



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 08:52 PM EDT

PDB ID : 6UDK
EMDB ID : EMD-20740
Title : HIV-1 bNAb 1-55 in complex with modified BG505 SOSIP-based immunogen RC1 and 10-1074
Authors : Abernathy, M.E.; Barnes, C.O.; Gristick, H.B.; Bjorkman, P.J.
Deposited on : 2019-09-19
Resolution : 3.90 Å (reported)
Based on initial models : 6MTJ, 4RWY, 5T3Z

This is a wwPDB EM Validation Summary 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

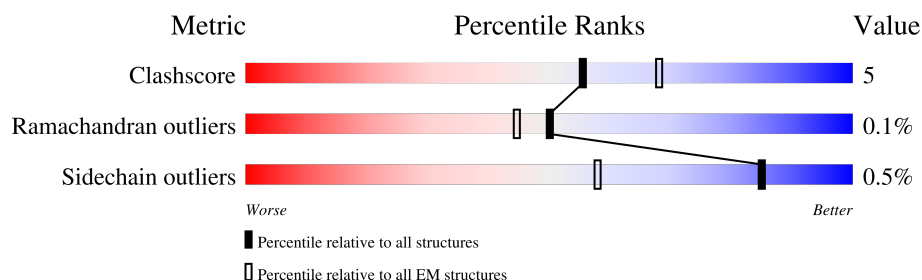
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	G	481	<div> <div>8%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
1	K	481	<div> <div>6%</div> <div>81%</div> <div>10%</div> <div>8%</div> </div>
1	R	481	<div> <div>8%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
2	A	238	<div> <div>31%</div> <div>49%</div> <div>7%</div> <div>44%</div> </div>
2	F	238	<div> <div>31%</div> <div>46%</div> <div>10%</div> <div>44%</div> </div>
2	O	238	<div> <div>30%</div> <div>50%</div> <div>5%</div> <div>44%</div> </div>
3	B	214	<div> <div>14%</div> <div>45%</div> <div>5%</div> <div>50%</div> </div>
3	I	214	<div> <div>14%</div> <div>43%</div> <div>7%</div> <div>50%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	214	
4	D	262	
4	H	262	
4	M	262	
5	E	234	
5	L	234	
5	N	234	
6	C	153	
6	J	153	
6	Q	153	
7	S	2	
7	W	2	
7	X	2	
7	b	2	
7	c	2	
7	f	2	
7	g	2	
8	T	6	
8	d	6	
9	U	3	
9	Z	3	
10	V	8	
10	a	8	
11	Y	7	
12	e	6	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25724 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 RC1 variant of HIV-1 Env glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		
1	K	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		
1	R	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		

- Molecule 2 is a protein called 10-1074 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
2	F	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
2	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 3 is a protein called 10-1074 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
3	I	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
3	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 4 is a protein called 1-55 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	130	Total	C	N	O	S	0	0
			1056	675	180	197	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	130	Total	C	N	O	S	0	0
			1056	675	180	197	4		
4	H	130	Total	C	N	O	S	0	0
			1056	675	180	197	4		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	221	HIS	-	expression tag	UNP S6C4S0
M	222	HIS	-	expression tag	UNP S6C4S0
M	223	HIS	-	expression tag	UNP S6C4S0
M	224	HIS	-	expression tag	UNP S6C4S0
M	225	HIS	-	expression tag	UNP S6C4S0
D	221	HIS	-	expression tag	UNP S6C4S0
D	222	HIS	-	expression tag	UNP S6C4S0
D	223	HIS	-	expression tag	UNP S6C4S0
D	224	HIS	-	expression tag	UNP S6C4S0
D	225	HIS	-	expression tag	UNP S6C4S0
H	221	HIS	-	expression tag	UNP S6C4S0
H	222	HIS	-	expression tag	UNP S6C4S0
H	223	HIS	-	expression tag	UNP S6C4S0
H	224	HIS	-	expression tag	UNP S6C4S0
H	225	HIS	-	expression tag	UNP S6C4S0

- Molecule 5 is a protein called 1-55 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	108	Total	C	N	O	S	0	0
			810	510	139	159	2		
5	E	108	Total	C	N	O	S	0	0
			810	510	139	159	2		
5	L	108	Total	C	N	O	S	0	0
			810	510	139	159	2		

- Molecule 6 is a protein called RC1 variant of HIV-1 Env glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	123	Total	C	N	O	S	0	0
			979	617	170	186	6		
6	J	123	Total	C	N	O	S	0	0
			979	617	170	186	6		

Continued on next page...

Continued from previous page...

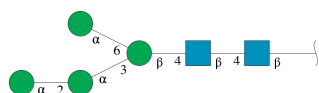
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	123	Total	C	N	O	S	0	0
			979	617	170	186	6		

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



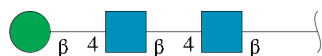
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



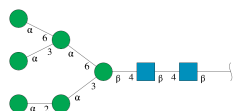
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	6	Total	C	N	O	0	0
			72	40	2	30		
8	d	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 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.



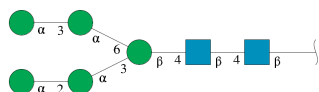
Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	3	Total	C	N	O	0	0
			39	22	2	15		
9	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



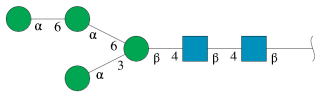
Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	8	Total	C	N	O	0	0
			94	52	2	40		
10	a	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



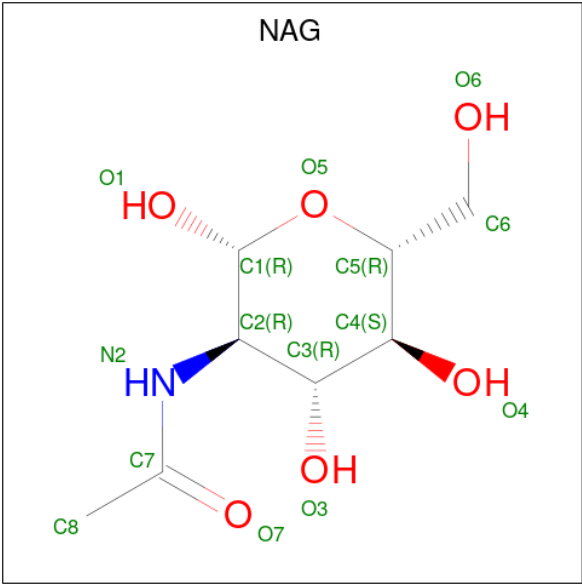
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 12 is an oligosaccharide called 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
12	e	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

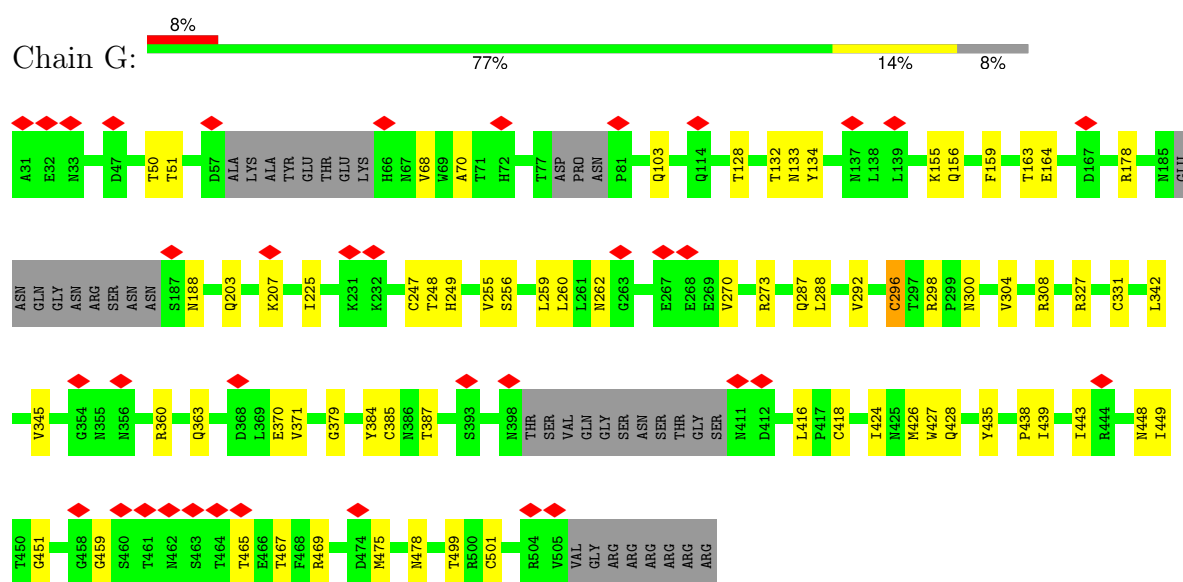
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	G	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	K	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0
13	R	1	Total 14	C 8	N 1	O 5	0

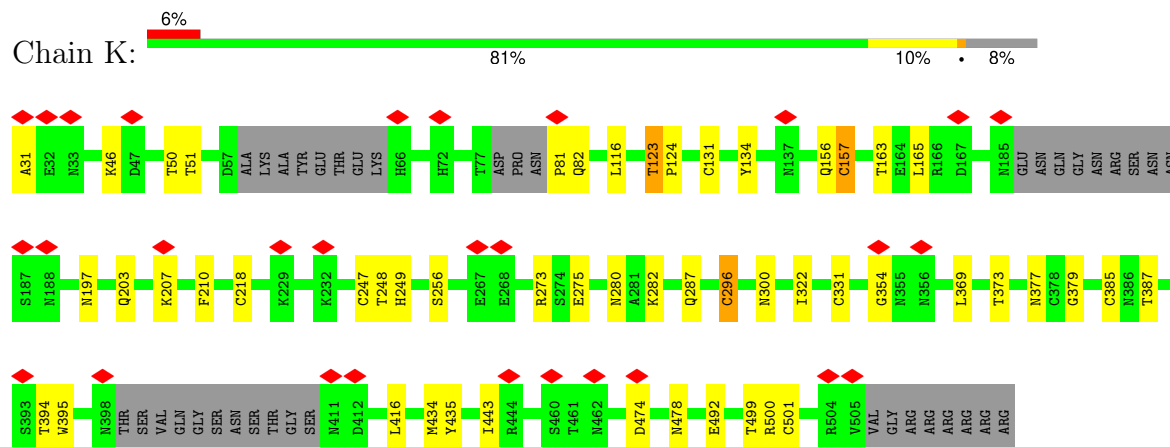
3 Residue-property plots

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

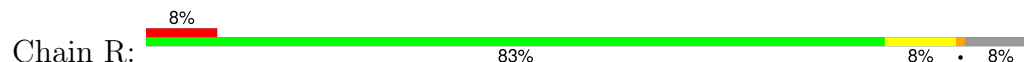
- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp120

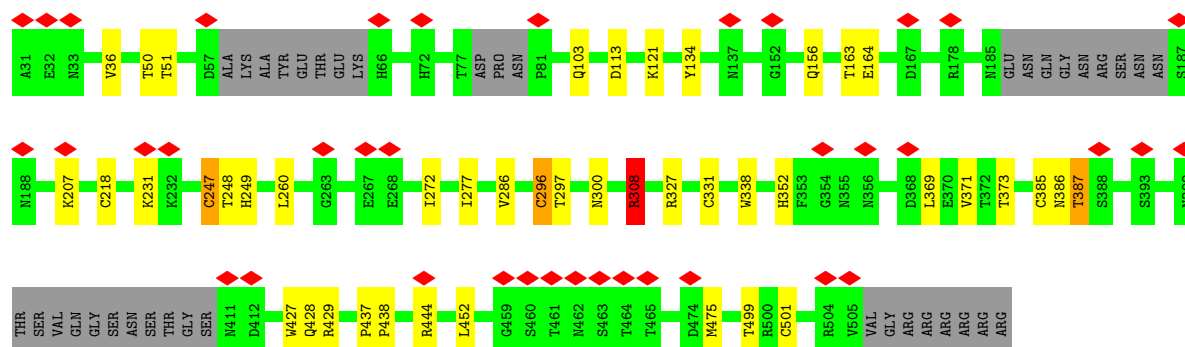


- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp120

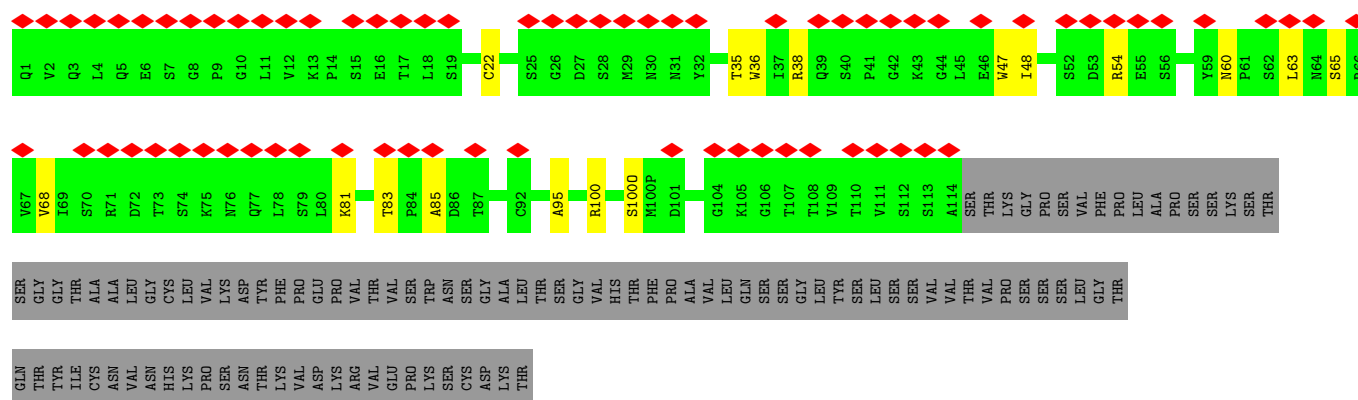


- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp120

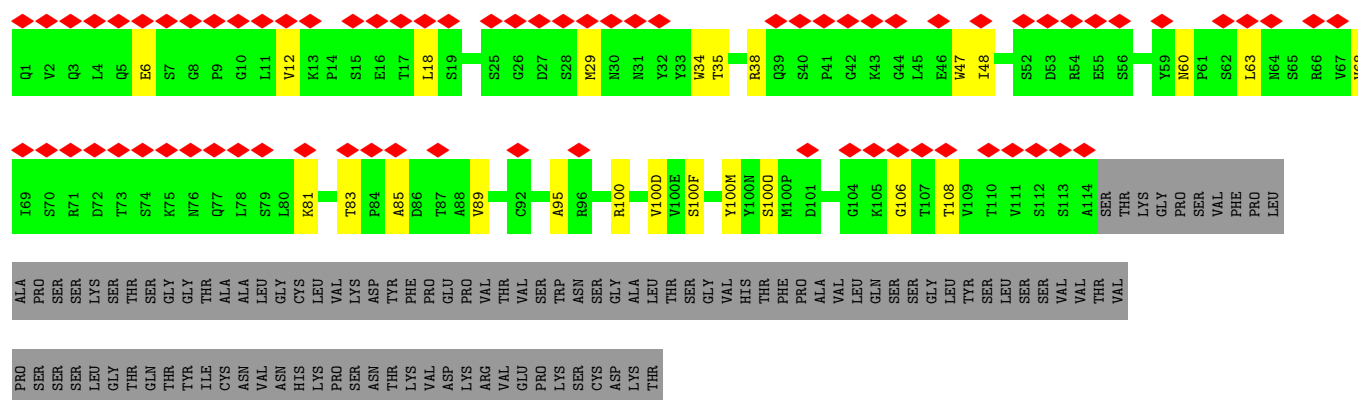




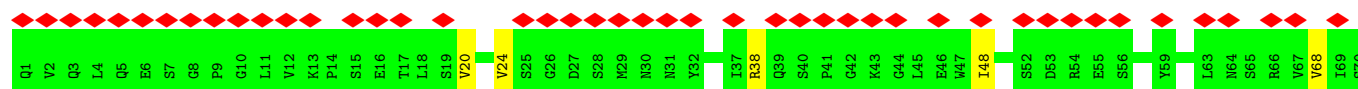
• Molecule 2: 10-1074 Fab Heavy Chain



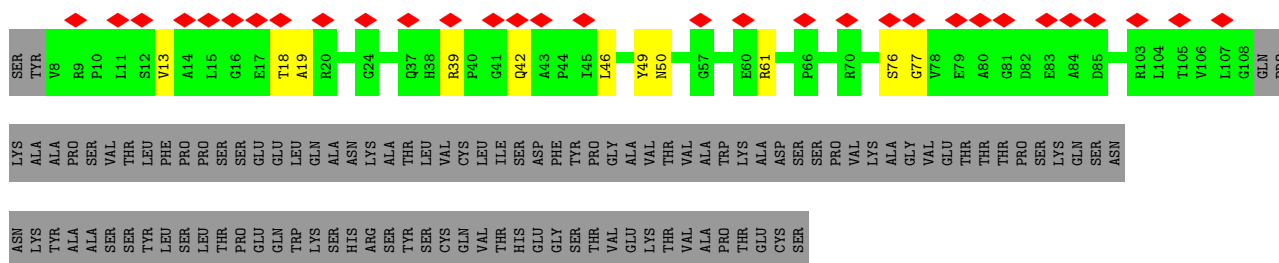
• Molecule 2: 10-1074 Fab Heavy Chain



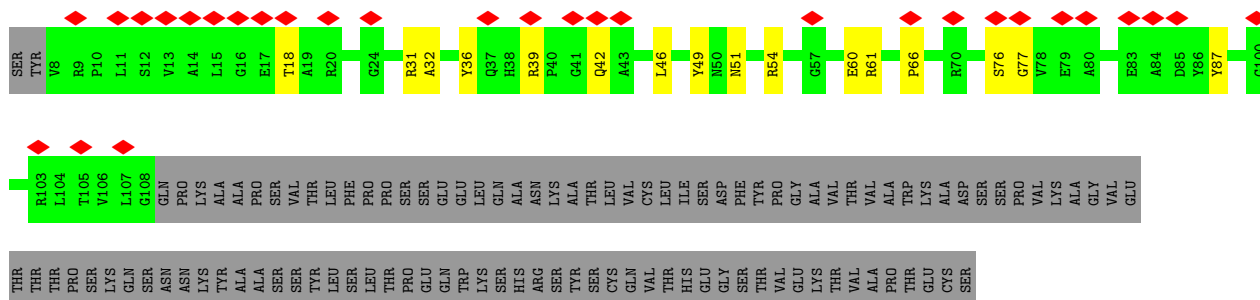
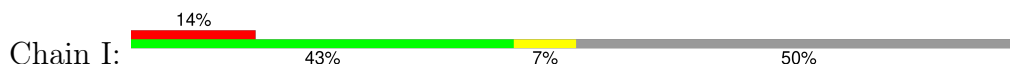
• Molecule 2: 10-1074 Fab Heavy Chain



