



## Full wwPDB EM Validation Report ⓘ

May 1, 2024 – 03:22 PM EDT

PDB ID : 8TNI  
EMDB ID : EMD-41417  
Title : Cryo-EM structure of HIV-1 Env BG505 DS-SOSIP in complex with broadly neutralizing bi-specific antibody CAP256L-R27 targeting the CD4-binding site and the V2-apex  
Authors : Zhou, T.; Morano, N.C.; Roark, R.S.; Kwong, P.D.; Xu, J.  
Deposited on : 2023-08-01  
Resolution : 3.61 Å (reported)  
Based on initial model : 7LPN

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

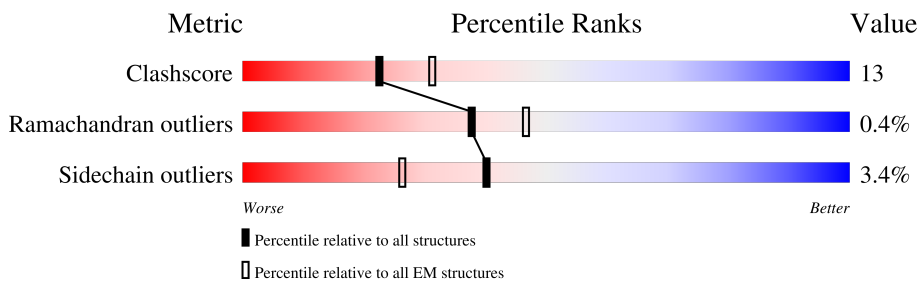
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.61 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	481	
1	C	481	
1	E	481	
2	B	153	
2	D	153	
2	F	153	
3	H	353	
3	I	353	

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Mol	Chain	Length	Quality of chain
3	J	353	 19% 49% 16% 34%
4	X	247	 20% 40% 17% 42%
5	G	2	 100%
5	K	2	 50% 50% 50%
5	M	2	 50% 50%
5	N	2	 100%
5	P	2	 100%
5	Q	2	 100%
5	S	2	 100%
5	T	2	 100%
5	U	2	 100%
5	V	2	 50% 50%
5	Z	2	 100%
5	a	2	 100%
6	L	3	 67% 33%
6	O	3	 33% 67%
6	W	3	 33% 67%
6	Y	3	 100%
7	R	4	 75% 25%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 19399 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 HIV-1 BG505 DS-SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	453	3567	2235	630	672	30	0	0
1	C	453	3567	2235	630	672	30	0	0
1	E	453	3567	2235	630	672	30	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
E	201	CYS	ILE	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	433	CYS	ALA	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 BG505 DS-SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	127	Total	C	N	O	S	0	0
			1009	639	173	191	6		
2	D	126	Total	C	N	O	S	0	0
			1002	634	172	190	6		
2	F	126	Total	C	N	O	S	0	0
			1002	634	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
D	559	PRO	ILE	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called Light chain of bi-specific antibody CAP256L-R27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	121	Total	C	N	O	S	0	0
			911	565	163	178	5		
3	I	121	Total	C	N	O	S	0	0
			911	565	163	178	5		
3	J	232	Total	C	N	O	S	0	0
			1730	1075	305	343	7		

- Molecule 4 is a protein called Heavy chain of bi-specific antibody CAP256L-R27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	144	Total	C	N	O	S	0	0
			1143	714	199	221	9		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	2	28	16	2	10	0	0
5	K	2	28	16	2	10	0	0
5	M	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	P	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0
5	S	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	V	2	28	16	2	10	0	0
5	Z	2	28	16	2	10	0	0
5	a	2	28	16	2	10	0	0

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



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

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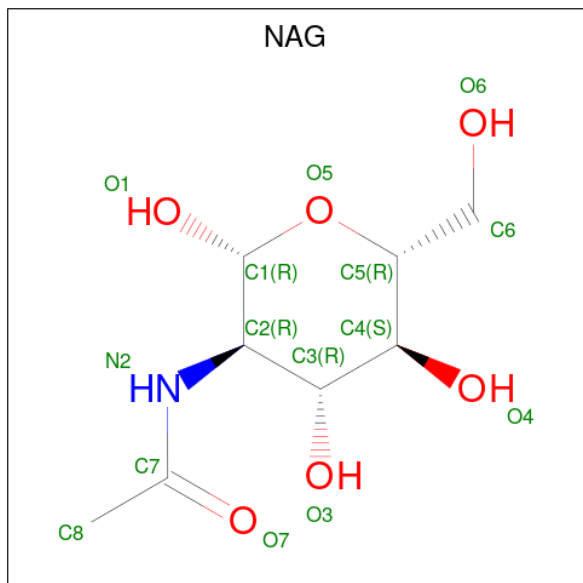
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	Y	3	39	22	2	15	0	0

- 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
			Total	C	N	O		
7	R	4	50	28	2	20	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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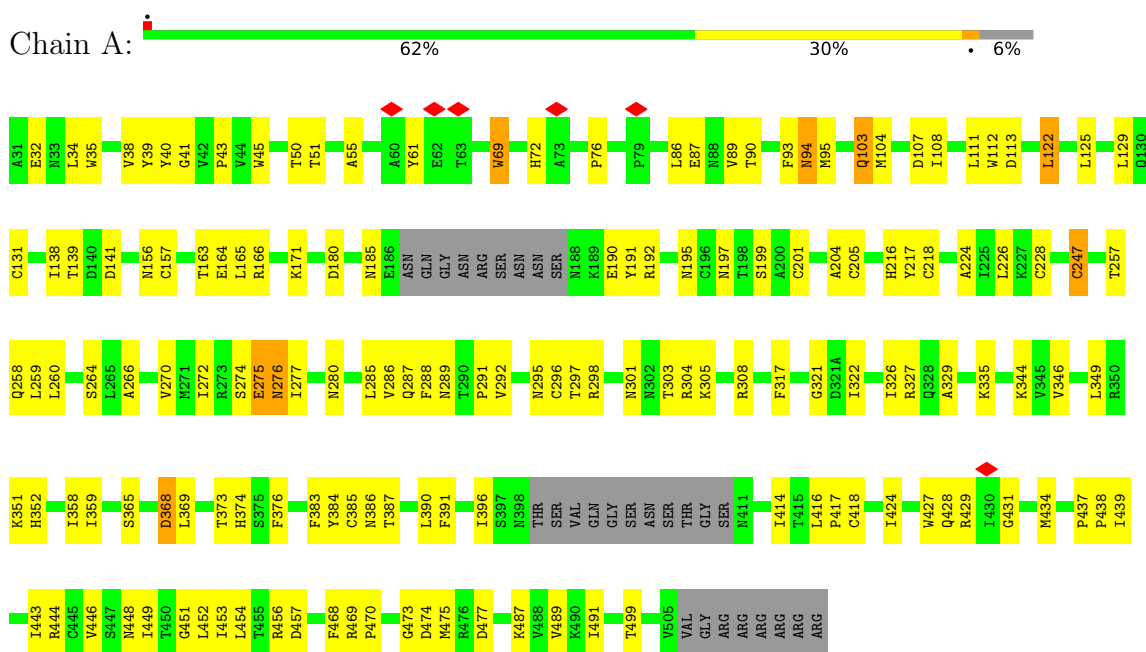
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	

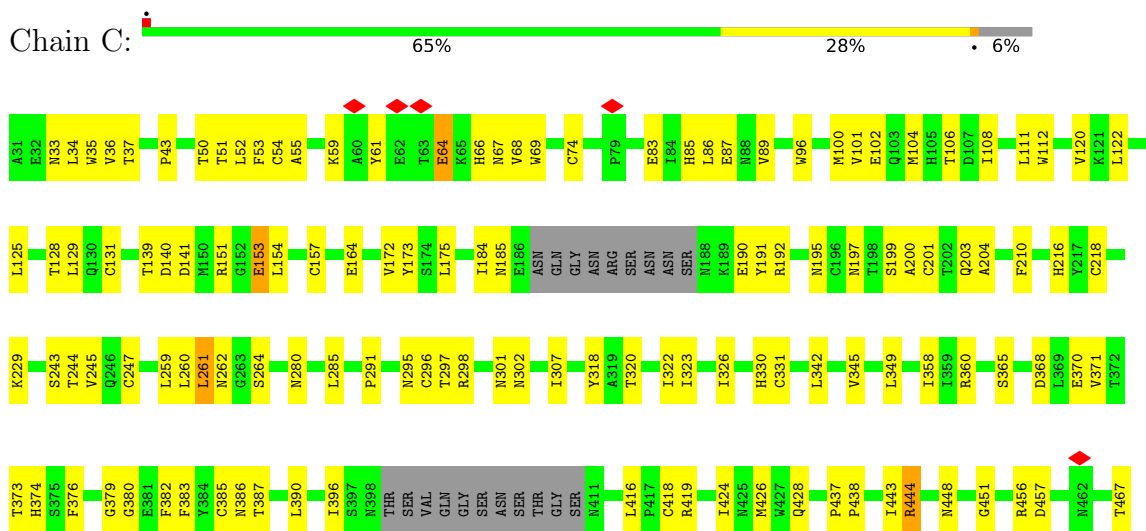
### 3 Residue-property plots [i](#)

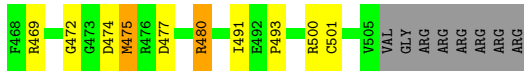
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: HIV-1 BG505 DS-SOSIP gp120

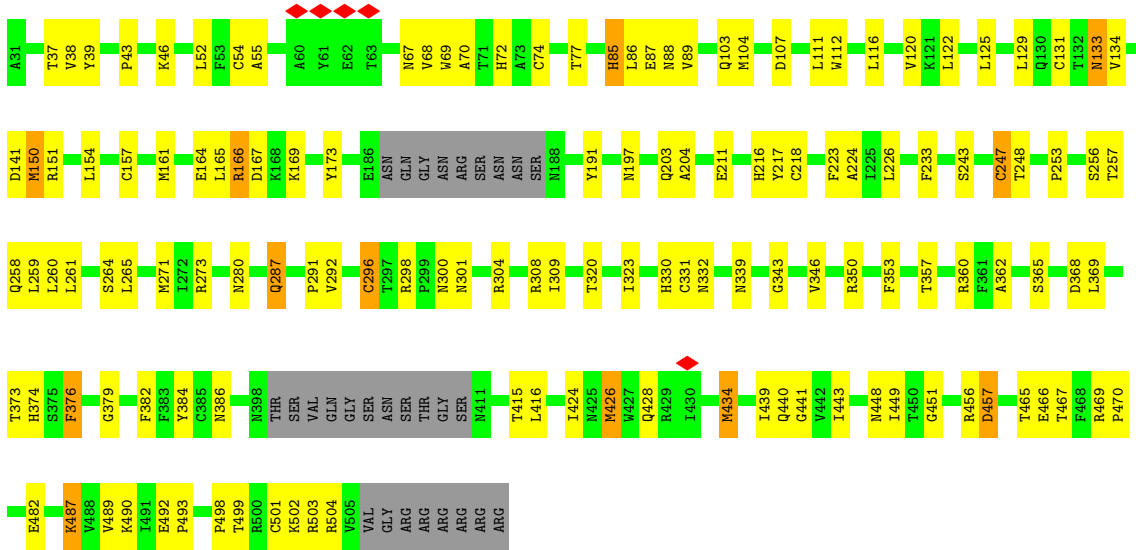


#### • Molecule 1: HIV-1 BG505 DS-SOSIP gp120

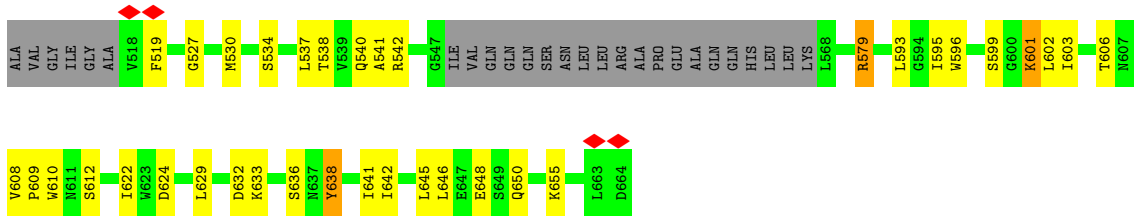




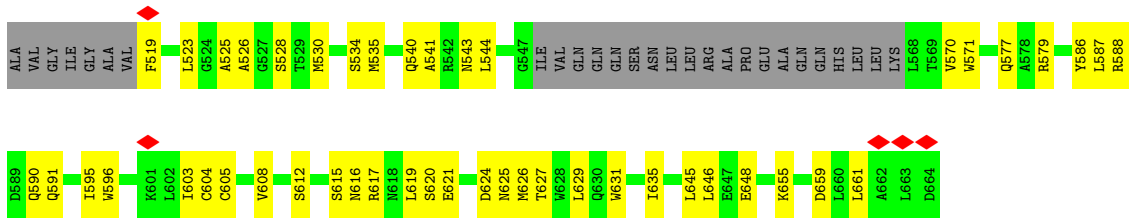
• Molecule 1: HIV-1 BG505 DS-SOSIP gp120



• Molecule 2: HIV-1 BG505 DS-SOSIP gp41

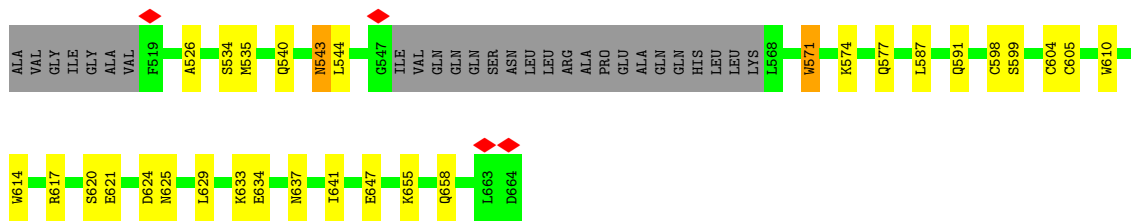


• Molecule 2: HIV-1 BG505 DS-SOSIP gp41

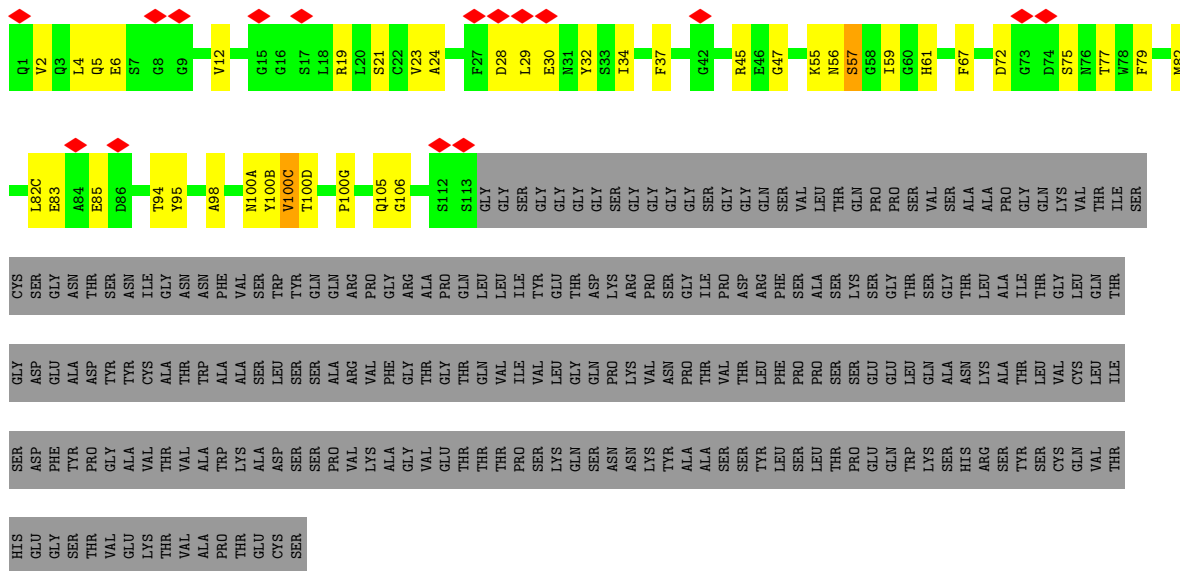


• Molecule 2: HIV-1 BG505 DS-SOSIP gp41

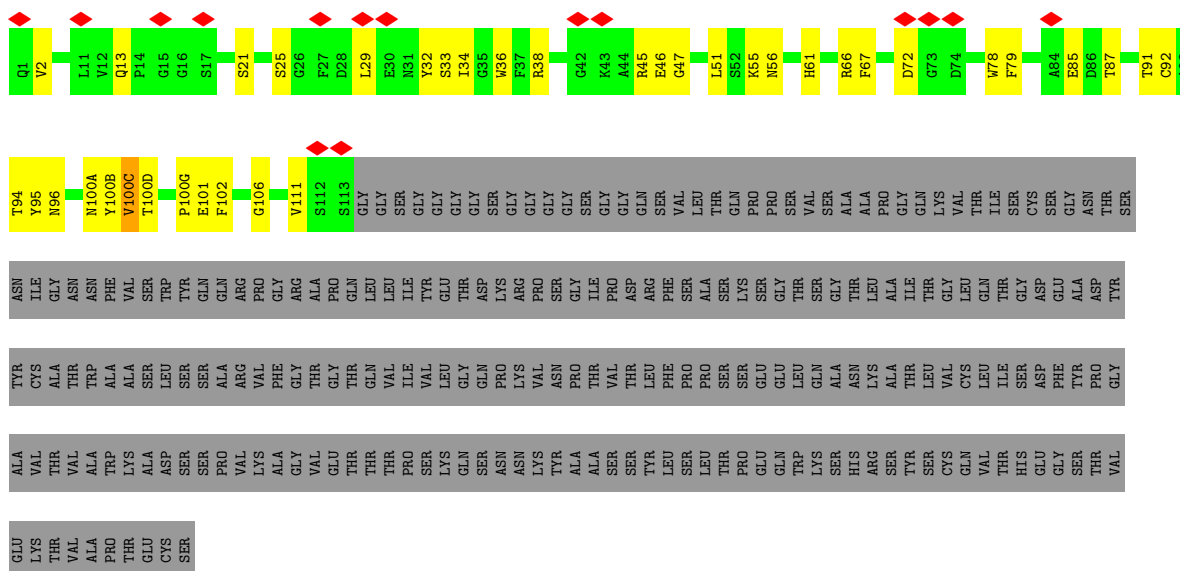




• Molecule 3: Light chain of bi-specific antibody CAP256L-R27



• Molecule 3: Light chain of bi-specific antibody CAP256L-R27







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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain P:  100%



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

Chain Q:  100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%

MAG1  
MAG2

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

Chain V:  50% 50%

MAG1  
MAG2

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

Chain Z:  100%

MAG1  
MAG2

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

Chain a:  100%

MAG1  
MAG2

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

Chain L:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain O:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain W:  33% 67%




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

Chain Y:  100%



- 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 R:  75% 25%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	236154	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.06	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.913	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.225	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.28	0/3641	0.55	1/4943 (0.0%)
1	C	0.29	0/3641	0.55	0/4943
1	E	0.29	0/3641	0.55	1/4943 (0.0%)
2	B	0.26	0/1027	0.51	0/1393
2	D	0.24	0/1020	0.52	0/1383
2	F	0.27	0/1020	0.50	0/1383
3	H	0.29	0/929	0.64	0/1257
3	I	0.29	0/929	0.61	0/1257
3	J	0.27	0/1765	0.55	0/2397
4	X	0.26	0/1137	0.57	0/1536
All	All	0.28	0/18750	0.55	2/25435 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	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(°)	Ideal(°)
1	A	122	LEU	CA-CB-CG	5.09	127.00	115.30
1	E	296	CYS	CA-CB-SG	5.01	123.02	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
1	C	261	LEU	Peptide
1	E	166	ARG	Sidechain

## 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	3567	0	3491	111	0
1	C	3567	0	3491	95	0
1	E	3567	0	3491	98	0
2	B	1009	0	989	28	0
2	D	1002	0	981	36	0
2	F	1002	0	981	27	0
3	H	911	0	869	34	0
3	I	911	0	869	32	0
3	J	1730	0	1665	41	0
4	X	1143	0	1073	29	0
5	G	28	0	25	0	0
5	K	28	0	25	1	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	1	0
5	T	28	0	25	1	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	Z	28	0	25	0	0
5	a	28	0	25	0	0
6	L	39	0	34	2	0
6	O	39	0	34	0	0
6	W	39	0	34	2	0
6	Y	39	0	34	0	0
7	R	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	140	0	130	4	0
8	B	14	0	13	0	0
8	C	140	0	130	3	0
8	E	154	0	143	6	0
All	All	19399	0	18795	479	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 13.

