



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:58 AM UTC

PDB ID : 7UGO / pdb_00007ugo
EMDB ID : EMD-26492
Title : Cryo-EM structure of BG24 inferred germline Fabs with mature CDR3s and 10-1074 Fabs in complex with HIV-1 Env immunogen BG505-SOSIPv4.1-GT1
Authors : Dam, K.A.; Bjorkman, P.J.
Deposited on : 2022-03-25
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

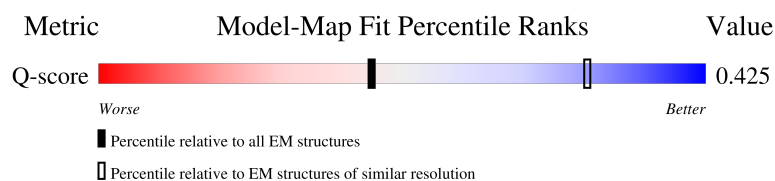
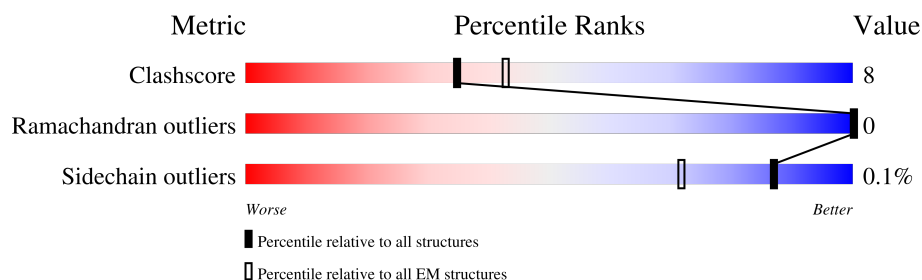
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



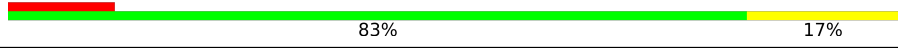
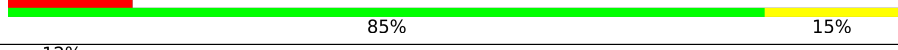
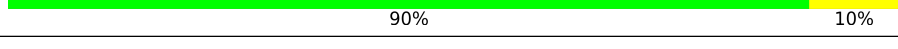
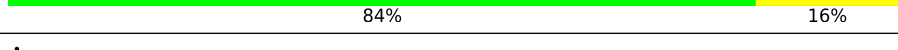
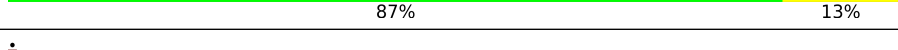
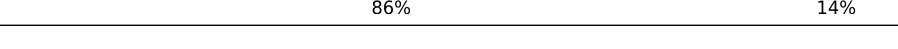
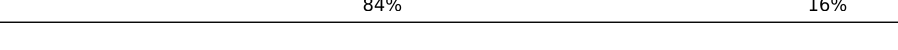
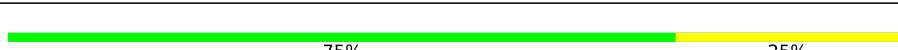
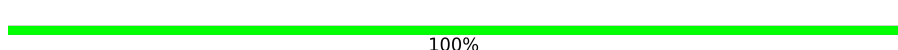
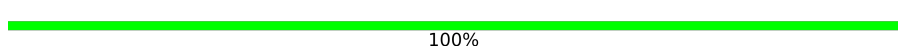
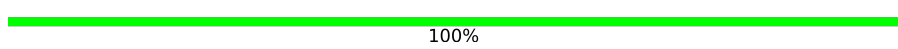
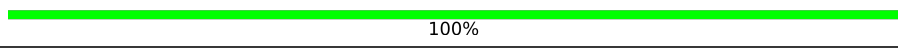
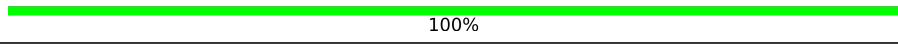
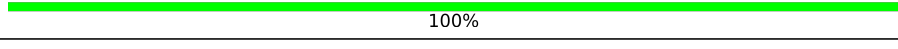
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	466	79% 16% .
1	B	466	83% 13% .
1	C	466	79% 17% .
2	D	129	84% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	129	
2	F	129	
3	M	133	
3	N	133	
3	O	133	
4	P	107	
4	Q	107	
4	R	107	
5	G	125	
5	H	125	
5	I	125	
6	J	106	
6	K	106	
6	L	106	
7	S	4	
7	g	4	
8	T	7	
9	U	2	
9	V	2	
9	W	2	
9	Y	2	
9	b	2	
9	c	2	
9	d	2	
9	f	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	2	 100%
9	j	2	 100%
9	k	2	 100%
9	l	2	 50% 50%
10	X	2	 100%
10	e	2	 100%
11	Z	3	 67% 33%
12	a	7	 29% 57% 14%
13	h	9	 44% 56%

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
10	MAN	e	1	-	-	X	-
10	MAN	e	2	X	-	-	-
11	BMA	Z	3	X	-	X	-
12	BMA	a	3	-	-	X	-
12	MAN	a	7	X	-	-	-
13	MAN	h	4	-	-	X	-
13	MAN	h	7	X	-	X	-
13	MAN	h	8	-	-	X	-
13	MAN	h	9	X	-	-	-
14	NAG	A	605	-	-	X	-
15	MAN	B	608	-	-	X	-
7	BMA	S	3	X	-	-	-
7	MAN	S	4	X	-	-	-
7	BMA	g	3	X	-	-	-
7	MAN	g	4	X	-	-	-
8	MAN	T	4	X	-	-	-
9	NAG	U	2	X	-	-	-
9	NAG	V	2	X	-	-	-
9	NAG	W	2	X	-	-	-
9	NAG	b	2	X	-	-	-
9	NAG	c	2	X	-	-	-
9	NAG	d	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	i	2	X	-	-	-
9	NAG	k	2	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 25590 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	447	Total	C	N	O	S	0	0
			3523	2218	622	656	27		
1	B	447	Total	C	N	O	S	0	0
			3523	2218	622	656	27		
1	C	447	Total	C	N	O	S	0	0
			3523	2218	622	656	27		

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LYS	GLU	conflict	UNP Q2N0S5
A	169	ARG	LYS	conflict	UNP Q2N0S5
A	173	HIS	TYR	conflict	UNP Q2N0S5
A	174	ALA	SER	conflict	UNP Q2N0S5
A	178	LYS	ARG	conflict	UNP Q2N0S5
A	181	ILE	VAL	conflict	UNP Q2N0S5
A	183	PRO	GLN	conflict	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ARG	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	189	THR	LYS	conflict	UNP Q2N0S5
A	190	SER	GLU	conflict	UNP Q2N0S5
A	199	ALA	SER	conflict	UNP Q2N0S5
A	276	ASP	ASN	conflict	UNP Q2N0S5
A	278	ARG	THR	conflict	UNP Q2N0S5
A	316	TRP	ALA	conflict	UNP Q2N0S5
A	332	ASN	THR	conflict	UNP Q2N0S5
A	386	ASP	ASN	conflict	UNP Q2N0S5
A	462	ASP	ASN	conflict	UNP Q2N0S5
A	471	SER	GLY	conflict	UNP Q2N0S5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	conflict	UNP Q2N0S5
B	64	LYS	GLU	conflict	UNP Q2N0S5
B	169	ARG	LYS	conflict	UNP Q2N0S5
B	173	HIS	TYR	conflict	UNP Q2N0S5
B	174	ALA	SER	conflict	UNP Q2N0S5
B	178	LYS	ARG	conflict	UNP Q2N0S5
B	181	ILE	VAL	conflict	UNP Q2N0S5
B	183	PRO	GLN	conflict	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	ARG	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	189	THR	LYS	conflict	UNP Q2N0S5
B	190	SER	GLU	conflict	UNP Q2N0S5
B	199	ALA	SER	conflict	UNP Q2N0S5
B	276	ASP	ASN	conflict	UNP Q2N0S5
B	278	ARG	THR	conflict	UNP Q2N0S5
B	316	TRP	ALA	conflict	UNP Q2N0S5
B	332	ASN	THR	conflict	UNP Q2N0S5
B	386	ASP	ASN	conflict	UNP Q2N0S5
B	462	ASP	ASN	conflict	UNP Q2N0S5
B	471	SER	GLY	conflict	UNP Q2N0S5
B	501	CYS	ALA	conflict	UNP Q2N0S5
C	64	LYS	GLU	conflict	UNP Q2N0S5
C	169	ARG	LYS	conflict	UNP Q2N0S5
C	173	HIS	TYR	conflict	UNP Q2N0S5
C	174	ALA	SER	conflict	UNP Q2N0S5
C	178	LYS	ARG	conflict	UNP Q2N0S5
C	181	ILE	VAL	conflict	UNP Q2N0S5
C	183	PRO	GLN	conflict	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ARG	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	189	THR	LYS	conflict	UNP Q2N0S5
C	190	SER	GLU	conflict	UNP Q2N0S5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ALA	SER	conflict	UNP Q2N0S5
C	276	ASP	ASN	conflict	UNP Q2N0S5
C	278	ARG	THR	conflict	UNP Q2N0S5
C	316	TRP	ALA	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	386	ASP	ASN	conflict	UNP Q2N0S5
C	462	ASP	ASN	conflict	UNP Q2N0S5
C	471	SER	GLY	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		
2	E	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		
2	F	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		

- Molecule 3 is a protein called 10-1074 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	N	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 4 is a protein called 10-1074 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
4	Q	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
4	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 5 is a protein called BG24 inferred germline Fab with mature CDR3s heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	125	Total	C	N	O	S	0	0
			960	603	164	186	7		
5	H	125	Total	C	N	O	S	0	0
			960	603	164	186	7		
5	I	125	Total	C	N	O	S	0	0
			960	603	164	186	7		

- Molecule 6 is a protein called BG24 inferred germline Fab with mature CDR3s light chain.

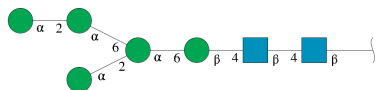
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	105	Total	C	N	O	S	0	0
			776	483	129	161	3		
6	K	105	Total	C	N	O	S	0	0
			776	483	129	161	3		
6	L	105	Total	C	N	O	S	0	0
			776	483	129	161	3		

- Molecule 7 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
7	S	4	Total	C	N	O	0	0
			50	28	2	20		
7	g	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]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	7	Total	C	N	O	0	0
			83	46	2	35		

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



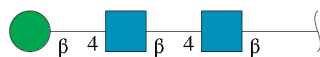
Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	2	Total	C	N	O	0	0
			28	16	2	10		
9	V	2	Total	C	N	O	0	0
			28	16	2	10		
9	W	2	Total	C	N	O	0	0
			28	16	2	10		
9	Y	2	Total	C	N	O	0	0
			28	16	2	10		
9	b	2	Total	C	N	O	0	0
			28	16	2	10		
9	c	2	Total	C	N	O	0	0
			28	16	2	10		
9	d	2	Total	C	N	O	0	0
			28	16	2	10		
9	f	2	Total	C	N	O	0	0
			28	16	2	10		
9	i	2	Total	C	N	O	0	0
			28	16	2	10		
9	j	2	Total	C	N	O	0	0
			28	16	2	10		
9	k	2	Total	C	N	O	0	0
			28	16	2	10		
9	l	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



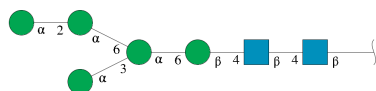
Mol	Chain	Residues	Atoms			AltConf	Trace
10	X	2	Total	C	O	0	0
			22	12	10		
10	e	2	Total	C	O	0	0
			22	12	10		

- Molecule 11 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.



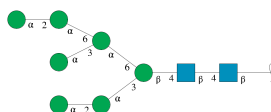
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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
13	h	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



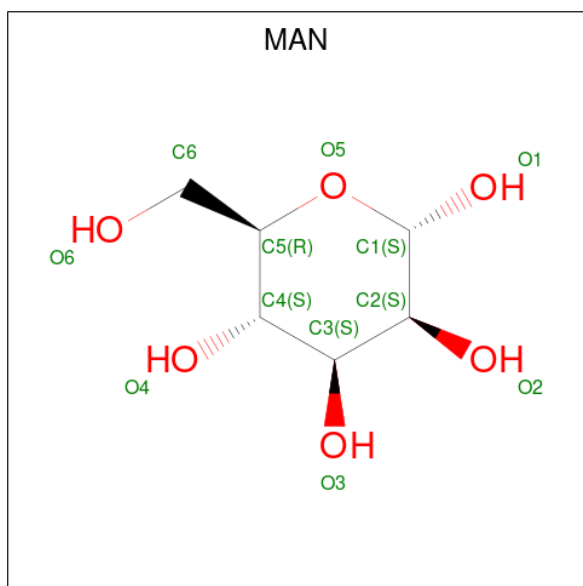
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	A	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14	8	1	5	
14	B	1	Total	C	N	O	0
			14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

Continued on next page...

Continued from previous page...

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

- Molecule 15 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

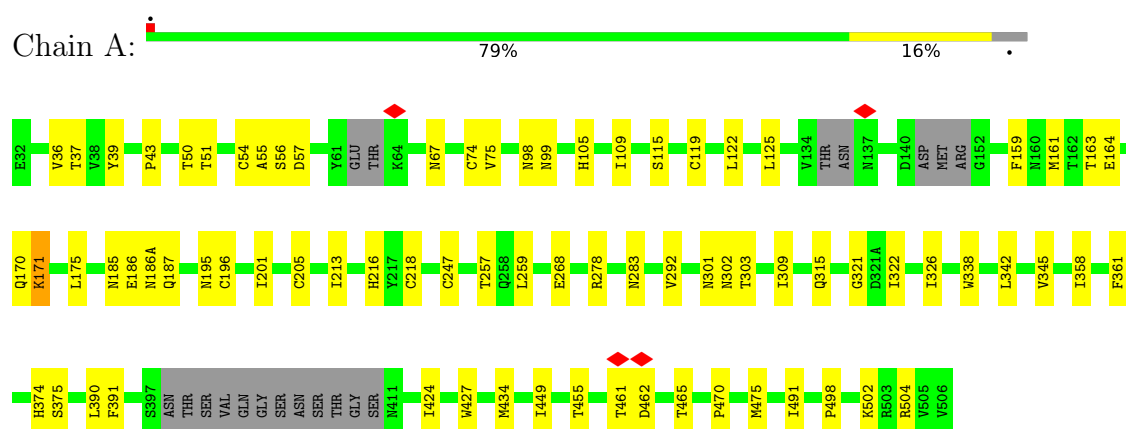


Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			11	6	5	
15	B	1	Total	C	O	0
			11	6	5	
15	B	1	Total	C	O	0
			11	6	5	
15	C	1	Total	C	O	0
			11	6	5	

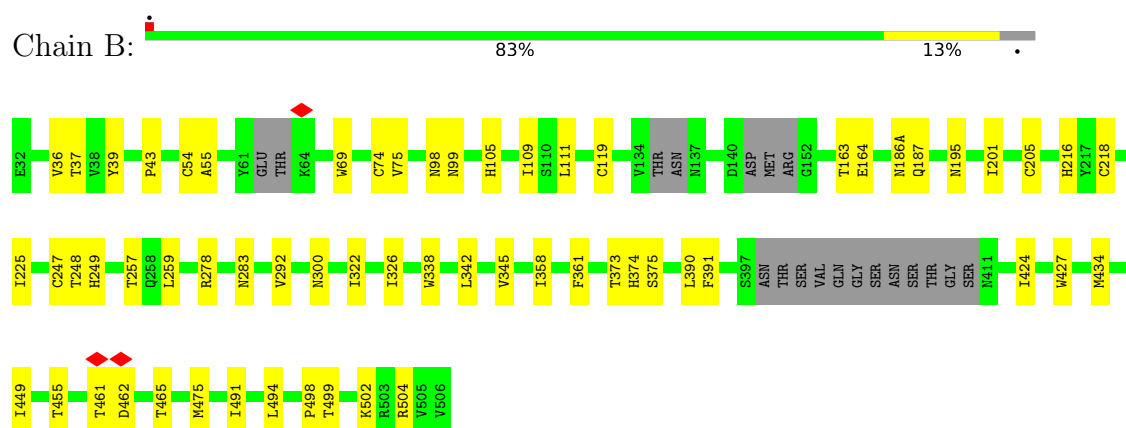
3 Residue-property plots

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

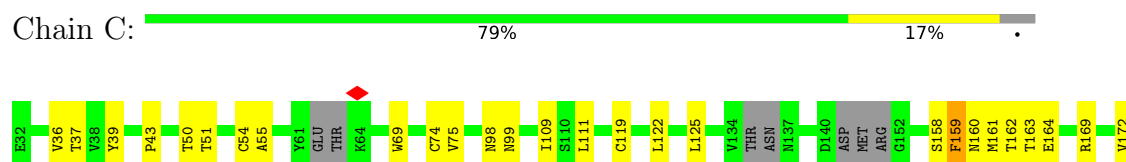
• Molecule 1: Envelope glycoprotein gp120

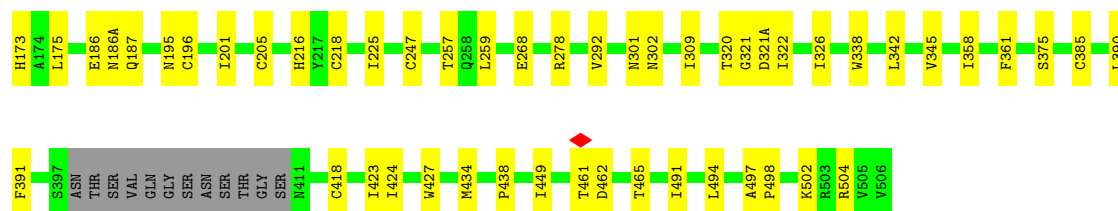


• Molecule 1: Envelope glycoprotein gp120

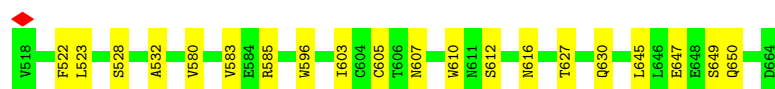
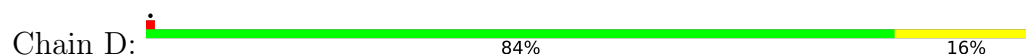


• Molecule 1: Envelope glycoprotein gp120

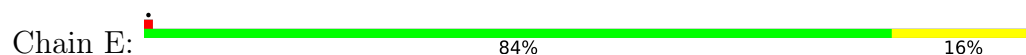




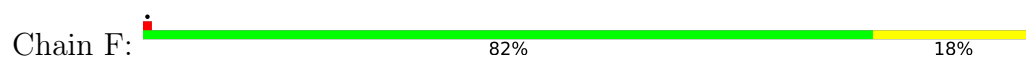
- Molecule 2: Envelope glycoprotein gp41



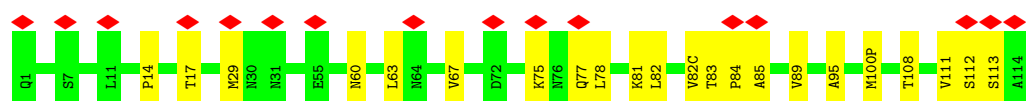
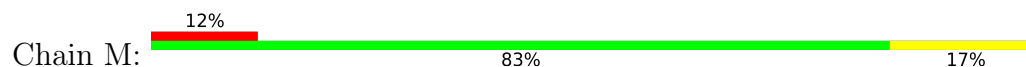
- Molecule 2: Envelope glycoprotein gp41



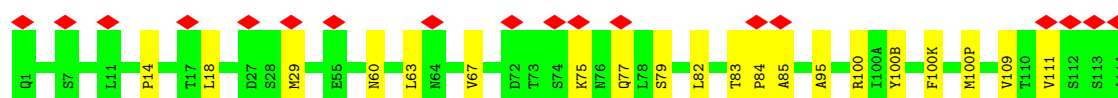
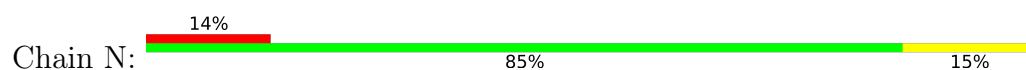
- Molecule 2: Envelope glycoprotein gp41



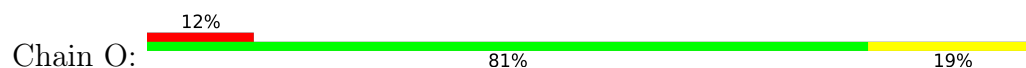
- Molecule 3: 10-1074 Fab heavy chain

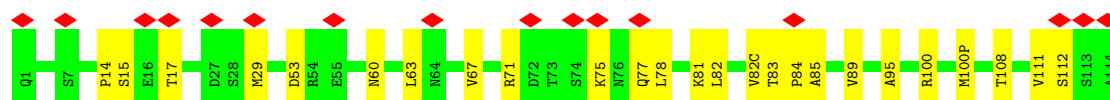


- Molecule 3: 10-1074 Fab heavy chain

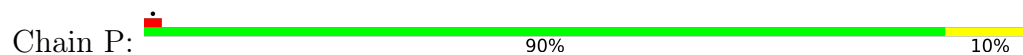


- Molecule 3: 10-1074 Fab heavy chain

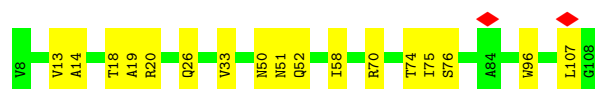
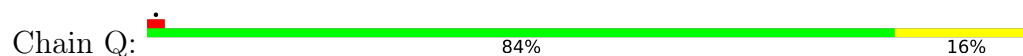




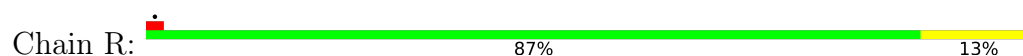
- Molecule 4: 10-1074 Fab light chain



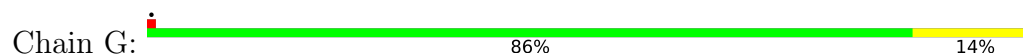
- Molecule 4: 10-1074 Fab light chain



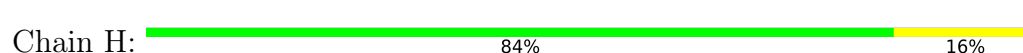
- Molecule 4: 10-1074 Fab light chain



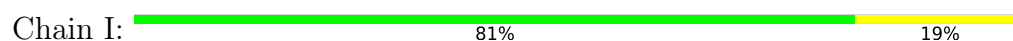
- Molecule 5: BG24 inferred germline Fab with mature CDR3s heavy chain



- Molecule 5: BG24 inferred germline Fab with mature CDR3s heavy chain

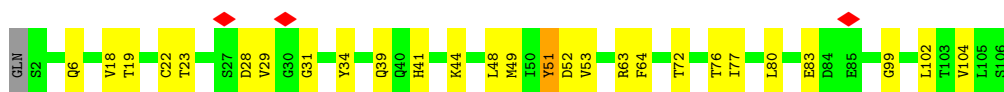


- Molecule 5: BG24 inferred germline Fab with mature CDR3s heavy chain



- Molecule 6: BG24 inferred germline Fab with mature CDR3s light chain

Chain J:  74% 25% ..



- Molecule 6: BG24 inferred germline Fab with mature CDR3s light chain

Chain K:  78% 20% ..



- Molecule 6: BG24 inferred germline Fab with mature CDR3s light chain

Chain L:  80% 18% ..