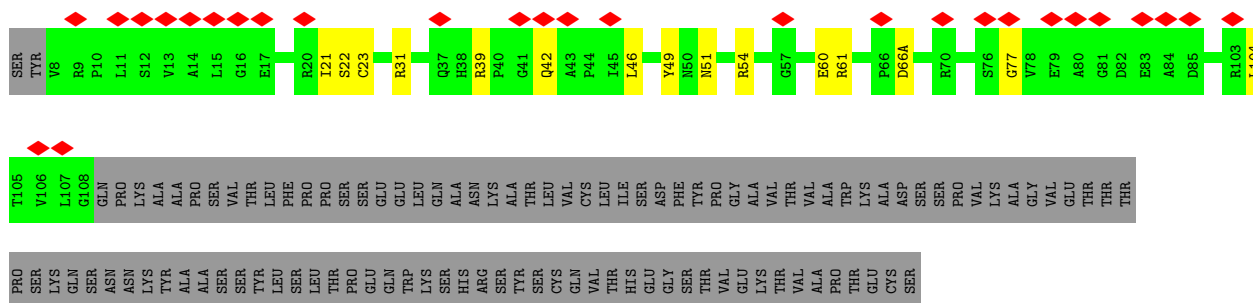
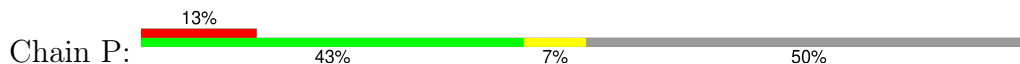
- Molecule 3: 10-1074 Fab Light Chain



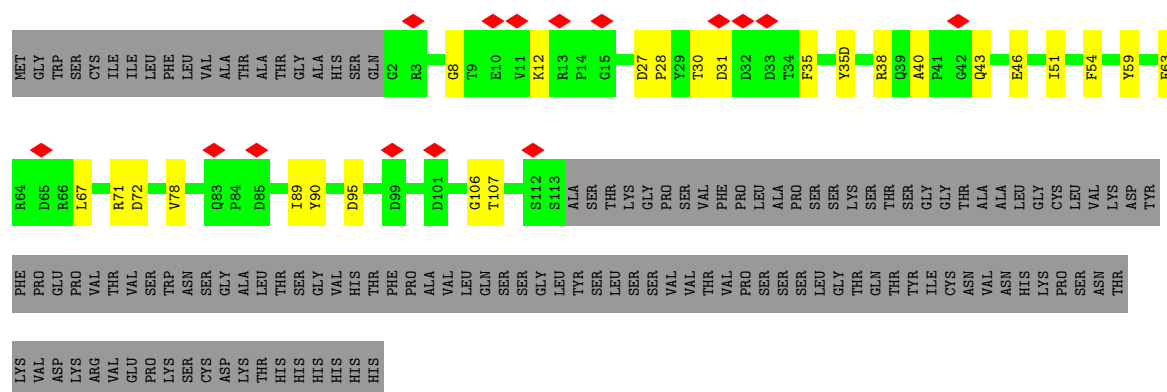
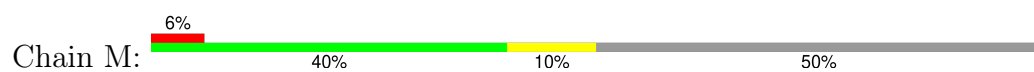
- Molecule 3: 10-1074 Fab Light Chain



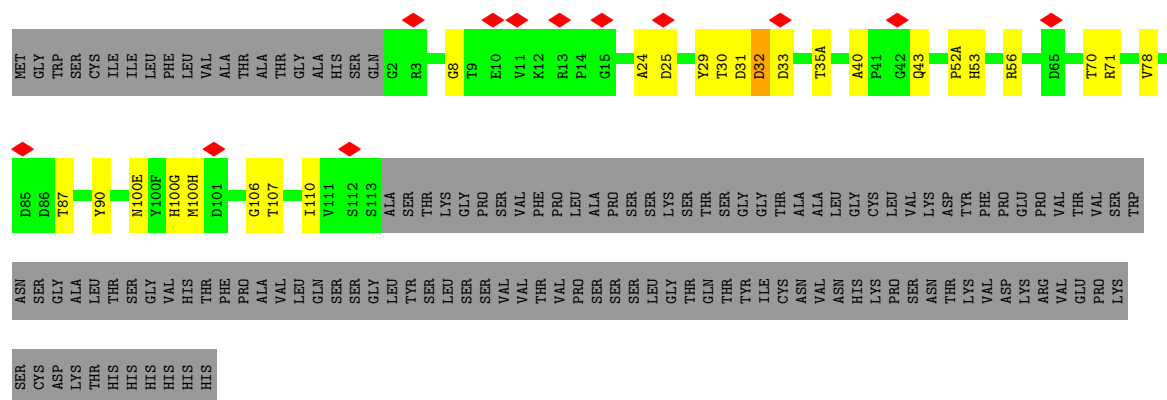
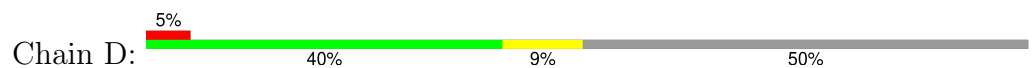
- Molecule 3: 10-1074 Fab Light Chain



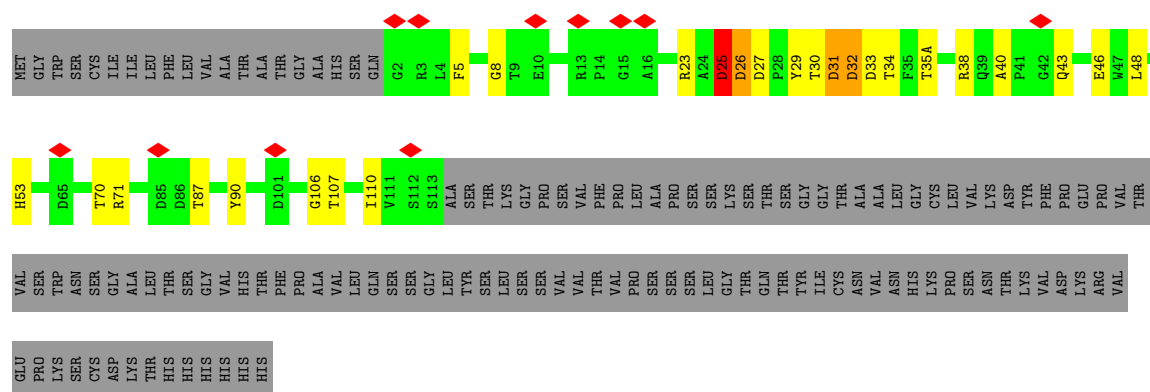
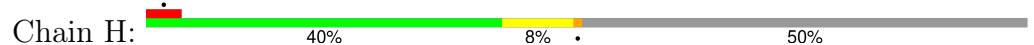
- Molecule 4: 1-55 Fab Heavy Chain



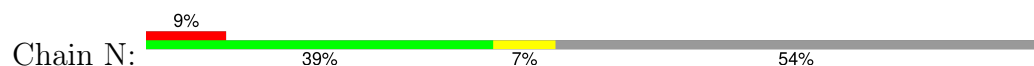
• Molecule 4: 1-55 Fab Heavy Chain

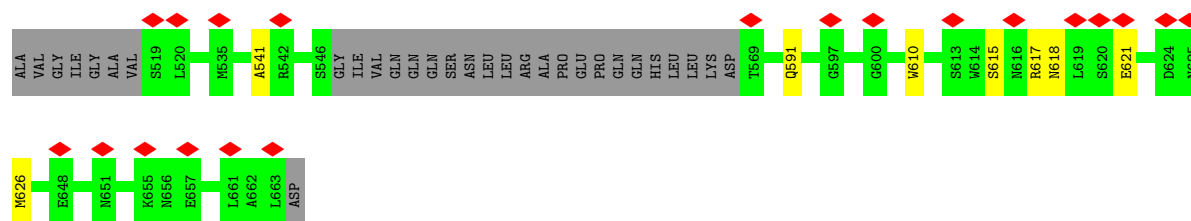


• Molecule 4: 1-55 Fab Heavy Chain

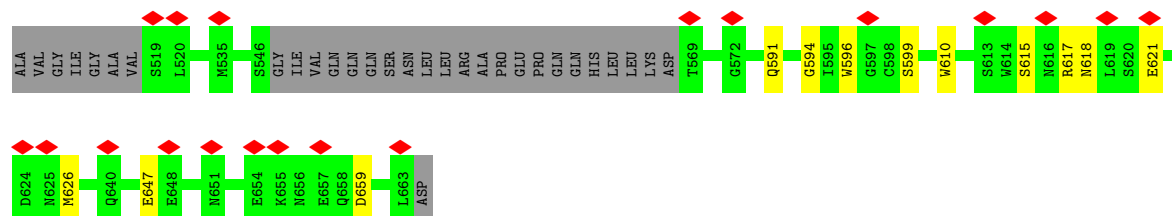


• Molecule 5: 1-55 Fab Light Chain

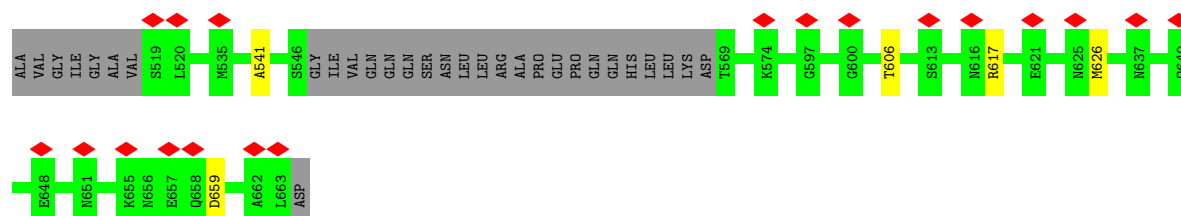
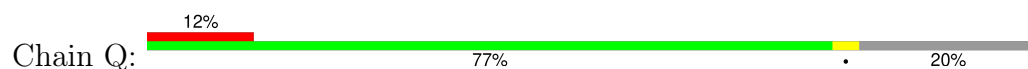




- Molecule 6: RC1 variant of HIV-1 Env glycoprotein gp41



- Molecule 6: RC1 variant of HIV-1 Env glycoprotein gp41



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



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



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



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



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



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



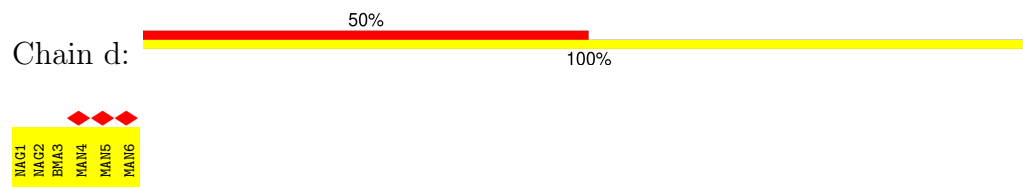
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



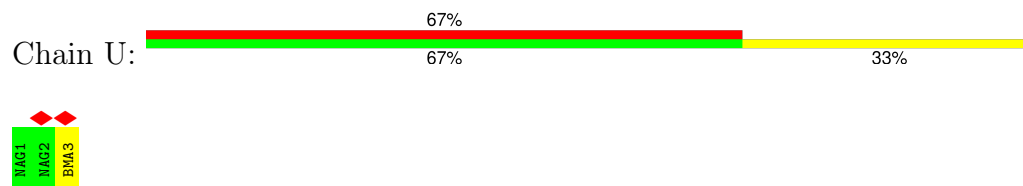
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



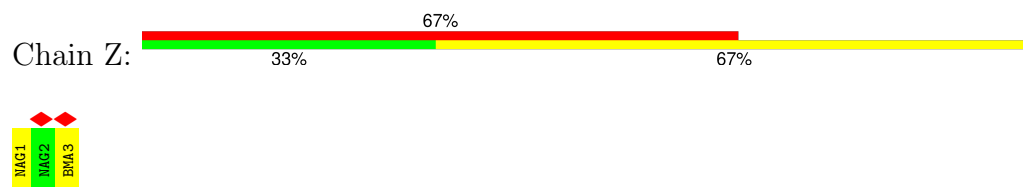
- Molecule 8: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



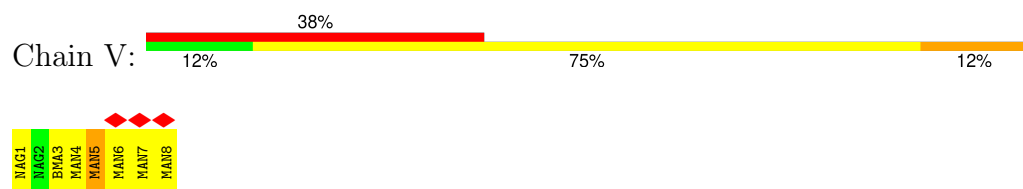
- Molecule 9: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



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



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



- Molecule 11: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

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



- Molecule 12: 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	110126	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	73000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.426	Depositor
Minimum map value	-0.263	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0717	Depositor
Map size (Å)	291.19998, 291.19998, 291.19998	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3999999, 1.3999999, 1.3999999	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.27	0/3558	0.51	0/4827
1	K	0.27	0/3558	0.50	0/4827
1	R	0.29	0/3558	0.52	0/4827
2	A	0.25	0/1066	0.49	0/1451
2	F	0.25	0/1066	0.50	0/1451
2	O	0.25	0/1066	0.47	0/1451
3	B	0.26	0/845	0.49	0/1148
3	I	0.25	0/845	0.47	0/1148
3	P	0.26	0/845	0.46	0/1148
4	D	0.47	0/1092	0.84	4/1488 (0.3%)
4	H	0.51	1/1092 (0.1%)	0.64	1/1488 (0.1%)
4	M	0.26	0/1092	0.53	0/1488
5	E	0.27	0/827	0.50	0/1120
5	L	0.27	0/827	0.52	0/1120
5	N	0.27	0/827	0.52	0/1120
6	C	0.23	0/998	0.39	0/1354
6	J	0.23	0/998	0.39	0/1354
6	Q	0.23	0/998	0.39	0/1354
All	All	0.29	1/25158 (0.0%)	0.52	5/34164 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	3
4	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	31	ASP	CB-CG	-6.28	1.38	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	33	ASP	CB-CG-OD1	-12.67	106.90	118.30
4	D	33	ASP	CB-CG-OD2	12.51	129.56	118.30
4	D	32	ASP	CB-CG-OD2	8.38	125.84	118.30
4	D	32	ASP	CB-CG-OD1	-7.20	111.82	118.30
4	H	26	ASP	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	23	ARG	Mainchain
1	R	308	ARG	Sidechain
1	R	386	ASN	Peptide
1	R	387	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3485	0	3436	43	0
1	K	3485	0	3436	33	0
1	R	3485	0	3436	29	0
2	A	1041	0	1005	10	0
2	F	1041	0	1005	12	0
2	O	1041	0	1005	7	0
3	B	824	0	788	6	0
3	I	824	0	788	8	0
3	P	824	0	788	8	0
4	D	1056	0	987	27	0
4	H	1056	0	986	21	0
4	M	1056	0	987	21	0
5	E	810	0	795	8	0
5	L	810	0	795	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	810	0	795	9	0
6	C	979	0	951	5	0
6	J	979	0	951	7	0
6	Q	979	0	951	4	0
7	S	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	f	28	0	25	0	0
7	g	28	0	25	0	0
8	T	72	0	61	0	0
8	d	72	0	61	0	0
9	U	39	0	34	0	0
9	Z	39	0	34	0	0
10	V	94	0	79	1	0
10	a	94	0	79	0	0
11	Y	83	0	70	0	0
12	e	72	0	61	0	0
13	G	126	0	117	1	0
13	K	126	0	117	1	0
13	R	126	0	117	0	0
All	All	25724	0	24890	244	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 5.