All (479) 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:E:296:CYS:HB3	1:E:331:CYS:HA	1.38	1.05
1:C:296:CYS:HB3	1:C:331:CYS:HA	1.37	1.04
8:A:609:NAG:H81	6:L:1:NAG:H62	1.62	0.80
3:H:4:LEU:HD13	3:H:24:ALA:HB2	1.62	0.80
1:E:55:ALA:HB3	1:E:216:HIS:HB2	1.65	0.77
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.66	0.75
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.66	0.75
1:C:291:PRO:HB3	1:C:448:ASN:OD1	1.87	0.74
1:A:218:CYS:HA	1:A:247:CYS:HB3	1.68	0.74
4:X:87:THR:HG22	4:X:111:VAL:H	1.53	0.73
1:C:83:GLU:HG3	1:C:245:VAL:HG23	1.70	0.72
1:E:151:ARG:HH21	8:E:605:NAG:H62	1.53	0.72
1:A:104:MET:SD	1:A:217:TYR:OH	2.47	0.71
2:B:655:LYS:NZ	2:F:534:SER:O	2.23	0.71
1:A:197:ASN:O	1:E:308:ARG:NH2	2.23	0.71
1:C:139:THR:O	1:C:141:ASP:N	2.23	0.70
2:D:621:GLU:HG2	2:D:625:ASN:HD21	1.56	0.70
3:H:5:GLN:HE21	3:H:23:VAL:HB	1.56	0.70
4:X:60:ALA:HB3	4:X:63:VAL:HG22	1.73	0.70
2:B:537:LEU:HB2	2:B:602:LEU:HD13	1.73	0.70
1:C:111:LEU:HD11	2:D:571:TRP:HE1	1.55	0.70
1:E:428:GLN:O	3:H:56:ASN:ND2	2.26	0.69
1:A:55:ALA:O	1:A:216:HIS:ND1	2.21	0.69
1:A:365:SER:OG	1:A:469:ARG:NH1	2.25	0.69
1:C:371:VAL:HG13	1:C:472:GLY:H	1.58	0.68
2:D:570:VAL:HG13	2:D:571:TRP:HD1	1.57	0.68
1:E:43:PRO:HG3	2:F:540:GLN:HE22	1.59	0.68
1:A:195:ASN:ND2	1:A:201:CYS:SG	2.67	0.67
1:E:258:GLN:HE21	1:E:470:PRO:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ALA:O	1:C:216:HIS:ND1	2.28	0.67
1:C:365:SER:OG	1:C:469:ARG:NH1	2.28	0.67
2:B:610:TRP:HD1	2:B:612:SER:H	1.43	0.66
1:A:297:THR:HG22	1:A:444:ARG:HG2	1.77	0.66
1:E:424:ILE:HD12	1:E:426:MET:HB2	1.78	0.66
1:E:55:ALA:O	1:E:216:HIS:ND1	2.27	0.66
1:E:218:CYS:HA	1:E:247:CYS:HB3	1.78	0.66
1:E:503:ARG:N	2:F:605:CYS:SG	2.69	0.65
4:X:29:PHE:O	4:X:71:ARG:NH2	2.29	0.65
4:X:35:HIS:NE2	4:X:95:ASP:OD1	2.29	0.65
1:A:272:ILE:HD13	1:A:286:VAL:HG22	1.79	0.65
1:A:303:THR:OG1	1:A:321:GLY:O	2.15	0.64
1:A:376:PHE:HB2	1:A:383:PHE:HB2	1.79	0.64
1:E:296:CYS:HB3	1:E:331:CYS:CA	2.20	0.64
4:X:20:LEU:HD12	4:X:80:LEU:HD23	1.79	0.64
1:A:259:LEU:HD22	1:A:449:ILE:HD11	1.79	0.64
3:H:83:GLU:OE1	3:H:83:GLU:N	2.31	0.64
3:J:1035:TRP:HE1	3:J:1086:TYR:HB3	1.62	0.64
1:A:277:ILE:HD12	1:A:352:HIS:HB3	1.80	0.64
1:E:469:ARG:HB2	3:H:100(A):ASN:HD21	1.63	0.64
2:B:534:SER:HA	2:B:537:LEU:HD21	1.80	0.63
2:B:608:VAL:HG21	2:B:645:LEU:HB3	1.80	0.62
3:H:67:PHE:HD1	3:H:82:MET:HG2	1.64	0.62
1:C:184:ILE:O	1:C:185:ASN:ND2	2.32	0.62
1:C:376:PHE:HB2	1:C:383:PHE:HB2	1.80	0.62
1:C:501:CYS:HB3	2:D:605:CYS:HB3	1.81	0.62
8:E:603:NAG:H81	6:W:1:NAG:H62	1.81	0.62
1:C:373:THR:HG22	1:C:386:ASN:HA	1.81	0.62
2:D:612:SER:OG	2:D:616:ASN:OD1	2.17	0.62
1:C:428:GLN:O	3:I:56:ASN:ND2	2.29	0.62
1:E:85:HIS:HA	1:E:243:SER:HB2	1.81	0.62
8:A:604:NAG:H3	8:A:604:NAG:H83	1.82	0.62
1:C:360:ARG:O	1:C:467:THR:HA	1.99	0.61
3:J:6:GLU:OE2	3:J:106:GLY:N	2.31	0.61
1:E:112:TRP:CZ2	1:E:434:MET:HE1	2.36	0.61
2:B:606:THR:HG21	2:B:646:LEU:HD22	1.80	0.61
1:E:226:LEU:HB2	1:E:487:LYS:HG2	1.82	0.61
3:J:100(B):TYR:O	3:J:100(C):VAL:HG22	2.01	0.61
4:X:39:GLN:HB2	4:X:45:LEU:HD23	1.82	0.61
1:A:264:SER:O	1:A:287:GLN:NE2	2.34	0.60
1:C:295:ASN:OD1	8:C:608:NAG:N2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ARG:NH1	1:E:466:GLU:OE1	2.32	0.60
3:J:63:VAL:HG13	3:J:64:LYS:HG2	1.82	0.60
1:E:264:SER:O	1:E:287:GLN:NE2	2.34	0.60
1:A:94:ASN:HD22	1:A:95:MET:N	2.00	0.60
1:A:104:MET:O	1:A:108:ILE:HG22	2.02	0.60
1:C:296:CYS:HB3	1:C:331:CYS:CA	2.24	0.59
1:A:165:LEU:HD21	1:C:192:ARG:HD3	1.84	0.59
2:F:629:LEU:O	2:F:633:LYS:HG2	2.02	0.59
1:A:270:VAL:HG22	1:A:288:PHE:HA	1.84	0.59
3:H:29:LEU:HD11	3:H:34:ILE:HD11	1.83	0.59
3:J:46:GLU:OE2	3:J:46:GLU:N	2.35	0.59
1:C:85:HIS:HA	1:C:243:SER:HB2	1.84	0.59
1:C:491:ILE:HD11	2:D:523:LEU:HD12	1.84	0.59
4:X:100(G):ASP:OD2	4:X:100(G):ASP:N	2.36	0.59
1:E:439:ILE:HG21	1:E:443:ILE:HD12	1.85	0.58
1:A:427:TRP:HZ3	1:A:475:MET:HG2	1.67	0.58
1:A:280:ASN:ND2	1:A:457:ASP:O	2.37	0.58
3:J:30:GLU:OE2	3:J:30:GLU:N	2.37	0.58
1:A:165:LEU:HD13	1:C:128:THR:HG22	1.84	0.58
1:C:320:THR:HA	1:C:438:PRO:HG2	1.86	0.58
3:H:47:GLY:HA3	3:H:100(C):VAL:HA	1.86	0.58
1:A:204:ALA:HB3	1:A:437:PRO:HD3	1.86	0.58
1:A:258:GLN:NE2	1:A:387:THR:OG1	2.37	0.58
1:A:301:ASN:OD1	8:A:603:NAG:N2	2.36	0.57
1:C:50:THR:OG1	1:C:51:THR:N	2.37	0.57
2:F:543:ASN:C	2:F:543:ASN:HD22	2.08	0.57
2:B:638:TYR:HB3	2:B:641:ILE:HD11	1.85	0.57
1:C:203:GLN:HE22	1:C:318:TYR:HD2	1.52	0.57
1:A:291:PRO:HB3	1:A:448:ASN:HB3	1.87	0.57
1:C:475:MET:O	1:C:475:MET:HG2	2.04	0.57
1:A:452:LEU:HD13	1:A:454:LEU:HD11	1.87	0.57
1:E:86:LEU:HB3	1:E:89:VAL:HG11	1.85	0.57
1:E:369:LEU:O	1:E:373:THR:OG1	2.23	0.57
2:D:530:MET:HG3	2:D:626:MET:HB2	1.87	0.56
1:A:439:ILE:HD12	1:A:443:ILE:HG21	1.86	0.56
2:F:614:TRP:HE1	2:F:641:ILE:HD11	1.71	0.56
1:A:335:LYS:HG3	1:A:414:ILE:HD11	1.87	0.56
2:B:632:ASP:OD2	2:B:636:SER:OG	2.23	0.56
1:C:218:CYS:HA	1:C:247:CYS:HB3	1.88	0.56
1:C:368:ASP:OD1	3:I:61:HIS:NE2	2.39	0.56
2:B:601:LYS:HE2	2:D:595:ILE:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ILE:HD13	1:C:192:ARG:HE	1.70	0.56
1:E:120:VAL:HG13	1:E:203:GLN:HB3	1.87	0.56
2:D:620:SER:O	2:D:624:ASP:HB2	2.06	0.56
1:E:69:TRP:HA	1:E:111:LEU:HD13	1.87	0.56
3:I:87:THR:HG22	3:I:111:VAL:HG12	1.87	0.56
3:J:45:ARG:NH2	3:J:100(D):THR:O	2.38	0.56
3:J:1090:THR:OG1	3:J:1095(C):ALA:O	2.22	0.56
1:C:469:ARG:HB2	3:I:100(A):ASN:HD21	1.71	0.55
1:E:69:TRP:CZ3	1:E:253:PRO:HG2	2.41	0.55
1:E:493:PRO:HG3	2:F:544:LEU:HD21	1.88	0.55
1:E:107:ASP:OD2	2:F:574:LYS:NZ	2.38	0.55
3:H:100(B):TYR:O	3:H:100(C):VAL:HG22	2.07	0.55
2:D:526:ALA:O	2:D:627:THR:OG1	2.24	0.55
1:A:112:TRP:HE1	1:A:434:MET:HE2	1.71	0.55
3:I:100(B):TYR:O	3:I:100(C):VAL:HG22	2.06	0.55
4:X:47:TRP:HD1	3:J:1098:PHE:HB2	1.72	0.55
3:I:34:ILE:HD12	3:I:78:TRP:CD2	2.42	0.55
3:J:96:ASN:OD1	3:J:97:ARG:N	2.38	0.55
1:A:141:ASP:OD1	1:A:141:ASP:N	2.38	0.55
1:C:33:ASN:OD1	1:C:35:TRP:NE1	2.40	0.55
1:C:69:TRP:HA	1:C:111:LEU:HD23	1.89	0.54
1:E:465:THR:O	1:E:465:THR:HG22	2.07	0.54
1:A:199:SER:HB2	1:A:431:GLY:HA2	1.88	0.54
1:C:379:GLY:HA3	1:C:443:ILE:HD11	1.89	0.54
1:E:131:CYS:HB3	1:E:191:TYR:HD2	1.73	0.54
2:D:541:ALA:O	2:F:591:GLN:NE2	2.41	0.54
3:I:85:GLU:OE2	3:I:85:GLU:N	2.31	0.54
1:E:38:VAL:HG13	2:F:604:CYS:HB3	1.90	0.54
4:X:34:MET:HG3	4:X:78:LEU:HD13	1.90	0.54
1:A:185:ASN:ND2	1:A:190:GLU:OE1	2.40	0.53
3:I:91:THR:HG22	3:I:106:GLY:HA3	1.90	0.53
1:A:298:ARG:HG3	1:A:329:ALA:HB2	1.89	0.53
2:B:579:ARG:NH2	2:D:577:GLN:OE1	2.41	0.53
1:E:379:GLY:HA3	1:E:443:ILE:HD11	1.90	0.53
3:H:32:TYR:HB3	3:H:94:THR:OG1	2.09	0.53
1:A:50:THR:OG1	1:A:51:THR:N	2.41	0.53
4:X:43:LYS:NZ	4:X:44:GLY:O	2.35	0.53
1:E:339:ASN:OD1	8:E:611:NAG:N2	2.42	0.53
1:E:68:VAL:HG13	1:E:69:TRP:CD1	2.44	0.53
3:I:32:TYR:HB3	3:I:94:THR:OG1	2.08	0.53
1:C:68:VAL:HG23	1:C:69:TRP:CE3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:ARG:HB2	3:H:100(A):ASN:ND2	2.23	0.53
3:H:67:PHE:CD1	3:H:82:MET:HG2	2.44	0.53
3:H:72:ASP:OD1	3:H:72:ASP:N	2.42	0.53
3:I:101:GLU:HG2	3:I:102:PHE:CD1	2.44	0.53
1:E:129:LEU:HD23	1:E:157:CYS:SG	2.49	0.52
1:E:46:LYS:NZ	1:E:492:GLU:OE1	2.34	0.52
1:E:298:ARG:O	1:E:300:ASN:N	2.40	0.52
1:E:298:ARG:NH2	1:E:441:GLY:O	2.43	0.52
1:A:131:CYS:HB2	1:A:191:TYR:HD2	1.75	0.52
1:A:368:ASP:OD1	3:J:57:SER:OG	2.26	0.52
1:E:291:PRO:HB3	1:E:448:ASN:HB3	1.92	0.52
1:A:45:TRP:HB2	1:A:489:VAL:HB	1.91	0.52
2:D:535:MET:SD	2:F:655:LYS:NZ	2.72	0.52
1:A:94:ASN:HD22	1:A:95:MET:H	1.58	0.52
4:X:40:ALA:HB3	4:X:43:LYS:HG2	1.92	0.52
3:J:1035:TRP:NE1	3:J:1086:TYR:HB3	2.24	0.52
3:I:72:ASP:N	3:I:72:ASP:OD1	2.42	0.52
1:E:166:ARG:O	1:E:166:ARG:HG2	2.10	0.51
1:E:265:LEU:HD21	1:E:291:PRO:HG3	1.91	0.51
3:H:5:GLN:NE2	3:H:23:VAL:HB	2.23	0.51
1:E:280:ASN:ND2	1:E:457:ASP:O	2.42	0.51
3:H:30:GLU:OE2	3:H:30:GLU:N	2.44	0.51
1:C:37:THR:OG1	2:D:604:CYS:O	2.19	0.51
1:A:369:LEU:O	1:A:373:THR:OG1	2.29	0.51
1:E:365:SER:HB3	3:H:100(C):VAL:HG22	1.93	0.51
1:C:501:CYS:SG	2:F:658:GLN:NE2	2.72	0.51
4:X:68:THR:HB	4:X:81:GLN:HB3	1.92	0.51
1:A:296:CYS:SG	1:A:376:PHE:HE2	2.33	0.51
2:D:631:TRP:CZ2	2:D:635:ILE:HD11	2.46	0.51
1:C:469:ARG:HB2	3:I:100(A):ASN:ND2	2.25	0.51
1:C:185:ASN:HD21	1:C:190:GLU:HB2	1.76	0.51
3:J:37:PHE:N	3:J:91:THR:O	2.38	0.51
1:A:38:VAL:HG21	2:B:596:TRP:HZ3	1.76	0.51
3:H:12:VAL:HG11	3:H:82(C):LEU:HD23	1.93	0.51
3:I:2:VAL:HB	3:I:102:PHE:HD2	1.76	0.51
2:F:624:ASP:OD2	2:F:625:ASN:N	2.44	0.50
1:A:358:ILE:HD12	1:A:396:ILE:HA	1.93	0.50
1:C:199:SER:OG	1:C:200:ALA:N	2.44	0.50
3:J:100(B):TYR:C	3:J:100(D):THR:H	2.14	0.50
1:A:131:CYS:HA	1:A:156:ASN:O	2.12	0.50
3:I:95:TYR:CE1	3:I:100(G):PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:66:ARG:HG3	3:I:67:PHE:CD1	2.46	0.50
3:I:2:VAL:HG12	3:I:2:VAL:O	2.12	0.50
1:A:266:ALA:N	1:A:287:GLN:HE21	2.10	0.50
1:E:151:ARG:NH2	8:E:605:NAG:H62	2.26	0.50
3:I:38:ARG:HB3	3:I:46:GLU:HG3	1.94	0.50
4:X:100(H):TYS:C	4:X:100(J):ASP:H	2.24	0.50
1:E:37:THR:HG1	1:E:39:TYR:HE1	1.60	0.49
3:H:95:TYR:CE1	3:H:100(G):PRO:HG3	2.48	0.49
3:J:105:GLN:OE1	3:J:105:GLN:N	2.41	0.49
1:C:385:CYS:HA	1:C:418:CYS:HA	1.93	0.49
1:E:332:ASN:OD1	1:E:415:THR:HG22	2.11	0.49
1:C:358:ILE:HD12	1:C:396:ILE:HD12	1.95	0.49
1:E:164:GLU:HG2	1:E:165:LEU:N	2.28	0.49
3:I:101:GLU:HG2	3:I:102:PHE:HD1	1.78	0.49
3:J:4:LEU:HD13	3:J:24:ALA:HB2	1.94	0.49
1:A:304:ARG:NH2	1:A:438:PRO:O	2.41	0.49
3:I:33:SER:OG	3:I:96:ASN:O	2.29	0.49
1:C:129:LEU:HD23	1:C:157:CYS:HB3	1.94	0.49
2:F:617:ARG:NH1	2:F:634:GLU:OE2	2.46	0.49
3:I:55:LYS:HG3	3:I:56:ASN:N	2.28	0.49
1:A:285:LEU:HD21	1:A:477:ASP:HB3	1.94	0.49
1:A:386:ASN:HB3	1:A:417:PRO:HD2	1.94	0.49
1:C:64:GLU:OE1	1:C:66:HIS:N	2.32	0.49
1:C:260:LEU:HB2	1:C:451:GLY:HA3	1.94	0.49
1:C:301:ASN:OD1	8:C:604:NAG:N2	2.45	0.49
1:E:111:LEU:HD11	2:F:571:TRP:CH2	2.47	0.49
1:A:358:ILE:HD11	1:A:396:ILE:HG22	1.95	0.49
1:E:122:LEU:HD13	1:E:125:LEU:HD13	1.93	0.49
1:E:70:ALA:HB1	1:E:72:HIS:CD2	2.47	0.48
1:E:169:LYS:HG3	4:X:100(F):SER:OG	2.13	0.48
1:E:498:PRO:HB3	2:F:610:TRP:CD2	2.48	0.48
3:J:1091:TRP:CE3	3:J:1096:ARG:HD3	2.47	0.48
1:E:43:PRO:HB2	2:F:526:ALA:HA	1.94	0.48
1:C:68:VAL:HG23	1:C:69:TRP:HE3	1.77	0.48
1:E:292:VAL:HB	1:E:449:ILE:HB	1.95	0.48
3:I:47:GLY:HA3	3:I:100(C):VAL:HA	1.94	0.48
1:A:473:GLY:HA2	3:J:98:ALA:HB3	1.95	0.48
1:A:474:ASP:OD1	1:A:474:ASP:N	2.43	0.48
1:C:131:CYS:HB2	1:C:191:TYR:CD1	2.47	0.48
1:C:153:GLU:OE1	1:C:419:ARG:NH2	2.46	0.48
3:H:105:GLN:N	3:H:105:GLN:OE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:29:LEU:HD11	3:I:34:ILE:HD11	1.96	0.48
1:A:139:THR:HG21	1:A:327:ARG:HG2	1.95	0.48
1:A:34:LEU:HA	1:A:499:THR:O	2.14	0.48
1:C:67:ASN:OD1	1:C:67:ASN:N	2.45	0.48
1:A:295:ASN:OD1	1:A:444:ARG:NH2	2.47	0.47
1:C:197:ASN:OD1	8:C:609:NAG:N2	2.47	0.47
1:E:55:ALA:HB1	1:E:77:THR:HB	1.96	0.47
1:E:122:LEU:HD12	1:E:122:LEU:O	2.14	0.47
4:X:100(G):ASP:O	4:X:100(K):PHE:N	2.47	0.47
3:I:21:SER:HB2	3:I:79:PHE:HD1	1.79	0.47
1:E:164:GLU:HG2	1:E:165:LEU:H	1.78	0.47
2:F:617:ARG:NH2	2:F:621:GLU:OE2	2.44	0.47
3:H:82:MET:HE2	3:H:82(C):LEU:HD21	1.96	0.47
2:B:632:ASP:O	2:B:636:SER:OG	2.26	0.47
1:E:482:GLU:N	1:E:482:GLU:OE1	2.48	0.47
3:J:1035:TRP:CZ3	3:J:1088:CYS:HB3	2.50	0.47
1:C:345:VAL:O	1:C:349:LEU:HB2	2.14	0.47
2:D:655:LYS:HD2	2:D:655:LYS:HA	1.64	0.47
2:D:526:ALA:HB1	2:D:629:LEU:HD11	1.97	0.47
1:E:112:TRP:HZ2	1:E:434:MET:HE1	1.78	0.47
1:E:353:PHE:O	1:E:357:THR:OG1	2.24	0.47
3:I:100(B):TYR:C	3:I:100(D):THR:H	2.18	0.47
1:A:446:VAL:O	6:L:1:NAG:H5	2.15	0.47
2:B:595:ILE:O	2:B:650:GLN:HG2	2.15	0.47
3:J:95:TYR:CE1	3:J:100(G):PRO:HG3	2.49	0.47
3:J:51:LEU:HD22	3:J:78:TRP:HE1	1.80	0.47
1:C:101:VAL:HG11	1:C:480:ARG:HE	1.80	0.46
1:E:280:ASN:OD1	1:E:456:ARG:NH2	2.48	0.46
2:F:637:ASN:OD1	2:F:637:ASN:N	2.40	0.46
3:I:87:THR:O	3:I:87:THR:OG1	2.33	0.46
1:E:261:LEU:HD11	1:E:376:PHE:CE1	2.51	0.46
3:H:2:VAL:HG12	3:H:2:VAL:O	2.15	0.46
1:A:274:SER:OG	1:A:276:ASN:O	2.31	0.46
3:J:3:GLN:N	3:J:3:GLN:OE1	2.47	0.46
2:B:655:LYS:NZ	2:F:535:MET:HA	2.31	0.46
1:C:59:LYS:O	1:C:61:TYR:N	2.48	0.46
1:C:387:THR:O	1:C:387:THR:OG1	2.34	0.46
2:D:579:ARG:NH2	2:F:577:GLN:OE1	2.49	0.46
1:A:39:TYR:CE1	2:B:603:ILE:HG12	2.50	0.46
1:C:204:ALA:HB3	1:C:437:PRO:HD3	1.97	0.46
3:I:2:VAL:HA	3:I:25:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:3:GLN:O	4:X:4:LEU:HD23	2.16	0.46
4:X:58:TYR:CE2	3:J:1095(A):SER:HA	2.51	0.46
1:E:116:LEU:HD21	1:E:434:MET:HE2	1.98	0.46
1:E:374:HIS:O	1:E:384:TYR:HA	2.16	0.46
1:E:301:ASN:HD22	1:E:323:ILE:HD11	1.81	0.46
1:A:131:CYS:HB2	1:A:191:TYR:CD2	2.51	0.46
1:A:192:ARG:NH2	8:A:604:NAG:HN2	2.14	0.46
1:C:172:VAL:HG21	1:C:307:ILE:HG21	1.97	0.46
1:C:301:ASN:HB2	1:C:323:ILE:HB	1.98	0.46
1:A:351:LYS:HD2	1:A:351:LYS:HA	1.70	0.45
1:E:256:SER:OG	1:E:257:THR:N	2.50	0.45
1:C:261:LEU:HB3	1:C:262:ASN:HB2	1.98	0.45
3:H:83:GLU:HB2	3:H:85:GLU:OE2	2.17	0.45
1:A:295:ASN:OD1	1:A:446:VAL:HG12	2.17	0.45
1:C:195:ASN:ND2	1:C:201:CYS:SG	2.89	0.45
1:E:382:PHE:CD2	1:E:424:ILE:HG21	2.51	0.45
1:E:218:CYS:HA	1:E:247:CYS:CB	2.46	0.45
3:J:47:GLY:N	3:J:100(C):VAL:HA	2.30	0.45
1:A:122:LEU:O	1:A:122:LEU:HD12	2.16	0.45
1:A:391:PHE:CZ	1:A:452:LEU:HD21	2.52	0.45
1:E:87:GLU:HG2	1:E:88:ASN:OD1	2.16	0.45
3:J:1027(B):ASN:OD1	3:J:1028:ILE:N	2.50	0.45
4:X:51:ILE:HG13	4:X:54:GLY:HA2	1.99	0.45
1:A:289:ASN:OD1	1:A:344:LYS:NZ	2.38	0.45
1:C:298:ARG:NH2	1:C:302:ASN:OD1	2.50	0.45
1:E:360:ARG:HH21	1:E:467:THR:HG21	1.81	0.45
4:X:63:VAL:HB	4:X:67:PHE:CD1	2.52	0.45
1:A:359:ILE:HD12	1:A:468:PHE:HE2	1.81	0.45
1:C:322:ILE:HG21	1:C:326:ILE:HG12	1.99	0.45
1:E:197:ASN:OD1	8:E:604:NAG:N2	2.50	0.45
3:J:62:SER:OG	3:J:64:LYS:O	2.33	0.45
2:D:608:VAL:HG12	2:D:608:VAL:O	2.17	0.45
3:H:21:SER:HB2	3:H:79:PHE:HD2	1.82	0.45
3:J:1027(B):ASN:HD22	3:J:1097:VAL:HG11	1.81	0.45
1:A:171:LYS:NZ	5:K:1:NAG:HN2	2.14	0.44
3:H:57:SER:OG	3:H:59:ILE:HG12	2.16	0.44
3:J:1035:TRP:CE2	3:J:1073:LEU:HD22	2.52	0.44
2:D:586:TYR:CE2	2:F:587:LEU:HD12	2.52	0.44
2:D:608:VAL:HG21	2:D:645:LEU:HB3	1.98	0.44
1:C:210:PHE:HD2	1:C:380:GLY:HA2	1.81	0.44
1:C:229:LYS:HE2	1:C:243:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:HG12	1:E:154:LEU:O	2.17	0.44
4:X:22:CYS:HB3	4:X:78:LEU:HB3	1.98	0.44
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.81	0.44
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.75	0.44
1:C:370:GLU:OE2	1:C:428:GLN:HG2	2.18	0.44
1:C:34:LEU:HD21	2:D:619:LEU:HD22	2.00	0.44
1:C:86:LEU:HD21	1:C:244:THR:HG22	1.99	0.44
2:D:525:ALA:O	2:D:528:SER:OG	2.35	0.44
2:D:661:LEU:HD23	2:D:661:LEU:HA	1.79	0.44
3:J:1088:CYS:O	3:J:1099:GLY:N	2.46	0.44
1:A:93:PHE:CE2	1:A:228:CYS:HB2	2.52	0.44
2:B:642:ILE:O	2:B:646:LEU:HG	2.17	0.44
1:C:259:LEU:HB3	1:C:374:HIS:NE2	2.33	0.44
1:E:343:GLY:O	1:E:346:VAL:HG12	2.17	0.44
3:H:55:LYS:HG3	3:H:56:ASN:N	2.33	0.44
3:I:55:LYS:O	3:I:56:ASN:HB3	2.17	0.44
1:A:259:LEU:HD13	1:A:449:ILE:HD11	2.00	0.44
1:A:260:LEU:HB2	1:A:451:GLY:HA3	1.99	0.44
2:D:534:SER:O	2:D:534:SER:OG	2.31	0.44
3:H:75:SER:OG	3:H:77:THR:HG22	2.18	0.44
1:A:292:VAL:O	1:A:449:ILE:HG22	2.18	0.43
1:A:424:ILE:HD11	1:A:434:MET:HE3	2.00	0.43
2:B:648:GLU:OE1	2:B:648:GLU:HA	2.18	0.43
1:C:477:ASP:OD1	1:C:477:ASP:N	2.51	0.43
1:A:32:GLU:O	1:A:34:LEU:N	2.47	0.43
1:A:129:LEU:HD23	1:A:157:CYS:SG	2.58	0.43
1:C:154:LEU:HD12	1:C:175:LEU:HD23	2.00	0.43
1:E:104:MET:HE3	1:E:217:TYR:HE2	1.83	0.43
1:E:386:ASN:O	1:E:416:LEU:HB3	2.18	0.43
1:E:502:LYS:N	2:F:605:CYS:SG	2.91	0.43
3:J:12:VAL:O	3:J:111:VAL:HA	2.18	0.43
1:C:101:VAL:HG21	1:C:480:ARG:HG3	2.00	0.43
1:A:224:ALA:HB3	1:A:489:VAL:HG23	2.00	0.43
1:A:428:GLN:HB3	3:J:56:ASN:O	2.17	0.43
1:E:43:PRO:HG3	2:F:540:GLN:NE2	2.30	0.43
3:J:6:GLU:N	3:J:6:GLU:OE1	2.51	0.43
1:E:233:PHE:O	1:E:273:ARG:NH1	2.52	0.43
3:J:52:SER:OG	3:J:57:SER:OG	2.26	0.43
1:A:43:PRO:HD3	2:B:540:GLN:HE21	1.84	0.43
1:A:427:TRP:CZ3	1:A:475:MET:HG2	2.50	0.43
2:B:542:ARG:O	2:D:591:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PRO:HG3	2:D:540:GLN:NE2	2.33	0.43
1:C:54:CYS:HB3	1:C:74:CYS:HB3	1.69	0.43
1:E:428:GLN:CD	1:E:428:GLN:H	2.22	0.43
1:A:113:ASP:CG	1:A:429:ARG:HH12	2.21	0.43
1:A:163:THR:OG1	1:A:164:GLU:OE1	2.37	0.43
1:A:280:ASN:OD1	1:A:456:ARG:NH2	2.51	0.43
1:A:429:ARG:H	1:A:429:ARG:HG3	1.59	0.43
1:C:280:ASN:ND2	1:C:457:ASP:O	2.51	0.43
2:D:621:GLU:O	2:D:625:ASN:ND2	2.51	0.43
1:E:133:ASN:HB3	8:E:605:NAG:N2	2.34	0.43
1:E:362:ALA:HB3	1:E:469:ARG:HG2	2.01	0.43
1:E:224:ALA:HB3	1:E:489:VAL:HG23	2.01	0.43
3:H:55:LYS:O	3:H:56:ASN:HB3	2.18	0.43
3:H:59:ILE:HB	3:H:61:HIS:CE1	2.54	0.43
3:I:51:LEU:HD23	3:I:78:TRP:CD1	2.54	0.43
4:X:89:LEU:HD23	4:X:91:TYR:CZ	2.54	0.43
4:X:97:ARG:NH2	4:X:100(W):GLY:O	2.52	0.43
1:E:217:TYR:H	1:E:248:THR:HG22	1.84	0.42
3:I:2:VAL:HB	3:I:102:PHE:CD2	2.53	0.42
3:I:91:THR:HG22	3:I:106:GLY:CA	2.49	0.42
3:J:4:LEU:HD12	3:J:92:CYS:SG	2.58	0.42
2:B:599:SER:O	2:B:599:SER:OG	2.29	0.42
1:C:36:VAL:HG11	2:D:646:LEU:HD21	2.00	0.42
1:E:304:ARG:HG2	1:E:440:GLN:HG2	2.00	0.42
3:I:13:GLN:H	3:I:13:GLN:CD	2.23	0.42
2:B:622:ILE:HD13	2:B:622:ILE:HA	1.88	0.42
2:B:629:LEU:O	2:B:633:LYS:HG2	2.20	0.42
1:E:350:ARG:NH1	1:E:357:THR:O	2.45	0.42
3:I:36:TRP:CZ3	3:I:92:CYS:HB3	2.54	0.42
5:T:1:NAG:H61	5:T:2:NAG:C7	2.50	0.42
1:C:204:ALA:HB1	1:C:210:PHE:HZ	1.85	0.42
1:E:457:ASP:HB2	1:E:467:THR:O	2.19	0.42
1:A:90:THR:O	1:A:90:THR:OG1	2.31	0.42
1:C:102:GLU:O	1:C:106:THR:HG23	2.19	0.42
4:X:66:ARG:HH12	4:X:83:ARG:HD2	1.84	0.42
1:C:104:MET:O	1:C:108:ILE:HG12	2.19	0.42
1:C:184:ILE:HD12	1:C:184:ILE:HA	1.96	0.42
1:E:501:CYS:HB3	2:F:605:CYS:SG	2.59	0.42
3:H:37:PHE:HZ	3:H:100(G):PRO:HD2	1.84	0.42
1:A:138:ILE:HD12	1:A:326:ILE:HB	2.00	0.42
1:C:96:TRP:HH2	1:C:285:LEU:HD13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ASP:OD1	1:E:150:MET:N	2.52	0.42
4:X:3:GLN:O	4:X:3:GLN:NE2	2.52	0.42
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.81	0.42
1:A:129:LEU:HB3	1:A:131:CYS:SG	2.60	0.42
1:A:166:ARG:HG2	4:X:100(I):TYS:HB2	2.01	0.42
2:B:538:THR:HG23	2:D:595:ILE:HD12	2.02	0.42
1:C:474:ASP:OD1	1:C:474:ASP:N	2.52	0.42
1:A:272:ILE:HD12	1:A:349:LEU:HD13	2.02	0.42
1:A:390:LEU:HD21	1:A:416:LEU:HD21	2.01	0.42
4:X:3:GLN:OE1	4:X:5:VAL:HG23	2.19	0.42
3:H:6:GLU:OE2	3:H:106:GLY:N	2.28	0.42
6:W:1:NAG:H61	6:W:2:NAG:N2	2.35	0.42
1:A:103:GLN:HE21	1:A:103:GLN:HB3	1.66	0.41
1:A:274:SER:OG	1:A:275:GLU:N	2.52	0.41
1:A:277:ILE:CD1	1:A:352:HIS:HB3	2.50	0.41
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.86	0.41
1:A:69:TRP:HA	1:A:111:LEU:HD13	2.01	0.41
1:E:67:ASN:ND2	1:E:69:TRP:O	2.53	0.41
1:E:223:PHE:CE1	1:E:490:LYS:HB2	2.55	0.41
1:E:257:THR:O	1:E:258:GLN:HG2	2.20	0.41
1:A:385:CYS:HA	1:A:418:CYS:HA	2.02	0.41
2:D:617:ARG:HG3	2:D:621:GLU:OE1	2.19	0.41
1:A:40:TYR:HB2	2:B:593:LEU:HD11	2.03	0.41
1:C:493:PRO:HG3	2:D:544:LEU:HD21	2.02	0.41
1:E:204:ALA:HB2	1:E:434:MET:SD	2.61	0.41
3:J:1018:LYS:HE3	3:J:1074:ALA:HB1	2.02	0.41
3:J:29:LEU:HD12	3:J:34:ILE:HD11	2.02	0.41
2:B:629:LEU:HD12	2:B:629:LEU:H	1.85	0.41
1:C:122:LEU:HD12	1:C:122:LEU:O	2.18	0.41
1:E:54:CYS:HB3	1:E:74:CYS:HB3	1.53	0.41
1:E:382:PHE:CZ	1:E:424:ILE:HD13	2.56	0.41
1:A:35:TRP:CD1	2:B:609:PRO:HB3	2.56	0.41
1:A:61:TYR:HE2	1:A:72:HIS:HB3	1.86	0.41
1:A:180:ASP:N	1:A:180:ASP:OD1	2.53	0.41
1:A:258:GLN:OE1	1:A:470:PRO:HB2	2.21	0.41
1:C:164:GLU:H	1:C:164:GLU:HG3	1.74	0.41
1:C:296:CYS:SG	1:C:376:PHE:HE1	2.43	0.41
1:E:37:THR:HG21	1:E:499:THR:HG22	2.01	0.41
1:E:259:LEU:HD23	1:E:259:LEU:HA	1.87	0.41
4:X:47:TRP:CD1	3:J:1098:PHE:HB2	2.54	0.41
3:J:1037:GLN:HB3	3:J:1047:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:LEU:HD21	1:C:416:LEU:HD21	2.01	0.41
1:E:260:LEU:HB2	1:E:451:GLY:HA3	2.02	0.41
3:H:100(B):TYR:C	3:H:100(D):THR:H	2.24	0.41
4:X:36:TRP:CD1	4:X:80:LEU:HD13	2.55	0.41
1:A:305:LYS:HB2	1:A:305:LYS:HE3	1.84	0.41
1:A:346:VAL:HG22	1:A:359:ILE:HG21	2.01	0.41
1:A:374:HIS:CE1	1:A:376:PHE:HE1	2.39	0.41
1:C:120:VAL:HG13	1:C:203:GLN:HB3	2.02	0.41
1:C:280:ASN:OD1	1:C:456:ARG:NH2	2.54	0.41
1:C:297:THR:OG1	1:C:444:ARG:HG2	2.21	0.41
1:C:382:PHE:CZ	1:C:424:ILE:HD13	2.54	0.41
2:D:523:LEU:HA	2:D:540:GLN:NE2	2.36	0.41
3:J:18:LEU:HB2	3:J:82:MET:HG3	2.02	0.41
1:A:224:ALA:HB2	1:A:491:ILE:HD11	2.02	0.41
1:A:226:LEU:HB2	1:A:487:LYS:HG2	2.03	0.41
1:C:297:THR:HA	1:C:443:ILE:O	2.21	0.41
1:C:424:ILE:HD12	1:C:426:MET:HB2	2.02	0.41
1:E:368:ASP:OD1	3:H:98:ALA:HB1	2.21	0.41
3:J:51:LEU:HD12	3:J:69:ILE:HG23	2.03	0.41
3:J:56:ASN:ND2	3:J:97:ARG:HE	2.19	0.41
1:A:86:LEU:HB2	1:A:89:VAL:HG11	2.02	0.40
1:C:285:LEU:HD21	1:C:477:ASP:HB3	2.02	0.40
1:A:41:GLY:HA3	2:B:541:ALA:HB2	2.04	0.40
1:A:164:GLU:HB3	1:A:308:ARG:HD2	2.03	0.40
1:A:322:ILE:HG21	1:A:326:ILE:HG12	2.03	0.40
2:D:645:LEU:HA	2:D:648:GLU:OE1	2.20	0.40
1:E:161:MET:HE3	1:E:309:ILE:HA	2.04	0.40
4:X:61:GLU:HA	4:X:64:TRP:CD2	2.56	0.40
1:A:87:GLU:O	2:B:527:GLY:HA3	2.22	0.40
1:A:427:TRP:O	1:A:429:ARG:N	2.54	0.40
1:C:87:GLU:O	1:C:89:VAL:HG23	2.21	0.40
3:H:45:ARG:HB3	3:H:45:ARG:CZ	2.51	0.40
2:D:586:TYR:HE2	2:F:587:LEU:HD12	1.86	0.40
2:F:647:GLU:OE1	2:F:647:GLU:HA	2.21	0.40
3:H:19:ARG:HG3	3:H:19:ARG:HH11	1.86	0.40
5:S:1:NAG:O6	5:S:2:NAG:N2	2.55	0.40
1:A:257:THR:O	1:A:258:GLN:HG2	2.22	0.40
1:A:260:LEU:HD21	1:A:453:ILE:HD11	2.04	0.40
1:A:374:HIS:O	1:A:384:TYR:HA	2.21	0.40
2:D:588:ARG:O	2:D:588:ARG:HD3	2.22	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	447/481 (93%)	397 (89%)	49 (11%)	1 (0%)	47	79
1	C	447/481 (93%)	400 (90%)	45 (10%)	2 (0%)	34	71
1	E	447/481 (93%)	399 (89%)	48 (11%)	0	100	100
2	B	123/153 (80%)	113 (92%)	9 (7%)	1 (1%)	19	58
2	D	122/153 (80%)	110 (90%)	11 (9%)	1 (1%)	19	58
2	F	122/153 (80%)	109 (89%)	12 (10%)	1 (1%)	19	58
3	H	119/353 (34%)	103 (87%)	15 (13%)	1 (1%)	19	58
3	I	119/353 (34%)	108 (91%)	10 (8%)	1 (1%)	19	58
3	J	228/353 (65%)	202 (89%)	25 (11%)	1 (0%)	34	71
4	X	140/247 (57%)	134 (96%)	5 (4%)	1 (1%)	22	61
All	All	2314/3208 (72%)	2075 (90%)	229 (10%)	10 (0%)	38	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	601	LYS
1	C	140	ASP
2	F	598	CYS
3	H	100(C)	VAL
3	I	100(C)	VAL
3	J	100(C)	VAL
1	A	276	ASN
2	D	603	ILE
1	C	153	GLU
4	X	100(Y)	VAL