- Molecule 7: 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:  50% 50%



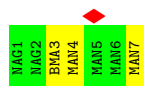
- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  75% 25%



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

Chain T:  14% 57% 43%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  100%



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

Chain Y:  50% 50%



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

Chain b:  100%



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

Chain c:  100%



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

Chain d:  100%



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

Chain f:  50% 50%

MAG1
MAG2

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

Chain i:  100%

MAG1
MAG2

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

Chain j:  100%

MAG1
MAG2

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

Chain k:  100%

MAG1
MAG2

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

Chain l:  50% 50%

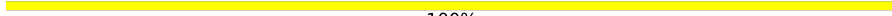
MAG1
MAG2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain X:  100%

MAY1
MAY2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain e:  100%



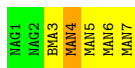
- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 67% 33%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 29% 57% 14%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 h: 44% 56%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225140	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0223	Depositor
Map size ($\text{\AA}$)	291.84, 291.84, 291.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.14, 1.14, 1.14	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/3598	0.36	0/4885
1	B	0.13	0/3598	0.36	0/4885
1	C	0.18	0/3598	0.44	2/4885 (0.0%)
2	D	0.11	0/1048	0.28	0/1421
2	E	0.12	0/1048	0.28	0/1421
2	F	0.11	0/1048	0.29	0/1421
3	M	0.11	0/1066	0.31	0/1451
3	N	0.11	0/1066	0.30	0/1451
3	O	0.11	0/1066	0.32	0/1451
4	P	0.10	0/845	0.30	0/1148
4	Q	0.10	0/845	0.30	0/1148
4	R	0.11	0/845	0.32	0/1148
5	G	0.10	0/983	0.27	0/1333
5	H	0.11	0/983	0.28	0/1333
5	I	0.10	0/983	0.28	0/1333
6	J	0.10	0/794	0.32	0/1077
6	K	0.10	0/794	0.31	0/1077
6	L	0.10	0/794	0.31	0/1077
All	All	0.13	0/25002	0.34	2/33945 (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
6	J	0	1
6	K	0	1
6	L	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	160	ASN	N-CA-C	8.14	120.15	111.28
1	C	159	PHE	N-CA-C	6.55	119.12	109.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	J	51	TYR	Peptide
6	K	51	TYR	Peptide
6	L	51	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3523	0	3462	69	0
1	B	3523	0	3462	45	0
1	C	3523	0	3462	71	0
2	D	1030	0	1020	15	0
2	E	1030	0	1020	15	0
2	F	1030	0	1020	17	0
3	M	1041	0	1005	14	0
3	N	1041	0	1005	14	0
3	O	1041	0	1005	20	0
4	P	824	0	788	8	0
4	Q	824	0	788	12	0
4	R	824	0	788	9	0
5	G	960	0	923	11	0
5	H	960	0	923	14	0
5	I	960	0	923	16	0
6	J	776	0	738	16	0
6	K	776	0	738	14	0
6	L	776	0	738	12	0
7	S	50	0	41	4	0
7	g	50	0	42	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	83	0	68	4	0
9	U	28	0	25	0	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0
9	Y	28	0	25	0	0
9	b	28	0	25	0	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
9	k	28	0	25	0	0
9	l	28	0	25	0	0
10	X	22	0	19	4	0
10	e	22	0	19	13	0
11	Z	39	0	34	10	0
12	a	83	0	70	9	0
13	h	105	0	87	16	0
14	A	84	0	78	10	0
14	B	84	0	75	0	0
14	C	84	0	78	2	0
14	D	14	0	13	0	0
14	E	14	0	13	0	0
14	F	14	0	13	0	0
15	A	11	0	10	4	0
15	B	22	0	20	10	0
15	C	11	0	10	2	0
All	All	25590	0	24798	403	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 8.

All (403) 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:C:161:MET:CE	1:C:309:ILE:CD1	1.96	1.42
15:B:608:MAN:C2	11:Z:3:BMA:O6	1.69	1.38
12:a:3:BMA:O3	10:e:1:MAN:C1	1.75	1.32
1:C:161:MET:CE	1:C:309:ILE:HD11	1.58	1.28
12:a:3:BMA:C3	10:e:1:MAN:C1	2.13	1.24
15:B:601:MAN:H2	11:Z:3:BMA:O3	1.40	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:CB	14:A:605:NAG:H82	1.77	1.15
1:A:301:ASN:O	1:A:322:ILE:CD1	1.95	1.14
1:C:161:MET:HE3	1:C:309:ILE:CG1	1.77	1.14
1:A:171:LYS:CB	14:A:605:NAG:C8	2.27	1.13
3:O:100:ARG:NH1	13:h:8:MAN:O3	1.82	1.11
1:C:161:MET:HE1	1:C:309:ILE:HD11	1.30	1.10
1:C:161:MET:HE2	1:C:309:ILE:CD1	1.79	1.10
1:A:171:LYS:HB2	14:A:605:NAG:C8	1.84	1.07
1:C:161:MET:CE	1:C:309:ILE:CG1	2.34	1.05
15:B:608:MAN:H2	11:Z:3:BMA:O6	0.88	1.04
1:C:161:MET:HE3	1:C:309:ILE:HG13	1.40	1.04
8:T:3:BMA:O3	10:X:1:MAN:C1	2.08	1.00
1:A:301:ASN:O	1:A:322:ILE:HD12	1.57	0.99
1:C:161:MET:HE2	1:C:309:ILE:HD12	1.41	0.99
1:C:161:MET:CE	1:C:309:ILE:HG13	1.93	0.99
1:C:161:MET:HE3	1:C:309:ILE:CD1	1.85	0.98
12:a:3:BMA:H3	10:e:1:MAN:O5	1.64	0.98
1:A:171:LYS:HB3	14:A:605:NAG:H82	1.45	0.98
1:A:171:LYS:HB2	14:A:605:NAG:H82	1.41	0.97
12:a:3:BMA:H3	10:e:1:MAN:C1	1.91	0.96
1:A:171:LYS:HB3	14:A:605:NAG:C8	1.93	0.95
1:C:301:ASN:O	1:C:322:ILE:HD12	1.66	0.95
1:C:301:ASN:O	1:C:322:ILE:CD1	2.15	0.94
1:C:385:CYS:HB3	1:C:418:CYS:HA	1.50	0.94
4:R:66(B):ILE:HD11	13:h:9:MAN:O3	1.69	0.92
15:B:601:MAN:C2	11:Z:3:BMA:O3	2.17	0.92
1:C:161:MET:CE	1:C:309:ILE:HD12	1.97	0.88
4:Q:50:ASN:OD1	10:e:2:MAN:O3	1.94	0.85
15:C:606:MAN:C1	7:g:3:BMA:O4	2.24	0.85
15:A:607:MAN:O2	7:S:3:BMA:O4	1.94	0.85
1:A:171:LYS:CB	14:A:605:NAG:H83	2.08	0.84
1:A:37:THR:HG22	2:D:605:CYS:HB3	1.58	0.82
1:A:171:LYS:HD2	1:A:171:LYS:O	1.79	0.81
1:A:301:ASN:C	1:A:322:ILE:CD1	2.53	0.80
15:A:607:MAN:O2	7:S:3:BMA:C4	2.31	0.78
15:B:608:MAN:H2	11:Z:3:BMA:HO6	0.98	0.78
1:C:175:LEU:HD12	1:C:321:GLY:O	1.84	0.77
13:h:4:MAN:O4	13:h:7:MAN:C2	2.33	0.77
3:O:100:ARG:HH12	13:h:8:MAN:HO3	1.32	0.76
8:T:3:BMA:H4	8:T:4:MAN:H2	1.66	0.76
1:C:37:THR:HG22	2:F:605:CYS:HB3	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:607:MAN:HO2	7:S:3:BMA:C4	1.99	0.75
13:h:3:BMA:O4	13:h:8:MAN:C1	2.33	0.75
4:Q:52:GLN:NE2	10:e:2:MAN:O6	2.20	0.74
1:C:161:MET:HE3	1:C:309:ILE:HD11	1.48	0.74
15:B:601:MAN:H2	11:Z:3:BMA:HO3	1.51	0.73
1:C:301:ASN:C	1:C:322:ILE:CD1	2.61	0.73
6:J:19:THR:HG22	6:J:76:THR:HG22	1.71	0.72
15:B:608:MAN:C2	11:Z:3:BMA:HO6	1.73	0.71
3:O:100:ARG:HH22	13:h:8:MAN:C3	2.03	0.70
1:B:300:ASN:HB3	1:B:322:ILE:HD11	1.73	0.70
6:L:29:VAL:HG12	6:L:31:GLY:H	1.56	0.70
1:C:322:ILE:HG21	1:C:326:ILE:HD11	1.73	0.70
6:K:19:THR:HG22	6:K:76:THR:HG22	1.72	0.69
3:O:100:ARG:CZ	13:h:8:MAN:O3	2.40	0.69
13:h:4:MAN:O4	13:h:7:MAN:C1	2.40	0.69
12:a:3:BMA:O4	10:e:1:MAN:C1	2.41	0.68
1:A:301:ASN:C	1:A:322:ILE:HD11	2.18	0.68
6:J:29:VAL:HG12	6:J:31:GLY:H	1.60	0.66
1:C:301:ASN:C	1:C:322:ILE:HD11	2.21	0.66
1:C:161:MET:HE2	1:C:309:ILE:CG1	2.15	0.66
1:A:301:ASN:O	1:A:322:ILE:HD11	1.92	0.66
6:K:48:LEU:HD21	6:K:51:TYR:HB3	1.77	0.66
3:N:83:THR:HG22	3:N:85:ALA:H	1.61	0.66
2:F:627:THR:H	2:F:630:GLN:HE21	1.45	0.65
1:B:322:ILE:HG21	1:B:326:ILE:HD11	1.79	0.64
1:C:159:PHE:N	1:C:172:VAL:O	2.28	0.64
2:E:627:THR:H	2:E:630:GLN:HE21	1.45	0.64
6:J:48:LEU:HD21	6:J:51:TYR:HB3	1.78	0.64
1:A:171:LYS:HB3	14:A:605:NAG:H83	1.73	0.63
2:D:627:THR:H	2:D:630:GLN:HE21	1.46	0.63
13:h:4:MAN:O4	13:h:7:MAN:H2	1.98	0.63
3:O:100:ARG:HH22	13:h:8:MAN:H3	1.61	0.63
12:a:3:BMA:C4	10:e:1:MAN:C1	2.77	0.63
15:A:607:MAN:O2	7:S:3:BMA:H4	1.99	0.62
3:O:83:THR:HG22	3:O:85:ALA:H	1.64	0.62
3:M:60:ASN:HB2	3:M:63:LEU:HD23	1.81	0.62
8:T:3:BMA:C3	10:X:1:MAN:C1	2.77	0.62
3:M:83:THR:HG22	3:M:85:ALA:H	1.65	0.61
4:P:19:ALA:HB3	4:P:75:ILE:HD11	1.82	0.61
6:L:48:LEU:HD21	6:L:51:TYR:HB3	1.82	0.61
1:B:491:ILE:O	2:E:585:ARG:NH2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HG22	2:E:605:CYS:HB3	1.81	0.60
1:A:491:ILE:O	2:D:585:ARG:NH2	2.34	0.60
3:M:84:PRO:HA	3:M:111:VAL:HG23	1.82	0.60
13:h:4:MAN:O4	13:h:7:MAN:H3	2.01	0.60
4:Q:26:GLN:HG2	4:Q:70:ARG:HH11	1.66	0.60
4:Q:19:ALA:HB3	4:Q:75:ILE:HD11	1.82	0.60
1:C:424:ILE:HD11	1:C:434:MET:HE3	1.82	0.60
3:N:60:ASN:HB2	3:N:63:LEU:HD23	1.84	0.60
3:O:100:ARG:NH2	13:h:8:MAN:O3	2.34	0.60
1:A:195:ASN:HD21	1:A:201:ILE:HD12	1.67	0.59
1:B:36:VAL:HG12	2:E:610:TRP:HE3	1.67	0.59
1:B:259:LEU:HD22	1:B:449:ILE:HD11	1.84	0.59
1:A:259:LEU:HD22	1:A:449:ILE:HD11	1.85	0.59
1:A:292:VAL:HB	1:A:449:ILE:HG23	1.85	0.59
1:C:164:GLU:OE1	1:C:164:GLU:N	2.28	0.59
3:O:67:VAL:HB	3:O:82:LEU:HD13	1.85	0.59
1:C:292:VAL:HB	1:C:449:ILE:HG23	1.83	0.59
3:O:84:PRO:HA	3:O:111:VAL:HG23	1.85	0.59
1:C:195:ASN:HD21	1:C:201:ILE:HD12	1.68	0.58
1:A:278:ARG:NH1	6:J:28:ASP:O	2.36	0.58
1:A:424:ILE:HD11	1:A:434:MET:HE3	1.83	0.58
3:N:84:PRO:HA	3:N:111:VAL:HG23	1.85	0.58
3:N:95:ALA:HB2	3:N:100(P):MET:HG3	1.86	0.58
1:B:424:ILE:HD11	1:B:434:MET:HE3	1.85	0.58
6:J:63:ARG:NH2	6:J:83:GLU:OE1	2.37	0.58
1:A:502:LYS:O	1:A:504:ARG:NH2	2.36	0.58
3:M:84:PRO:HB3	3:M:112:SER:HA	1.85	0.58
15:B:608:MAN:C1	11:Z:3:BMA:O6	2.49	0.58
3:N:67:VAL:HB	3:N:82:LEU:HD13	1.86	0.58
1:B:292:VAL:HB	1:B:449:ILE:HG23	1.86	0.58
6:J:34:TYR:HB3	6:J:52:ASP:HB2	1.86	0.58
1:C:491:ILE:O	2:F:585:ARG:NH2	2.36	0.57
3:M:67:VAL:HB	3:M:82:LEU:HD13	1.85	0.57
1:B:361:PHE:HB3	1:B:391:PHE:HB3	1.86	0.57
1:A:322:ILE:HG21	1:A:326:ILE:HD11	1.85	0.57
1:B:257:THR:OG1	1:B:375:SER:OG	2.23	0.57
1:B:502:LYS:O	1:B:504:ARG:NH2	2.37	0.57
3:N:100:ARG:HH22	10:e:1:MAN:H4	1.68	0.57
3:O:95:ALA:HB2	3:O:100(P):MET:HG3	1.86	0.57
1:A:175:LEU:HD12	1:A:321:GLY:O	2.04	0.57
4:R:26:GLN:HG2	4:R:70:ARG:HH11	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:66(B):ILE:HD11	13:h:9:MAN:C3	2.35	0.56
1:B:300:ASN:HB3	1:B:322:ILE:CD1	2.35	0.56
1:B:322:ILE:HG23	1:B:322:ILE:O	2.05	0.56
4:P:26:GLN:HG2	4:P:70:ARG:HH11	1.68	0.56
1:A:361:PHE:HB3	1:A:391:PHE:HB3	1.87	0.56
1:C:385:CYS:HB3	1:C:418:CYS:CA	2.29	0.56
1:B:195:ASN:HD21	1:B:201:ILE:HD12	1.72	0.55
2:D:645:LEU:O	2:D:649:SER:OG	2.23	0.55
1:C:361:PHE:HB3	1:C:391:PHE:HB3	1.88	0.55
1:B:186(A):ASN:N	1:B:187:GLN:HA	2.22	0.55
3:M:95:ALA:HB2	3:M:100(P):MET:HG3	1.89	0.55
6:K:52:ASP:OD1	6:K:53:VAL:N	2.40	0.55
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.89	0.55
1:C:502:LYS:O	1:C:504:ARG:NH2	2.40	0.55
2:D:580:VAL:HA	2:D:583:VAL:HG12	1.88	0.55
5:H:17:SER:HB3	5:H:82(A):SER:HB2	1.89	0.55
1:A:186(A):ASN:N	1:A:187:GLN:HA	2.22	0.55
1:B:278:ARG:NH1	6:K:28:ASP:O	2.40	0.55
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.88	0.55
6:L:19:THR:HG22	6:L:76:THR:HG22	1.88	0.54
1:A:301:ASN:H	1:A:322:ILE:HD11	1.72	0.54
1:A:36:VAL:HG12	2:D:610:TRP:HE3	1.72	0.54
2:E:580:VAL:HA	2:E:583:VAL:HG12	1.89	0.54
2:F:607:ASN:HB2	2:F:650:GLN:HE22	1.73	0.54
3:O:60:ASN:HB2	3:O:63:LEU:HD23	1.89	0.54
6:K:63:ARG:NH2	6:K:83:GLU:OE1	2.40	0.54
1:B:55:ALA:HB3	1:B:216:HIS:HB2	1.90	0.54
3:N:75:LYS:HD3	3:N:77:GLN:HG2	1.89	0.54
1:C:301:ASN:H	1:C:322:ILE:HD11	1.73	0.54
4:R:54:ARG:NH1	4:R:60:GLU:OE1	2.40	0.54
3:N:29:MET:N	3:N:29:MET:SD	2.79	0.53
6:J:52:ASP:OD1	6:J:53:VAL:N	2.40	0.53
3:O:17:THR:HB	3:O:81:LYS:HE3	1.91	0.53
13:h:4:MAN:O4	13:h:7:MAN:C3	2.57	0.53
2:F:580:VAL:HA	2:F:583:VAL:HG12	1.89	0.53
4:Q:14:ALA:HA	4:Q:107:LEU:H	1.73	0.53
12:a:3:BMA:HO3	10:e:1:MAN:C1	2.12	0.53
6:J:23:THR:HG21	6:J:72:THR:HA	1.89	0.53
6:L:34:TYR:HB3	6:L:52:ASP:HB2	1.88	0.53
1:C:195:ASN:HD22	1:C:423:ILE:HG21	1.73	0.53
1:C:186(A):ASN:N	1:C:187:GLN:HA	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100(F):PHE:O	6:K:38:TYR:OH	2.21	0.52
6:L:52:ASP:OD1	6:L:53:VAL:N	2.42	0.52
6:L:25:THR:HG22	6:L:27:SER:H	1.74	0.52
3:O:14:PRO:HG3	3:O:84:PRO:HG3	1.92	0.52
1:B:163:THR:HG22	1:B:164:GLU:H	1.74	0.52
6:J:41:HIS:HB2	6:J:44:LYS:HB2	1.91	0.52
1:C:74:CYS:SG	1:C:75:VAL:N	2.83	0.52
6:J:39:GLN:HB3	6:J:49:MET:HE3	1.90	0.52
1:C:278:ARG:NH1	6:L:28:ASP:O	2.43	0.52
4:R:14:ALA:HA	4:R:107:LEU:H	1.75	0.52
4:P:14:ALA:HA	4:P:107:LEU:H	1.74	0.52
1:B:461:THR:OG1	1:B:462:ASP:N	2.42	0.51
1:C:161:MET:HE2	1:C:309:ILE:HG13	1.81	0.51
1:B:74:CYS:SG	1:B:75:VAL:N	2.83	0.51
1:B:54:CYS:SG	1:B:55:ALA:N	2.84	0.51
1:C:461:THR:OG1	1:C:462:ASP:N	2.43	0.51
1:A:163:THR:HG22	1:A:164:GLU:H	1.75	0.51
5:G:51:ILE:HG13	5:G:57:THR:HG22	1.93	0.51
6:L:41:HIS:HB2	6:L:44:LYS:HB2	1.91	0.51
1:A:119:CYS:SG	1:A:205:CYS:N	2.68	0.51
6:K:41:HIS:HB2	6:K:44:LYS:HB2	1.93	0.51
1:A:185:ASN:O	1:A:186(A):ASN:ND2	2.43	0.51
4:Q:18:THR:HG22	4:Q:76:SER:HA	1.92	0.51
5:H:51:ILE:HG13	5:H:57:THR:HG22	1.93	0.51
2:F:656:ASN:O	2:F:660:LEU:HG	2.10	0.50
5:G:18:VAL:HG13	5:G:82(C):LEU:HD11	1.93	0.50
2:E:652:GLN:NE2	2:E:653:GLN:HG3	2.26	0.50
1:A:74:CYS:SG	1:A:75:VAL:N	2.85	0.50
1:C:54:CYS:SG	1:C:55:ALA:N	2.85	0.50
6:J:6:GLN:HB3	6:J:22:CYS:SG	2.51	0.50
1:C:257:THR:OG1	1:C:375:SER:OG	2.23	0.50
5:G:17:SER:HB3	5:G:82(A):SER:HB2	1.92	0.50
1:A:257:THR:OG1	1:A:375:SER:OG	2.27	0.50
3:N:77:GLN:OE1	3:N:79:SER:OG	2.28	0.50
1:C:36:VAL:HG12	2:F:610:TRP:HE3	1.76	0.50
3:O:84:PRO:HB3	3:O:112:SER:HA	1.93	0.50
5:G:48:MET:HG2	5:G:63:PHE:HE2	1.77	0.50
5:H:18:VAL:HG13	5:H:82(C):LEU:HD11	1.92	0.50
13:h:4:MAN:C4	13:h:7:MAN:H2	2.40	0.50
6:K:39:GLN:HB3	6:K:49:MET:HE3	1.94	0.49
12:a:3:BMA:C3	10:e:1:MAN:O5	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:OG1	1:A:462:ASP:N	2.44	0.49
6:L:63:ARG:NH2	6:L:83:GLU:OE1	2.44	0.49
4:R:18:THR:HG22	4:R:76:SER:HA	1.94	0.49
5:I:17:SER:HB3	5:I:82(A):SER:HB2	1.94	0.49
5:I:100(F):PHE:O	6:L:38:TYR:OH	2.24	0.49
6:J:18:VAL:HG21	6:J:102:LEU:HD11	1.95	0.49
1:B:342:LEU:HA	1:B:345:VAL:HG12	1.95	0.49
1:C:342:LEU:HA	1:C:345:VAL:HG12	1.95	0.49
5:I:17:SER:HA	5:I:82:LEU:O	2.13	0.49
4:P:54:ARG:NH1	4:P:60:GLU:OE1	2.45	0.49
4:Q:13:VAL:HG21	4:Q:19:ALA:HB2	1.95	0.49
5:H:1:GLN:HE21	5:H:3:GLN:HG2	1.78	0.49
1:A:498:PRO:HB3	2:D:610:TRP:CD2	2.48	0.49
1:C:259:LEU:HD22	1:C:449:ILE:HD11	1.93	0.49
1:A:170:GLN:HG3	1:A:170:GLN:O	2.13	0.49
5:G:1:GLN:HE21	5:G:3:GLN:HG2	1.77	0.49
5:G:67:VAL:HG12	5:G:82:LEU:HD13	1.95	0.49
5:I:18:VAL:HG13	5:I:82(C):LEU:HD11	1.95	0.49
1:A:462:ASP:N	1:A:462:ASP:OD1	2.46	0.49
5:H:48:MET:HG2	5:H:63:PHE:HE2	1.78	0.49
1:C:119:CYS:SG	1:C:205:CYS:N	2.70	0.48
1:A:171:LYS:CG	14:A:605:NAG:H83	2.43	0.48
1:B:498:PRO:HB3	2:E:610:TRP:CD2	2.49	0.48
6:K:34:TYR:HB3	6:K:52:ASP:HB2	1.95	0.48
3:M:75:LYS:HD3	3:M:77:GLN:HG2	1.96	0.48
1:C:195:ASN:OD1	1:C:196:CYS:N	2.47	0.48
1:B:248:THR:OG1	1:B:249:HIS:N	2.46	0.48
3:O:29:MET:SD	3:O:29:MET:N	2.80	0.48
1:C:338:TRP:CE2	1:C:390:LEU:HD22	2.49	0.48
4:P:13:VAL:HG21	4:P:19:ALA:HB2	1.95	0.48
15:B:601:MAN:C1	11:Z:3:BMA:O3	2.62	0.47
3:O:71:ARG:HG3	3:O:78:LEU:HG	1.96	0.47
4:P:66(B):ILE:HD12	10:X:1:MAN:O3	2.14	0.47
2:F:612:SER:OG	2:F:616:ASN:OD1	2.26	0.47
5:H:67:VAL:HG12	5:H:82:LEU:HD13	1.96	0.47
6:K:29:VAL:HG13	6:K:33:ASN:HD21	1.77	0.47
1:A:54:CYS:SG	1:A:55:ALA:N	2.87	0.47
1:A:342:LEU:HA	1:A:345:VAL:HG12	1.95	0.47
15:B:608:MAN:O2	11:Z:3:BMA:O6	2.28	0.47
5:H:17:SER:HA	5:H:82:LEU:O	2.15	0.47
5:I:48:MET:HG2	5:I:63:PHE:HE2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:607:NAG:O7	14:C:607:NAG:O3	2.33	0.47
4:R:13:VAL:HG21	4:R:19:ALA:HB2	1.96	0.47
1:B:195:ASN:ND2	1:B:201:ILE:HB	2.29	0.47
1:B:257:THR:HG1	1:B:375:SER:HG	1.56	0.47
1:C:498:PRO:HB3	2:F:610:TRP:CD2	2.49	0.47
5:I:1:GLN:HE21	5:I:3:GLN:HG2	1.80	0.47
1:B:462:ASP:N	1:B:462:ASP:OD1	2.46	0.46
1:A:303:THR:O	1:A:321:GLY:N	2.47	0.46
6:K:29:VAL:HA	6:K:33:ASN:ND2	2.30	0.46
4:P:66(B):ILE:CD1	10:X:1:MAN:O3	2.64	0.46
4:Q:52:GLN:CD	10:e:2:MAN:O6	2.59	0.46
1:A:109:ILE:HD13	1:A:427:TRP:CD1	2.51	0.46
1:A:171:LYS:HG2	14:A:605:NAG:H83	1.97	0.46
1:C:37:THR:OG1	1:C:497:ALA:O	2.34	0.46
3:M:17:THR:HB	3:M:81:LYS:HE3	1.96	0.46
1:C:320:THR:HG22	1:C:438:PRO:HB3	1.96	0.46
1:B:195:ASN:HD21	1:B:201:ILE:HB	1.81	0.46
3:M:29:MET:SD	3:M:29:MET:N	2.84	0.46
5:G:17:SER:HA	5:G:82:LEU:O	2.15	0.46
5:H:47:TRP:HZ2	5:H:50:TRP:HD1	1.63	0.46
1:A:67:ASN:HD21	1:A:213:ILE:HD13	1.81	0.45
1:B:119:CYS:SG	1:B:205:CYS:N	2.70	0.45
1:A:98:ASN:OD1	1:A:99:ASN:N	2.50	0.45
2:E:528:SER:HB3	2:E:532:ALA:HB3	1.99	0.45
5:I:47:TRP:HZ2	5:I:50:TRP:HD1	1.62	0.45
2:D:607:ASN:HB2	2:D:650:GLN:HE22	1.81	0.45
1:C:186(A):ASN:O	1:C:186(A):ASN:ND2	2.50	0.45
1:A:338:TRP:CE2	1:A:390:LEU:HD22	2.52	0.45
2:E:645:LEU:O	2:E:649:SER:OG	2.24	0.45
5:I:51:ILE:HG13	5:I:57:THR:HG22	1.99	0.45
1:C:43:PRO:HB3	2:F:523:LEU:HD13	1.99	0.45
5:I:50:TRP:CE2	5:I:58:ASN:HB3	2.51	0.45
1:B:109:ILE:HD13	1:B:427:TRP:CD1	2.52	0.45
1:C:301:ASN:N	1:C:322:ILE:HD11	2.32	0.45
1:C:358:ILE:HB	1:C:465:THR:HG22	1.99	0.45
2:D:612:SER:OG	2:D:616:ASN:OD1	2.26	0.45
2:D:528:SER:HB3	2:D:532:ALA:HB3	1.99	0.45
5:H:50:TRP:CE2	5:H:58:ASN:HB3	2.52	0.45
5:H:82(A):SER:OG	5:H:82(B):ARG:N	2.50	0.45
6:L:29:VAL:HA	6:L:33:ASN:ND2	2.32	0.45
1:B:43:PRO:HB3	2:E:523:LEU:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ILE:HD13	1:C:427:TRP:CD1	2.52	0.44
2:E:612:SER:OG	2:E:616:ASN:OD1	2.26	0.44
1:C:50:THR:OG1	1:C:51:THR:N	2.50	0.44
1:C:195:ASN:ND2	1:C:201:ILE:HD12	2.30	0.44
5:G:47:TRP:HZ2	5:G:50:TRP:HD1	1.64	0.44
1:C:161:MET:HE1	1:C:309:ILE:CD1	1.99	0.44
3:M:89:VAL:HA	3:M:108:THR:HA	1.98	0.44
6:K:18:VAL:HG23	6:K:77:ILE:HB	2.00	0.44
1:B:98:ASN:OD1	1:B:99:ASN:N	2.50	0.44
1:B:218:CYS:HA	1:B:247:CYS:CB	2.48	0.44
1:A:39:TYR:HE1	2:D:603:ILE:HG23	1.82	0.44
1:B:338:TRP:CE2	1:B:390:LEU:HD22	2.52	0.44
1:B:494:LEU:HD21	2:E:593:LEU:HD21	2.00	0.44
2:F:528:SER:HB3	2:F:532:ALA:HB3	1.99	0.44
5:G:50:TRP:CE2	5:G:58:ASN:HB3	2.53	0.44
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.84	0.43
1:B:37:THR:HG21	1:B:499:THR:HG22	2.00	0.43
1:C:494:LEU:HD21	2:F:593:LEU:HD21	2.00	0.43
1:A:43:PRO:HB3	2:D:523:LEU:HD13	2.00	0.43
1:A:218:CYS:HA	1:A:247:CYS:CB	2.48	0.43
1:C:218:CYS:HA	1:C:247:CYS:CB	2.48	0.43
3:N:100(B):TYR:CB	10:e:1:MAN:O6	2.66	0.43
3:O:75:LYS:HD3	3:O:77:GLN:HG2	2.00	0.43
5:G:82(A):SER:OG	5:G:82(B):ARG:N	2.51	0.43
1:C:39:TYR:HE1	2:F:603:ILE:HG23	1.82	0.43
1:C:98:ASN:OD1	1:C:99:ASN:N	2.50	0.43
15:C:606:MAN:C2	7:g:3:BMA:O4	2.65	0.43
3:O:53:ASP:OD1	3:O:71:ARG:NH2	2.44	0.43
6:J:28:ASP:OD1	6:J:28:ASP:N	2.48	0.43
3:N:100:ARG:HD2	3:N:100(K):PHE:HE1	1.83	0.43
1:C:169:ARG:HA	1:C:169:ARG:HD3	1.78	0.43
6:K:18:VAL:HG21	6:K:102:LEU:HD11	2.01	0.43
1:A:195:ASN:ND2	1:A:201:ILE:HB	2.33	0.43
1:A:268:GLU:O	1:A:268:GLU:HG2	2.19	0.43
1:B:39:TYR:HE1	2:E:603:ILE:HG23	1.84	0.43
5:I:82(A):SER:OG	5:I:82(B):ARG:N	2.51	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.86	0.43
1:B:358:ILE:HD12	1:B:465:THR:HG22	2.00	0.43
1:C:302:ASN:HA	1:C:322:ILE:HD13	2.01	0.43
3:O:89:VAL:HA	3:O:108:THR:HA	2.01	0.43
1:A:195:ASN:OD1	1:A:196:CYS:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HD12	1:A:465:THR:HG22	2.00	0.42
1:A:122:LEU:HD13	1:A:125:LEU:HD22	1.99	0.42
3:M:82:LEU:HG	3:M:82(C):VAL:HG12	2.02	0.42
4:R:19:ALA:HB3	4:R:75:ILE:HD11	2.00	0.42
2:E:607:ASN:HB2	2:E:650:GLN:HE22	1.83	0.42
5:I:6:GLN:HE21	5:I:107:THR:HG23	1.85	0.42
5:I:97:LYS:HE3	5:I:97:LYS:HB2	1.90	0.42
6:K:20:ILE:HG23	6:K:75:LEU:HB3	2.00	0.42
6:L:18:VAL:HG21	6:L:102:LEU:HD11	2.00	0.42
1:A:50:THR:OG1	1:A:51:THR:N	2.51	0.42
2:E:522:PHE:CE2	2:E:523:LEU:HD23	2.54	0.42
5:I:50:TRP:HE1	5:I:58:ASN:HD22	1.67	0.42
1:A:301:ASN:N	1:A:322:ILE:HD11	2.34	0.42
2:D:596:TRP:CD1	2:D:647:GLU:HB3	2.55	0.42
1:A:56:SER:OG	1:A:57:ASP:N	2.53	0.42
1:C:322:ILE:HG23	1:C:322:ILE:O	2.19	0.42
2:F:546:SER:O	2:F:546:SER:OG	2.35	0.42
3:M:14:PRO:HD3	3:M:113:SER:HA	2.01	0.42
1:C:69:TRP:HA	1:C:111:LEU:HD21	2.02	0.42
1:C:186:GLU:C	1:C:187:GLN:HA	2.45	0.42
1:B:283:ASN:HD22	1:B:455:THR:HG22	1.85	0.42
1:A:115:SER:O	1:A:115:SER:OG	2.34	0.42
1:B:373:THR:OG1	1:B:374:HIS:N	2.52	0.42
4:Q:33:VAL:HB	4:Q:51:ASN:OD1	2.20	0.42
5:I:87:THR:HG22	5:I:111:VAL:H	1.85	0.42
12:a:4:MAN:HO4	12:a:7:MAN:HO2	0.43	0.42
1:A:186:GLU:C	1:A:187:GLN:HA	2.45	0.41
1:C:268:GLU:O	1:C:268:GLU:HG2	2.19	0.41
5:H:115:SER:O	5:H:115:SER:OG	2.32	0.41
2:F:652:GLN:HA	2:F:655:LYS:HE3	2.02	0.41
6:J:80:LEU:HD21	6:J:104:VAL:HG12	2.02	0.41
1:A:302:ASN:HA	1:A:322:ILE:HD13	2.03	0.41
1:C:158:SER:HA	1:C:173:HIS:HA	2.03	0.41
2:D:522:PHE:CE2	2:D:523:LEU:HD23	2.55	0.41
2:F:522:PHE:CE2	2:F:523:LEU:HD23	2.55	0.41
4:R:78:VAL:HG23	4:R:82:ASP:HB2	2.02	0.41
5:H:50:TRP:HE1	5:H:58:ASN:HD22	1.69	0.41
1:A:391:PHE:CE2	1:A:470:PRO:HG3	2.56	0.41
6:J:64:PHE:HB2	6:J:77:ILE:HA	2.02	0.41
3:O:15:SER:H	3:O:82(C):VAL:HG22	1.85	0.41
13:h:4:MAN:H3	13:h:7:MAN:H2	1.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:HD22	1:A:455:THR:HG22	1.86	0.41
1:B:69:TRP:HA	1:B:111:LEU:HD21	2.01	0.41
1:B:259:LEU:HB2	1:B:374:HIS:CD2	2.56	0.41
1:C:122:LEU:HD13	1:C:125:LEU:HD22	2.02	0.41
1:C:225:ILE:HD12	1:C:247:CYS:HA	2.02	0.41
14:C:607:NAG:HO3	14:C:607:NAG:C7	2.33	0.41
3:M:60:ASN:ND2	4:P:96:TRP:HB3	2.36	0.41
3:M:77:GLN:C	3:M:78:LEU:HD12	2.46	0.41
3:N:14:PRO:HG3	3:N:84:PRO:HG3	2.02	0.41
5:I:75:ILE:HG13	5:I:77:THR:HG23	2.02	0.41
1:A:159:PHE:HE1	1:A:161:MET:HE2	1.87	0.41
1:A:309:ILE:HG22	1:A:315:GLN:HB2	2.03	0.41
2:F:608:VAL:N	2:F:650:GLN:HE21	2.18	0.41
3:N:60:ASN:ND2	4:Q:96:TRP:HB3	2.36	0.41
5:I:34:MET:HE2	5:I:34:MET:HB3	2.00	0.41
1:C:195:ASN:HD22	1:C:423:ILE:CG2	2.35	0.40
8:T:3:BMA:C4	8:T:4:MAN:H2	2.43	0.40
1:A:36:VAL:HG12	2:D:610:TRP:CE3	2.54	0.40
1:A:105:HIS:NE2	1:A:475:MET:HE3	2.36	0.40
1:B:105:HIS:NE2	1:B:475:MET:HE3	2.36	0.40
1:B:225:ILE:HD12	1:B:247:CYS:HA	2.02	0.40
4:Q:20:ARG:HG2	4:Q:74:THR:HB	2.03	0.40
4:Q:58:ILE:HD12	4:Q:58:ILE:HA	1.94	0.40
1:A:259:LEU:HB2	1:A:374:HIS:CD2	2.56	0.40
5:G:87:THR:HG22	5:G:111:VAL:H	1.87	0.40
5:H:20:VAL:HB	5:H:80:MET:HB3	2.03	0.40
3:N:18:LEU:HD21	3:N:109:VAL:HG11	2.03	0.40
6:J:6:GLN:HG3	6:J:99:GLY:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/466 (94%)	399 (91%)	38 (9%)	0	100	100
1	B	437/466 (94%)	402 (92%)	35 (8%)	0	100	100
1	C	437/466 (94%)	399 (91%)	38 (9%)	0	100	100
2	D	125/129 (97%)	120 (96%)	5 (4%)	0	100	100
2	E	125/129 (97%)	120 (96%)	5 (4%)	0	100	100
2	F	125/129 (97%)	122 (98%)	3 (2%)	0	100	100
3	M	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
3	N	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
3	O	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
4	P	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
4	Q	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
4	R	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
5	G	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
5	H	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
5	I	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
6	J	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
6	K	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
6	L	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
All	All	3072/3198 (96%)	2892 (94%)	180 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/416 (96%)	397 (100%)	1 (0%)	86	85
1	B	398/416 (96%)	398 (100%)	0	100	100
1	C	398/416 (96%)	395 (99%)	3 (1%)	73	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	112/112 (100%)	112 (100%)	0	100	100
2	E	112/112 (100%)	112 (100%)	0	100	100
2	F	112/112 (100%)	112 (100%)	0	100	100
3	M	116/116 (100%)	116 (100%)	0	100	100
3	N	116/116 (100%)	116 (100%)	0	100	100
3	O	116/116 (100%)	116 (100%)	0	100	100
4	P	85/85 (100%)	85 (100%)	0	100	100
4	Q	85/85 (100%)	85 (100%)	0	100	100
4	R	85/85 (100%)	85 (100%)	0	100	100
5	G	102/102 (100%)	102 (100%)	0	100	100
5	H	102/102 (100%)	102 (100%)	0	100	100
5	I	102/102 (100%)	102 (100%)	0	100	100
6	J	86/87 (99%)	86 (100%)	0	100	100
6	K	86/87 (99%)	86 (100%)	0	100	100
6	L	86/87 (99%)	86 (100%)	0	100	100
All	All	2697/2754 (98%)	2693 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LYS
1	C	162	THR
1	C	163	THR
1	C	321(A)	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	315	GLN
1	A	374	HIS
1	B	186(A)	ASN
1	B	203	GLN
1	B	283	ASN
1	B	374	HIS
1	C	186(A)	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	ASN
1	C	283	ASN
2	D	630	GLN
2	D	650	GLN
2	E	630	GLN
2	E	652	GLN
2	F	630	GLN
2	F	650	GLN
3	M	1	GLN
3	M	5	GLN
3	M	39	GLN
3	M	60	ASN
3	M	64	ASN
3	N	39	GLN
3	N	60	ASN
3	O	1	GLN
3	O	5	GLN
3	O	39	GLN
3	O	60	ASN
4	Q	52	GLN
5	G	6	GLN
5	G	58	ASN
5	H	6	GLN
5	H	58	ASN
5	I	6	GLN
5	I	58	ASN
6	J	81	GLN
6	K	41	HIS
6	K	81	GLN
6	L	81	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 ⓘ