The worst 5 of 244 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:R:207:LYS:HE3	4:D:31:ASP:O	1.16	1.31
4:D:25:ASP:OD2	4:D:32:ASP:HB3	1.22	1.27
1:R:207:LYS:CE	4:D:31:ASP:O	2.05	1.04
4:D:25:ASP:OD2	4:D:32:ASP:CB	2.07	1.01
4:D:25:ASP:HB3	4:D:30:THR:HG21	1.44	0.97

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	G	432/481 (90%)	406 (94%)	26 (6%)	0	100	100
1	K	432/481 (90%)	412 (95%)	20 (5%)	0	100	100
1	R	432/481 (90%)	401 (93%)	30 (7%)	1 (0%)	44	75
2	A	131/238 (55%)	127 (97%)	4 (3%)	0	100	100
2	F	131/238 (55%)	131 (100%)	0	0	100	100
2	O	131/238 (55%)	129 (98%)	2 (2%)	0	100	100
3	B	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
3	I	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
3	P	105/214 (49%)	102 (97%)	3 (3%)	0	100	100
4	D	128/262 (49%)	116 (91%)	12 (9%)	0	100	100
4	H	128/262 (49%)	114 (89%)	13 (10%)	1 (1%)	16	51
4	M	128/262 (49%)	115 (90%)	13 (10%)	0	100	100
5	E	106/234 (45%)	99 (93%)	7 (7%)	0	100	100
5	L	106/234 (45%)	98 (92%)	8 (8%)	0	100	100
5	N	106/234 (45%)	97 (92%)	9 (8%)	0	100	100
6	C	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
6	J	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
6	Q	119/153 (78%)	118 (99%)	1 (1%)	0	100	100
All	All	3063/4746 (64%)	2901 (95%)	160 (5%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	25	ASP
1	R	387	THR

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	G	395/428 (92%)	393 (100%)	2 (0%)	86	90
1	K	395/428 (92%)	391 (99%)	4 (1%)	73	81
1	R	395/428 (92%)	391 (99%)	4 (1%)	73	81
2	A	116/208 (56%)	115 (99%)	1 (1%)	75	83
2	F	116/208 (56%)	116 (100%)	0	100	100
2	O	116/208 (56%)	116 (100%)	0	100	100
3	B	85/178 (48%)	85 (100%)	0	100	100
3	I	85/178 (48%)	85 (100%)	0	100	100
3	P	85/178 (48%)	85 (100%)	0	100	100
4	D	113/226 (50%)	113 (100%)	0	100	100
4	H	113/226 (50%)	111 (98%)	2 (2%)	54	71
4	M	113/226 (50%)	113 (100%)	0	100	100
5	E	87/199 (44%)	87 (100%)	0	100	100
5	L	87/199 (44%)	87 (100%)	0	100	100
5	N	87/199 (44%)	87 (100%)	0	100	100
6	C	106/130 (82%)	106 (100%)	0	100	100
6	J	106/130 (82%)	106 (100%)	0	100	100
6	Q	106/130 (82%)	106 (100%)	0	100	100
All	All	2706/4107 (66%)	2693 (100%)	13 (0%)	85	90

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	296	CYS
1	R	308	ARG
4	H	32	ASP
2	A	100	ARG
4	H	25	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	50	ASN
6	Q	543	ASN
3	P	89	HIS
6	C	543	ASN
3	P	52	GLN

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 ⓘ

61 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	S	1	7,1	14,14,15	0.32	0	17,19,21	0.49	0
7	NAG	S	2	7	14,14,15	0.40	0	17,19,21	0.48	0
8	NAG	T	1	8,1	14,14,15	0.37	0	17,19,21	0.76	0
8	NAG	T	2	8	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
8	BMA	T	3	8	11,11,12	0.76	0	15,15,17	0.94	1 (6%)
8	MAN	T	4	8	11,11,12	0.80	0	15,15,17	1.04	2 (13%)
8	MAN	T	5	8	11,11,12	0.83	0	15,15,17	1.01	2 (13%)
8	MAN	T	6	8	11,11,12	0.81	0	15,15,17	1.08	2 (13%)
9	NAG	U	1	9,1	14,14,15	0.27	0	17,19,21	0.56	0
9	NAG	U	2	9	14,14,15	0.30	0	17,19,21	0.52	0
9	BMA	U	3	9	11,11,12	0.76	0	15,15,17	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	V	1	10,1	14,14,15	0.36	0	17,19,21	1.09	1 (5%)
10	NAG	V	2	10	14,14,15	0.32	0	17,19,21	0.59	0
10	BMA	V	3	10	11,11,12	0.92	0	15,15,17	1.14	2 (13%)
10	MAN	V	4	10	11,11,12	0.86	0	15,15,17	1.28	1 (6%)
10	MAN	V	5	10	11,11,12	1.04	1 (9%)	15,15,17	1.24	2 (13%)
10	MAN	V	6	10	11,11,12	0.85	0	15,15,17	0.96	2 (13%)
10	MAN	V	7	10	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
10	MAN	V	8	10	11,11,12	0.82	0	15,15,17	1.10	2 (13%)
7	NAG	W	1	7,1	14,14,15	0.47	0	17,19,21	1.09	1 (5%)
7	NAG	W	2	7	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
7	NAG	X	1	7,1	14,14,15	0.34	0	17,19,21	0.67	0
7	NAG	X	2	7	14,14,15	0.41	0	17,19,21	0.56	0
11	NAG	Y	1	1,11	14,14,15	0.31	0	17,19,21	0.63	0
11	NAG	Y	2	11	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
11	BMA	Y	3	11	11,11,12	0.78	0	15,15,17	0.98	1 (6%)
11	MAN	Y	4	11	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
11	MAN	Y	5	11	11,11,12	0.84	0	15,15,17	0.97	2 (13%)
11	MAN	Y	6	11	11,11,12	0.85	0	15,15,17	1.05	2 (13%)
11	MAN	Y	7	11	11,11,12	0.80	0	15,15,17	1.07	2 (13%)
9	NAG	Z	1	9,1	14,14,15	0.78	0	17,19,21	2.41	3 (17%)
9	NAG	Z	2	9	14,14,15	0.27	0	17,19,21	0.54	0
9	BMA	Z	3	9	11,11,12	0.76	0	15,15,17	0.84	1 (6%)
10	NAG	a	1	10,1	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	a	2	10	14,14,15	0.32	0	17,19,21	0.57	0
10	BMA	a	3	10	11,11,12	1.00	0	15,15,17	1.09	1 (6%)
10	MAN	a	4	10	11,11,12	0.82	0	15,15,17	1.21	1 (6%)
10	MAN	a	5	10	11,11,12	1.53	3 (27%)	15,15,17	2.11	3 (20%)
10	MAN	a	6	10	11,11,12	1.31	2 (18%)	15,15,17	1.90	3 (20%)
10	MAN	a	7	10	11,11,12	1.00	1 (9%)	15,15,17	1.36	2 (13%)
10	MAN	a	8	10	11,11,12	1.81	2 (18%)	15,15,17	2.17	4 (26%)
7	NAG	b	1	7,1	14,14,15	0.40	0	17,19,21	1.08	1 (5%)
7	NAG	b	2	7	14,14,15	0.39	0	17,19,21	0.63	1 (5%)
7	NAG	c	1	7,1	14,14,15	0.54	0	17,19,21	1.08	2 (11%)
7	NAG	c	2	7	14,14,15	0.39	0	17,19,21	0.61	0
8	NAG	d	1	8,1	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
8	NAG	d	2	8	14,14,15	0.82	1 (7%)	17,19,21	2.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	d	3	8	11,11,12	0.82	0	15,15,17	1.03	1 (6%)
8	MAN	d	4	8	11,11,12	0.86	0	15,15,17	1.08	2 (13%)
8	MAN	d	5	8	11,11,12	0.87	0	15,15,17	0.99	2 (13%)
8	MAN	d	6	8	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
12	NAG	e	1	12,1	14,14,15	0.29	0	17,19,21	0.57	0
12	NAG	e	2	12	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
12	BMA	e	3	12	11,11,12	0.92	1 (9%)	15,15,17	0.88	0
12	MAN	e	4	12	11,11,12	0.83	0	15,15,17	1.10	2 (13%)
12	MAN	e	5	12	11,11,12	1.09	1 (9%)	15,15,17	1.29	2 (13%)
12	MAN	e	6	12	11,11,12	0.88	0	15,15,17	1.28	2 (13%)
7	NAG	f	1	7,1	14,14,15	0.42	0	17,19,21	1.09	1 (5%)
7	NAG	f	2	7	14,14,15	0.34	0	17,19,21	0.62	1 (5%)
7	NAG	g	1	7,1	14,14,15	0.28	0	17,19,21	0.49	0
7	NAG	g	2	7	14,14,15	0.55	0	17,19,21	1.04	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
7	NAG	S	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
8	NAG	T	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	BMA	T	3	8	-	2/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
8	MAN	T	6	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	0/2/19/22	0/1/1/1
10	NAG	V	1	10,1	-	4/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
10	MAN	V	4	10	-	0/2/19/22	0/1/1/1
10	MAN	V	5	10	-	1/2/19/22	1/1/1/1
10	MAN	V	6	10	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	e	5	12	-	1/2/19/22	1/1/1/1
12	MAN	e	6	12	-	1/2/19/22	0/1/1/1
7	NAG	f	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	NAG	g	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	4/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	8	MAN	C1-C2	4.47	1.62	1.52
10	a	8	MAN	O5-C1	3.13	1.49	1.43
10	a	5	MAN	C1-C2	3.10	1.59	1.52
10	a	6	MAN	O3-C3	2.57	1.49	1.43
10	a	5	MAN	O5-C5	2.49	1.48	1.43

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	1	NAG	C2-N2-C7	8.40	134.16	122.90
8	d	2	NAG	C2-N2-C7	8.32	134.04	122.90
10	a	8	MAN	C1-O5-C5	6.46	120.85	112.19
10	a	5	MAN	C1-O5-C5	6.35	120.69	112.19
10	a	6	MAN	C1-O5-C5	4.80	118.62	112.19

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	b	2	NAG	C4-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	V	5	MAN	C1-C2-C3-C4-C5-O5
12	e	5	MAN	C1-C2-C3-C4-C5-O5

Continued on next page...

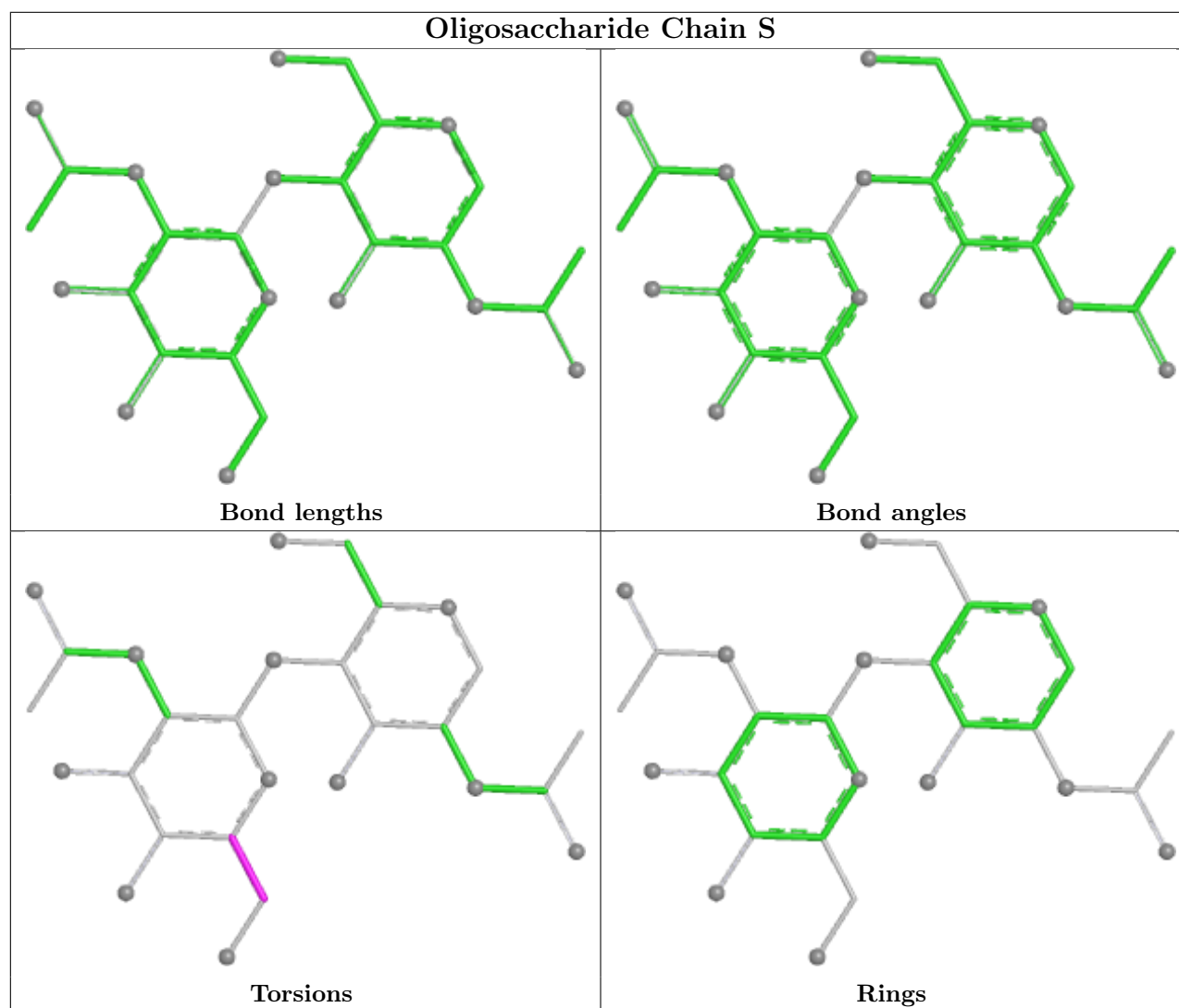
Continued from previous page...

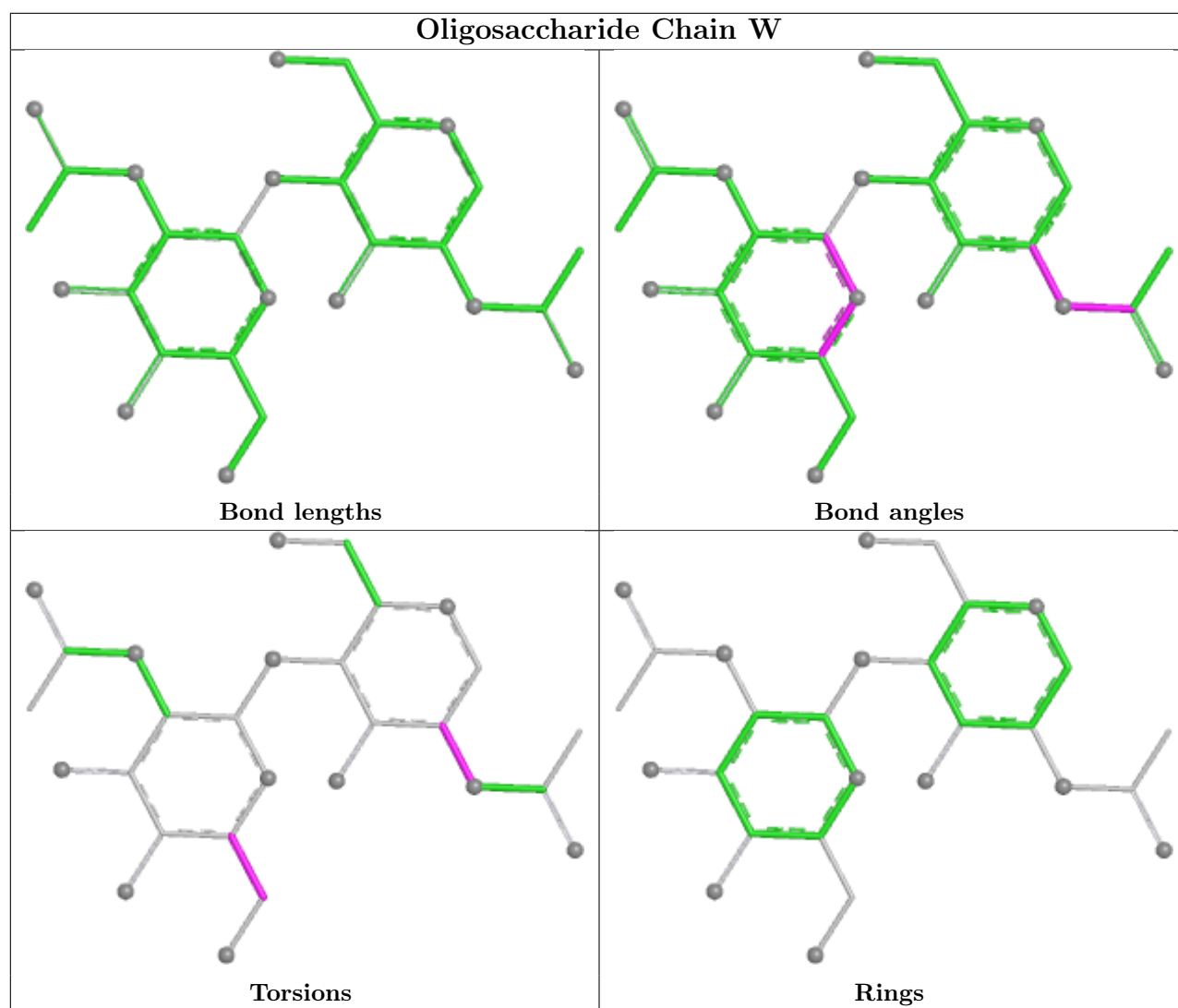
Mol	Chain	Res	Type	Atoms
10	a	7	MAN	C1-C2-C3-C4-C5-O5

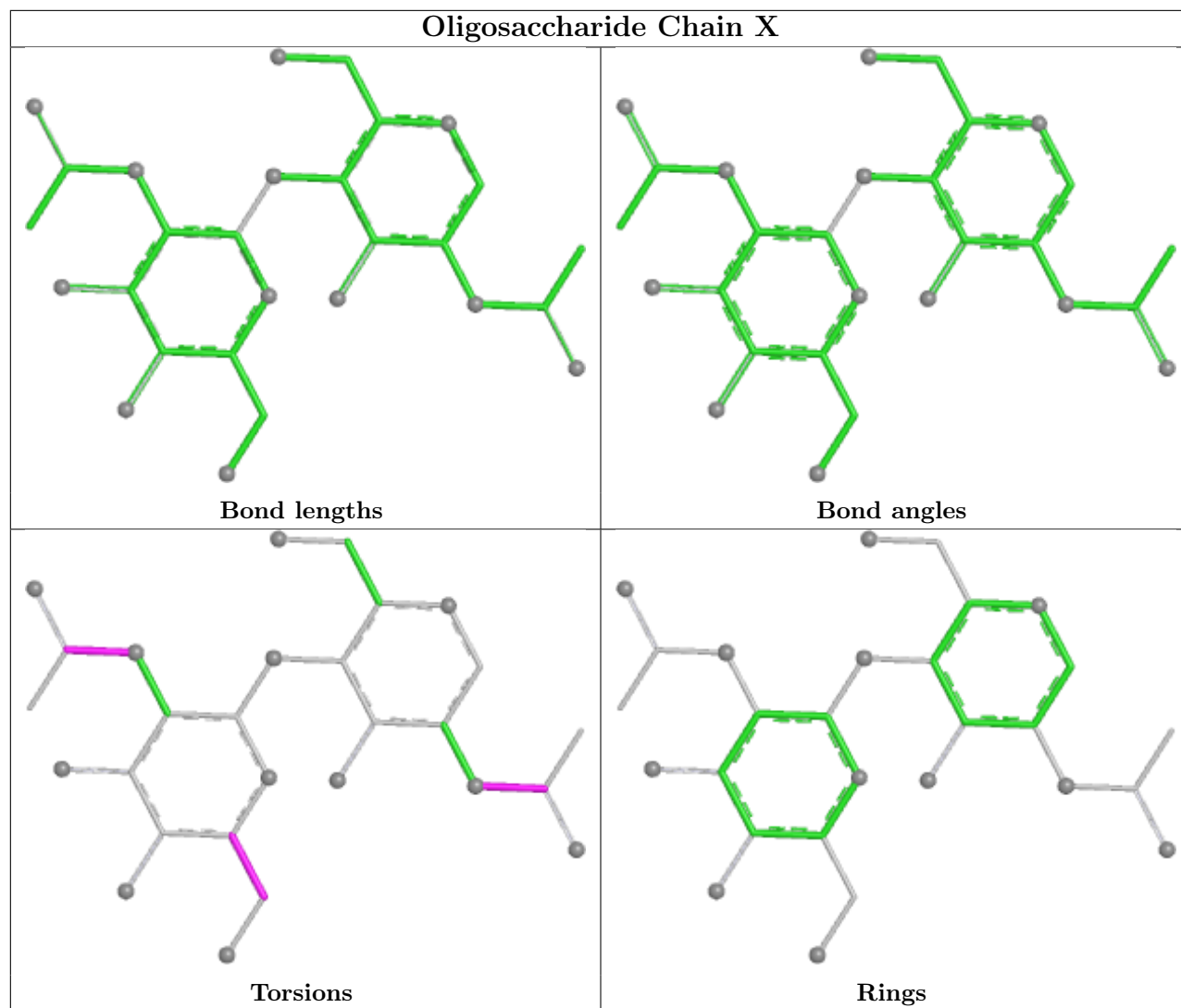
1 monomer is involved in 1 short contact:

