



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 12:04 PM UTC

PDB ID : 8DUA / pdb_00008dua
EMDB ID : EMD-27718
Title : SIV E660.CR54 SOS-2P Env Trimer with ITS92.02
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2022-07-27
Resolution : 4.32 Å(reported)
Based on initial model : 6TYB

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:

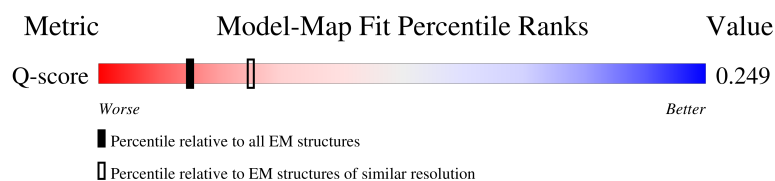
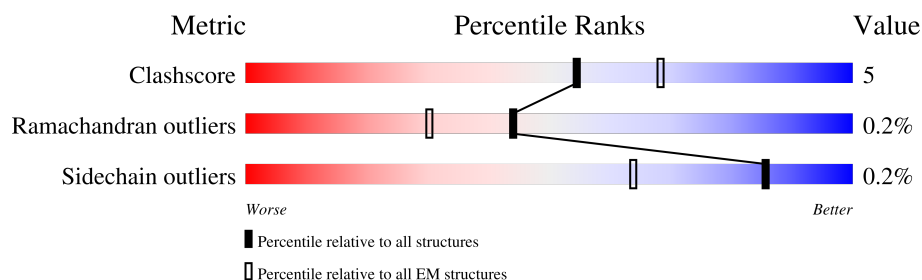
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 4.32 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.



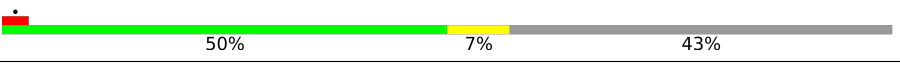
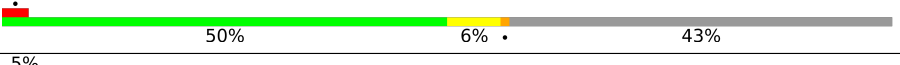
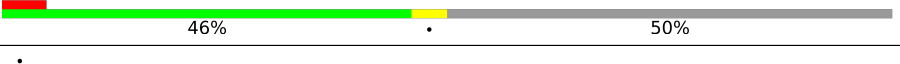
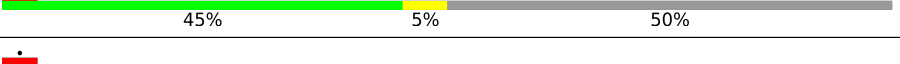
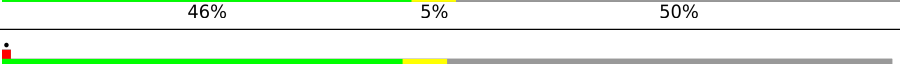
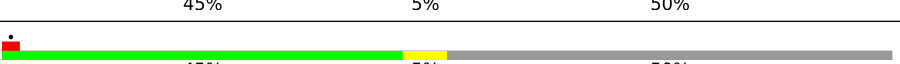
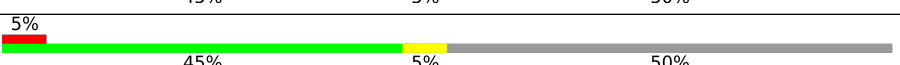
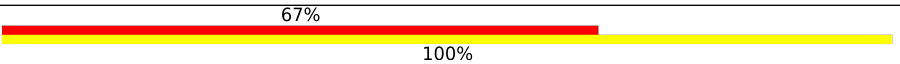
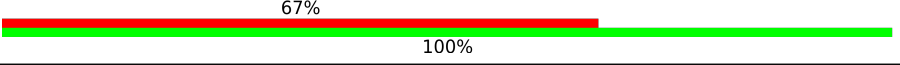
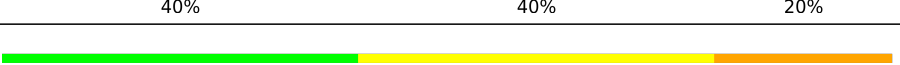
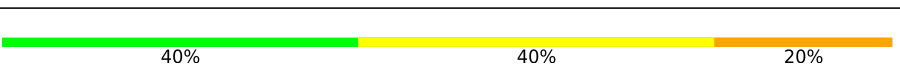
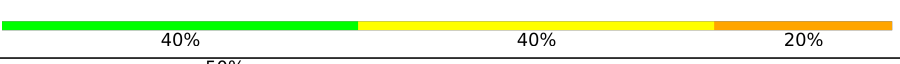
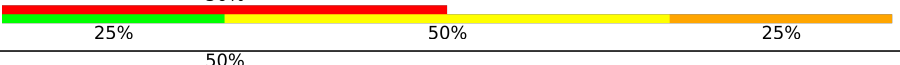
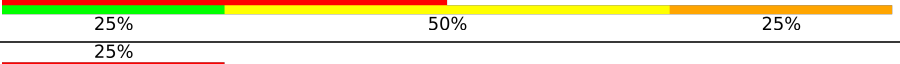
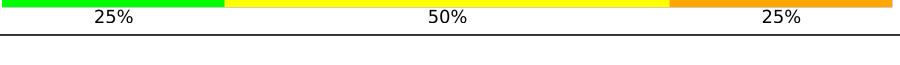
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3853 (3.83 - 4.82)

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	148	
1	B	148	
1	F	148	
2	C	512	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	512	
2	I	512	
3	D	228	
3	H	228	
3	J	228	
4	E	214	
4	K	214	
4	L	214	
5	M	3	
5	O	3	
5	R	3	
5	T	3	
5	W	3	
5	Y	3	
6	N	5	
6	Q	5	
6	S	5	
6	V	5	
6	X	5	
6	a	5	
7	P	4	
7	U	4	
7	Z	4	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15612 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 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	91	Total	C	N	O	S	0	0
			762	483	130	144	5		
1	A	91	Total	C	N	O	S	0	0
			762	483	130	144	5		
1	F	91	Total	C	N	O	S	0	0
			762	483	130	144	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	VAL	conflict	UNP V9PL68
B	569	PRO	THR	conflict	UNP V9PL68
B	605	CYS	HIS	conflict	UNP V9PL68
A	559	PRO	VAL	conflict	UNP V9PL68
A	569	PRO	THR	conflict	UNP V9PL68
A	605	CYS	HIS	conflict	UNP V9PL68
F	559	PRO	VAL	conflict	UNP V9PL68
F	569	PRO	THR	conflict	UNP V9PL68
F	605	CYS	HIS	conflict	UNP V9PL68

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	292	Total	C	N	O	S	0	0
			2354	1490	400	446	18		
2	C	292	Total	C	N	O	S	0	0
			2354	1490	400	446	18		
2	I	292	Total	C	N	O	S	0	0
			2354	1490	400	446	18		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	VAL	conflict	UNP C4NR77
G	512	ARG	ASN	conflict	UNP C4NR77
G	513	ARG	LYS	conflict	UNP C4NR77
G	515	ARG	-	expression tag	UNP C4NR77
C	501	CYS	VAL	conflict	UNP C4NR77
C	512	ARG	ASN	conflict	UNP C4NR77
C	513	ARG	LYS	conflict	UNP C4NR77
C	515	ARG	-	expression tag	UNP C4NR77
I	501	CYS	VAL	conflict	UNP C4NR77
I	512	ARG	ASN	conflict	UNP C4NR77
I	513	ARG	LYS	conflict	UNP C4NR77
I	515	ARG	-	expression tag	UNP C4NR77

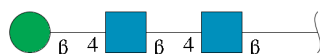
- Molecule 3 is a protein called ITS92.02 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	115	Total	C	N	O	S	0	0
			888	564	152	170	2		
3	D	115	Total	C	N	O	S	0	0
			888	564	152	170	2		
3	J	115	Total	C	N	O	S	0	0
			888	564	152	170	2		

- Molecule 4 is a protein called ITS92.02 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			824	519	139	163	3		
4	E	107	Total	C	N	O	S	0	0
			824	519	139	163	3		
4	K	107	Total	C	N	O	S	0	0
			824	519	139	163	3		

- Molecule 5 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.



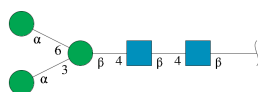
Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	3	Total	C	N	O		0	0
			39	22	2	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	R	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		

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



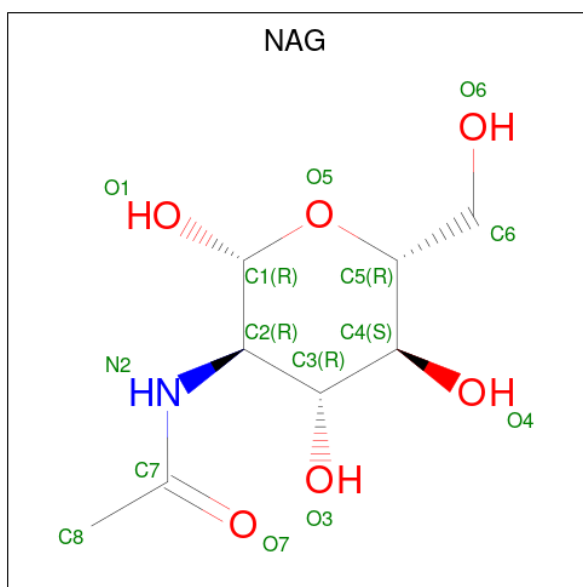
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	Q	5	Total	C	N	O	0	0
			61	34	2	25		
6	S	5	Total	C	N	O	0	0
			61	34	2	25		
6	V	5	Total	C	N	O	0	0
			61	34	2	25		
6	X	5	Total	C	N	O	0	0
			61	34	2	25		
6	a	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	P	4	Total	C	N	O	0	0
			50	28	2	20		
7	U	4	Total	C	N	O	0	0
			50	28	2	20		
7	Z	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

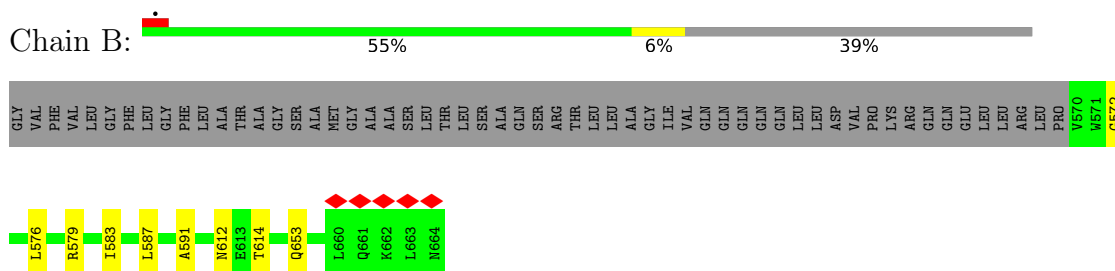
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total 14	C 8	N 1	O 5	0
8	A	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	C	1	Total 14	C 8	N 1	O 5	0
8	F	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0
8	I	1	Total 14	C 8	N 1	O 5	0

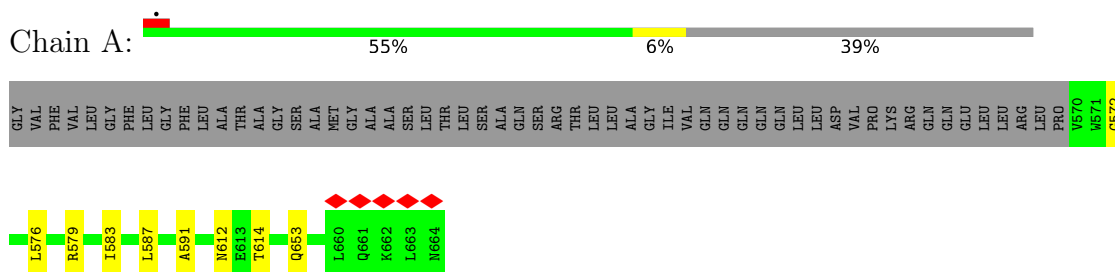
3 Residue-property plots [i](#)

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

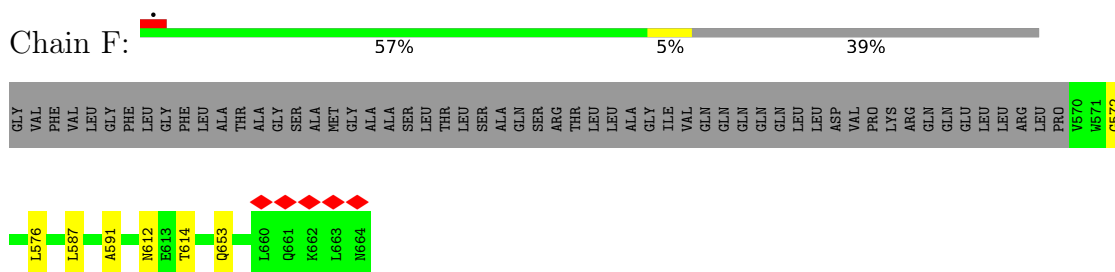
- Molecule 1: Envelope glycoprotein gp41



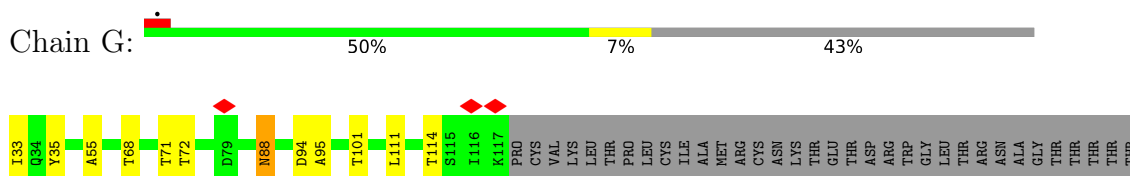
- Molecule 1: Envelope glycoprotein gp41



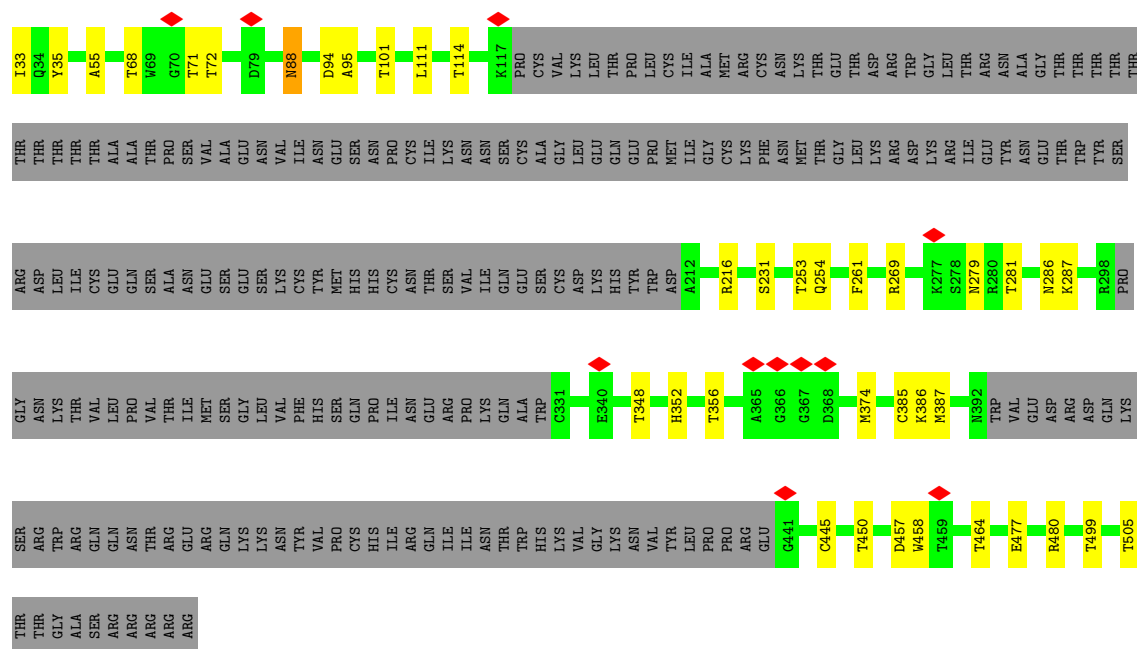
- Molecule 1: Envelope glycoprotein gp41



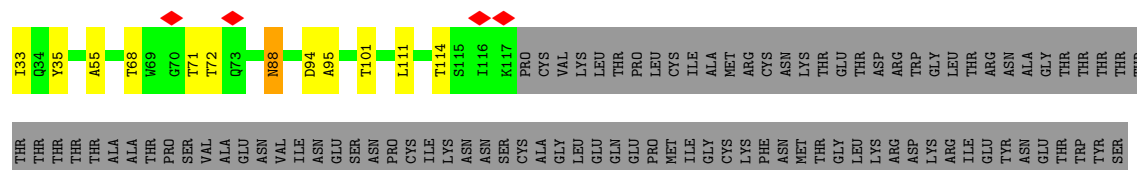
- Molecule 2: Envelope glycoprotein gp120



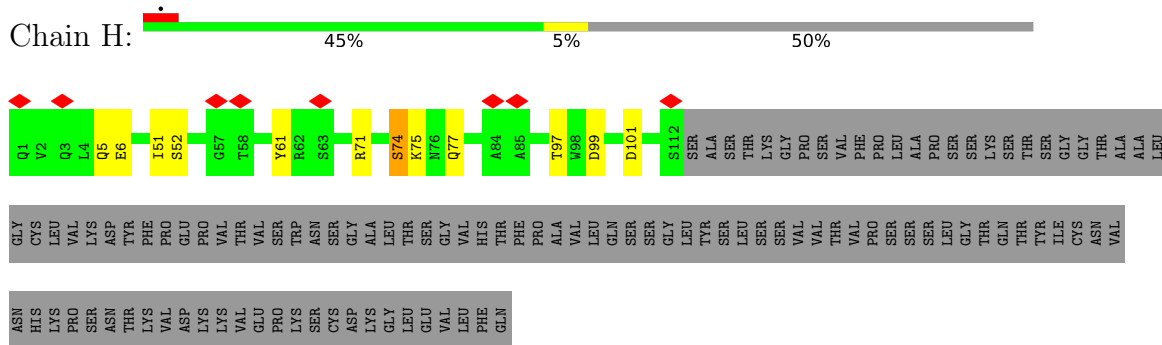
- Molecule 2: Envelope glycoprotein gp120



