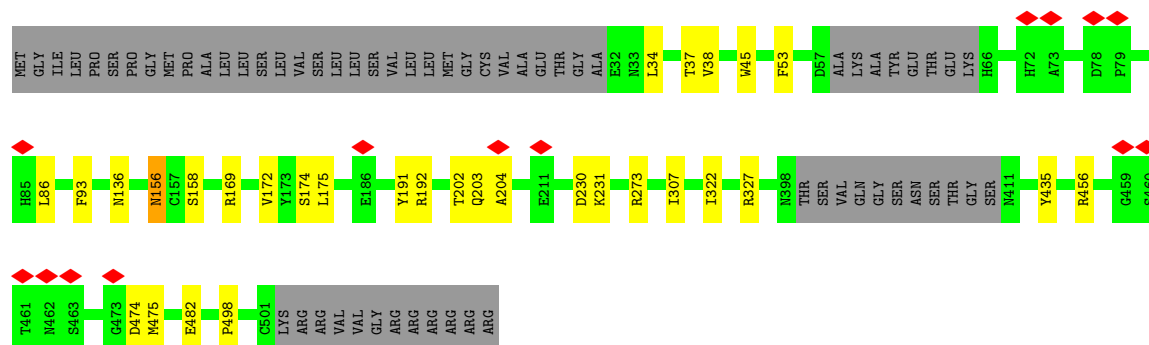
- Molecule 3: HIV Envelope ApexGT2.2MUT gp120

Chain C:  81% 14%



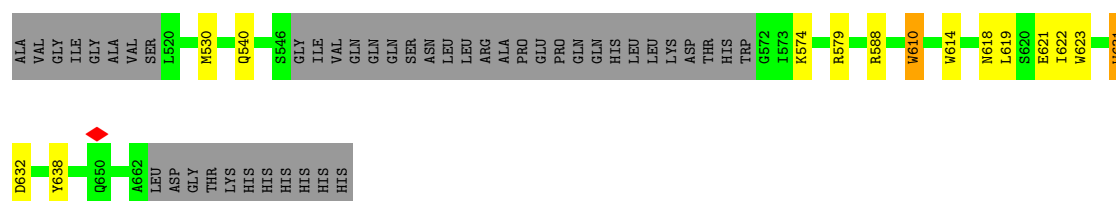
- Molecule 3: HIV Envelope ApexGT2.2MUT gp120

Chain E:  81% 6% 12%

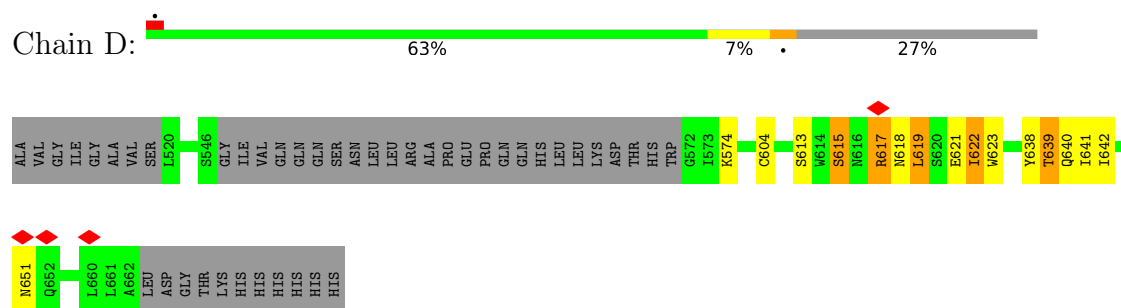


- Molecule 4: HIV Envelope ApexGT2.2MUT gp41

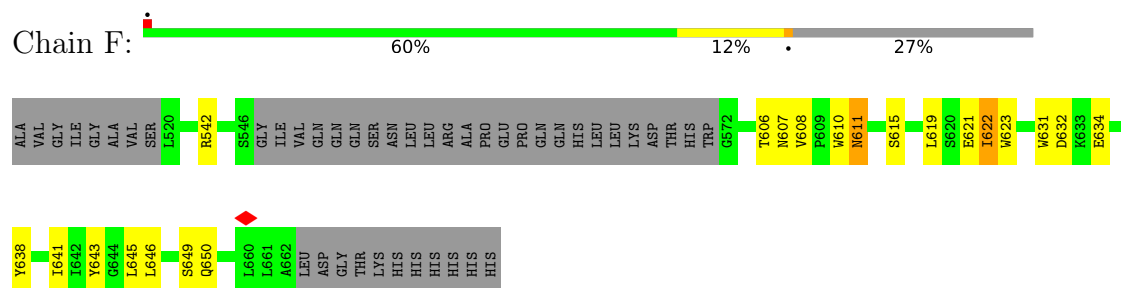
Chain B: 



- Molecule 4: HIV Envelope ApexGT2.2MUT gp41



- Molecule 4: HIV Envelope ApexGT2.2MUT gp41



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



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



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



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





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

Chain O:  100%



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

Chain Q:  100%



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

Chain T:  50% 100%



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

Chain U:  100%



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

Chain J:  100%



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

Chain P:  100%



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

Chain S:  100%

NAG1  
NAG2  
BMA3  
MAN4

- 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%

NAG1  
NAG2  
BMA3

- 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:  33% 67% 33%

  
NAG1  
NAG2  
BMA3

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

Chain V:  14% 29% 71%

  
NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	238078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.894	Depositor
Minimum map value	-4.530	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.689	Depositor
Map size (Å)	322.0, 322.0, 322.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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: NAG, TYS, MAN, 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	H	0.96	2/1038 (0.2%)	1.05	3/1405 (0.2%)
2	L	0.93	0/820	0.97	1/1114 (0.1%)
3	A	1.04	8/3532 (0.2%)	0.92	6/4804 (0.1%)
3	C	1.03	5/3462 (0.1%)	0.90	4/4706 (0.1%)
3	E	1.05	7/3532 (0.2%)	0.97	11/4804 (0.2%)
4	B	1.05	2/950 (0.2%)	0.95	2/1287 (0.2%)
4	D	0.96	1/950 (0.1%)	0.87	0/1287
4	F	0.92	0/950	0.90	4/1287 (0.3%)
All	All	1.02	25/15234 (0.2%)	0.94	31/20694 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	157	CYS	CB-SG	10.58	2.00	1.82
3	E	174	SER	CA-CB	-9.85	1.38	1.52
3	E	158	SER	CA-CB	-9.14	1.39	1.52
3	A	157	CYS	CB-SG	8.36	1.96	1.82
3	E	169	ARG	CG-CD	-7.33	1.33	1.51
4	D	604	CYS	CB-SG	-6.66	1.71	1.82
3	E	45	TRP	CB-CG	-6.30	1.39	1.50
3	E	482	GLU	CD-OE1	-6.25	1.18	1.25
3	A	112	TRP	CB-CG	-6.18	1.39	1.50
3	A	482	GLU	CD-OE1	-5.73	1.19	1.25
1	H	6	GLU	CD-OE2	-5.72	1.19	1.25
3	A	482	GLU	CG-CD	-5.68	1.43	1.51
4	B	540	GLN	CG-CD	-5.56	1.38	1.51
1	H	6	GLU	CD-OE1	-5.24	1.19	1.25
3	A	164	GLU	CD-OE1	-5.23	1.19	1.25
3	C	435	TYR	CD2-CE2	-5.20	1.31	1.39
4	B	631	TRP	CZ3-CH2	-5.17	1.31	1.40
3	E	53	PHE	CB-CG	-5.12	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	298	ARG	CG-CD	-5.11	1.39	1.51
3	A	93	PHE	CB-CG	-5.11	1.42	1.51
3	E	482	GLU	CG-CD	-5.09	1.44	1.51
3	C	199	SER	CB-OG	-5.08	1.35	1.42
3	A	32	GLU	CB-CG	5.07	1.61	1.52
3	A	199	SER	CB-OG	-5.05	1.35	1.42
3	C	45	TRP	CB-CG	-5.04	1.41	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	156	ASN	CB-CA-C	-10.94	88.52	110.40
3	E	169	ARG	NE-CZ-NH1	-10.29	115.15	120.30
3	A	327	ARG	NE-CZ-NH2	-8.65	115.97	120.30
3	A	456	ARG	NE-CZ-NH2	-8.39	116.10	120.30
3	E	327	ARG	NE-CZ-NH2	-8.31	116.14	120.30
3	E	435	TYR	CB-CG-CD2	-8.06	116.17	121.00
3	E	456	ARG	NE-CZ-NH2	-7.71	116.45	120.30
3	C	498	PRO	N-CA-CB	-7.29	94.55	103.30
3	A	419	ARG	NE-CZ-NH2	-7.27	116.66	120.30
4	B	588	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	L	61	ARG	NE-CZ-NH2	-6.93	116.83	120.30
3	E	174	SER	N-CA-CB	-6.93	100.11	110.50
1	H	100(J)	TYR	CA-CB-CG	6.67	126.06	113.40
3	E	136	ASN	CB-CA-C	-6.42	97.56	110.40
4	B	579	ARG	NE-CZ-NH2	-6.29	117.15	120.30
3	C	435	TYR	CB-CG-CD2	-6.29	117.22	121.00
4	F	542	ARG	NE-CZ-NH2	-5.86	117.37	120.30
3	E	273	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	H	19	ARG	NE-CZ-NH2	-5.77	117.42	120.30
3	A	93	PHE	CB-CG-CD2	-5.69	116.82	120.80
3	A	166	ARG	NE-CZ-NH2	-5.40	117.60	120.30
4	F	643	TYR	CB-CG-CD2	-5.40	117.76	121.00
3	E	93	PHE	CB-CG-CD2	-5.34	117.06	120.80
3	E	191	TYR	CB-CG-CD1	-5.27	117.84	121.00
3	C	39	TYR	CB-CG-CD2	-5.26	117.84	121.00
3	E	435	TYR	CB-CG-CD1	5.24	124.15	121.00
4	F	542	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	H	91	TYR	CB-CG-CD1	-5.17	117.90	121.00
3	C	173	TYR	CB-CG-CD2	-5.16	117.91	121.00
4	F	611	ASN	CB-CA-C	5.04	120.47	110.40
3	A	435	TYR	CB-CG-CD2	-5.01	117.99	121.00



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1046	0	978	1	0
2	L	801	0	774	3	0
3	A	3458	0	3375	11	0
3	C	3392	0	3323	14	0
3	E	3458	0	3379	11	0
4	B	934	0	907	9	0
4	D	934	0	907	18	0
4	F	934	0	906	12	0
5	G	28	0	25	0	0
5	I	28	0	24	0	0
5	K	28	0	25	0	0
5	M	28	0	25	0	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	24	0	0
6	J	50	0	43	0	0
6	P	50	0	43	0	0
6	S	50	0	43	0	0
7	N	39	0	34	0	0
7	R	39	0	34	1	0
8	V	83	0	70	1	0
9	A	154	0	141	1	0
9	B	42	0	39	0	0
9	C	140	0	130	0	0
9	D	42	0	39	0	0
9	E	98	0	91	1	0
9	F	42	0	39	0	0
All	All	16010	0	15493	69	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 2.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:THR:HG21	3:C:190:ASN:ND2	1.75	0.99
3:C:128:THR:CG2	3:C:190:ASN:ND2	2.44	0.80
3:E:175:LEU:HD11	7:R:1:NAG:H82	1.68	0.75
4:F:608:VAL:HG21	4:F:646:LEU:HA	1.70	0.73
4:F:621:GLU:C	4:F:623:TRP:H	1.92	0.73
3:C:128:THR:HG21	3:C:190:ASN:HD21	1.58	0.69
4:F:608:VAL:HG22	4:F:649:SER:HB2	1.78	0.66
3:C:498:PRO:HG2	4:D:622:ILE:HD13	1.80	0.62
3:C:107:ASP:OD1	4:D:574:LYS:NZ	2.35	0.60
3:C:131:CYS:HB3	3:C:157:CYS:HA	1.86	0.58
3:A:107:ASP:OD1	4:B:574:LYS:NZ	2.37	0.58
3:A:36:VAL:HG22	4:B:610:TRP:HD1	1.69	0.57
4:D:617:ARG:HH12	4:D:621:GLU:HB3	1.69	0.57
4:F:621:GLU:C	4:F:623:TRP:N	2.59	0.56
4:B:621:GLU:O	4:B:623:TRP:N	2.39	0.55
4:D:639:THR:O	4:D:642:ILE:N	2.38	0.55
2:L:31:SER:O	2:L:50:GLY:HA2	2.07	0.54
3:C:496:VAL:HG11	4:D:642:ILE:HG21	1.91	0.53
4:D:619:LEU:HD22	4:D:622:ILE:HD11	1.90	0.53
4:F:621:GLU:O	4:F:623:TRP:N	2.43	0.51
2:L:34:ALA:HB2	2:L:91:TYR:HE2	1.75	0.51
3:E:156:ASN:HA	3:E:175:LEU:HD23	1.92	0.51
4:D:615:SER:OG	4:D:617:ARG:HG2	2.11	0.51
4:D:617:ARG:NH1	4:D:618:ASN:H	2.08	0.51
3:A:36:VAL:HG22	4:B:610:TRP:CD1	2.45	0.51
3:A:131:CYS:HB3	3:A:157:CYS:HA	1.93	0.51
4:D:622:ILE:HD12	4:D:623:TRP:CD1	2.45	0.50
4:D:639:THR:O	4:D:641:ILE:N	2.45	0.49
4:D:615:SER:OG	4:D:617:ARG:NE	2.46	0.49
1:H:22:CYS:O	1:H:23:ALA:CB	2.61	0.48
3:C:187:ASN:C	3:C:189:ALA:H	2.17	0.48
3:E:498:PRO:HD2	4:F:622:ILE:HD13	1.95	0.48
3:C:187:ASN:O	3:C:189:ALA:N	2.46	0.48
4:D:617:ARG:HH11	4:D:618:ASN:H	1.61	0.48
4:F:631:TRP:O	4:F:634:GLU:N	2.46	0.48
3:A:46:LYS:NZ	4:B:632:ASP:OD2	2.47	0.47
4:B:621:GLU:O	4:B:622:ILE:C	2.53	0.47
3:E:474:ASP:OD1	3:E:475:MET:N	2.48	0.46
4:D:617:ARG:NH1	4:D:617:ARG:HA	2.30	0.46
4:D:618:ASN:O	4:D:621:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:606:THR:OG1	4:F:607:ASN:N	2.49	0.45
3:E:498:PRO:HG3	4:F:610:TRP:CZ2	2.51	0.45
3:A:474:ASP:OD1	3:A:475:MET:N	2.50	0.45
3:A:97:LYS:NZ	3:A:275:GLU:OE2	2.51	0.44
8:V:3:BMA:H62	8:V:4:MAN:H2	1.53	0.44
3:C:34:LEU:CD1	4:D:617:ARG:HG3	2.48	0.44
3:C:205:CYS:N	3:C:206:PRO:CD	2.81	0.44
3:E:172:VAL:HG11	3:E:307:ILE:HD13	2.00	0.43
4:D:617:ARG:NH1	4:D:622:ILE:HG12	2.33	0.43
4:D:638:TYR:O	4:D:639:THR:C	2.56	0.43
2:L:34:ALA:HB2	2:L:91:TYR:CE2	2.52	0.43
4:F:631:TRP:O	4:F:632:ASP:C	2.53	0.43
3:A:370:GLU:OE2	3:A:421:LYS:NZ	2.52	0.42
4:B:614:TRP:CD1	4:B:638:TYR:CE2	3.07	0.42
4:B:622:ILE:HG13	4:B:631:TRP:CZ3	2.53	0.42
4:B:530:MET:SD	4:B:622:ILE:O	2.78	0.41
3:C:37:THR:OG1	3:C:499:THR:HG22	2.20	0.41
3:E:37:THR:OG1	3:E:38:VAL:N	2.53	0.41
3:E:192:ARG:HD3	9:E:1001:NAG:H81	2.03	0.41
3:E:230:ASP:OD1	3:E:231:LYS:N	2.53	0.41
4:F:638:TYR:HA	4:F:641:ILE:HD12	2.03	0.41
4:D:617:ARG:HD3	4:D:622:ILE:HG12	2.02	0.41
3:E:34:LEU:HD13	4:F:619:LEU:HD23	2.02	0.41
3:E:202:THR:O	3:E:203:GLN:HB2	2.21	0.41
3:A:123:THR:N	3:A:124:PRO:CD	2.84	0.40
3:C:131:CYS:HB3	3:C:157:CYS:CA	2.51	0.40
3:C:183:PRO:HA	3:C:191:TYR:CD2	2.56	0.40
3:A:93:PHE:HB3	3:A:487:LYS:HD2	2.03	0.40
3:A:279:ASN:CG	9:A:603:NAG:H82	2.42	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	H	128/238 (54%)	119 (93%)	8 (6%)	1 (1%)	19	58
2	L	104/214 (49%)	98 (94%)	4 (4%)	2 (2%)	8	40
3	A	435/504 (86%)	417 (96%)	18 (4%)	0	100	100
3	C	427/504 (85%)	409 (96%)	14 (3%)	4 (1%)	17	55
3	E	435/504 (86%)	419 (96%)	14 (3%)	2 (0%)	29	67
4	B	114/162 (70%)	110 (96%)	4 (4%)	0	100	100
4	D	114/162 (70%)	109 (96%)	1 (1%)	4 (4%)	3	29
4	F	114/162 (70%)	110 (96%)	2 (2%)	2 (2%)	8	41
All	All	1871/2450 (76%)	1791 (96%)	65 (4%)	15 (1%)	24	58

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	23	ALA
4	D	639	THR
4	D	640	GLN
3	C	85	HIS
3	C	188	SER
4	F	622	ILE
2	L	9	GLY
2	L	51	ALA
3	E	86	LEU
4	D	651	ASN
3	E	204	ALA
4	F	650	GLN
4	D	613	SER
3	C	187	ASN
3	C	498	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	H	107/199 (54%)	105 (98%)	2 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	88/185 (48%)	83 (94%)	5 (6%)	20	49
3	A	393/444 (88%)	392 (100%)	1 (0%)	92	95
3	C	387/444 (87%)	385 (100%)	2 (0%)	88	93
3	E	393/444 (88%)	392 (100%)	1 (0%)	92	95
4	B	101/138 (73%)	98 (97%)	3 (3%)	41	64
4	D	101/138 (73%)	97 (96%)	4 (4%)	31	57
4	F	101/138 (73%)	98 (97%)	3 (3%)	41	64
All	All	1671/2130 (78%)	1650 (99%)	21 (1%)	70	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	53	ASP
1	H	100(J)	TYR
2	L	6	GLN
2	L	31	SER
2	L	52	SER
2	L	56	THR
2	L	97	THR
3	A	133	ASN
4	B	610	TRP
4	B	618	ASN
4	B	619	LEU
3	C	184	MET
3	C	498	PRO
3	E	322	ILE
4	D	615	SER
4	D	617	ARG
4	D	619	LEU
4	D	622	ILE
4	F	611	ASN
4	F	615	SER
4	F	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	6	GLN