### 5.3.2 Protein sidechains [i](#)

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	405/429 (94%)	396 (98%)	9 (2%)	52 77
1	C	405/429 (94%)	392 (97%)	13 (3%)	39 69
1	E	405/429 (94%)	386 (95%)	19 (5%)	26 60
2	B	109/129 (84%)	104 (95%)	5 (5%)	27 61
2	D	108/129 (84%)	101 (94%)	7 (6%)	17 51
2	F	108/129 (84%)	104 (96%)	4 (4%)	34 66
3	H	95/281 (34%)	93 (98%)	2 (2%)	53 78
3	I	95/281 (34%)	94 (99%)	1 (1%)	73 87
3	J	184/281 (66%)	176 (96%)	8 (4%)	29 63
4	X	116/205 (57%)	114 (98%)	2 (2%)	60 82
All	All	2030/2722 (75%)	1960 (97%)	70 (3%)	40 68

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	TRP
1	A	76	PRO
1	A	94	ASN
1	A	103	GLN
1	A	107	ASP
1	A	205	CYS
1	A	247	CYS
1	A	317	PHE
1	A	368	ASP
2	B	519	PHE
2	B	530	MET
2	B	579	ARG
2	B	624	ASP
2	B	638	TYR
1	C	52	LEU
1	C	53	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	64	GLU
1	C	100	MET
1	C	112	TRP
1	C	151	ARG
1	C	173	TYR
1	C	264	SER
1	C	330	HIS
1	C	444	ARG
1	C	475	MET
1	C	480	ARG
1	C	500	ARG
2	D	519	PHE
2	D	543	ASN
2	D	587	LEU
2	D	590	GLN
2	D	596	TRP
2	D	615	SER
2	D	659	ASP
1	E	52	LEU
1	E	85	HIS
1	E	103	GLN
1	E	133	ASN
1	E	150	MET
1	E	167	ASP
1	E	173	TYR
1	E	211	GLU
1	E	247	CYS
1	E	271	MET
1	E	287	GLN
1	E	320	THR
1	E	330	HIS
1	E	376	PHE
1	E	426	MET
1	E	434	MET
1	E	457	ASP
1	E	487	LYS
1	E	504	ARG
2	F	543	ASN
2	F	571	TRP
2	F	599	SER
2	F	620	SER
3	H	28	ASP

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Mol	Chain	Res	Type
3	H	57	SER
3	I	45	ARG
4	X	3	GLN
4	X	108	MET
3	J	7	SER
3	J	22	CYS
3	J	45	ARG
3	J	55	LYS
3	J	72	ASP
3	J	83	GLU
3	J	92	CYS
3	J	1098	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	287	GLN
1	C	185	ASN
1	C	287	GLN
2	D	625	ASN
1	E	280	ASN
1	E	287	GLN
2	F	543	ASN
3	H	5	GLN
4	X	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TYS	X	100(H)	1,4	15,16,17	1.49	2 (13%)	18,22,24	3.43	7 (38%)
4	TYS	X	100(I)	4	15,16,17	1.33	3 (20%)	18,22,24	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TYS	X	100(H)	1,4	-	4/10/11/13	0/1/1/1
4	TYS	X	100(I)	4	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	100(H)	TYS	O2-S	4.30	1.63	1.45
4	X	100(I)	TYS	OH-CZ	-3.15	1.37	1.42
4	X	100(I)	TYS	OH-S	-2.79	1.54	1.58
4	X	100(H)	TYS	OH-CZ	-2.67	1.38	1.42
4	X	100(I)	TYS	O3-S	2.22	1.64	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	100(H)	TYS	OH-S-O2	-7.58	85.59	107.71
4	X	100(H)	TYS	O2-S-O1	-7.08	83.78	112.22
4	X	100(H)	TYS	O3-S-O2	-5.68	88.75	108.49
4	X	100(H)	TYS	OH-S-O1	5.31	123.18	107.71
4	X	100(H)	TYS	O3-S-OH	4.68	117.11	105.83
4	X	100(I)	TYS	CG-CB-CA	-3.31	107.40	114.10
4	X	100(H)	TYS	O3-S-O1	2.81	118.25	108.49
4	X	100(H)	TYS	CB-CA-C	-2.10	107.54	111.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	100(H)	TYS	CZ-OH-S-O1

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Mol	Chain	Res	Type	Atoms
4	X	100(H)	TYS	CZ-OH-S-O3
4	X	100(H)	TYS	CA-CB-CG-CD1
4	X	100(H)	TYS	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	100(H)	TYS	1	0
4	X	100(I)	TYS	1	0