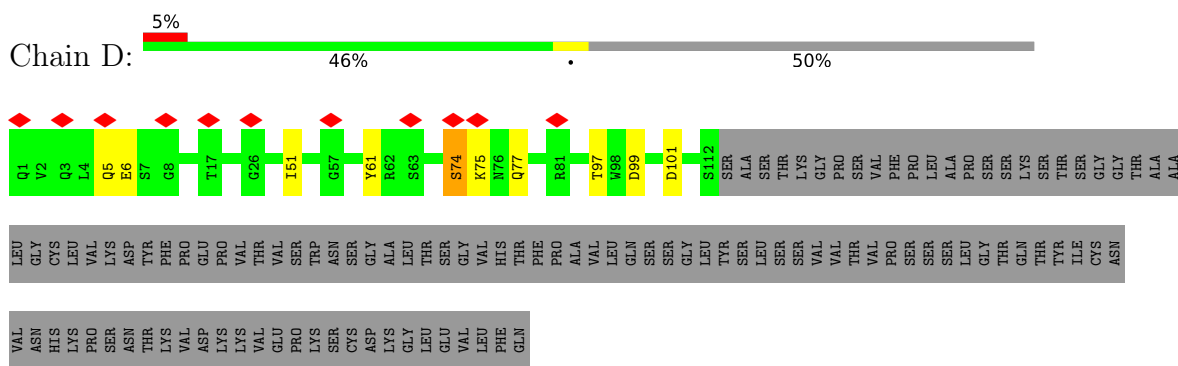
- Molecule 2: Envelope glycoprotein gp120



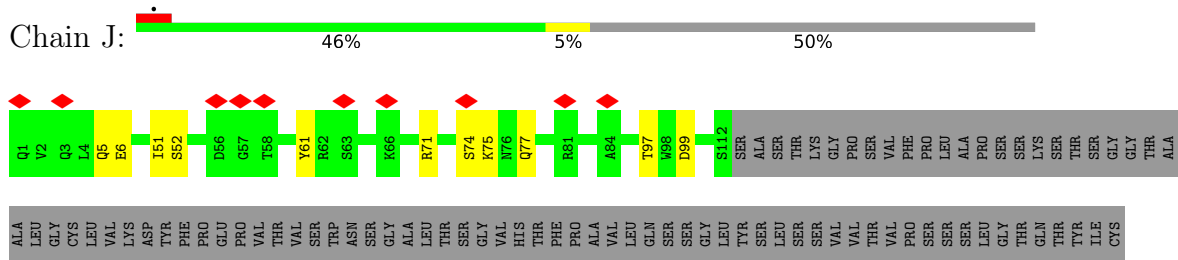
- Molecule 3: ITS92.02 Heavy Chain



- Molecule 3: ITS92.02 Heavy Chain

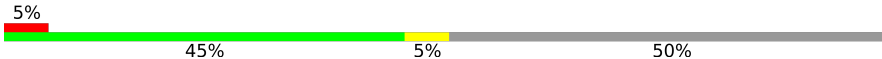


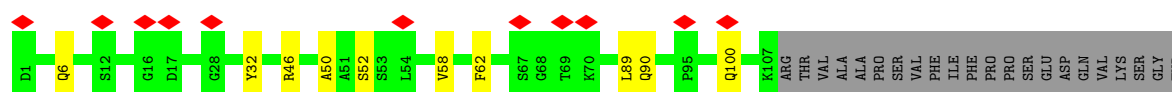
- Molecule 3: ITS92.02 Heavy Chain



ASN VAL
ASN HIS
LYS PRO
SER SER
ASN THR
LYS VAL
ASP VAL
LYS LYS
VAL VAL
GLU VAL
PRO PRO
LYS LYS
SER SER
CYS ASP
LYS LYS
GLY GLY
LEU LEU
GLU VAL
PHE PHE
GLN

• Molecule 4: ITS92.02 Light Chain

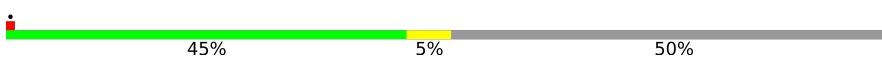
Chain L: 

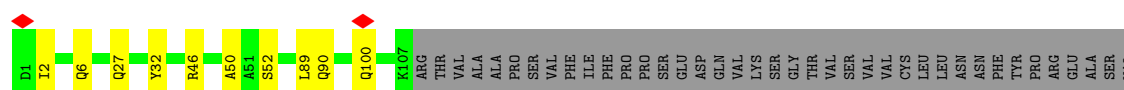


LYS VAL
SER VAL
VAL VAL
CYS VAL
LEU LEU
ASN ASN
PHE PHE
TYR TYR
PRO PRO
ARG ARG
GLU GLU
ALA ALA
SER SER
VAL VAL
THR THR
LYS LYS
TRP TRP
LYS LYS
VAL VAL
ASP ASP
GLY GLY
ALA ALA
LEU LEU
LYS LYS
THR THR

LYS VAL
TYR VAL
ALA VAL
CYS VAL
GLY VAL
THR THR
HIS HIS
GLN GLN
LEU LEU
SER SER
SER SER
PRO PRO
VAL VAL
THR THR
LYS LYS
PHE PHE
ASN ASN
ARG ARG
GLY GLY
CYS CYS

• Molecule 4: ITS92.02 Light Chain

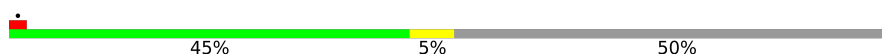
Chain E: 

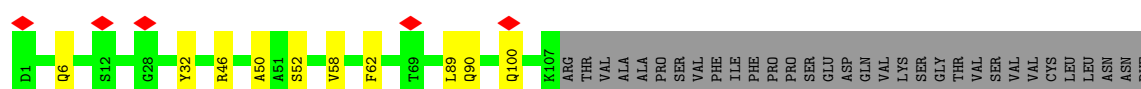


LYS TRP
VAL VAL
LYS VAL
ASP VAL
GLY VAL
ALA VAL
LEU VAL
THR THR
LYS LYS
ASN ASN
SER SER
GLN GLN
GLU GLU
SER SER
VAL VAL
THR THR
GLY GLY
GLN GLN
ASP ASP
SER SER
LYS LYS
VAL VAL
ASN ASN
THR THR
TYR TYR
SER SER
LEU LEU
SER SER
SER SER
THR THR
THR THR
GLY GLY
TYR TYR
GLN GLN
SER SER
HIS HIS
LYS LYS
VAL VAL
THR THR
VAL VAL
CYS CYS
VAL VAL
THR THR
SER SER
PRO PRO
VAL VAL
THR THR

LYS SER
PHE PHE
ASN ASN
ARG ARG
GLY GLY
CYS CYS

• Molecule 4: ITS92.02 Light Chain

Chain K: 



TYR PRO
ARG ARG
GLU GLU
SER SER
VAL VAL
LYS LYS
TRP TRP
LYS LYS
VAL VAL
ASP ASP
GLY GLY
ALA ALA
LEU LEU
LYS LYS
THR THR
GLY GLY
ASN ASN
SER SER
GLN GLN
GLU GLU
VAL VAL
SER SER
THR THR
GLY GLY
GLN GLN
ASP ASP
LYS LYS
ASN ASN
THR THR
TYR TYR
SER SER
LEU LEU
SER SER
SER SER
THR THR
THR THR
PHE PHE
PHE PHE
PRO PRO
PRO PRO
SER SER
SER SER
THR THR
GLU GLU
GLN GLN
VAL VAL
LYS LYS
SER SER
HIS HIS
LYS LYS
VAL VAL
THR THR
SER SER
VAL VAL
CYS CYS
VAL VAL
THR THR
THR THR
HIS HIS
ASN ASN
GLN GLN

GLY LEU
SER SER
SER SER
PRO PRO
VAL VAL
THR THR
LYS LYS
SER SER
PHE PHE
ASN ASN
ARG ARG
GLY GLY
CYS CYS

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

Chain M: 



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



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



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



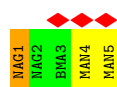
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



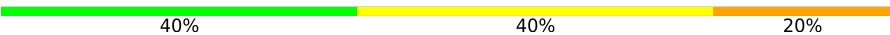
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

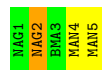


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



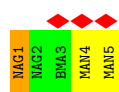
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 

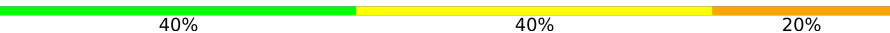


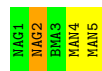
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 



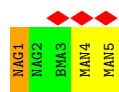
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



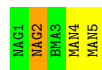
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

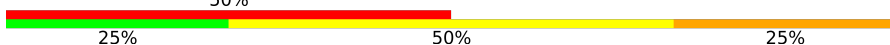


- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 



- 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 P: 



- 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



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.16	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	346.56, 346.56, 346.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.10	0/780	0.21	0/1063
1	B	0.09	0/780	0.22	0/1063
1	F	0.10	0/780	0.22	0/1063
2	C	0.22	0/2412	0.45	2/3283 (0.1%)
2	G	0.19	0/2412	0.40	1/3283 (0.0%)
2	I	0.17	0/2412	0.38	2/3283 (0.1%)
3	D	0.11	0/912	0.26	0/1245
3	H	0.11	0/912	0.26	0/1245
3	J	0.11	0/912	0.26	0/1245
4	E	0.12	0/843	0.28	0/1142
4	K	0.12	0/843	0.27	0/1142
4	L	0.12	0/843	0.27	0/1142
All	All	0.16	0/14841	0.34	5/20199 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	279	ASN	CA-CB-CG	-10.78	101.82	112.60
2	C	279	ASN	N-CA-C	-8.46	103.07	112.72
2	I	279	ASN	N-CA-C	-6.64	103.86	112.23
2	I	279	ASN	CB-CA-C	5.37	121.33	110.38
2	C	281	THR	N-CA-C	5.04	116.64	109.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	762	0	728	5	0
1	B	762	0	728	5	0
1	F	762	0	728	4	0
2	C	2354	0	2233	27	0
2	G	2354	0	2232	27	0
2	I	2354	0	2233	26	0
3	D	888	0	869	8	0
3	H	888	0	869	9	0
3	J	888	0	869	8	0
4	E	824	0	804	8	0
4	K	824	0	804	7	0
4	L	824	0	804	7	0
5	M	39	0	34	2	0
5	O	39	0	34	0	0
5	R	39	0	34	1	0
5	T	39	0	34	0	0
5	W	39	0	34	1	0
5	Y	39	0	34	0	0
6	N	61	0	52	2	0
6	Q	61	0	52	2	0
6	S	61	0	52	2	0
6	V	61	0	52	2	0
6	X	61	0	52	2	0
6	a	61	0	52	2	0
7	P	50	0	43	3	0
7	U	50	0	43	3	0
7	Z	50	0	43	3	0
8	A	14	0	13	2	0
8	B	14	0	13	2	0
8	C	112	0	104	6	0
8	F	14	0	13	2	0
8	G	112	0	104	2	0
8	I	112	0	104	2	0
All	All	15612	0	14897	155	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.

All (155) 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)
8:C:1003:NAG:O3	8:C:1003:NAG:O7	1.89	0.89
3:D:75:LYS:NZ	3:D:77:GLN:OE1	2.26	0.69
3:H:75:LYS:NZ	3:H:77:GLN:OE1	2.25	0.68
2:I:261:PHE:CD2	7:Z:1:NAG:H81	2.29	0.67
3:J:99:ASP:O	4:K:46:ARG:NH1	2.27	0.67
4:E:27:GLN:N	4:E:27:GLN:OE1	2.28	0.66
3:D:99:ASP:O	4:E:46:ARG:NH1	2.29	0.66
1:B:612:ASN:OD1	1:B:614:THR:OG1	2.13	0.66
2:C:458:TRP:HB3	2:C:464:THR:HG23	1.77	0.66
1:A:612:ASN:OD1	1:A:614:THR:OG1	2.12	0.66
3:H:99:ASP:O	4:L:46:ARG:NH1	2.29	0.66
3:J:75:LYS:NZ	3:J:77:GLN:OE1	2.26	0.66
2:G:253:THR:O	2:G:254:GLN:NE2	2.29	0.65
2:C:261:PHE:CD2	7:U:1:NAG:H81	2.31	0.65
2:I:253:THR:O	2:I:254:GLN:NE2	2.29	0.65
3:H:5:GLN:N	3:H:5:GLN:OE1	2.30	0.65
2:C:261:PHE:HD2	7:U:1:NAG:H81	1.62	0.64
1:F:612:ASN:OD1	1:F:614:THR:OG1	2.14	0.64
3:J:5:GLN:N	3:J:5:GLN:OE1	2.30	0.64
2:G:261:PHE:CD2	7:P:1:NAG:H81	2.33	0.63
3:D:5:GLN:OE1	3:D:5:GLN:N	2.31	0.63
2:G:261:PHE:HD2	7:P:1:NAG:H81	1.63	0.63
2:C:253:THR:O	2:C:254:GLN:NE2	2.32	0.63
1:B:587:LEU:O	1:B:591:ALA:N	2.30	0.63
3:J:97:THR:O	4:K:46:ARG:NH2	2.31	0.63
2:I:261:PHE:HD2	7:Z:1:NAG:H81	1.63	0.63
2:G:33:ILE:N	4:L:32:TYR:HH	1.97	0.62
3:D:97:THR:O	4:E:46:ARG:NH2	2.32	0.62
3:H:97:THR:O	4:L:46:ARG:NH2	2.33	0.62
1:A:587:LEU:O	1:A:591:ALA:N	2.32	0.62
2:G:111:LEU:O	2:G:114:THR:OG1	2.17	0.61
1:F:587:LEU:O	1:F:591:ALA:N	2.34	0.61
2:I:111:LEU:O	2:I:114:THR:OG1	2.19	0.61
2:I:33:ILE:N	4:K:32:TYR:HH	1.99	0.60
2:C:111:LEU:O	2:C:114:THR:OG1	2.19	0.60
4:K:6:GLN:OE1	4:K:100:GLN:N	2.35	0.59
4:L:6:GLN:OE1	4:L:100:GLN:N	2.36	0.59
2:C:33:ILE:N	4:E:32:TYR:HH	1.99	0.59
2:G:261:PHE:O	2:G:450:THR:OG1	2.20	0.59
2:I:88:ASN:OD1	2:I:88:ASN:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ASN:N	2:C:88:ASN:OD1	2.36	0.58
2:C:261:PHE:O	2:C:450:THR:OG1	2.21	0.58
2:G:55:ALA:O	2:G:216:ARG:N	2.37	0.58
4:E:6:GLN:OE1	4:E:100:GLN:N	2.36	0.57
2:I:279:ASN:H	8:I:1008:NAG:H82	1.69	0.57
2:G:88:ASN:N	2:G:88:ASN:OD1	2.37	0.57
2:I:261:PHE:O	2:I:450:THR:OG1	2.22	0.56
8:C:1003:NAG:HO3	8:C:1003:NAG:C7	2.09	0.56
2:C:348:THR:O	2:C:352:HIS:N	2.39	0.56
2:I:477:GLU:OE1	2:I:477:GLU:N	2.39	0.56
2:C:55:ALA:O	2:C:216:ARG:N	2.39	0.55
2:C:477:GLU:N	2:C:477:GLU:OE1	2.39	0.55
3:H:51:ILE:HD13	3:H:61:TYR:OH	2.07	0.55
2:I:55:ALA:O	2:I:216:ARG:N	2.39	0.55
3:J:51:ILE:HD13	3:J:61:TYR:OH	2.07	0.55
3:D:51:ILE:HD13	3:D:61:TYR:OH	2.07	0.54
2:G:348:THR:O	2:G:352:HIS:N	2.41	0.54
8:C:1003:NAG:O6	8:C:1003:NAG:O4	2.22	0.54
2:G:94:ASP:OD1	2:G:95:ALA:N	2.41	0.54
2:I:445:CYS:HB2	7:Z:2:NAG:H81	1.88	0.54
2:G:477:GLU:N	2:G:477:GLU:OE1	2.39	0.54
5:R:2:NAG:O3	5:R:3:BMA:O5	2.24	0.54
5:W:2:NAG:O3	5:W:3:BMA:O5	2.24	0.53
2:I:94:ASP:OD1	2:I:95:ALA:N	2.41	0.53
2:C:94:ASP:OD1	2:C:95:ALA:N	2.40	0.53
2:G:286:ASN:OD1	2:G:287:LYS:N	2.43	0.52
2:I:286:ASN:OD1	2:I:287:LYS:N	2.43	0.52
2:I:385:CYS:SG	2:I:386:LYS:N	2.82	0.52
2:C:445:CYS:HB2	7:U:2:NAG:H81	1.90	0.52
2:G:445:CYS:HB2	7:P:2:NAG:H81	1.93	0.51
2:C:286:ASN:OD1	2:C:287:LYS:N	2.43	0.51
2:G:385:CYS:SG	2:G:386:LYS:N	2.83	0.51
2:C:385:CYS:SG	2:C:386:LYS:N	2.83	0.51
2:G:231:SER:O	2:G:269:ARG:NE	2.45	0.50
2:I:348:THR:O	2:I:352:HIS:N	2.45	0.50
3:H:74:SER:OG	3:H:75:LYS:N	2.44	0.50
3:J:74:SER:OG	3:J:75:LYS:N	2.44	0.49
8:A:701:NAG:C1	8:A:701:NAG:H82	2.43	0.49
8:B:701:NAG:C1	8:B:701:NAG:H82	2.43	0.49
8:F:701:NAG:C1	8:F:701:NAG:H82	2.43	0.49
2:C:356:THR:HG23	2:C:356:THR:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:356:THR:HG23	2:I:356:THR:O	2.13	0.49
5:M:2:NAG:O3	5:M:3:BMA:O5	2.24	0.49
6:S:1:NAG:C1	6:S:1:NAG:H82	2.43	0.49
6:Q:2:NAG:C1	6:Q:2:NAG:H82	2.43	0.48
8:C:1003:NAG:O3	8:C:1003:NAG:C7	2.58	0.48
6:N:1:NAG:C1	6:N:1:NAG:H82	2.43	0.48
2:G:35:TYR:N	2:G:499:THR:O	2.45	0.48
6:V:2:NAG:C1	6:V:2:NAG:H82	2.43	0.48
6:a:2:NAG:C1	6:a:2:NAG:H82	2.43	0.48
4:L:89:LEU:HD23	4:L:90:GLN:N	2.29	0.48
2:C:458:TRP:CD1	8:C:1003:NAG:H81	2.47	0.48
6:X:1:NAG:C1	6:X:1:NAG:H82	2.43	0.48
2:G:356:THR:O	2:G:356:THR:HG23	2.13	0.48
3:D:74:SER:OG	3:D:75:LYS:N	2.44	0.47
1:A:572:GLY:O	1:A:576:LEU:HD23	2.14	0.47
1:F:572:GLY:O	1:F:576:LEU:HD23	2.15	0.47
1:B:572:GLY:O	1:B:576:LEU:HD23	2.15	0.47
2:G:352(B):ARG:HH22	8:G:1008:NAG:C8	2.28	0.47
4:E:89:LEU:HD23	4:E:90:GLN:N	2.29	0.47
2:I:101:THR:HG21	2:I:480:ARG:HG2	1.97	0.46
2:G:72:THR:HG22	2:G:72:THR:O	2.16	0.46
2:G:352(B):ARG:HH22	8:G:1008:NAG:C7	2.29	0.46
1:A:653:GLN:NE2	2:C:505:THR:O	2.48	0.46
4:K:89:LEU:HD23	4:K:90:GLN:N	2.29	0.46
2:C:72:THR:HG22	2:C:72:THR:O	2.15	0.46
1:F:653:GLN:NE2	2:I:505:THR:O	2.49	0.46
2:G:101:THR:HG21	2:G:480:ARG:HG2	1.97	0.46
2:I:35:TYR:N	2:I:499:THR:O	2.46	0.46
2:C:374:MET:HE2	2:C:387:MET:HE3	1.98	0.45
2:I:374:MET:HE2	2:I:387:MET:HE3	1.99	0.45
2:I:72:THR:HG22	2:I:72:THR:O	2.16	0.45
2:C:35:TYR:N	2:C:499:THR:O	2.45	0.45
2:C:101:THR:HG21	2:C:480:ARG:HG2	1.98	0.45
2:C:71:THR:O	2:C:71:THR:HG22	2.18	0.45
2:C:231:SER:O	2:C:269:ARG:NE	2.51	0.44
2:I:231:SER:O	2:I:269:ARG:NE	2.50	0.44
1:B:653:GLN:NE2	2:G:505:THR:O	2.51	0.44
4:E:2:ILE:HD13	4:E:27:GLN:HE22	1.81	0.44
4:L:58:VAL:HG21	4:L:62:PHE:HD2	1.82	0.44
1:A:579:ARG:O	1:A:583:ILE:HD12	2.18	0.44
2:I:279:ASN:O	2:I:280:ARG:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:374:MET:HE2	2:G:387:MET:HE3	1.99	0.44
2:I:71:THR:HG22	2:I:71:THR:O	2.17	0.44
2:C:457:ASP:N	2:C:457:ASP:OD1	2.51	0.43
4:E:50:ALA:O	4:E:52:SER:N	2.52	0.43
4:K:58:VAL:HG21	4:K:62:PHE:HD2	1.83	0.43
5:M:1:NAG:O3	5:M:2:NAG:O5	2.27	0.43
8:A:701:NAG:C1	8:A:701:NAG:C8	2.97	0.43
8:F:701:NAG:C1	8:F:701:NAG:C8	2.97	0.43
6:N:1:NAG:C1	6:N:1:NAG:C8	2.97	0.43
2:G:234:SER:OG	2:G:272:ILE:O	2.36	0.43
8:B:701:NAG:C1	8:B:701:NAG:C8	2.97	0.43
2:G:71:THR:O	2:G:71:THR:HG22	2.17	0.42
6:X:1:NAG:C1	6:X:1:NAG:C8	2.97	0.42
6:V:2:NAG:C1	6:V:2:NAG:C8	2.97	0.42
2:C:458:TRP:CG	8:C:1003:NAG:H81	2.54	0.42
6:a:2:NAG:C1	6:a:2:NAG:C8	2.97	0.42
4:K:50:ALA:O	4:K:52:SER:N	2.51	0.42
6:S:1:NAG:C1	6:S:1:NAG:C8	2.97	0.42
3:D:6:GLU:N	3:D:6:GLU:OE1	2.53	0.42
4:L:50:ALA:O	4:L:52:SER:N	2.51	0.41
1:B:579:ARG:O	1:B:583:ILE:HD12	2.19	0.41
3:H:52:SER:O	3:H:71:ARG:NH2	2.49	0.41
6:Q:2:NAG:C1	6:Q:2:NAG:C8	2.98	0.41
2:C:68:THR:O	2:C:72:THR:OG1	2.38	0.41
2:G:68:THR:O	2:G:72:THR:OG1	2.39	0.41
2:I:279:ASN:N	8:I:1008:NAG:H82	2.33	0.41
2:G:280:ARG:NH1	2:G:477:GLU:OE2	2.54	0.41
2:I:68:THR:O	2:I:72:THR:OG1	2.39	0.41
3:H:101:ASP:OD1	3:H:101:ASP:N	2.52	0.41
3:J:6:GLU:OE1	3:J:6:GLU:N	2.54	0.41
3:J:52:SER:O	3:J:71:ARG:NH2	2.49	0.41
3:D:101:ASP:N	3:D:101:ASP:OD1	2.53	0.40
3:H:6:GLU:OE1	3:H:6:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/148 (60%)	85 (96%)	4 (4%)	0	100	100
1	B	89/148 (60%)	85 (96%)	4 (4%)	0	100	100
1	F	89/148 (60%)	85 (96%)	4 (4%)	0	100	100
2	C	284/512 (56%)	268 (94%)	16 (6%)	0	100	100
2	G	284/512 (56%)	270 (95%)	14 (5%)	0	100	100
2	I	284/512 (56%)	270 (95%)	13 (5%)	1 (0%)	30	66
3	D	113/228 (50%)	104 (92%)	8 (7%)	1 (1%)	14	49
3	H	113/228 (50%)	104 (92%)	8 (7%)	1 (1%)	14	49
3	J	113/228 (50%)	104 (92%)	9 (8%)	0	100	100
4	E	105/214 (49%)	98 (93%)	7 (7%)	0	100	100
4	K	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
4	L	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
All	All	1773/3306 (54%)	1671 (94%)	99 (6%)	3 (0%)	44	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	280	ARG
3	H	74	SER
3	D	74	SER