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Mol	Chain	Res	Type
3	C	190	ASN
3	C	258	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TYS	H	100(I)	1	15,16,17	2.77	6 (40%)	18,22,24	0.87	0
1	TYS	H	100(E)	1	15,16,17	3.08	7 (46%)	18,22,24	0.75	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
1	TYS	H	100(I)	1	-	1/10/11/13	0/1/1/1
1	TYS	H	100(E)	1	-	0/10/11/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100(I)	TYS	CE2-CZ	5.18	1.49	1.38
1	H	100(I)	TYS	CE1-CZ	5.01	1.48	1.38
1	H	100(E)	TYS	CD2-CG	4.79	1.49	1.38
1	H	100(E)	TYS	CD1-CG	4.77	1.49	1.38
1	H	100(I)	TYS	CD2-CG	4.70	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100(E)	TYS	CE2-CD2	4.69	1.47	1.38
1	H	100(E)	TYS	CE2-CZ	4.62	1.47	1.38
1	H	100(E)	TYS	CE1-CZ	4.61	1.47	1.38
1	H	100(I)	TYS	CD1-CG	4.30	1.48	1.38
1	H	100(E)	TYS	CE1-CD1	3.80	1.45	1.38
1	H	100(E)	TYS	CB-CG	3.34	1.59	1.51
1	H	100(I)	TYS	CE2-CD2	3.11	1.44	1.38
1	H	100(I)	TYS	CE1-CD1	2.78	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	100(E)	TYS	CB-CA-C	2.06	115.33	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	100(I)	TYS	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

41 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	G	1	5,3	14,14,15	2.03	6 (42%)	17,19,21	1.13	2 (11%)
5	NAG	G	2	5	14,14,15	1.95	6 (42%)	17,19,21	0.91	1 (5%)
5	NAG	I	1	5,3	14,14,15	1.95	5 (35%)	17,19,21	6.43	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	I	2	5	14,14,15	1.97	6 (42%)	17,19,21	0.85	1 (5%)
6	NAG	J	1	6,3	14,14,15	2.01	6 (42%)	17,19,21	1.12	2 (11%)
6	NAG	J	2	6	14,14,15	1.89	6 (42%)	17,19,21	1.91	2 (11%)
6	BMA	J	3	6	11,11,12	0.86	1 (9%)	15,15,17	1.39	3 (20%)
6	MAN	J	4	6	11,11,12	2.06	6 (54%)	15,15,17	0.64	0
5	NAG	K	1	5,3	14,14,15	2.19	7 (50%)	17,19,21	1.45	3 (17%)
5	NAG	K	2	5	14,14,15	1.99	4 (28%)	17,19,21	0.96	2 (11%)
5	NAG	M	1	5,3	14,14,15	2.21	7 (50%)	17,19,21	1.27	1 (5%)
5	NAG	M	2	5	14,14,15	2.01	6 (42%)	17,19,21	0.86	1 (5%)
7	NAG	N	1	3,7	14,14,15	1.28	2 (14%)	17,19,21	2.54	6 (35%)
7	NAG	N	2	7	14,14,15	0.78	0	17,19,21	2.01	6 (35%)
7	BMA	N	3	7	11,11,12	0.38	0	15,15,17	0.79	1 (6%)
5	NAG	O	1	5,3	14,14,15	2.10	4 (28%)	17,19,21	1.15	1 (5%)
5	NAG	O	2	5	14,14,15	1.95	6 (42%)	17,19,21	0.93	1 (5%)
6	NAG	P	1	6,3	14,14,15	2.13	7 (50%)	17,19,21	1.24	2 (11%)
6	NAG	P	2	6	14,14,15	1.91	6 (42%)	17,19,21	0.98	1 (5%)
6	BMA	P	3	6	11,11,12	0.80	0	15,15,17	0.90	1 (6%)
6	MAN	P	4	6	11,11,12	1.97	6 (54%)	15,15,17	0.64	0
5	NAG	Q	1	5,3	14,14,15	2.05	6 (42%)	17,19,21	1.03	1 (5%)
5	NAG	Q	2	5	14,14,15	1.96	6 (42%)	17,19,21	0.94	1 (5%)
7	NAG	R	1	3,7	14,14,15	1.07	2 (14%)	17,19,21	2.57	4 (23%)
7	NAG	R	2	7	14,14,15	0.48	0	17,19,21	1.45	3 (17%)
7	BMA	R	3	7	11,11,12	0.23	0	15,15,17	0.99	1 (6%)
6	NAG	S	1	6,3	14,14,15	2.02	4 (28%)	17,19,21	1.15	2 (11%)
6	NAG	S	2	6	14,14,15	2.00	6 (42%)	17,19,21	2.13	3 (17%)
6	BMA	S	3	6	11,11,12	0.85	0	15,15,17	0.79	1 (6%)
6	MAN	S	4	6	11,11,12	2.01	6 (54%)	15,15,17	0.64	0
5	NAG	T	1	5,3	14,14,15	2.04	7 (50%)	17,19,21	1.18	3 (17%)
5	NAG	T	2	5	14,14,15	1.94	6 (42%)	17,19,21	0.92	1 (5%)
5	NAG	U	1	5,3	14,14,15	1.90	6 (42%)	17,19,21	6.83	1 (5%)
5	NAG	U	2	5	14,14,15	1.97	6 (42%)	17,19,21	0.97	1 (5%)
8	NAG	V	1	3,8	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
8	NAG	V	2	8	14,14,15	0.36	0	17,19,21	0.71	0
8	BMA	V	3	8	11,11,12	0.24	0	15,15,17	0.85	0
8	MAN	V	4	8	11,11,12	0.22	0	15,15,17	0.89	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	V	5	8	11,11,12	0.18	0	15,15,17	0.80	1 (6%)
8	MAN	V	6	8	11,11,12	0.24	0	15,15,17	0.89	1 (6%)
8	MAN	V	7	8	11,11,12	0.19	0	15,15,17	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
6	NAG	J	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
7	NAG	N	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
6	NAG	P	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
6	MAN	P	4	6	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	1/6/23/26	0/1/1/1
7	NAG	R	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	5/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
6	NAG	S	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	1/2/19/22	0/1/1/1
6	MAN	S	4	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	T	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1
5	NAG	U	1	5,3	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
8	NAG	V	1	3,8	-	3/6/23/26	0/1/1/1
8	NAG	V	2	8	-	0/6/23/26	0/1/1/1
8	BMA	V	3	8	-	2/2/19/22	0/1/1/1
8	MAN	V	4	8	-	0/2/19/22	0/1/1/1
8	MAN	V	5	8	-	0/2/19/22	0/1/1/1
8	MAN	V	6	8	-	0/2/19/22	0/1/1/1
8	MAN	V	7	8	-	0/2/19/22	0/1/1/1

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	1	NAG	C1-C2	5.30	1.60	1.52
5	O	1	NAG	C1-C2	5.20	1.60	1.52
5	M	1	NAG	C1-C2	5.04	1.59	1.52
6	J	1	NAG	C1-C2	5.02	1.59	1.52
5	K	1	NAG	C1-C2	4.98	1.59	1.52
5	G	1	NAG	C1-C2	4.84	1.59	1.52
6	P	1	NAG	C1-C2	4.76	1.59	1.52
5	K	2	NAG	C1-C2	4.68	1.59	1.52
5	T	1	NAG	C1-C2	4.67	1.59	1.52
5	I	1	NAG	C1-C2	4.65	1.59	1.52
5	Q	1	NAG	C1-C2	4.63	1.59	1.52
5	M	2	NAG	C1-C2	4.53	1.59	1.52
5	U	2	NAG	C1-C2	4.53	1.59	1.52
5	Q	2	NAG	C1-C2	4.45	1.59	1.52
5	I	2	NAG	C1-C2	4.44	1.59	1.52
5	G	2	NAG	C1-C2	4.38	1.58	1.52
5	U	1	NAG	C1-C2	4.38	1.58	1.52
5	T	2	NAG	C1-C2	4.25	1.58	1.52
5	O	2	NAG	C1-C2	4.23	1.58	1.52
6	P	2	NAG	C1-C2	4.19	1.58	1.52
6	S	2	NAG	C1-C2	4.11	1.58	1.52
6	J	2	NAG	C1-C2	3.94	1.58	1.52
6	J	4	MAN	O5-C5	3.39	1.50	1.43
5	M	1	NAG	O5-C5	3.28	1.50	1.43
6	S	4	MAN	O5-C5	3.26	1.50	1.43
6	P	4	MAN	C2-C3	3.22	1.57	1.52
6	S	4	MAN	C2-C3	3.21	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	4	MAN	O5-C5	3.18	1.49	1.43
5	M	2	NAG	O5-C5	3.16	1.49	1.43
6	J	4	MAN	C2-C3	3.11	1.57	1.52
5	G	2	NAG	O5-C5	3.08	1.49	1.43
5	Q	1	NAG	O5-C5	3.08	1.49	1.43
5	I	2	NAG	O5-C5	3.06	1.49	1.43
5	Q	2	NAG	O5-C5	3.02	1.49	1.43
5	T	2	NAG	O5-C5	3.01	1.49	1.43
6	J	2	NAG	O5-C5	3.00	1.49	1.43
5	O	2	NAG	O5-C5	2.98	1.49	1.43
5	U	2	NAG	O5-C5	2.94	1.49	1.43
6	S	2	NAG	O5-C5	2.94	1.49	1.43
5	I	1	NAG	O5-C5	2.94	1.49	1.43
6	J	4	MAN	C1-C2	2.92	1.58	1.52
5	K	1	NAG	O5-C5	2.91	1.49	1.43
5	O	1	NAG	O5-C5	2.88	1.49	1.43
5	K	2	NAG	O5-C5	2.86	1.49	1.43
5	T	1	NAG	O5-C5	2.83	1.49	1.43
5	M	1	NAG	O5-C1	2.80	1.48	1.43
6	P	2	NAG	O5-C5	2.79	1.49	1.43
6	P	4	MAN	C1-C2	2.74	1.58	1.52
5	U	1	NAG	C3-C2	2.74	1.58	1.52
6	P	1	NAG	O5-C1	2.70	1.48	1.43
6	S	4	MAN	C1-C2	2.70	1.58	1.52
5	K	2	NAG	C3-C2	2.68	1.58	1.52
6	S	1	NAG	O5-C5	2.67	1.48	1.43
5	K	1	NAG	C4-C5	2.67	1.58	1.53
6	P	1	NAG	O5-C5	2.67	1.48	1.43
5	O	1	NAG	O5-C1	2.62	1.47	1.43
6	P	1	NAG	C3-C2	2.58	1.58	1.52
6	S	2	NAG	C3-C2	2.58	1.58	1.52
5	G	1	NAG	C3-C2	2.56	1.57	1.52
5	T	2	NAG	C3-C2	2.54	1.57	1.52
5	M	2	NAG	C3-C2	2.54	1.57	1.52
5	U	1	NAG	O5-C5	2.53	1.48	1.43
5	K	1	NAG	C3-C2	2.53	1.57	1.52
6	S	2	NAG	C4-C5	2.53	1.58	1.53
6	S	2	NAG	C4-C3	2.51	1.58	1.52
6	S	4	MAN	C4-C5	2.50	1.58	1.53
5	O	2	NAG	C4-C5	2.50	1.58	1.53
6	J	1	NAG	O5-C5	2.50	1.48	1.43
5	G	1	NAG	O5-C5	2.49	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	2	NAG	C3-C2	2.49	1.57	1.52
5	Q	2	NAG	C4-C5	2.48	1.58	1.53
5	M	1	NAG	C4-C3	2.48	1.58	1.52
5	G	2	NAG	C3-C2	2.48	1.57	1.52
5	I	2	NAG	C3-C2	2.47	1.57	1.52
5	Q	1	NAG	C3-C2	2.47	1.57	1.52
7	N	1	NAG	O5-C5	-2.46	1.38	1.43
6	P	1	NAG	C2-N2	2.46	1.50	1.46
6	S	1	NAG	O5-C1	2.45	1.47	1.43
5	O	2	NAG	C3-C2	2.44	1.57	1.52
5	Q	2	NAG	C3-C2	2.43	1.57	1.52
6	J	4	MAN	C4-C5	2.43	1.58	1.53
5	M	1	NAG	C4-C5	2.42	1.58	1.53
5	T	2	NAG	C4-C5	2.42	1.58	1.53
6	J	4	MAN	O5-C1	2.42	1.47	1.43
5	K	1	NAG	O5-C1	2.42	1.47	1.43
5	G	1	NAG	C4-C3	2.41	1.58	1.52
5	U	2	NAG	C3-C2	2.40	1.57	1.52
5	T	1	NAG	C4-C3	2.40	1.58	1.52
5	I	1	NAG	O5-C1	2.40	1.47	1.43
6	P	1	NAG	C4-C3	2.37	1.58	1.52
5	I	1	NAG	C4-C5	2.36	1.58	1.53
6	J	2	NAG	C4-C5	2.36	1.58	1.53
5	Q	1	NAG	O5-C1	2.36	1.47	1.43
5	M	2	NAG	C4-C5	2.34	1.58	1.53
5	O	1	NAG	C3-C2	2.34	1.57	1.52
5	U	1	NAG	C4-C3	2.34	1.58	1.52
6	P	1	NAG	C4-C5	2.33	1.58	1.53
5	Q	1	NAG	C4-C5	2.33	1.57	1.53
5	Q	1	NAG	C4-C3	2.32	1.58	1.52
5	U	2	NAG	C2-N2	2.31	1.50	1.46
5	K	1	NAG	C4-C3	2.31	1.58	1.52
6	P	4	MAN	C4-C5	2.30	1.57	1.53
5	G	2	NAG	C4-C5	2.29	1.57	1.53
5	I	2	NAG	C4-C5	2.28	1.57	1.53
6	P	2	NAG	C4-C3	2.28	1.58	1.52
5	U	2	NAG	C4-C5	2.28	1.57	1.53
5	K	1	NAG	O4-C4	2.28	1.48	1.43
5	T	1	NAG	C3-C2	2.27	1.57	1.52
5	T	1	NAG	C4-C5	2.27	1.57	1.53
5	O	2	NAG	C4-C3	2.24	1.58	1.52
5	K	2	NAG	C4-C5	2.24	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	NAG	C3-C2	2.22	1.57	1.52
5	T	1	NAG	O5-C1	2.22	1.47	1.43
5	M	1	NAG	C3-C2	2.22	1.57	1.52
5	O	2	NAG	C2-N2	2.18	1.50	1.46
6	S	2	NAG	C2-N2	2.18	1.50	1.46
5	T	2	NAG	C4-C3	2.17	1.57	1.52
6	J	2	NAG	C4-C3	2.16	1.57	1.52
6	P	2	NAG	C2-N2	2.16	1.50	1.46
6	P	2	NAG	C4-C5	2.16	1.57	1.53
6	J	1	NAG	C4-C3	2.16	1.57	1.52
5	U	1	NAG	C4-C5	2.16	1.57	1.53
6	S	4	MAN	O5-C1	2.15	1.47	1.43
5	G	1	NAG	C4-C5	2.14	1.57	1.53
5	M	2	NAG	O5-C1	2.14	1.47	1.43
6	J	1	NAG	O5-C1	2.13	1.47	1.43
5	G	2	NAG	C4-C3	2.12	1.57	1.52
5	G	1	NAG	O5-C1	2.11	1.47	1.43
6	J	2	NAG	C2-N2	2.11	1.49	1.46
6	J	3	BMA	O3-C3	2.11	1.47	1.43
5	Q	2	NAG	C4-C3	2.10	1.57	1.52
5	U	2	NAG	C4-C3	2.09	1.57	1.52
5	I	1	NAG	C3-C2	2.08	1.56	1.52
5	I	2	NAG	C2-N2	2.07	1.49	1.46
5	U	1	NAG	O5-C1	2.07	1.47	1.43
6	P	4	MAN	O5-C1	2.07	1.47	1.43
6	J	2	NAG	C3-C2	2.07	1.56	1.52
5	G	2	NAG	C2-N2	2.07	1.49	1.46
5	T	2	NAG	C2-N2	2.07	1.49	1.46
6	P	4	MAN	C4-C3	2.06	1.57	1.52
5	I	2	NAG	C4-C3	2.06	1.57	1.52
6	J	4	MAN	C4-C3	2.05	1.57	1.52
5	M	2	NAG	C4-C3	2.05	1.57	1.52
6	S	4	MAN	C4-C3	2.04	1.57	1.52
7	N	1	NAG	O5-C1	-2.03	1.40	1.43
7	R	1	NAG	C1-C2	-2.03	1.49	1.52
5	T	1	NAG	C2-N2	2.03	1.49	1.46
6	S	1	NAG	C3-C2	2.03	1.56	1.52
5	M	1	NAG	O4-C4	2.03	1.47	1.43
5	Q	2	NAG	C2-N2	2.02	1.49	1.46
7	R	1	NAG	O5-C1	-2.02	1.40	1.43
6	J	1	NAG	C4-C5	2.01	1.57	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	1	NAG	C2-N2-C7	27.88	162.61	122.90
5	I	1	NAG	C2-N2-C7	26.12	160.09	122.90
7	R	1	NAG	C2-N2-C7	-6.94	113.03	122.90
6	S	2	NAG	C8-C7-N2	6.73	127.50	116.10
6	J	2	NAG	C8-C7-N2	6.03	126.30	116.10
7	N	1	NAG	O5-C1-C2	-5.51	102.59	111.29
7	R	1	NAG	C3-C4-C5	-4.83	101.63	110.24
7	N	1	NAG	O4-C4-C5	-4.37	98.45	109.30
6	S	2	NAG	O7-C7-N2	-4.00	114.61	121.95
7	N	1	NAG	O5-C5-C6	-3.93	101.04	107.20
6	J	2	NAG	O7-C7-N2	-3.77	115.02	121.95
7	R	1	NAG	C1-C2-N2	3.72	116.83	110.49
7	N	1	NAG	C3-C4-C5	-3.62	103.78	110.24
7	R	2	NAG	C2-N2-C7	3.53	127.93	122.90
5	K	1	NAG	O4-C4-C5	3.48	117.94	109.30
7	N	2	NAG	C6-C5-C4	-3.46	104.91	113.00
7	N	2	NAG	C1-O5-C5	3.45	116.86	112.19
7	N	2	NAG	O3-C3-C2	-3.39	102.44	109.47
7	N	2	NAG	O4-C4-C5	-3.36	100.97	109.30
7	N	1	NAG	C1-O5-C5	3.30	116.67	112.19
6	J	3	BMA	O3-C3-C4	3.24	117.85	110.35
7	N	1	NAG	C2-N2-C7	-3.14	118.43	122.90
7	R	1	NAG	C1-O5-C5	-3.02	108.10	112.19
5	Q	1	NAG	C1-C2-N2	-2.91	105.52	110.49
5	O	1	NAG	C8-C7-N2	2.84	120.91	116.10
7	N	2	NAG	O6-C6-C5	-2.84	101.56	111.29
5	T	1	NAG	C8-C7-N2	2.76	120.78	116.10
5	I	1	NAG	C8-C7-N2	2.75	120.76	116.10
6	P	1	NAG	C2-N2-C7	2.70	126.74	122.90
6	S	1	NAG	C8-C7-N2	2.64	120.57	116.10
5	K	1	NAG	C1-O5-C5	2.63	115.75	112.19
7	R	3	BMA	C1-O5-C5	2.57	115.68	112.19
5	T	1	NAG	C1-C2-N2	-2.54	106.16	110.49
7	N	2	NAG	O5-C5-C6	-2.52	103.26	107.20
6	J	3	BMA	O3-C3-C2	2.46	114.71	109.99
8	V	5	MAN	C1-O5-C5	2.39	115.42	112.19
7	R	2	NAG	O3-C3-C2	-2.36	104.58	109.47
6	J	1	NAG	C8-C7-N2	2.30	120.00	116.10
5	M	1	NAG	O4-C4-C5	2.29	114.98	109.30
5	O	2	NAG	C8-C7-N2	2.28	119.96	116.10
6	P	3	BMA	C2-C3-C4	-2.27	106.97	110.89
6	S	2	NAG	O7-C7-C8	-2.24	117.90	122.06
5	G	1	NAG	C1-C2-N2	-2.24	106.66	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	2	NAG	C8-C7-N2	2.24	119.89	116.10
6	S	1	NAG	O7-C7-C8	-2.23	117.91	122.06
6	J	3	BMA	C1-C2-C3	-2.21	106.95	109.67
5	G	1	NAG	C8-C7-N2	2.19	119.81	116.10
6	P	1	NAG	C8-C7-N2	2.19	119.80	116.10
5	K	1	NAG	C8-C7-N2	2.17	119.78	116.10
5	K	2	NAG	C8-C7-N2	2.15	119.73	116.10
6	P	2	NAG	C8-C7-N2	2.13	119.71	116.10
6	S	3	BMA	C2-C3-C4	-2.10	107.26	110.89
5	I	2	NAG	C8-C7-N2	2.10	119.66	116.10
7	N	3	BMA	C2-C3-C4	-2.10	107.27	110.89
8	V	1	NAG	C2-N2-C7	2.09	125.88	122.90
5	T	1	NAG	O7-C7-C8	-2.07	118.21	122.06
7	R	2	NAG	C4-C3-C2	-2.06	107.99	111.02
6	J	1	NAG	C1-C2-N2	-2.05	106.98	110.49
5	K	2	NAG	C1-O5-C5	2.05	114.97	112.19
5	Q	2	NAG	C8-C7-N2	2.05	119.56	116.10
5	T	2	NAG	C8-C7-N2	2.02	119.52	116.10
5	M	2	NAG	C8-C7-N2	2.02	119.52	116.10
8	V	6	MAN	C1-O5-C5	2.02	114.92	112.19
5	G	2	NAG	C8-C7-N2	2.01	119.51	116.10