## 5.5 Carbohydrates [i](#)

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	1	5,1	14,14,15	0.20	0	17,19,21	0.57	0
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	K	1	5,1	14,14,15	0.24	0	17,19,21	0.59	0
5	NAG	K	2	5	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	L	1	1,6	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
6	NAG	L	2	6	14,14,15	0.31	0	17,19,21	0.46	0
6	BMA	L	3	6	11,11,12	0.55	0	15,15,17	0.70	0
5	NAG	M	1	5,1	14,14,15	0.69	1 (7%)	17,19,21	0.79	1 (5%)
5	NAG	M	2	5	14,14,15	0.39	0	17,19,21	0.34	0
5	NAG	N	1	5,1	14,14,15	0.18	0	17,19,21	0.38	0
5	NAG	N	2	5	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	O	1	1,6	14,14,15	0.24	0	17,19,21	0.94	1 (5%)
6	NAG	O	2	6	14,14,15	0.34	0	17,19,21	0.73	0
6	BMA	O	3	6	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
5	NAG	P	1	5,1	14,14,15	0.39	0	17,19,21	0.66	0
5	NAG	P	2	5	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	Q	1	5,1	14,14,15	0.30	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	Q	2	5	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	R	1	1,7	14,14,15	0.30	0	17,19,21	0.44	0
7	NAG	R	2	7	14,14,15	0.20	0	17,19,21	0.62	0
7	BMA	R	3	7	11,11,12	0.57	0	15,15,17	0.75	0
7	MAN	R	4	7	11,11,12	1.55	3 (27%)	15,15,17	2.20	4 (26%)
5	NAG	S	1	5,1	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	S	2	5	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	T	1	5,1	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	T	2	5	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	U	1	5,1	14,14,15	0.21	0	17,19,21	0.53	0
5	NAG	U	2	5	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	V	1	5,1	14,14,15	0.39	0	17,19,21	0.82	0
5	NAG	V	2	5	14,14,15	0.25	0	17,19,21	0.60	1 (5%)
6	NAG	W	1	1,6	14,14,15	0.45	0	17,19,21	0.47	0
6	NAG	W	2	6	14,14,15	0.32	0	17,19,21	0.38	0
6	BMA	W	3	6	11,11,12	0.53	0	15,15,17	0.68	0
6	NAG	Y	1	1,6	14,14,15	0.23	0	17,19,21	0.60	0
6	NAG	Y	2	6	14,14,15	0.31	0	17,19,21	0.53	0
6	BMA	Y	3	6	11,11,12	0.61	0	15,15,17	0.74	0
5	NAG	Z	1	5,1	14,14,15	0.24	0	17,19,21	0.69	0
5	NAG	Z	2	5	14,14,15	0.24	0	17,19,21	0.63	0
5	NAG	a	1	5,1	14,14,15	0.22	0	17,19,21	0.56	0
5	NAG	a	2	5	14,14,15	0.24	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
5	NAG	G	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	4	MAN	C1-C2	3.54	1.60	1.52
7	R	4	MAN	O5-C1	2.97	1.48	1.43
5	M	1	NAG	O5-C1	-2.35	1.40	1.43
7	R	4	MAN	O5-C5	2.00	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	4	MAN	C1-O5-C5	6.62	121.17	112.19
7	R	4	MAN	O5-C1-C2	3.14	115.62	110.77
6	O	1	NAG	C1-O5-C5	3.12	116.43	112.19
7	R	4	MAN	C1-C2-C3	2.51	112.75	109.67
6	L	1	NAG	C1-O5-C5	2.39	115.43	112.19
6	O	3	BMA	C1-O5-C5	2.31	115.33	112.19
7	R	4	MAN	O2-C2-C3	-2.30	105.53	110.14
5	M	1	NAG	C1-O5-C5	2.19	115.16	112.19
5	V	2	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
6	Y	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
7	R	2	NAG	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
6	Y	1	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	N	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	P	1	NAG	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	V	1	NAG	C3-C2-N2-C7
5	T	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
5	Z	2	NAG	C3-C2-N2-C7
5	a	1	NAG	C3-C2-N2-C7
6	O	1	NAG	C3-C2-N2-C7
6	O	2	NAG	C3-C2-N2-C7
5	T	1	NAG	O5-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 7 short contacts:

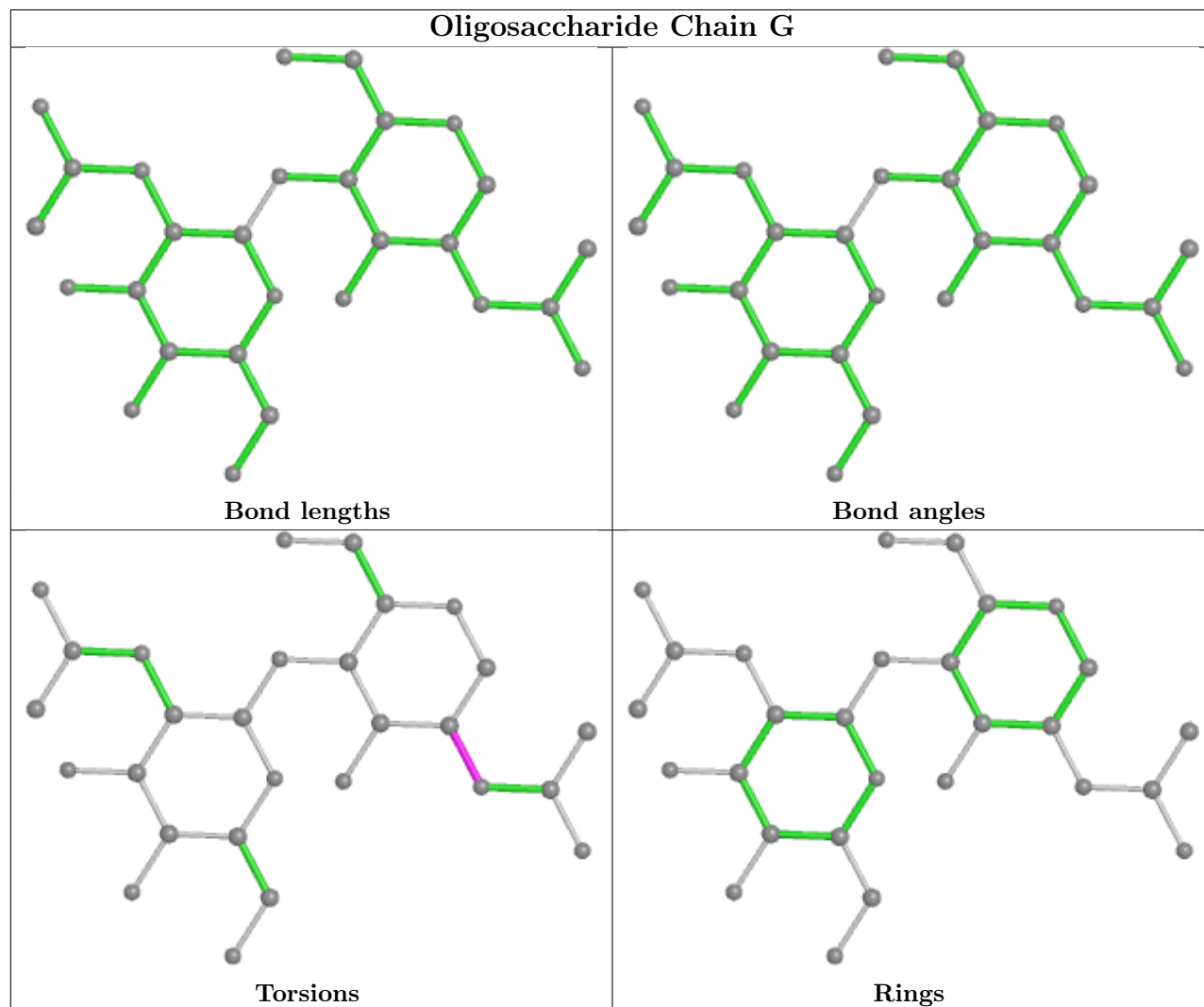
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	2	NAG	1	0
6	W	1	NAG	2	0
5	T	2	NAG	1	0
5	S	1	NAG	1	0
5	K	1	NAG	1	0
6	L	1	NAG	2	0
6	W	2	NAG	1	0

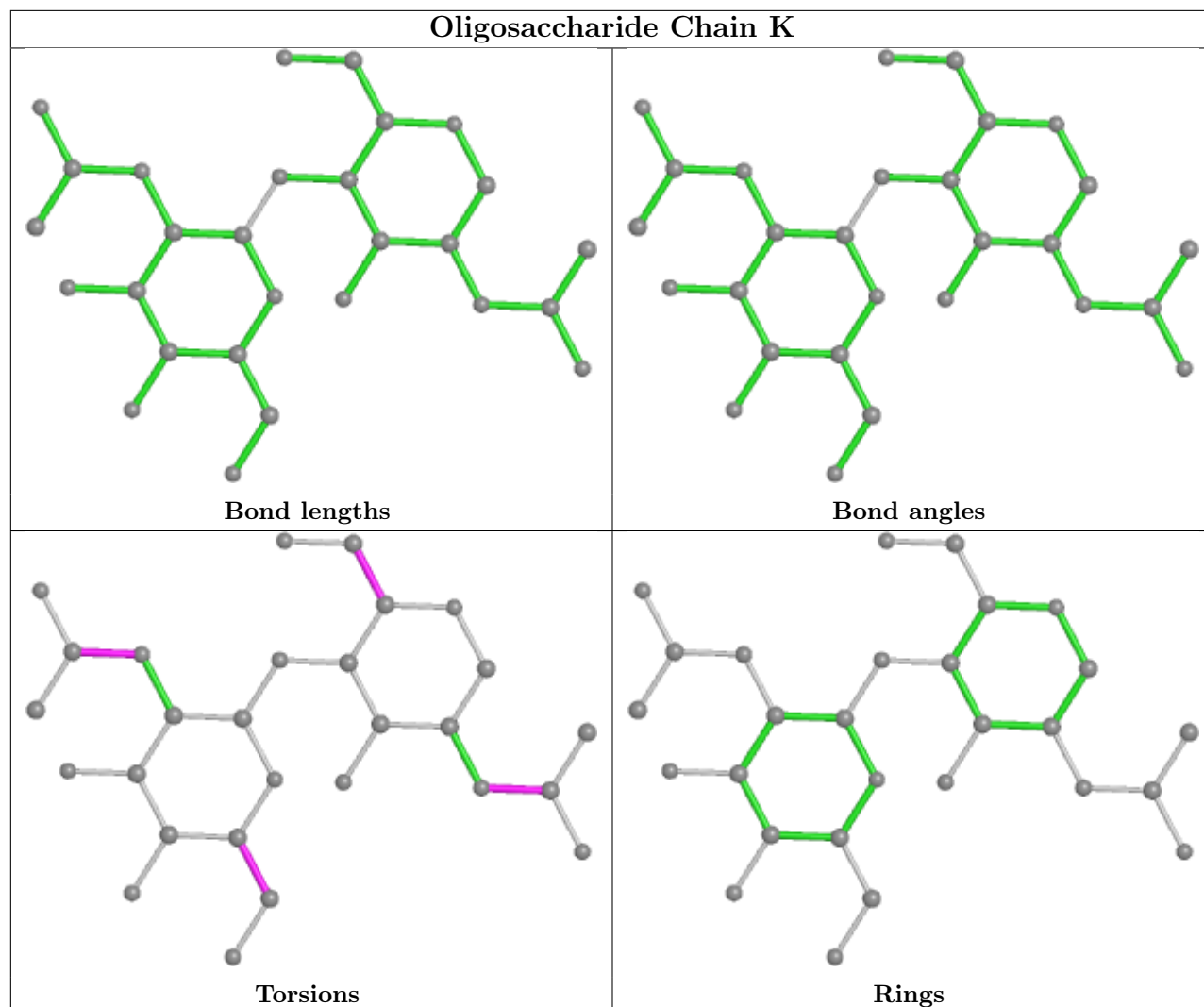
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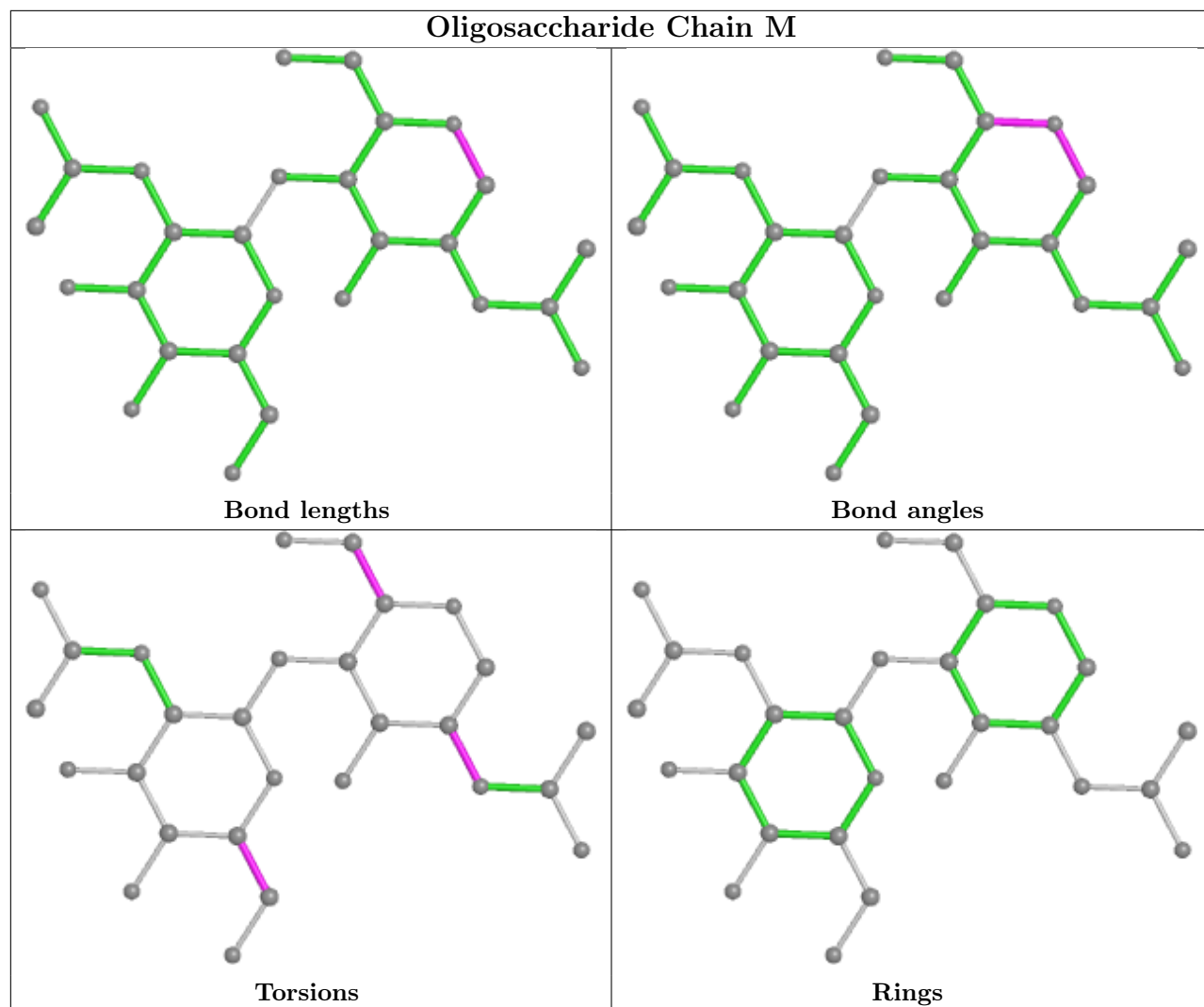
Continued from previous page...

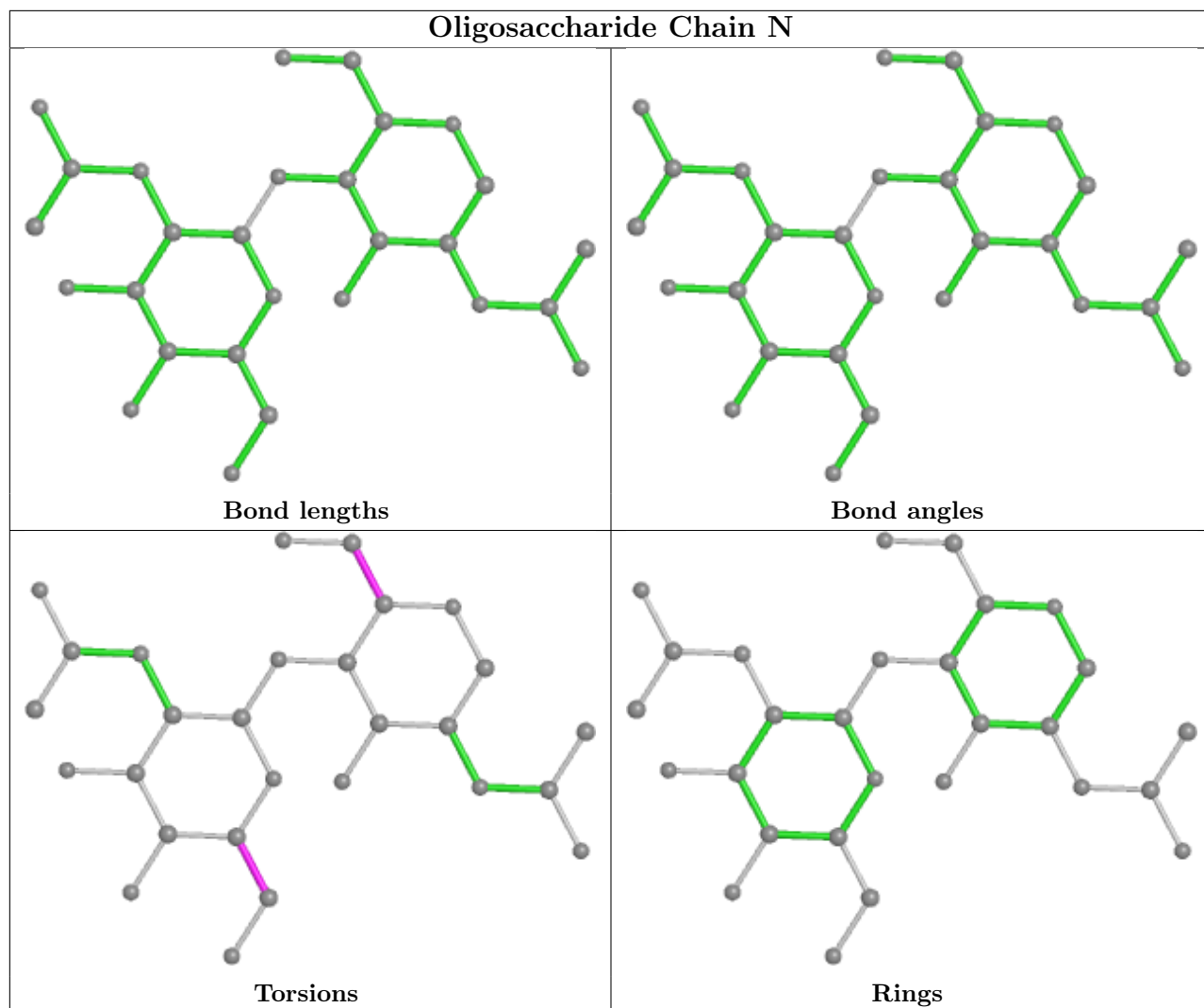
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1	NAG	1	0

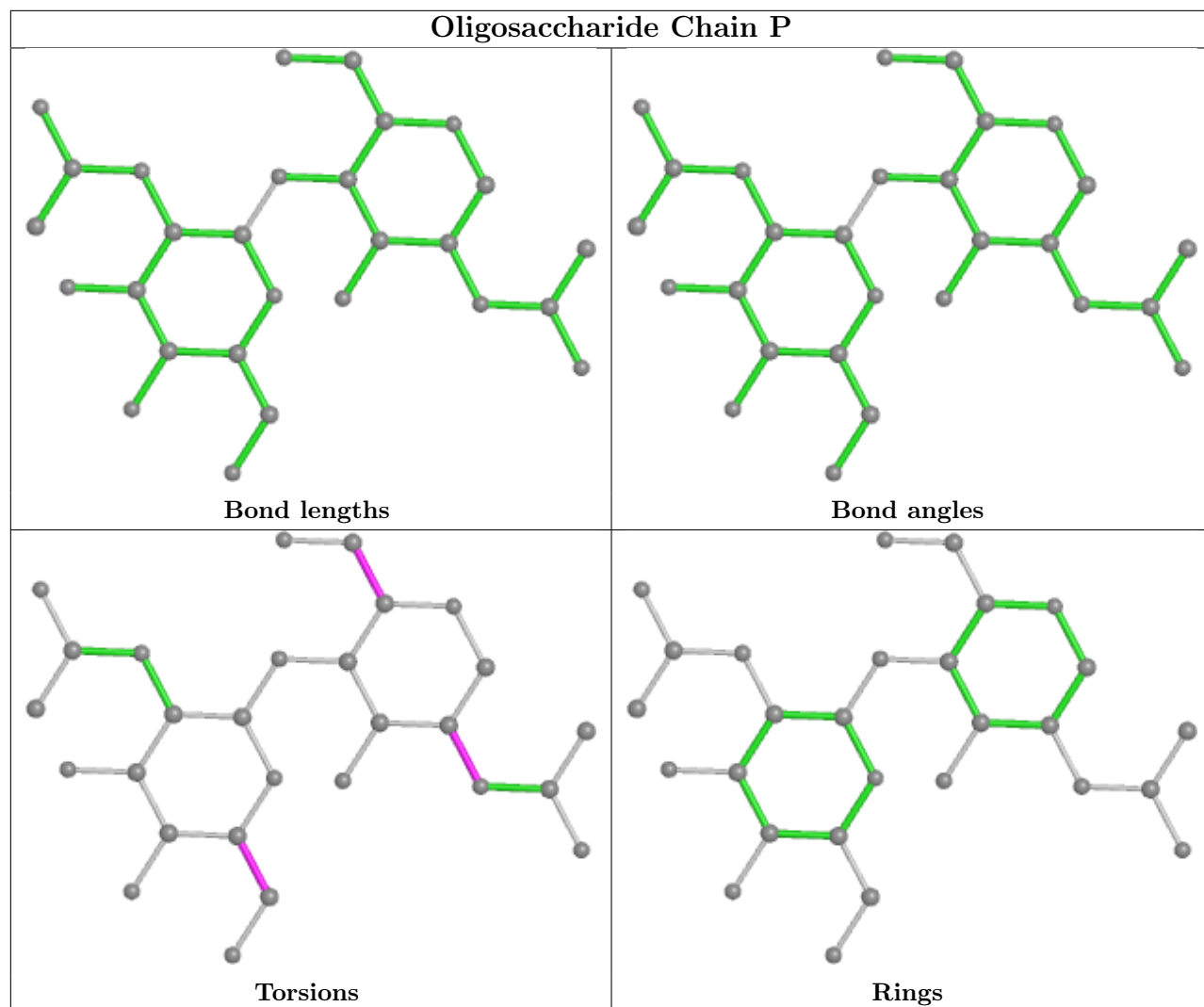
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