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	84/128 (66%)	84 (100%)	0	100	100
1	B	84/128 (66%)	84 (100%)	0	100	100
1	F	84/128 (66%)	84 (100%)	0	100	100
2	C	257/459 (56%)	256 (100%)	1 (0%)	84	82
2	G	257/459 (56%)	256 (100%)	1 (0%)	84	82
2	I	257/459 (56%)	256 (100%)	1 (0%)	84	82
3	D	98/196 (50%)	98 (100%)	0	100	100
3	H	98/196 (50%)	98 (100%)	0	100	100
3	J	98/196 (50%)	98 (100%)	0	100	100
4	E	92/189 (49%)	92 (100%)	0	100	100
4	K	92/189 (49%)	92 (100%)	0	100	100
4	L	92/189 (49%)	92 (100%)	0	100	100
All	All	1593/2916 (55%)	1590 (100%)	3 (0%)	85	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	88	ASN
2	C	88	ASN
2	I	88	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	594	ASN
2	G	360	ASN
4	L	3	GLN
2	C	360	ASN
4	E	3	GLN
1	F	594	ASN
2	I	360	ASN
3	J	82(A)	ASN
4	K	3	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	M	1	1,5	14,14,15	0.25	0	17,19,21	0.63	0
5	NAG	M	2	5	14,14,15	0.25	0	17,19,21	0.46	0
5	BMA	M	3	5	11,11,12	0.54	0	15,15,17	0.71	0
6	NAG	N	1	6,1	14,14,15	0.38	0	17,19,21	1.17	2 (11%)
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.54	0
6	BMA	N	3	6	11,11,12	0.57	0	15,15,17	0.69	0
6	MAN	N	4	6	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
6	MAN	N	5	6	11,11,12	0.63	0	15,15,17	1.14	2 (13%)
5	NAG	O	1	2,5	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	O	2	5	14,14,15	0.23	0	17,19,21	0.47	0
5	BMA	O	3	5	11,11,12	0.54	0	15,15,17	0.74	0
7	NAG	P	1	2,7	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
7	NAG	P	2	7	14,14,15	0.23	0	17,19,21	0.60	0
7	BMA	P	3	7	11,11,12	0.56	0	15,15,17	0.67	0
7	MAN	P	4	7	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
6	NAG	Q	1	2,6	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	Q	2	6	14,14,15	0.40	0	17,19,21	1.20	2 (11%)
6	BMA	Q	3	6	11,11,12	0.68	0	15,15,17	0.89	0
6	MAN	Q	4	6	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
6	MAN	Q	5	6	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
5	NAG	R	1	1,5	14,14,15	0.25	0	17,19,21	0.63	0
5	NAG	R	2	5	14,14,15	0.25	0	17,19,21	0.47	0
5	BMA	R	3	5	11,11,12	0.53	0	15,15,17	0.71	0
6	NAG	S	1	6,1	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	S	3	6	11,11,12	0.58	0	15,15,17	0.70	0
6	MAN	S	4	6	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
6	MAN	S	5	6	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
5	NAG	T	1	2,5	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	T	2	5	14,14,15	0.24	0	17,19,21	0.46	0
5	BMA	T	3	5	11,11,12	0.53	0	15,15,17	0.76	0
7	NAG	U	1	2,7	14,14,15	0.59	0	17,19,21	0.91	1 (5%)
7	NAG	U	2	7	14,14,15	0.22	0	17,19,21	0.58	0
7	BMA	U	3	7	11,11,12	0.54	0	15,15,17	0.67	0
7	MAN	U	4	7	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
6	NAG	V	1	2,6	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	V	2	6	14,14,15	0.39	0	17,19,21	1.18	2 (11%)
6	BMA	V	3	6	11,11,12	0.68	0	15,15,17	0.90	0
6	MAN	V	4	6	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
6	MAN	V	5	6	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
5	NAG	W	1	1,5	14,14,15	0.25	0	17,19,21	0.63	0
5	NAG	W	2	5	14,14,15	0.24	0	17,19,21	0.47	0
5	BMA	W	3	5	11,11,12	0.54	0	15,15,17	0.71	0
6	NAG	X	1	6,1	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
6	NAG	X	2	6	14,14,15	0.24	0	17,19,21	0.55	0
6	BMA	X	3	6	11,11,12	0.57	0	15,15,17	0.69	0
6	MAN	X	4	6	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
6	MAN	X	5	6	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
5	NAG	Y	1	2,5	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	Y	2	5	14,14,15	0.21	0	17,19,21	0.46	0
5	BMA	Y	3	5	11,11,12	0.54	0	15,15,17	0.74	0
7	NAG	Z	1	2,7	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
7	NAG	Z	2	7	14,14,15	0.23	0	17,19,21	0.59	0
7	BMA	Z	3	7	11,11,12	0.54	0	15,15,17	0.67	0
7	MAN	Z	4	7	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
6	NAG	a	1	2,6	14,14,15	0.25	0	17,19,21	0.50	0
6	NAG	a	2	6	14,14,15	0.39	0	17,19,21	1.18	2 (11%)
6	BMA	a	3	6	11,11,12	0.67	0	15,15,17	0.90	0
6	MAN	a	4	6	11,11,12	0.60	0	15,15,17	0.94	2 (13%)
6	MAN	a	5	6	11,11,12	0.61	0	15,15,17	0.94	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	W	2	5	-	4/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
6	NAG	X	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	BMA	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	0/2/19/22	0/1/1/1
6	MAN	X	5	6	-	1/2/19/22	1/1/1/1
5	NAG	Y	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
7	NAG	Z	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	4/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	0/1/1/1
6	NAG	a	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	3/6/23/26	0/1/1/1
6	BMA	a	3	6	-	2/2/19/22	0/1/1/1
6	MAN	a	4	6	-	0/2/19/22	0/1/1/1
6	MAN	a	5	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	1	NAG	C2-N2-C7	3.89	128.12	122.90
6	X	1	NAG	C2-N2-C7	3.88	128.10	122.90
6	Q	2	NAG	C2-N2-C7	3.87	128.09	122.90
6	N	1	NAG	C2-N2-C7	3.87	128.08	122.90
6	V	2	NAG	C2-N2-C7	3.86	128.07	122.90
6	a	2	NAG	C2-N2-C7	3.85	128.07	122.90
6	X	5	MAN	C1-O5-C5	3.45	116.81	112.19
6	N	5	MAN	C1-O5-C5	3.43	116.79	112.19
6	S	5	MAN	C1-O5-C5	3.41	116.76	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Z	1	NAG	C1-O5-C5	3.09	116.33	112.19
7	P	1	NAG	C1-O5-C5	3.05	116.28	112.19
7	U	1	NAG	C1-O5-C5	3.04	116.26	112.19
6	X	4	MAN	C1-O5-C5	2.54	115.58	112.19
6	N	4	MAN	C1-O5-C5	2.53	115.58	112.19
6	S	4	MAN	C1-O5-C5	2.51	115.55	112.19
7	Z	4	MAN	C1-O5-C5	2.30	115.27	112.19
7	U	4	MAN	C1-O5-C5	2.27	115.23	112.19
7	P	4	MAN	C1-O5-C5	2.27	115.22	112.19
6	Q	2	NAG	C1-C2-N2	2.22	113.93	110.43
6	X	4	MAN	O2-C2-C3	-2.21	105.56	110.15
6	V	4	MAN	C1-O5-C5	2.21	115.15	112.19
6	N	4	MAN	O2-C2-C3	-2.21	105.57	110.15
6	Q	4	MAN	C1-O5-C5	2.20	115.14	112.19
6	a	5	MAN	C1-O5-C5	2.19	115.12	112.19
6	S	4	MAN	O2-C2-C3	-2.18	105.63	110.15
6	a	2	NAG	C1-C2-N2	2.18	113.87	110.43
6	a	5	MAN	O2-C2-C3	-2.17	105.65	110.15
6	Q	5	MAN	C1-O5-C5	2.17	115.10	112.19
6	a	4	MAN	C1-O5-C5	2.17	115.09	112.19
6	V	2	NAG	C1-C2-N2	2.17	113.84	110.43
6	V	5	MAN	C1-O5-C5	2.16	115.08	112.19
6	a	4	MAN	O2-C2-C3	-2.15	105.69	110.15
6	V	4	MAN	O2-C2-C3	-2.15	105.70	110.15
6	V	5	MAN	O2-C2-C3	-2.15	105.70	110.15
6	Q	4	MAN	O2-C2-C3	-2.15	105.71	110.15
6	S	5	MAN	O2-C2-C3	-2.15	105.71	110.15
7	Z	4	MAN	O2-C2-C3	-2.13	105.73	110.15
6	X	5	MAN	O2-C2-C3	-2.13	105.74	110.15
7	P	4	MAN	O2-C2-C3	-2.13	105.74	110.15
6	Q	5	MAN	O2-C2-C3	-2.13	105.74	110.15
6	N	5	MAN	O2-C2-C3	-2.12	105.75	110.15
7	U	4	MAN	O2-C2-C3	-2.12	105.76	110.15
6	S	1	NAG	C1-C2-N2	2.10	113.74	110.43
6	N	1	NAG	C1-C2-N2	2.09	113.73	110.43
6	X	1	NAG	C1-C2-N2	2.09	113.72	110.43

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	Q	2	NAG	C1-C2-N2-C7
6	S	1	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7
6	X	1	NAG	C1-C2-N2-C7
6	a	2	NAG	C1-C2-N2-C7
5	M	3	BMA	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6
6	X	3	BMA	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	a	2	NAG	C8-C7-N2-C2
6	a	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
6	S	5	MAN	O5-C5-C6-O6
6	X	5	MAN	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	R	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C1-C2-N2-C7
7	P	2	NAG	C1-C2-N2-C7
7	U	2	NAG	C1-C2-N2-C7
7	Z	2	NAG	C1-C2-N2-C7
5	W	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C3-C2-N2-C7
5	R	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7
6	S	1	NAG	O5-C5-C6-O6
7	P	2	NAG	C3-C2-N2-C7
6	N	2	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	5	MAN	C1-C2-C3-C4-C5-O5
6	X	5	MAN	C1-C2-C3-C4-C5-O5
6	S	5	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 25 short contacts:

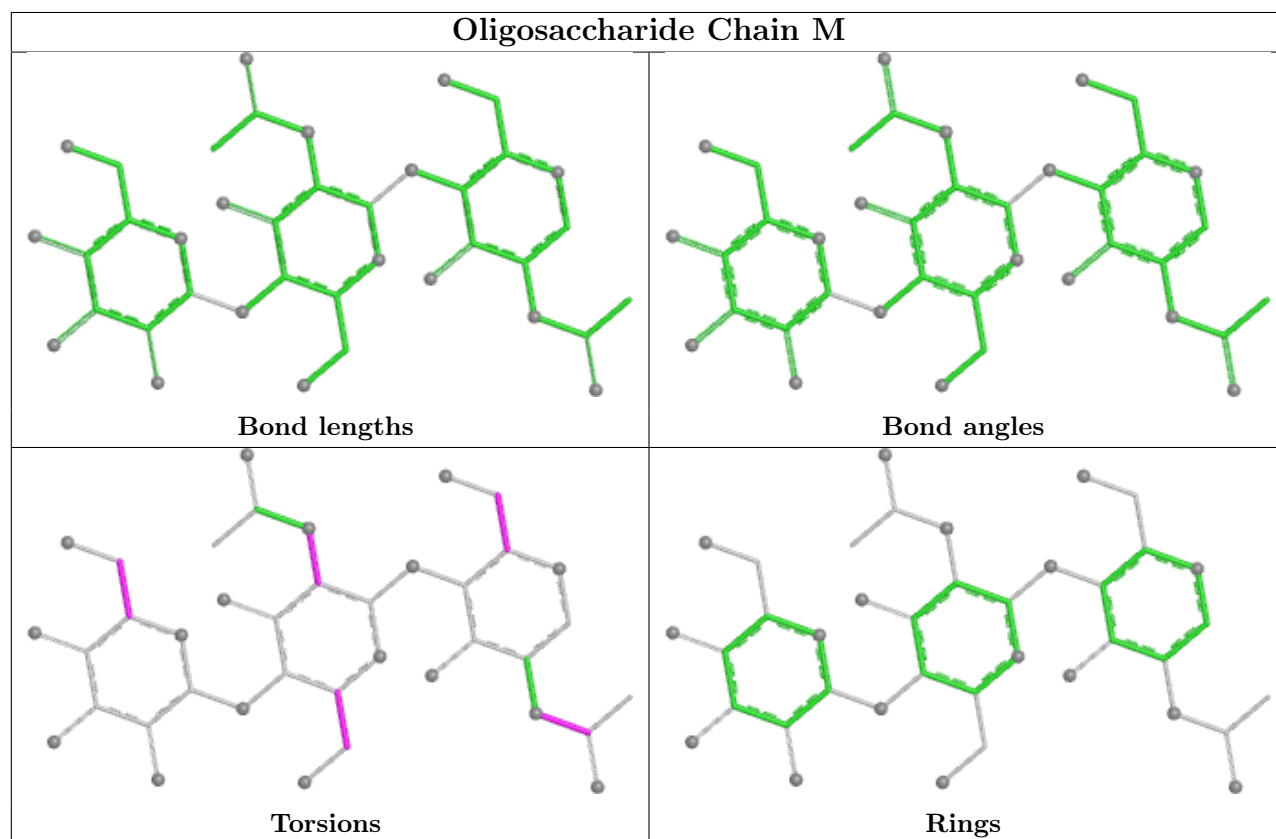
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1	NAG	2	0
5	M	3	BMA	1	0
5	M	1	NAG	1	0
7	P	2	NAG	1	0
6	N	1	NAG	2	0
5	R	3	BMA	1	0