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	U	1	NAG	C3-C2-N2-C7
6	P	1	NAG	C3-C2-N2-C7
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
7	R	2	NAG	C8-C7-N2-C2
7	R	2	NAG	O7-C7-N2-C2
7	R	1	NAG	C8-C7-N2-C2
7	R	1	NAG	O7-C7-N2-C2
7	N	3	BMA	O5-C5-C6-O6
8	V	1	NAG	C8-C7-N2-C2
8	V	1	NAG	O7-C7-N2-C2
7	N	3	BMA	C4-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2

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

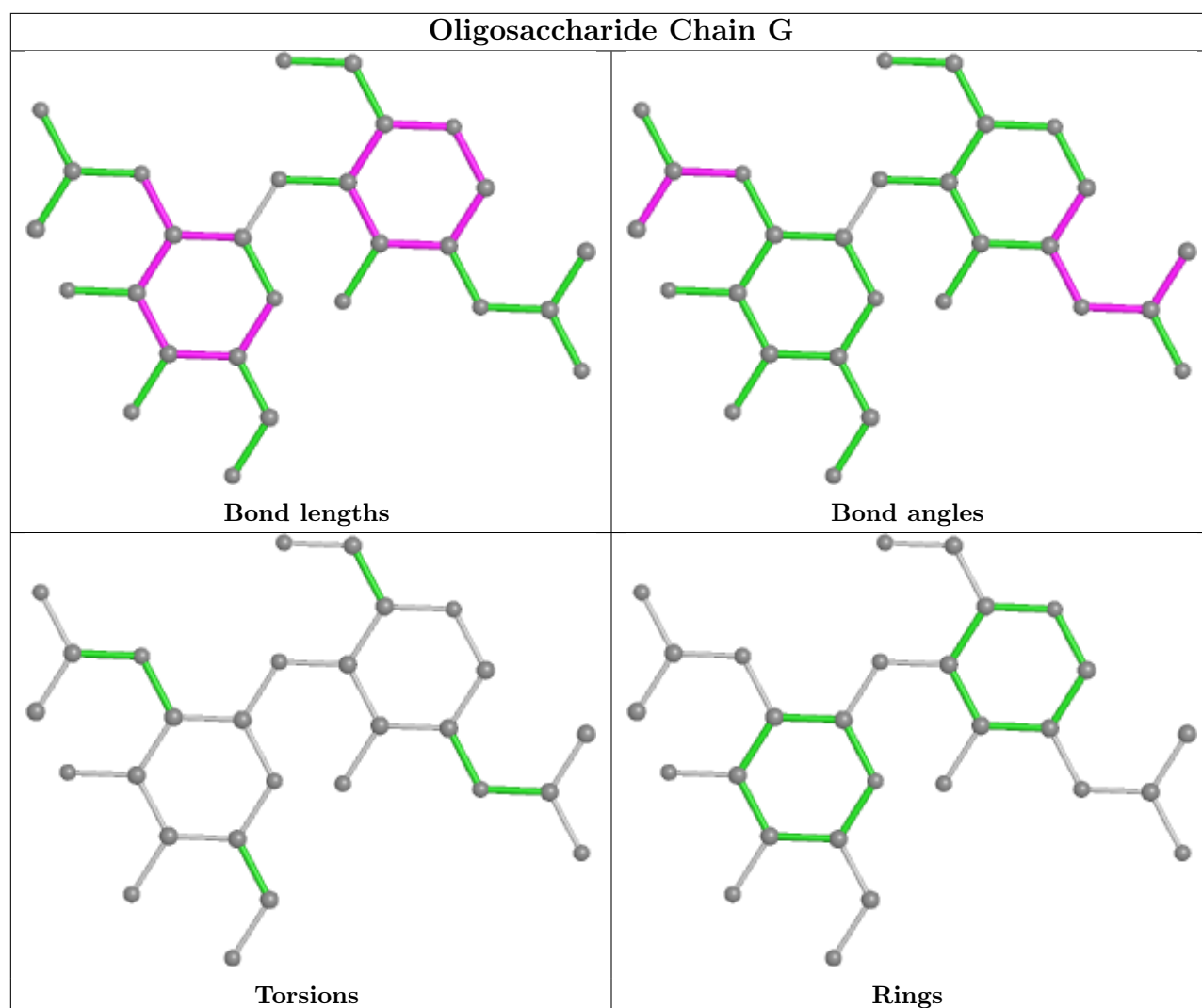
There are no ring outliers.

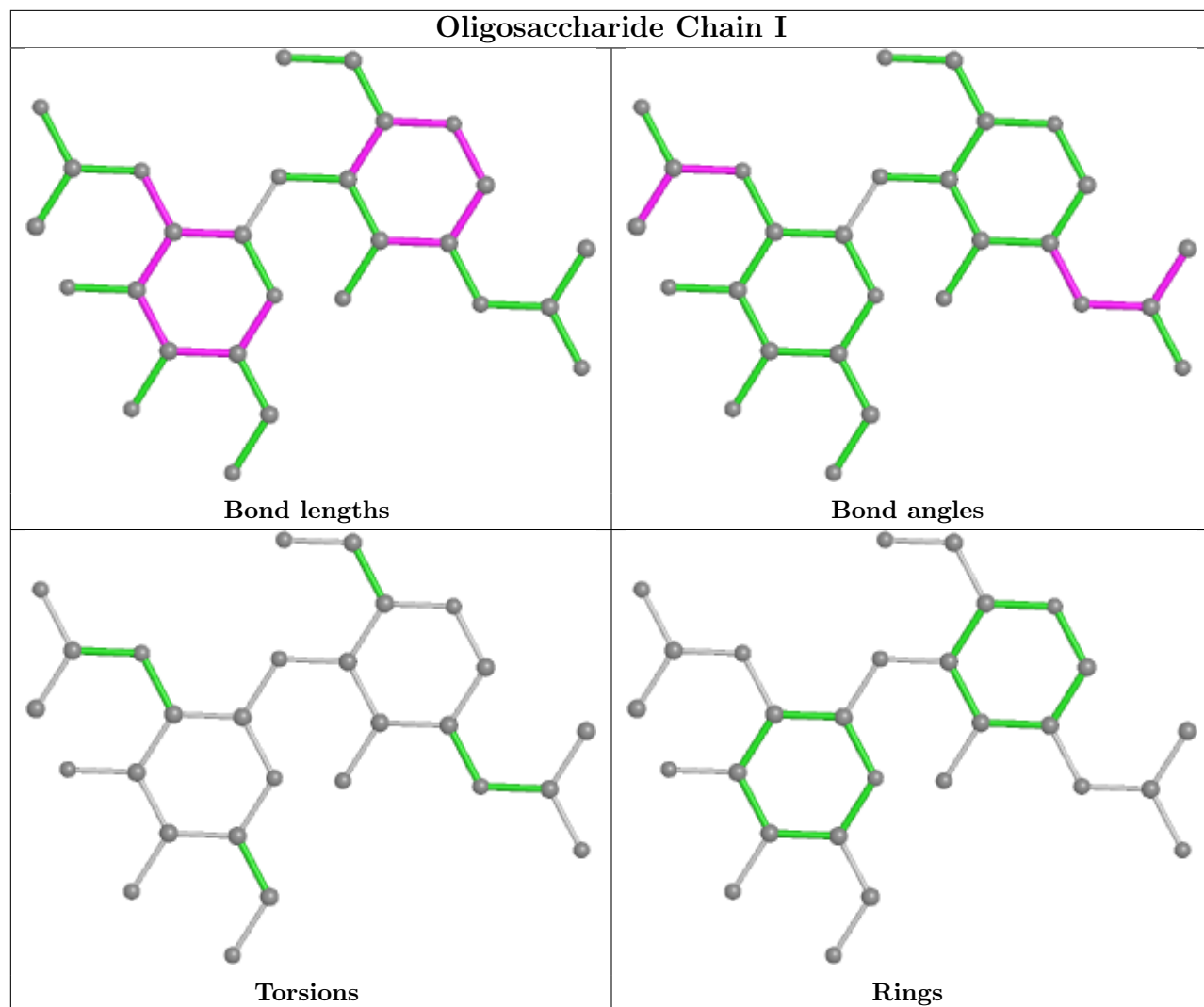
3 monomers are involved in 2 short contacts:

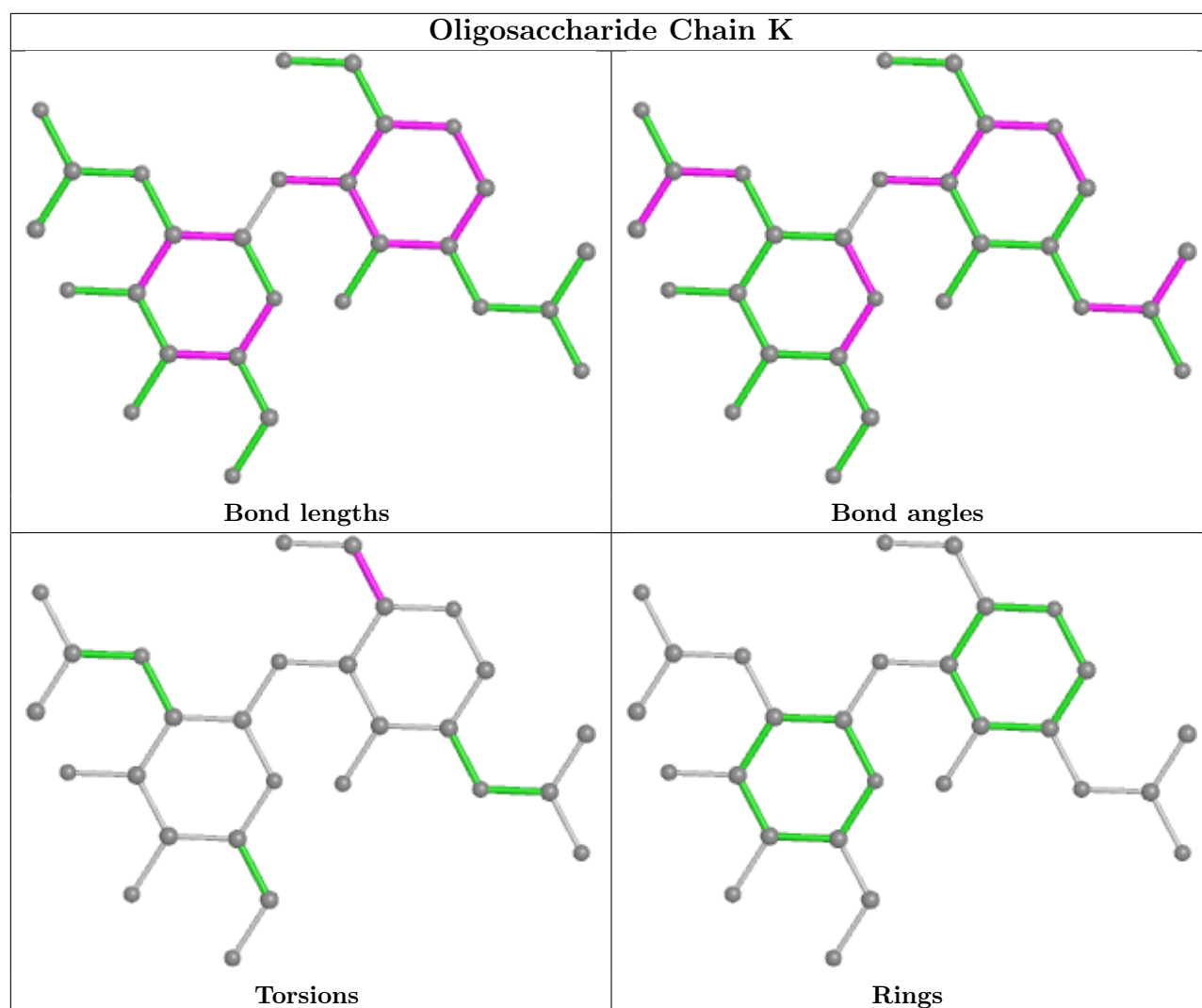
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	V	3	BMA	1	0
8	V	4	MAN	1	0
7	R	1	NAG	1	0

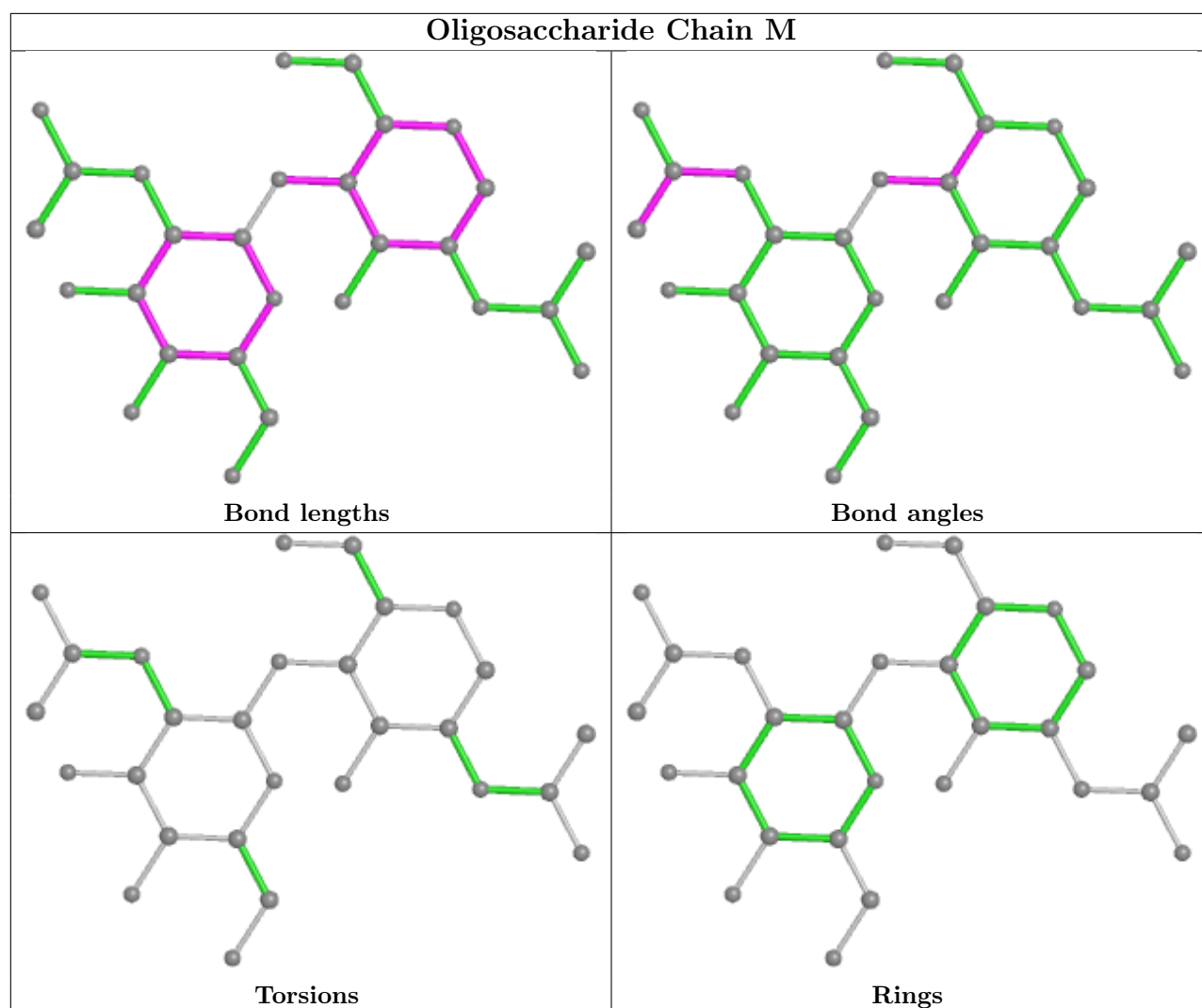
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