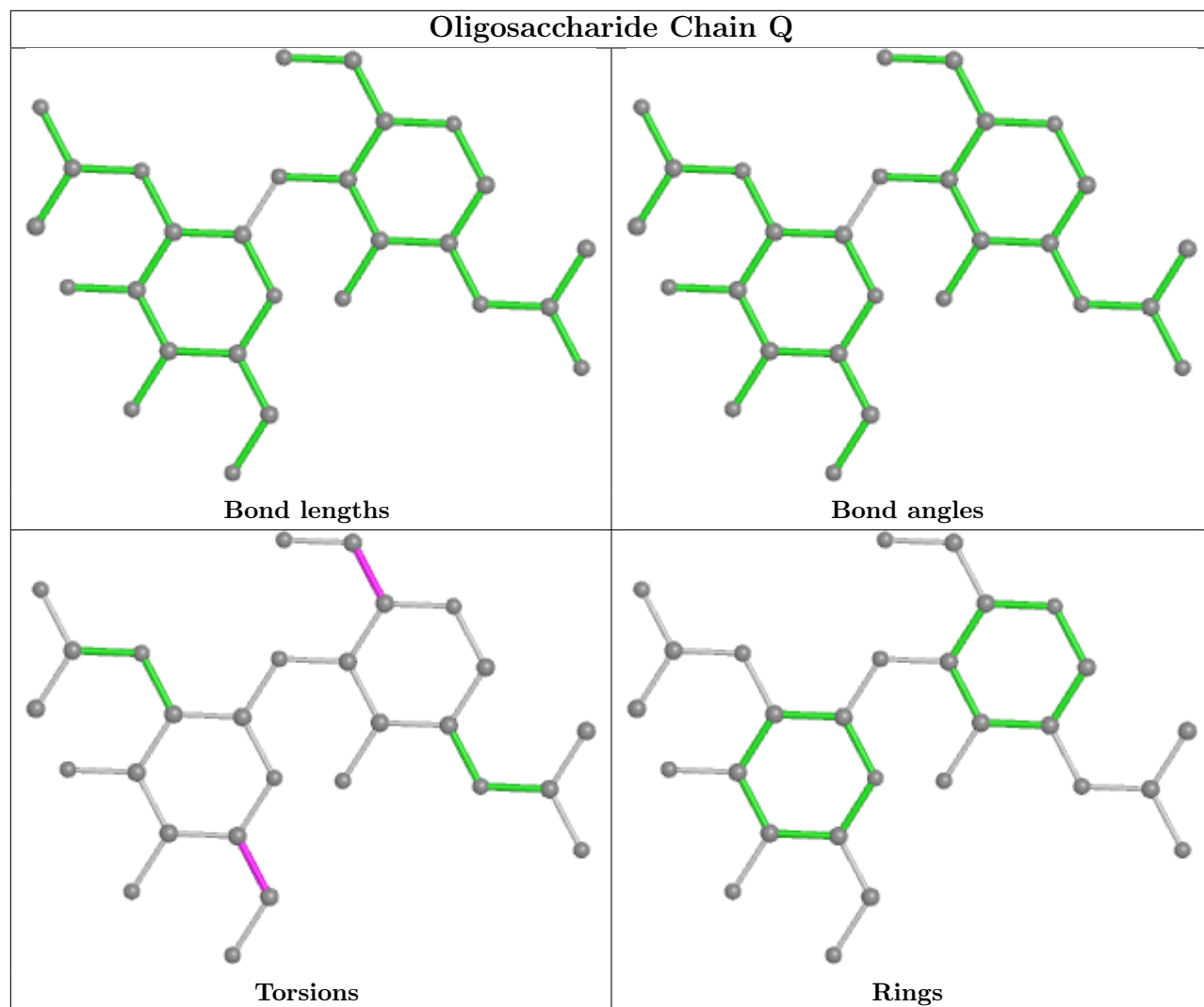


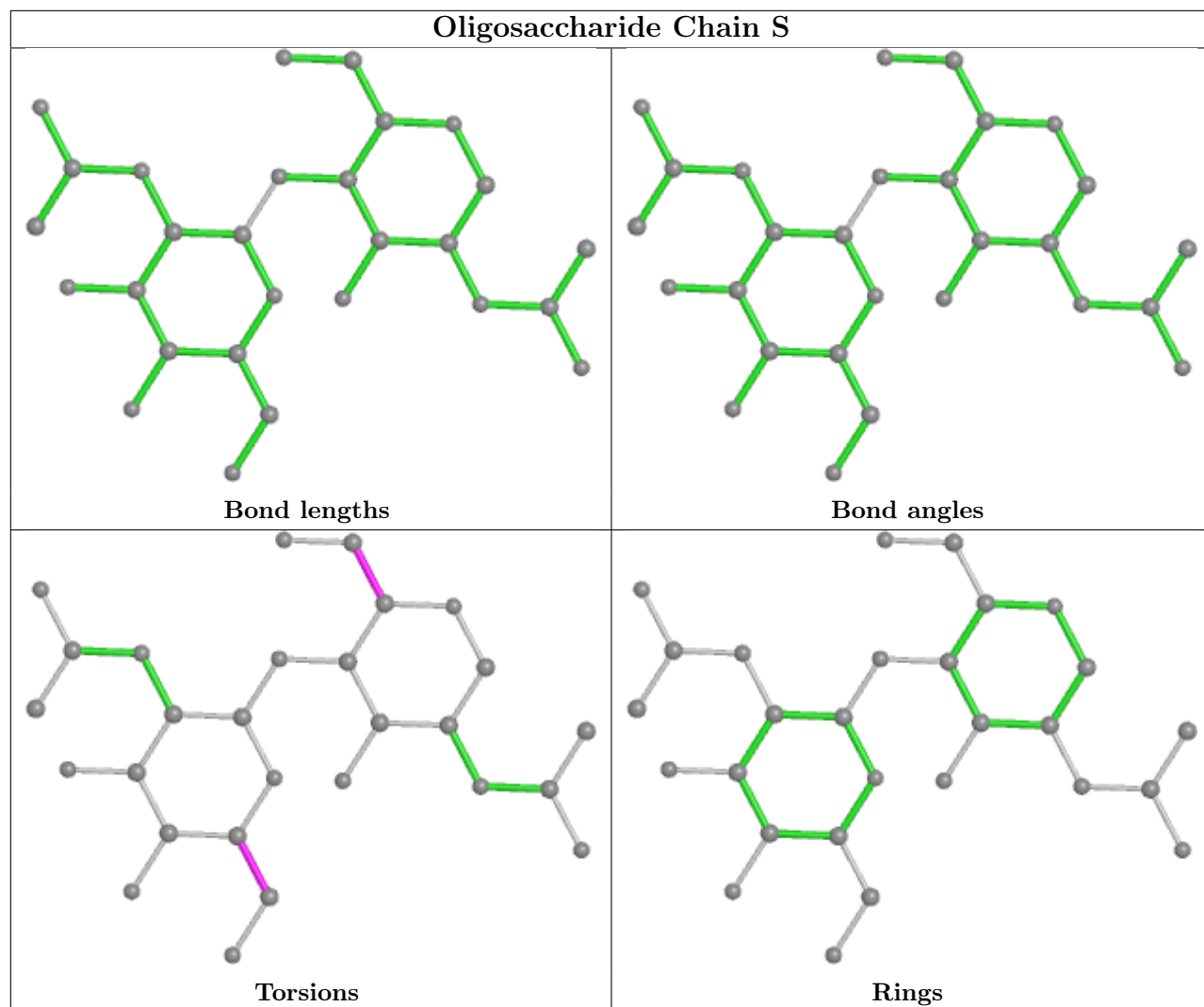




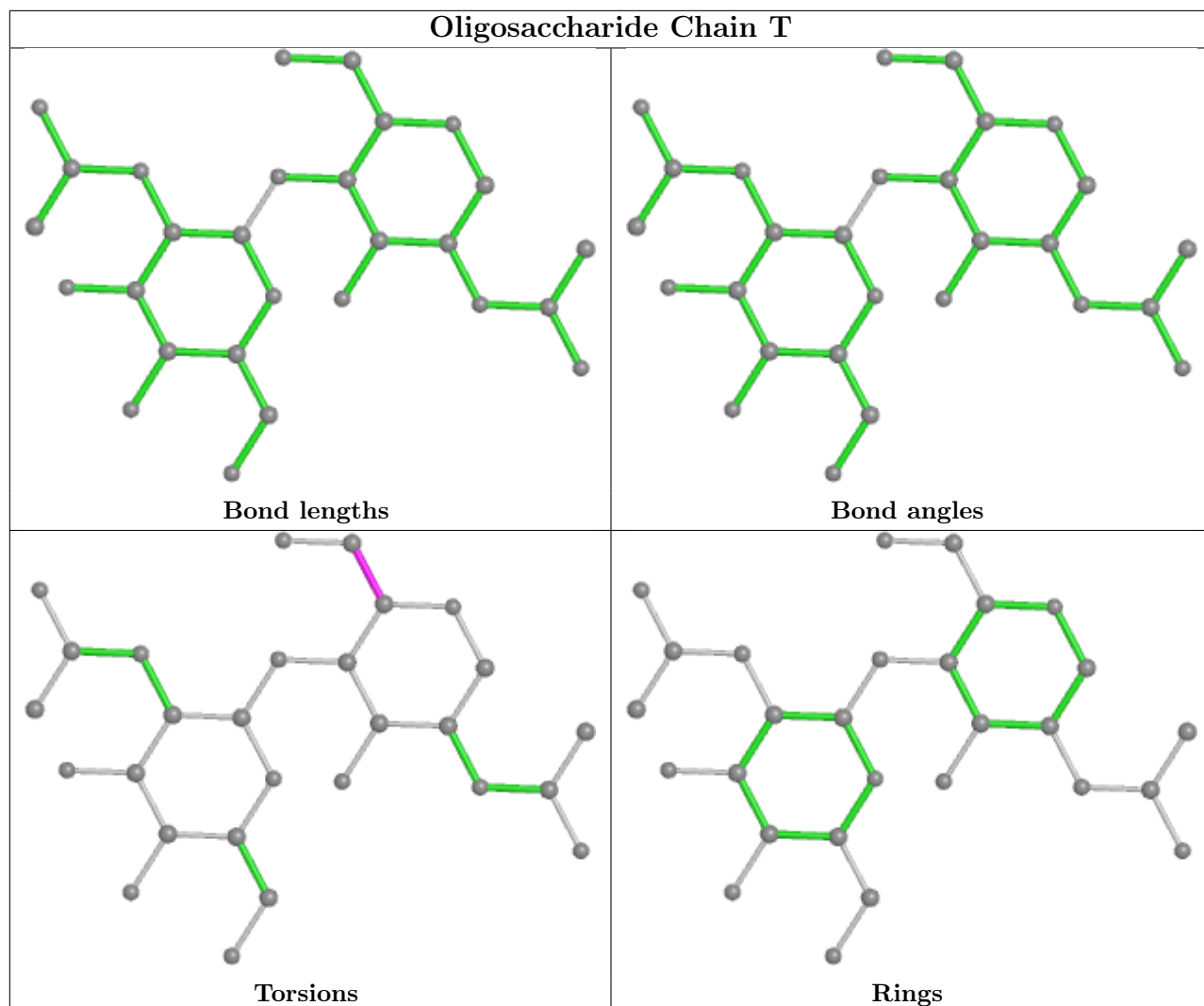


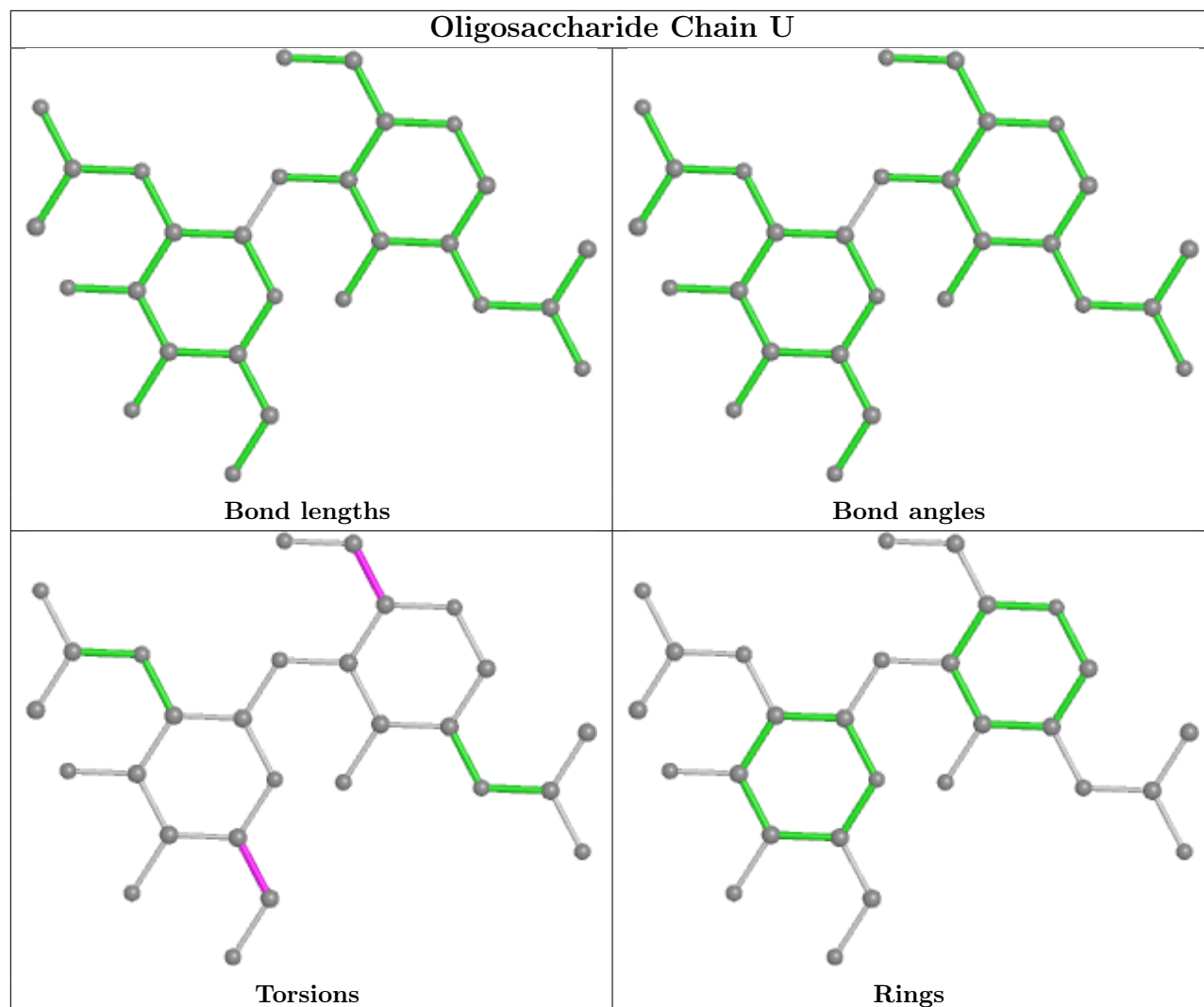


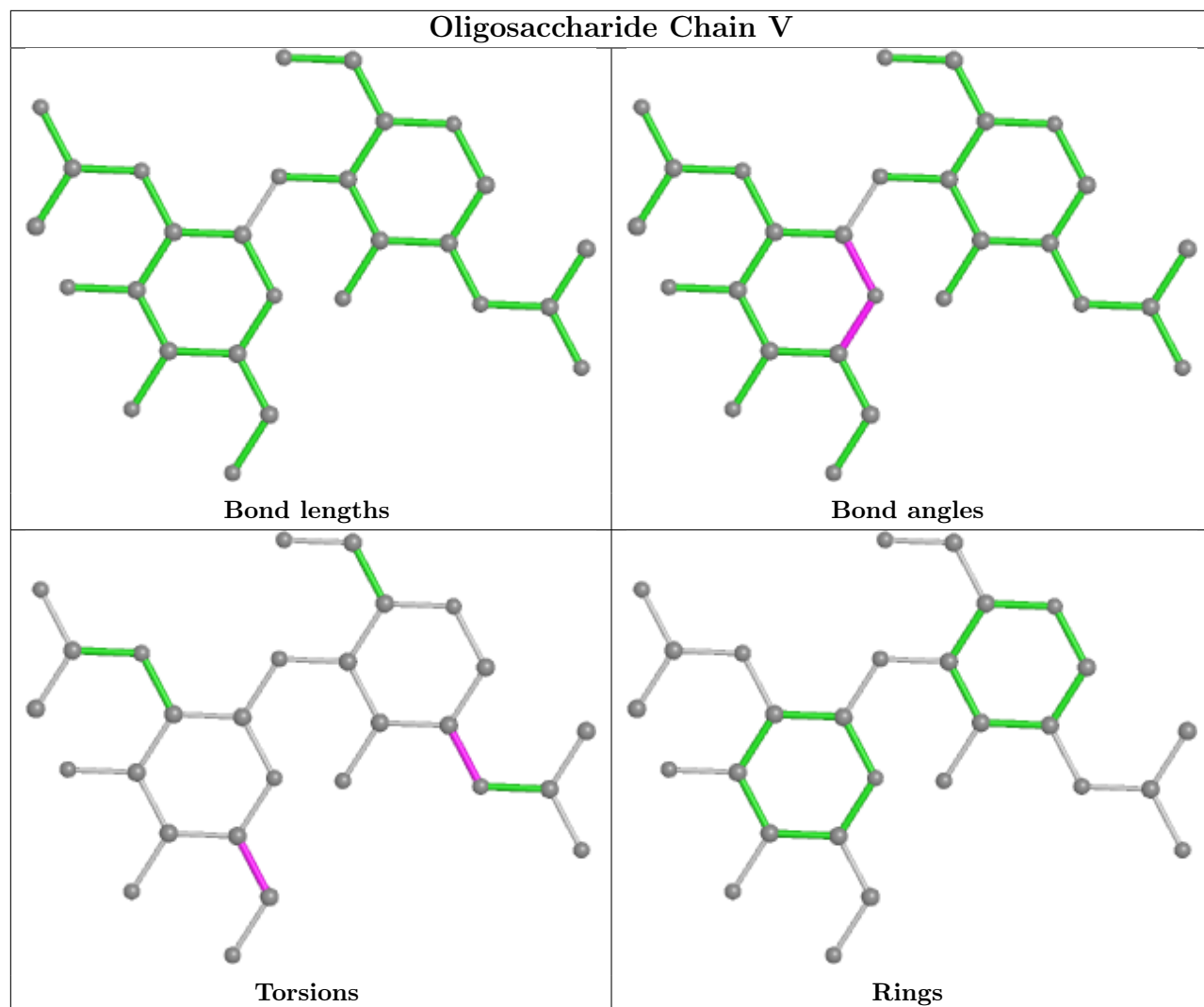


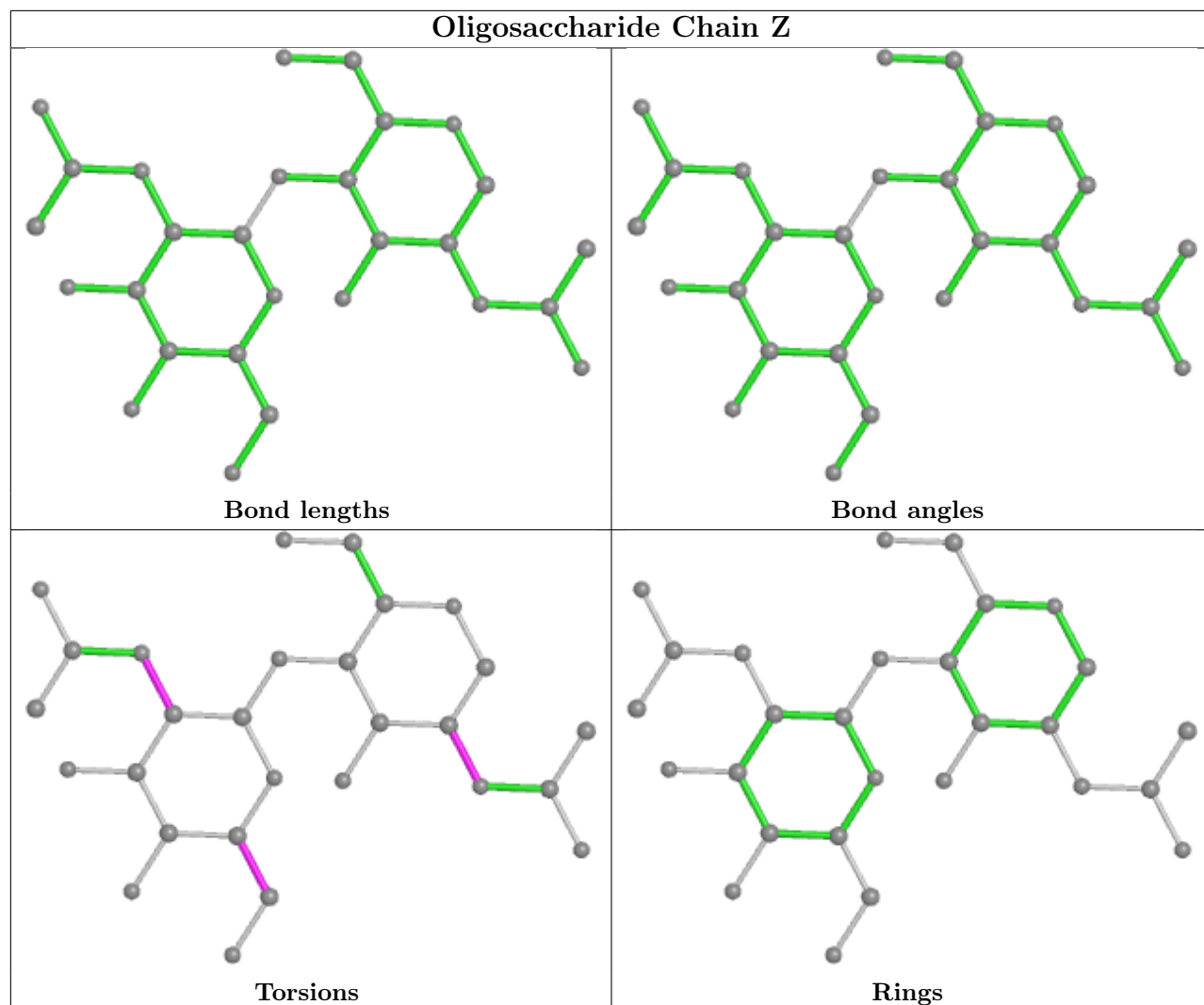


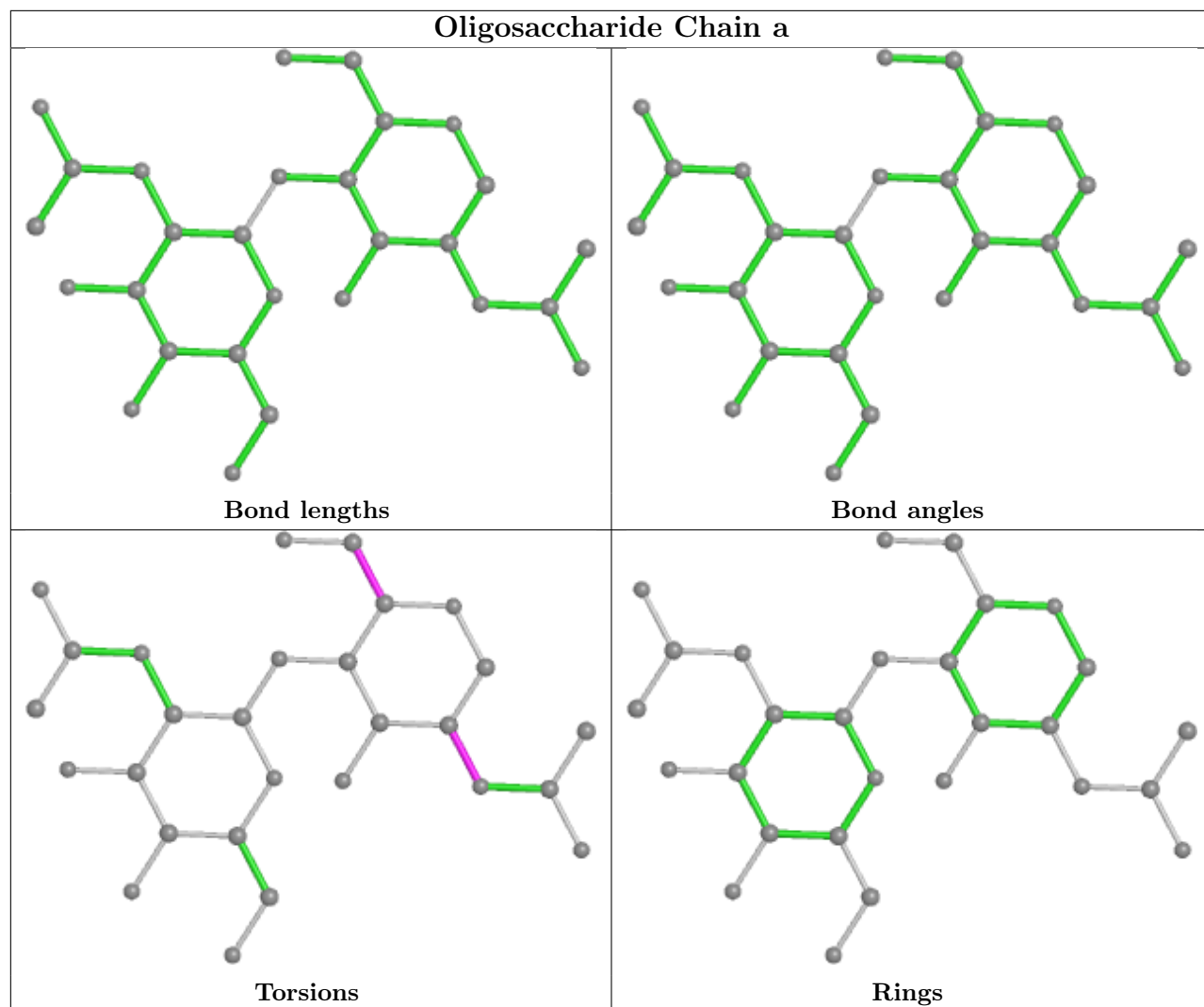


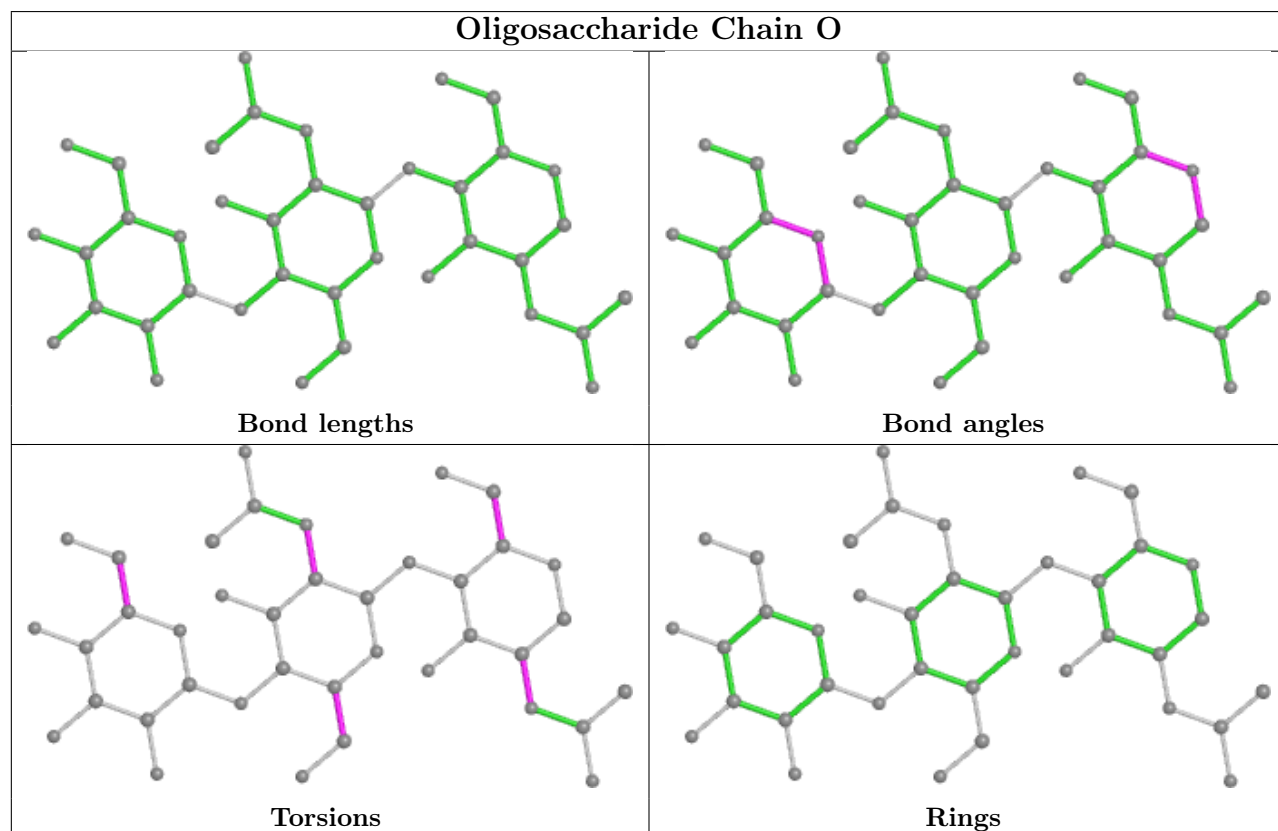
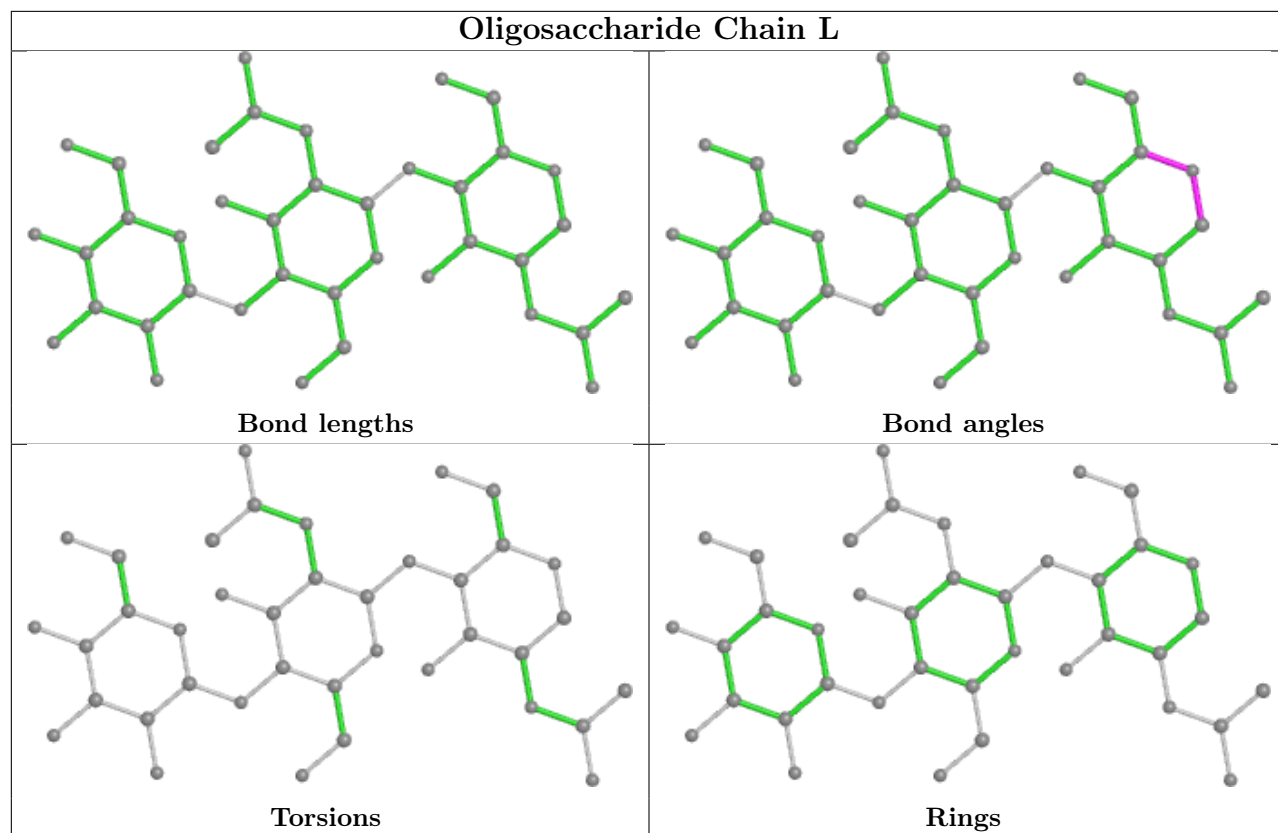


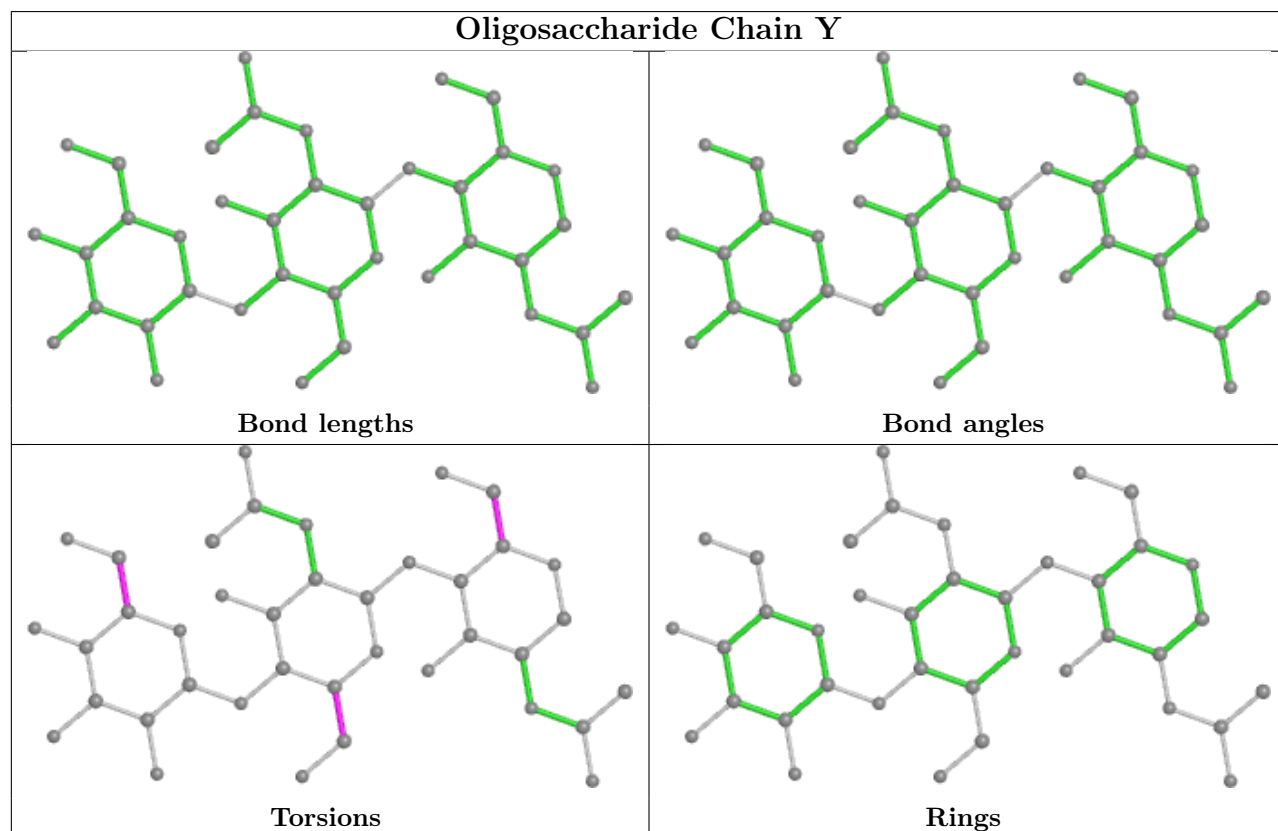
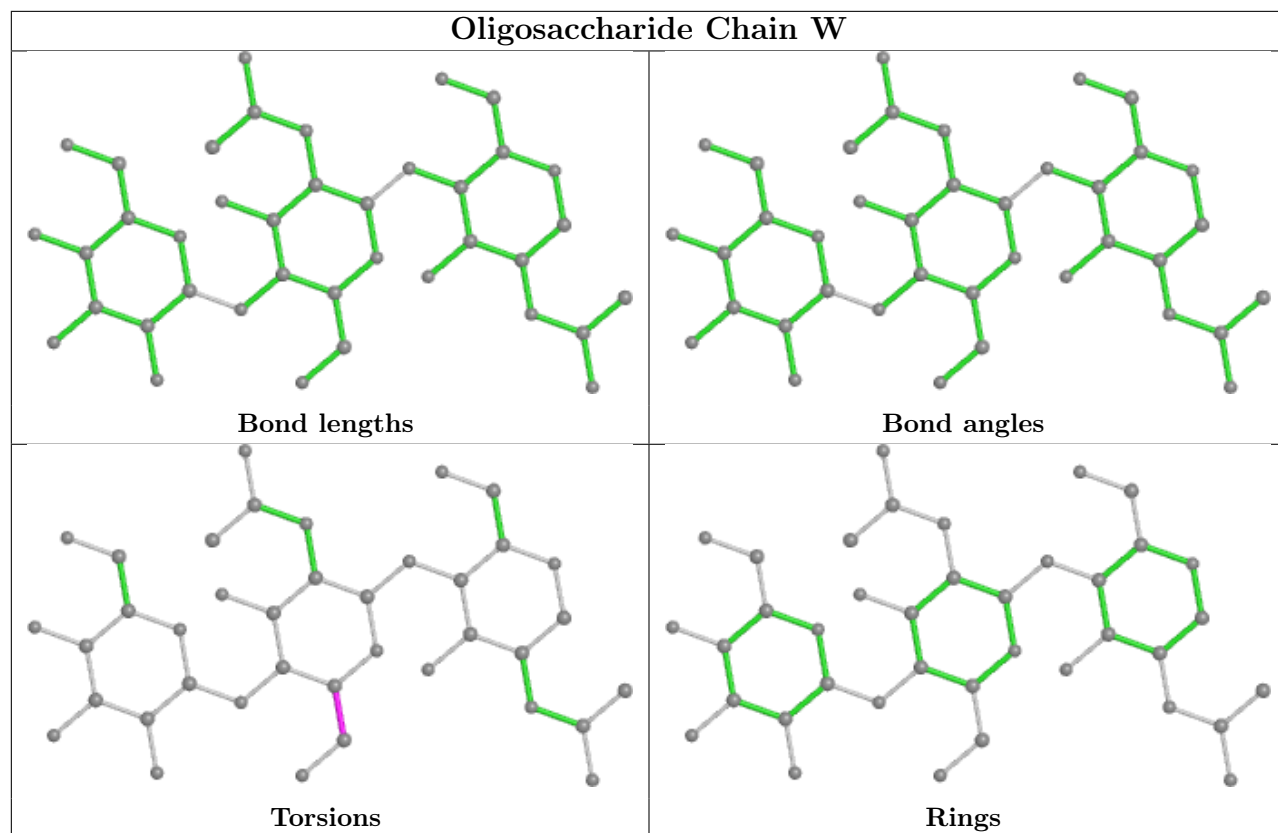


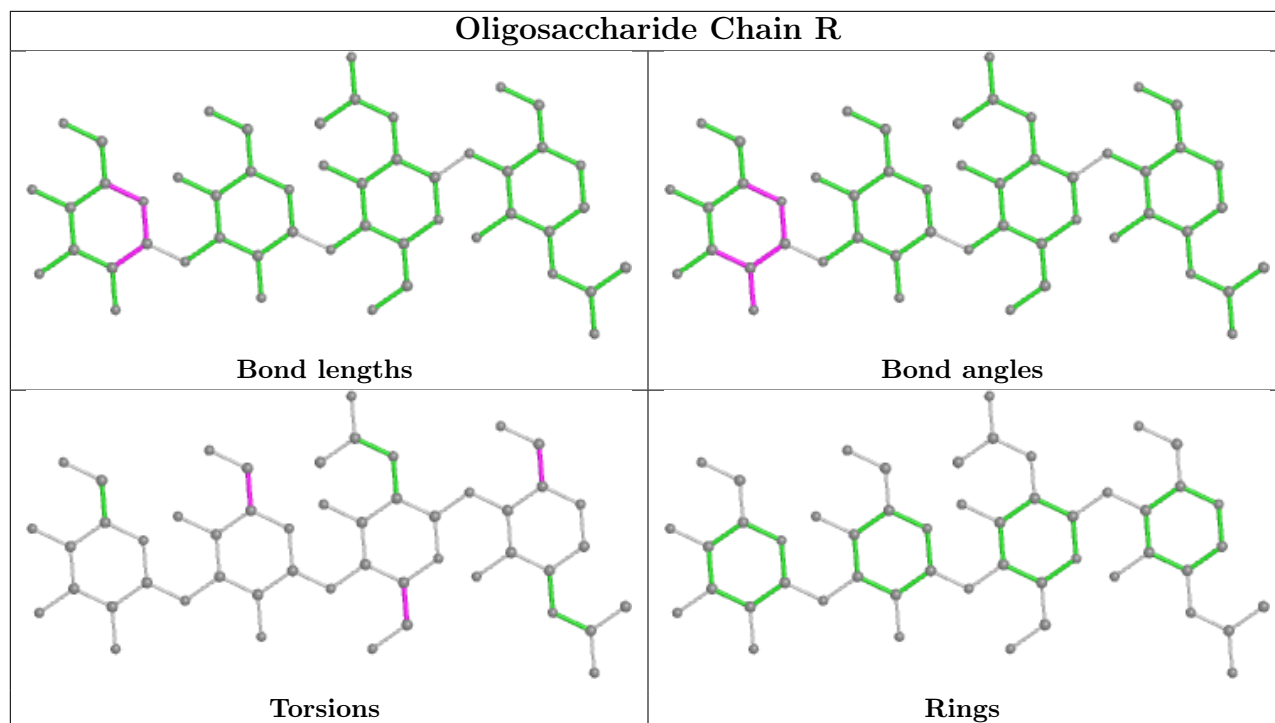












## 5.6 Ligand geometry [i](#)

32 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	C	601	1	14,14,15	0.28	0	17,19,21	0.38	0
8	NAG	A	609	1	14,14,15	0.16	0	17,19,21	0.72	1 (5%)
8	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.39	0
8	NAG	E	607	1	14,14,15	0.18	0	17,19,21	0.54	0
8	NAG	C	603	1	14,14,15	0.58	0	17,19,21	0.86	1 (5%)
8	NAG	E	601	1	14,14,15	0.31	0	17,19,21	0.46	0
8	NAG	E	608	1	14,14,15	0.29	0	17,19,21	0.46	0
8	NAG	E	603	1	14,14,15	0.38	0	17,19,21	0.52	0
8	NAG	E	605	1	14,14,15	0.83	1 (7%)	17,19,21	0.84	1 (5%)
8	NAG	A	610	1	14,14,15	0.39	0	17,19,21	0.50	0
8	NAG	A	603	1	14,14,15	0.33	0	17,19,21	0.48	0
8	NAG	A	602	1	14,14,15	0.21	0	17,19,21	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	E	606	1	14,14,15	0.17	0	17,19,21	0.78	1 (5%)
8	NAG	A	605	1	14,14,15	0.23	0	17,19,21	0.40	0
8	NAG	A	608	1	14,14,15	0.27	0	17,19,21	0.61	0
8	NAG	B	701	2	14,14,15	0.83	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	C	608	1	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
8	NAG	E	610	1	14,14,15	0.34	0	17,19,21	0.37	0
8	NAG	A	606	1	14,14,15	0.15	0	17,19,21	0.39	0
8	NAG	C	609	1	14,14,15	0.33	0	17,19,21	0.62	0
8	NAG	C	605	1	14,14,15	0.22	0	17,19,21	0.54	0
8	NAG	E	611	1	14,14,15	0.36	0	17,19,21	0.53	0
8	NAG	C	606	1	14,14,15	0.40	0	17,19,21	0.55	0
8	NAG	A	604	1	14,14,15	0.62	0	17,19,21	1.29	2 (11%)
8	NAG	E	609	1	14,14,15	0.33	0	17,19,21	0.34	0
8	NAG	C	604	1	14,14,15	0.63	0	17,19,21	0.56	0