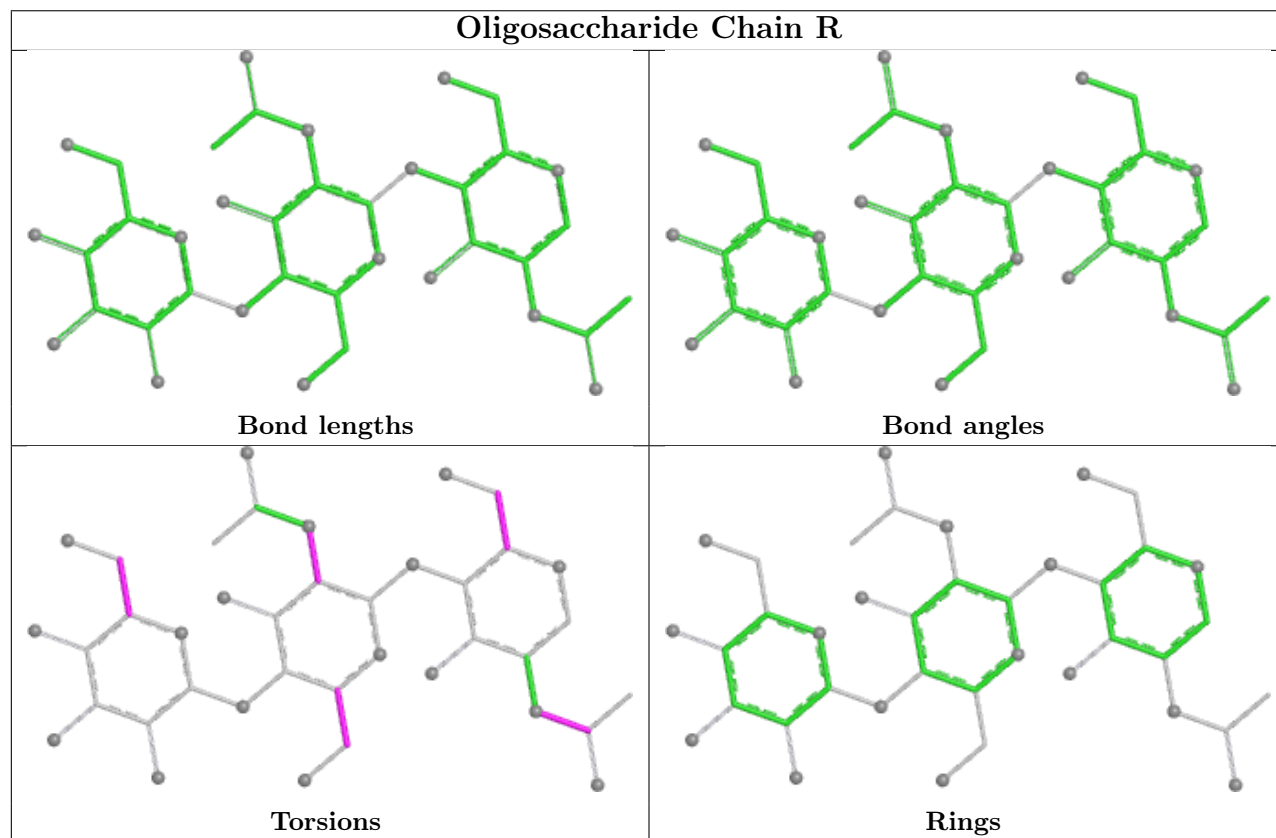
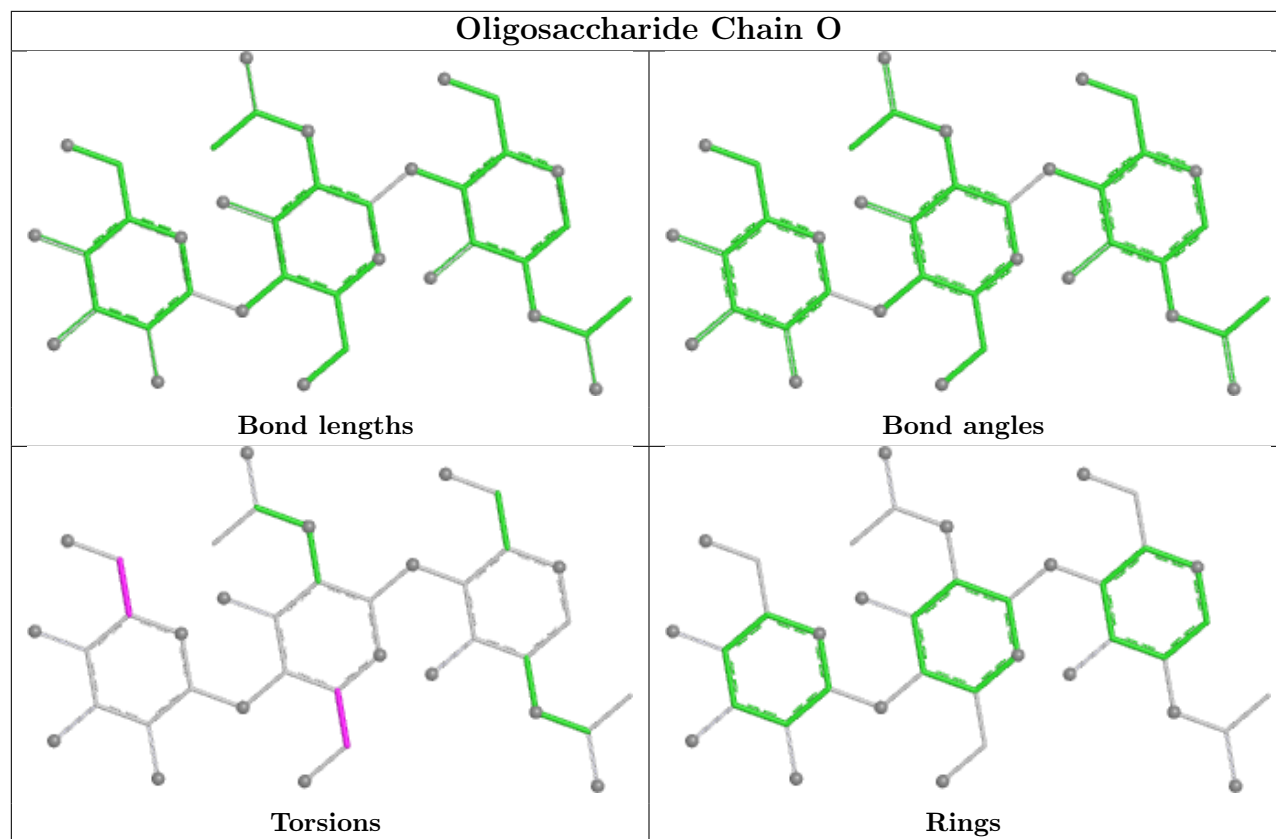
Continued on next page...

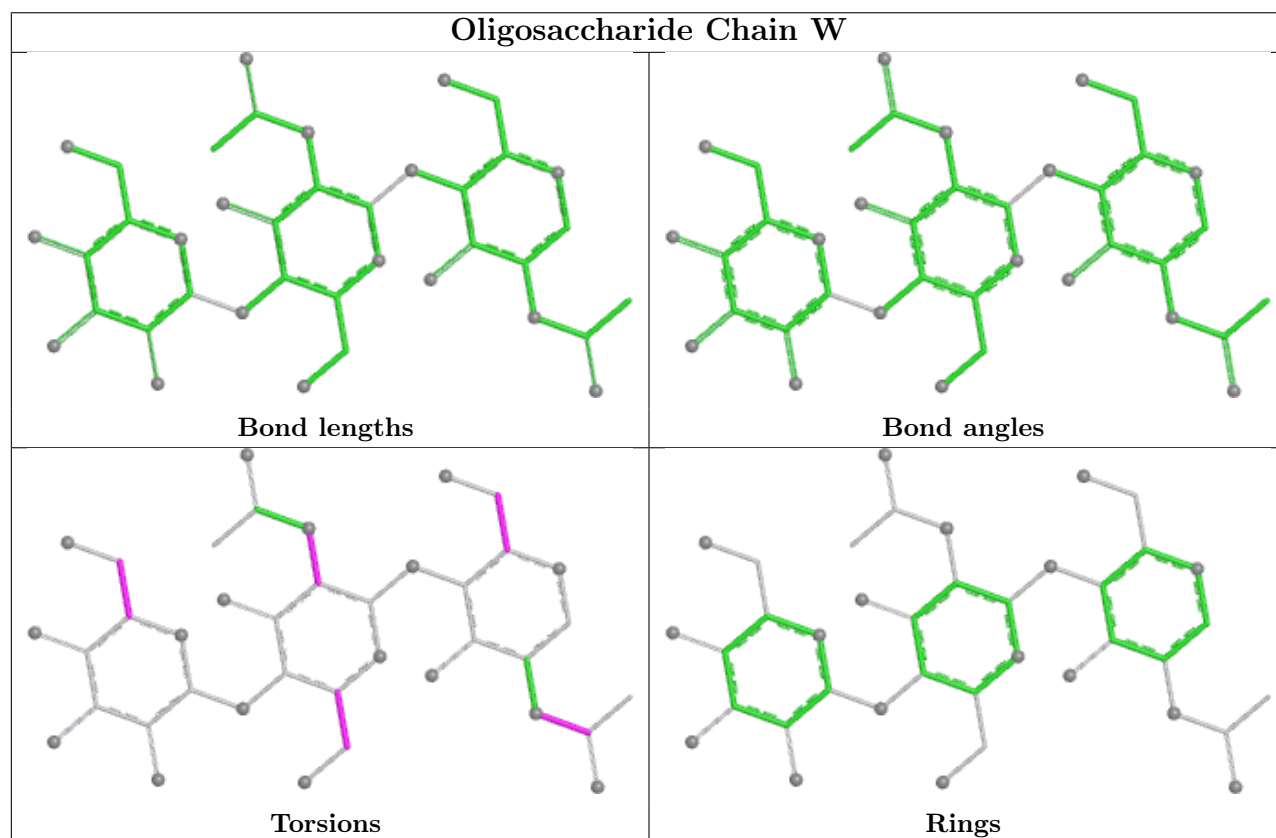
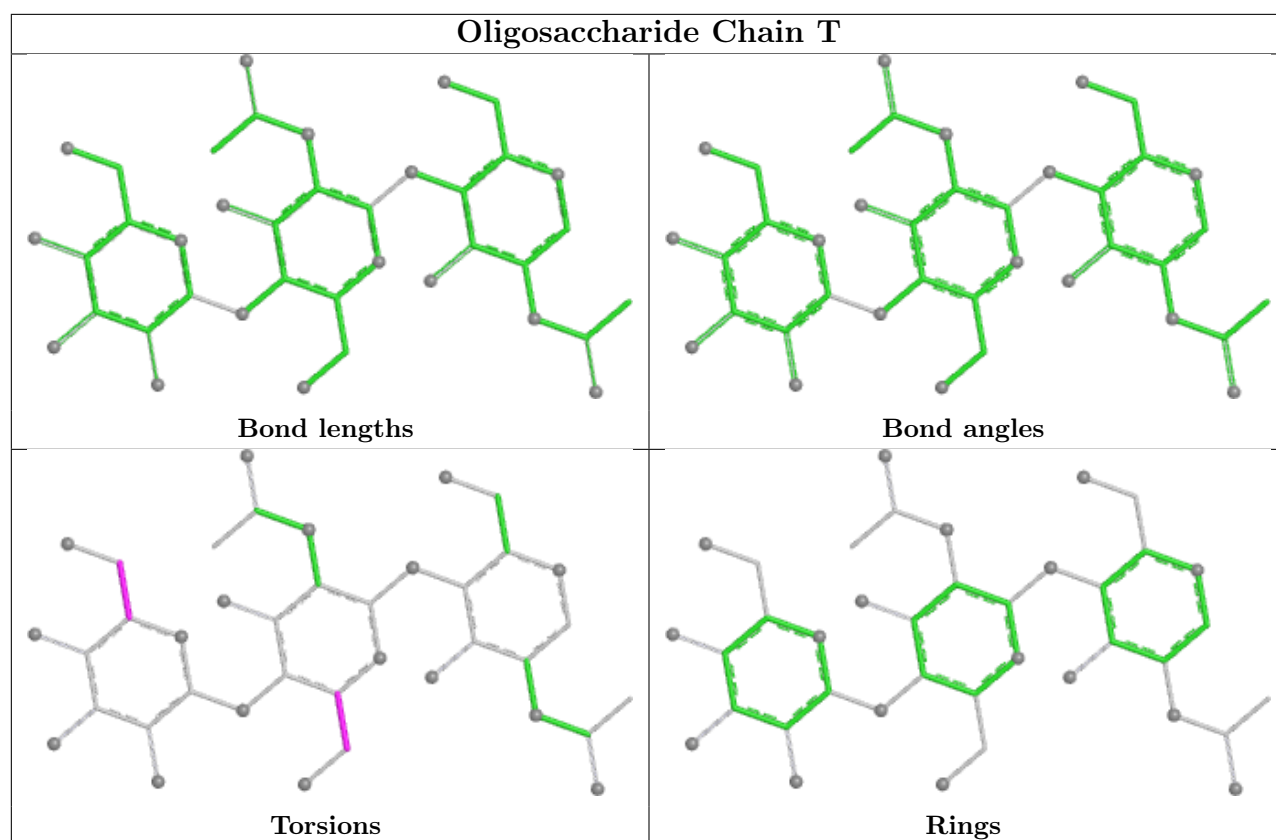
Continued from previous page...

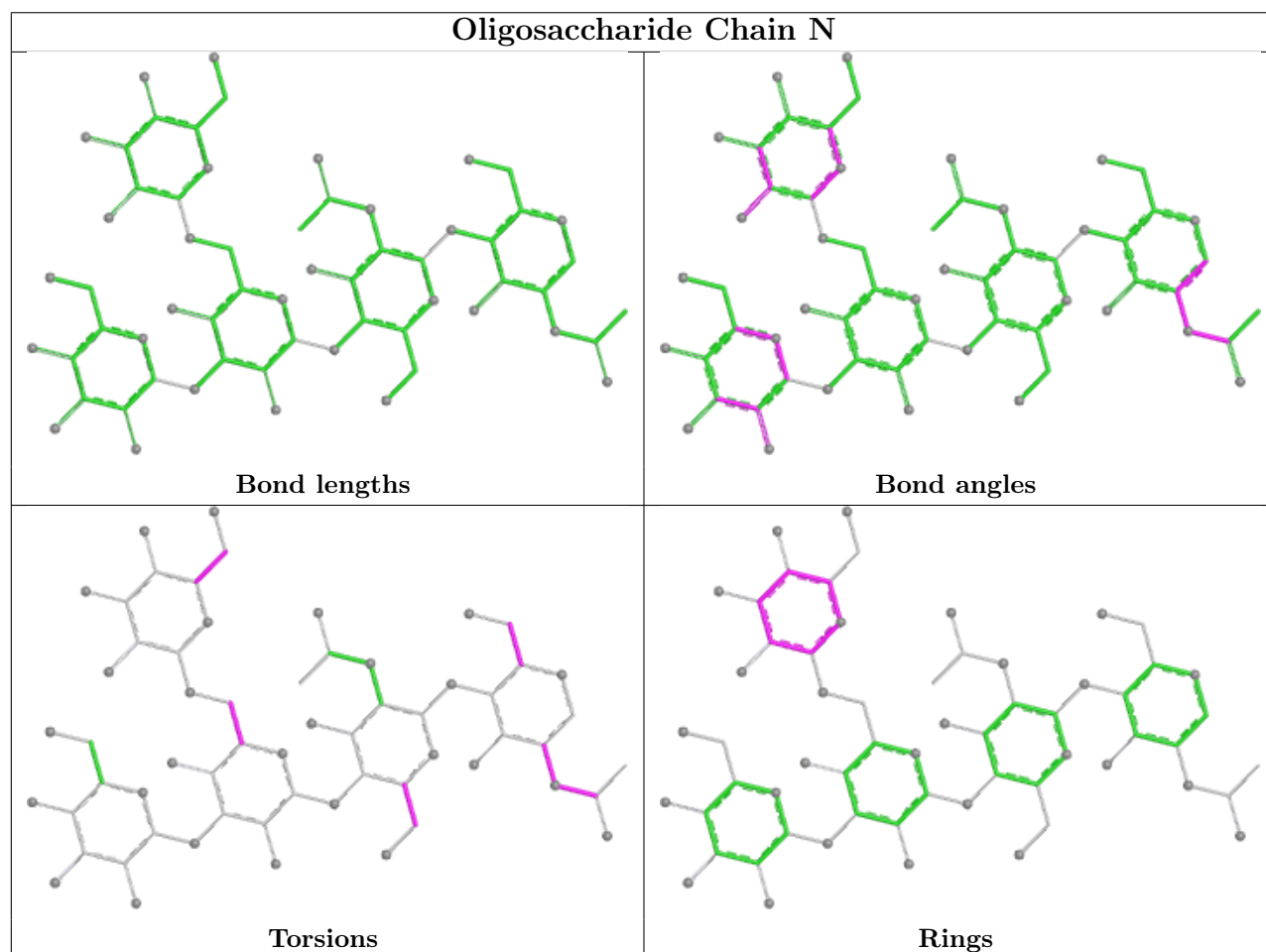
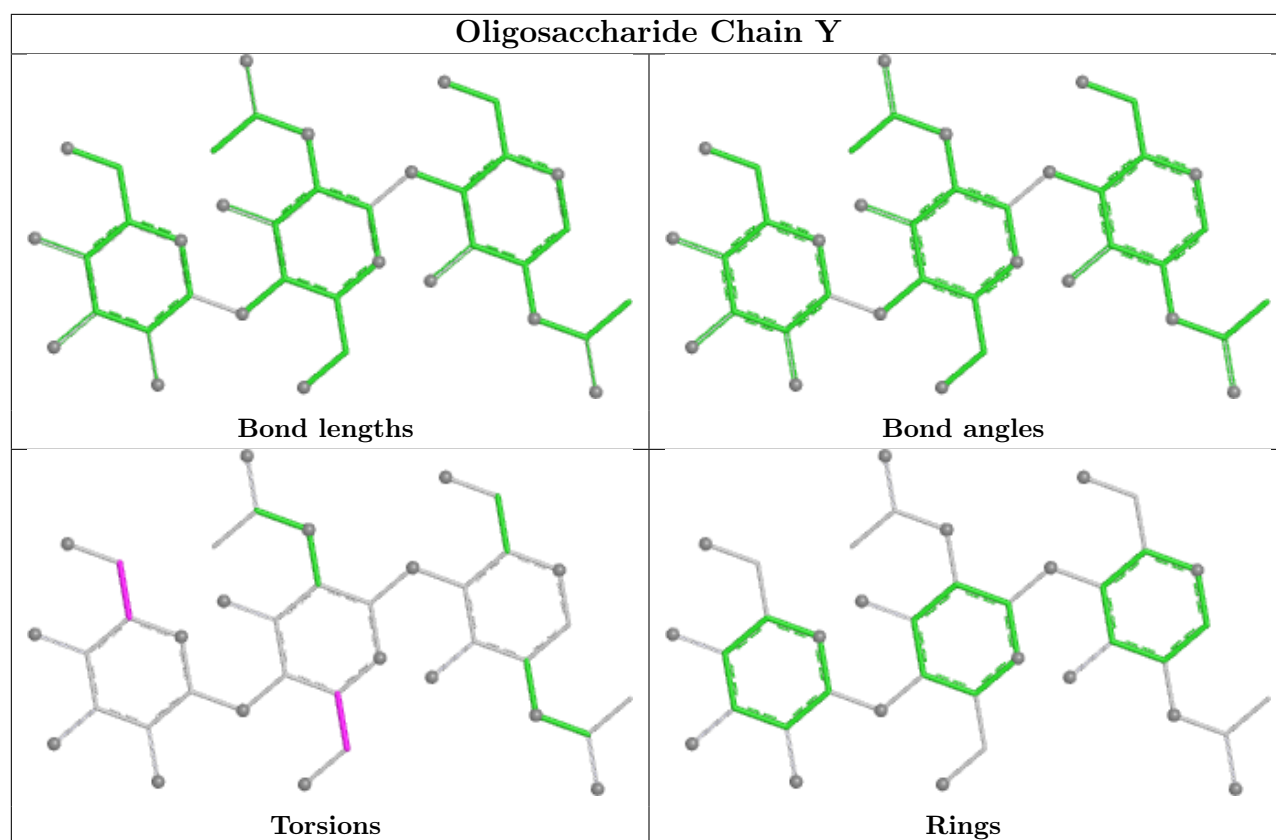
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	1	NAG	2	0
6	V	2	NAG	2	0
5	R	2	NAG	1	0
7	Z	1	NAG	2	0
5	M	2	NAG	2	0
7	U	1	NAG	2	0
5	W	3	BMA	1	0
6	Q	2	NAG	2	0
5	W	2	NAG	1	0
7	U	2	NAG	1	0
7	Z	2	NAG	1	0
6	a	2	NAG	2	0
6	X	1	NAG	2	0