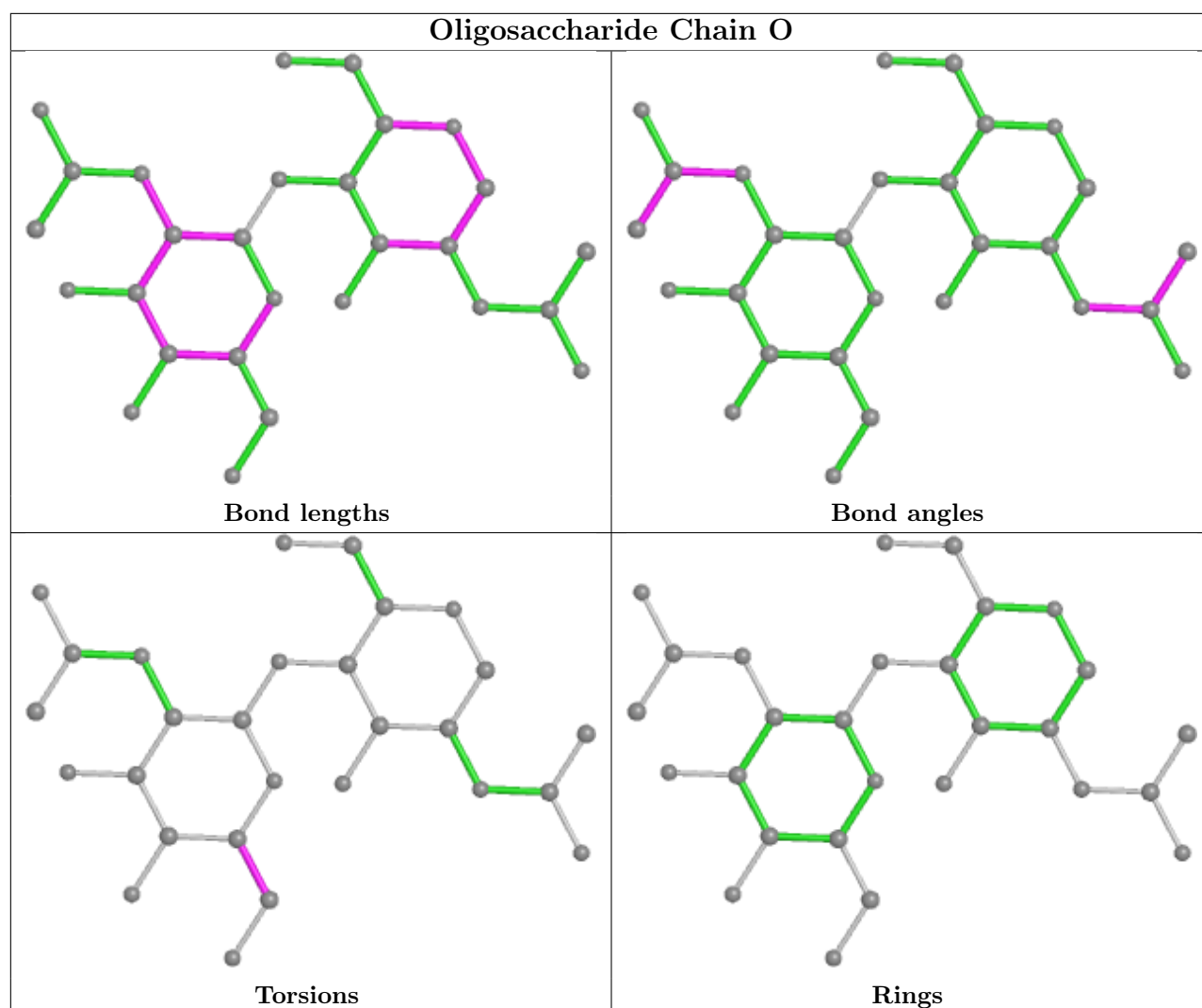


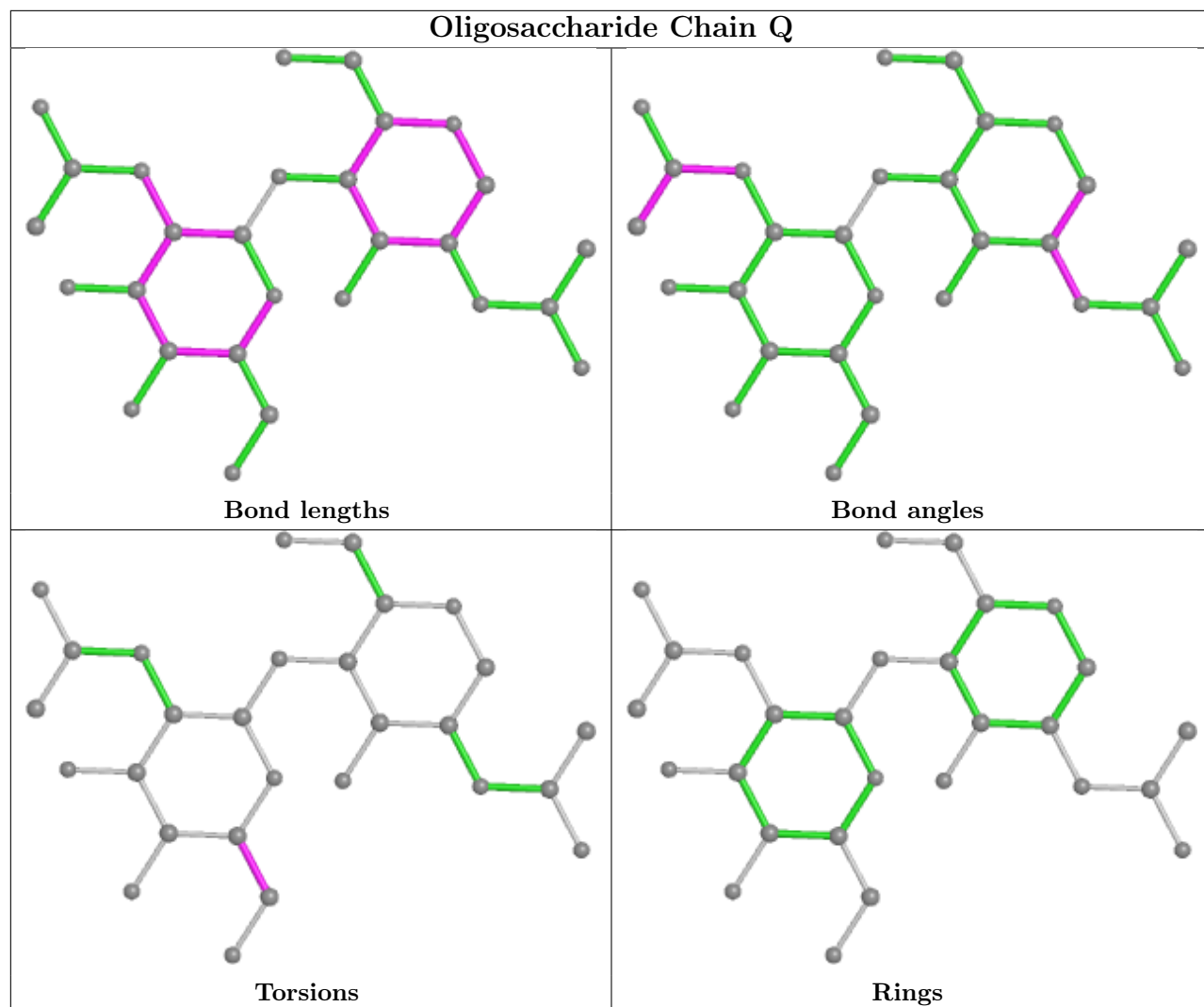


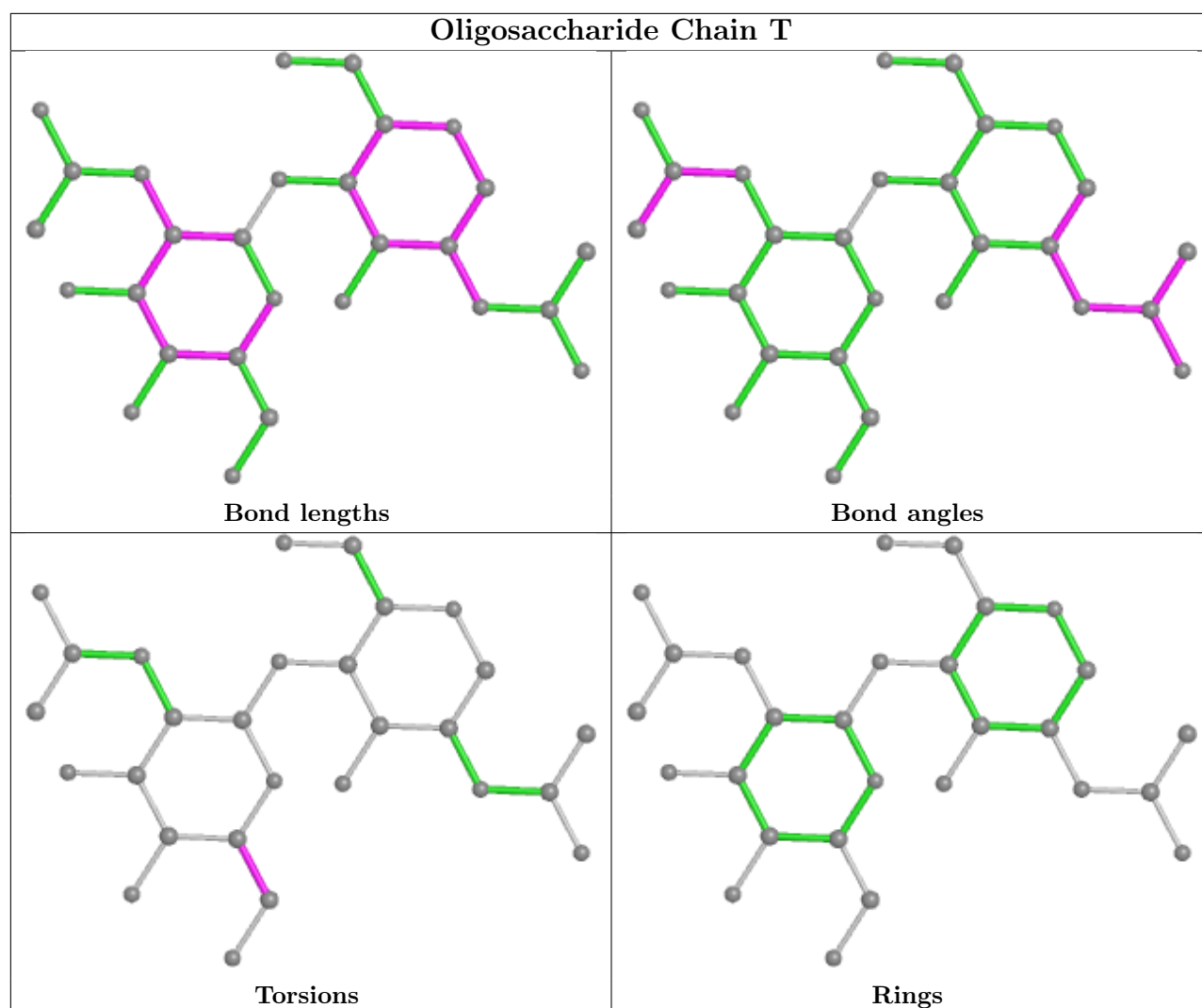


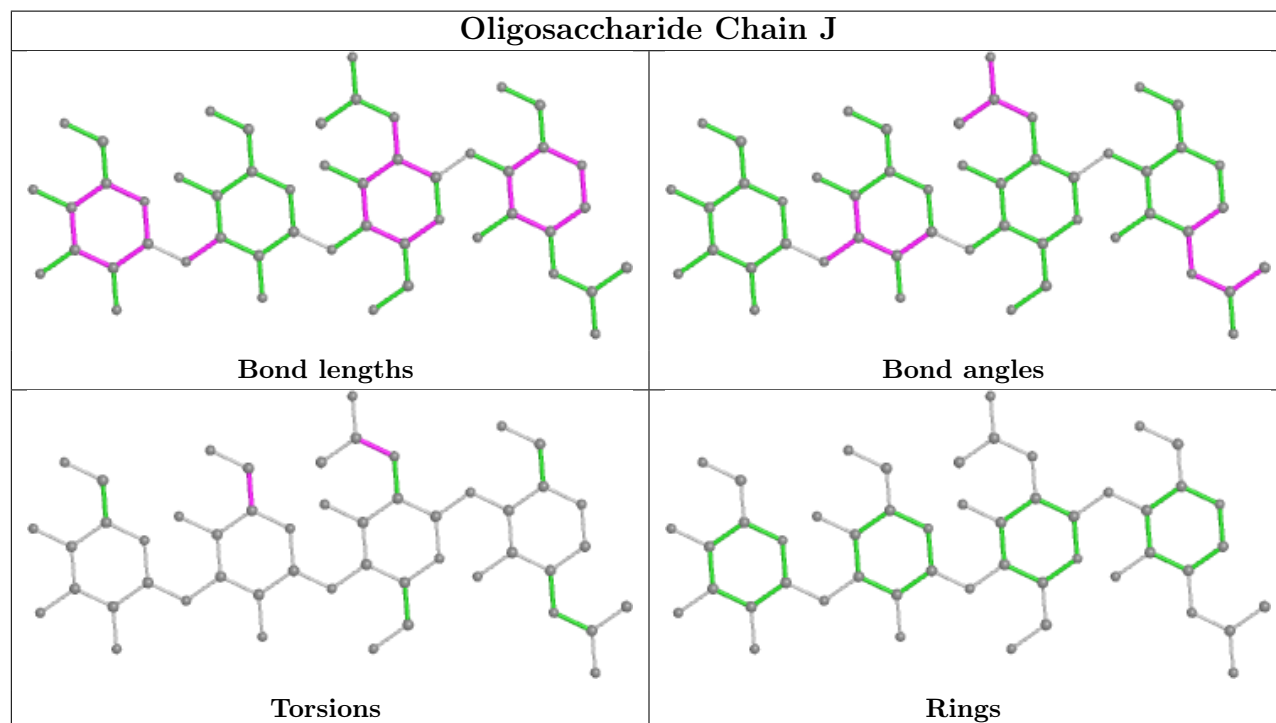
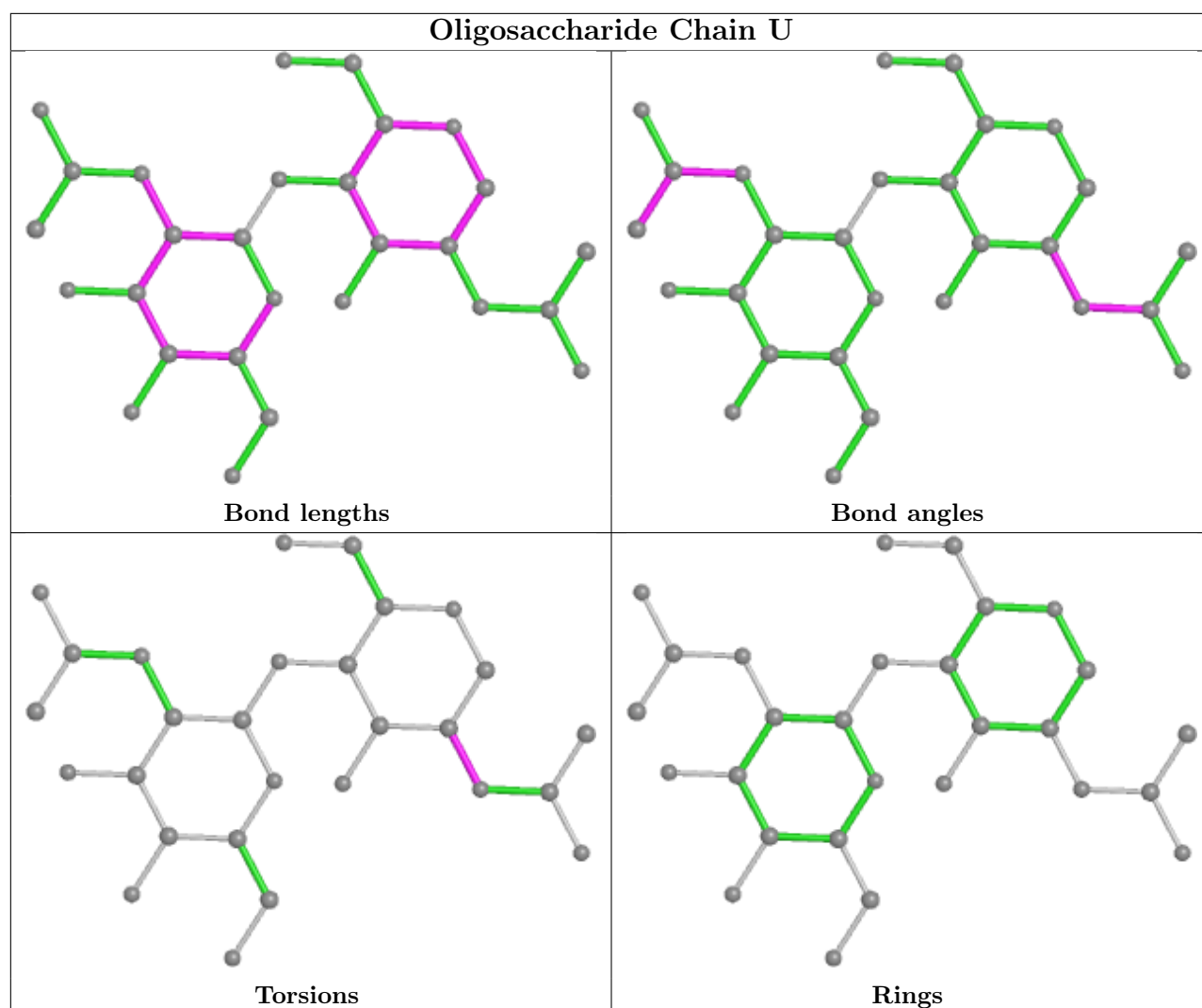