62 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	S	1	1,7	14,14,15	0.21	0	17,19,21	0.45	0
7	NAG	S	2	7	14,14,15	0.27	0	17,19,21	0.54	0
7	BMA	S	3	7	11,11,12	0.57	0	15,15,17	0.73	0
7	MAN	S	4	7	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
8	NAG	T	1	1,8	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	T	2	8	14,14,15	0.22	0	17,19,21	0.58	0
8	BMA	T	3	8	11,11,12	0.55	0	15,15,17	0.75	0
8	MAN	T	4	8	11,11,12	0.23	0	15,15,17	0.46	0
8	MAN	T	5	8	11,11,12	0.23	0	15,15,17	0.48	0
8	MAN	T	6	8	11,11,12	0.23	0	15,15,17	0.47	0
8	MAN	T	7	8	11,11,12	0.30	0	15,15,17	0.91	1 (6%)
9	NAG	U	1	1,9	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	U	2	9	14,14,15	0.22	0	17,19,21	0.43	0
9	NAG	V	1	1,9	14,14,15	0.21	0	17,19,21	0.50	0
9	NAG	V	2	9	14,14,15	0.19	0	17,19,21	0.44	0
9	NAG	W	1	1,9	14,14,15	0.23	0	17,19,21	0.45	0
9	NAG	W	2	9	14,14,15	0.20	0	17,19,21	0.44	0
10	MAN	X	1	10	11,11,12	0.24	0	15,15,17	0.46	0
10	MAN	X	2	10	11,11,12	0.70	0	15,15,17	0.94	2 (13%)
9	NAG	Y	1	1,9	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
9	NAG	Y	2	9	14,14,15	0.27	0	17,19,21	0.55	0
11	NAG	Z	1	11,1	14,14,15	0.22	0	17,19,21	0.45	0
11	NAG	Z	2	11	14,14,15	0.26	0	17,19,21	0.54	0
11	BMA	Z	3	11	11,11,12	0.22	0	15,15,17	0.57	0
12	NAG	a	1	12,1	14,14,15	0.24	0	17,19,21	0.42	0
12	NAG	a	2	12	14,14,15	0.21	0	17,19,21	0.59	0
12	BMA	a	3	12	11,11,12	0.55	0	15,15,17	0.75	0
12	MAN	a	4	12	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
12	MAN	a	5	12	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
12	MAN	a	6	12	11,11,12	0.66	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	a	7	12	11,11,12	0.23	0	15,15,17	0.50	0
9	NAG	b	1	1,9	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	b	2	9	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	c	1	1,9	14,14,15	0.22	0	17,19,21	0.49	0
9	NAG	c	2	9	14,14,15	0.20	0	17,19,21	0.44	0
9	NAG	d	1	1,9	14,14,15	0.22	0	17,19,21	0.45	0
9	NAG	d	2	9	14,14,15	0.21	0	17,19,21	0.44	0
10	MAN	e	1	10	11,11,12	0.24	0	15,15,17	0.46	0
10	MAN	e	2	10	11,11,12	0.23	0	15,15,17	0.47	0
9	NAG	f	1	1,9	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
9	NAG	f	2	9	14,14,15	0.28	0	17,19,21	0.56	0
7	NAG	g	1	1,7	14,14,15	0.21	0	17,19,21	0.46	0
7	NAG	g	2	7	14,14,15	0.26	0	17,19,21	0.53	0
7	BMA	g	3	7	11,11,12	0.22	0	15,15,17	0.57	0
7	MAN	g	4	7	11,11,12	0.24	0	15,15,17	0.47	0
13	NAG	h	1	1,13	14,14,15	0.21	0	17,19,21	0.43	0
13	NAG	h	2	13	14,14,15	0.21	0	17,19,21	0.58	0
13	BMA	h	3	13	11,11,12	0.55	0	15,15,17	0.75	0
13	MAN	h	4	13	11,11,12	0.23	0	15,15,17	0.47	0
13	MAN	h	5	13	11,11,12	0.24	0	15,15,17	0.47	0
13	MAN	h	6	13	11,11,12	0.23	0	15,15,17	0.47	0
13	MAN	h	7	13	11,11,12	0.24	0	15,15,17	0.47	0
13	MAN	h	8	13	11,11,12	0.22	0	15,15,17	0.49	0
13	MAN	h	9	13	11,11,12	0.23	0	15,15,17	0.47	0
9	NAG	i	1	1,9	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	i	2	9	14,14,15	0.24	0	17,19,21	0.43	0
9	NAG	j	1	1,9	14,14,15	0.21	0	17,19,21	0.48	0
9	NAG	j	2	9	14,14,15	0.19	0	17,19,21	0.43	0
9	NAG	k	1	1,9	14,14,15	0.23	0	17,19,21	0.45	0
9	NAG	k	2	9	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	l	1	1,9	14,14,15	0.30	0	17,19,21	0.63	1 (5%)
9	NAG	l	2	9	14,14,15	0.28	0	17,19,21	0.55	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
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	4/6/23/26	0/1/1/1
7	BMA	S	3	7	1/1/4/5	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	g	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	4/6/23/26	0/1/1/1
7	BMA	g	3	7	1/1/4/5	1/2/19/22	0/1/1/1
7	MAN	g	4	7	1/1/4/5	0/2/19/22	0/1/1/1
13	NAG	h	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	h	2	13	-	4/6/23/26	0/1/1/1
13	BMA	h	3	13	-	0/2/19/22	0/1/1/1
13	MAN	h	4	13	-	0/2/19/22	0/1/1/1
13	MAN	h	5	13	-	0/2/19/22	0/1/1/1
13	MAN	h	6	13	-	0/2/19/22	0/1/1/1
13	MAN	h	7	13	1/1/4/5	0/2/19/22	0/1/1/1
13	MAN	h	8	13	-	0/2/19/22	0/1/1/1
13	MAN	h	9	13	1/1/4/5	0/2/19/22	0/1/1/1
9	NAG	i	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	i	2	9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	j	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	j	2	9	-	2/6/23/26	0/1/1/1
9	NAG	k	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	k	2	9	1/1/5/7	2/6/23/26	0/1/1/1
9	NAG	l	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	l	2	9	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	6	MAN	C1-O5-C5	2.35	115.33	112.19
7	S	4	MAN	C1-O5-C5	2.29	115.25	112.19
12	a	5	MAN	C1-O5-C5	2.27	115.23	112.19
8	T	7	MAN	C1-C2-C3	2.25	112.92	109.64
12	a	4	MAN	C1-O5-C5	2.24	115.19	112.19
7	S	4	MAN	O2-C2-C3	-2.24	105.52	110.15
12	a	4	MAN	O2-C2-C3	-2.23	105.54	110.15
12	a	6	MAN	O2-C2-C3	-2.22	105.56	110.15
10	X	2	MAN	O2-C2-C3	-2.21	105.58	110.15
12	a	5	MAN	O2-C2-C3	-2.11	105.78	110.15
10	X	2	MAN	C1-O5-C5	2.06	114.95	112.19
9	Y	1	NAG	C1-O5-C5	2.03	114.91	112.19
9	f	1	NAG	C1-O5-C5	2.01	114.89	112.19
9	l	1	NAG	C1-O5-C5	2.01	114.88	112.19

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	S	3	BMA	C1
7	S	4	MAN	C1
7	g	3	BMA	C1
7	g	4	MAN	C1
8	T	4	MAN	C1
9	U	2	NAG	C1
9	V	2	NAG	C1
9	W	2	NAG	C1
9	b	2	NAG	C1
9	c	2	NAG	C1
9	d	2	NAG	C1
9	i	2	NAG	C1
9	k	2	NAG	C1
10	e	2	MAN	C1
11	Z	3	BMA	C1
12	a	7	MAN	C1
13	h	7	MAN	C1
13	h	9	MAN	C1

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	T	1	NAG	C4-C5-C6-O6
13	h	1	NAG	C4-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	j	2	NAG	O5-C5-C6-O6
9	k	2	NAG	O5-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
9	l	2	NAG	O5-C5-C6-O6
13	h	1	NAG	O5-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
12	a	1	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
11	Z	2	NAG	C4-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
11	Z	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	T	2	NAG	O5-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
12	a	2	NAG	O5-C5-C6-O6
13	h	2	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	d	1	NAG	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
11	Z	1	NAG	C4-C5-C6-O6
9	k	2	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
9	k	1	NAG	O5-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
9	k	1	NAG	C4-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
9	Y	2	NAG	C4-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
11	Z	2	NAG	O5-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	f	2	NAG	C4-C5-C6-O6
9	j	2	NAG	C4-C5-C6-O6
9	l	2	NAG	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
9	d	1	NAG	C4-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
12	a	2	NAG	C4-C5-C6-O6
13	h	2	NAG	C4-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6
9	f	1	NAG	C4-C5-C6-O6
9	l	1	NAG	O5-C5-C6-O6
9	l	1	NAG	C4-C5-C6-O6
7	g	3	BMA	O5-C5-C6-O6
10	e	2	MAN	O5-C5-C6-O6
8	T	7	MAN	O5-C5-C6-O6
11	Z	3	BMA	O5-C5-C6-O6
9	Y	1	NAG	C4-C5-C6-O6
9	Y	1	NAG	O5-C5-C6-O6
8	T	4	MAN	O5-C5-C6-O6
8	T	2	NAG	C1-C2-N2-C7
12	a	2	NAG	C1-C2-N2-C7
13	h	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