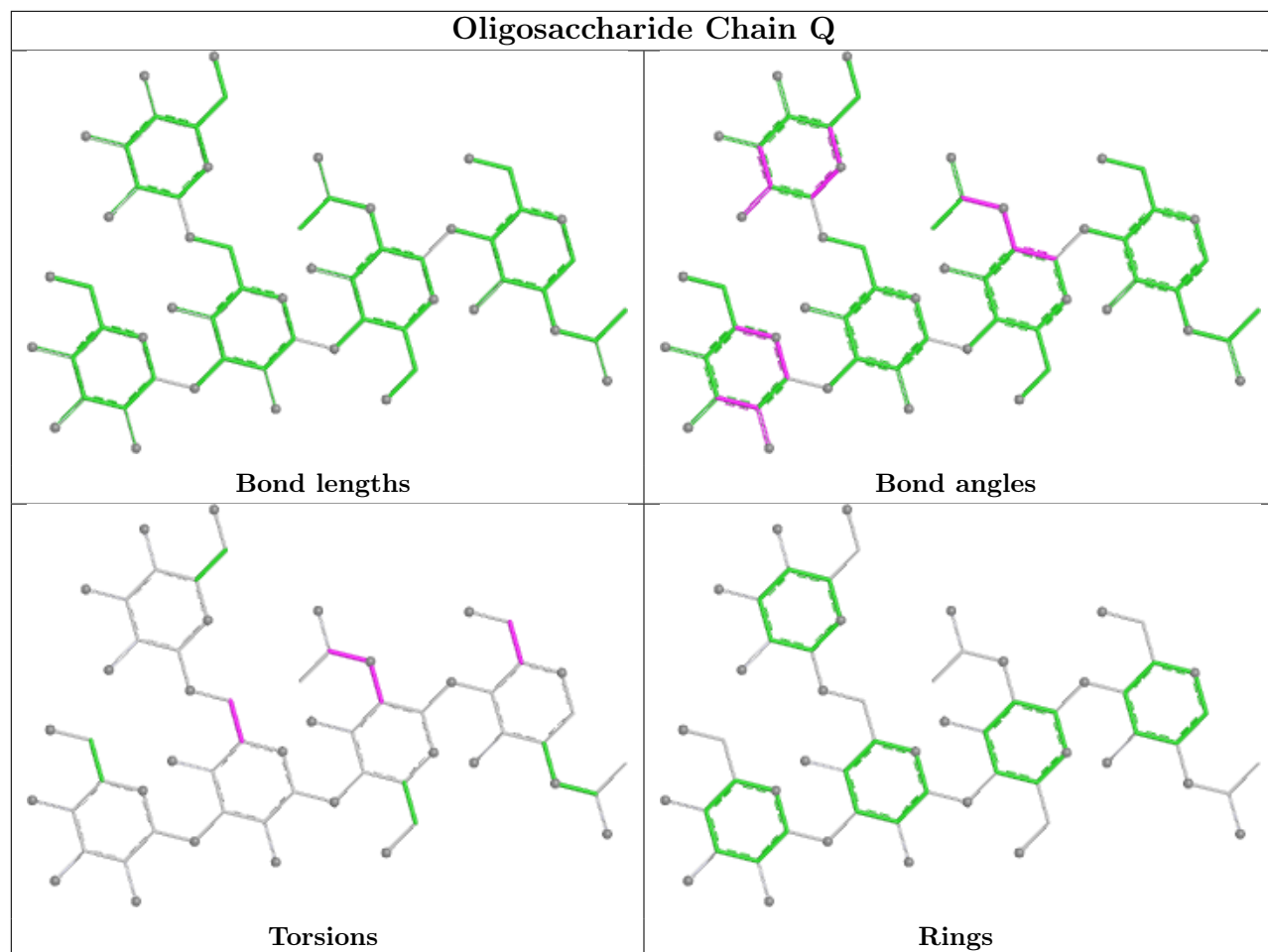
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