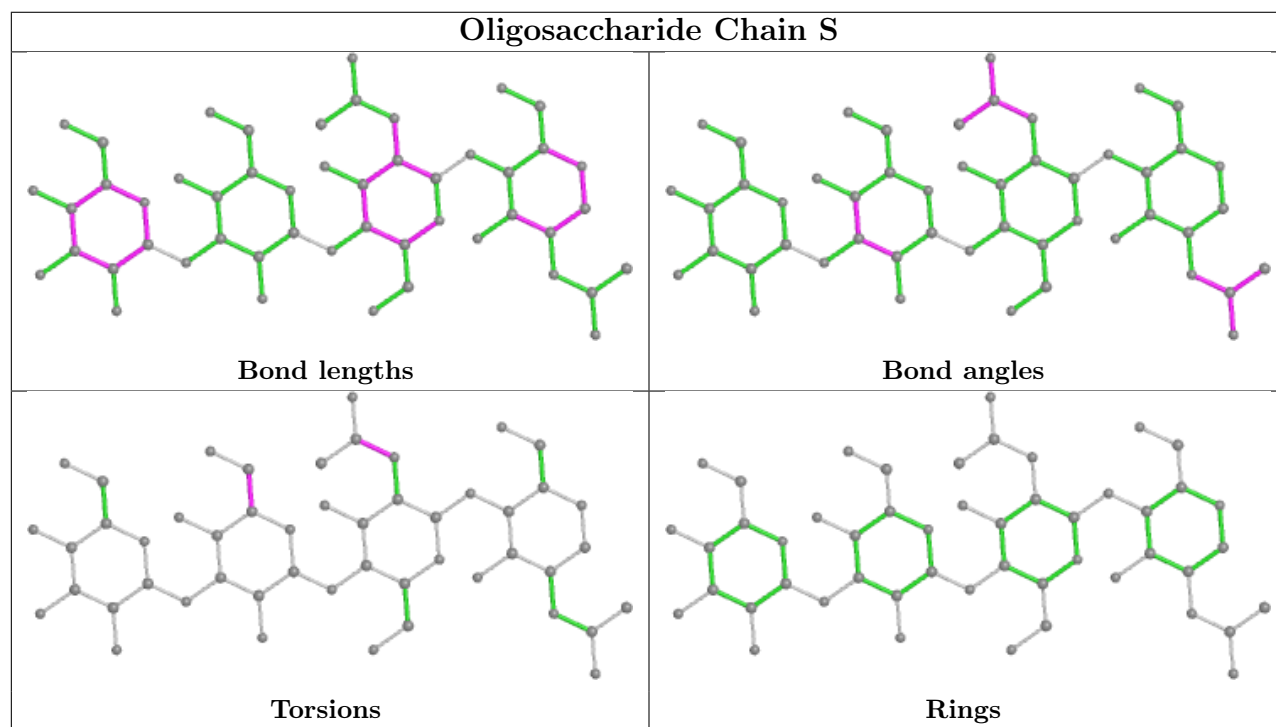
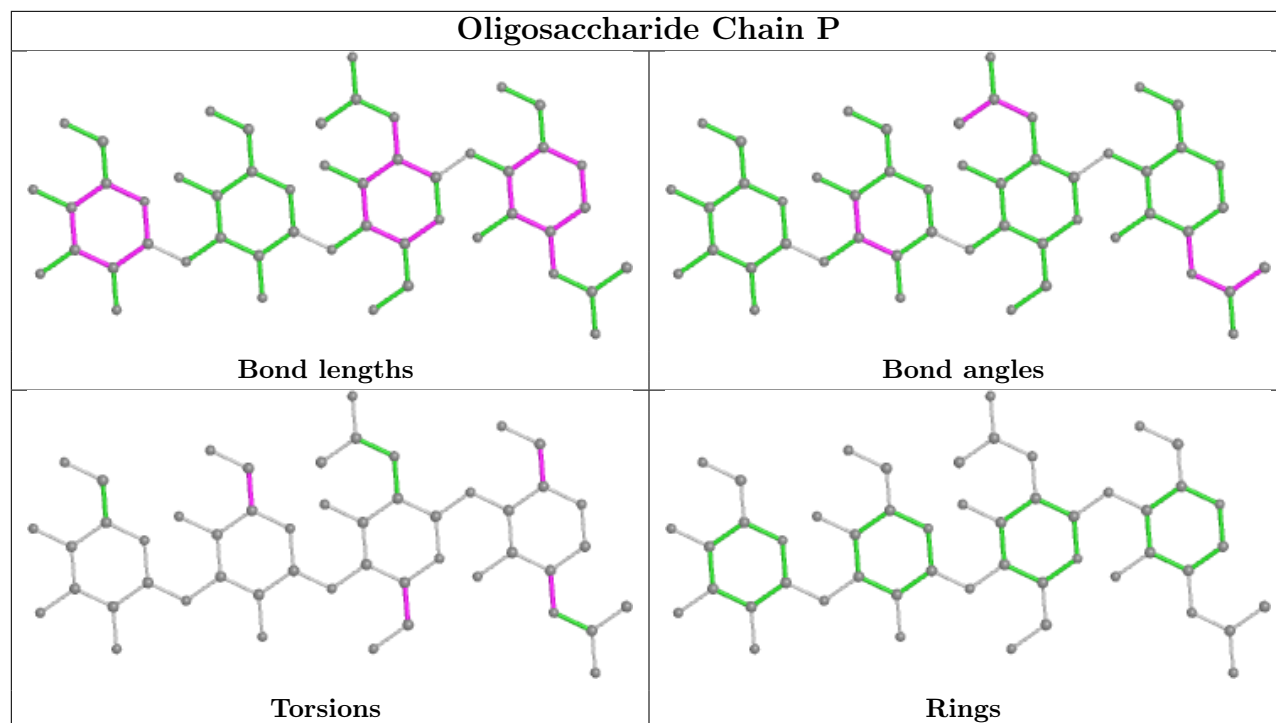


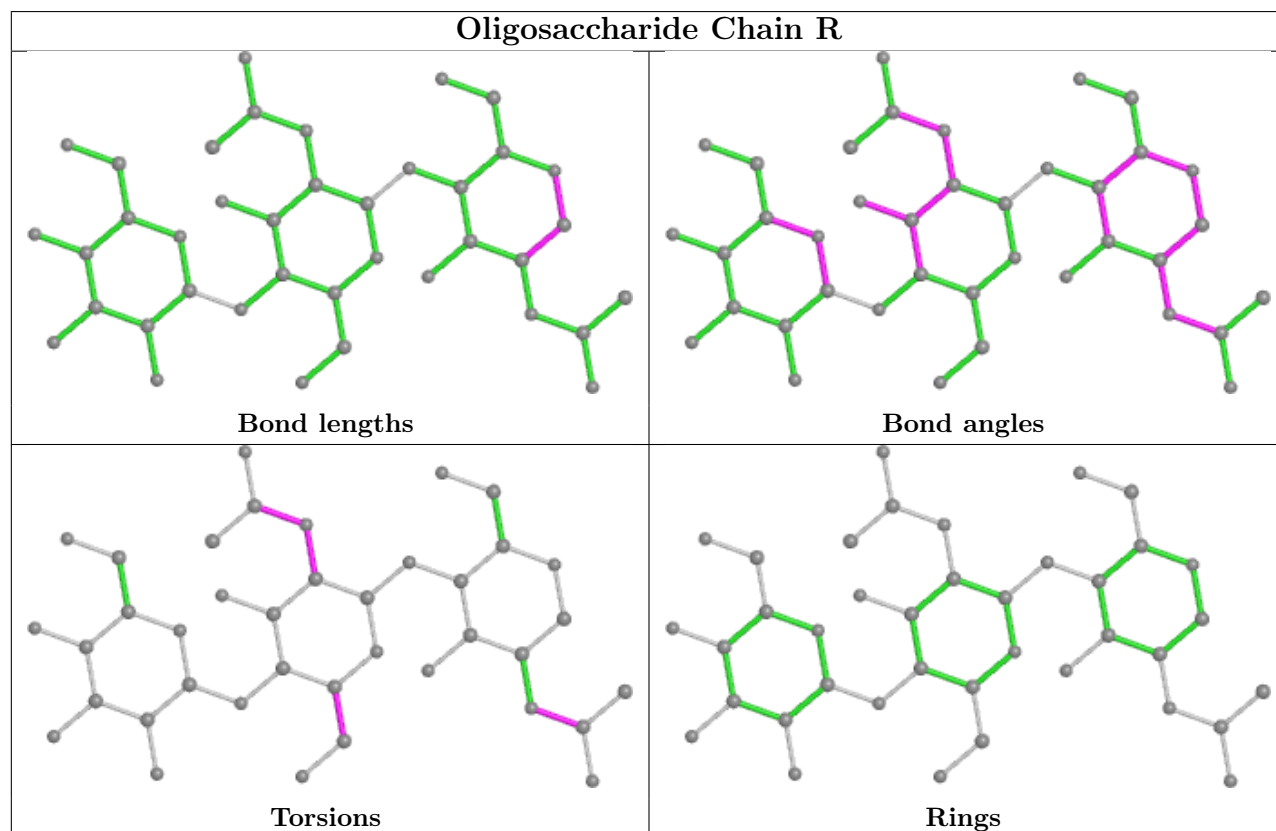
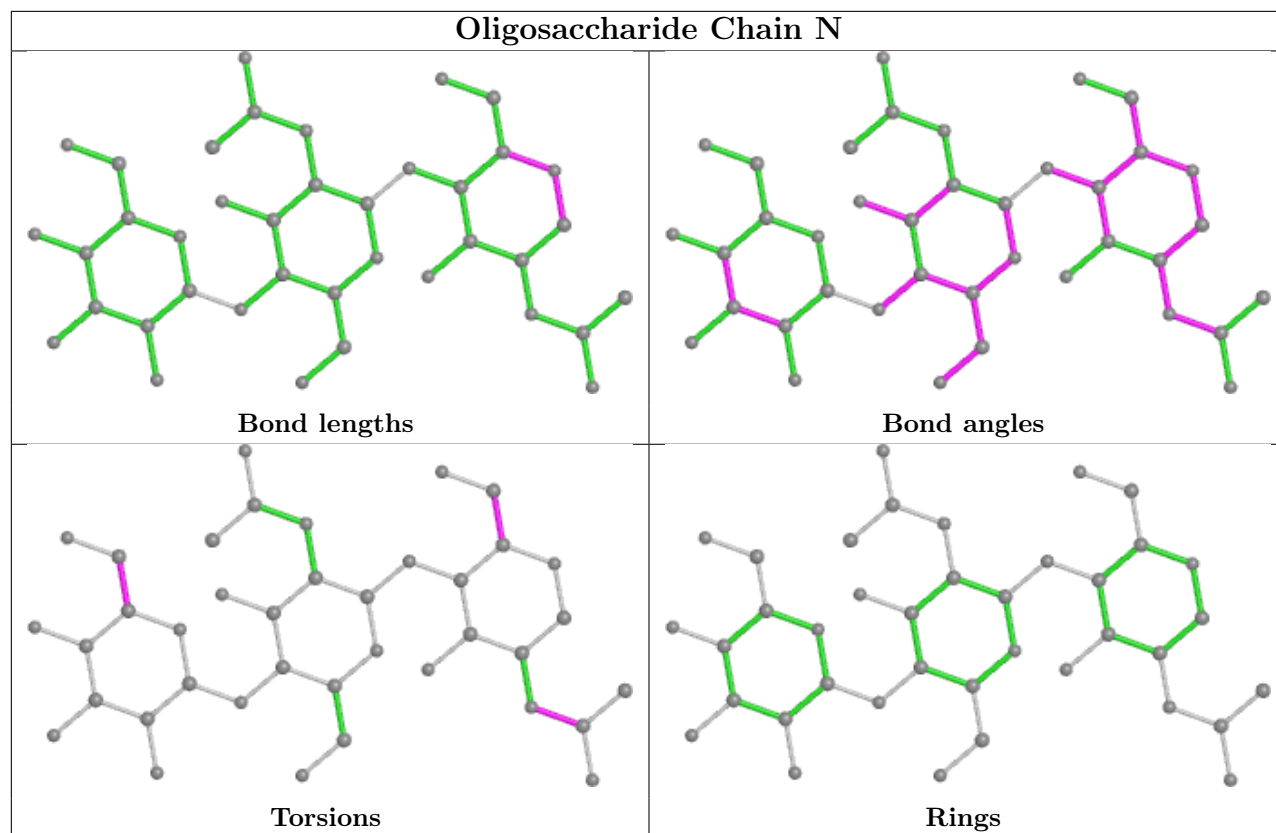


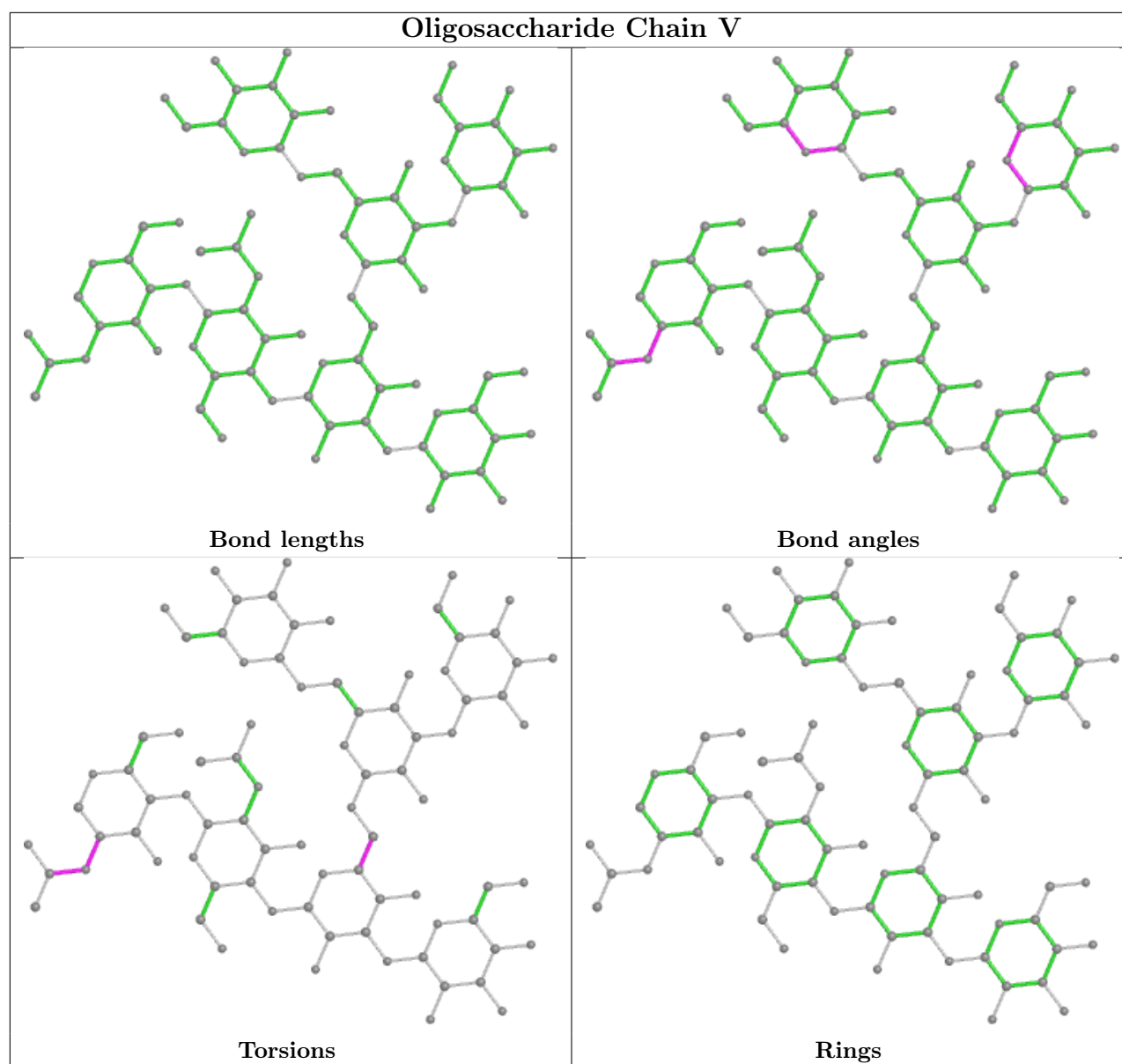












## 5.6 Ligand geometry [i](#)

37 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	E	1002	3	14,14,15	2.14	5 (35%)	17,19,21	0.93	0
9	NAG	A	611	3	14,14,15	2.21	7 (50%)	17,19,21	1.02	2 (11%)
9	NAG	A	610	3	14,14,15	2.16	6 (42%)	17,19,21	1.03	1 (5%)
9	NAG	B	701	4	14,14,15	0.36	0	17,19,21	1.15	3 (17%)
9	NAG	B	703	4	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
9	NAG	A	602	3	14,14,15	2.08	6 (42%)	17,19,21	1.04	0
9	NAG	C	603	3	14,14,15	2.17	6 (42%)	17,19,21	1.00	1 (5%)
9	NAG	C	609	3	14,14,15	2.14	5 (35%)	17,19,21	1.03	1 (5%)
9	NAG	E	1007	3	14,14,15	2.11	6 (42%)	17,19,21	1.11	2 (11%)
9	NAG	A	604	3	14,14,15	2.19	6 (42%)	17,19,21	0.97	1 (5%)
9	NAG	D	703	4	14,14,15	0.27	0	17,19,21	0.69	0
9	NAG	C	606	3	14,14,15	2.11	6 (42%)	17,19,21	1.05	1 (5%)
9	NAG	A	601	3	14,14,15	2.17	6 (42%)	17,19,21	0.95	1 (5%)
9	NAG	C	608	3	14,14,15	2.11	6 (42%)	17,19,21	0.94	0
9	NAG	E	1006	3	14,14,15	2.10	5 (35%)	17,19,21	1.02	1 (5%)
9	NAG	C	604	3	14,14,15	2.09	7 (50%)	17,19,21	1.30	3 (17%)
9	NAG	C	602	3	14,14,15	2.17	5 (35%)	17,19,21	0.94	0
9	NAG	A	603	3	14,14,15	2.15	5 (35%)	17,19,21	6.26	3 (17%)
9	NAG	A	605	3	14,14,15	2.17	5 (35%)	17,19,21	0.98	1 (5%)
9	NAG	A	607	3	14,14,15	2.05	6 (42%)	17,19,21	1.22	3 (17%)
9	NAG	C	605	3	14,14,15	2.12	6 (42%)	17,19,21	0.98	1 (5%)
9	NAG	A	609	3	14,14,15	1.96	4 (28%)	17,19,21	6.61	2 (11%)
9	NAG	D	702	4	14,14,15	0.30	0	17,19,21	0.57	0
9	NAG	E	1005	3	14,14,15	2.15	5 (35%)	17,19,21	1.10	1 (5%)
9	NAG	E	1001	3	14,14,15	2.13	5 (35%)	17,19,21	0.87	1 (5%)
9	NAG	F	701	4	14,14,15	0.92	1 (7%)	17,19,21	2.90	6 (35%)
9	NAG	A	608	3	14,14,15	2.23	5 (35%)	17,19,21	0.96	0
9	NAG	F	702	4	14,14,15	0.29	0	17,19,21	0.64	0
9	NAG	F	703	4	14,14,15	0.28	0	17,19,21	0.87	0
9	NAG	E	1003	3	14,14,15	2.02	5 (35%)	17,19,21	1.00	0
9	NAG	C	610	3	14,14,15	2.23	6 (42%)	17,19,21	1.07	2 (11%)
9	NAG	D	701	4	14,14,15	0.31	0	17,19,21	0.88	2 (11%)
9	NAG	A	606	3	14,14,15	2.07	6 (42%)	17,19,21	1.05	1 (5%)
9	NAG	C	607	3	14,14,15	2.26	6 (42%)	17,19,21	1.01	1 (5%)
9	NAG	B	702	4	14,14,15	0.54	0	17,19,21	1.64	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	C	601	3	14,14,15	2.09	5 (35%)	17,19,21	1.10	1 (5%)
9	NAG	E	1004	3	14,14,15	2.17	5 (35%)	17,19,21	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	E	1002	3	-	1/6/23/26	0/1/1/1
9	NAG	A	611	3	-	2/6/23/26	0/1/1/1
9	NAG	A	610	3	-	0/6/23/26	0/1/1/1
9	NAG	B	701	4	-	3/6/23/26	0/1/1/1
9	NAG	B	703	4	-	2/6/23/26	0/1/1/1
9	NAG	A	602	3	-	2/6/23/26	0/1/1/1
9	NAG	C	603	3	-	0/6/23/26	0/1/1/1
9	NAG	C	609	3	-	2/6/23/26	0/1/1/1
9	NAG	E	1007	3	-	0/6/23/26	0/1/1/1
9	NAG	A	604	3	-	0/6/23/26	0/1/1/1
9	NAG	D	703	4	-	2/6/23/26	0/1/1/1
9	NAG	C	606	3	-	1/6/23/26	0/1/1/1
9	NAG	A	601	3	-	0/6/23/26	0/1/1/1
9	NAG	C	608	3	-	0/6/23/26	0/1/1/1
9	NAG	E	1006	3	-	2/6/23/26	0/1/1/1
9	NAG	C	604	3	-	2/6/23/26	0/1/1/1
9	NAG	C	602	3	-	0/6/23/26	0/1/1/1
9	NAG	A	603	3	-	2/6/23/26	0/1/1/1
9	NAG	A	605	3	-	0/6/23/26	0/1/1/1
9	NAG	A	607	3	-	1/6/23/26	0/1/1/1
9	NAG	C	605	3	-	0/6/23/26	0/1/1/1
9	NAG	A	609	3	-	2/6/23/26	0/1/1/1
9	NAG	D	702	4	-	3/6/23/26	0/1/1/1
9	NAG	E	1005	3	-	0/6/23/26	0/1/1/1
9	NAG	E	1001	3	-	0/6/23/26	0/1/1/1
9	NAG	F	701	4	1/1/5/7	1/6/23/26	0/1/1/1
9	NAG	A	608	3	-	0/6/23/26	0/1/1/1
9	NAG	F	702	4	-	0/6/23/26	0/1/1/1
9	NAG	F	703	4	-	2/6/23/26	0/1/1/1
9	NAG	E	1003	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	610	3	-	0/6/23/26	0/1/1/1
9	NAG	D	701	4	-	3/6/23/26	0/1/1/1
9	NAG	A	606	3	-	0/6/23/26	0/1/1/1
9	NAG	C	607	3	-	0/6/23/26	0/1/1/1
9	NAG	B	702	4	-	4/6/23/26	0/1/1/1
9	NAG	C	601	3	-	0/6/23/26	0/1/1/1
9	NAG	E	1004	3	-	1/6/23/26	0/1/1/1