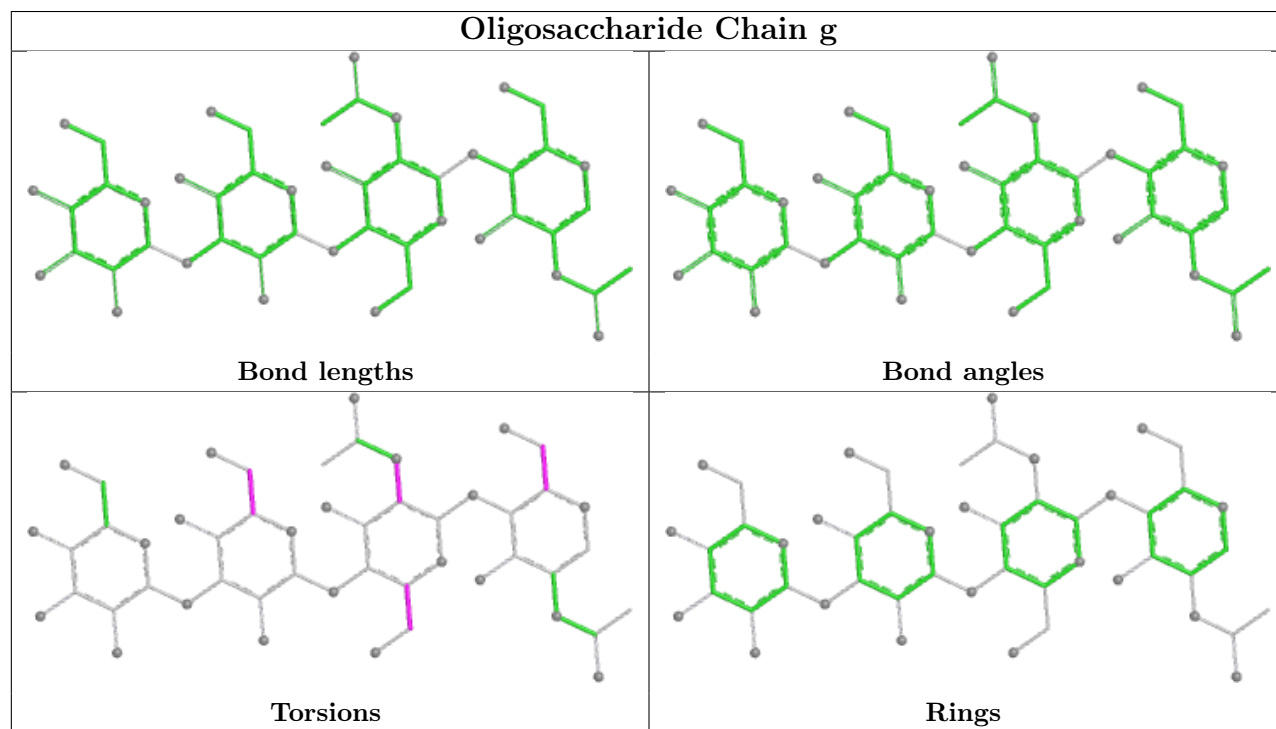
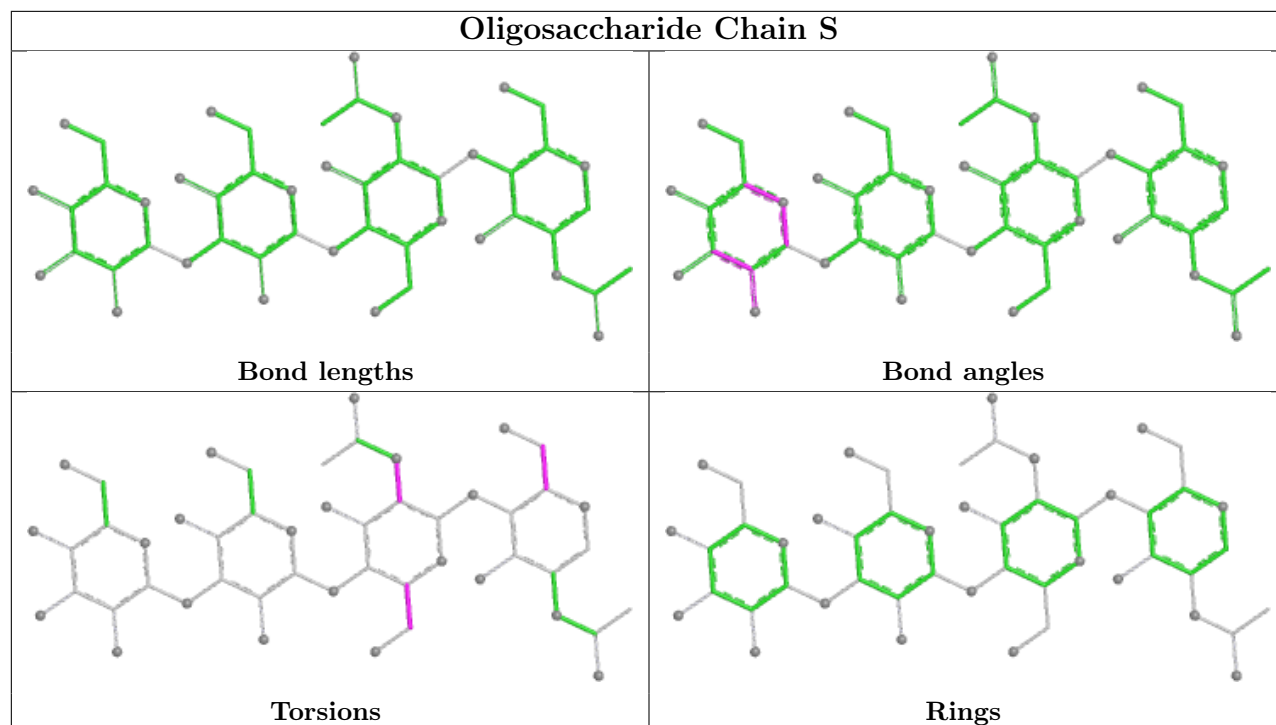
Mol	Chain	Res	Type	Atoms
7	S	2	NAG	C3-C2-N2-C7
7	g	2	NAG	C3-C2-N2-C7
9	Y	2	NAG	C3-C2-N2-C7
9	f	2	NAG	C3-C2-N2-C7
9	l	2	NAG	C3-C2-N2-C7
11	Z	2	NAG	C3-C2-N2-C7
7	S	2	NAG	C1-C2-N2-C7
7	g	2	NAG	C1-C2-N2-C7
9	Y	2	NAG	C1-C2-N2-C7
9	f	2	NAG	C1-C2-N2-C7
9	l	2	NAG	C1-C2-N2-C7
11	Z	2	NAG	C1-C2-N2-C7
8	T	2	NAG	C3-C2-N2-C7
12	a	2	NAG	C3-C2-N2-C7
13	h	2	NAG	C3-C2-N2-C7
9	U	2	NAG	C4-C5-C6-O6

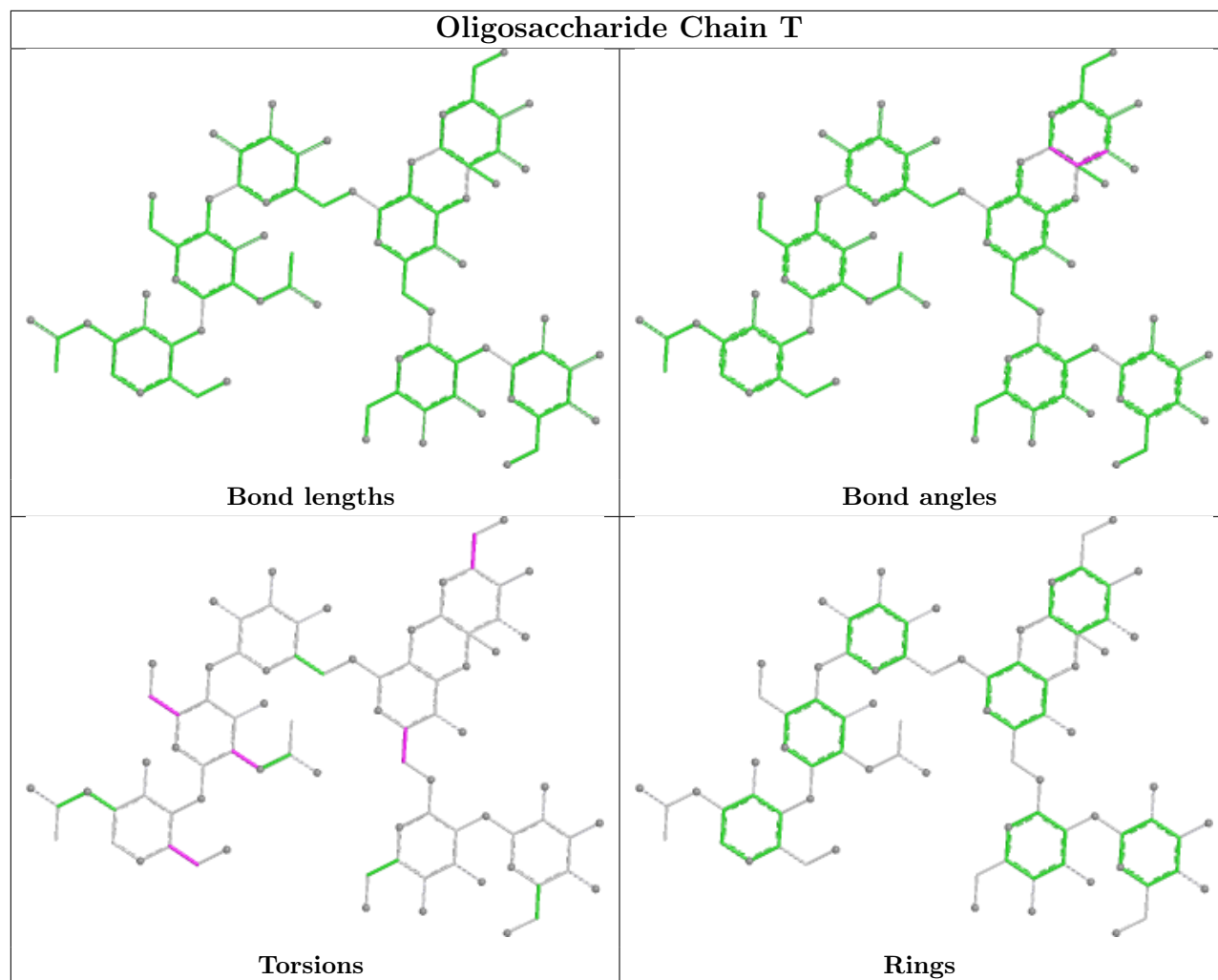
There are no ring outliers.

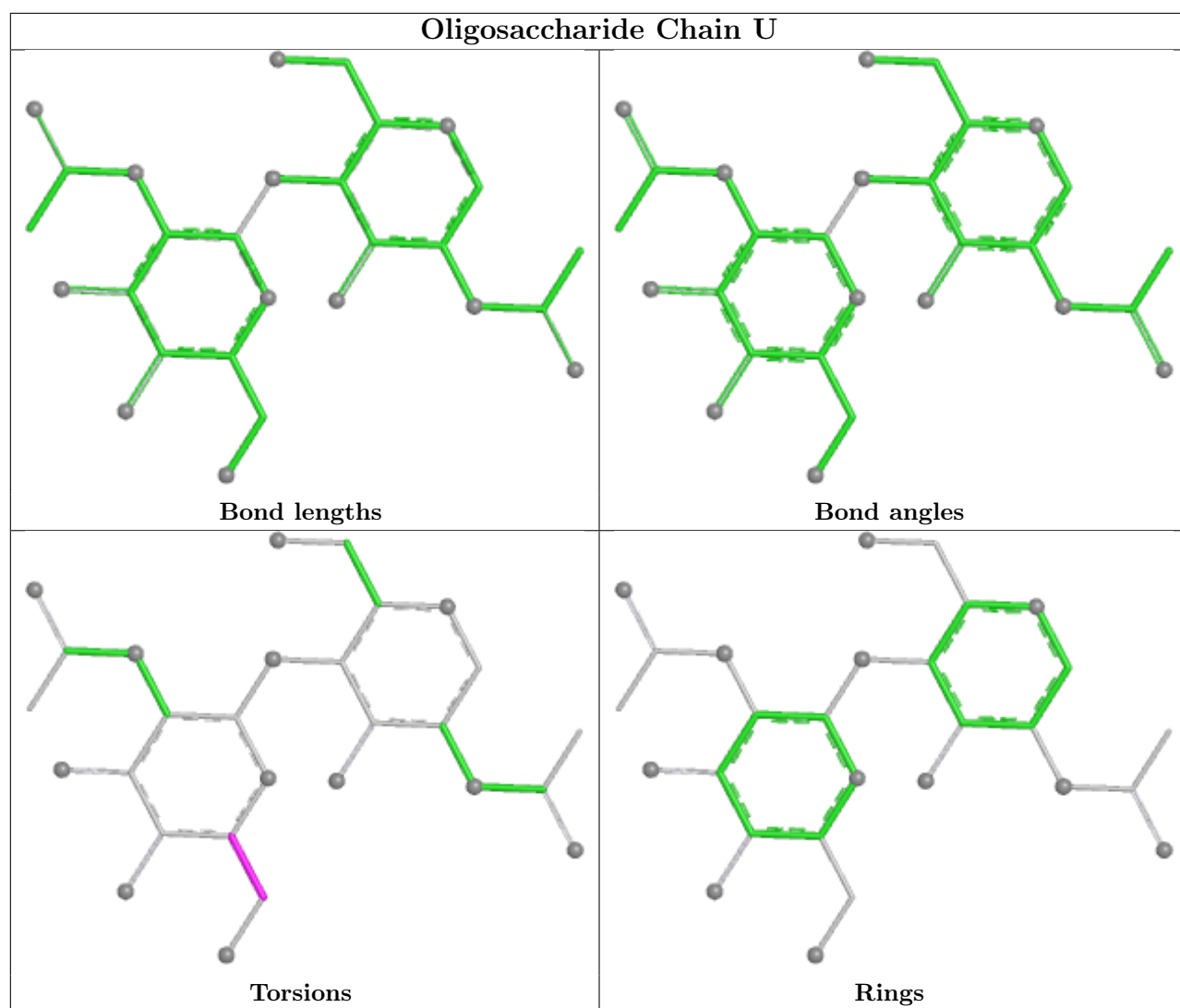
16 monomers are involved in 52 short contacts:

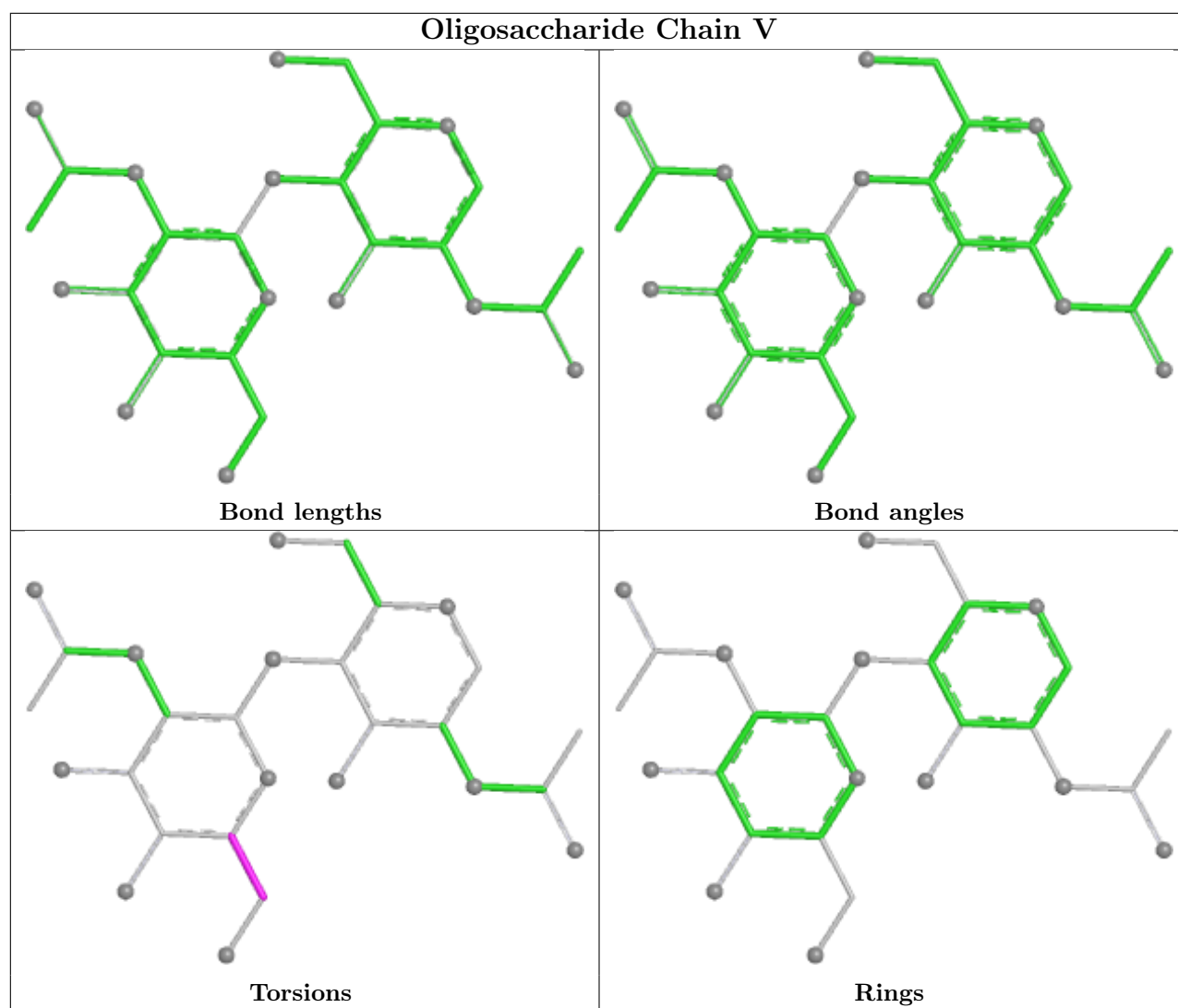
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	3	BMA	4	0
13	h	4	MAN	7	0
7	g	3	BMA	2	0
11	Z	3	BMA	10	0
7	S	3	BMA	4	0
10	X	1	MAN	4	0
12	a	7	MAN	1	0
12	a	4	MAN	1	0
13	h	3	BMA	1	0
13	h	7	MAN	7	0
10	e	1	MAN	10	0
12	a	3	BMA	8	0
13	h	8	MAN	7	0
10	e	2	MAN	3	0
13	h	9	MAN	2	0
8	T	4	MAN	2	0

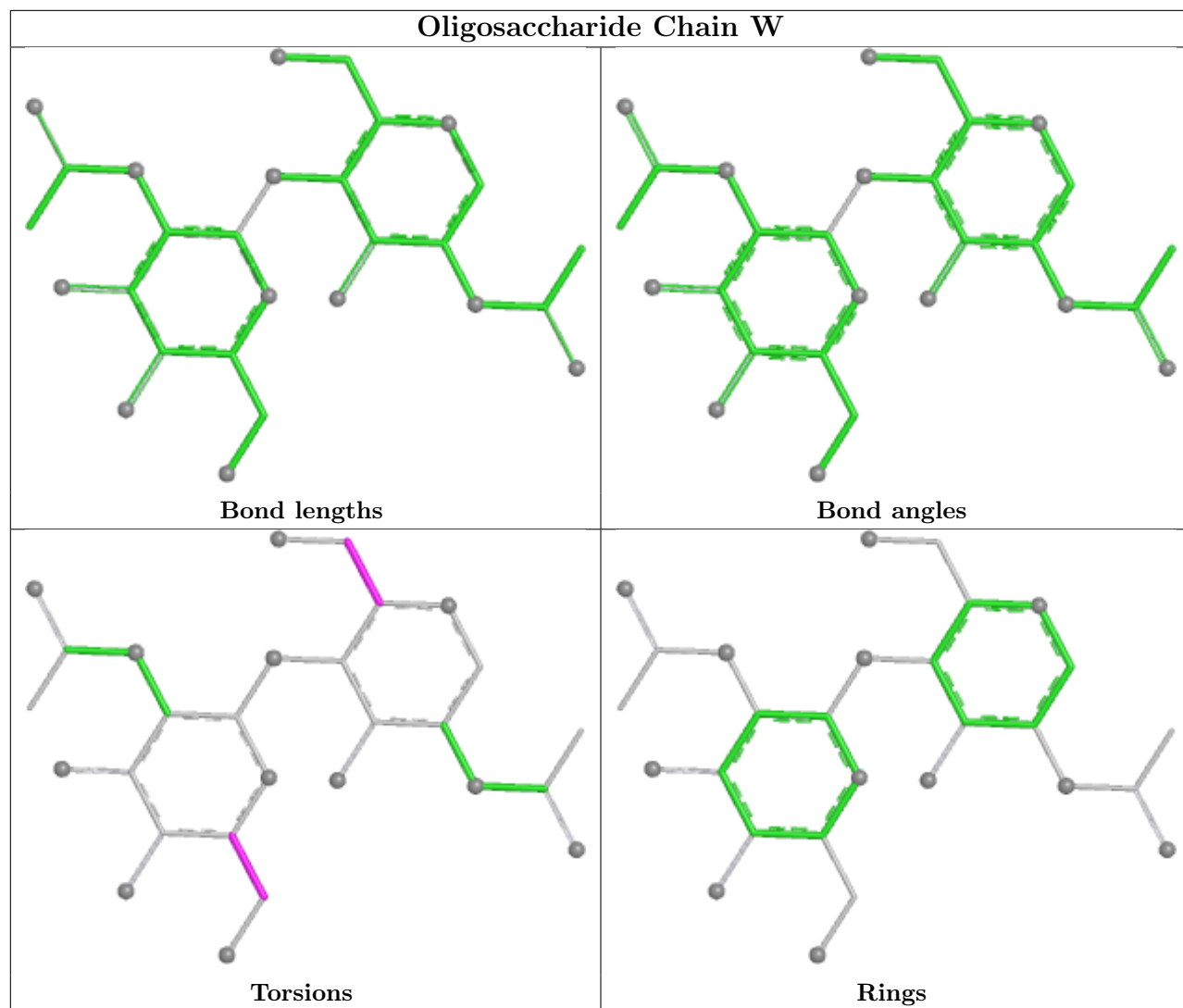
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