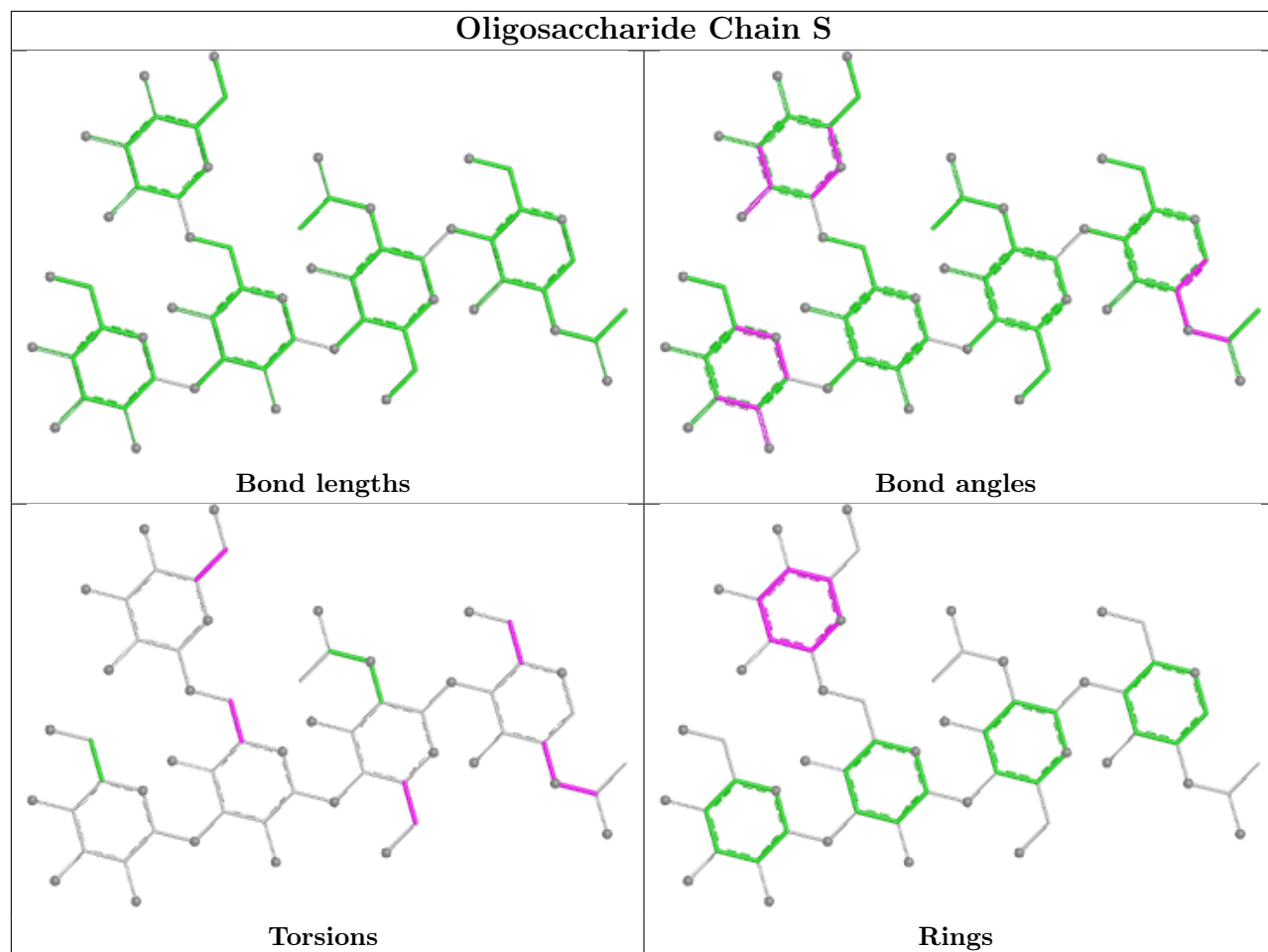


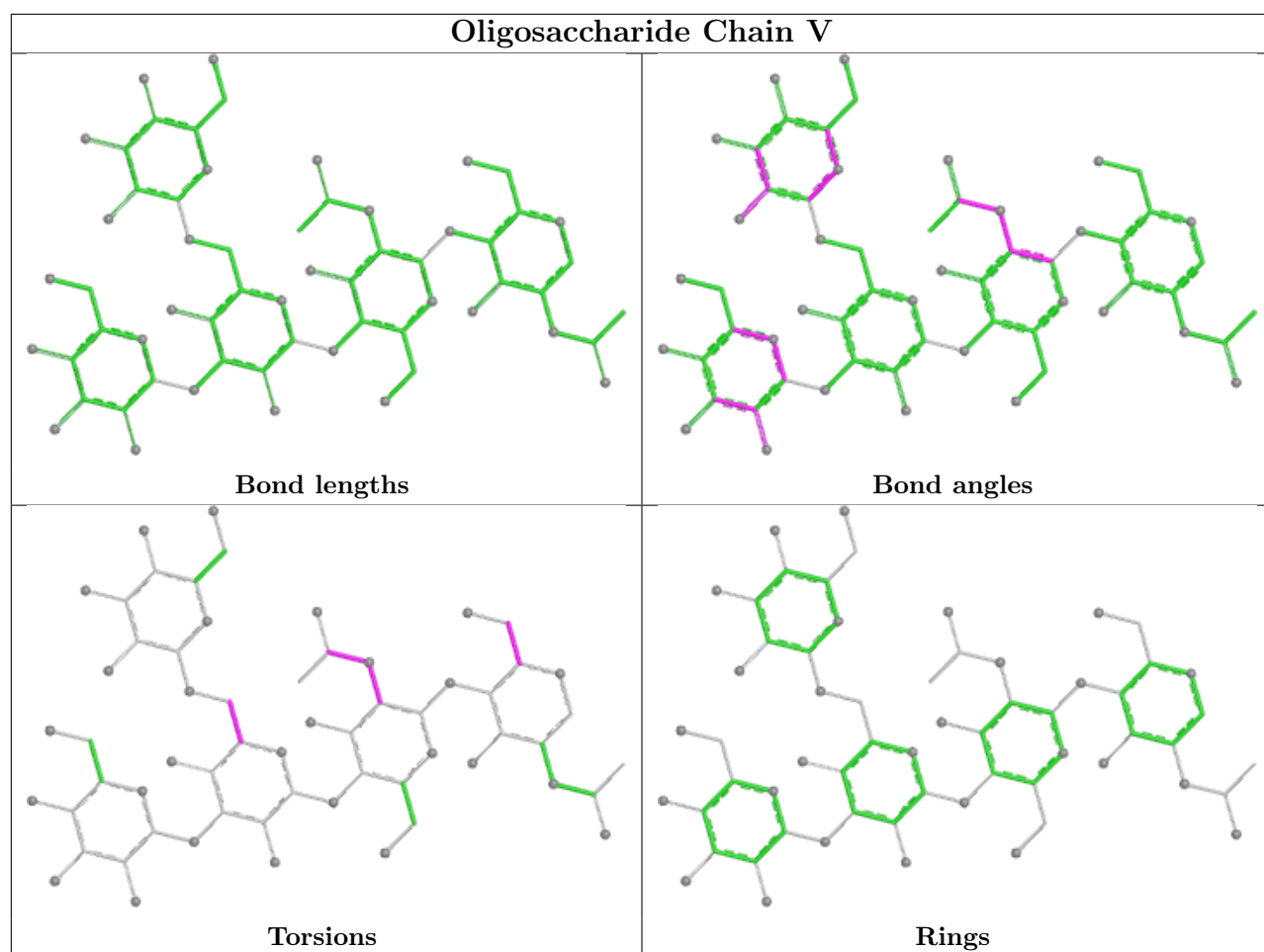


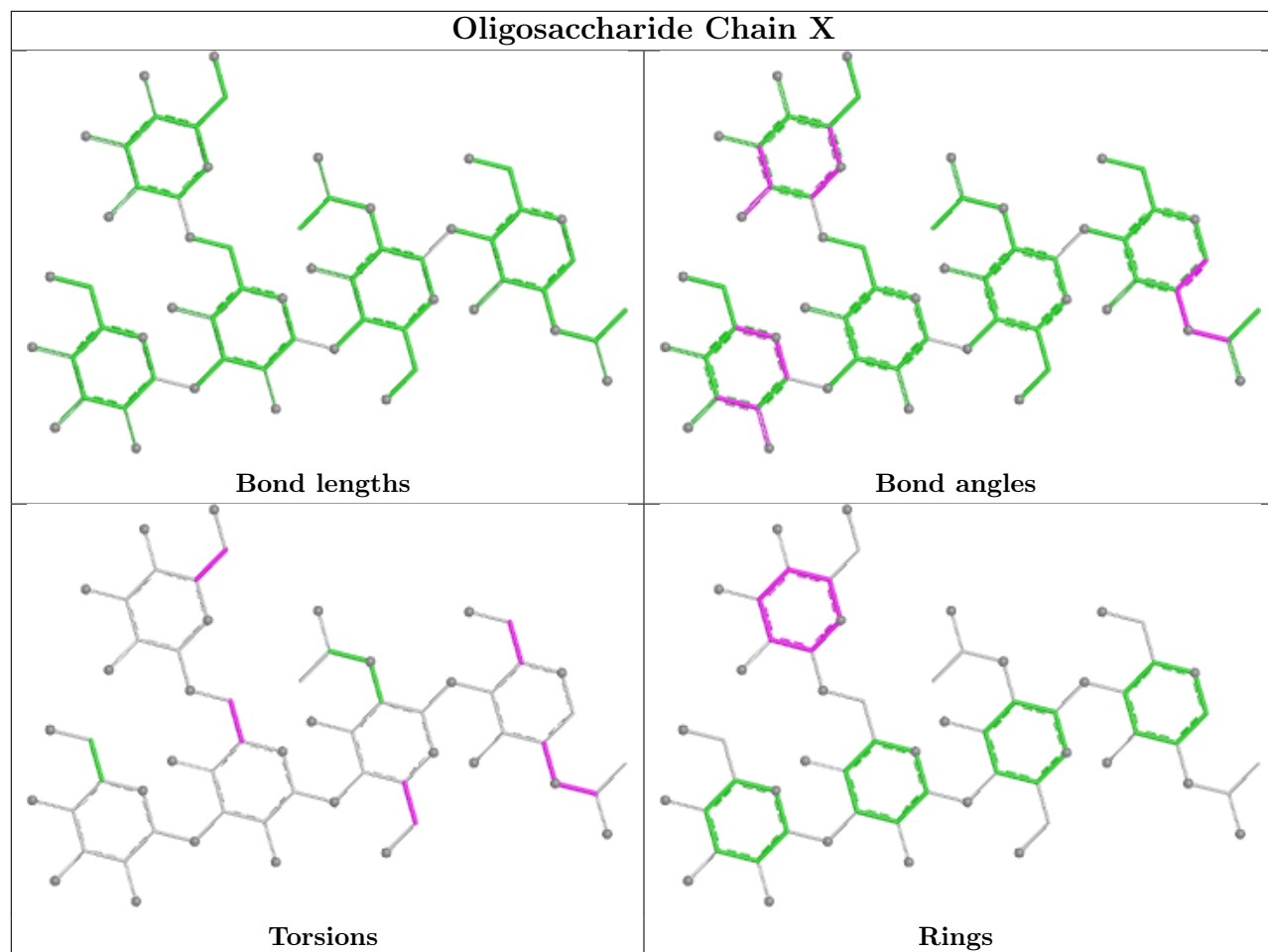


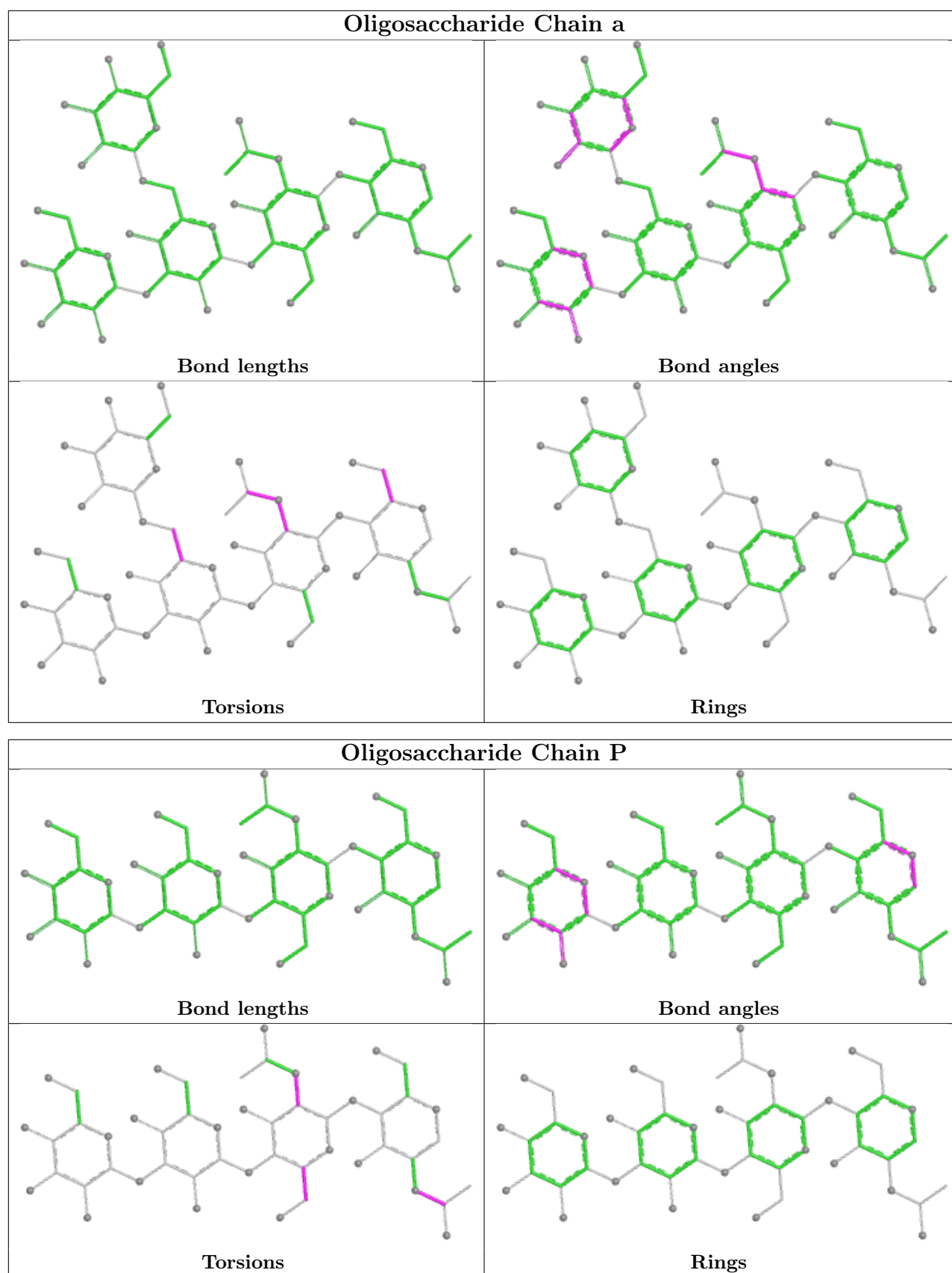


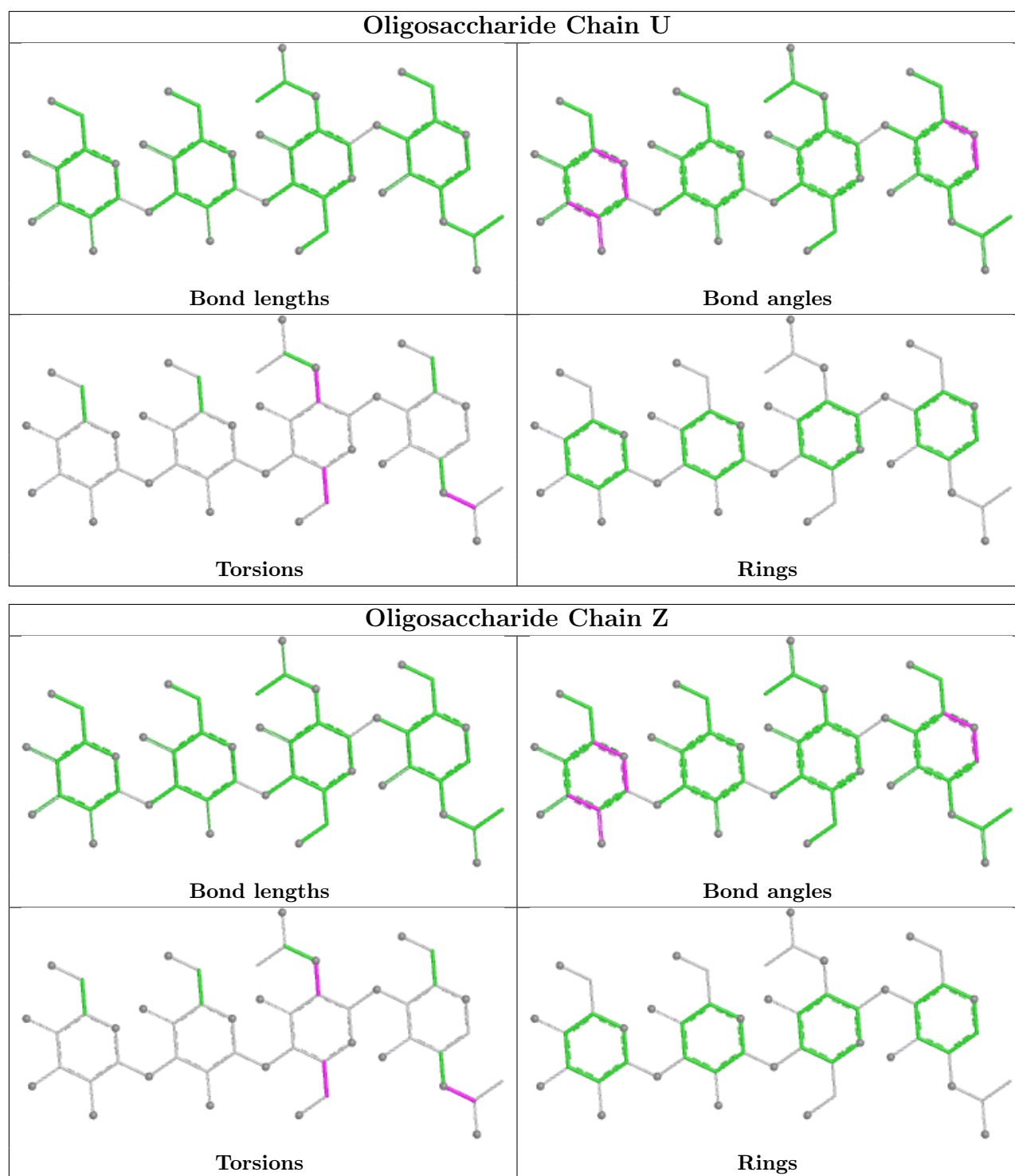












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
8	NAG	G	1004	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	I	1004	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	I	1003	2	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	I	1005	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	G	1005	2	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	G	1003	2	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	G	1008	2	14,14,15	0.40	0	17,19,21	0.75	0
8	NAG	C	1006	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	F	701	1	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
8	NAG	C	1003	2	14,14,15	0.28	0	17,19,21	1.25	1 (5%)
8	NAG	I	1008	2	14,14,15	0.32	0	17,19,21	1.16	3 (17%)
8	NAG	G	1001	2	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
8	NAG	C	1004	2	14,14,15	0.23	0	17,19,21	0.43	0
8	NAG	I	1001	2	14,14,15	0.31	0	17,19,21	0.67	0
8	NAG	G	1006	2	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	C	1002	2	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	C	1001	2	14,14,15	0.30	0	17,19,21	0.66	0
8	NAG	C	1008	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	B	701	1	14,14,15	0.42	0	17,19,21	1.19	2 (11%)
8	NAG	I	1002	2	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	A	701	1	14,14,15	0.43	0	17,19,21	1.19	2 (11%)
8	NAG	C	1007	2	14,14,15	0.24	0	17,19,21	0.44	0
8	NAG	G	1002	2	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	I	1007	2	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	C	1005	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	I	1006	2	14,14,15	0.24	0	17,19,21	0.43	0
8	NAG	G	1007	2	14,14,15	0.22	0	17,19,21	0.42	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
8	NAG	G	1004	2	-	3/6/23/26	0/1/1/1
8	NAG	I	1004	2	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	I	1003	2	-	0/6/23/26	0/1/1/1
8	NAG	I	1005	2	-	4/6/23/26	0/1/1/1
8	NAG	G	1005	2	-	4/6/23/26	0/1/1/1
8	NAG	G	1003	2	-	0/6/23/26	0/1/1/1
8	NAG	G	1008	2	-	3/6/23/26	0/1/1/1
8	NAG	C	1006	2	-	4/6/23/26	0/1/1/1
8	NAG	F	701	1	-	5/6/23/26	0/1/1/1
8	NAG	C	1003	2	-	4/6/23/26	0/1/1/1
8	NAG	I	1008	2	-	4/6/23/26	0/1/1/1
8	NAG	G	1001	2	-	4/6/23/26	0/1/1/1
8	NAG	C	1004	2	-	0/6/23/26	0/1/1/1
8	NAG	I	1001	2	-	4/6/23/26	0/1/1/1
8	NAG	G	1006	2	-	2/6/23/26	0/1/1/1
8	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
8	NAG	C	1001	2	-	4/6/23/26	0/1/1/1
8	NAG	C	1008	2	-	4/6/23/26	0/1/1/1
8	NAG	B	701	1	-	5/6/23/26	0/1/1/1
8	NAG	I	1002	2	-	0/6/23/26	0/1/1/1
8	NAG	A	701	1	-	5/6/23/26	0/1/1/1
8	NAG	C	1007	2	-	2/6/23/26	0/1/1/1
8	NAG	G	1002	2	-	0/6/23/26	0/1/1/1
8	NAG	I	1007	2	-	4/6/23/26	0/1/1/1
8	NAG	C	1005	2	-	3/6/23/26	0/1/1/1
8	NAG	I	1006	2	-	2/6/23/26	0/1/1/1
8	NAG	G	1007	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	NAG	C2-N2-C7	3.92	128.15	122.90
8	A	701	NAG	C2-N2-C7	3.88	128.10	122.90
8	F	701	NAG	C2-N2-C7	3.86	128.08	122.90
8	I	1008	NAG	C6-C5-C4	-2.45	107.00	113.02
8	I	1008	NAG	C2-N2-C7	-2.39	119.69	122.90
8	C	1003	NAG	O5-C1-C2	-2.35	107.65	111.29
8	F	701	NAG	C1-C2-N2	2.17	113.86	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	701	NAG	C1-C2-N2	2.16	113.84	110.43
8	B	701	NAG	C1-C2-N2	2.14	113.81	110.43
8	G	1001	NAG	C2-N2-C7	2.04	125.63	122.90
8	I	1008	NAG	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	701	NAG	C1-C2-N2-C7
8	A	701	NAG	C1-C2-N2-C7
8	F	701	NAG	C1-C2-N2-C7
8	G	1008	NAG	C4-C5-C6-O6
8	G	1004	NAG	O5-C5-C6-O6
8	C	1005	NAG	O5-C5-C6-O6
8	I	1004	NAG	O5-C5-C6-O6
8	G	1006	NAG	O5-C5-C6-O6
8	I	1006	NAG	O5-C5-C6-O6
8	I	1008	NAG	O5-C5-C6-O6
8	C	1007	NAG	O5-C5-C6-O6
8	G	1001	NAG	O5-C5-C6-O6
8	C	1001	NAG	O5-C5-C6-O6
8	C	1003	NAG	O5-C5-C6-O6
8	G	1008	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	F	701	NAG	O5-C5-C6-O6
8	I	1001	NAG	O5-C5-C6-O6
8	F	701	NAG	C4-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	A	701	NAG	C4-C5-C6-O6
8	G	1001	NAG	C4-C5-C6-O6
8	C	1001	NAG	C4-C5-C6-O6
8	I	1001	NAG	C4-C5-C6-O6
8	I	1007	NAG	O5-C5-C6-O6
8	B	701	NAG	C8-C7-N2-C2
8	B	701	NAG	O7-C7-N2-C2
8	G	1001	NAG	C8-C7-N2-C2
8	G	1001	NAG	O7-C7-N2-C2
8	G	1005	NAG	C8-C7-N2-C2
8	G	1005	NAG	O7-C7-N2-C2
8	A	701	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	O7-C7-N2-C2
8	C	1001	NAG	C8-C7-N2-C2
8	C	1001	NAG	O7-C7-N2-C2
8	C	1006	NAG	C8-C7-N2-C2
8	C	1006	NAG	O7-C7-N2-C2
8	F	701	NAG	C8-C7-N2-C2
8	F	701	NAG	O7-C7-N2-C2
8	I	1001	NAG	C8-C7-N2-C2
8	I	1001	NAG	O7-C7-N2-C2
8	I	1005	NAG	C8-C7-N2-C2
8	I	1005	NAG	O7-C7-N2-C2
8	I	1008	NAG	C8-C7-N2-C2
8	C	1008	NAG	O5-C5-C6-O6
8	G	1007	NAG	O5-C5-C6-O6
8	I	1004	NAG	C4-C5-C6-O6
8	C	1005	NAG	C4-C5-C6-O6
8	G	1004	NAG	C4-C5-C6-O6
8	I	1008	NAG	O7-C7-N2-C2
8	I	1006	NAG	C4-C5-C6-O6
8	C	1007	NAG	C4-C5-C6-O6
8	I	1008	NAG	C4-C5-C6-O6
8	G	1006	NAG	C4-C5-C6-O6
8	I	1005	NAG	C4-C5-C6-O6
8	C	1006	NAG	C4-C5-C6-O6
8	G	1005	NAG	C4-C5-C6-O6
8	C	1003	NAG	C4-C5-C6-O6
8	I	1005	NAG	O5-C5-C6-O6
8	G	1007	NAG	C1-C2-N2-C7
8	C	1003	NAG	C1-C2-N2-C7
8	C	1008	NAG	C1-C2-N2-C7
8	I	1007	NAG	C1-C2-N2-C7
8	G	1005	NAG	O5-C5-C6-O6
8	C	1006	NAG	O5-C5-C6-O6
8	G	1007	NAG	C3-C2-N2-C7
8	C	1003	NAG	C3-C2-N2-C7
8	C	1008	NAG	C3-C2-N2-C7
8	I	1007	NAG	C3-C2-N2-C7
8	I	1007	NAG	C4-C5-C6-O6
8	G	1004	NAG	C1-C2-N2-C7
8	G	1008	NAG	C1-C2-N2-C7
8	C	1005	NAG	C1-C2-N2-C7
8	I	1004	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	1007	NAG	C4-C5-C6-O6
8	C	1008	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	1008	NAG	2	0
8	F	701	NAG	2	0
8	C	1003	NAG	6	0
8	I	1008	NAG	2	0
8	B	701	NAG	2	0
8	A	701	NAG	2	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.

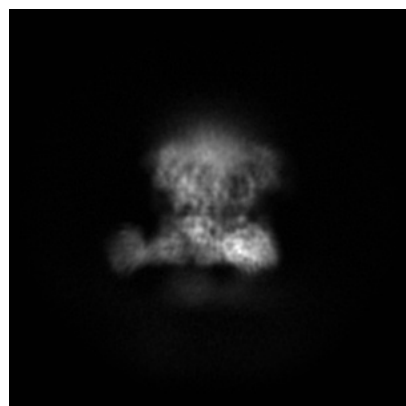
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27718. These allow visual inspection of the internal detail of the map and identification of artifacts.

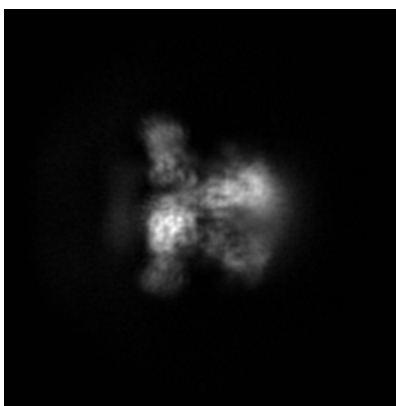
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

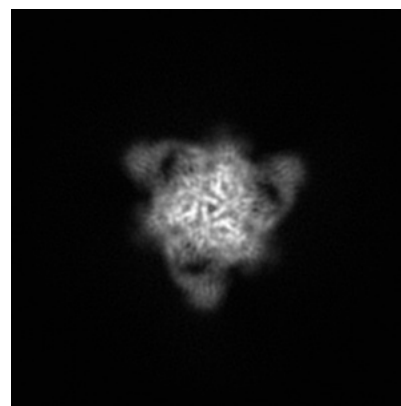
6.1.1 Primary map



X

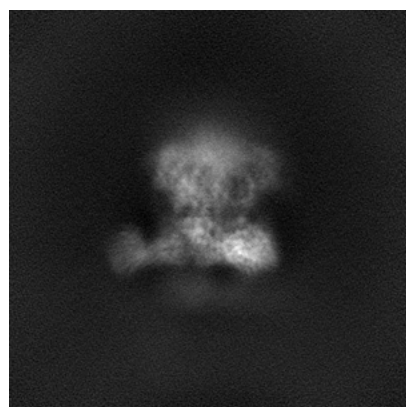


Y

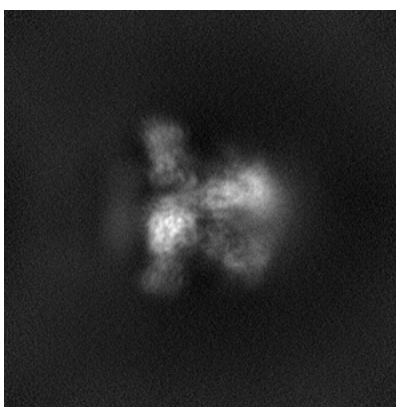


Z

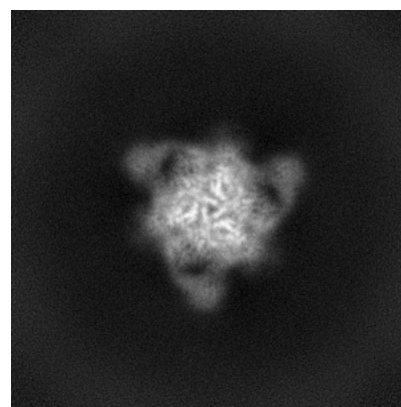
6.1.2 Raw map



X



Y

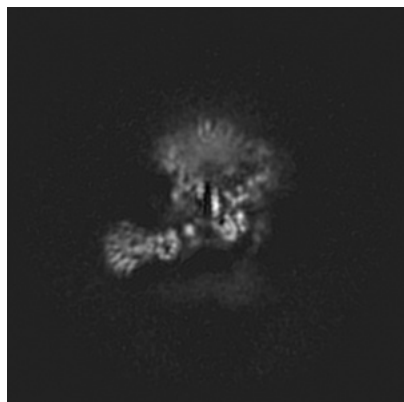


Z

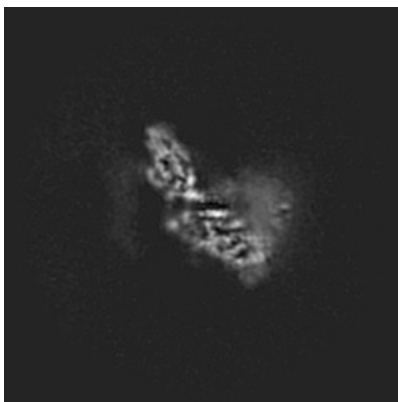
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