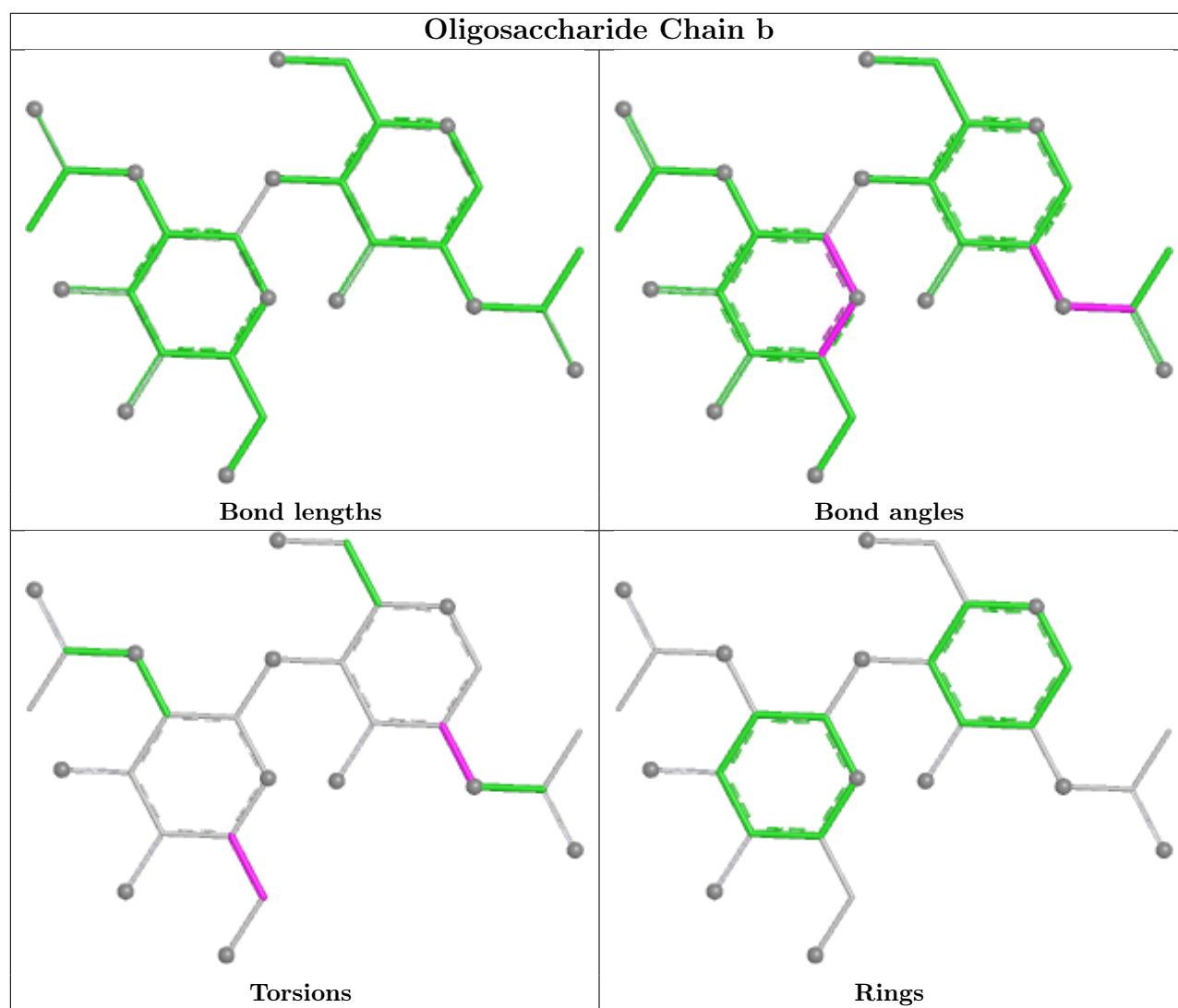
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	V	5	MAN	1	0

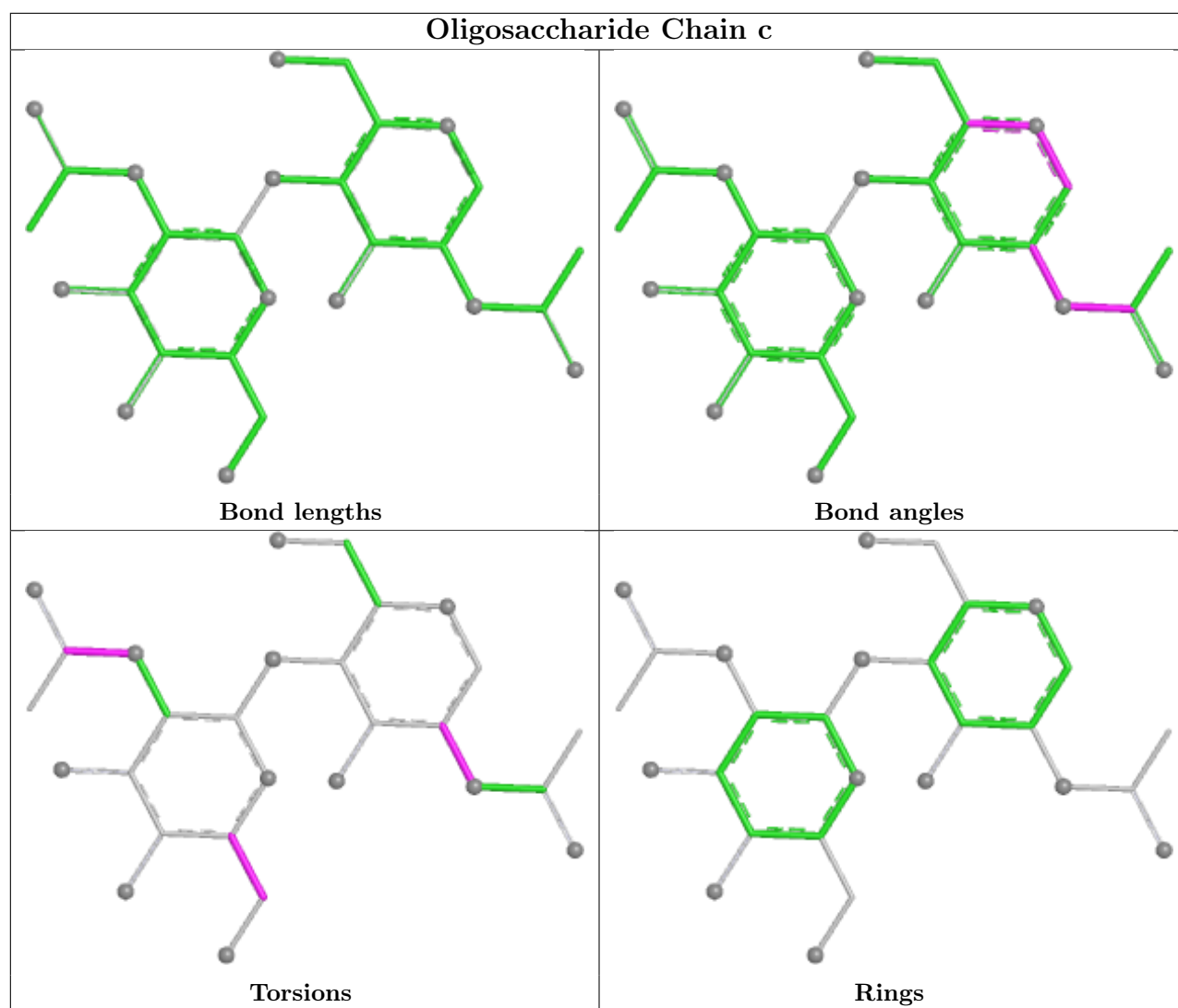
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