8	NAG	E	602	1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	A	607	1	14,14,15	0.33	0	17,19,21	0.39	0
8	NAG	C	602	1	14,14,15	0.38	0	17,19,21	0.51	0
8	NAG	E	604	1	14,14,15	0.30	0	17,19,21	0.47	0
8	NAG	C	607	1	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
8	NAG	C	610	1	14,14,15	0.31	0	17,19,21	0.36	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	C	601	1	-	2/6/23/26	0/1/1/1
8	NAG	A	609	1	-	3/6/23/26	0/1/1/1
8	NAG	A	601	1	-	2/6/23/26	0/1/1/1
8	NAG	E	607	1	-	2/6/23/26	0/1/1/1
8	NAG	C	603	1	-	1/6/23/26	0/1/1/1
8	NAG	E	601	1	-	4/6/23/26	0/1/1/1
8	NAG	E	608	1	-	3/6/23/26	0/1/1/1
8	NAG	E	603	1	-	4/6/23/26	0/1/1/1
8	NAG	E	605	1	-	2/6/23/26	0/1/1/1
8	NAG	A	610	1	-	4/6/23/26	0/1/1/1
8	NAG	A	603	1	-	2/6/23/26	0/1/1/1
8	NAG	A	602	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	606	1	-	3/6/23/26	0/1/1/1
8	NAG	A	605	1	-	2/6/23/26	0/1/1/1
8	NAG	A	608	1	-	4/6/23/26	0/1/1/1
8	NAG	B	701	2	-	3/6/23/26	0/1/1/1
8	NAG	C	608	1	-	0/6/23/26	0/1/1/1
8	NAG	E	610	1	-	0/6/23/26	0/1/1/1
8	NAG	A	606	1	-	4/6/23/26	0/1/1/1
8	NAG	C	609	1	-	3/6/23/26	0/1/1/1
8	NAG	C	605	1	-	3/6/23/26	0/1/1/1
8	NAG	E	611	1	-	1/6/23/26	0/1/1/1
8	NAG	C	606	1	-	3/6/23/26	0/1/1/1
8	NAG	A	604	1	-	5/6/23/26	0/1/1/1
8	NAG	E	609	1	-	1/6/23/26	0/1/1/1
8	NAG	C	604	1	-	2/6/23/26	0/1/1/1
8	NAG	E	602	1	-	2/6/23/26	0/1/1/1
8	NAG	A	607	1	-	0/6/23/26	0/1/1/1
8	NAG	C	602	1	-	4/6/23/26	0/1/1/1
8	NAG	E	604	1	-	2/6/23/26	0/1/1/1
8	NAG	C	607	1	-	3/6/23/26	0/1/1/1
8	NAG	C	610	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	NAG	O5-C1	2.66	1.48	1.43
8	E	605	NAG	C1-C2	2.37	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	604	NAG	C2-N2-C7	4.33	129.07	122.90
8	B	701	NAG	C1-O5-C5	3.81	117.35	112.19
8	C	603	NAG	C1-O5-C5	3.12	116.41	112.19
8	C	607	NAG	C1-O5-C5	2.81	115.99	112.19
8	E	605	NAG	C1-O5-C5	2.80	115.98	112.19
8	E	606	NAG	C1-O5-C5	2.38	115.42	112.19
8	A	609	NAG	C1-O5-C5	2.19	115.17	112.19
8	C	608	NAG	C1-O5-C5	2.14	115.10	112.19
8	A	604	NAG	C1-C2-N2	2.11	114.09	110.49