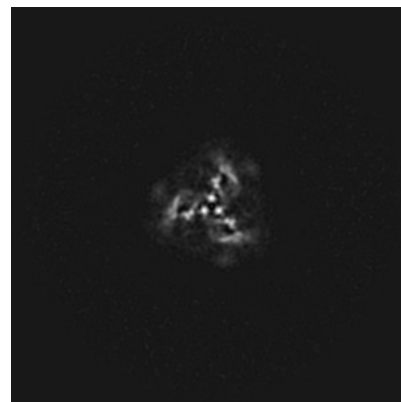
6.2.1 Primary map



X Index: 160

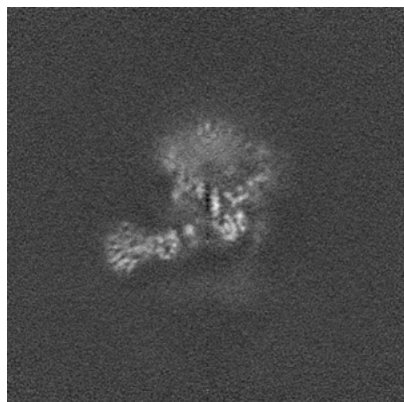


Y Index: 160



Z Index: 160

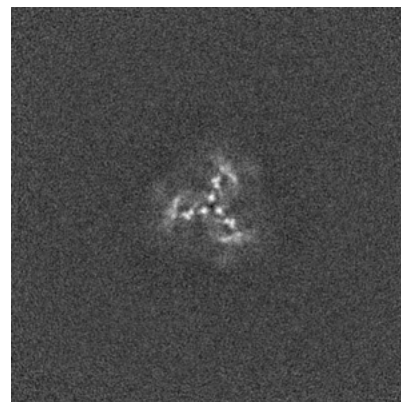
6.2.2 Raw map



X Index: 160



Y Index: 160

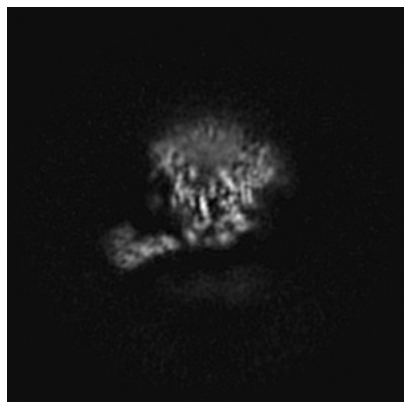


Z Index: 160

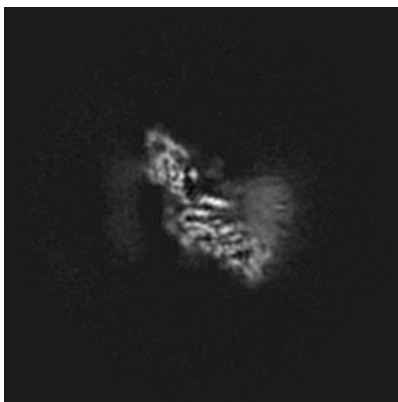
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

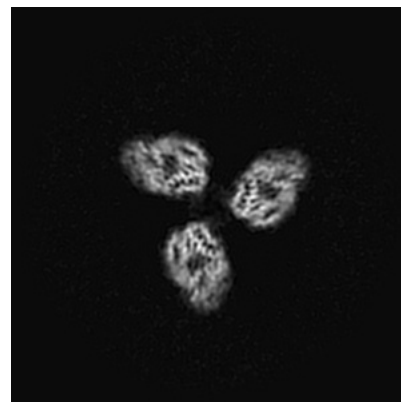
6.3.1 Primary map



X Index: 166

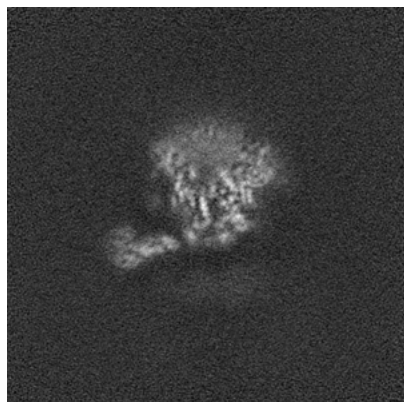


Y Index: 155

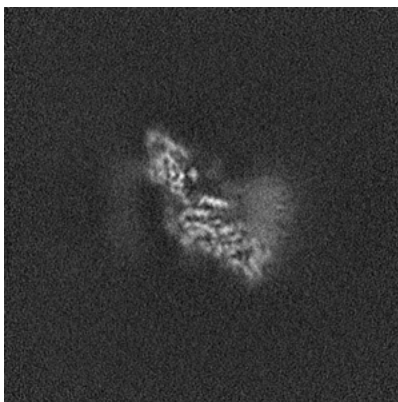


Z Index: 125

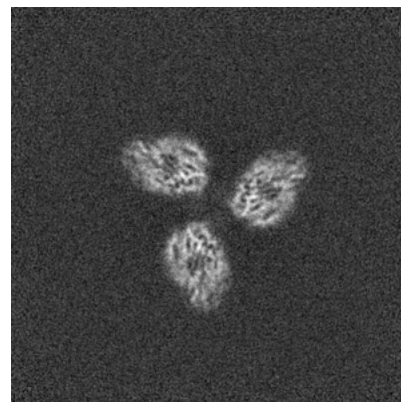
6.3.2 Raw map



X Index: 166



Y Index: 155

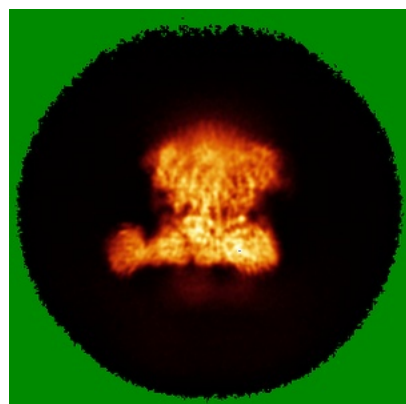


Z Index: 125

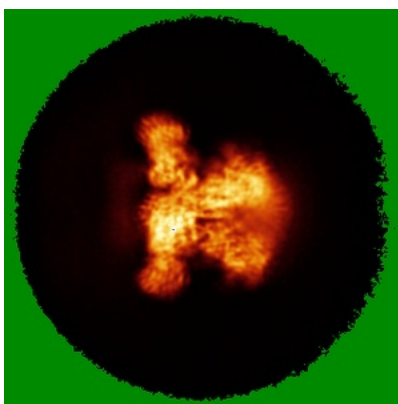
The images above show the largest variance slices of the map in three orthogonal directions.

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

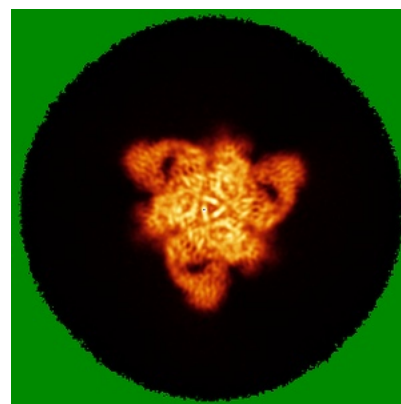
6.4.1 Primary map



X

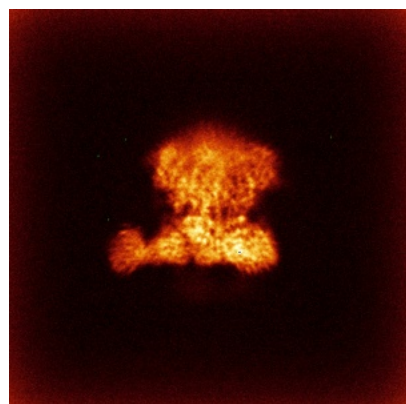


Y

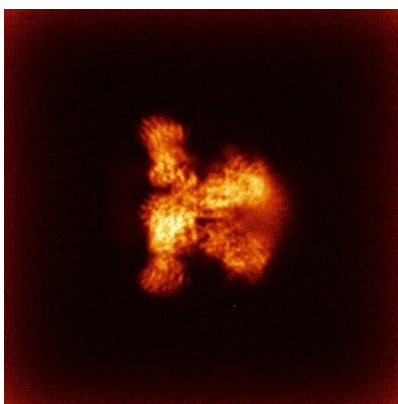


Z

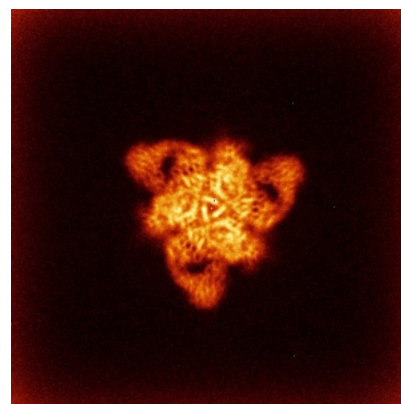
6.4.2 Raw map



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.

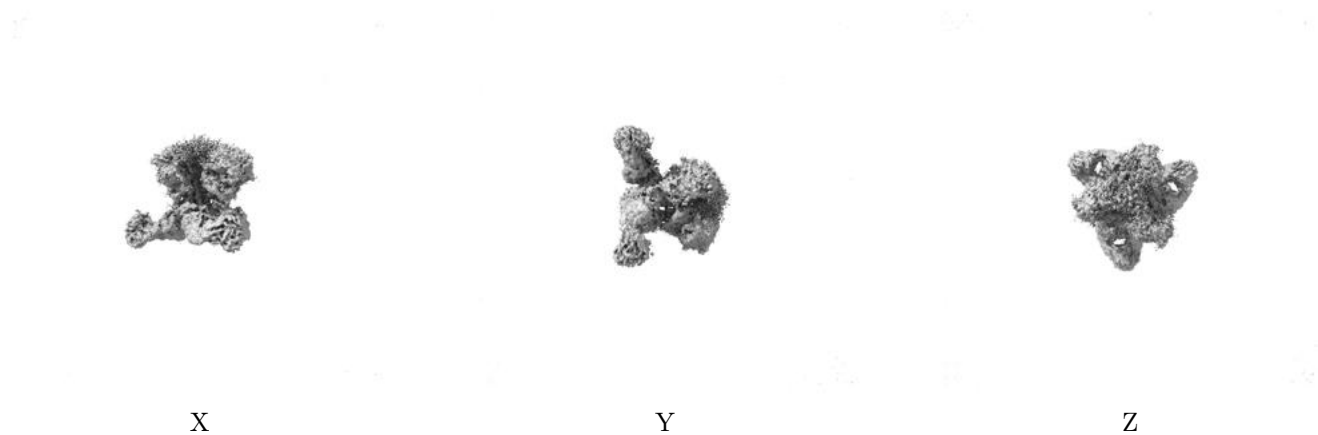
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

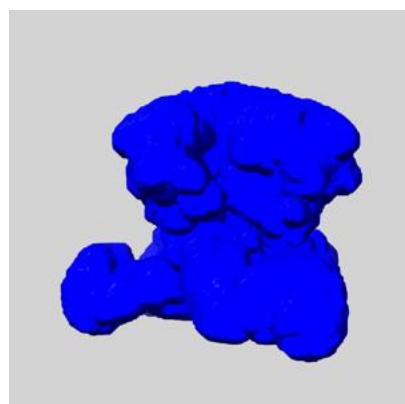
6.6 Mask visualisation [i](#)

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

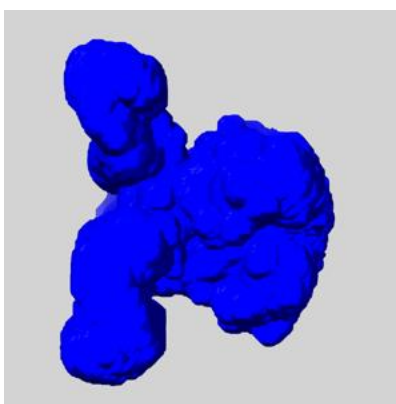
A mask typically either:

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

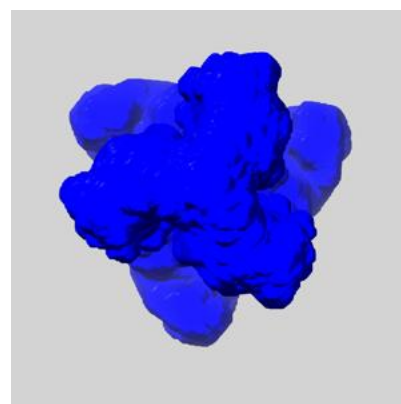
6.6.1 emd_27718_msk_1.map [i](#)



X



Y

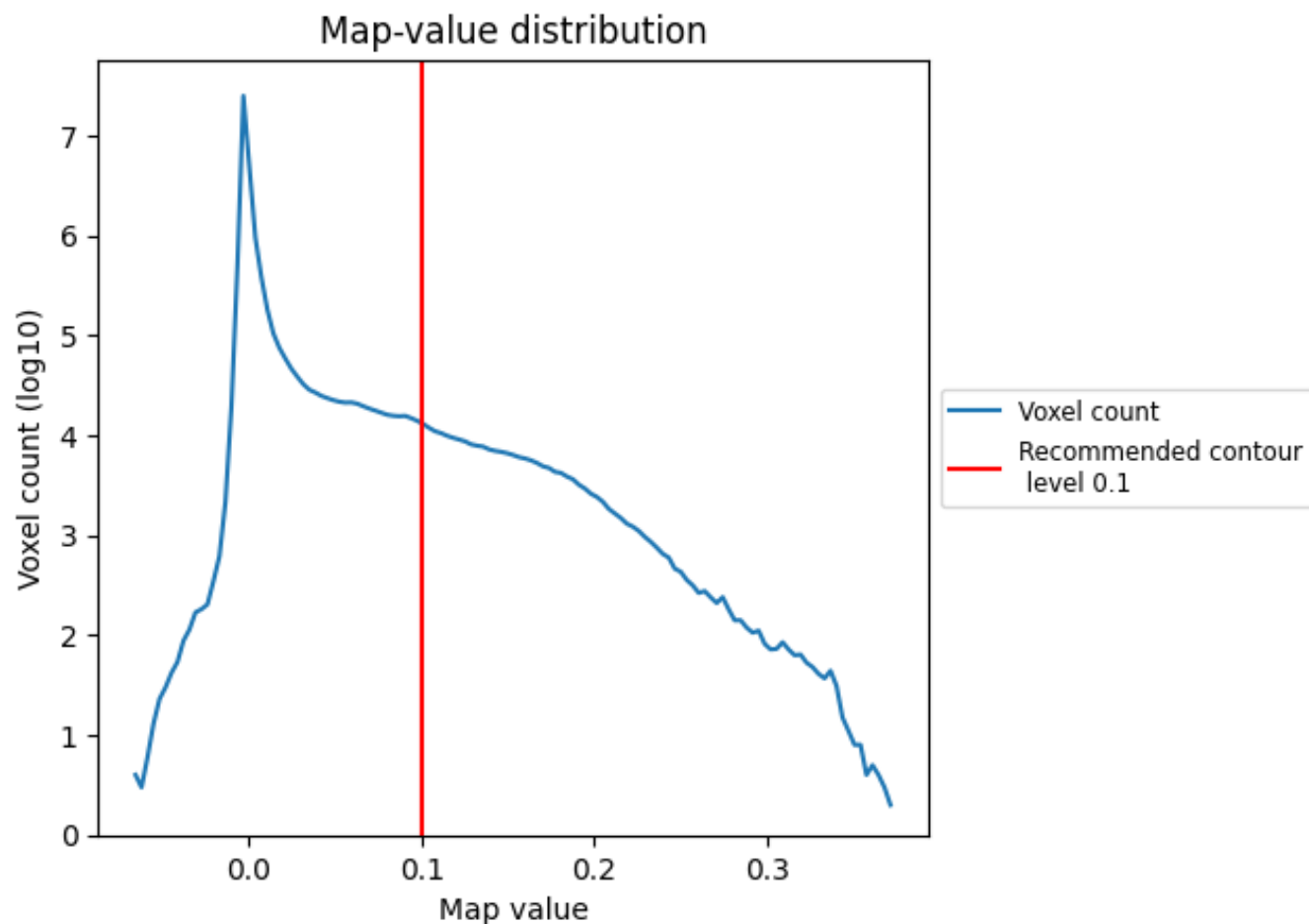


Z

7 Map analysis [i](#)

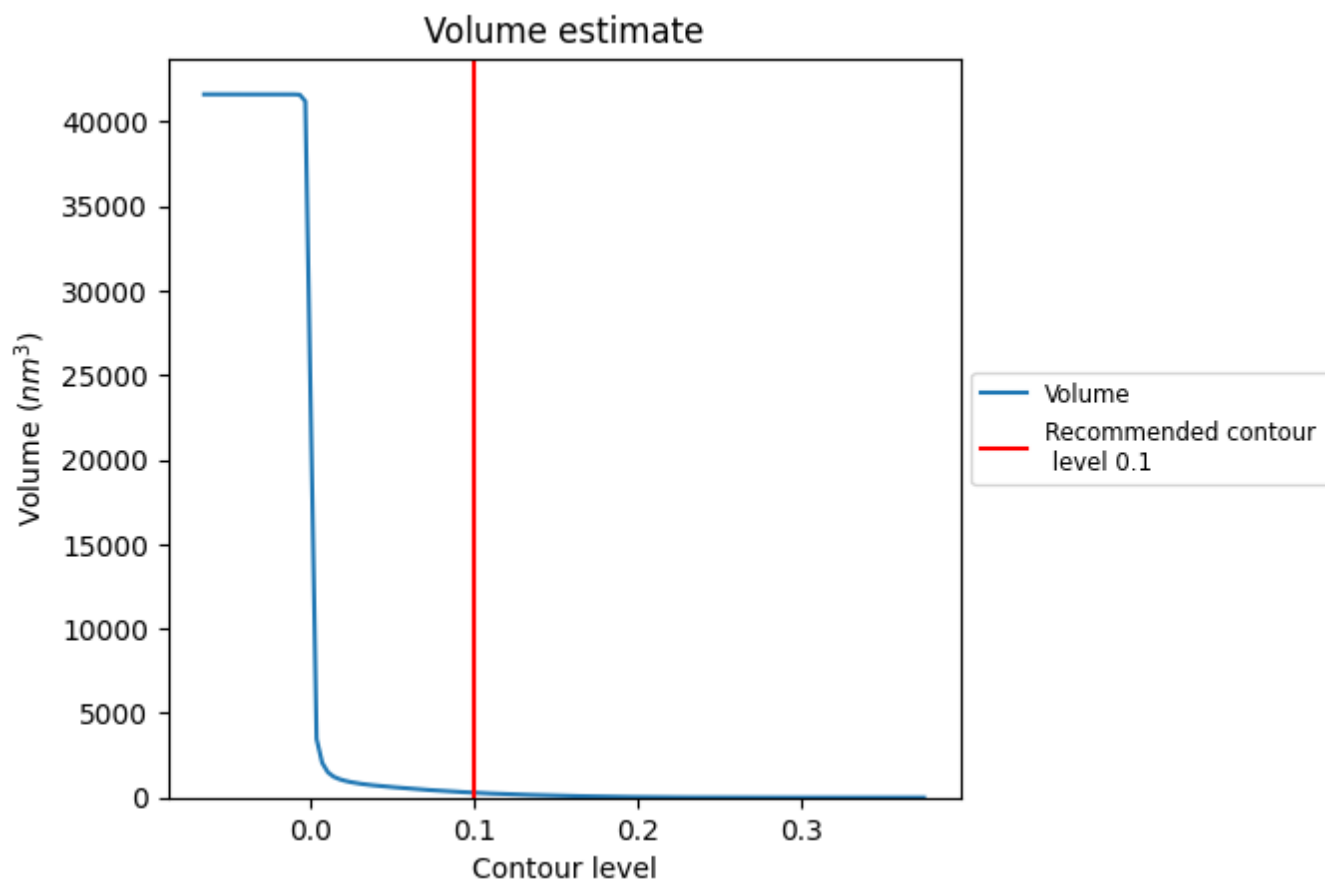
This section contains the results of statistical analysis of the map.