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	603	NAG	C1-C2	5.91	1.61	1.52
9	A	608	NAG	C1-C2	5.66	1.60	1.52
9	C	610	NAG	C1-C2	5.61	1.60	1.52
9	E	1001	NAG	C1-C2	5.51	1.60	1.52
9	A	611	NAG	C1-C2	5.50	1.60	1.52
9	E	1004	NAG	C1-C2	5.50	1.60	1.52
9	A	604	NAG	C1-C2	5.42	1.60	1.52
9	E	1005	NAG	C1-C2	5.38	1.60	1.52
9	A	601	NAG	C1-C2	5.38	1.60	1.52
9	C	602	NAG	C1-C2	5.35	1.60	1.52
9	C	603	NAG	C1-C2	5.34	1.60	1.52
9	A	602	NAG	C1-C2	5.31	1.60	1.52
9	E	1002	NAG	C1-C2	5.31	1.60	1.52
9	A	605	NAG	C1-C2	5.28	1.60	1.52
9	C	607	NAG	C1-C2	5.22	1.60	1.52
9	A	610	NAG	C1-C2	5.18	1.60	1.52
9	C	609	NAG	C1-C2	5.17	1.60	1.52
9	C	605	NAG	C1-C2	5.12	1.60	1.52
9	E	1006	NAG	C1-C2	5.12	1.60	1.52
9	A	606	NAG	C1-C2	5.11	1.60	1.52
9	E	1007	NAG	C1-C2	5.06	1.59	1.52
9	C	606	NAG	C1-C2	4.97	1.59	1.52
9	E	1003	NAG	C1-C2	4.87	1.59	1.52
9	C	601	NAG	C1-C2	4.82	1.59	1.52
9	C	608	NAG	C1-C2	4.75	1.59	1.52
9	C	604	NAG	C1-C2	4.68	1.59	1.52
9	A	607	NAG	C1-C2	4.61	1.59	1.52
9	A	609	NAG	C1-C2	4.54	1.59	1.52
9	C	607	NAG	O5-C5	3.55	1.50	1.43
9	C	601	NAG	O5-C5	3.38	1.50	1.43
9	C	604	NAG	O5-C5	3.36	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	609	NAG	O5-C5	3.34	1.50	1.43
9	C	608	NAG	O5-C5	3.31	1.50	1.43
9	A	610	NAG	O5-C5	3.29	1.50	1.43
9	C	602	NAG	O5-C5	3.29	1.50	1.43
9	A	605	NAG	O5-C5	3.26	1.50	1.43
9	C	606	NAG	O5-C5	3.25	1.50	1.43
9	E	1002	NAG	O5-C5	3.22	1.50	1.43
9	C	609	NAG	O5-C5	3.22	1.50	1.43
9	C	610	NAG	O5-C5	3.19	1.49	1.43
9	F	701	NAG	C1-C2	3.19	1.57	1.52
9	A	608	NAG	O5-C5	3.17	1.49	1.43
9	A	601	NAG	O5-C5	3.17	1.49	1.43
9	C	605	NAG	O5-C5	3.17	1.49	1.43
9	C	601	NAG	O5-C1	3.16	1.48	1.43
9	E	1005	NAG	O5-C5	3.16	1.49	1.43
9	A	607	NAG	O5-C5	3.15	1.49	1.43
9	E	1003	NAG	O5-C5	3.13	1.49	1.43
9	A	611	NAG	O5-C5	3.13	1.49	1.43
9	E	1004	NAG	O5-C5	3.11	1.49	1.43
9	A	604	NAG	O5-C5	3.10	1.49	1.43
9	C	603	NAG	O5-C5	3.09	1.49	1.43
9	E	1007	NAG	O5-C5	3.07	1.49	1.43
9	E	1006	NAG	O5-C5	3.04	1.49	1.43
9	C	608	NAG	O5-C1	2.95	1.48	1.43
9	C	602	NAG	O5-C1	2.88	1.48	1.43
9	A	610	NAG	O5-C1	2.88	1.48	1.43
9	C	603	NAG	O5-C1	2.88	1.48	1.43
9	A	608	NAG	O5-C1	2.86	1.48	1.43
9	C	607	NAG	C4-C5	2.86	1.59	1.53
9	E	1001	NAG	O5-C5	2.85	1.49	1.43
9	A	609	NAG	O5-C1	2.84	1.48	1.43
9	A	605	NAG	O5-C1	2.82	1.48	1.43
9	A	611	NAG	O5-C1	2.82	1.48	1.43
9	C	606	NAG	O5-C1	2.81	1.48	1.43
9	E	1002	NAG	O5-C1	2.80	1.48	1.43
9	C	610	NAG	O5-C1	2.78	1.48	1.43
9	A	606	NAG	O5-C5	2.77	1.49	1.43
9	E	1007	NAG	O5-C1	2.76	1.48	1.43
9	C	609	NAG	O5-C1	2.74	1.48	1.43
9	E	1004	NAG	O5-C1	2.74	1.48	1.43
9	E	1003	NAG	O5-C1	2.73	1.48	1.43
9	A	602	NAG	O5-C5	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1006	NAG	O5-C1	2.71	1.48	1.43
9	E	1005	NAG	O5-C1	2.71	1.48	1.43
9	A	603	NAG	O5-C5	2.71	1.48	1.43
9	A	607	NAG	O5-C1	2.70	1.48	1.43
9	A	604	NAG	O5-C1	2.69	1.48	1.43
9	A	601	NAG	O5-C1	2.68	1.48	1.43
9	C	605	NAG	O5-C1	2.64	1.47	1.43
9	C	604	NAG	O5-C1	2.62	1.47	1.43
9	A	603	NAG	C3-C2	2.56	1.57	1.52
9	A	606	NAG	C3-C2	2.56	1.57	1.52
9	C	604	NAG	C4-C5	2.50	1.58	1.53
9	C	607	NAG	O5-C1	2.49	1.47	1.43
9	A	602	NAG	O5-C1	2.47	1.47	1.43
9	A	606	NAG	O5-C1	2.44	1.47	1.43
9	E	1001	NAG	O5-C1	2.42	1.47	1.43
9	A	604	NAG	C4-C5	2.40	1.58	1.53
9	A	607	NAG	C4-C5	2.40	1.58	1.53
9	C	602	NAG	C3-C2	2.40	1.57	1.52
9	A	603	NAG	O5-C1	2.38	1.47	1.43
9	E	1004	NAG	C3-C2	2.35	1.57	1.52
9	C	609	NAG	C3-C2	2.35	1.57	1.52
9	A	608	NAG	C3-C2	2.34	1.57	1.52
9	A	605	NAG	C3-C2	2.33	1.57	1.52
9	E	1007	NAG	C4-C5	2.33	1.57	1.53
9	C	610	NAG	C4-C5	2.32	1.57	1.53
9	A	611	NAG	C3-C2	2.32	1.57	1.52
9	C	608	NAG	C4-C5	2.31	1.57	1.53
9	C	606	NAG	C4-C5	2.31	1.57	1.53
9	A	609	NAG	C4-C5	2.31	1.57	1.53
9	A	611	NAG	C4-C5	2.30	1.57	1.53
9	C	605	NAG	C4-C5	2.30	1.57	1.53
9	C	610	NAG	C3-C2	2.30	1.57	1.52
9	E	1001	NAG	C4-C5	2.29	1.57	1.53
9	E	1005	NAG	C3-C2	2.29	1.57	1.52
9	C	609	NAG	C4-C5	2.28	1.57	1.53
9	A	601	NAG	C3-C2	2.27	1.57	1.52
9	E	1006	NAG	C3-C2	2.26	1.57	1.52
9	A	602	NAG	C4-C5	2.26	1.57	1.53
9	E	1002	NAG	C3-C2	2.26	1.57	1.52
9	E	1007	NAG	C3-C2	2.26	1.57	1.52
9	A	601	NAG	C4-C5	2.26	1.57	1.53
9	A	604	NAG	C3-C2	2.26	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	607	NAG	C3-C2	2.26	1.57	1.52
9	C	606	NAG	C3-C2	2.25	1.57	1.52
9	E	1005	NAG	C4-C5	2.24	1.57	1.53
9	C	603	NAG	C4-C5	2.24	1.57	1.53
9	C	605	NAG	C3-C2	2.23	1.57	1.52
9	E	1006	NAG	C4-C5	2.23	1.57	1.53
9	C	607	NAG	C4-C3	2.23	1.58	1.52
9	C	603	NAG	C3-C2	2.23	1.57	1.52
9	E	1001	NAG	C3-C2	2.22	1.57	1.52
9	A	602	NAG	C3-C2	2.22	1.57	1.52
9	C	608	NAG	C3-C2	2.22	1.57	1.52
9	E	1004	NAG	C4-C5	2.22	1.57	1.53
9	A	610	NAG	C4-C5	2.21	1.57	1.53
9	A	608	NAG	C4-C5	2.20	1.57	1.53
9	A	605	NAG	C4-C5	2.20	1.57	1.53
9	A	610	NAG	C3-C2	2.20	1.57	1.52
9	A	604	NAG	C4-C3	2.18	1.57	1.52
9	A	603	NAG	C4-C5	2.17	1.57	1.53
9	C	604	NAG	C2-N2	2.15	1.50	1.46
9	E	1003	NAG	C4-C5	2.14	1.57	1.53
9	C	604	NAG	C3-C2	2.14	1.57	1.52
9	C	602	NAG	C4-C5	2.13	1.57	1.53
9	C	604	NAG	C4-C3	2.11	1.57	1.52
9	C	607	NAG	C3-C2	2.11	1.57	1.52
9	C	601	NAG	C4-C5	2.11	1.57	1.53
9	E	1002	NAG	C4-C5	2.11	1.57	1.53
9	A	606	NAG	C4-C5	2.10	1.57	1.53
9	C	608	NAG	C4-C3	2.08	1.57	1.52
9	C	601	NAG	C3-C2	2.07	1.56	1.52
9	A	601	NAG	C4-C3	2.07	1.57	1.52
9	A	611	NAG	C2-N2	2.06	1.49	1.46
9	C	610	NAG	C2-N2	2.06	1.49	1.46
9	C	603	NAG	C4-C3	2.06	1.57	1.52
9	A	610	NAG	C4-C3	2.05	1.57	1.52
9	A	611	NAG	C4-C3	2.05	1.57	1.52
9	A	607	NAG	C2-N2	2.03	1.49	1.46
9	A	606	NAG	C4-C3	2.02	1.57	1.52
9	C	606	NAG	C4-C3	2.02	1.57	1.52
9	E	1003	NAG	C3-C2	2.02	1.56	1.52
9	A	602	NAG	C4-C3	2.01	1.57	1.52
9	C	605	NAG	C4-C3	2.00	1.57	1.52
9	E	1007	NAG	C4-C3	2.00	1.57	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	609	NAG	C2-N2-C7	26.95	161.28	122.90
9	A	603	NAG	C2-N2-C7	25.27	158.89	122.90
9	F	701	NAG	O5-C1-C2	-8.71	97.54	111.29
9	B	702	NAG	O5-C5-C6	-5.16	99.12	107.20
9	F	701	NAG	C4-C3-C2	-4.31	104.70	111.02
9	F	701	NAG	C2-N2-C7	-3.97	117.25	122.90
9	A	603	NAG	C8-C7-N2	3.46	121.95	116.10
9	C	604	NAG	C8-C7-N2	3.41	121.88	116.10
9	F	701	NAG	C1-C2-N2	3.36	116.23	110.49
9	A	607	NAG	C8-C7-N2	3.10	121.34	116.10
9	F	701	NAG	C3-C4-C5	-3.05	104.80	110.24
9	C	610	NAG	C8-C7-N2	2.84	120.90	116.10
9	E	1007	NAG	C8-C7-N2	2.69	120.66	116.10
9	B	701	NAG	O5-C5-C6	2.58	111.24	107.20
9	E	1005	NAG	C8-C7-N2	2.56	120.43	116.10
9	C	604	NAG	O7-C7-C8	-2.56	117.31	122.06
9	B	703	NAG	C2-N2-C7	-2.54	119.29	122.90
9	C	604	NAG	C1-C2-N2	-2.54	106.15	110.49
9	A	611	NAG	C8-C7-N2	2.48	120.30	116.10
9	B	702	NAG	C1-O5-C5	2.43	115.49	112.19
9	C	606	NAG	C8-C7-N2	2.43	120.21	116.10
9	A	609	NAG	C8-C7-N2	2.43	120.21	116.10
9	D	701	NAG	O5-C5-C6	2.36	110.90	107.20
9	E	1001	NAG	C8-C7-N2	2.32	120.03	116.10
9	B	701	NAG	C2-N2-C7	-2.32	119.60	122.90
9	F	701	NAG	O5-C5-C6	2.31	110.83	107.20
9	A	605	NAG	C8-C7-N2	2.30	119.99	116.10
9	C	605	NAG	C8-C7-N2	2.28	119.96	116.10
9	A	607	NAG	O7-C7-C8	-2.28	117.83	122.06
9	A	610	NAG	C8-C7-N2	2.26	119.93	116.10
9	C	601	NAG	C8-C7-N2	2.26	119.92	116.10
9	C	610	NAG	O7-C7-C8	-2.24	117.90	122.06
9	E	1006	NAG	C8-C7-N2	2.20	119.82	116.10
9	E	1007	NAG	O7-C7-C8	-2.15	118.06	122.06
9	A	606	NAG	C8-C7-N2	2.15	119.74	116.10
9	D	701	NAG	C4-C3-C2	-2.14	107.88	111.02
9	A	603	NAG	C1-O5-C5	2.14	115.09	112.19
9	C	609	NAG	C8-C7-N2	2.09	119.64	116.10
9	A	601	NAG	C8-C7-N2	2.07	119.61	116.10
9	A	604	NAG	C8-C7-N2	2.07	119.61	116.10
9	A	607	NAG	C1-C2-N2	-2.04	107.01	110.49
9	C	603	NAG	C8-C7-N2	2.03	119.54	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	607	NAG	C8-C7-N2	2.02	119.52	116.10
9	A	611	NAG	O7-C7-C8	-2.01	118.32	122.06
9	B	701	NAG	O5-C1-C2	-2.01	108.12	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	F	701	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	701	NAG	C8-C7-N2-C2
9	B	701	NAG	O7-C7-N2-C2
9	B	703	NAG	C8-C7-N2-C2
9	B	703	NAG	O7-C7-N2-C2
9	D	702	NAG	C8-C7-N2-C2
9	D	702	NAG	O7-C7-N2-C2
9	D	703	NAG	C8-C7-N2-C2
9	D	703	NAG	O7-C7-N2-C2
9	B	702	NAG	C8-C7-N2-C2
9	B	702	NAG	O7-C7-N2-C2
9	D	701	NAG	C8-C7-N2-C2
9	D	701	NAG	O7-C7-N2-C2
9	F	703	NAG	C8-C7-N2-C2
9	B	702	NAG	O5-C5-C6-O6
9	C	604	NAG	O5-C5-C6-O6
9	B	702	NAG	C4-C5-C6-O6
9	F	703	NAG	O7-C7-N2-C2
9	A	611	NAG	O5-C5-C6-O6
9	A	602	NAG	O5-C5-C6-O6
9	A	607	NAG	O5-C5-C6-O6
9	A	609	NAG	C1-C2-N2-C7
9	C	606	NAG	O5-C5-C6-O6
9	A	603	NAG	O5-C5-C6-O6
9	E	1004	NAG	O5-C5-C6-O6
9	D	702	NAG	O5-C5-C6-O6
9	C	609	NAG	C4-C5-C6-O6
9	A	603	NAG	C1-C2-N2-C7
9	D	701	NAG	O5-C5-C6-O6
9	F	701	NAG	O5-C5-C6-O6
9	E	1006	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	609	NAG	O5-C5-C6-O6
9	C	604	NAG	C4-C5-C6-O6
9	E	1006	NAG	O5-C5-C6-O6
9	B	701	NAG	C4-C5-C6-O6
9	E	1002	NAG	C4-C5-C6-O6
9	A	602	NAG	C4-C5-C6-O6
9	A	609	NAG	C3-C2-N2-C7
9	A	611	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	603	NAG	1	0
9	E	1001	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

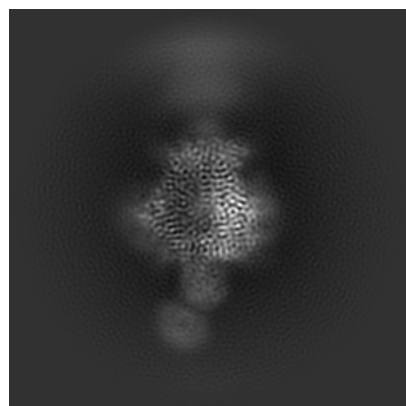
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25732. These allow visual inspection of the internal detail of the map and identification of artifacts.