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	602	NAG	C4-C5-C6-O6
8	A	605	NAG	O5-C5-C6-O6
8	C	604	NAG	O5-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	A	609	NAG	C4-C5-C6-O6
8	E	605	NAG	C4-C5-C6-O6
8	C	607	NAG	O5-C5-C6-O6
8	C	607	NAG	C4-C5-C6-O6
8	E	602	NAG	C4-C5-C6-O6
8	A	606	NAG	O5-C5-C6-O6
8	A	608	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	C	601	NAG	O5-C5-C6-O6
8	C	602	NAG	O5-C5-C6-O6
8	C	601	NAG	C4-C5-C6-O6
8	A	610	NAG	O5-C5-C6-O6
8	E	603	NAG	O5-C5-C6-O6
8	A	604	NAG	C4-C5-C6-O6
8	E	602	NAG	O5-C5-C6-O6
8	A	608	NAG	C4-C5-C6-O6
8	C	604	NAG	C4-C5-C6-O6
8	A	609	NAG	O5-C5-C6-O6
8	E	605	NAG	O5-C5-C6-O6
8	A	601	NAG	C4-C5-C6-O6
8	A	605	NAG	C4-C5-C6-O6
8	C	606	NAG	C4-C5-C6-O6
8	E	601	NAG	O5-C5-C6-O6
8	A	602	NAG	C8-C7-N2-C2
8	A	602	NAG	O7-C7-N2-C2
8	A	604	NAG	C8-C7-N2-C2
8	A	604	NAG	O7-C7-N2-C2
8	A	606	NAG	C8-C7-N2-C2
8	A	606	NAG	O7-C7-N2-C2
8	A	610	NAG	C8-C7-N2-C2
8	A	610	NAG	O7-C7-N2-C2
8	C	602	NAG	C8-C7-N2-C2
8	C	602	NAG	O7-C7-N2-C2
8	E	601	NAG	C8-C7-N2-C2
8	E	601	NAG	O7-C7-N2-C2
8	E	603	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	E	603	NAG	O7-C7-N2-C2
8	A	604	NAG	O5-C5-C6-O6
8	C	606	NAG	O5-C5-C6-O6
8	C	605	NAG	O5-C5-C6-O6
8	C	609	NAG	O5-C5-C6-O6
8	A	602	NAG	O5-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	E	606	NAG	C4-C5-C6-O6
8	C	605	NAG	C4-C5-C6-O6
8	C	609	NAG	C4-C5-C6-O6
8	E	608	NAG	O5-C5-C6-O6
8	A	606	NAG	C4-C5-C6-O6
8	A	610	NAG	C4-C5-C6-O6
8	E	603	NAG	C4-C5-C6-O6
8	E	607	NAG	O5-C5-C6-O6
8	E	607	NAG	C4-C5-C6-O6
8	E	604	NAG	C4-C5-C6-O6
8	E	604	NAG	O5-C5-C6-O6
8	A	603	NAG	C1-C2-N2-C7
8	E	606	NAG	O5-C5-C6-O6
8	E	608	NAG	C1-C2-N2-C7
8	E	608	NAG	C4-C5-C6-O6
8	E	601	NAG	C4-C5-C6-O6
8	A	604	NAG	C3-C2-N2-C7
8	C	603	NAG	C3-C2-N2-C7
8	C	606	NAG	C3-C2-N2-C7
8	C	607	NAG	C3-C2-N2-C7
8	C	609	NAG	C3-C2-N2-C7
8	E	606	NAG	C3-C2-N2-C7
8	E	611	NAG	C4-C5-C6-O6
8	B	701	NAG	C1-C2-N2-C7
8	E	609	NAG	O5-C5-C6-O6
8	A	603	NAG	C3-C2-N2-C7
8	A	608	NAG	C3-C2-N2-C7
8	A	609	NAG	C3-C2-N2-C7
8	C	605	NAG	C3-C2-N2-C7
8	A	608	NAG	C1-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	609	NAG	1	0
8	E	603	NAG	1	0
8	E	605	NAG	3	0
8	A	603	NAG	1	0
8	C	608	NAG	1	0
8	C	609	NAG	1	0
8	E	611	NAG	1	0
8	A	604	NAG	2	0
8	C	604	NAG	1	0
8	E	604	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

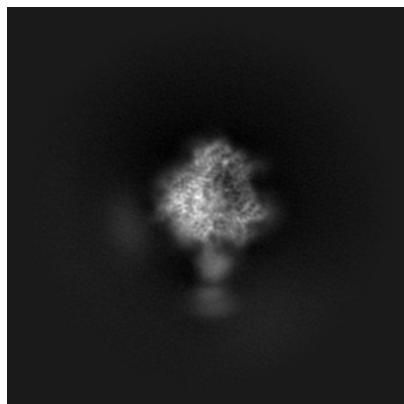
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41417. These allow visual inspection of the internal detail of the map and identification of artifacts.

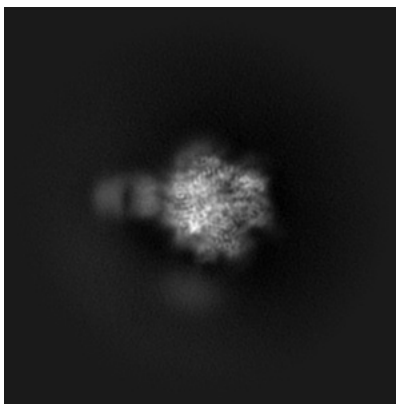
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

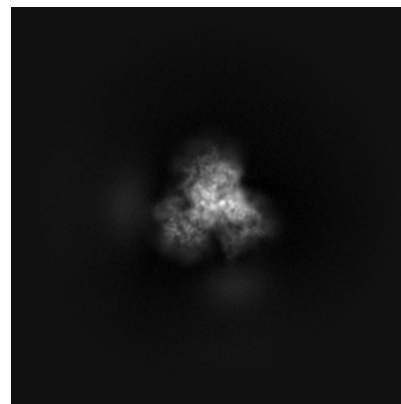
#### 6.1.1 Primary map



X

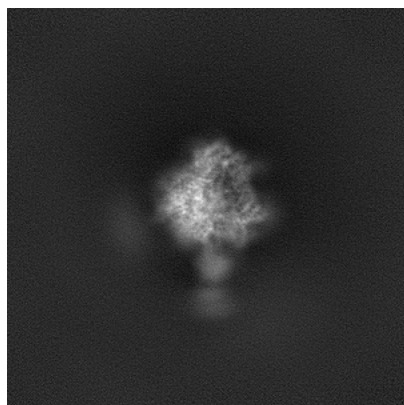


Y

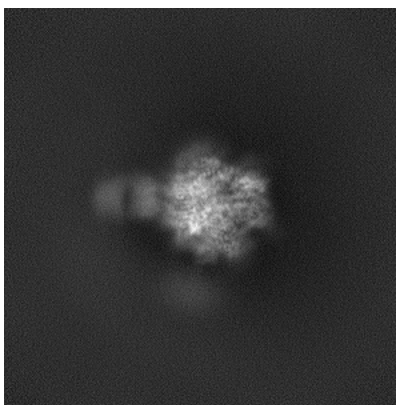


Z

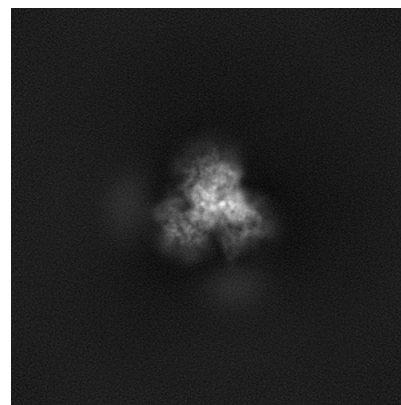
#### 6.1.2 Raw map



X



Y

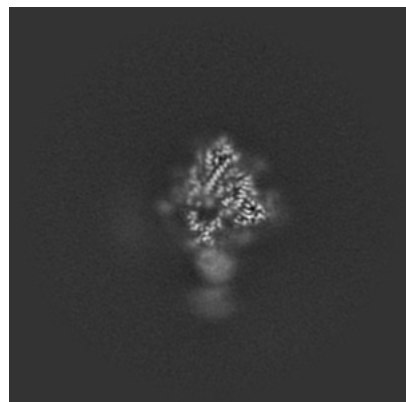


Z

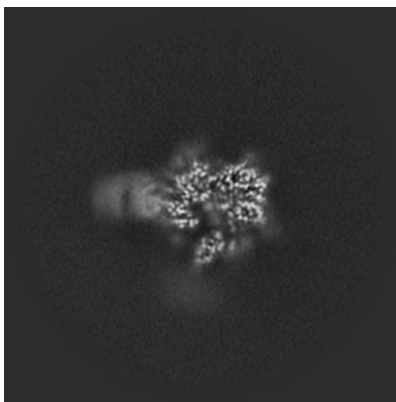
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

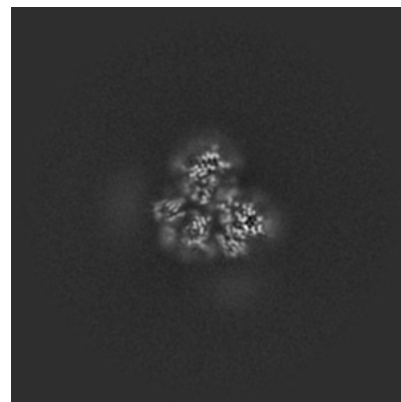
### 6.2.1 Primary map



X Index: 250



Y Index: 250

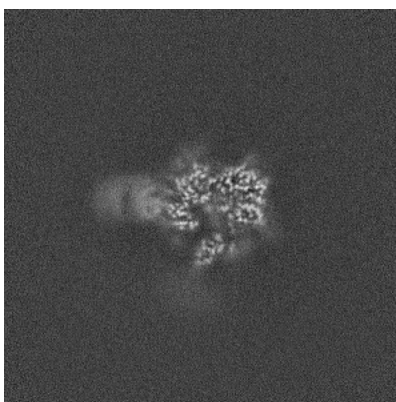


Z Index: 250

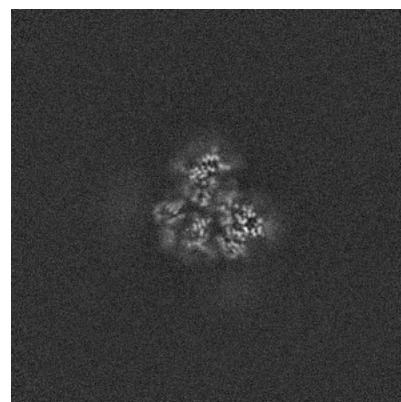
### 6.2.2 Raw map



X Index: 250



Y Index: 250



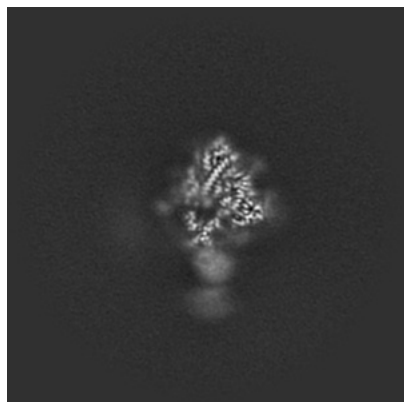
Z Index: 250

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

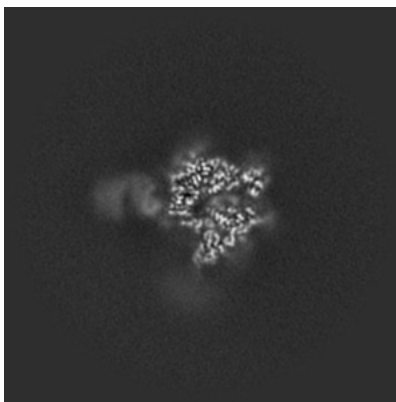


## 6.3 Largest variance slices [i](#)

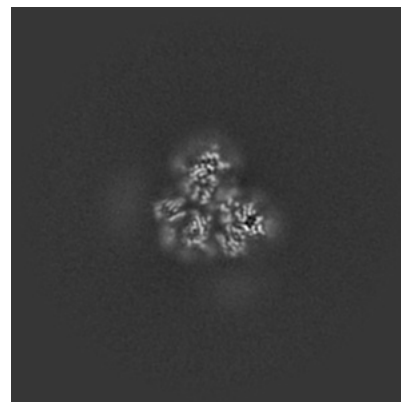
### 6.3.1 Primary map



X Index: 251

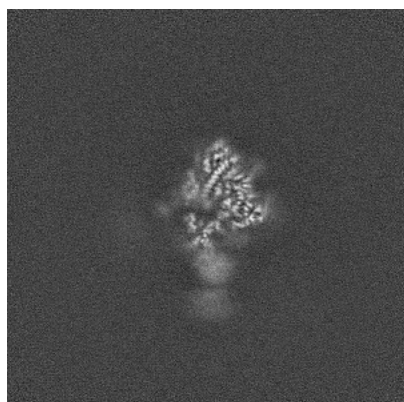


Y Index: 242

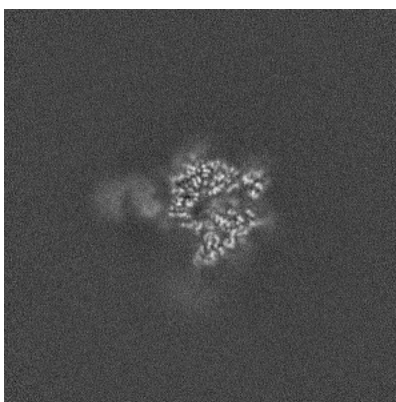


Z Index: 251

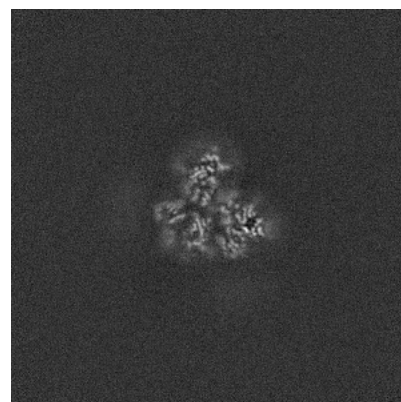
### 6.3.2 Raw map



X Index: 252



Y Index: 242



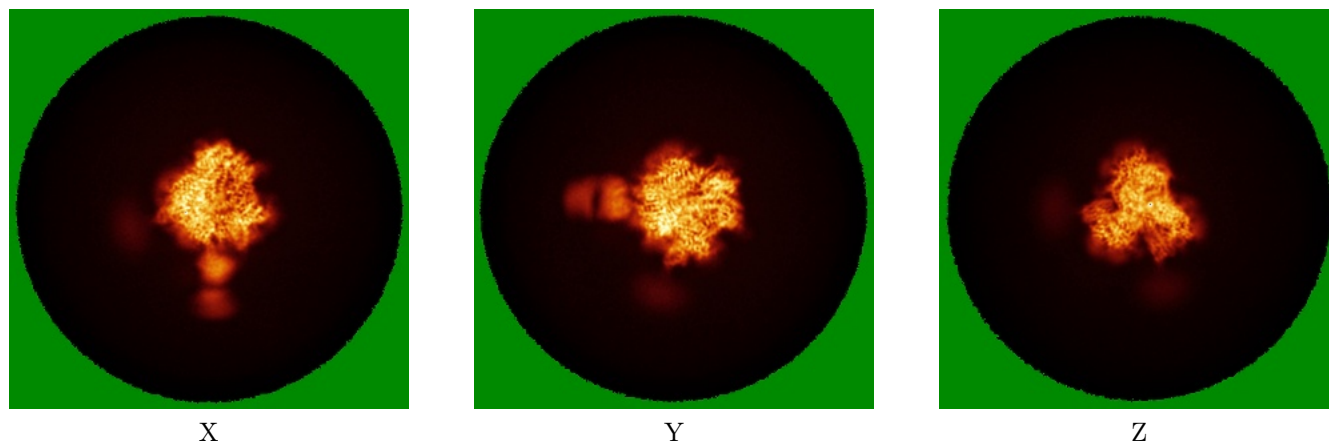
Z Index: 251

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

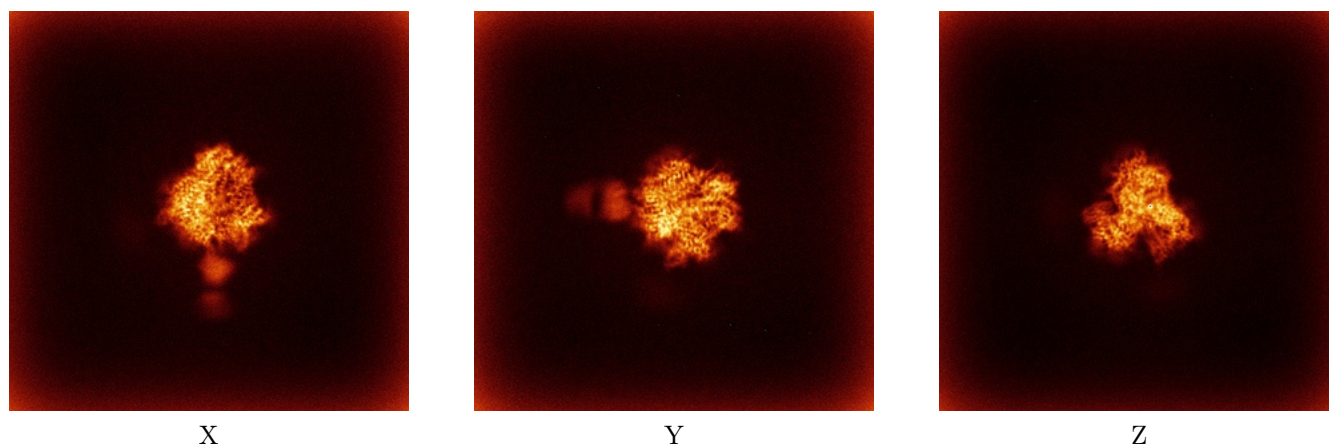


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



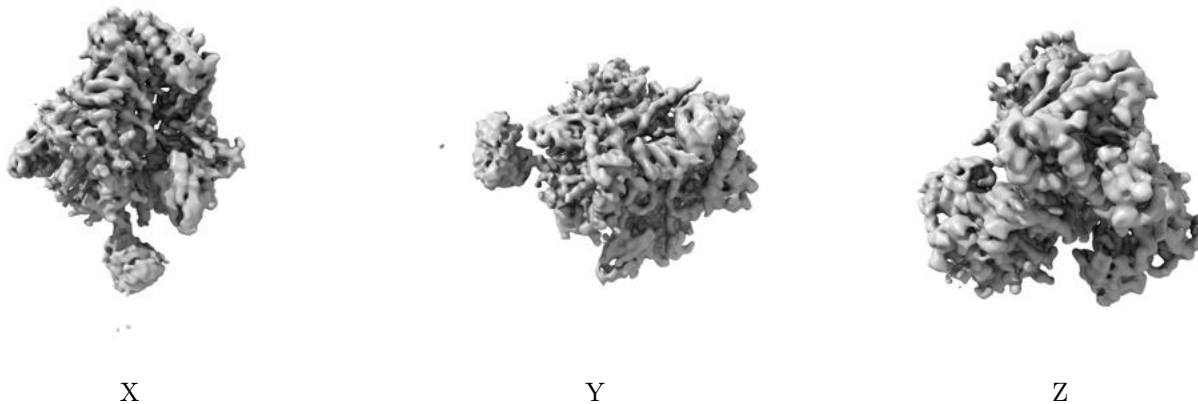
### 6.4.2 Raw map



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.

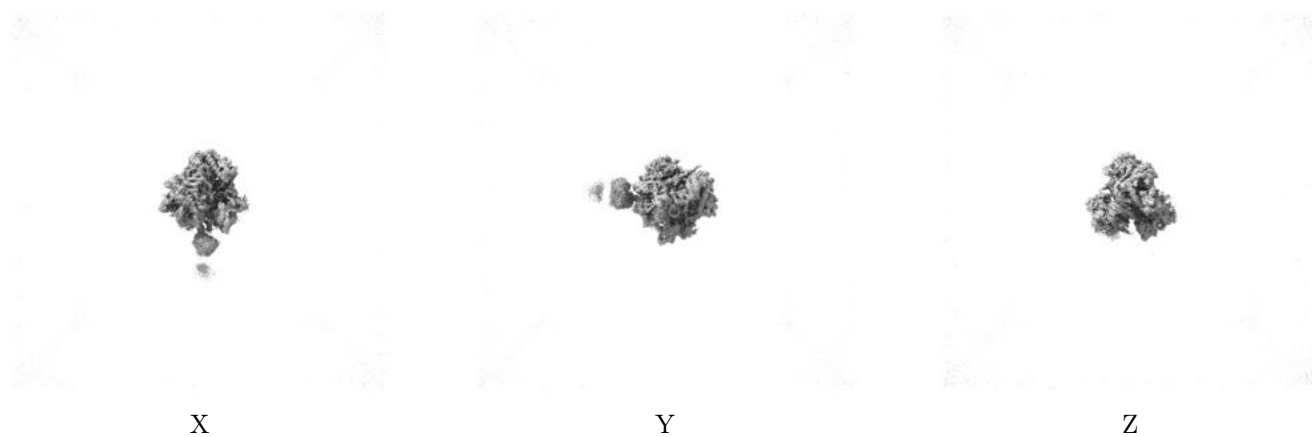
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.225. 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.