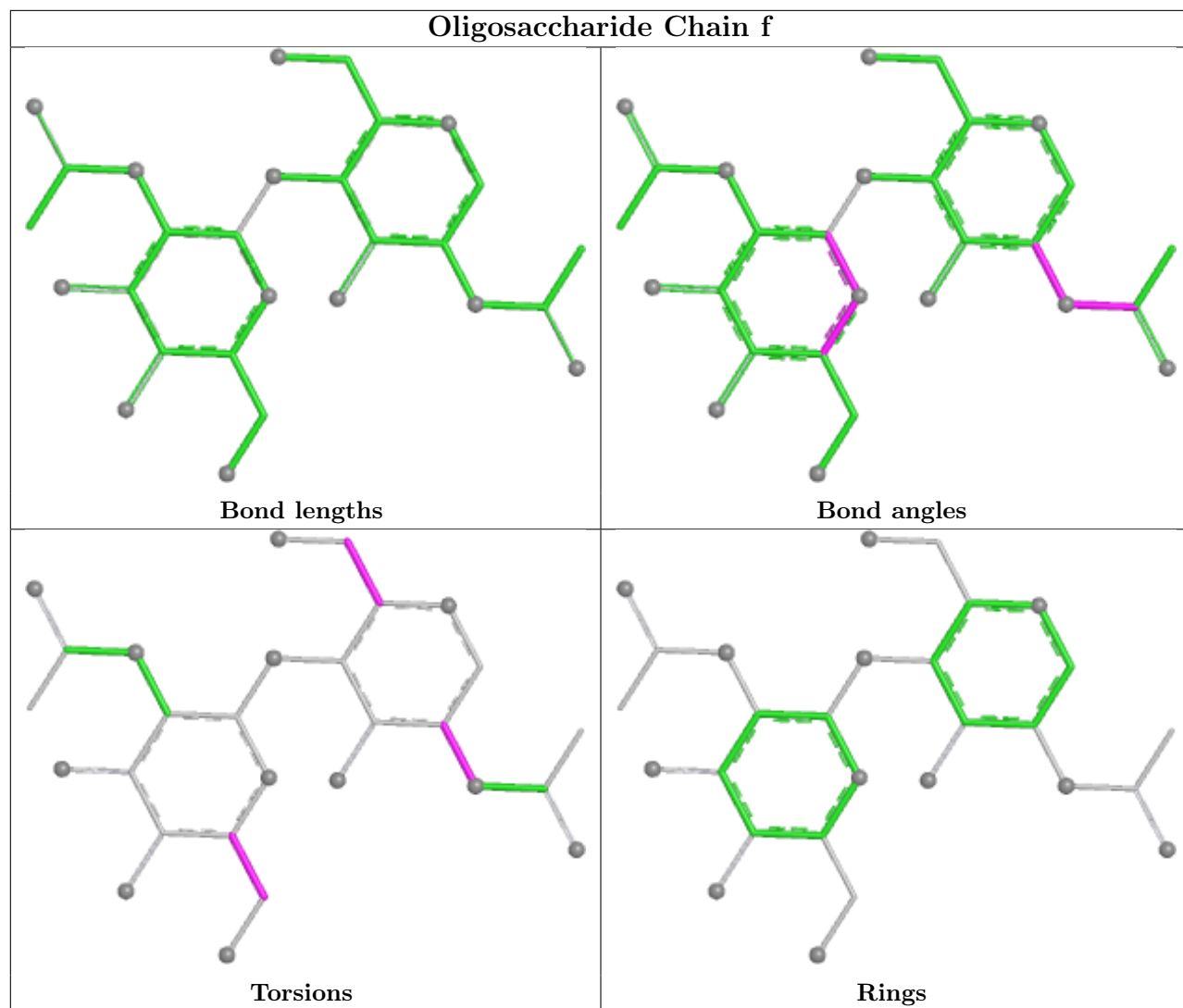


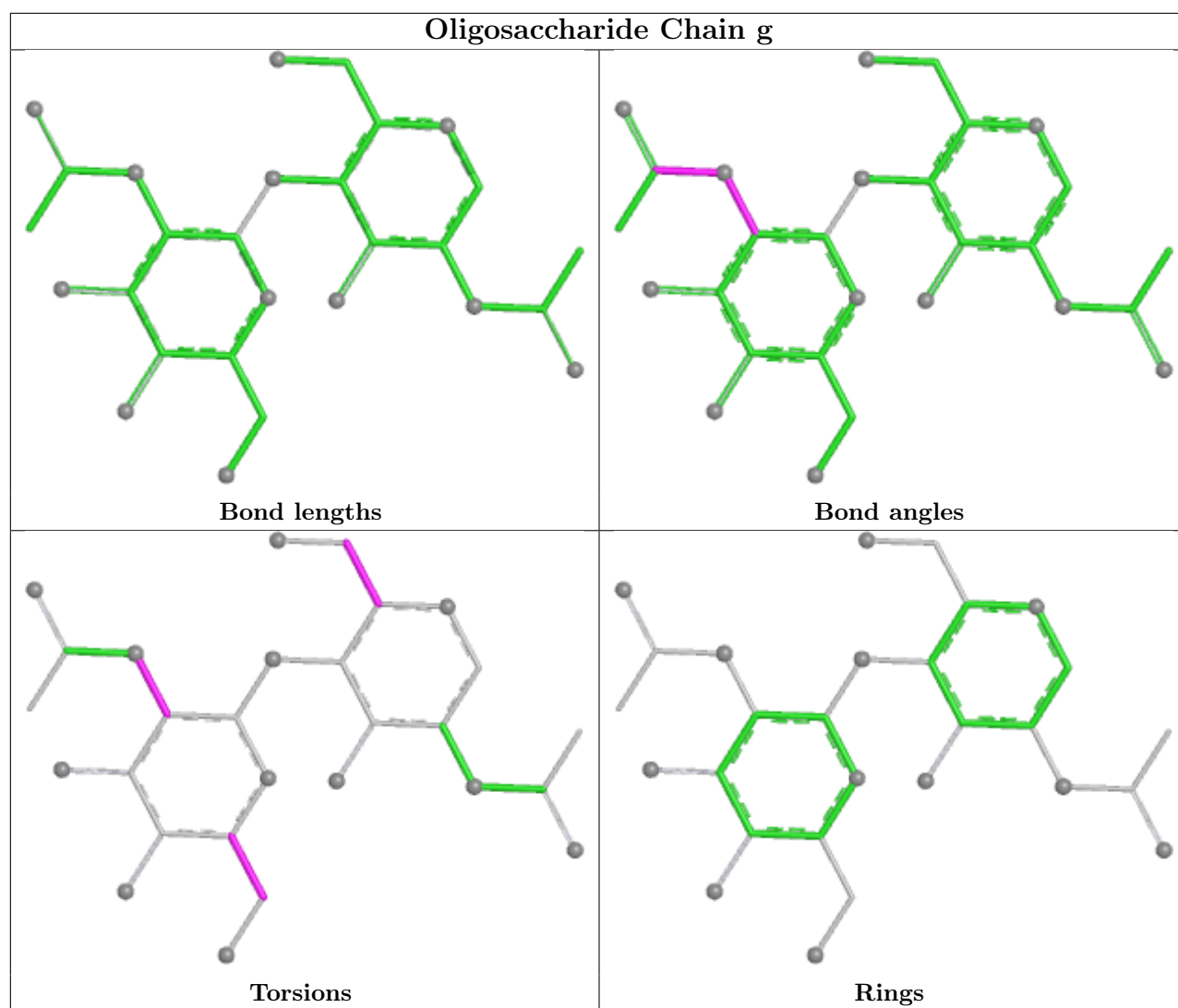


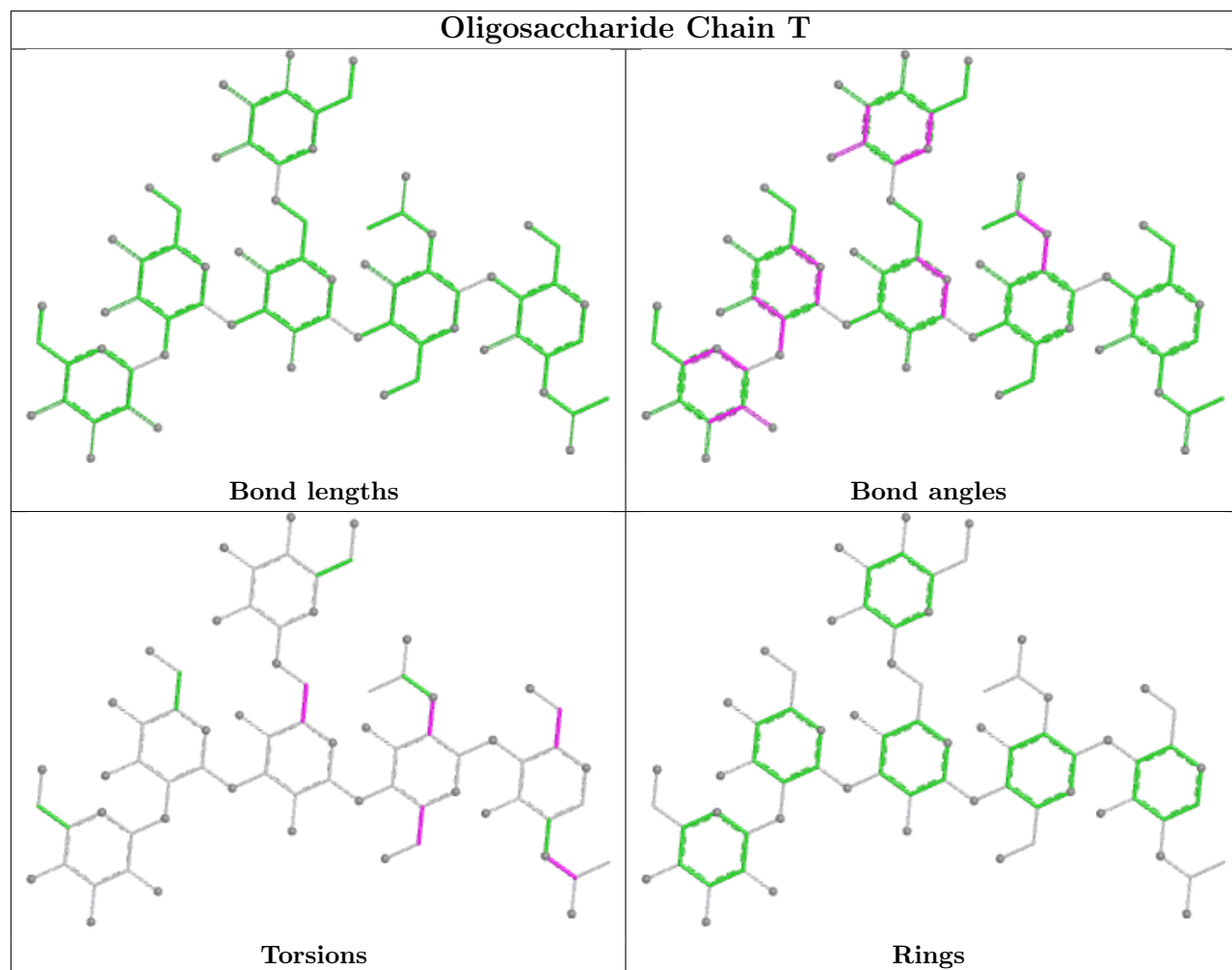


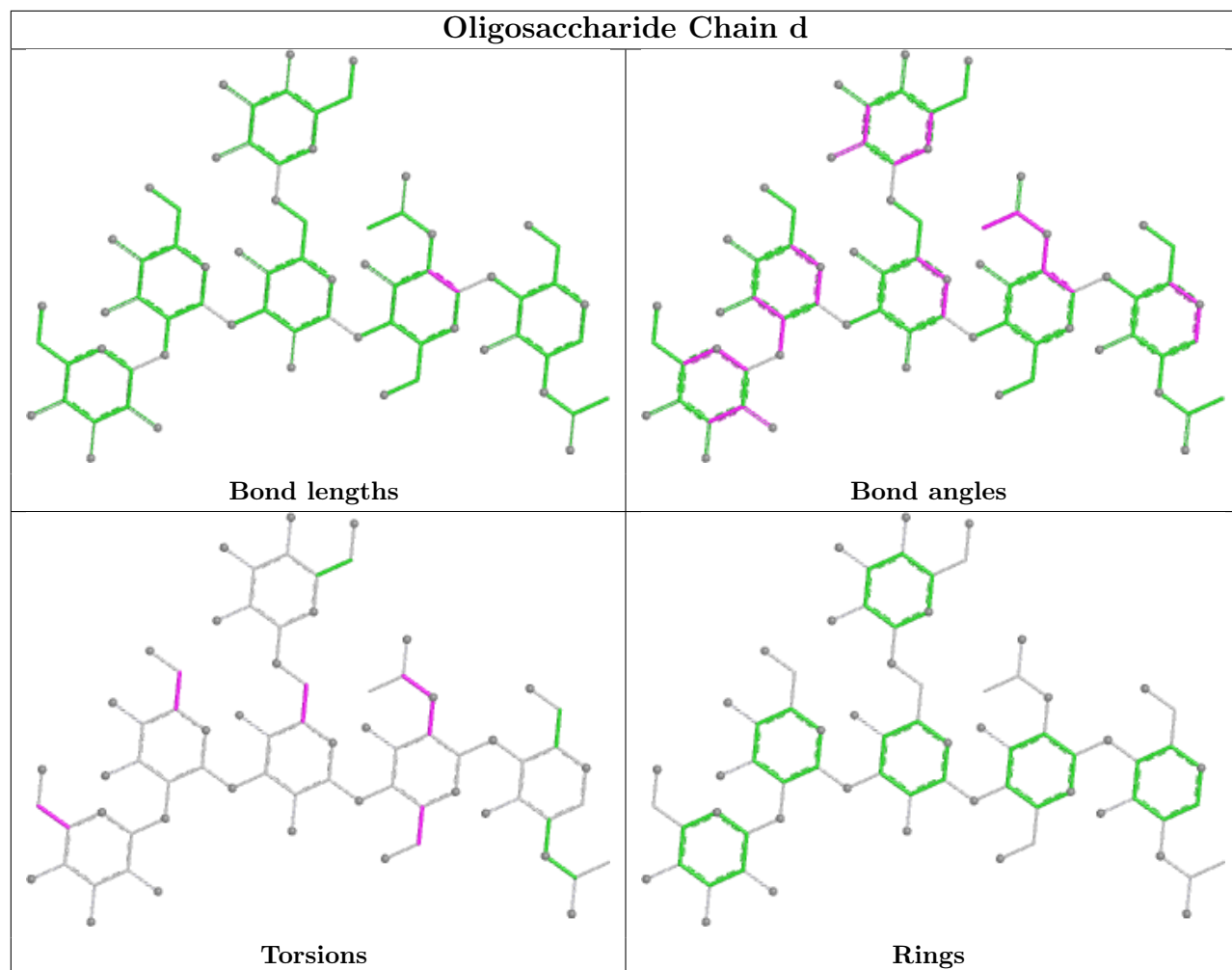


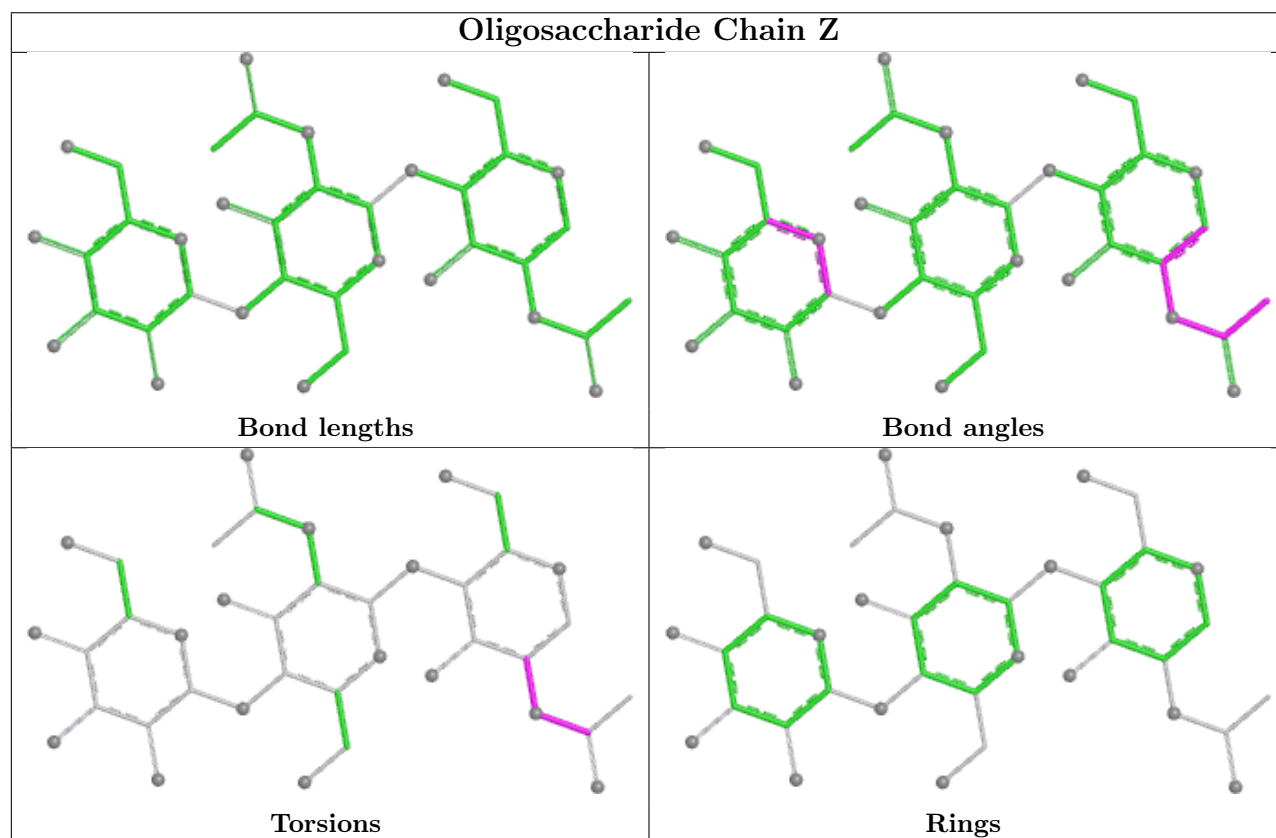
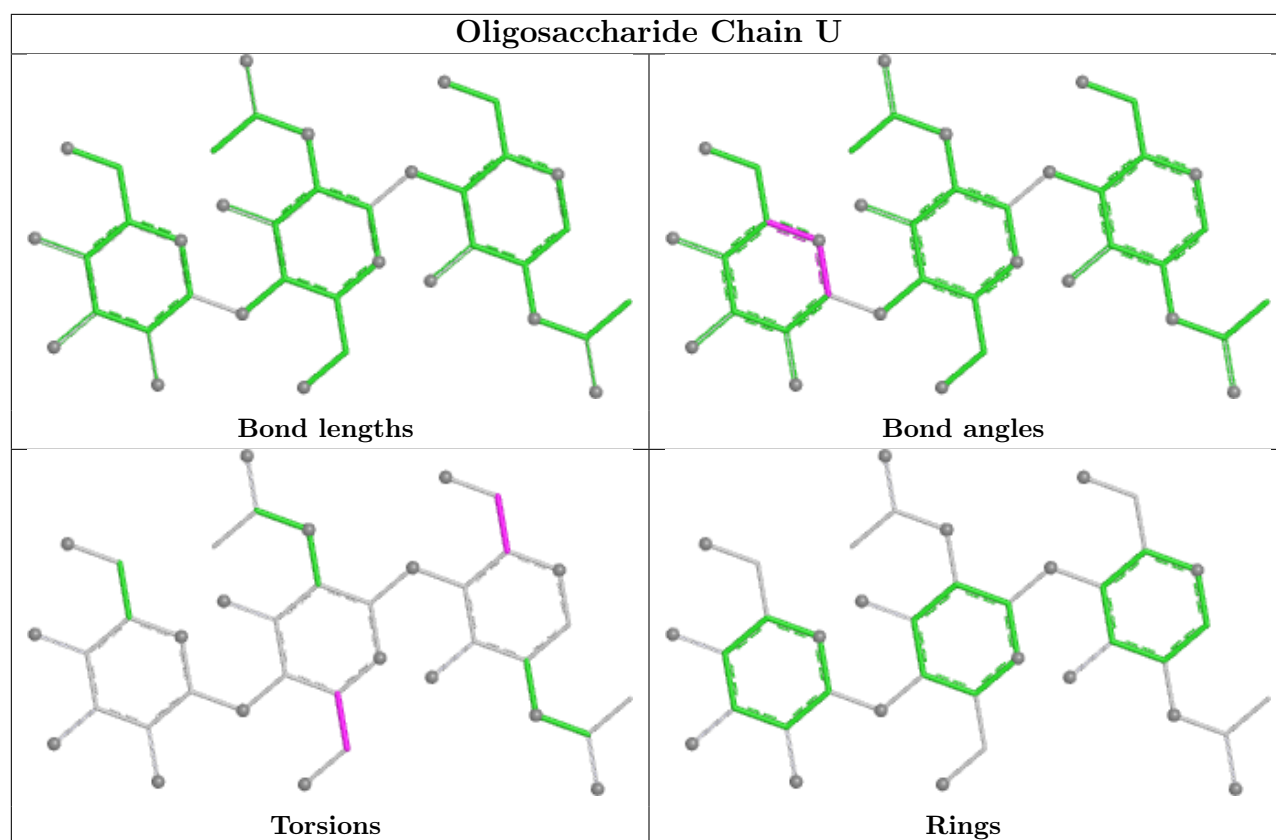