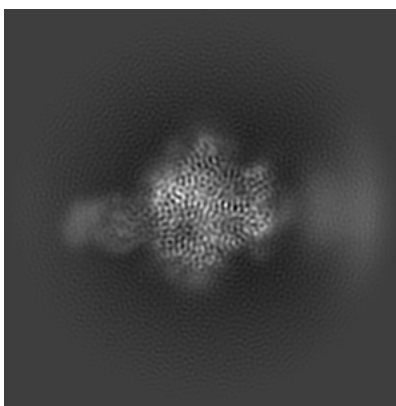
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

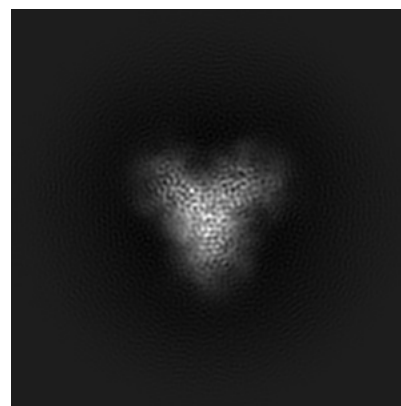
#### 6.1.1 Primary map



X

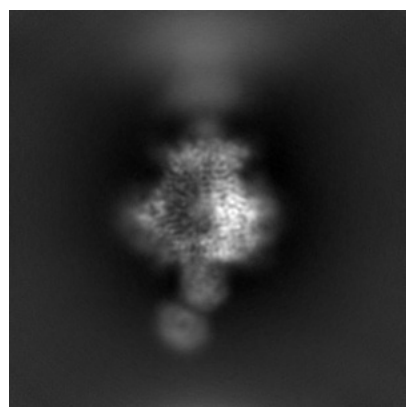


Y

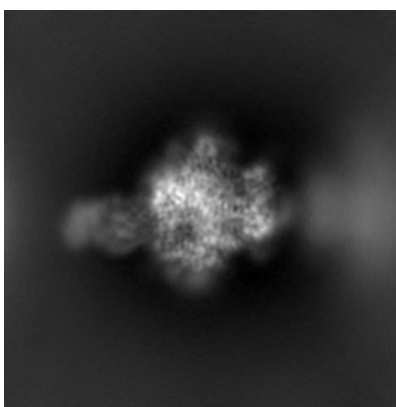


Z

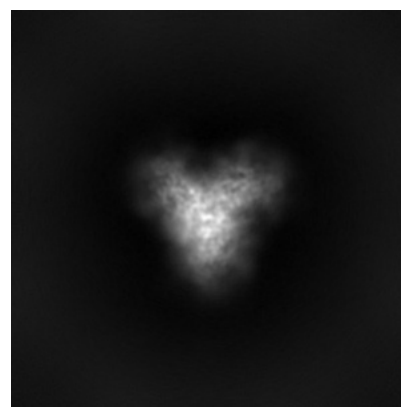
#### 6.1.2 Raw map



X



Y

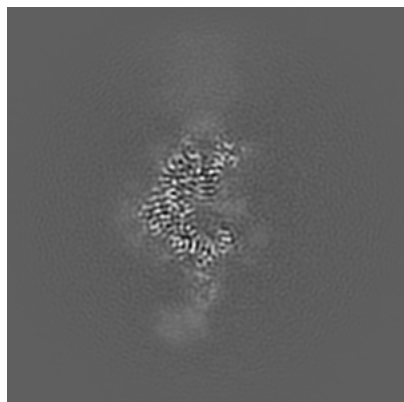


Z

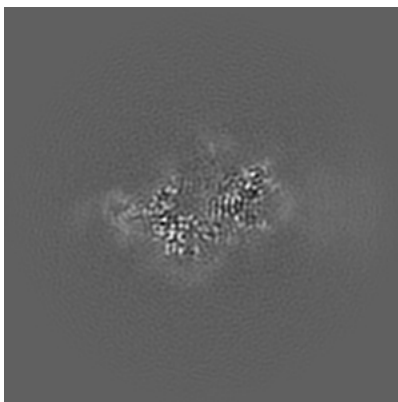
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

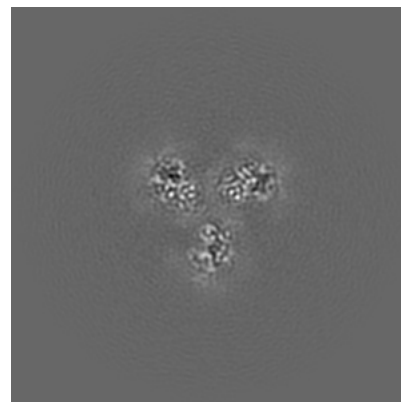
### 6.2.1 Primary map



X Index: 140

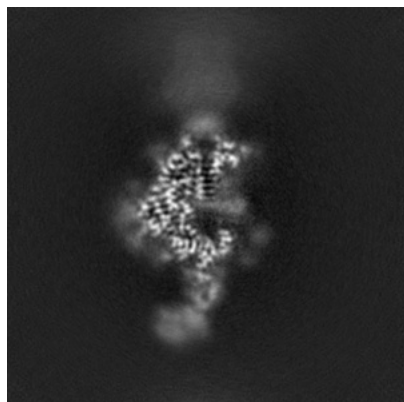


Y Index: 140

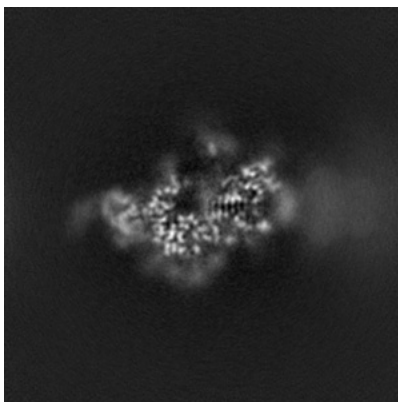


Z Index: 140

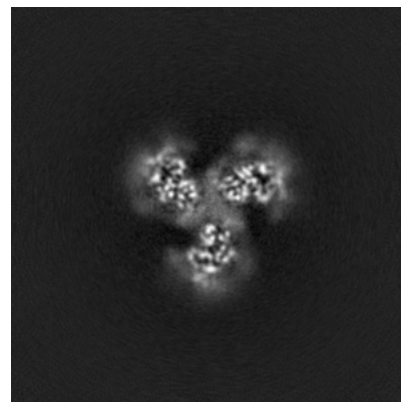
### 6.2.2 Raw map



X Index: 140



Y Index: 140

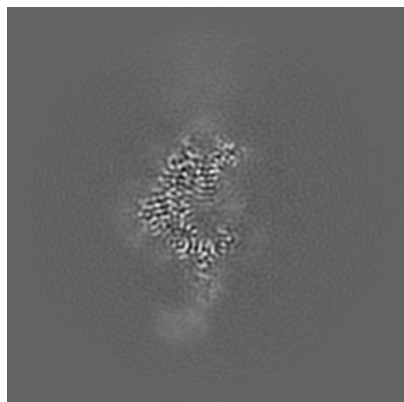


Z Index: 140

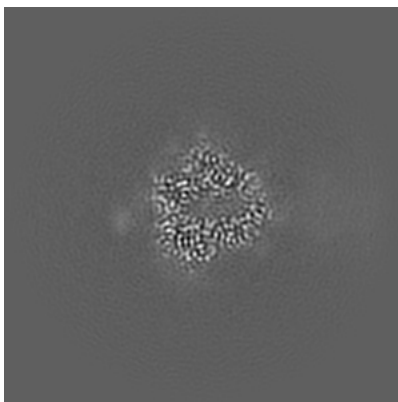
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

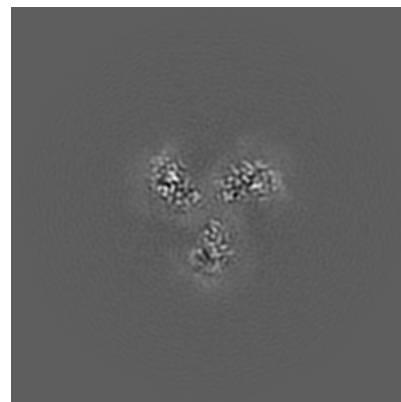
### 6.3.1 Primary map



X Index: 139

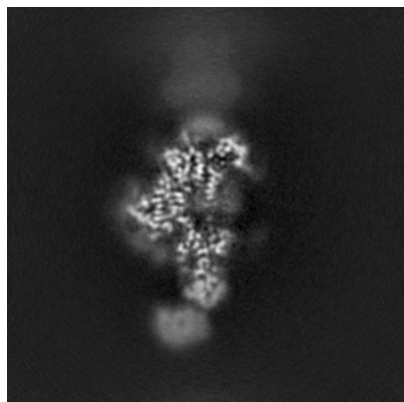


Y Index: 151

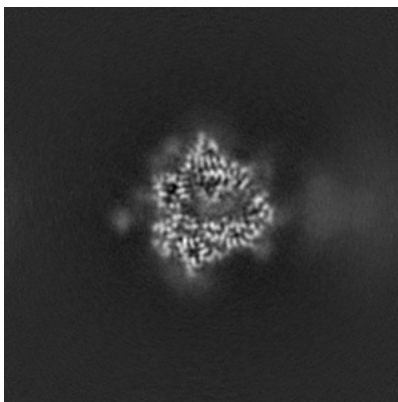


Z Index: 138

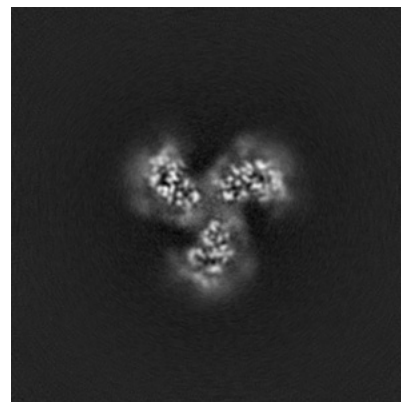
### 6.3.2 Raw map



X Index: 135



Y Index: 153



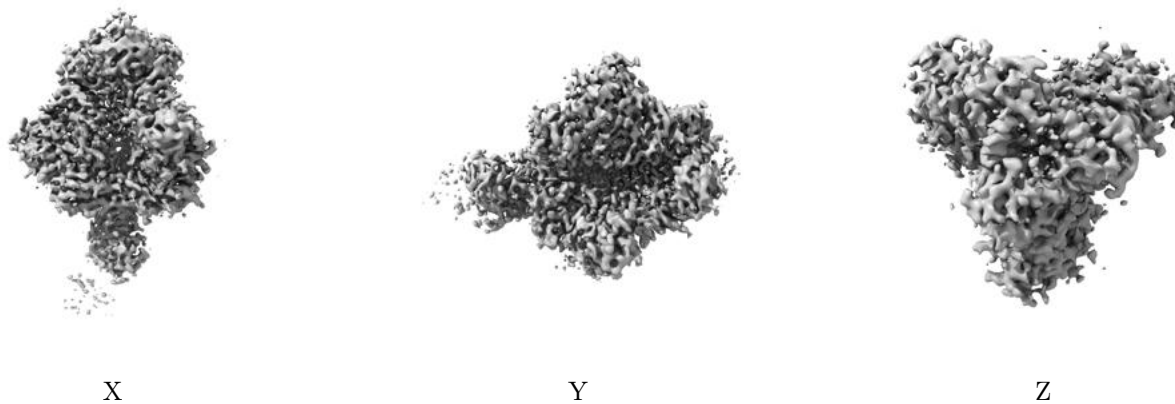
Z Index: 138

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



## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.689. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

## 6.5 Mask visualisation [i](#)

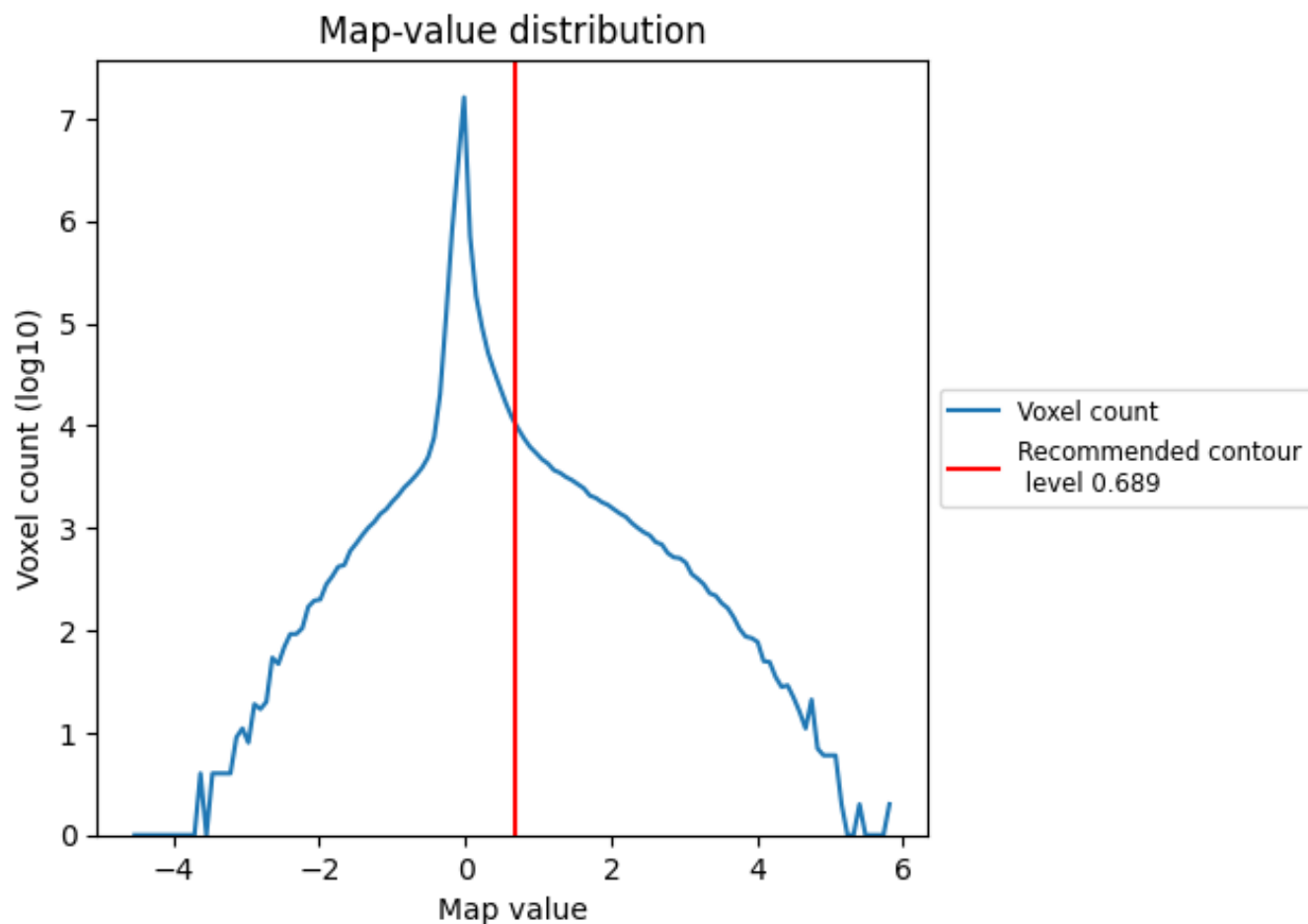
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

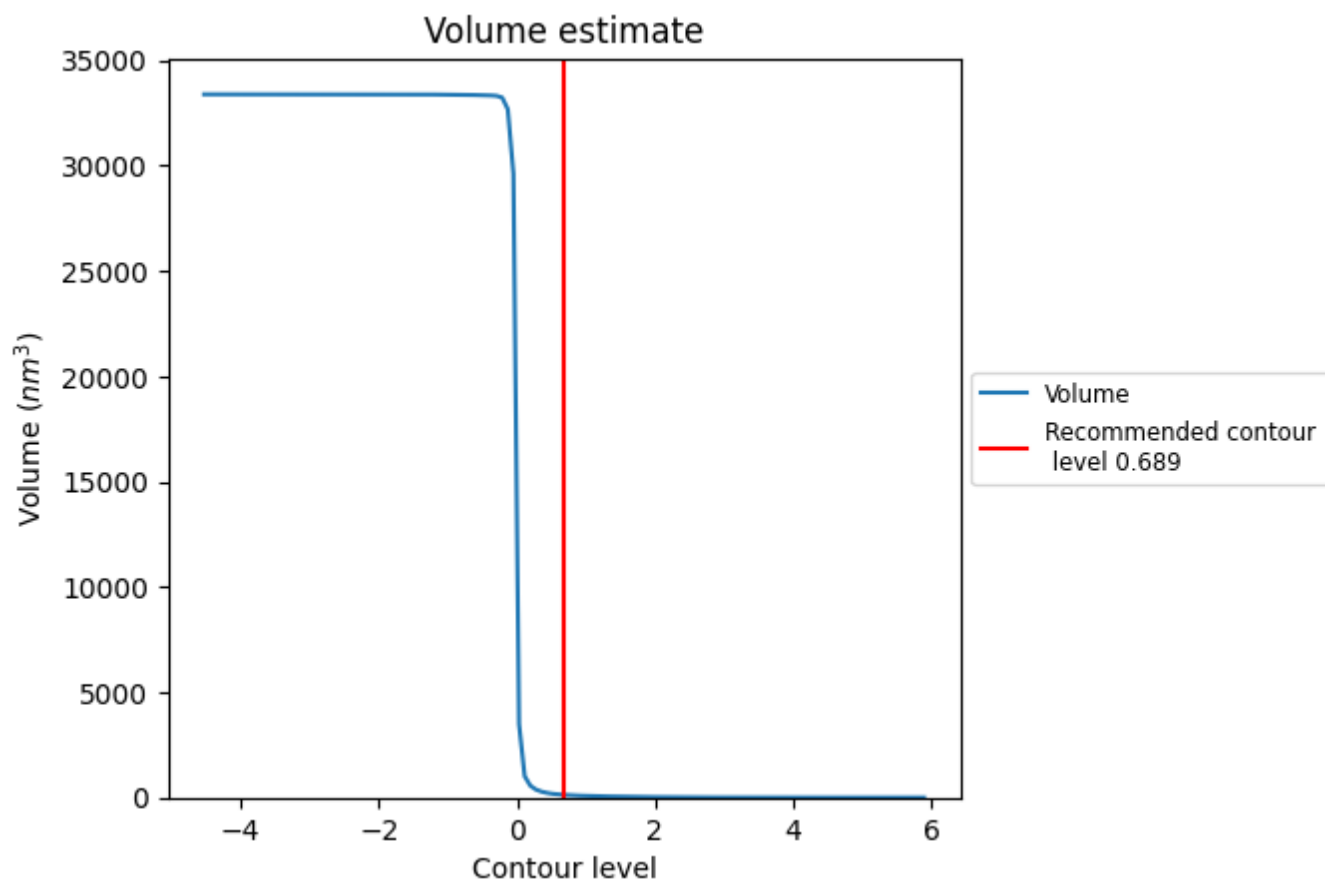
This section contains the results of statistical analysis of the map.