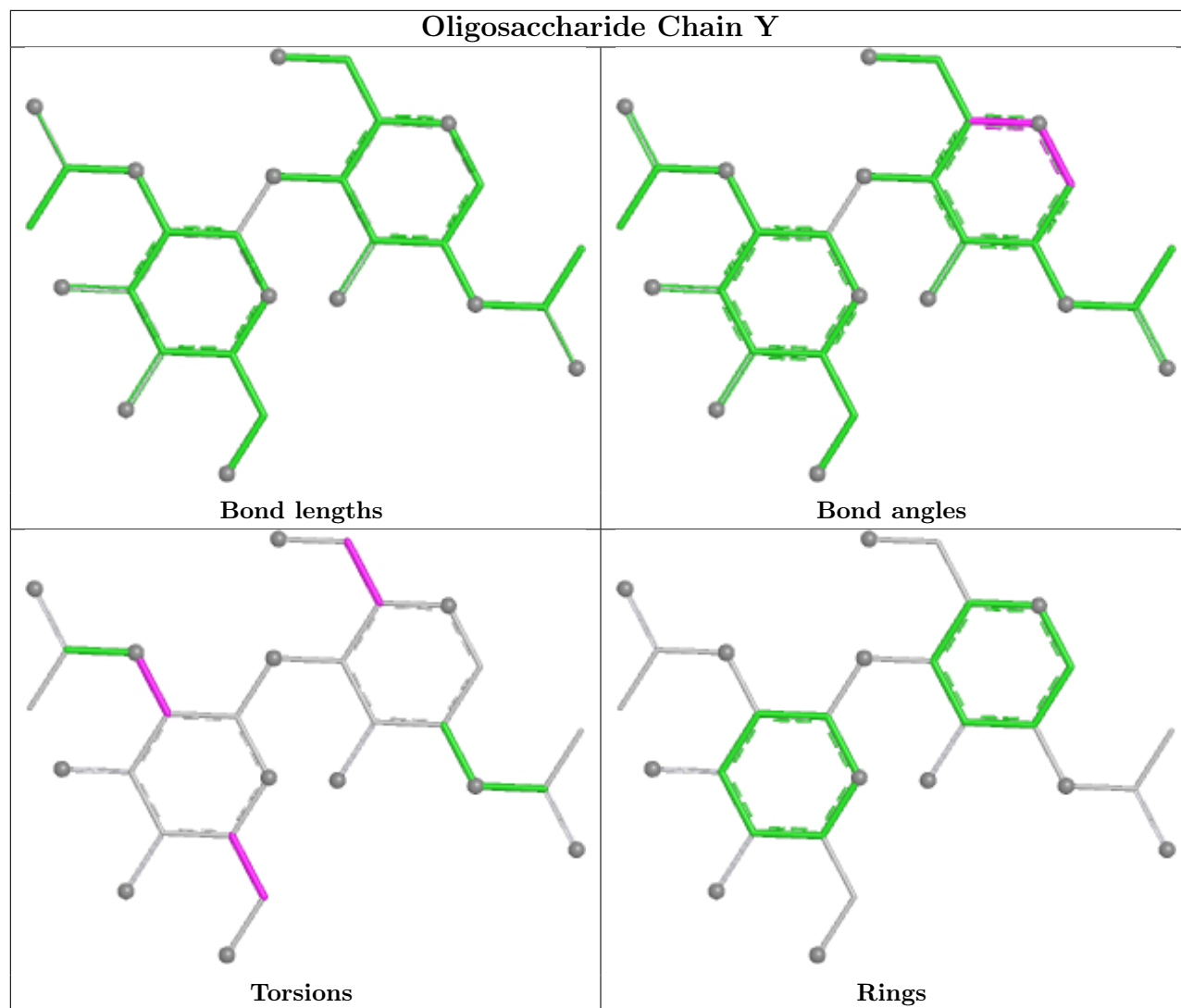


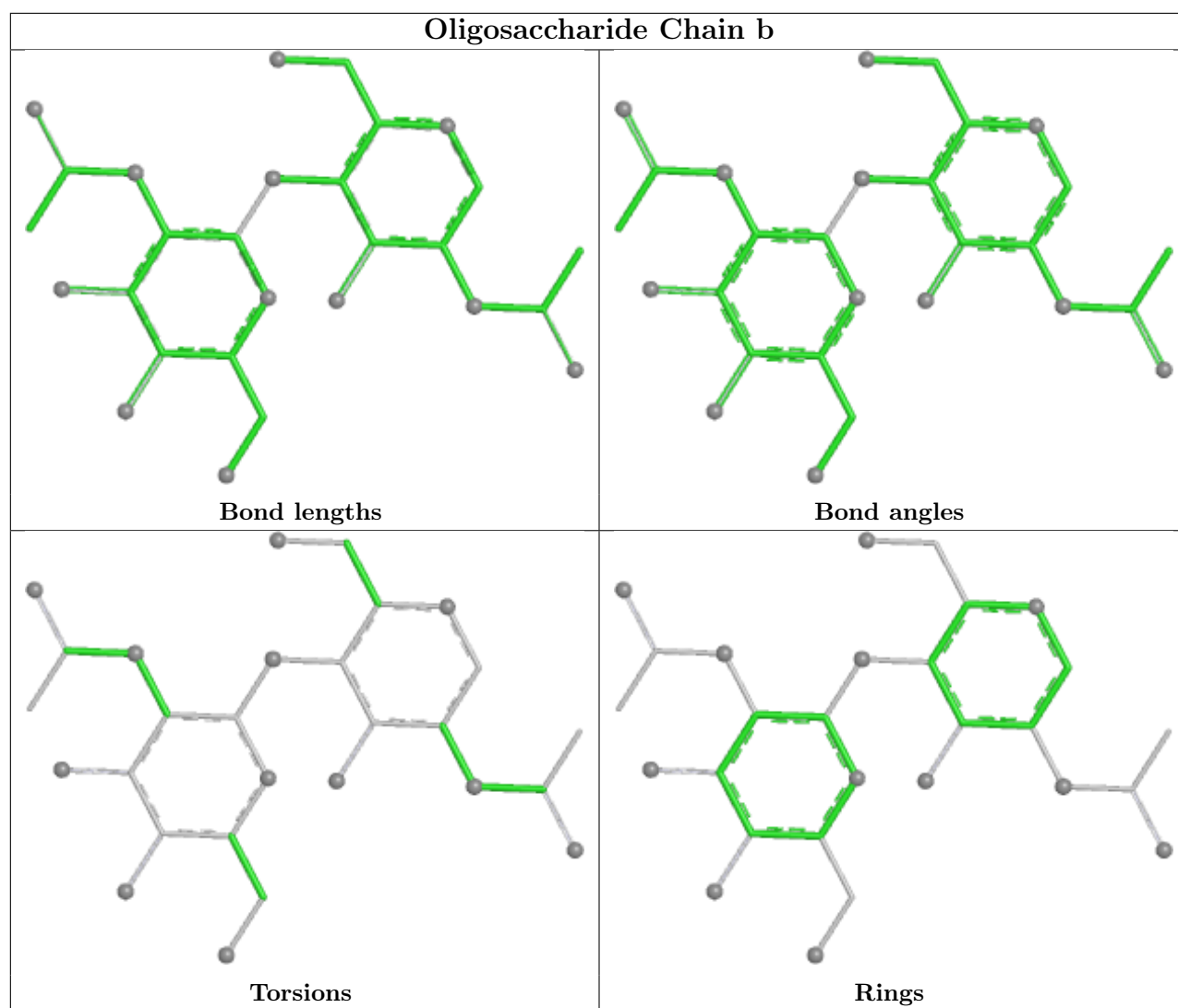


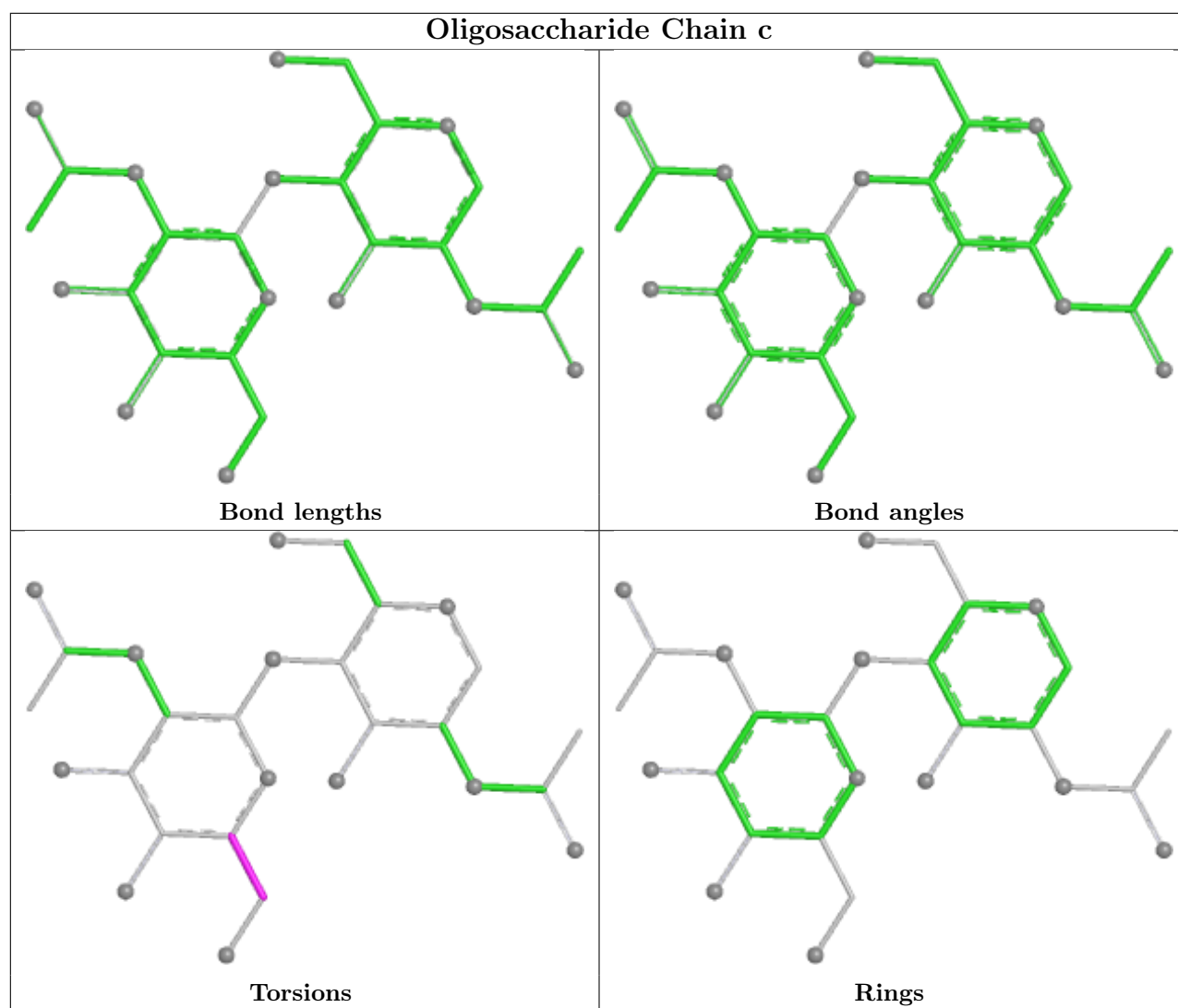


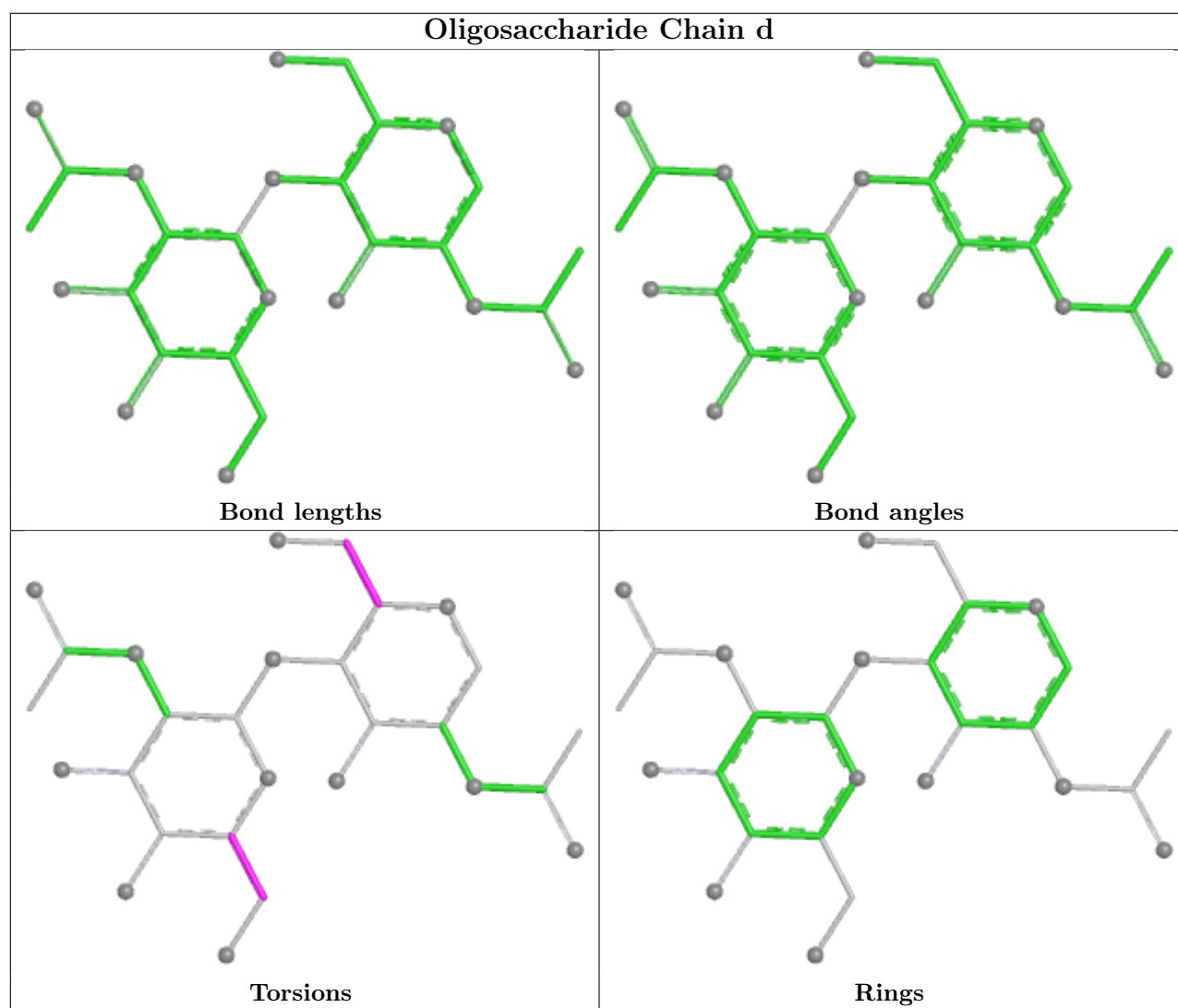


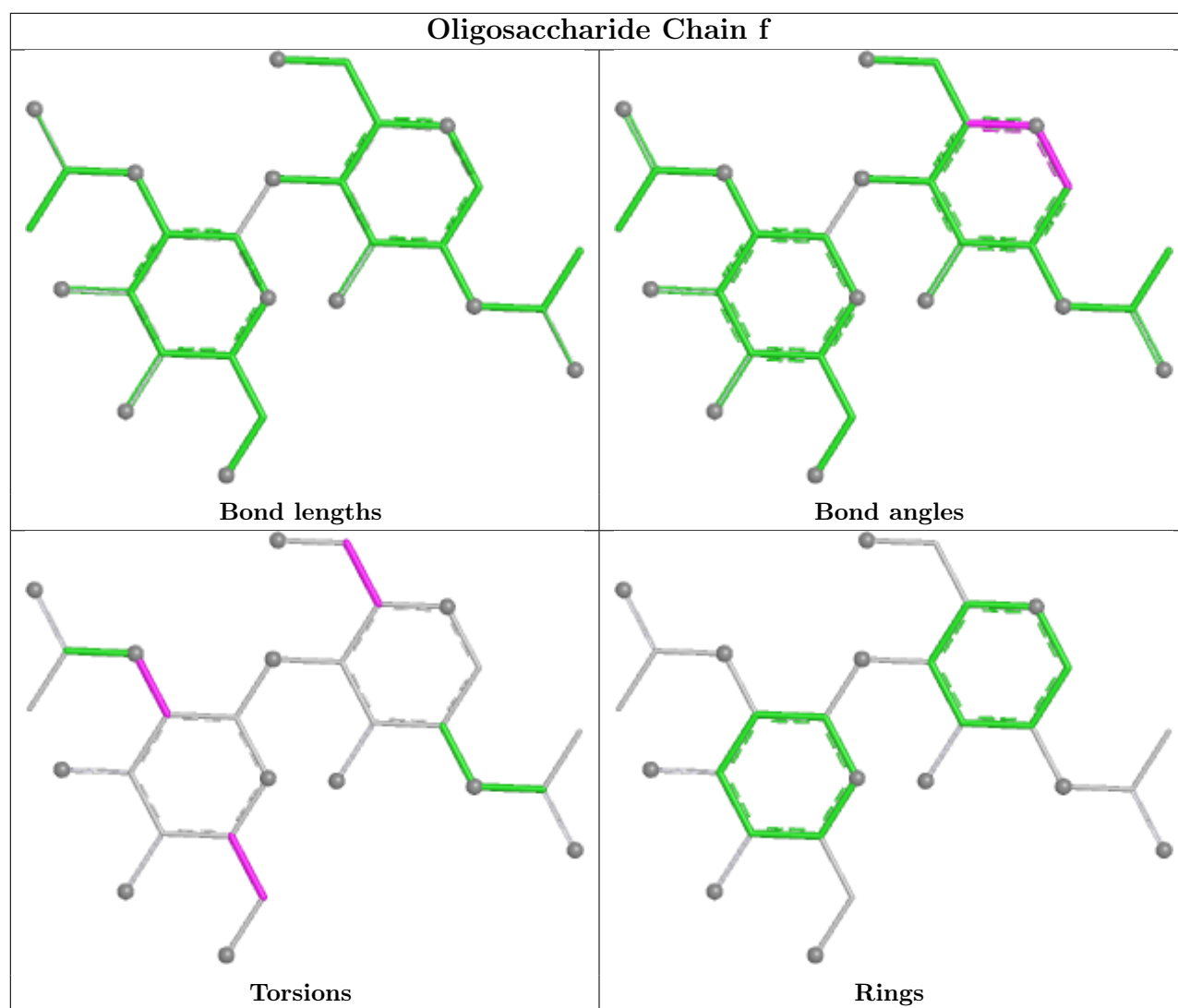