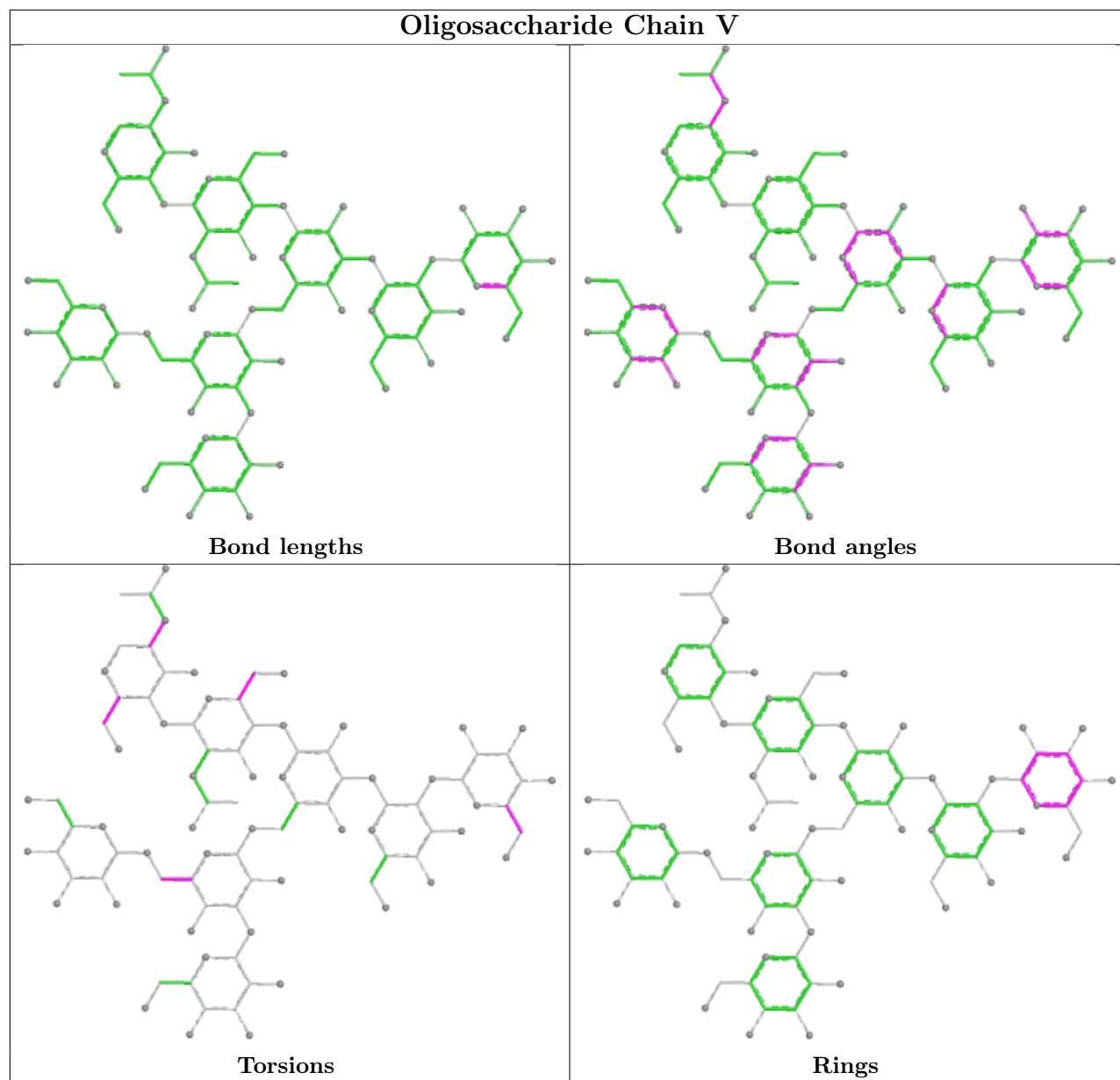


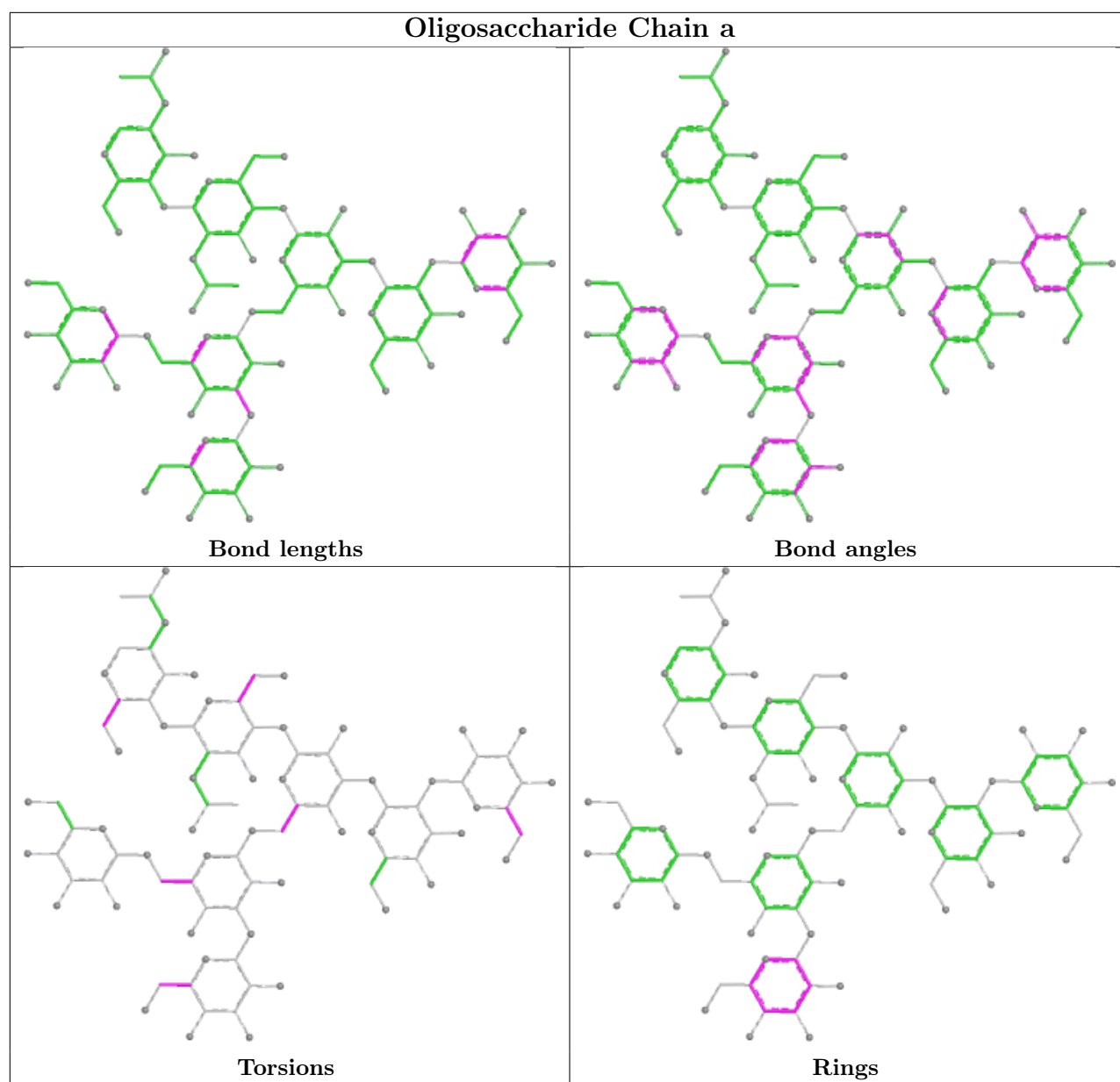


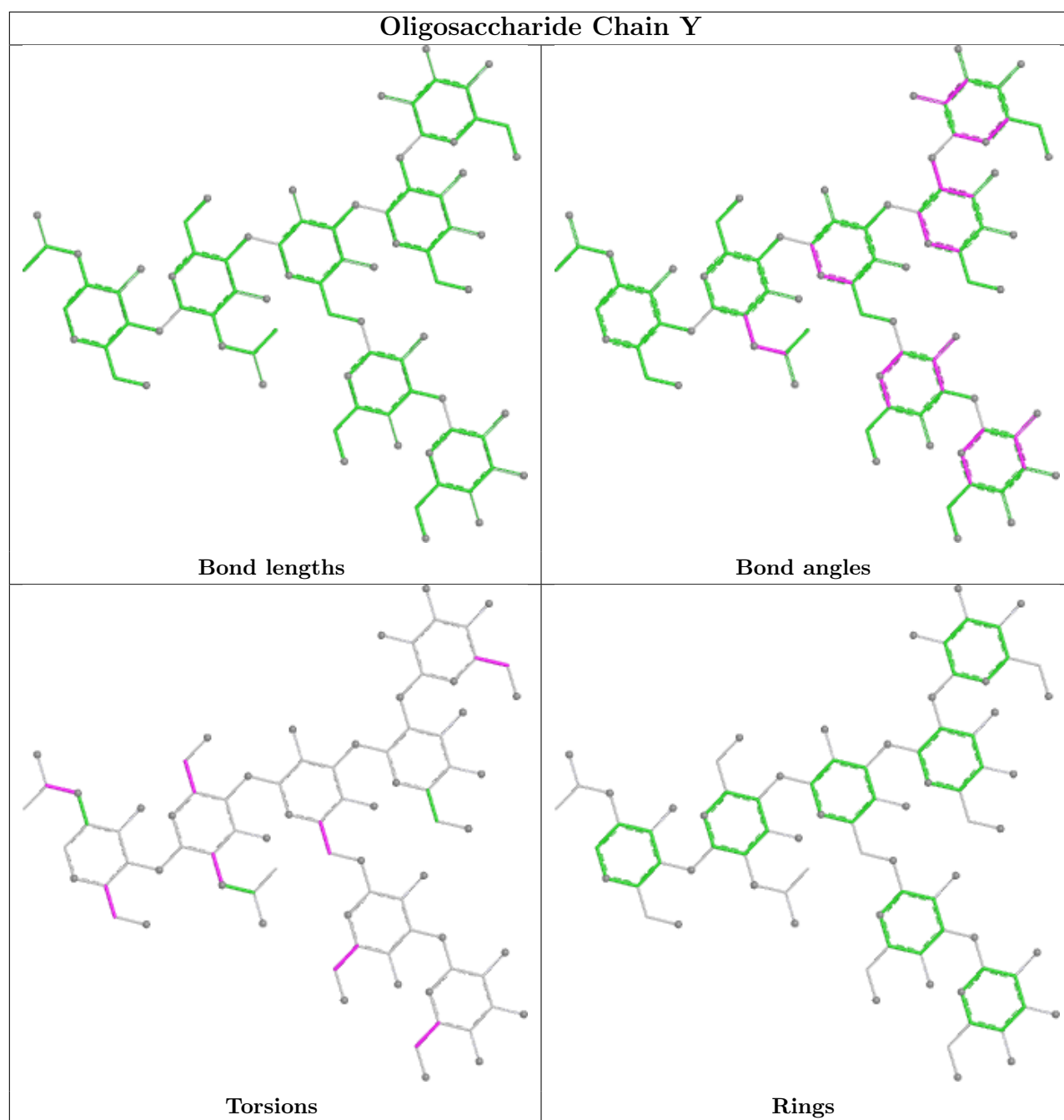


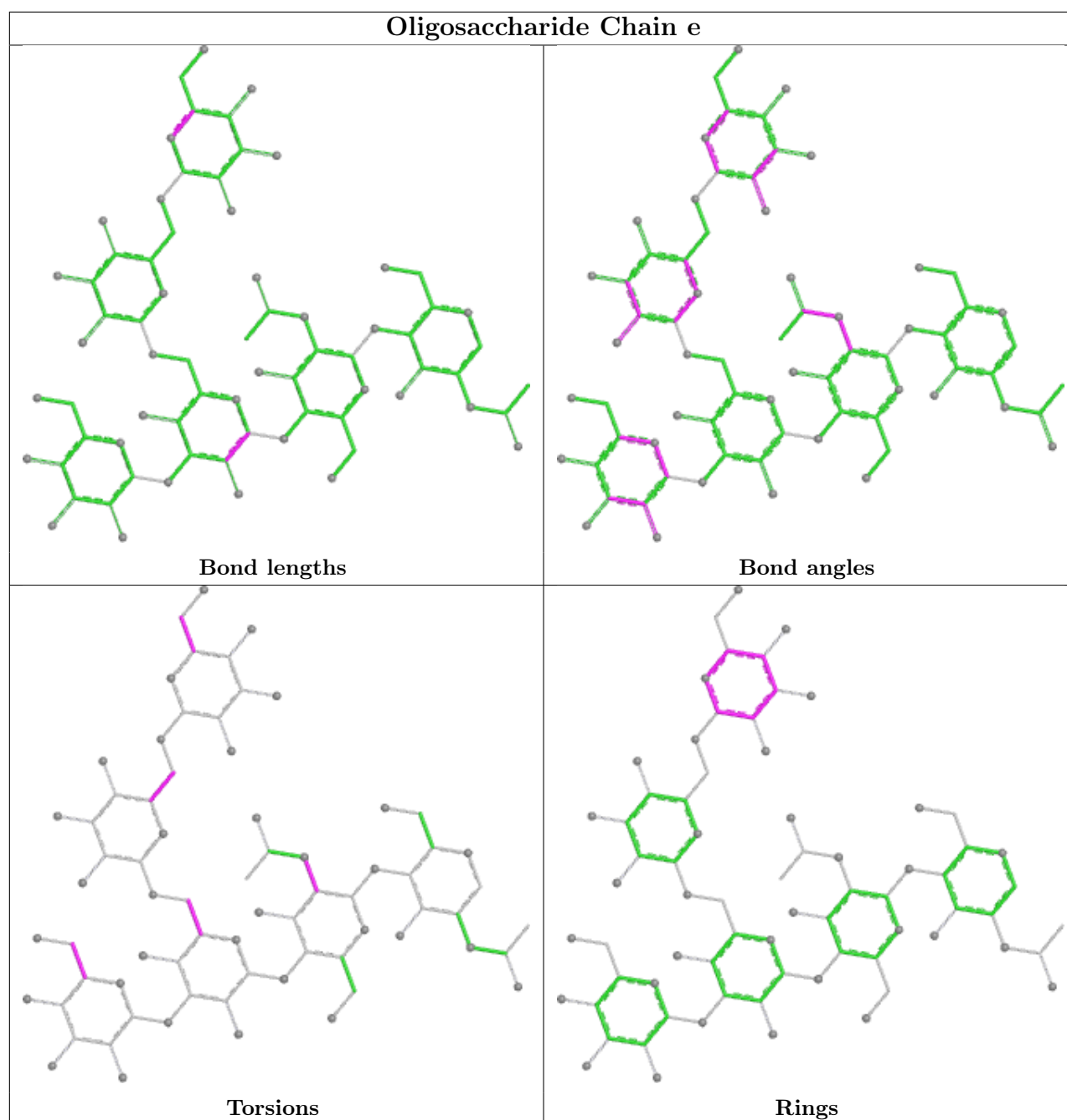












5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	R	605	1	14,14,15	0.38	0	17,19,21	0.53	0
13	NAG	K	626	1	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
13	NAG	G	623	1	14,14,15	0.38	0	17,19,21	0.48	0
13	NAG	R	601	1	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
13	NAG	R	602	1	14,14,15	0.49	0	17,19,21	0.57	0
13	NAG	G	628	1	14,14,15	0.98	1 (7%)	17,19,21	2.37	3 (17%)
13	NAG	G	630	1	14,14,15	0.38	0	17,19,21	0.53	0
13	NAG	G	629	1	14,14,15	0.36	0	17,19,21	0.60	0
13	NAG	G	613	1	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
13	NAG	G	626	1	14,14,15	0.38	0	17,19,21	0.53	0
13	NAG	K	602	1	14,14,15	0.35	0	17,19,21	0.50	0
13	NAG	R	620	1	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
13	NAG	R	625	1	14,14,15	0.50	0	17,19,21	1.04	1 (5%)
13	NAG	K	617	1	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
13	NAG	G	627	1	14,14,15	0.56	0	17,19,21	1.05	1 (5%)
13	NAG	R	613	1	14,14,15	0.38	0	17,19,21	0.52	0
13	NAG	R	612	1	14,14,15	0.37	0	17,19,21	0.62	0
13	NAG	K	630	1	14,14,15	0.39	0	17,19,21	0.53	0
13	NAG	K	605	1	14,14,15	0.36	0	17,19,21	0.52	0
13	NAG	G	622	1	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
13	NAG	R	621	1	14,14,15	0.38	0	17,19,21	0.55	0
13	NAG	K	627	1	14,14,15	0.43	0	17,19,21	0.49	0
13	NAG	K	601	1	14,14,15	0.41	0	17,19,21	0.65	0
13	NAG	G	612	1	14,14,15	0.48	0	17,19,21	1.06	1 (5%)
13	NAG	R	624	1	14,14,15	0.39	0	17,19,21	0.54	0
13	NAG	K	631	1	14,14,15	0.45	0	17,19,21	0.57	0
13	NAG	K	616	1	14,14,15	0.48	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	R	605	1	-	0/6/23/26	0/1/1/1
13	NAG	K	626	1	-	4/6/23/26	0/1/1/1
13	NAG	G	623	1	-	0/6/23/26	0/1/1/1
13	NAG	R	601	1	-	4/6/23/26	0/1/1/1
13	NAG	R	602	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	G	628	1	-	6/6/23/26	0/1/1/1
13	NAG	G	630	1	-	2/6/23/26	0/1/1/1
13	NAG	G	629	1	-	4/6/23/26	0/1/1/1
13	NAG	G	613	1	-	3/6/23/26	0/1/1/1
13	NAG	G	626	1	-	2/6/23/26	0/1/1/1
13	NAG	K	602	1	-	2/6/23/26	0/1/1/1
13	NAG	R	620	1	-	4/6/23/26	0/1/1/1
13	NAG	R	625	1	-	2/6/23/26	0/1/1/1
13	NAG	K	617	1	-	4/6/23/26	0/1/1/1
13	NAG	G	627	1	-	4/6/23/26	0/1/1/1
13	NAG	R	613	1	-	1/6/23/26	0/1/1/1
13	NAG	R	612	1	-	2/6/23/26	0/1/1/1
13	NAG	K	630	1	-	2/6/23/26	0/1/1/1
13	NAG	K	605	1	-	2/6/23/26	0/1/1/1
13	NAG	G	622	1	-	4/6/23/26	0/1/1/1
13	NAG	R	621	1	-	0/6/23/26	0/1/1/1
13	NAG	K	627	1	-	1/6/23/26	0/1/1/1
13	NAG	K	601	1	-	4/6/23/26	0/1/1/1
13	NAG	G	612	1	-	4/6/23/26	0/1/1/1
13	NAG	R	624	1	-	1/6/23/26	0/1/1/1
13	NAG	K	631	1	-	2/6/23/26	0/1/1/1
13	NAG	K	616	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	628	NAG	C1-C2	3.03	1.56	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	628	NAG	C2-N2-C7	8.29	134.00	122.90
13	G	628	NAG	C1-C2-N2	3.87	116.53	110.43
13	K	616	NAG	C2-N2-C7	3.29	127.31	122.90
13	R	601	NAG	C2-N2-C7	3.27	127.28	122.90
13	G	622	NAG	C2-N2-C7	3.25	127.26	122.90

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	627	NAG	O5-C5-C6-O6
13	G	628	NAG	O5-C5-C6-O6
13	R	601	NAG	O5-C5-C6-O6
13	K	601	NAG	C4-C5-C6-O6
13	K	631	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	630	NAG	1	0
13	K	627	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.

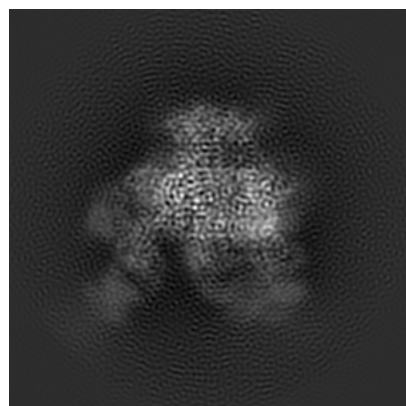
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20740. These allow visual inspection of the internal detail of the map and identification of artifacts.

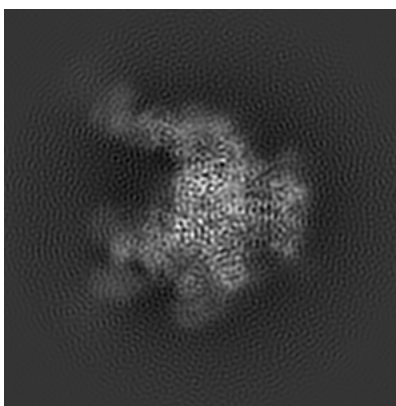
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

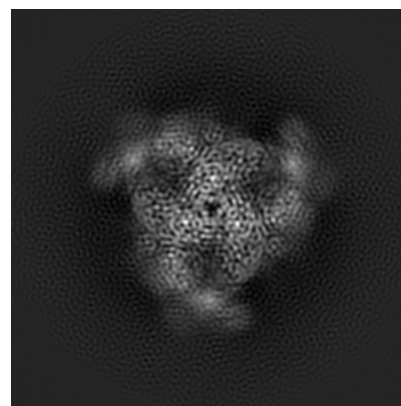
6.1.1 Primary map



X

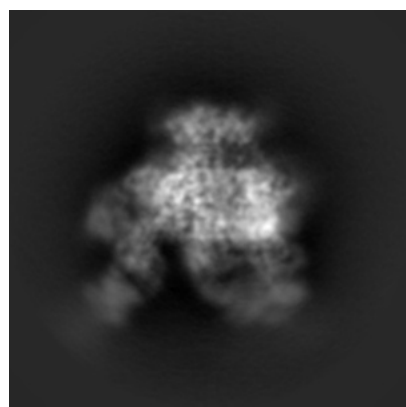


Y

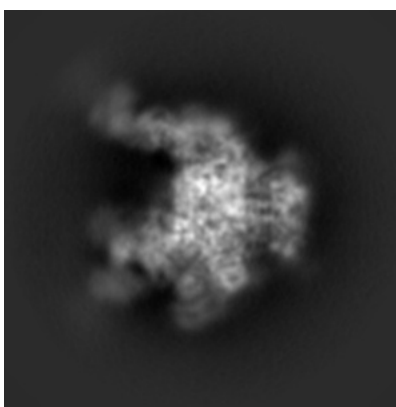


Z

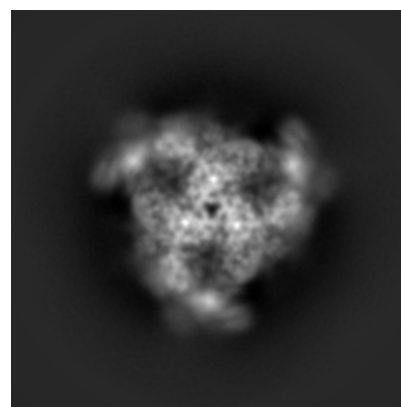
6.1.2 Raw map



X



Y

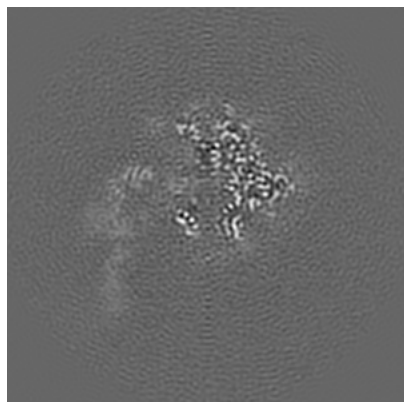


Z

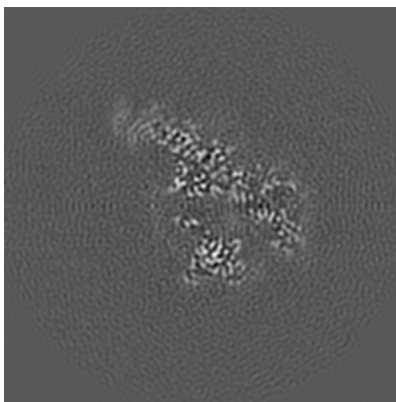
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