### 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.

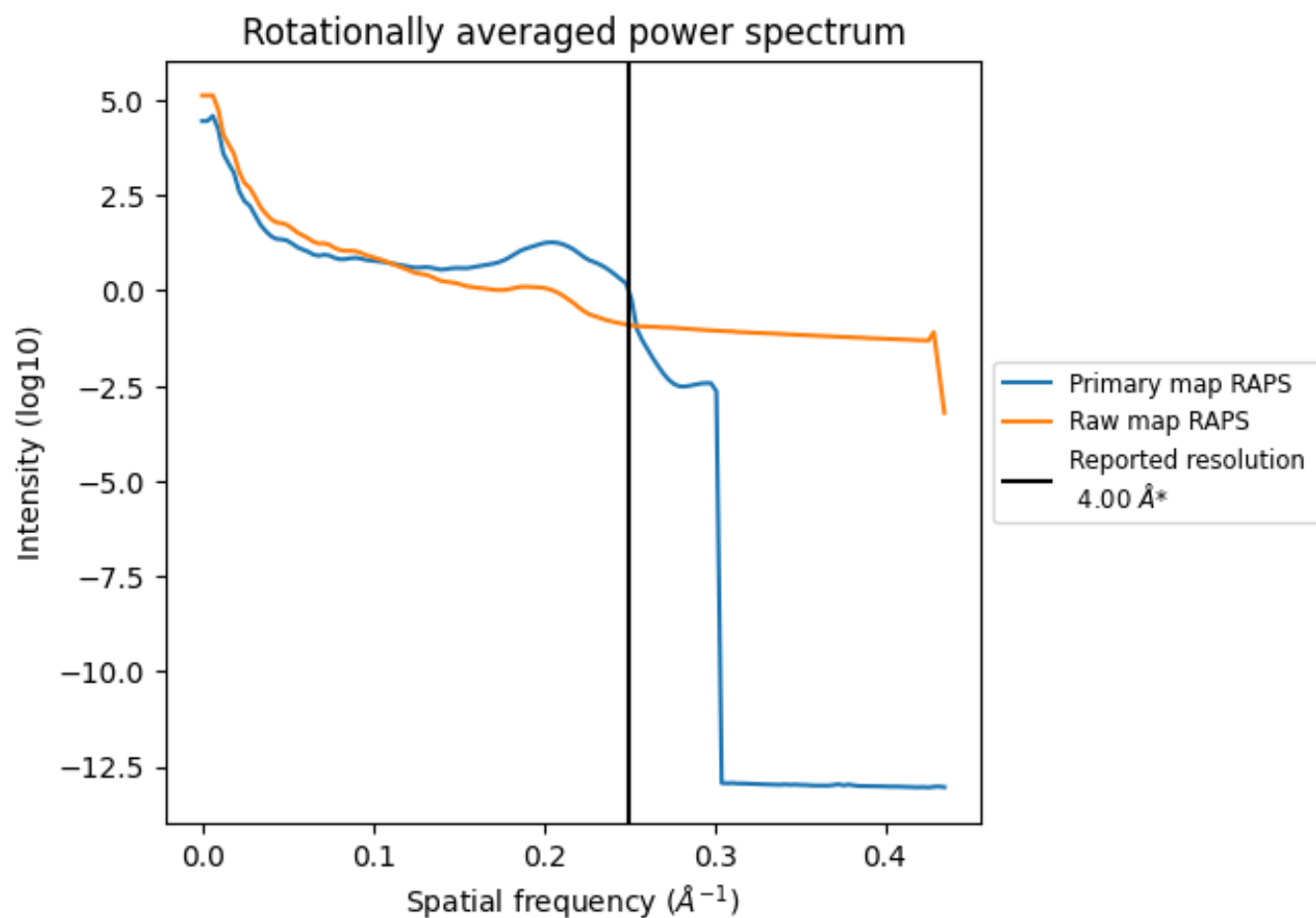
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm<sup>3</sup>; this corresponds to an approximate mass of 113 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 ⓘ

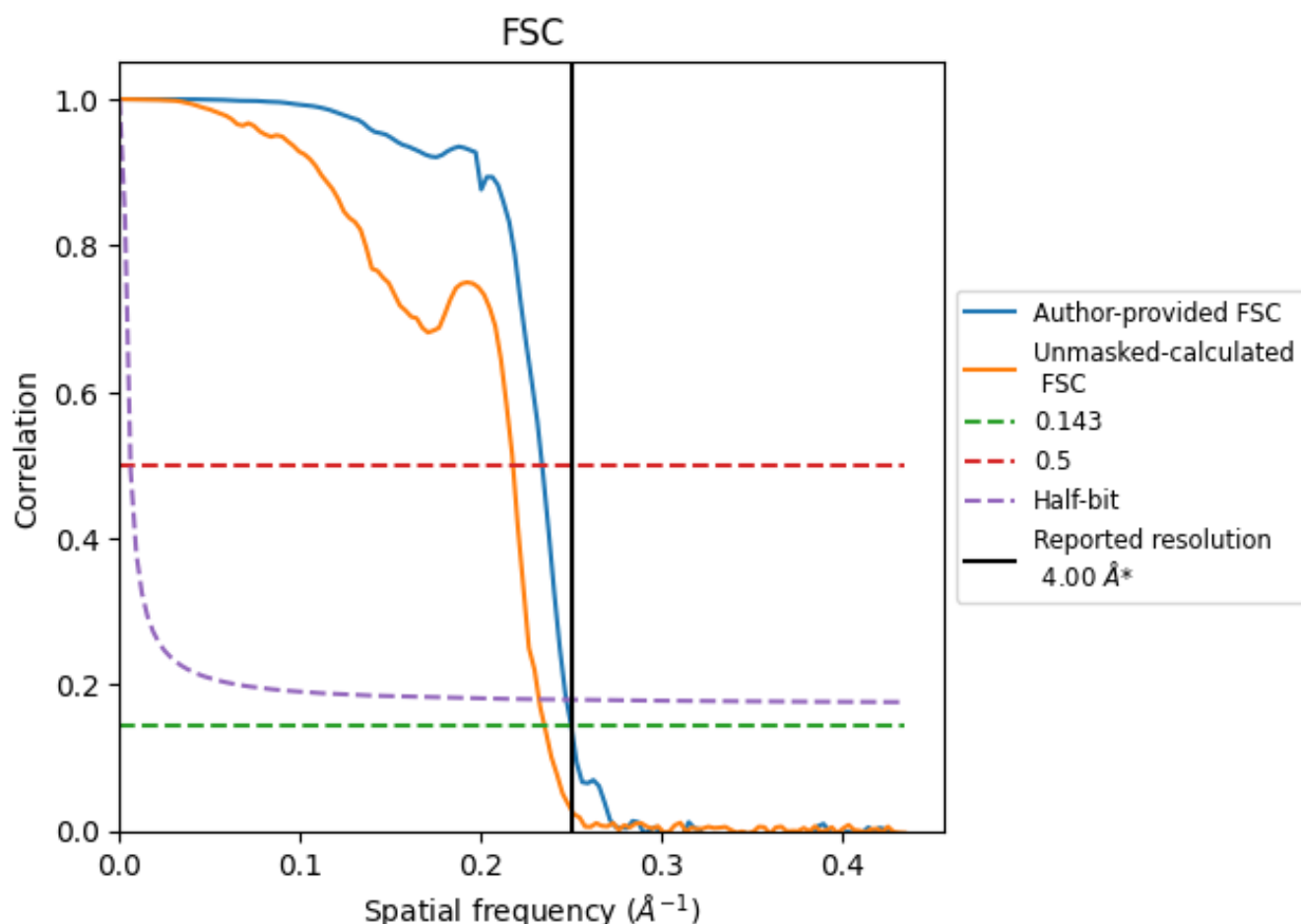


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

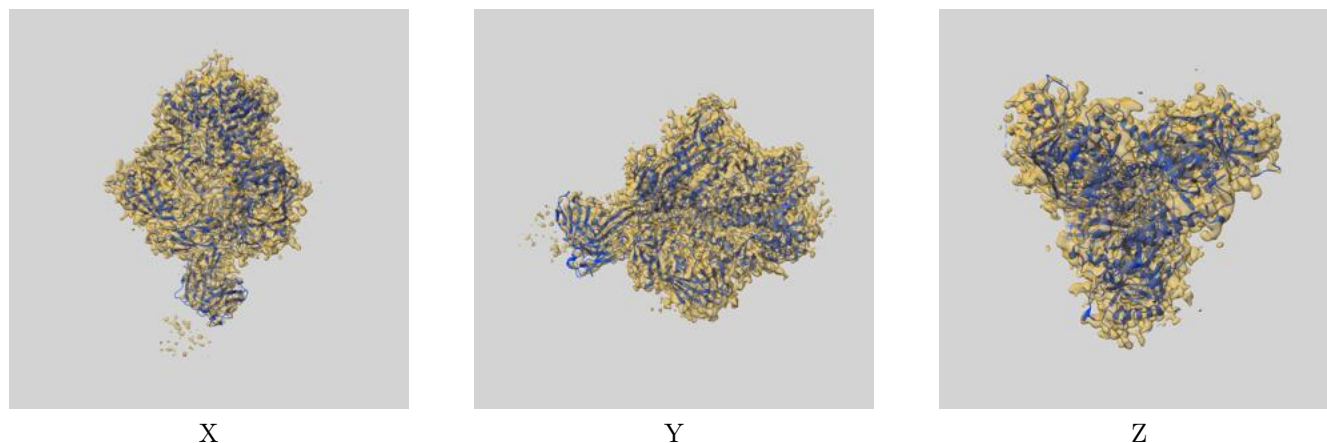
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	4.28	4.04
Unmasked-calculated*	4.25	4.59	4.30

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

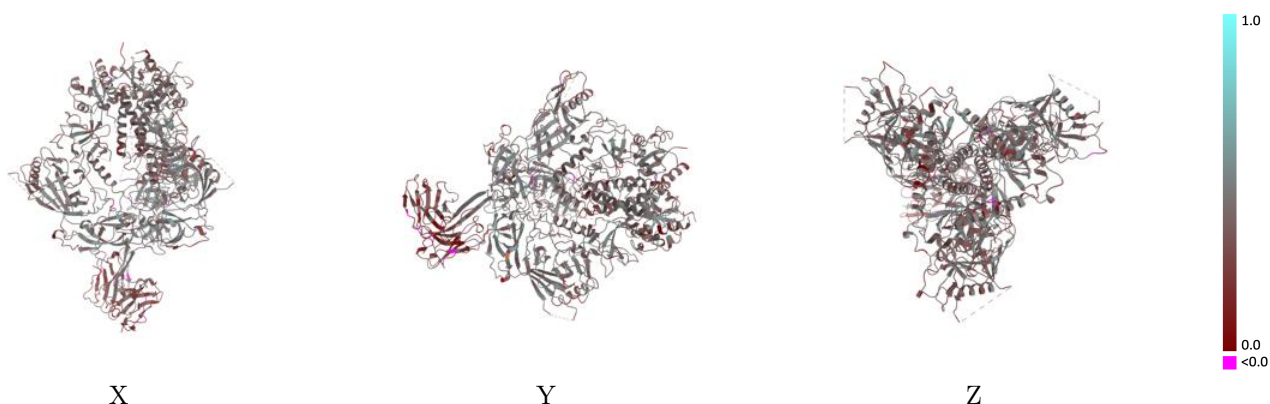
This section contains information regarding the fit between EMDB map EMD-25732 and PDB model 7T73. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



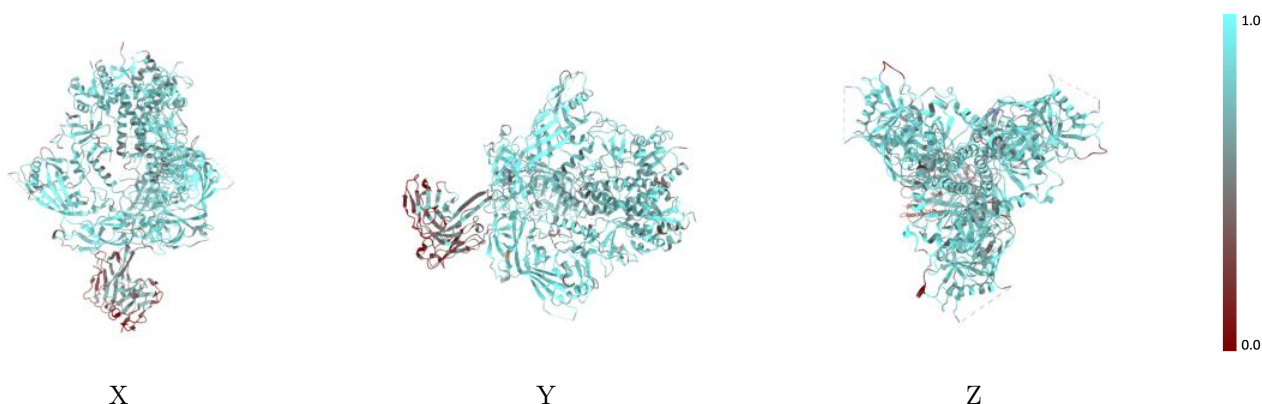
The images above show the 3D surface view of the map at the recommended contour level 0.689 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



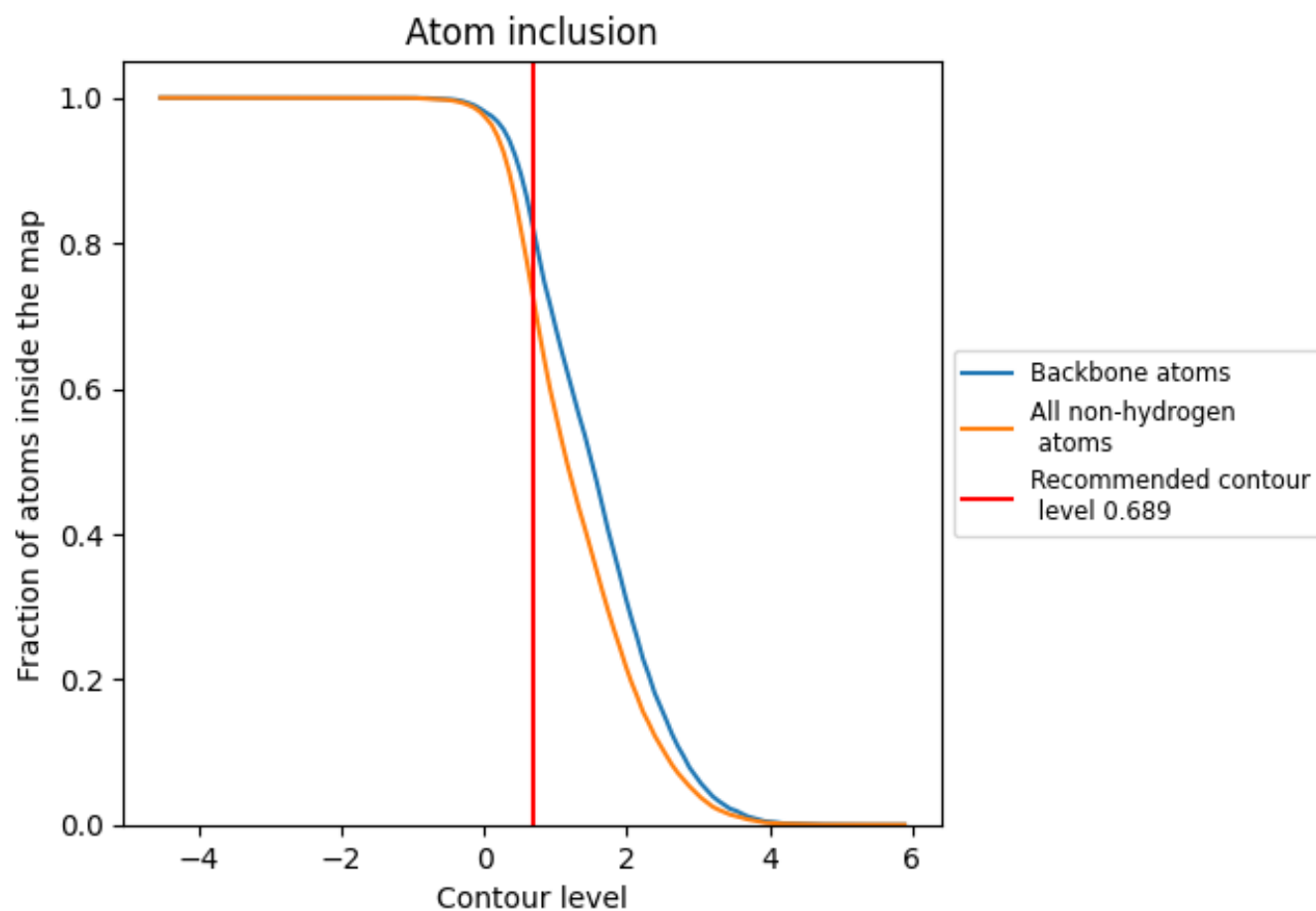
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.689).

## 9.4 Atom inclusion [i](#)

















































At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.689) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7262	 0.3880
A	 0.7836	 0.4140
B	 0.7477	 0.3830
C	 0.7648	 0.4040
D	 0.7414	 0.3770
E	 0.7944	 0.4200
F	 0.7508	 0.3870
G	 0.5714	 0.3220
H	 0.4092	 0.2540
I	 0.6071	 0.3190
J	 0.7000	 0.3700
K	 0.6786	 0.3640
L	 0.3913	 0.2640
M	 0.3214	 0.2720
N	 0.7692	 0.4870
O	 0.6071	 0.3130
P	 0.6800	 0.3790
Q	 0.6429	 0.3940
R	 0.5128	 0.4850
S	 0.7000	 0.4210
T	 0.5714	 0.2880
U	 0.7143	 0.3670
V	 0.6386	 0.4020