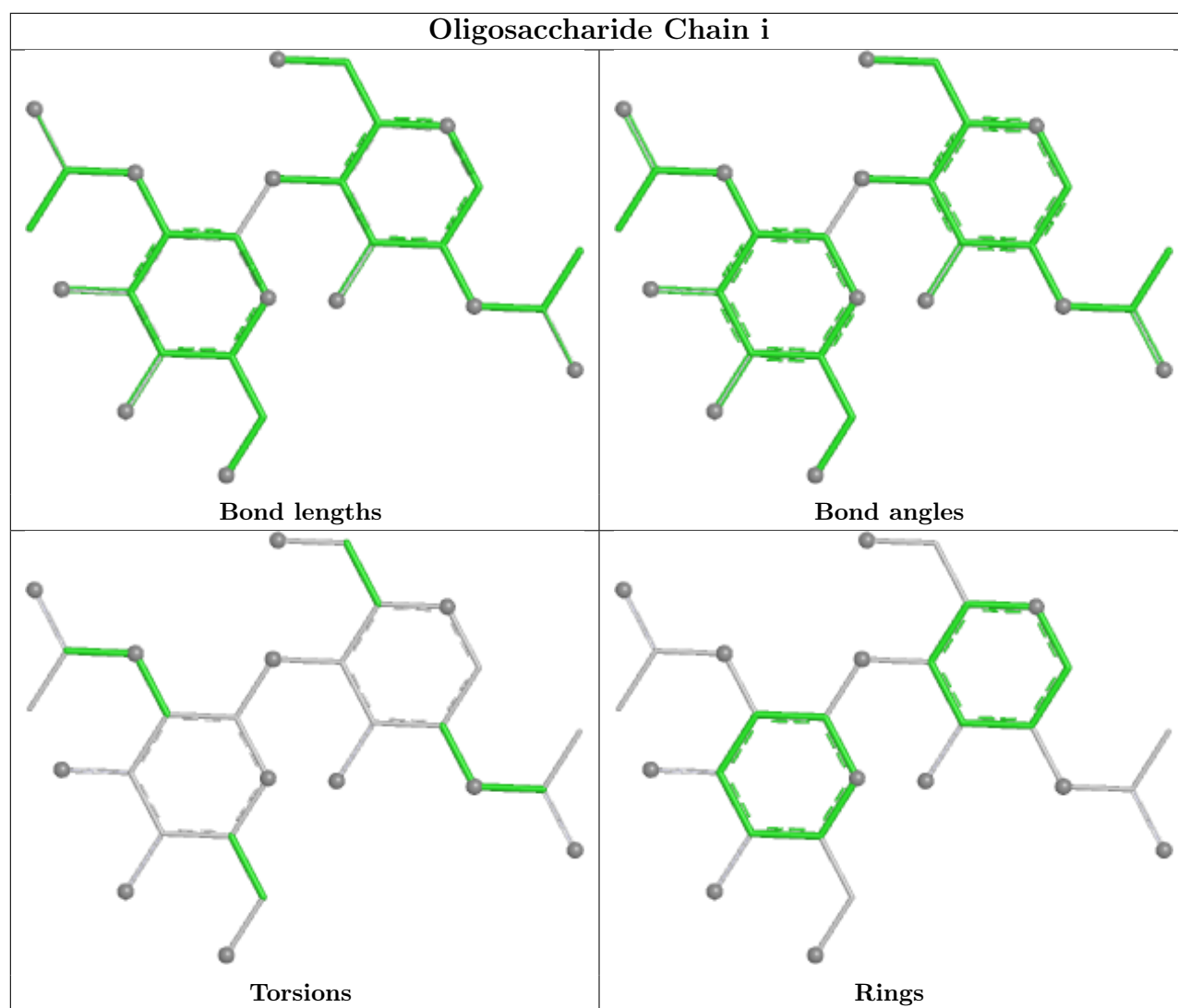


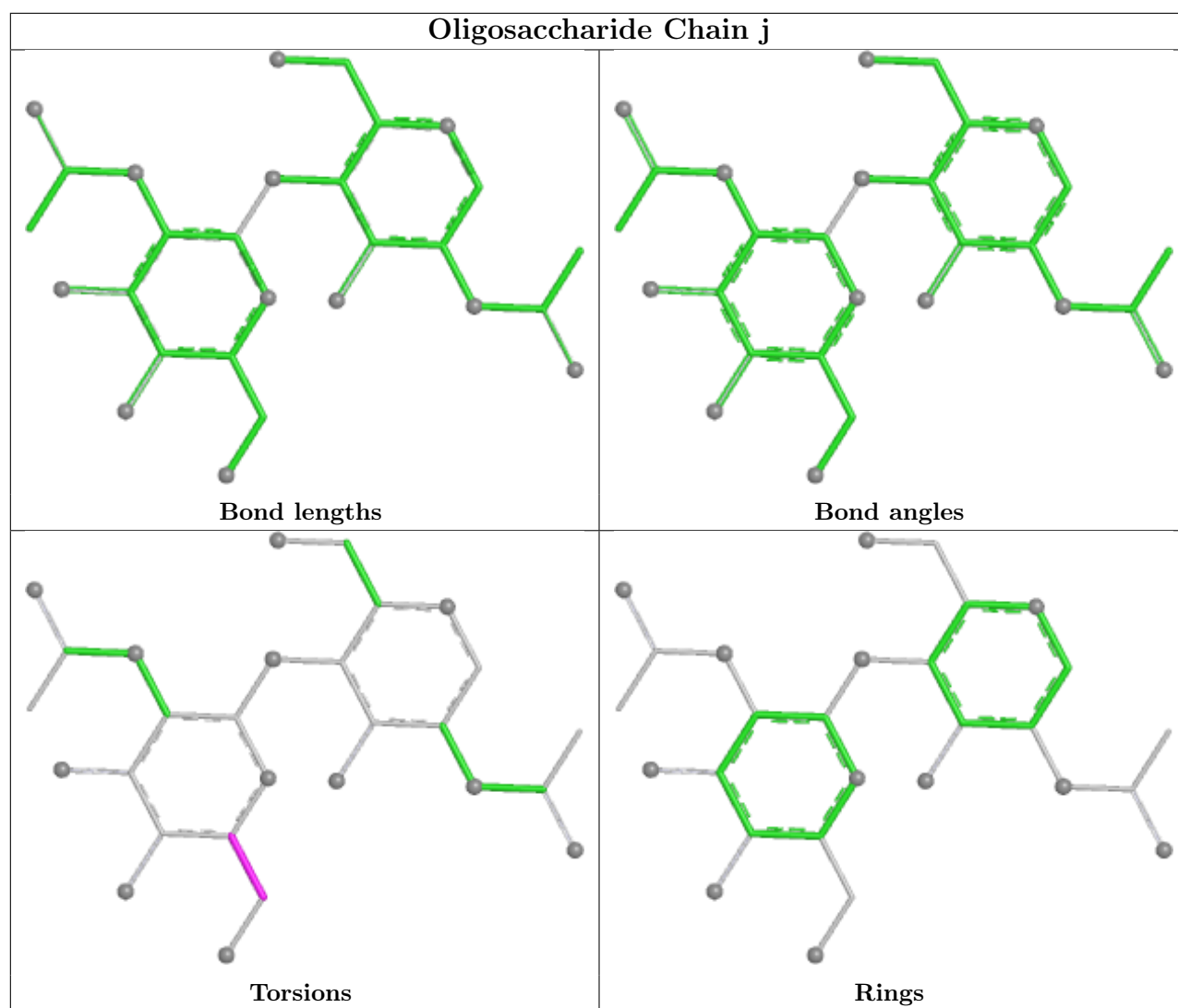


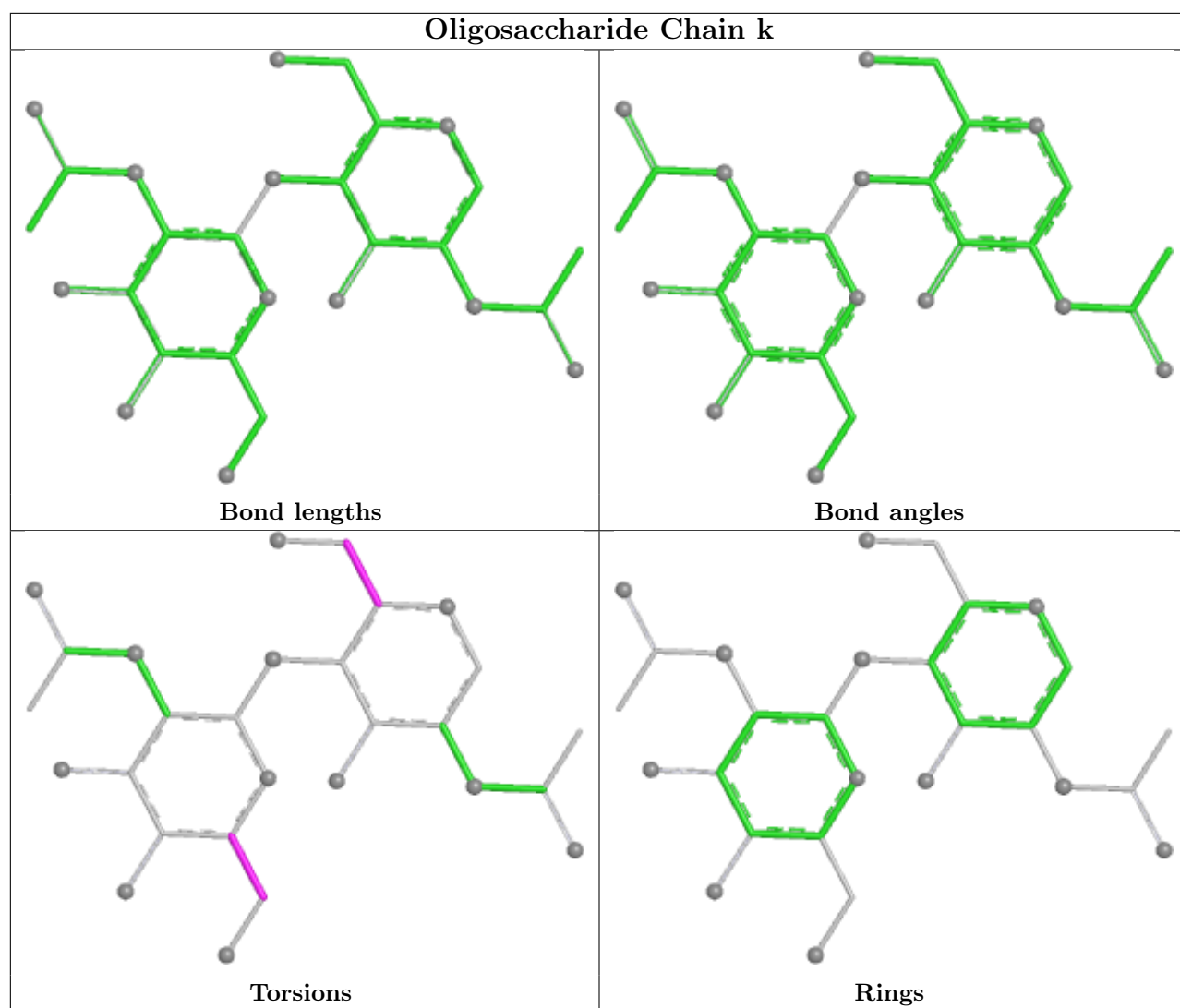


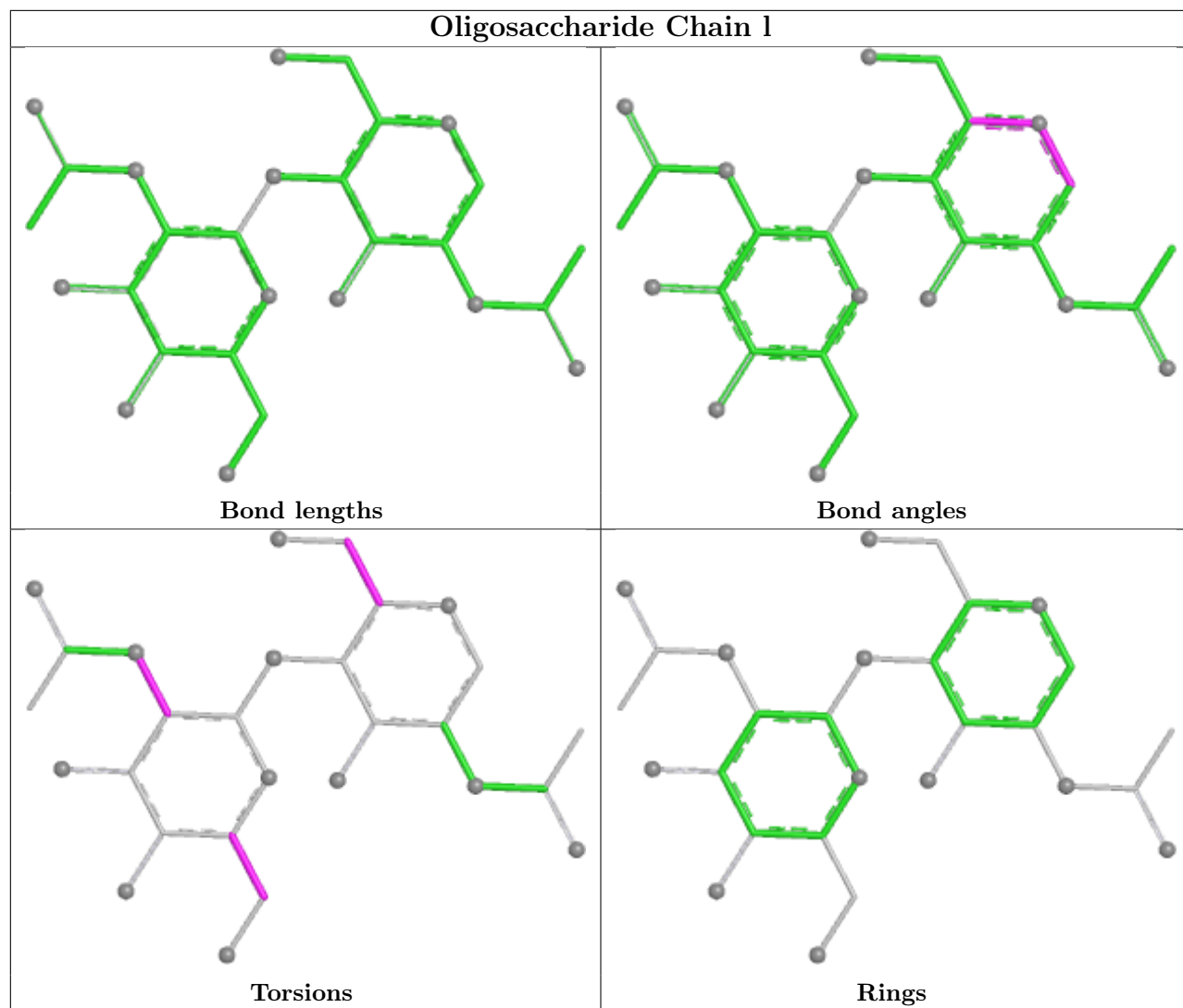


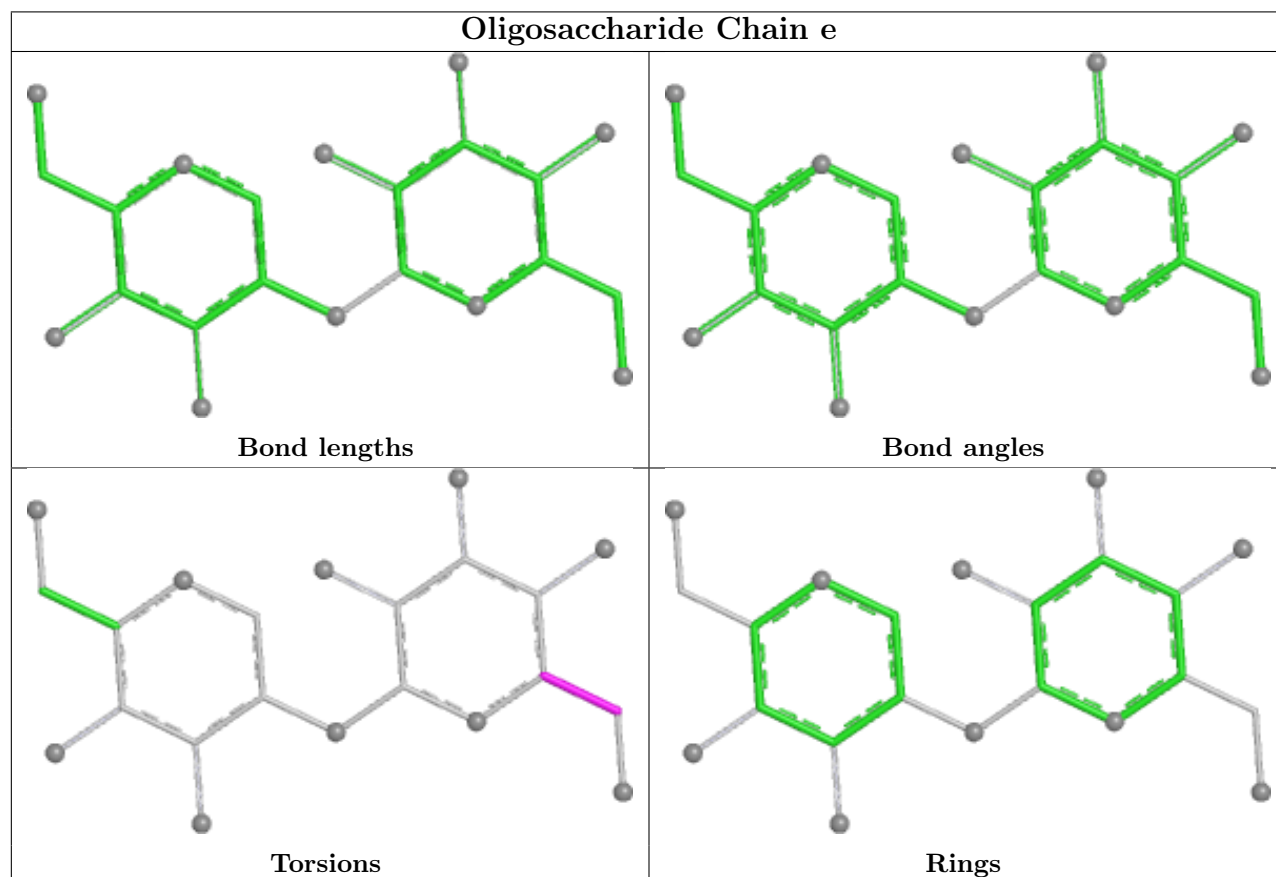
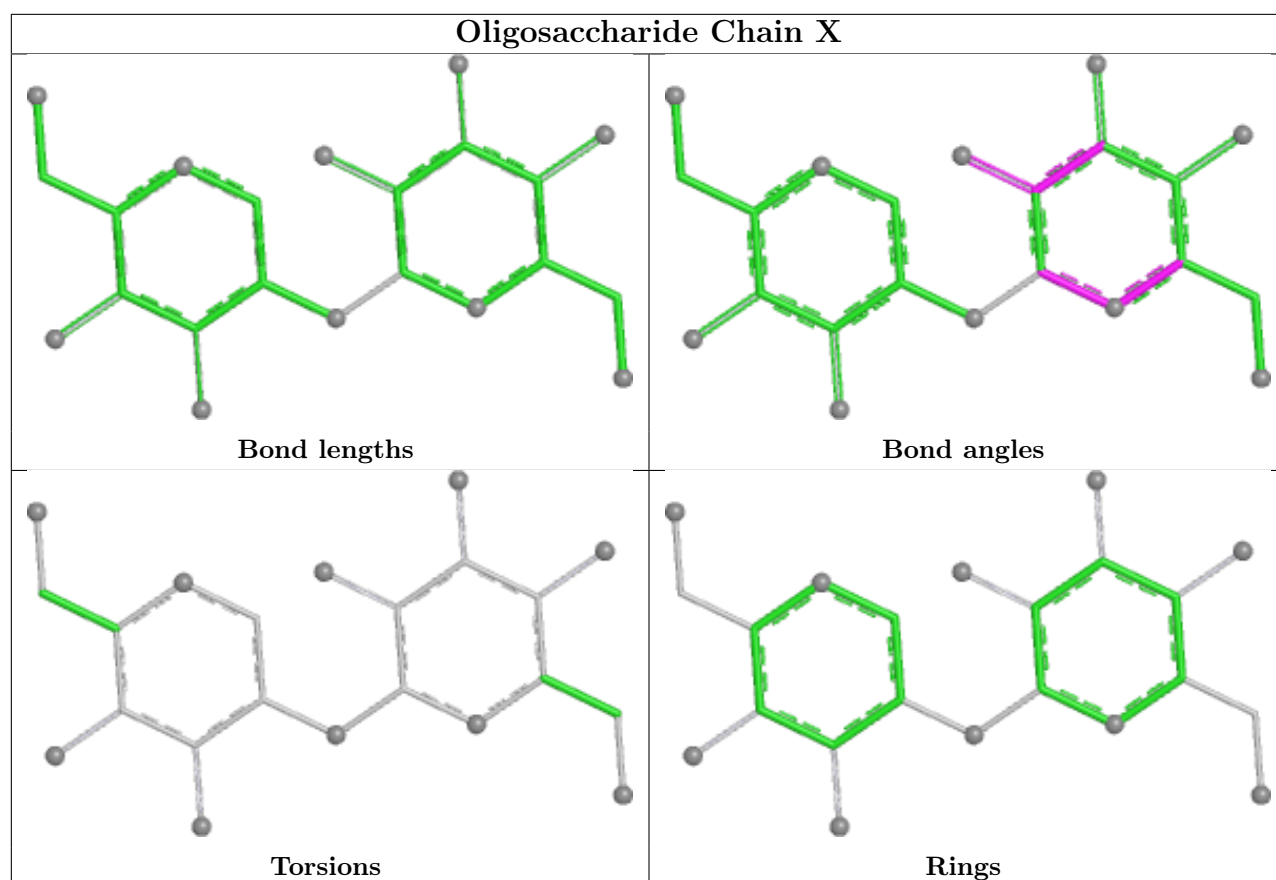