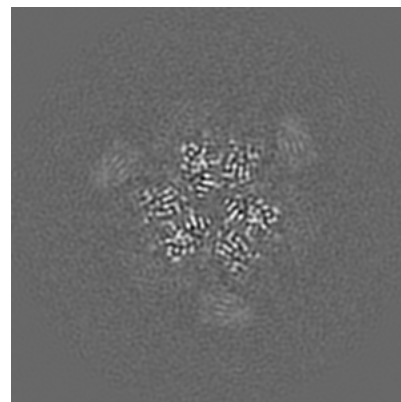
6.2.1 Primary map



X Index: 104

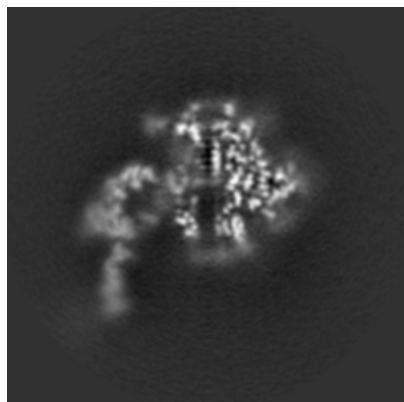


Y Index: 104

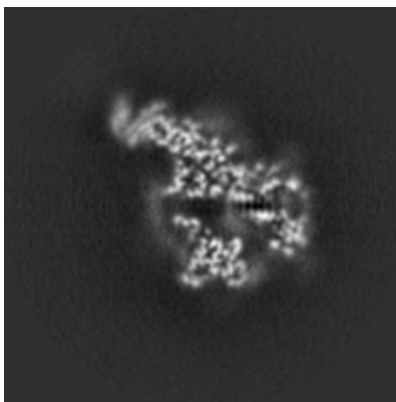


Z Index: 104

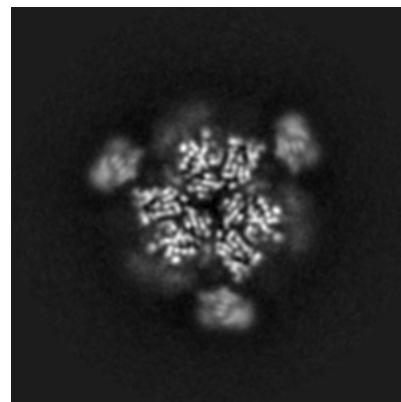
6.2.2 Raw map



X Index: 104



Y Index: 104

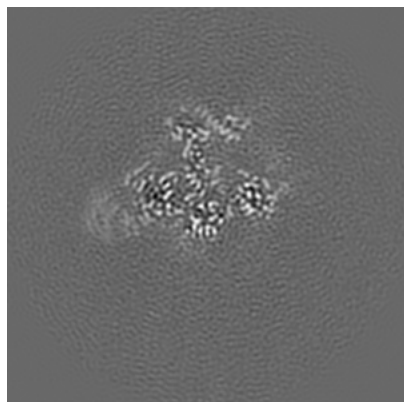


Z Index: 104

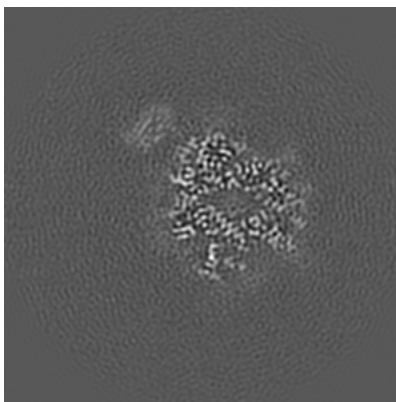
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

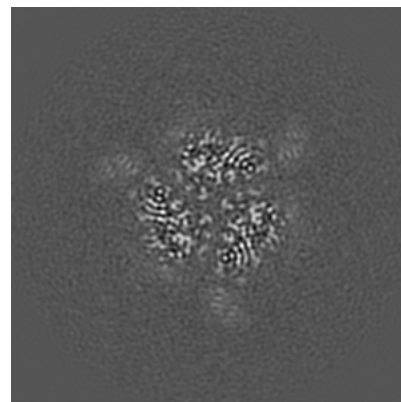
6.3.1 Primary map



X Index: 116

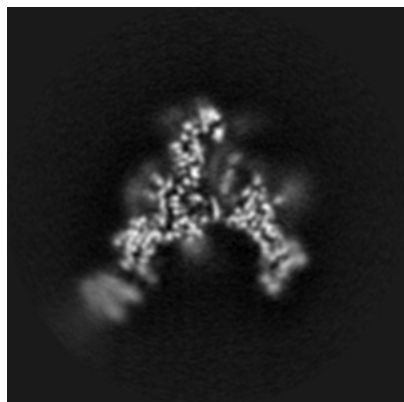


Y Index: 97

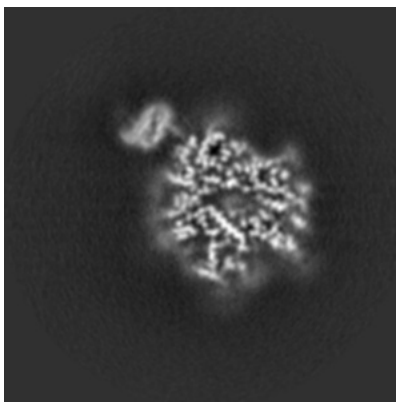


Z Index: 108

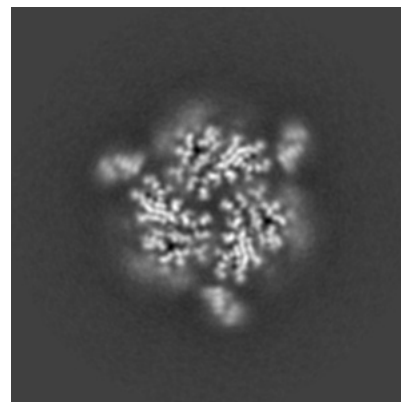
6.3.2 Raw map



X Index: 89



Y Index: 97

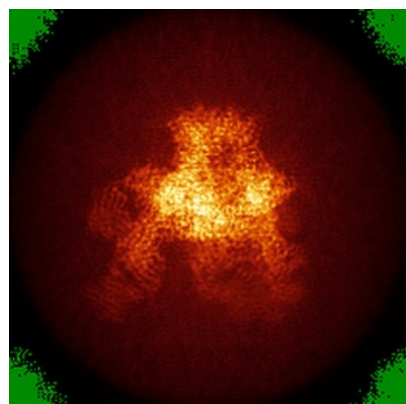


Z Index: 109

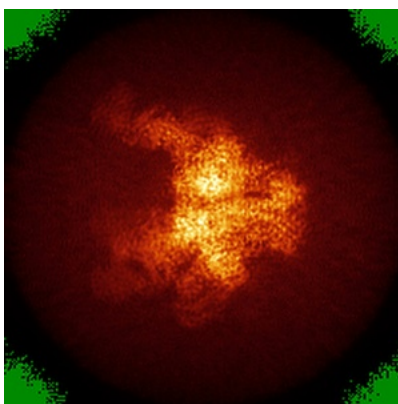
The images above show the largest variance slices of the map in three orthogonal directions.

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

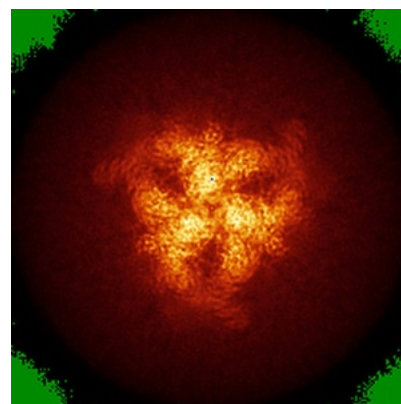
6.4.1 Primary map



X

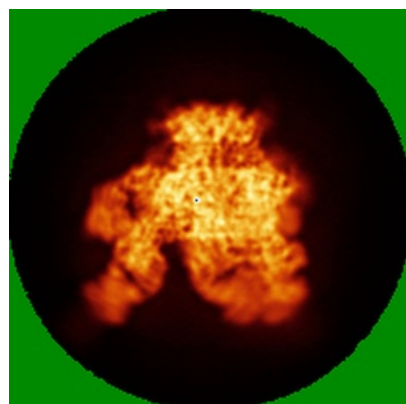


Y

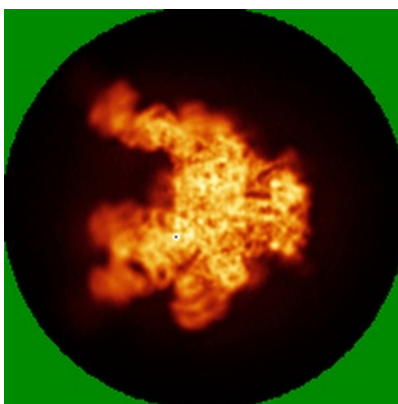


Z

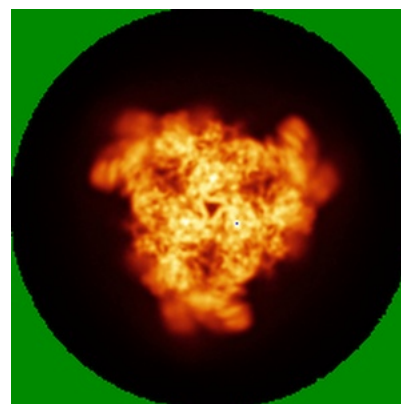
6.4.2 Raw map



X



Y

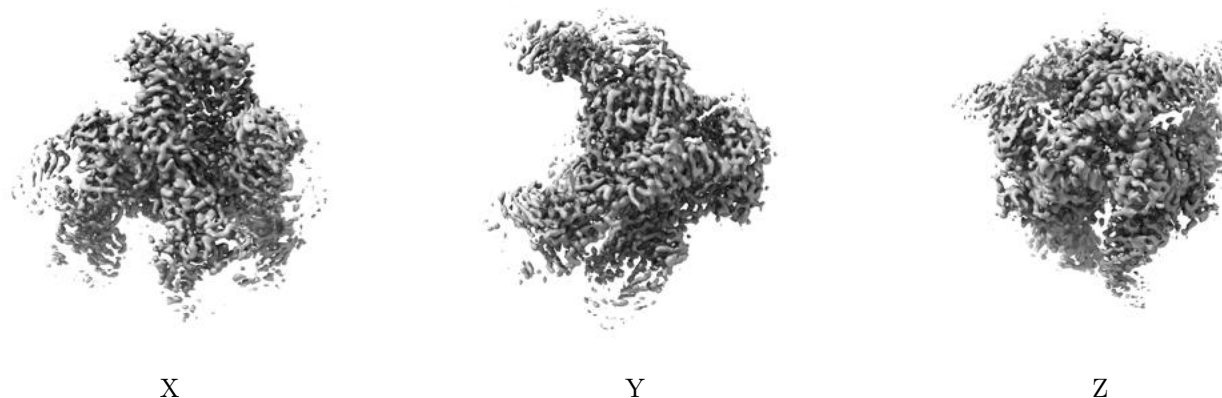


Z

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 0.0717. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

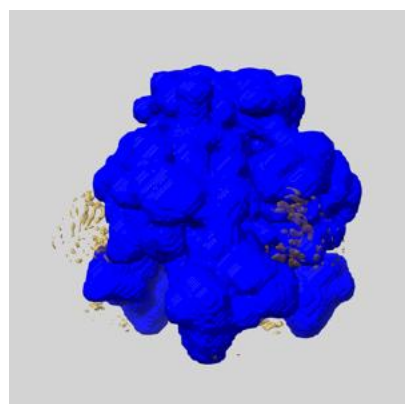
6.6 Mask visualisation [i](#)

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

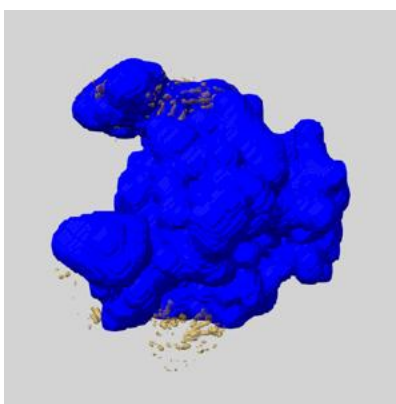
A mask typically either:

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

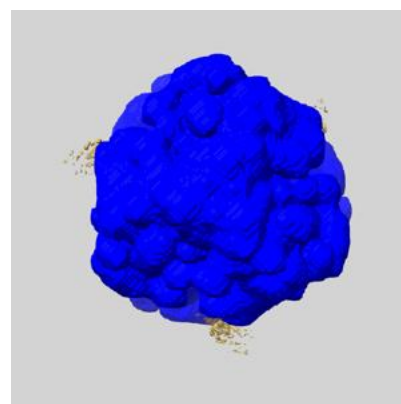
6.6.1 emd_20740_msk_1.map [i](#)



X



Y

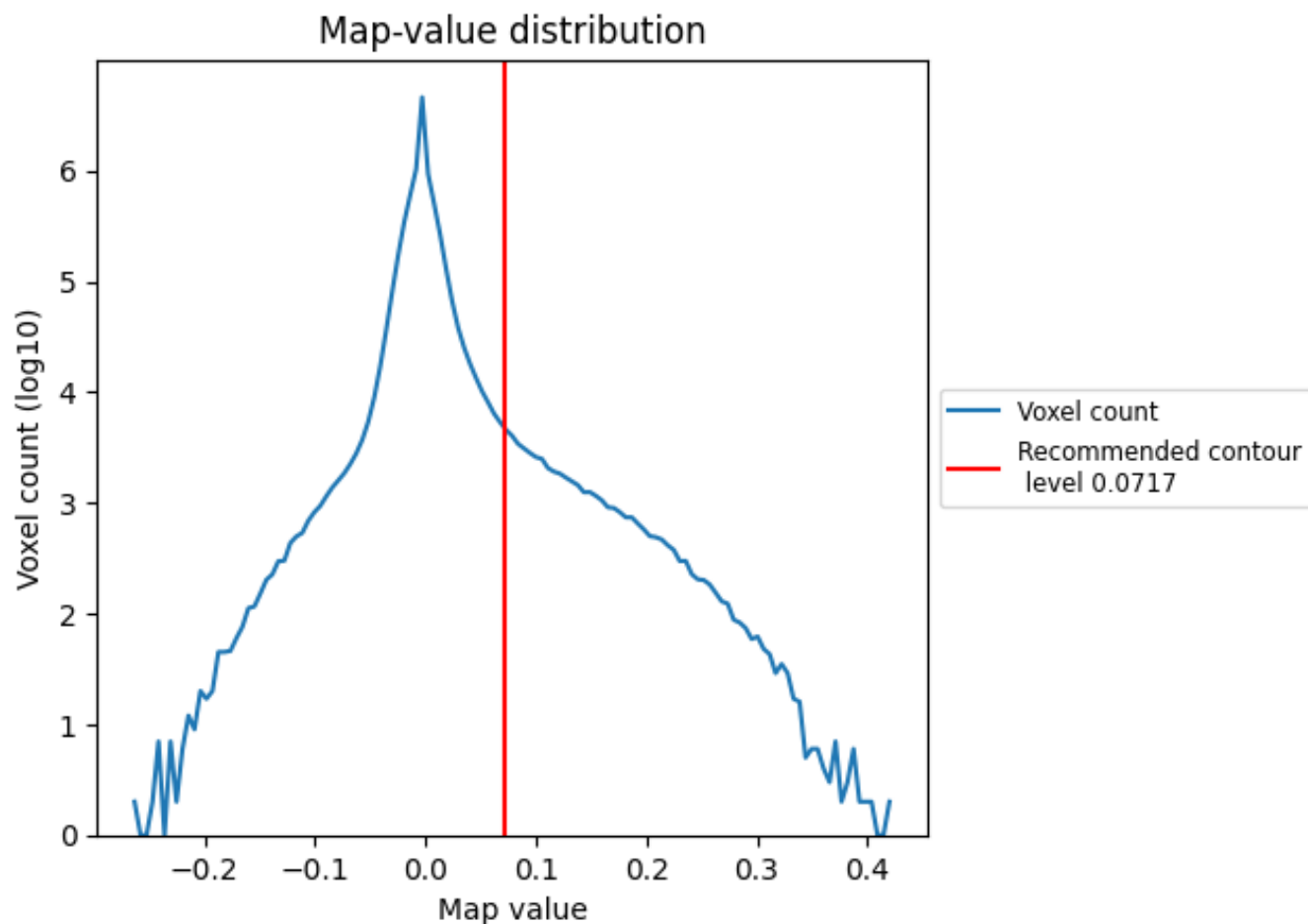


Z

7 Map analysis [i](#)

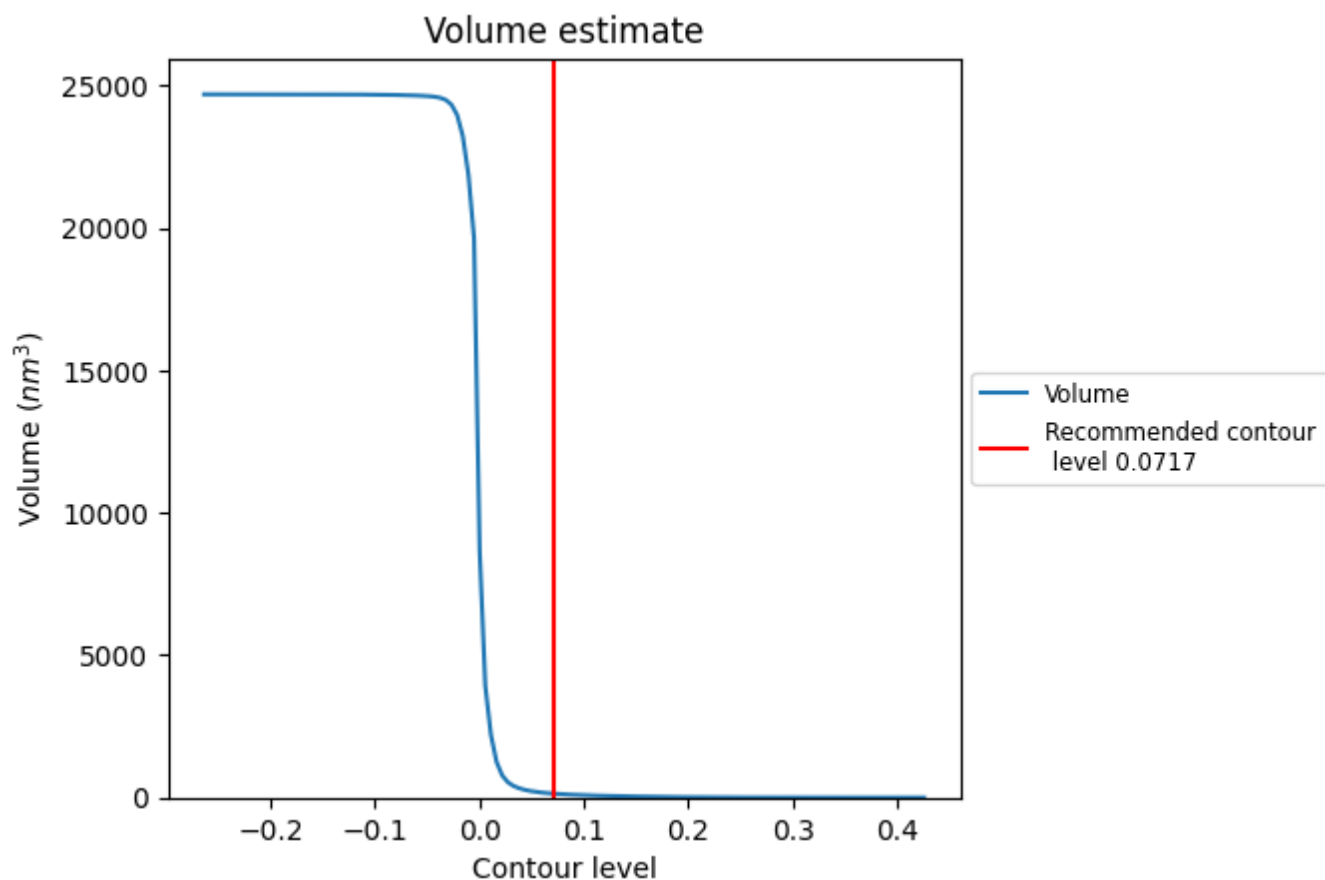
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