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.

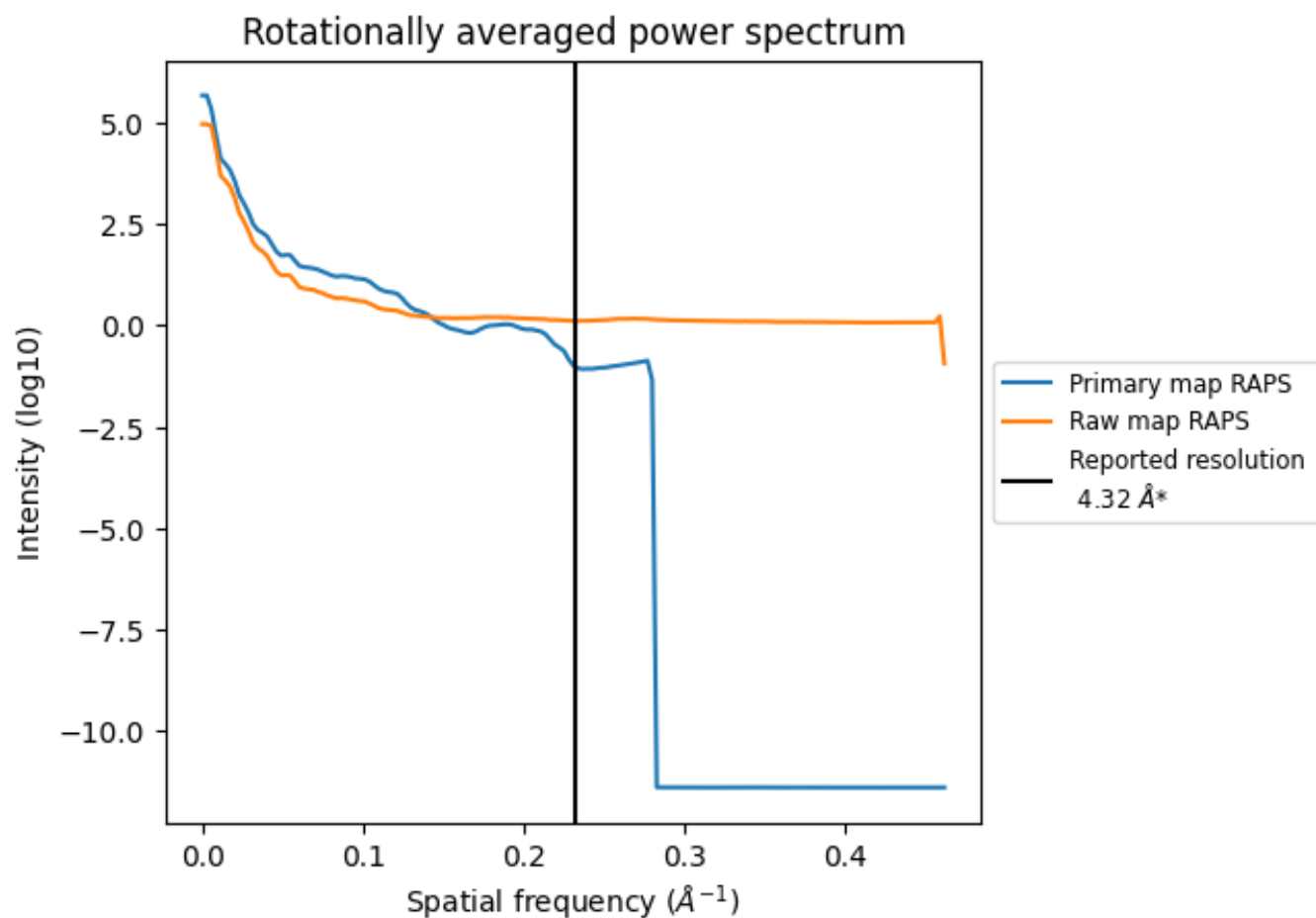
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm^3 ; this corresponds to an approximate mass of 257 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 ⓘ

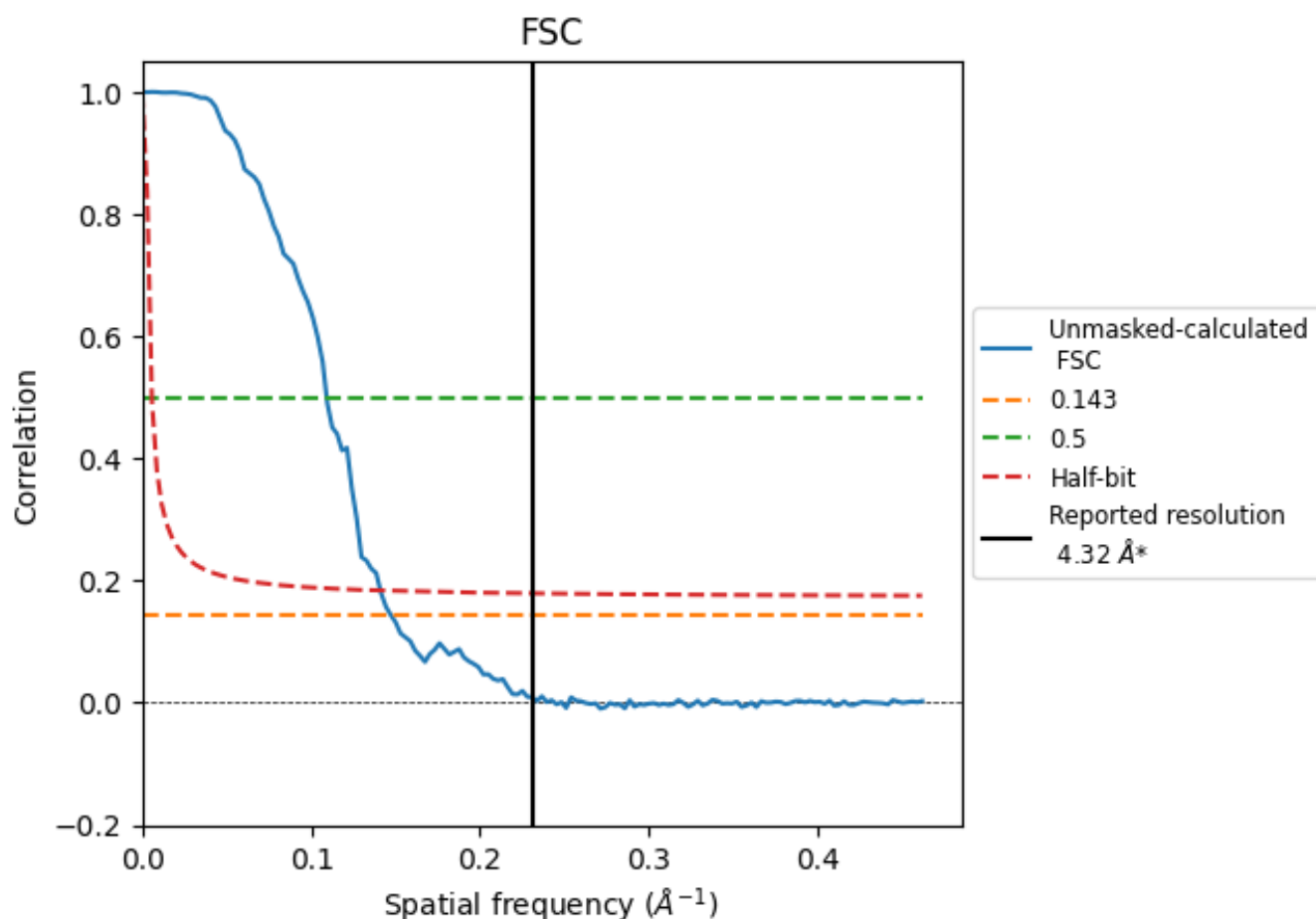


*Reported resolution corresponds to spatial frequency of 0.231 $\text{\AA}^{-1}$

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 0.231 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

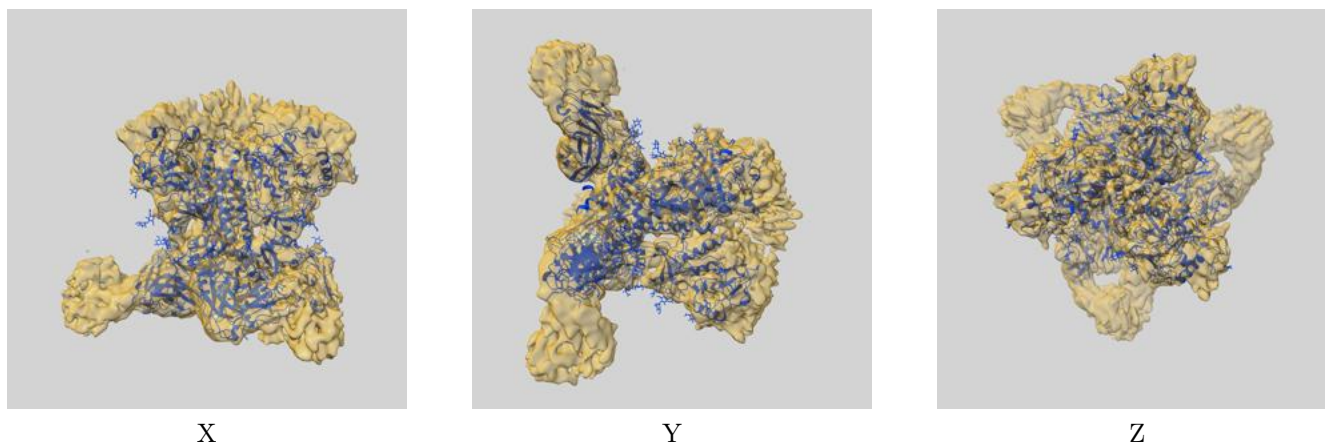
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.79	9.16	7.09

*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 6.79 differs from the reported value 4.32 by more than 10 %

9 Map-model fit [i](#)

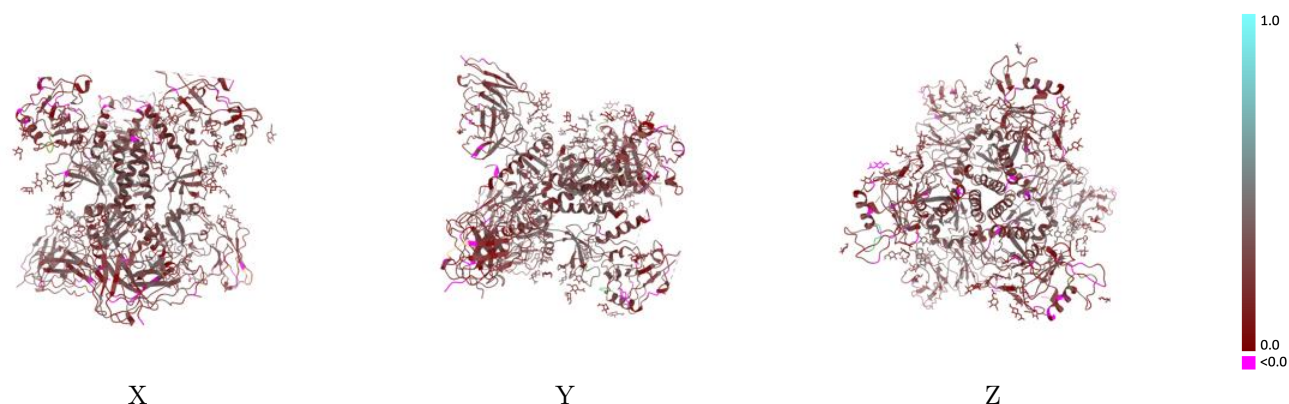
This section contains information regarding the fit between EMDB map EMD-27718 and PDB model 8DUA. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



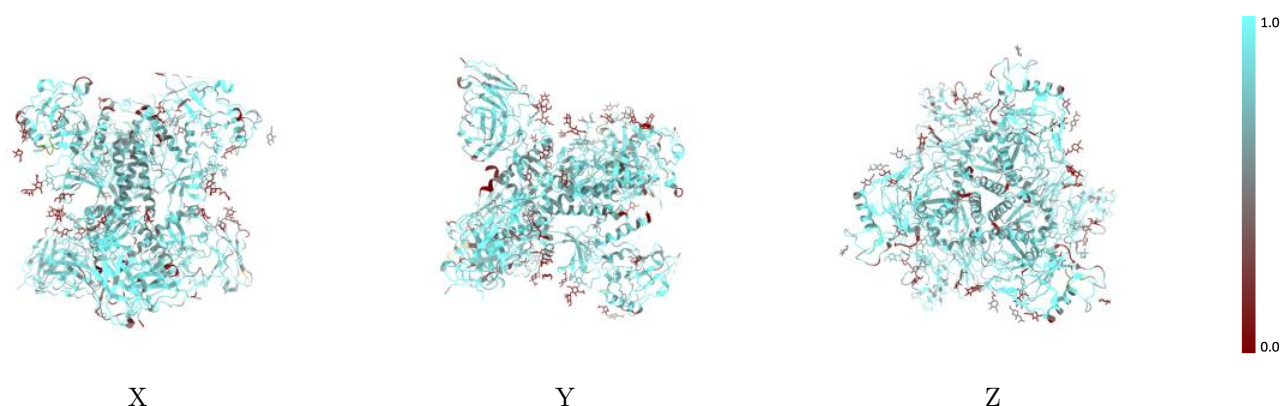
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



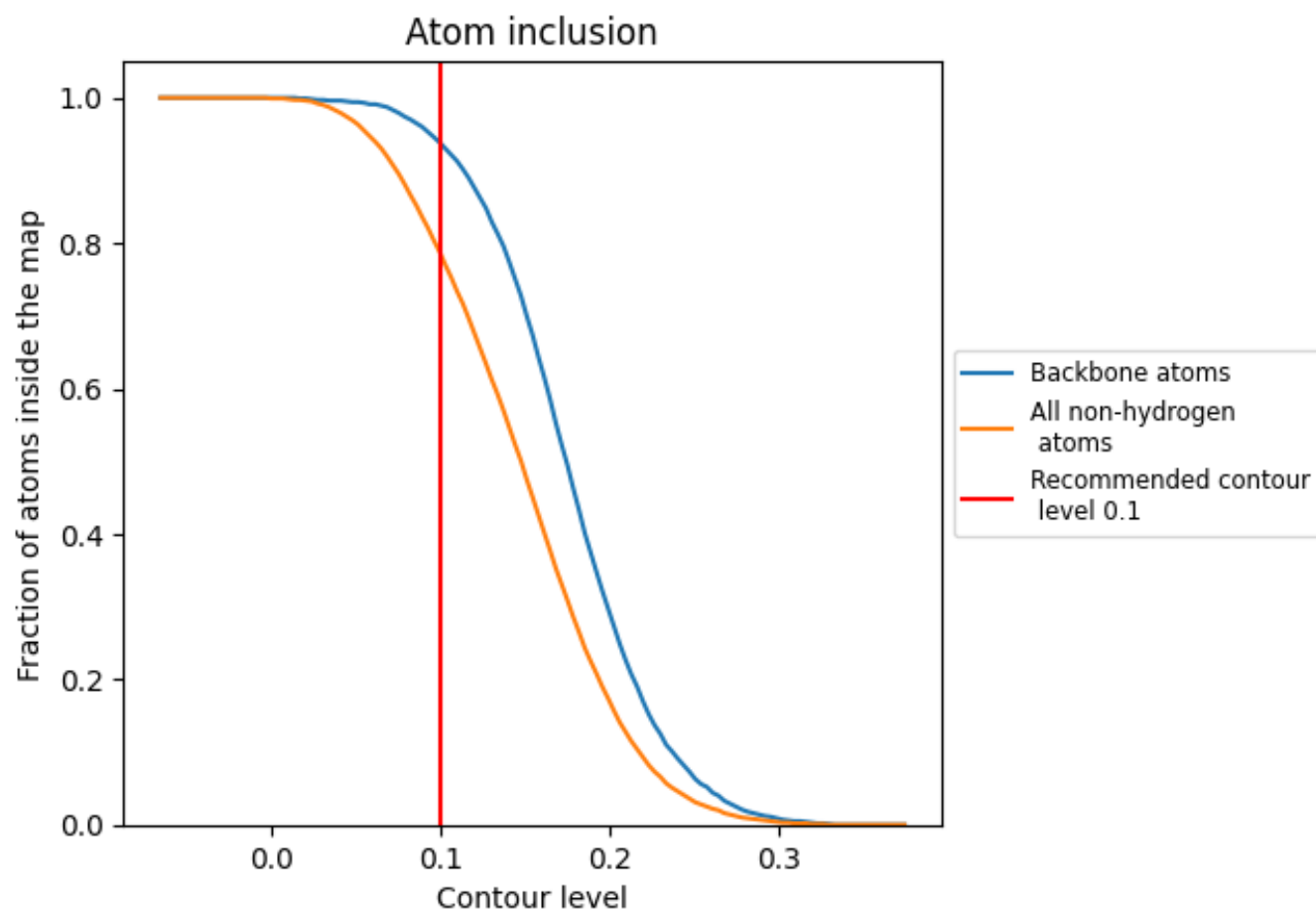
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.2490
A	 0.7480	 0.2640
B	 0.7390	 0.2620
C	 0.8160	 0.2540
D	 0.7900	 0.1990
E	 0.8350	 0.2490
F	 0.7440	 0.2620
G	 0.8110	 0.2430
H	 0.8150	 0.2430
I	 0.8170	 0.2500
J	 0.8080	 0.2400
K	 0.8190	 0.2550
L	 0.8060	 0.2600
M	 0.4360	 0.3240
N	 0.4430	 0.1770
O	 0.2560	 0.1650
P	 0.4800	 0.1620
Q	 0.7380	 0.3770
R	 0.4100	 0.3390
S	 0.3610	 0.2550
T	 0.2310	 0.1770
U	 0.4400	 0.1840
V	 0.7540	 0.3320
W	 0.4360	 0.3550
X	 0.4430	 0.2620
Y	 0.2560	 0.2030
Z	 0.4400	 0.1360
a	 0.7540	 0.3540