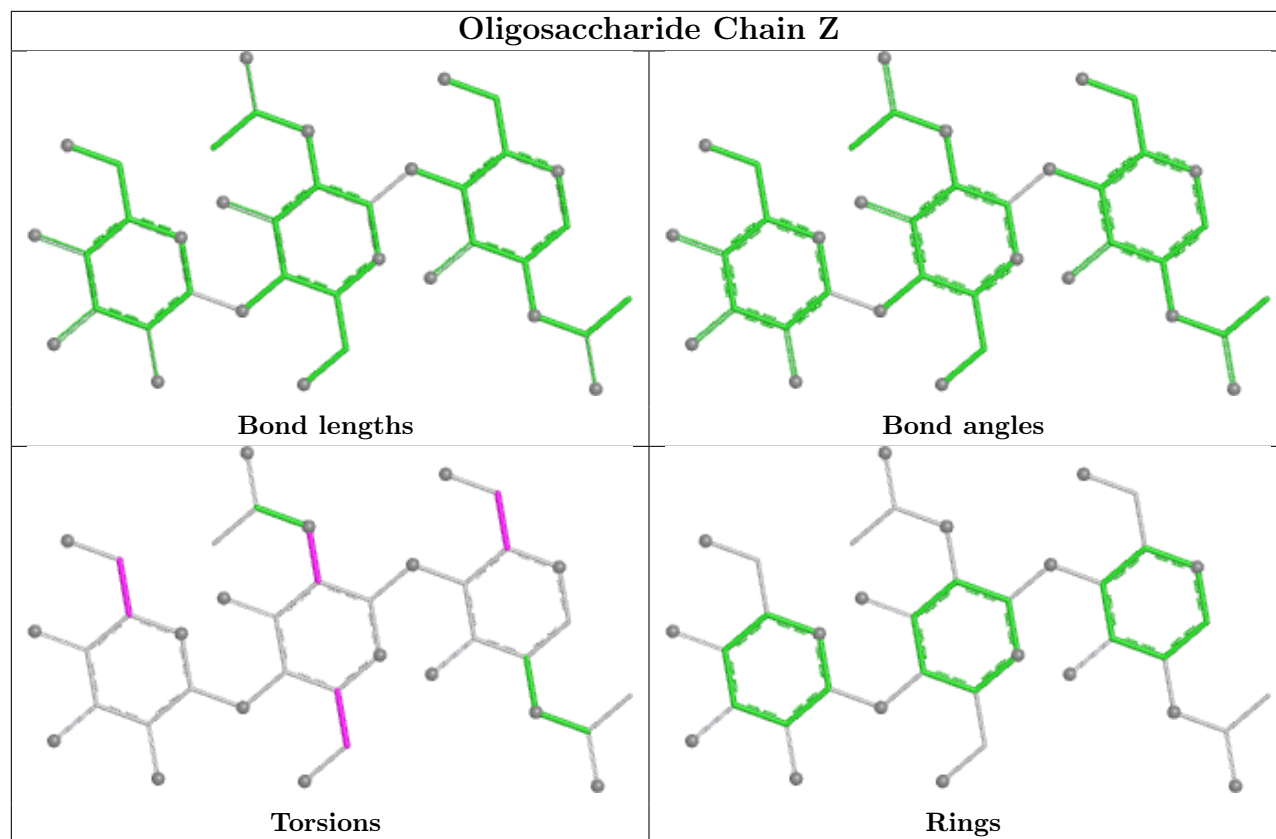


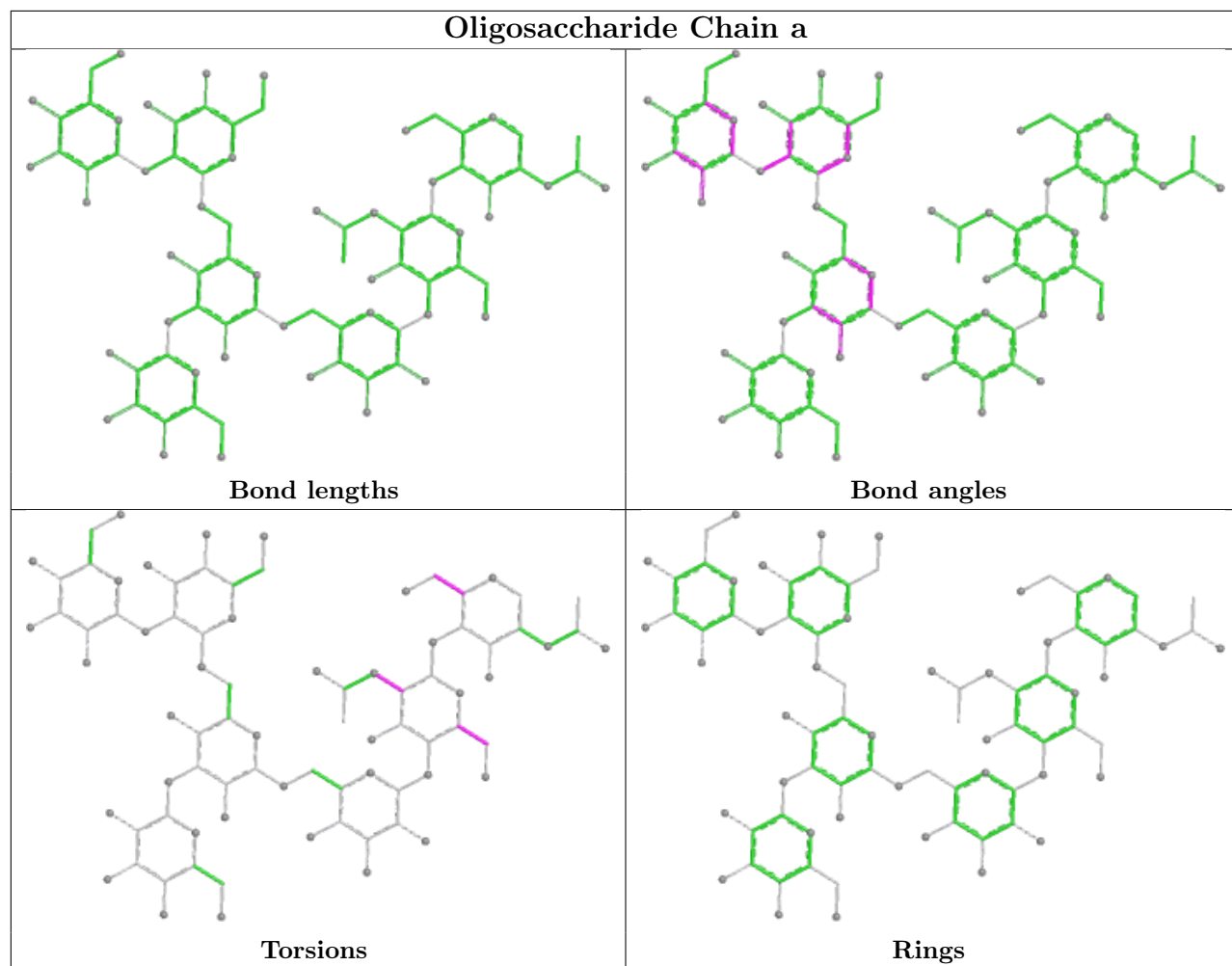


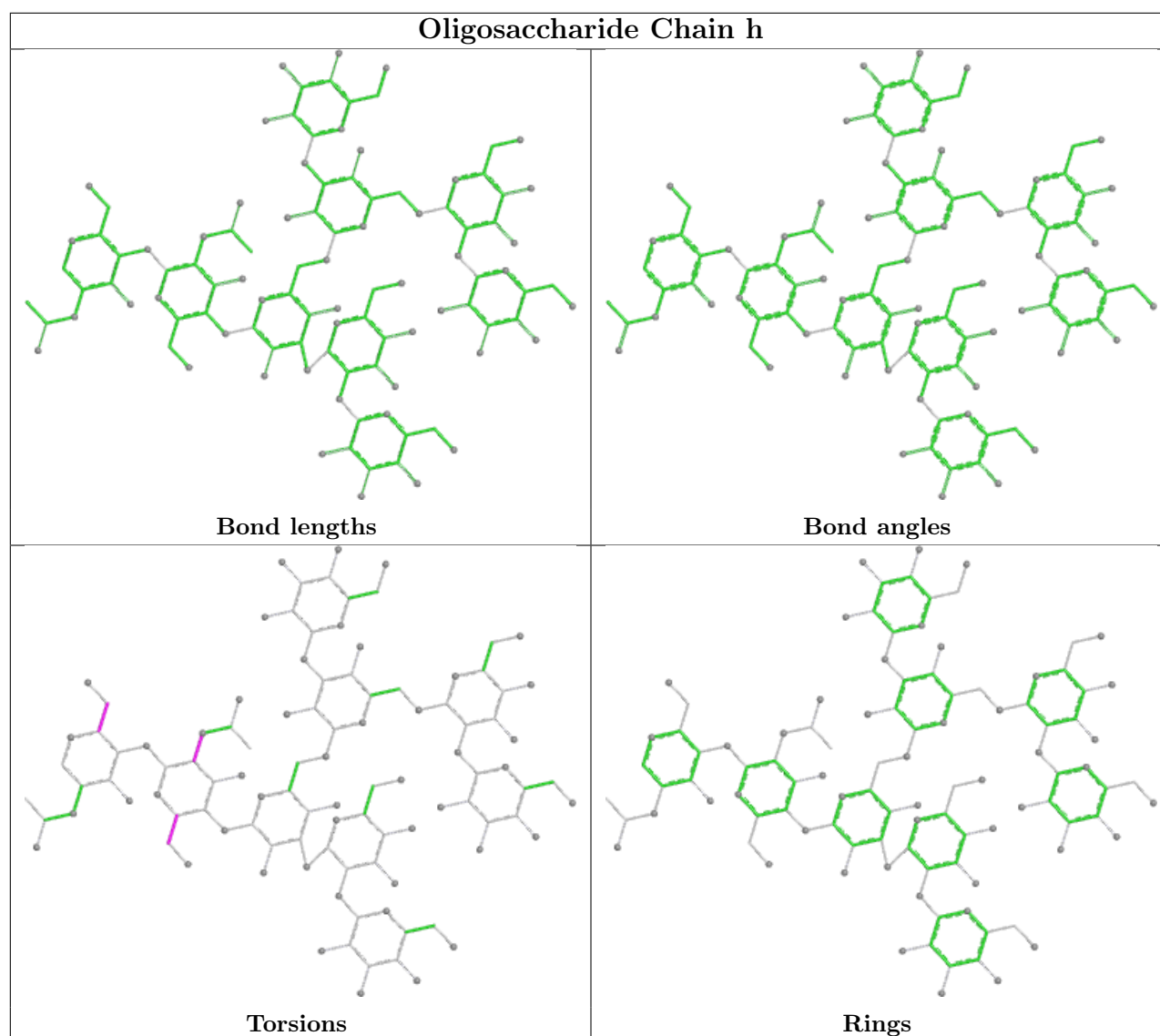












5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
15	MAN	A	607	-	11,11,12	0.29	0	15,15,17	0.92	1 (6%)
14	NAG	C	603	1	14,14,15	0.19	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	604	1	14,14,15	0.19	0	17,19,21	0.48	0
14	NAG	B	606	1	14,14,15	0.24	0	17,19,21	0.46	0
14	NAG	C	604	1	14,14,15	0.22	0	17,19,21	0.46	0
15	MAN	B	601	-	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
14	NAG	B	607	1	14,14,15	0.24	0	17,19,21	0.45	0
14	NAG	E	701	2	14,14,15	0.21	0	17,19,21	0.39	0
14	NAG	B	603	1	14,14,15	0.21	0	17,19,21	0.46	0
14	NAG	A	602	1	14,14,15	0.21	0	17,19,21	0.46	0
14	NAG	A	603	1	14,14,15	0.18	0	17,19,21	0.48	0
15	MAN	C	606	-	11,11,12	0.23	0	15,15,17	0.50	0
14	NAG	A	606	1	14,14,15	0.25	0	17,19,21	0.44	0
14	NAG	C	605	1	14,14,15	0.25	0	17,19,21	0.45	0
15	MAN	B	608	-	11,11,12	0.30	0	15,15,17	0.91	1 (6%)
14	NAG	C	602	1	14,14,15	0.22	0	17,19,21	0.45	0
14	NAG	A	604	1	14,14,15	0.22	0	17,19,21	0.46	0
14	NAG	A	601	1	14,14,15	0.18	0	17,19,21	0.44	0
14	NAG	C	607	1	14,14,15	0.29	0	17,19,21	0.50	0
14	NAG	B	605	1	14,14,15	0.21	0	17,19,21	0.46	0
14	NAG	D	701	2	14,14,15	0.23	0	17,19,21	0.40	0
14	NAG	A	605	1	14,14,15	0.26	0	17,19,21	0.47	0
14	NAG	F	701	2	14,14,15	0.26	0	17,19,21	0.49	0
14	NAG	B	602	1	14,14,15	0.20	0	17,19,21	0.44	0
14	NAG	C	601	1	14,14,15	0.19	0	17,19,21	0.44	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
15	MAN	A	607	-	-	1/2/19/22	0/1/1/1
14	NAG	C	603	1	-	0/6/23/26	0/1/1/1
14	NAG	B	604	1	-	0/6/23/26	0/1/1/1
14	NAG	B	606	1	-	2/6/23/26	0/1/1/1
14	NAG	C	604	1	-	2/6/23/26	0/1/1/1
15	MAN	B	601	-	-	0/2/19/22	0/1/1/1
14	NAG	B	607	1	-	2/6/23/26	0/1/1/1
14	NAG	E	701	2	-	2/6/23/26	0/1/1/1
14	NAG	B	603	1	-	2/6/23/26	0/1/1/1
14	NAG	A	602	1	-	2/6/23/26	0/1/1/1
14	NAG	A	603	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MAN	C	606	-	-	1/2/19/22	0/1/1/1
14	NAG	A	606	1	-	2/6/23/26	0/1/1/1
14	NAG	C	605	1	-	2/6/23/26	0/1/1/1
15	MAN	B	608	-	-	1/2/19/22	0/1/1/1
14	NAG	C	602	1	-	2/6/23/26	0/1/1/1
14	NAG	A	604	1	-	2/6/23/26	0/1/1/1
14	NAG	A	601	1	-	0/6/23/26	0/1/1/1
14	NAG	C	607	1	-	4/6/23/26	0/1/1/1
14	NAG	B	605	1	-	2/6/23/26	0/1/1/1
14	NAG	D	701	2	-	2/6/23/26	0/1/1/1
14	NAG	A	605	1	-	2/6/23/26	0/1/1/1
14	NAG	F	701	2	-	2/6/23/26	0/1/1/1
14	NAG	B	602	1	-	0/6/23/26	0/1/1/1
14	NAG	C	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	607	MAN	C1-C2-C3	2.28	112.97	109.64
15	B	601	MAN	C1-O5-C5	2.27	115.23	112.19
15	B	608	MAN	C1-C2-C3	2.23	112.89	109.64
15	B	601	MAN	O2-C2-C3	-2.22	105.55	110.15

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	607	NAG	C3-C2-N2-C7
14	B	607	NAG	C4-C5-C6-O6
14	C	605	NAG	C4-C5-C6-O6
14	A	606	NAG	C4-C5-C6-O6
14	B	606	NAG	O5-C5-C6-O6
14	C	605	NAG	O5-C5-C6-O6
14	B	607	NAG	O5-C5-C6-O6
14	A	605	NAG	O5-C5-C6-O6
14	A	602	NAG	C4-C5-C6-O6
14	B	603	NAG	C4-C5-C6-O6
14	C	602	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	606	NAG	O5-C5-C6-O6
14	C	607	NAG	C8-C7-N2-C2
14	C	607	NAG	O7-C7-N2-C2
14	A	602	NAG	O5-C5-C6-O6
14	E	701	NAG	O5-C5-C6-O6
14	F	701	NAG	O5-C5-C6-O6
14	B	606	NAG	C4-C5-C6-O6
14	A	604	NAG	O5-C5-C6-O6
14	B	603	NAG	O5-C5-C6-O6
14	B	605	NAG	O5-C5-C6-O6
14	C	602	NAG	O5-C5-C6-O6
14	A	605	NAG	C4-C5-C6-O6
14	C	604	NAG	O5-C5-C6-O6
14	D	701	NAG	O5-C5-C6-O6
14	E	701	NAG	C4-C5-C6-O6
14	F	701	NAG	C4-C5-C6-O6
14	A	604	NAG	C4-C5-C6-O6
14	D	701	NAG	C4-C5-C6-O6
15	B	608	MAN	O5-C5-C6-O6
15	C	606	MAN	O5-C5-C6-O6
15	A	607	MAN	O5-C5-C6-O6
14	C	604	NAG	C4-C5-C6-O6
14	C	607	NAG	O5-C5-C6-O6
14	B	605	NAG	C4-C5-C6-O6
14	C	601	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	607	MAN	4	0
15	B	601	MAN	4	0
15	C	606	MAN	2	0
15	B	608	MAN	6	0
14	C	607	NAG	2	0
14	A	605	NAG	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	E	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	546:SER	C	565:LEU	N	27.68
1	E	546:SER	C	565:LEU	N	27.64
1	F	546:SER	C	565:LEU	N	27.60

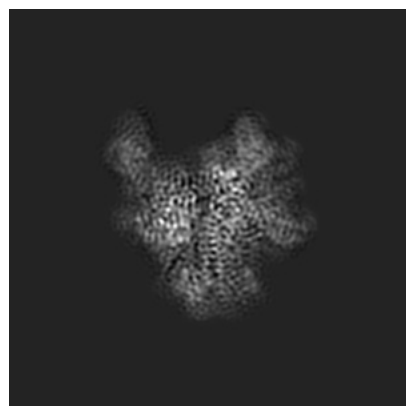
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26492. These allow visual inspection of the internal detail of the map and identification of artifacts.

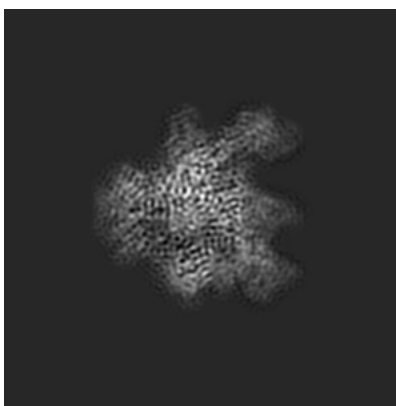
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

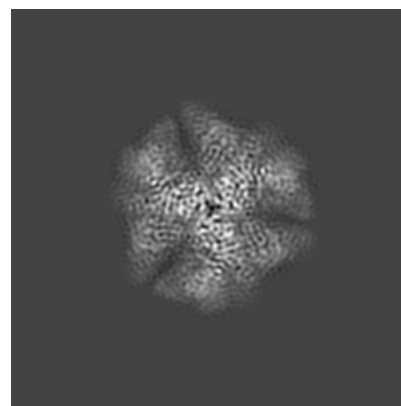
6.1.1 Primary map



X

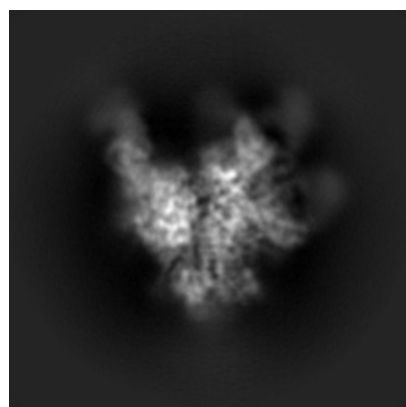


Y

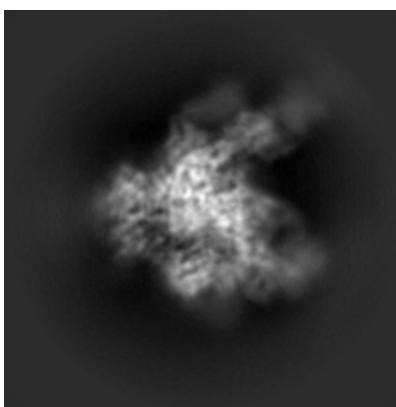


Z

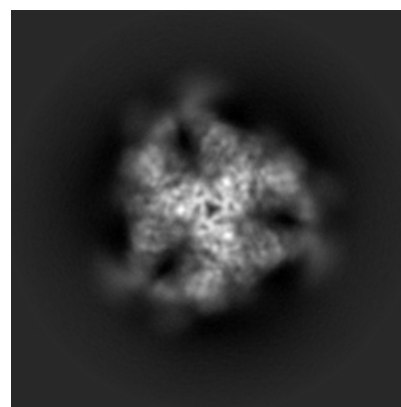
6.1.2 Raw map



X



Y

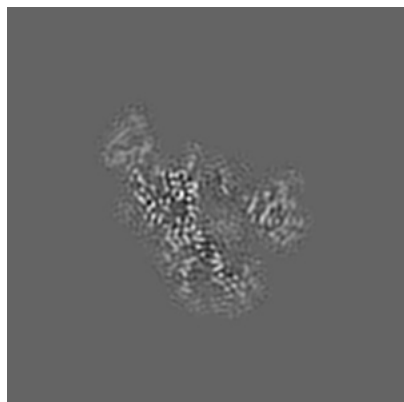


Z

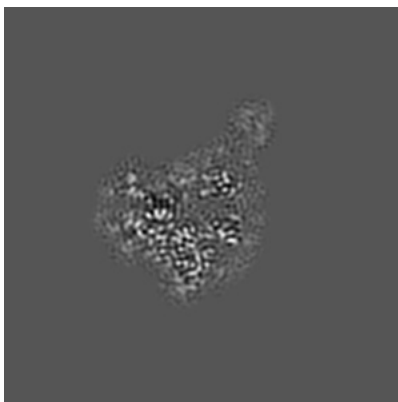
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

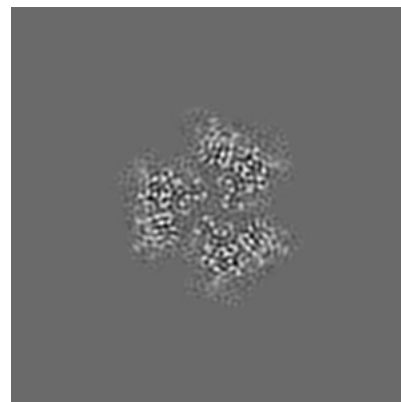
6.2.1 Primary map



X Index: 128

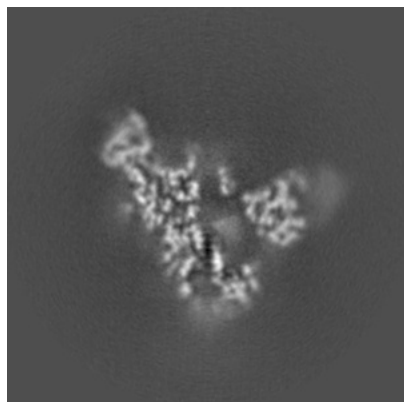


Y Index: 128

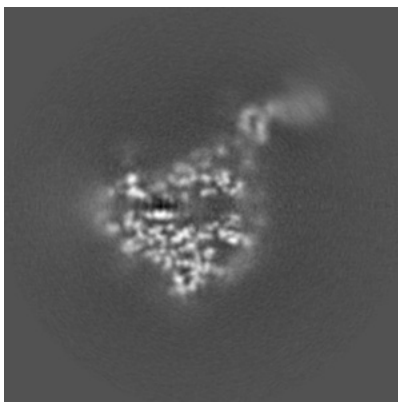


Z Index: 128

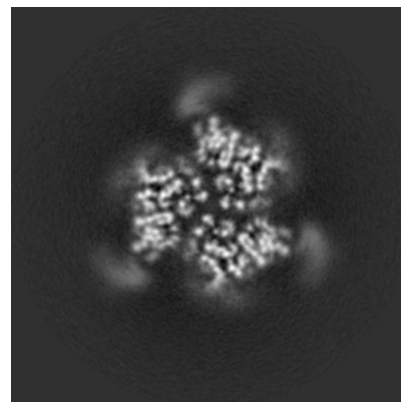
6.2.2 Raw map



X Index: 128



Y Index: 128

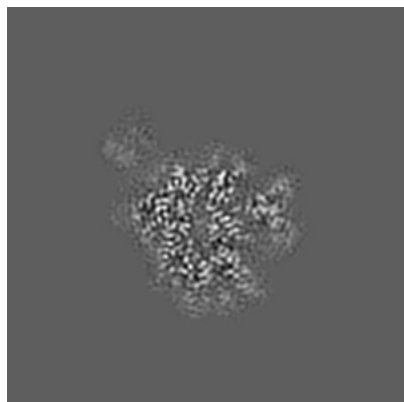


Z Index: 128

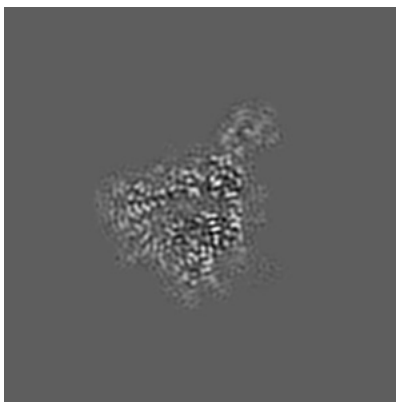
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

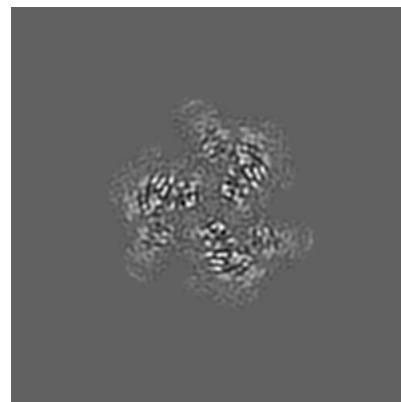
6.3.1 Primary map



X Index: 136

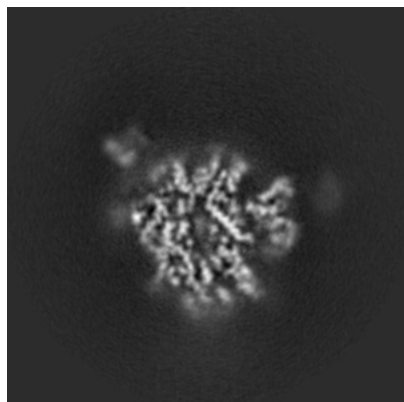


Y Index: 136

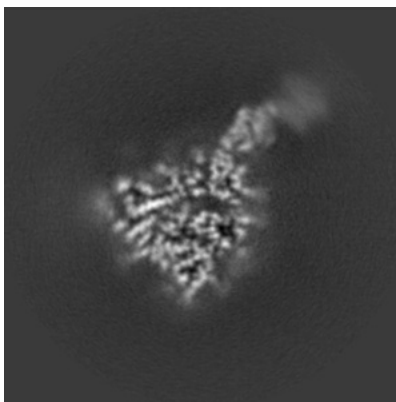


Z Index: 120

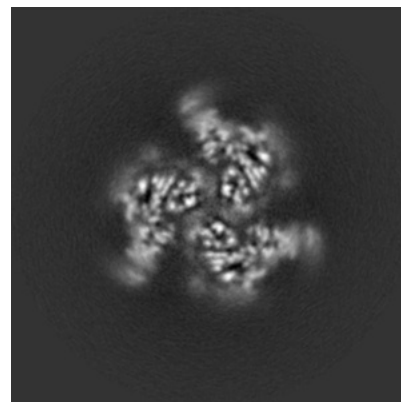
6.3.2 Raw map



X Index: 137



Y Index: 134

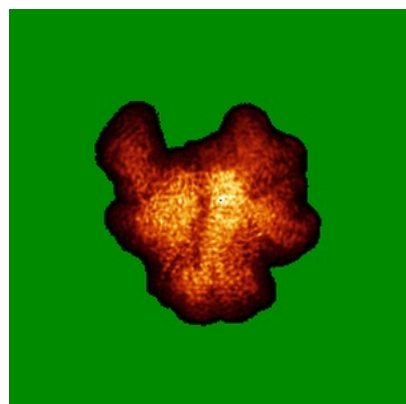


Z Index: 119

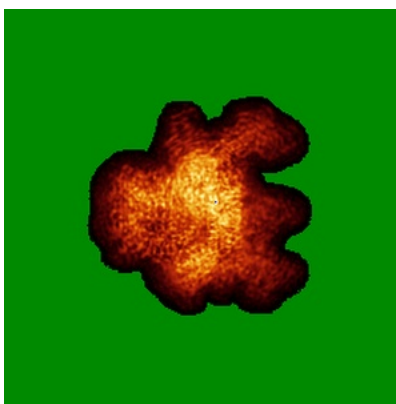
The images above show the largest variance slices of the map in three orthogonal directions.

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

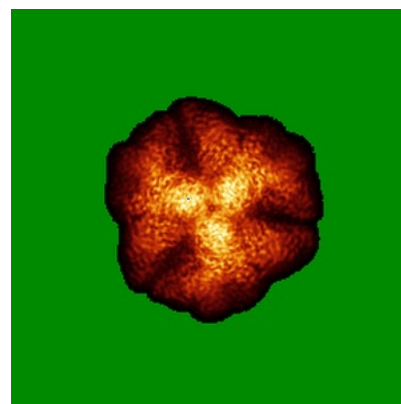
6.4.1 Primary map



X

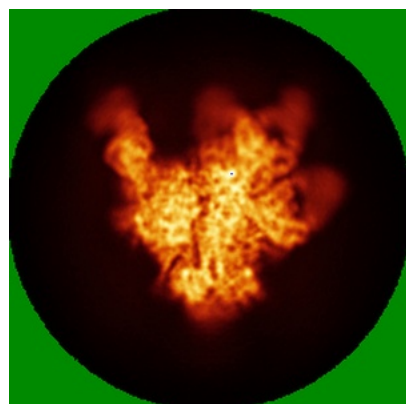


Y

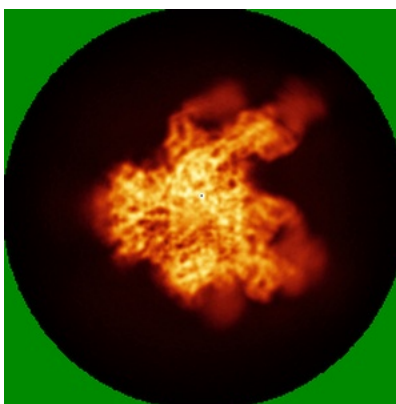


Z

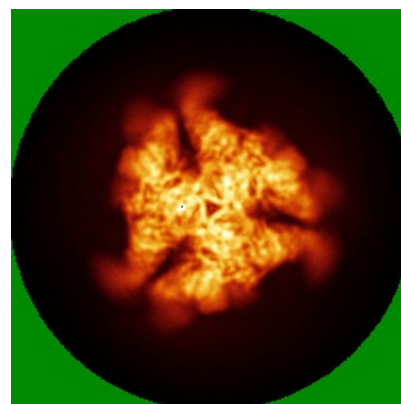
6.4.2 Raw map



X



Y

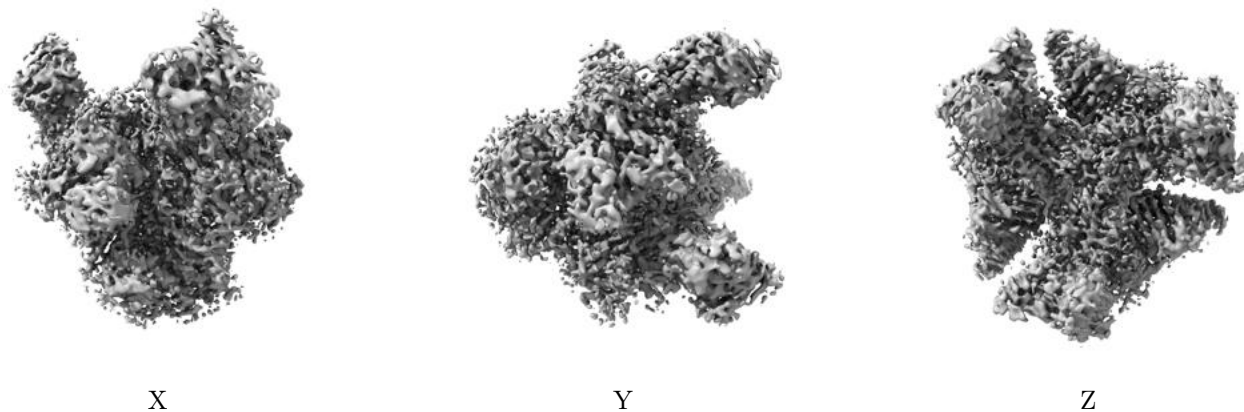


Z

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 0.0223. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