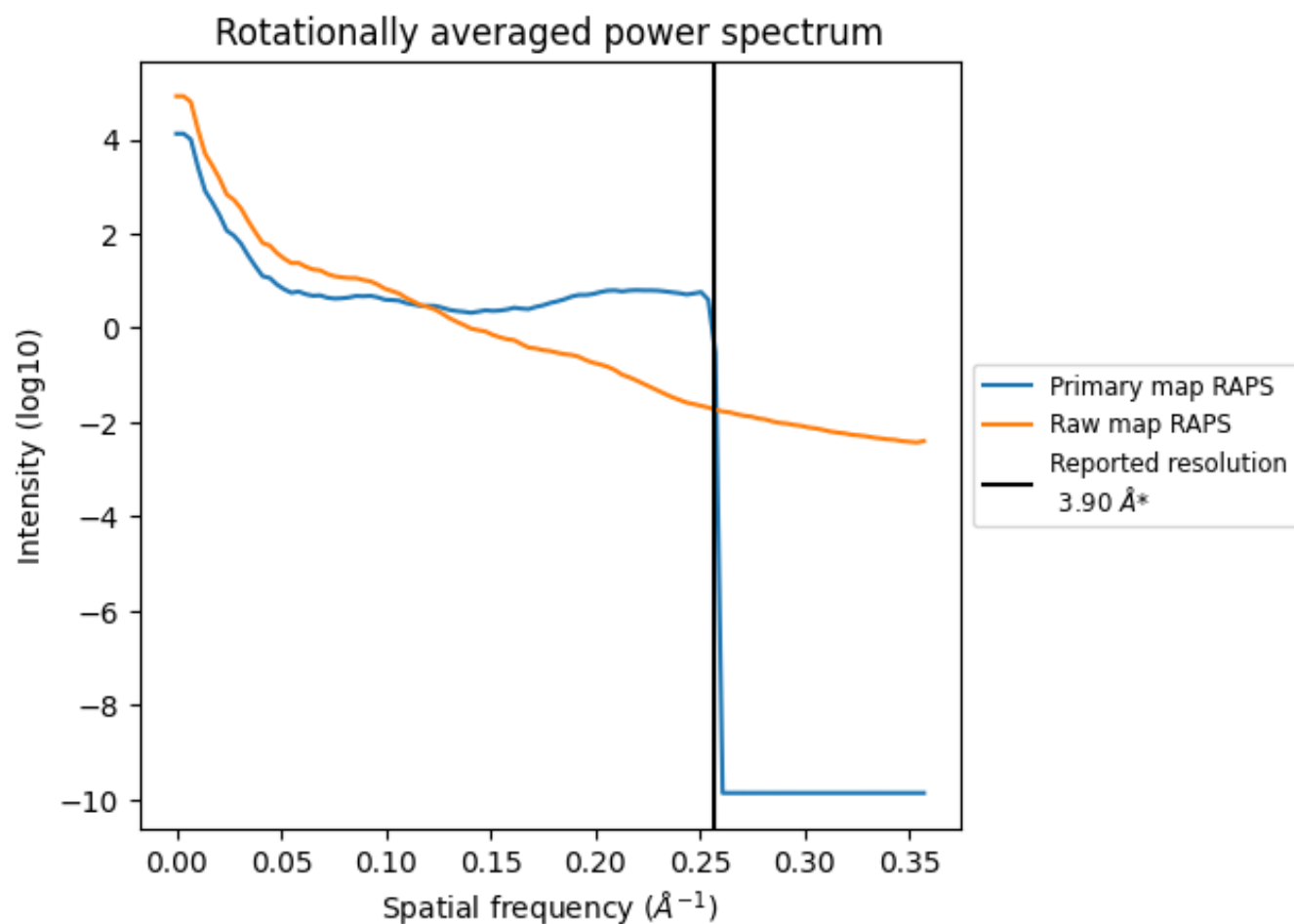
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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 ⓘ

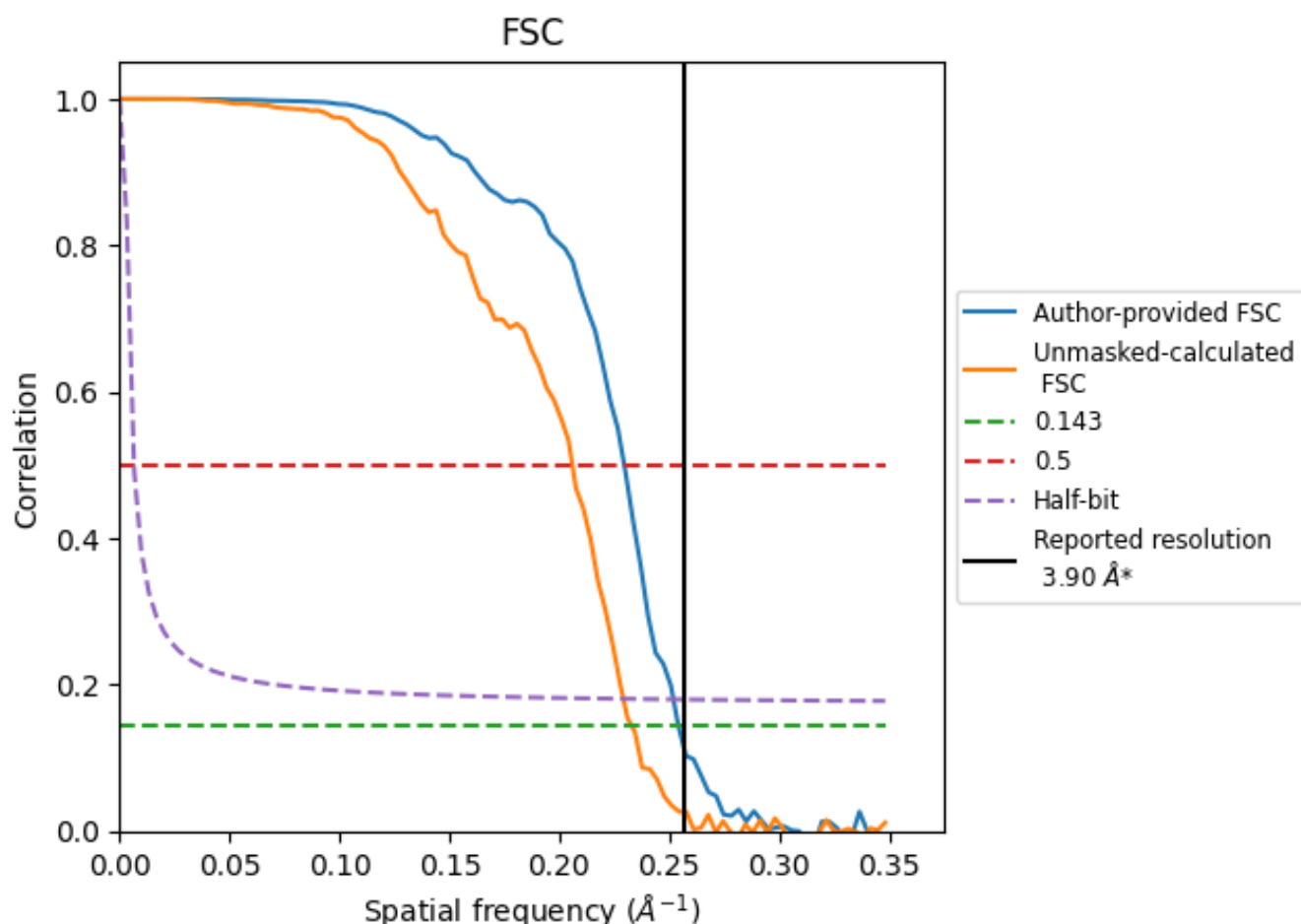


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates

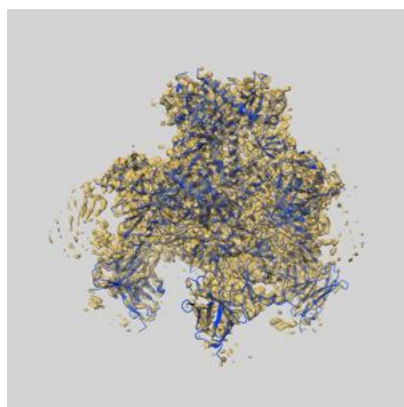
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.36	3.97
Unmasked-calculated*	4.29	4.86	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.29 differs from the reported value 3.9 by more than 10 %

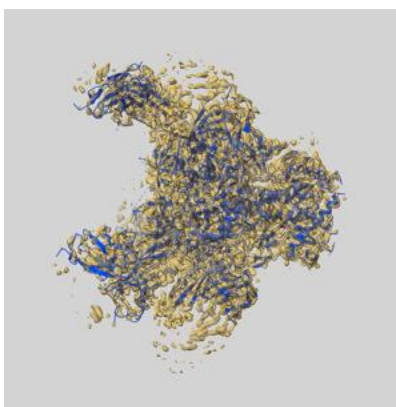
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20740 and PDB model 6UDK. Per-residue inclusion information can be found in section [3](#) on page [10](#).

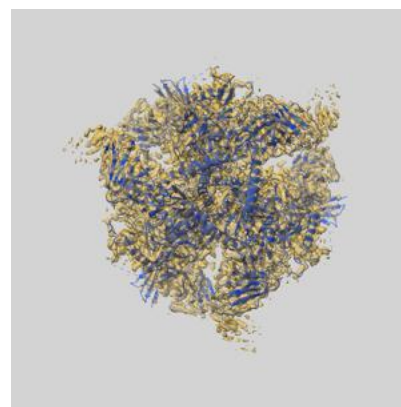
9.1 Map-model overlay [i](#)



X



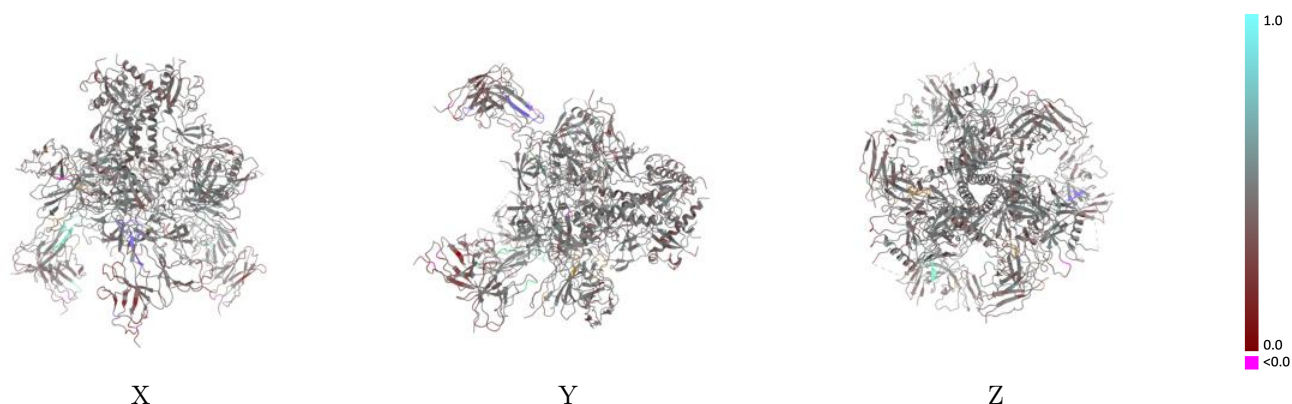
Y



Z

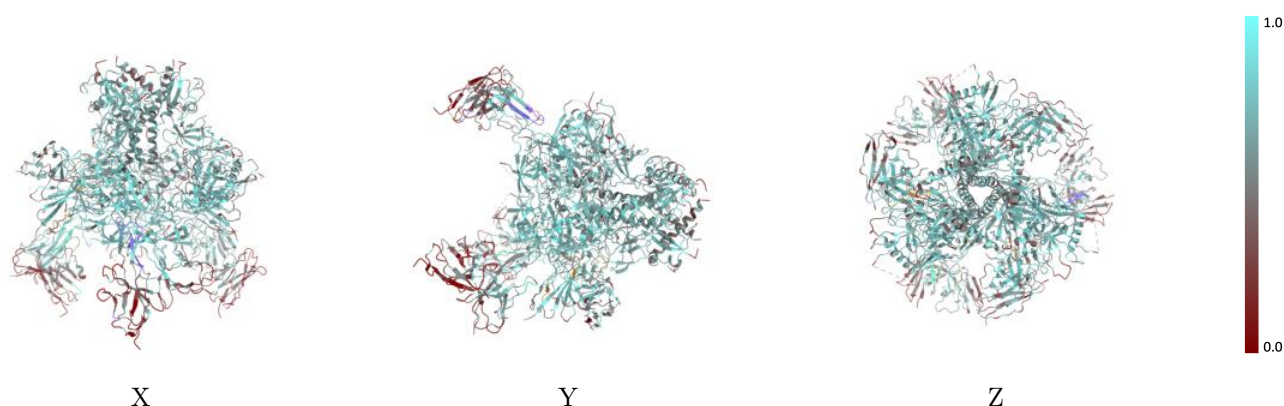
The images above show the 3D surface view of the map at the recommended contour level 0.0717 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



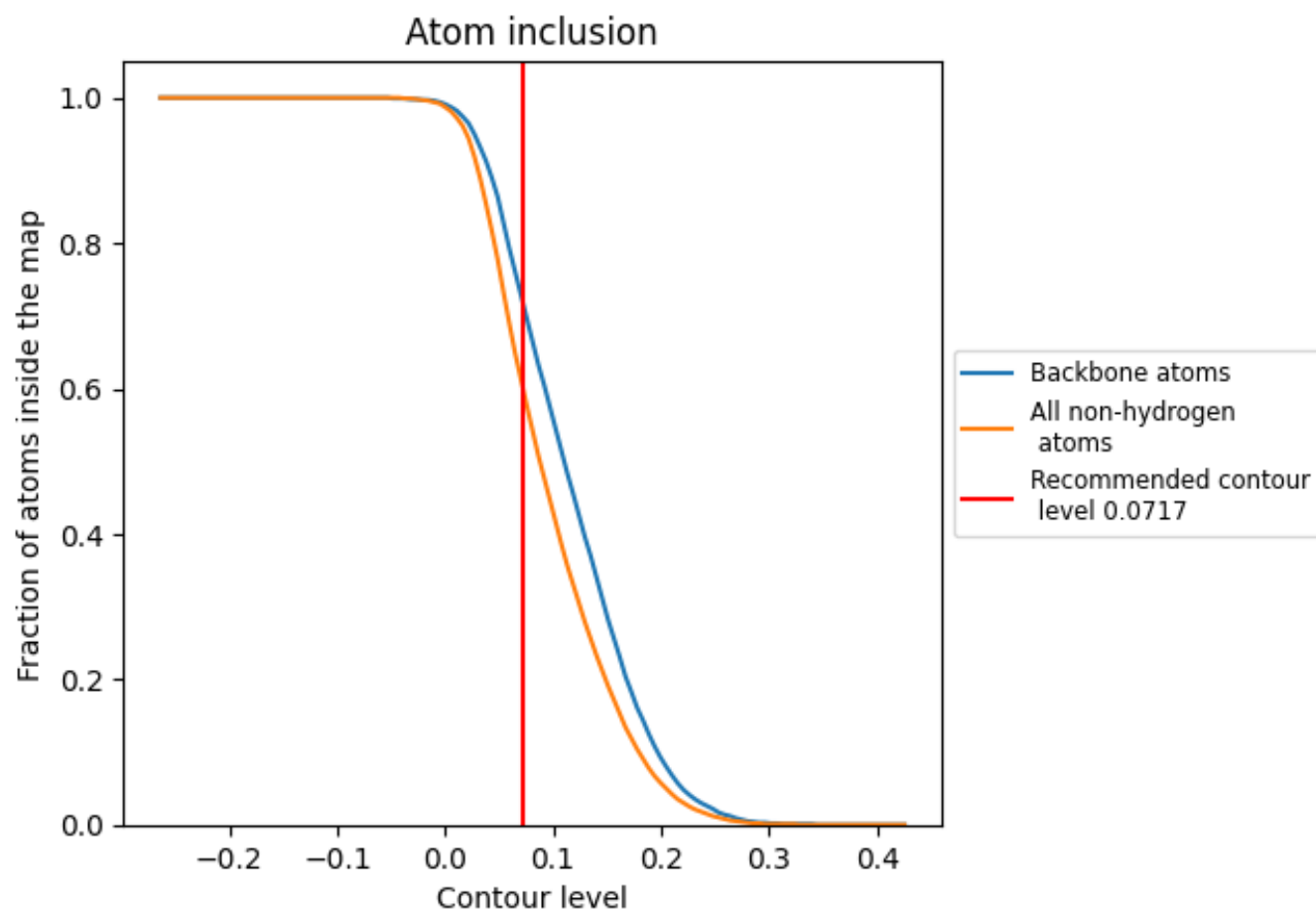
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0717).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.0717) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6030	 0.4420
A	 0.3800	 0.3810
B	 0.5410	 0.4360
C	 0.6040	 0.4470
D	 0.6790	 0.4620
E	 0.5830	 0.4390
F	 0.3840	 0.3860
G	 0.6690	 0.4550
H	 0.6830	 0.4660
I	 0.5360	 0.4370
J	 0.6150	 0.4500
K	 0.6710	 0.4590
L	 0.5750	 0.4360
M	 0.6770	 0.4570
N	 0.5890	 0.4350
O	 0.3790	 0.3960
P	 0.5460	 0.4380
Q	 0.6110	 0.4480
R	 0.6680	 0.4550
S	 0.3930	 0.3800
T	 0.5560	 0.4390
U	 0.2820	 0.3240
V	 0.5960	 0.4440
W	 0.5360	 0.3820
X	 0.2860	 0.4460
Y	 0.4460	 0.4350
Z	 0.2820	 0.3190
a	 0.5530	 0.3640
b	 0.5000	 0.3600
c	 0.3570	 0.4190
d	 0.5000	 0.4660
e	 0.6110	 0.3370
f	 0.5000	 0.3210
g	 0.3210	 0.3470