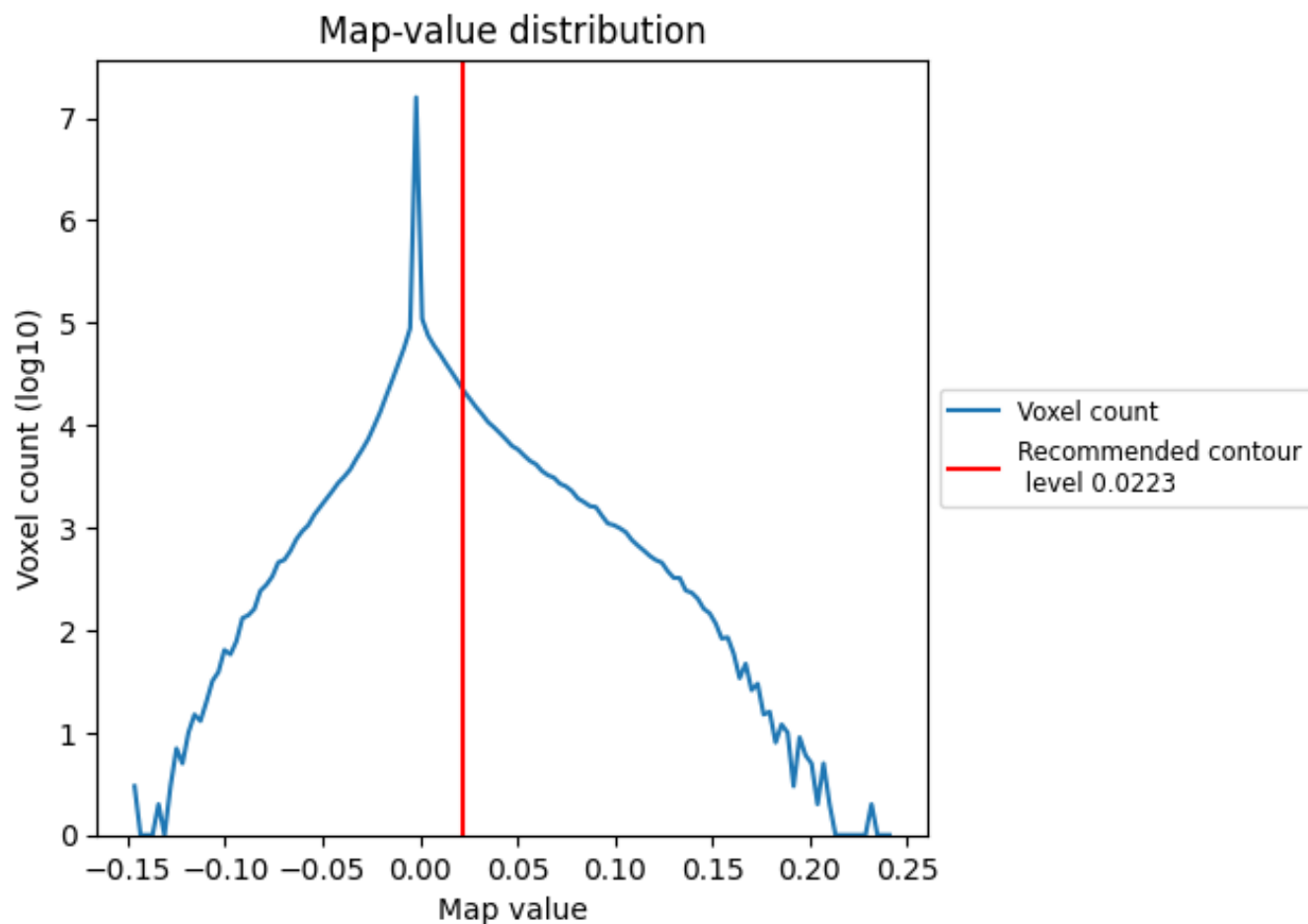
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

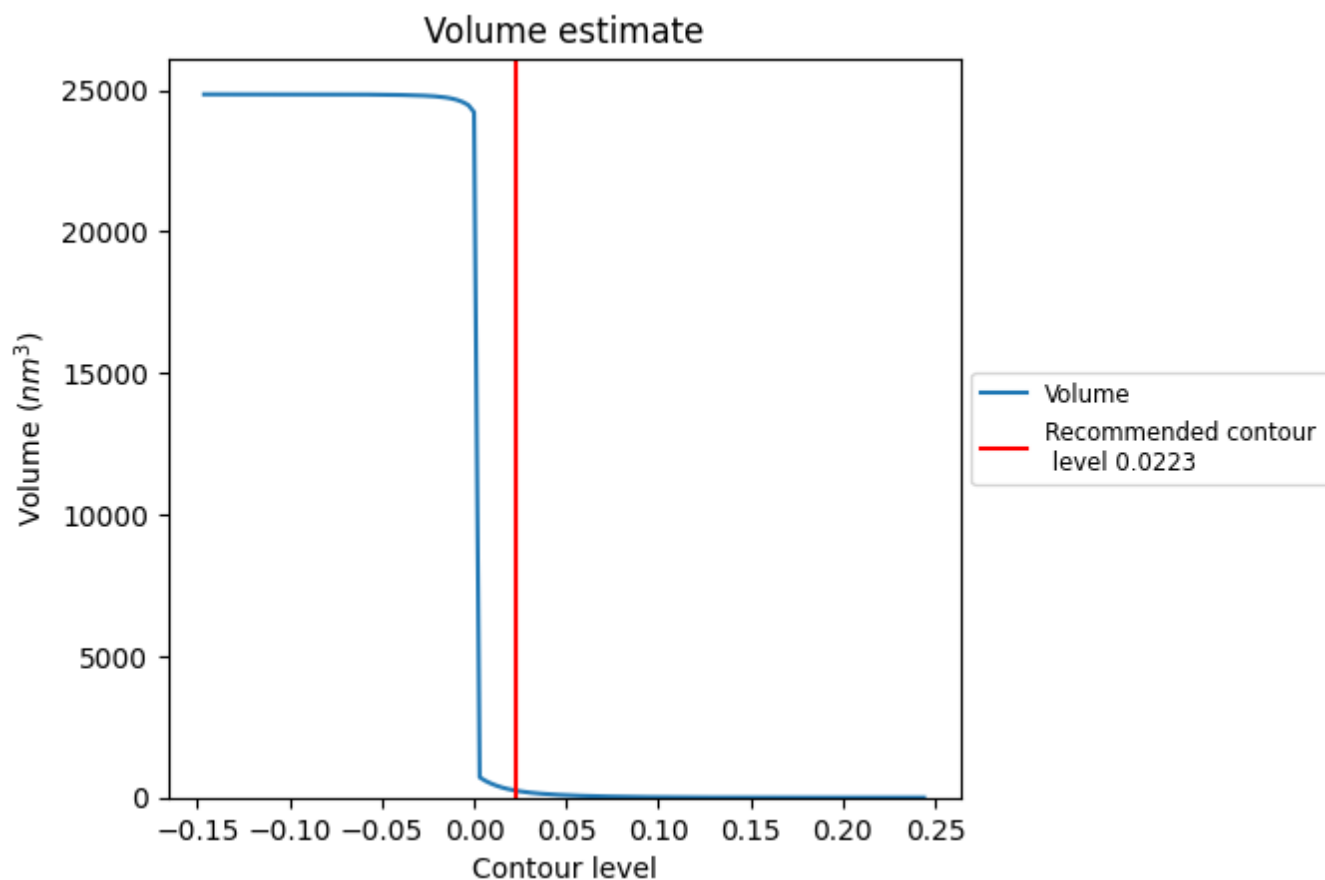
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

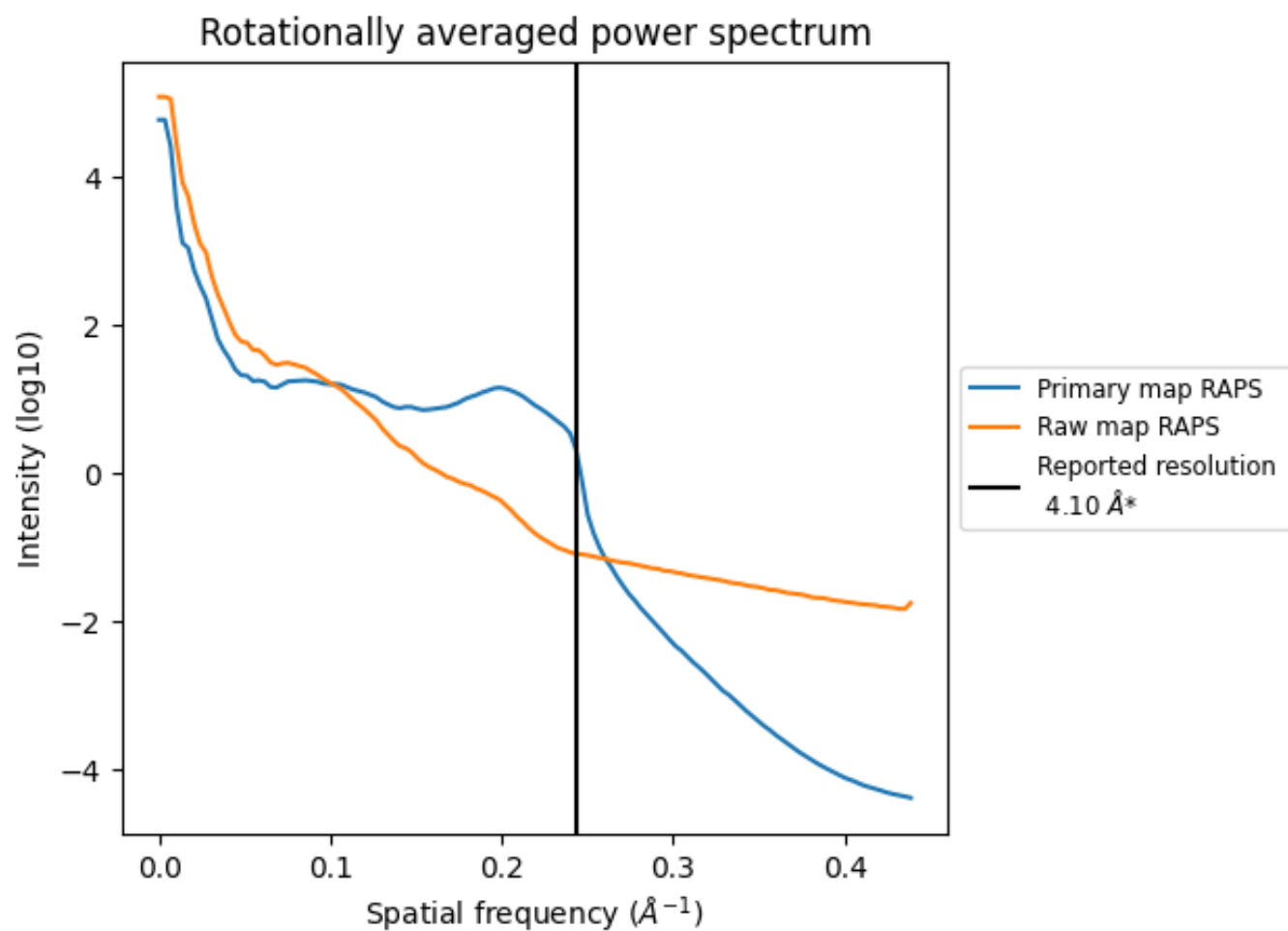
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 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 ⓘ

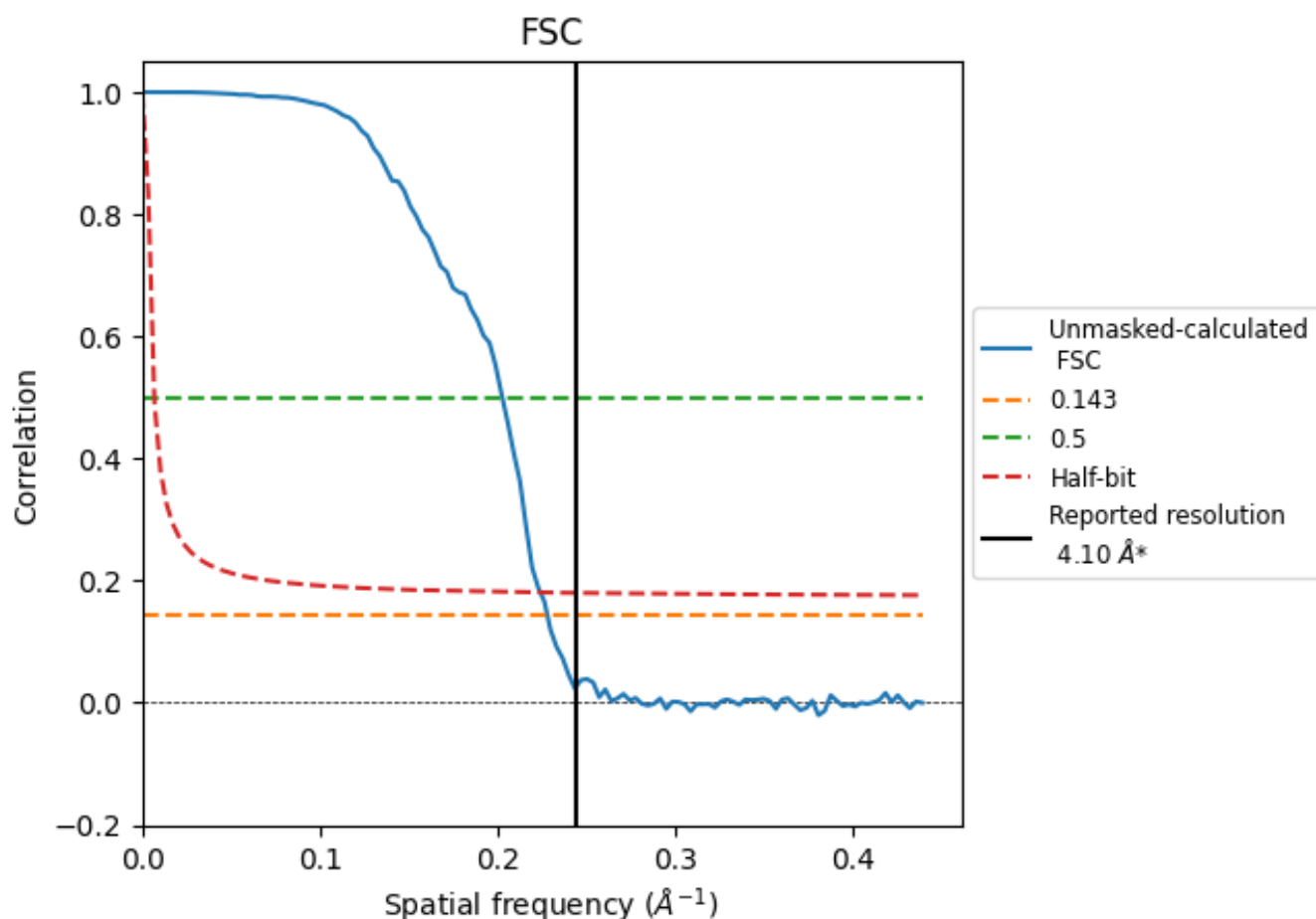


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

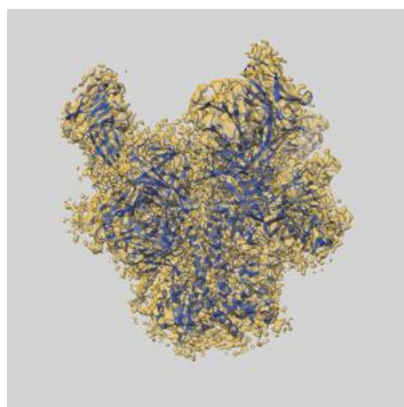
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	4.94	4.47

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

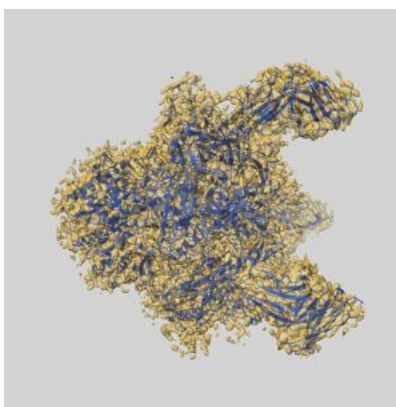
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26492 and PDB model 7UGO. Per-residue inclusion information can be found in section [3](#) on page [14](#).

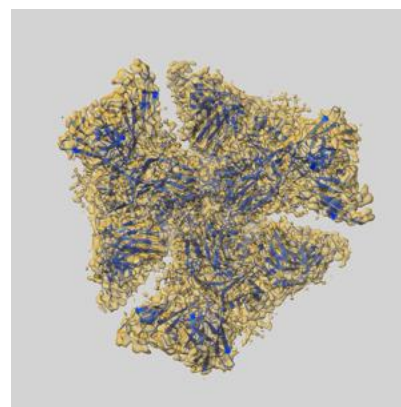
9.1 Map-model overlay [i](#)



X



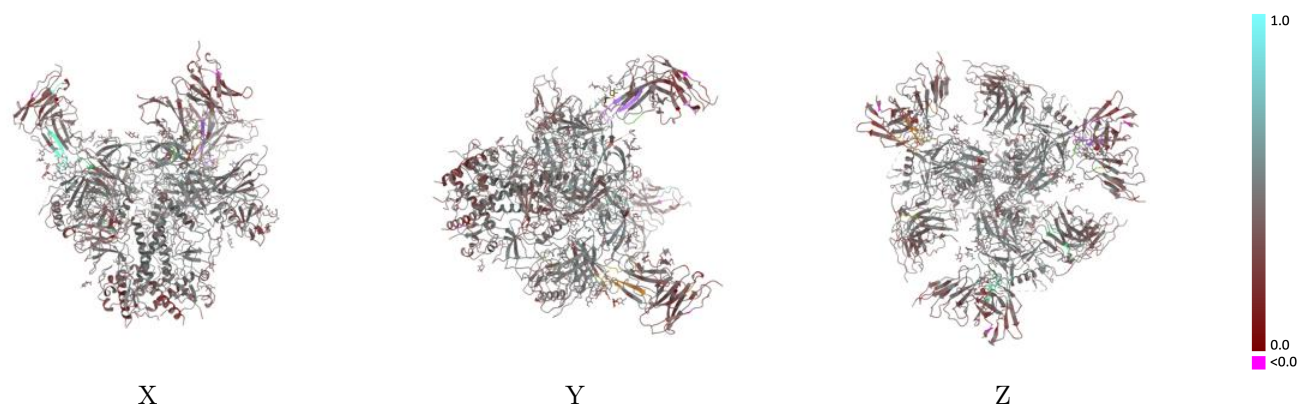
Y



Z

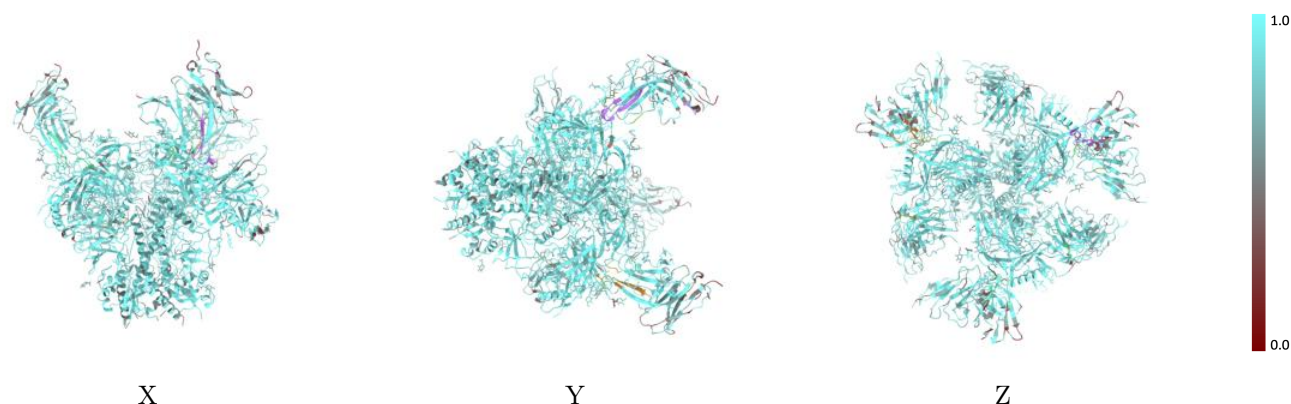
The images above show the 3D surface view of the map at the recommended contour level 0.0223 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



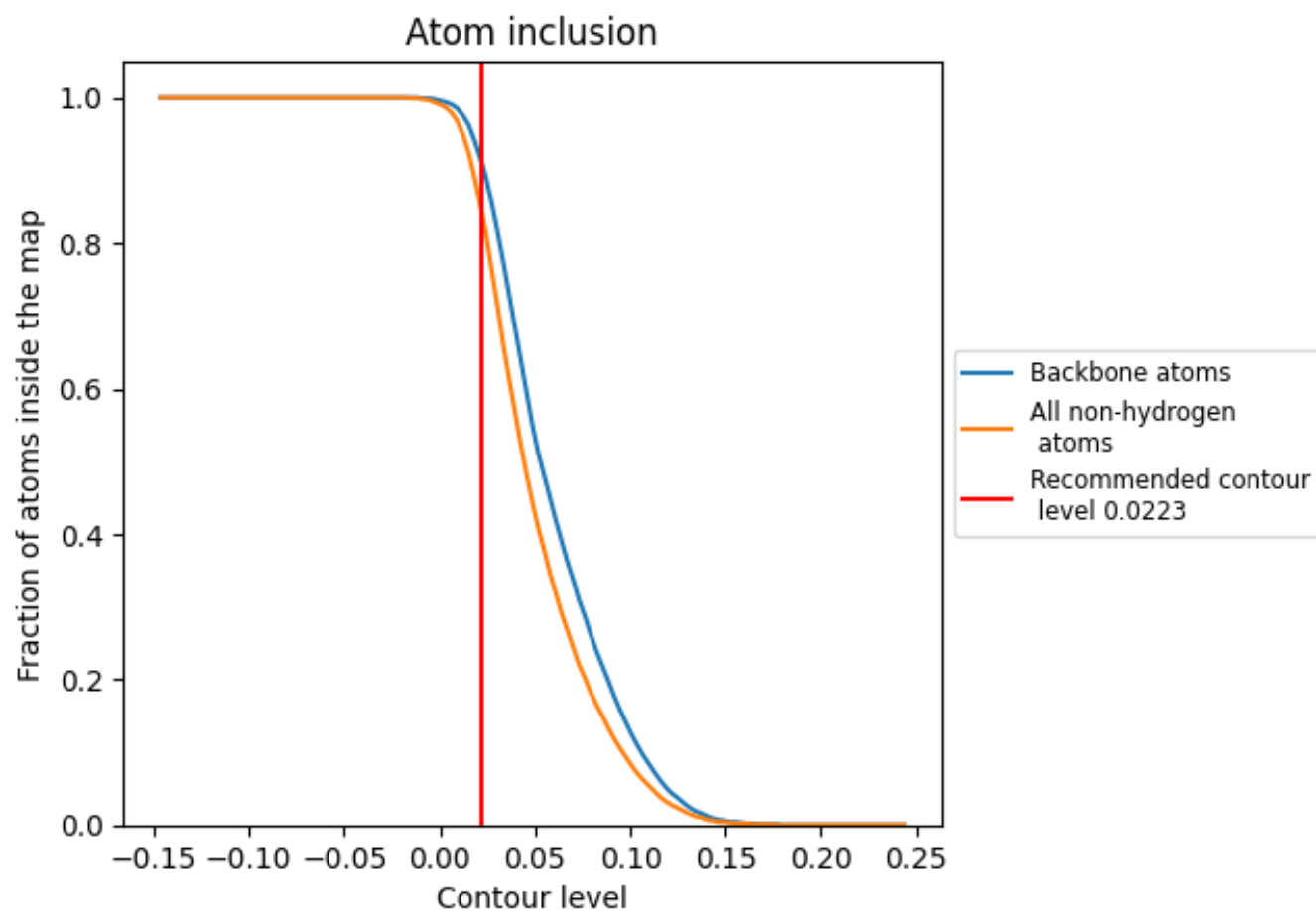
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0223).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0223) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4250
A	 0.8790	 0.4620
B	 0.8830	 0.4650
C	 0.8820	 0.4620
D	 0.8510	 0.4090
E	 0.8470	 0.4070
F	 0.8480	 0.4060
G	 0.8560	 0.4400
H	 0.8590	 0.4410
I	 0.8610	 0.4380
J	 0.7700	 0.3620
K	 0.7740	 0.3650
L	 0.7720	 0.3630
M	 0.7410	 0.3550
N	 0.7300	 0.3560
O	 0.7350	 0.3590
P	 0.8430	 0.4100
Q	 0.8390	 0.4100
R	 0.8370	 0.4100
S	 0.9200	 0.4800
T	 0.7710	 0.3880
U	 0.8210	 0.4270
V	 0.7140	 0.4420
W	 0.8210	 0.4840
X	 0.9550	 0.4360
Y	 0.7860	 0.3990
Z	 0.8210	 0.4140
a	 0.8550	 0.4670
b	 0.8210	 0.4290
c	 0.7140	 0.4270
d	 0.8210	 0.4870
e	 0.6360	 0.1710
f	 0.7500	 0.4010
g	 0.9000	 0.4340
h	 0.8000	 0.3930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8210	 0.4520
j	 0.7500	 0.4370
k	 0.8210	 0.4780
l	 0.7860	 0.4130