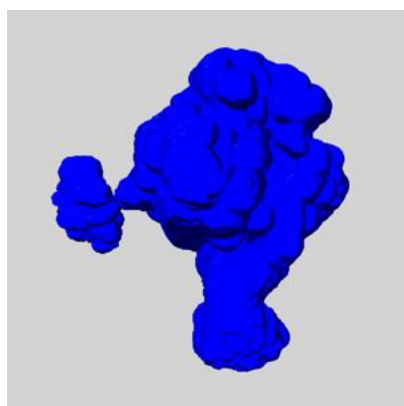
## 6.6 Mask visualisation [i](#)

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

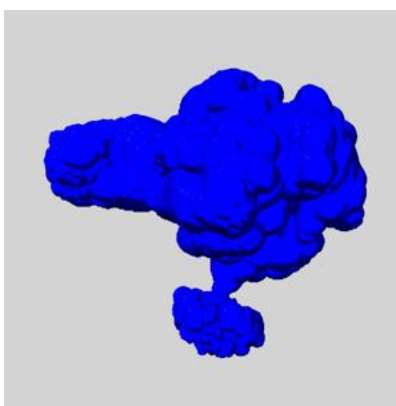
A mask typically either:

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

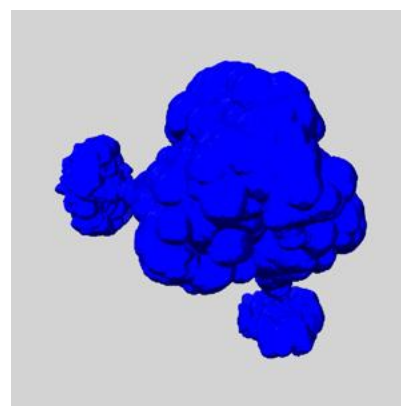
### 6.6.1 emd\_41417\_msk\_1.map [i](#)



X



Y

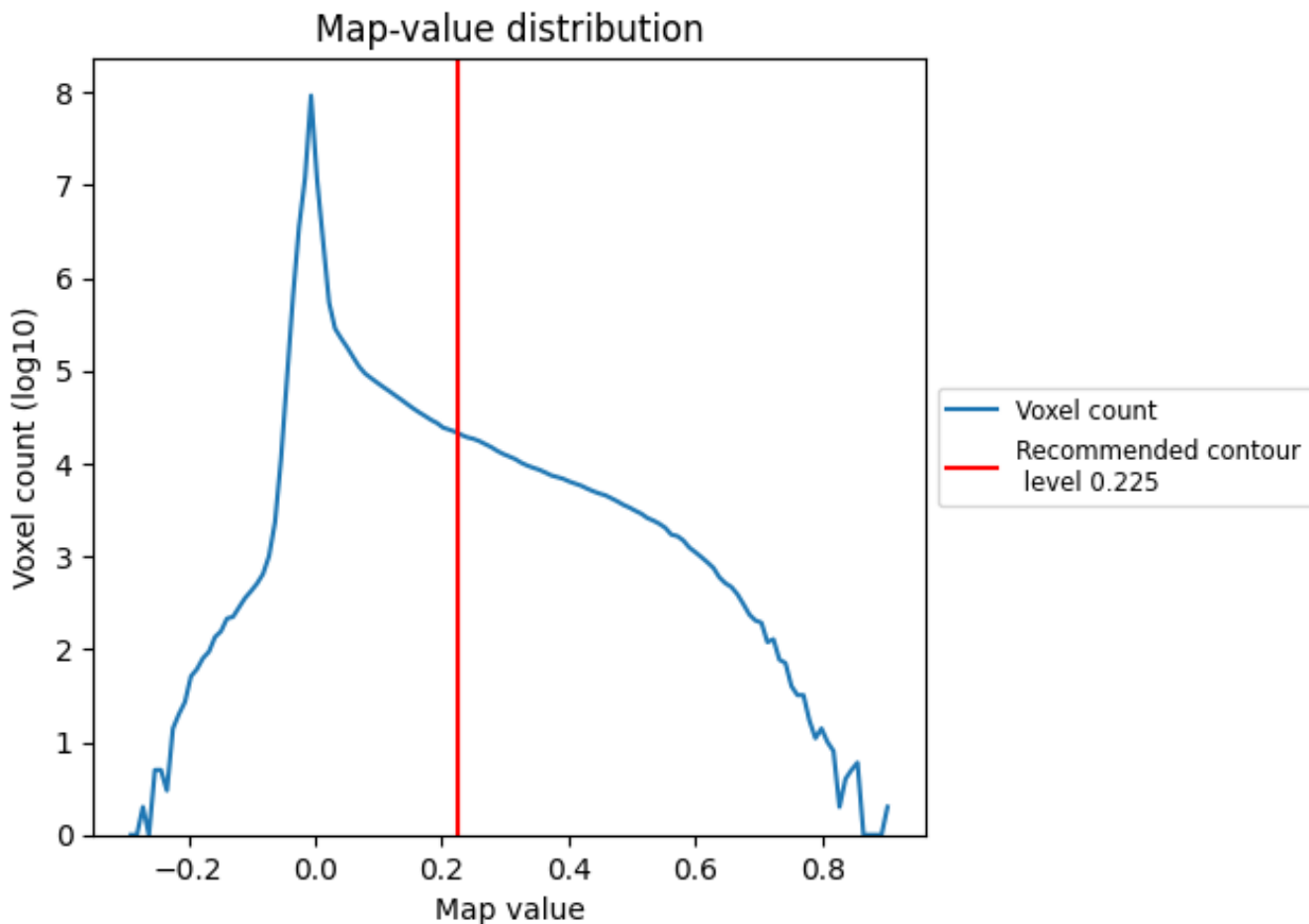


Z

## 7 Map analysis [i](#)

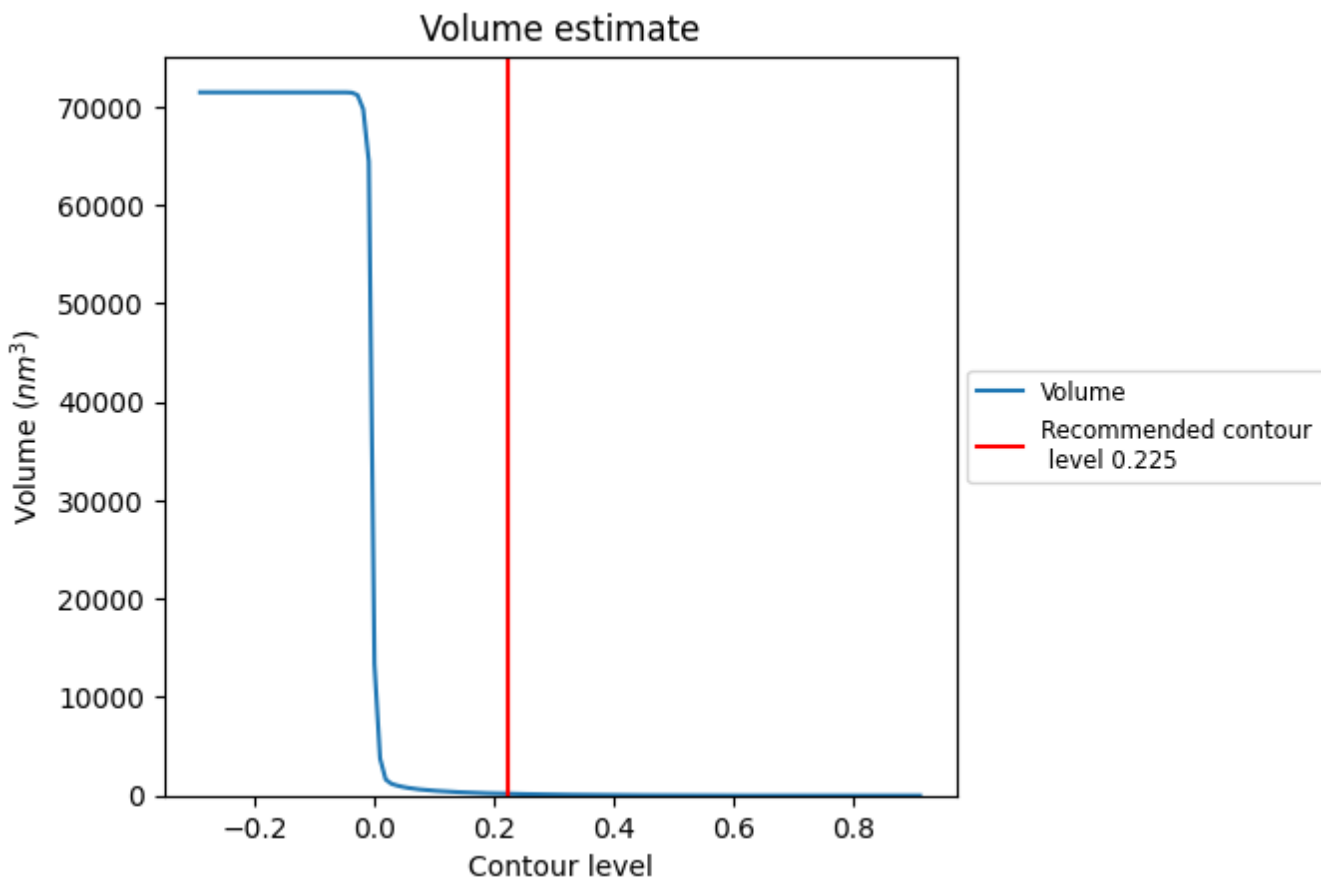
This section contains the results of statistical analysis of the map.

### 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.

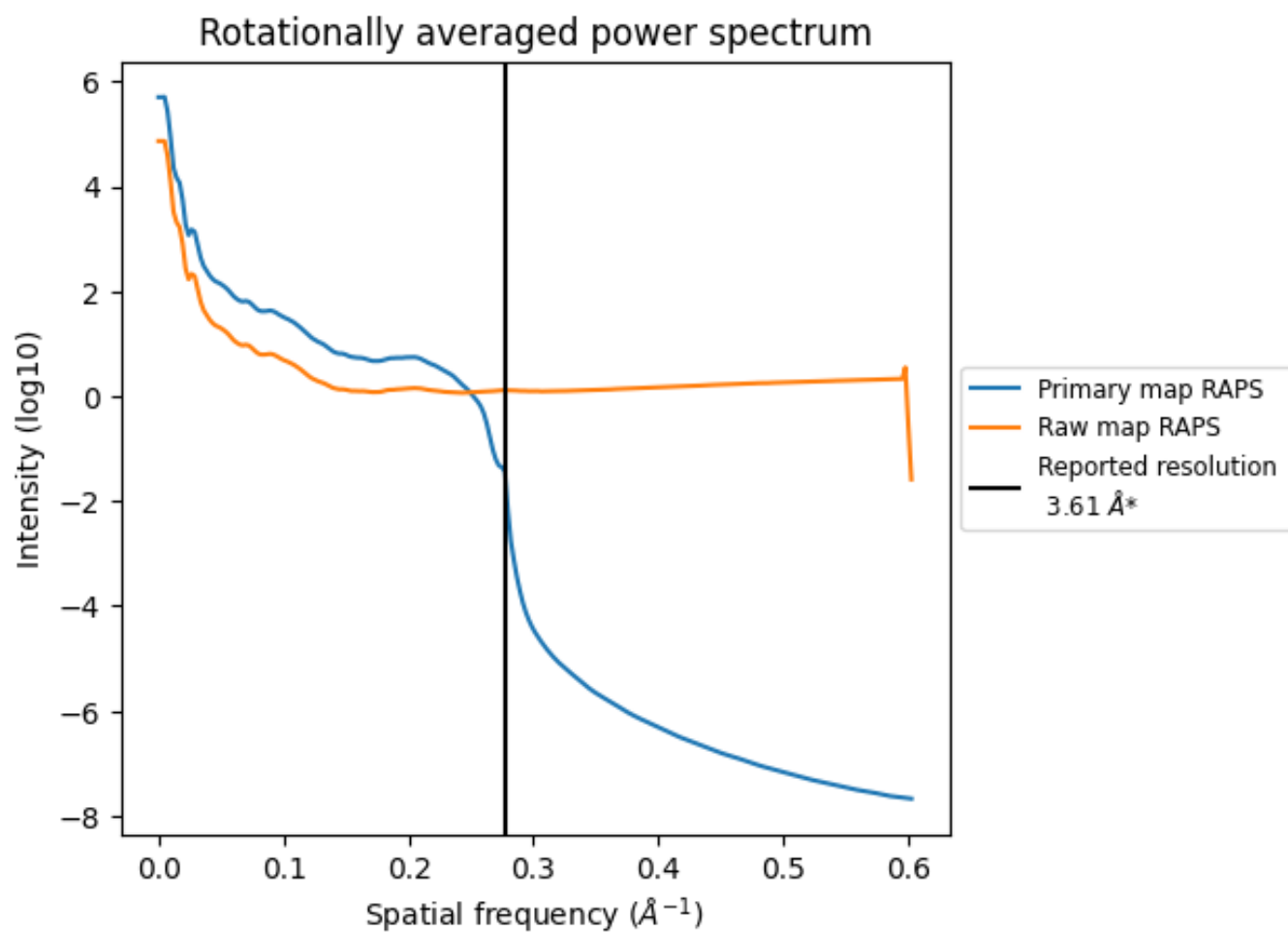
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181  $\text{nm}^3$ ; this corresponds to an approximate mass of 164 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 [i](#)

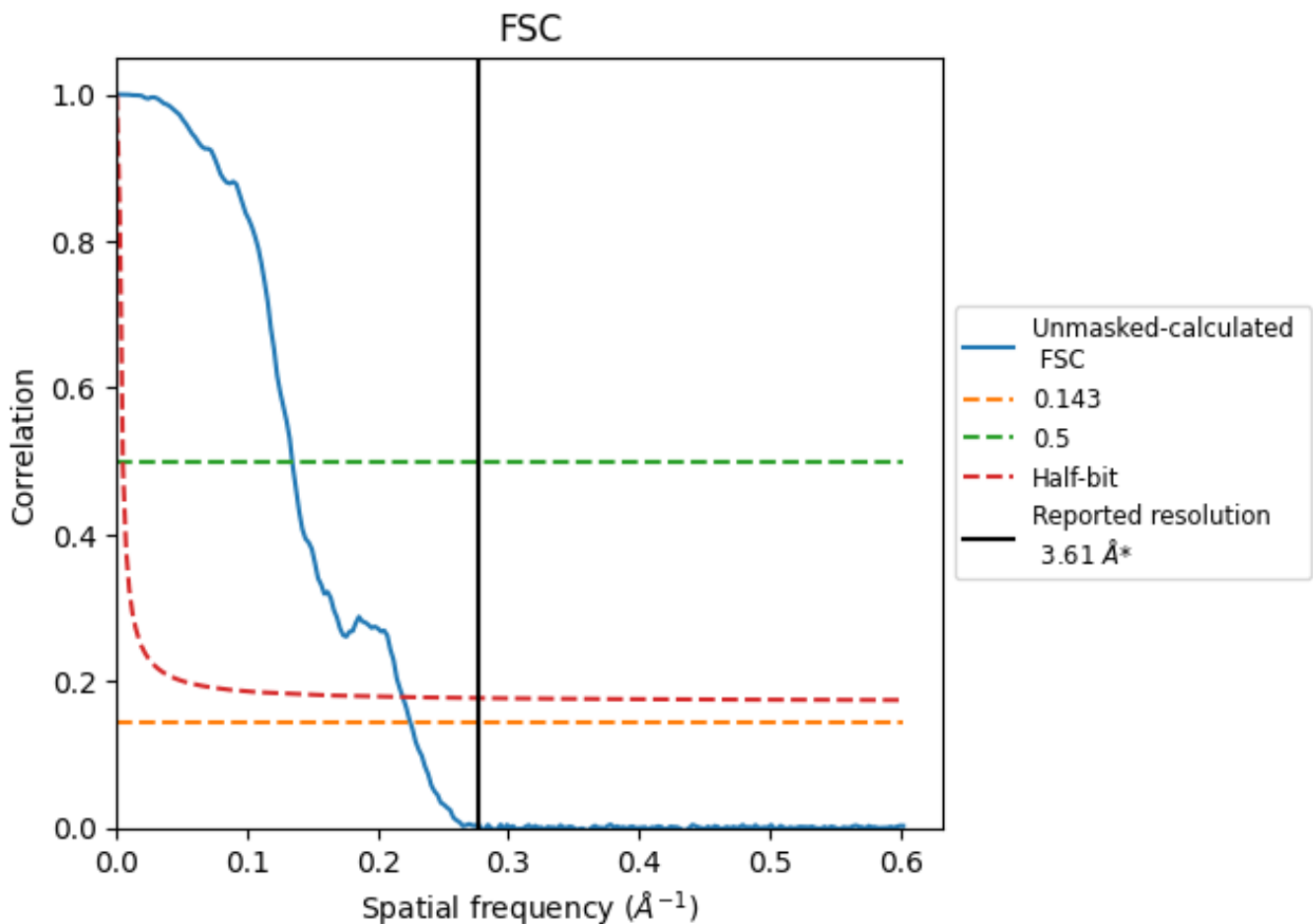


\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.61	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.45	7.43	4.56

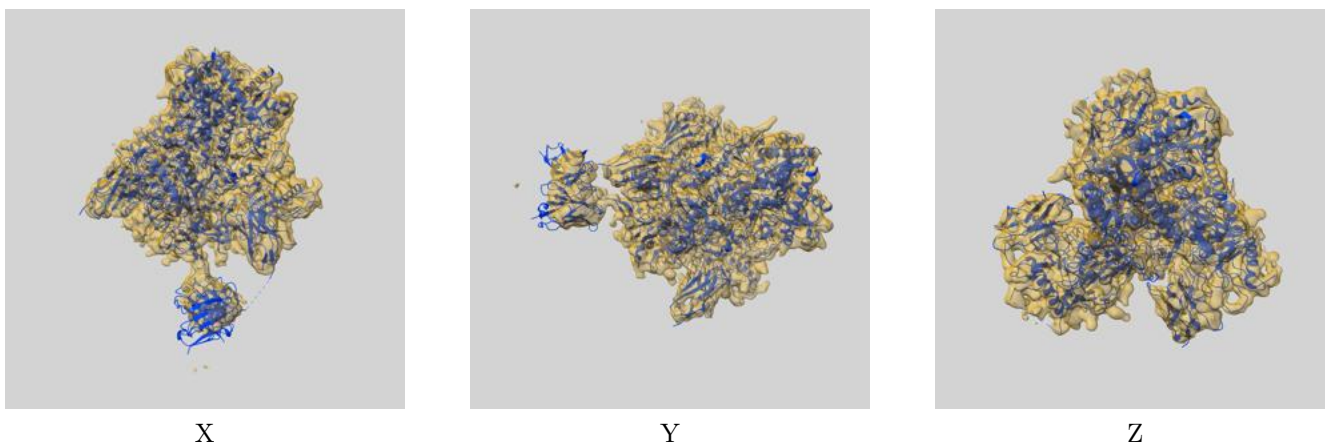
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 7.43 differs from the reported value 3.61 by more than 10 %



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

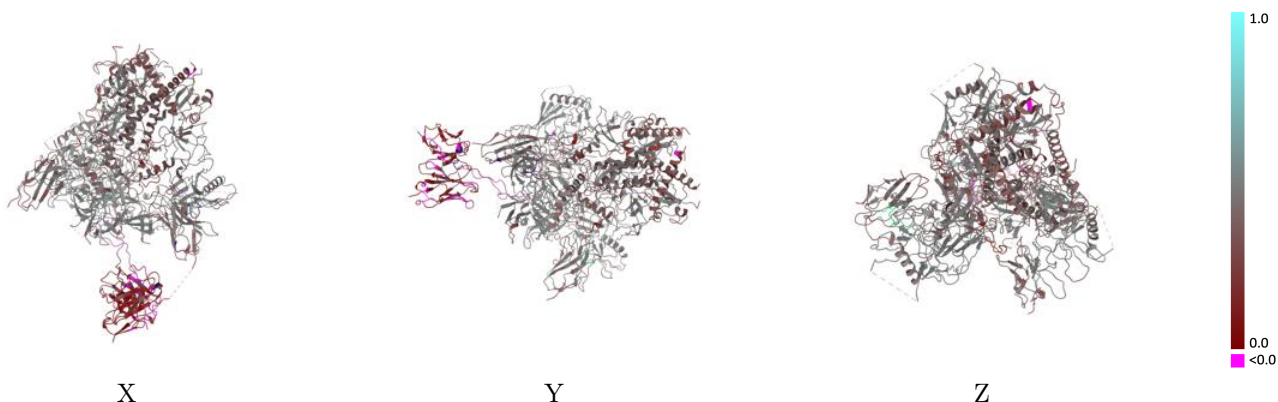
This section contains information regarding the fit between EMDB map EMD-41417 and PDB model 8TNI. Per-residue inclusion information can be found in section 3 on page 10.

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



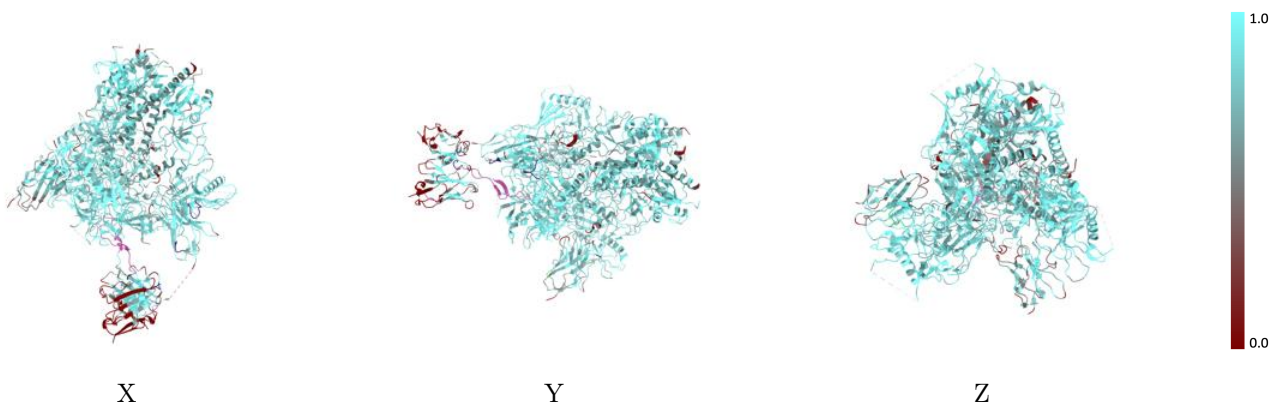
The images above show the 3D surface view of the map at the recommended contour level 0.225 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



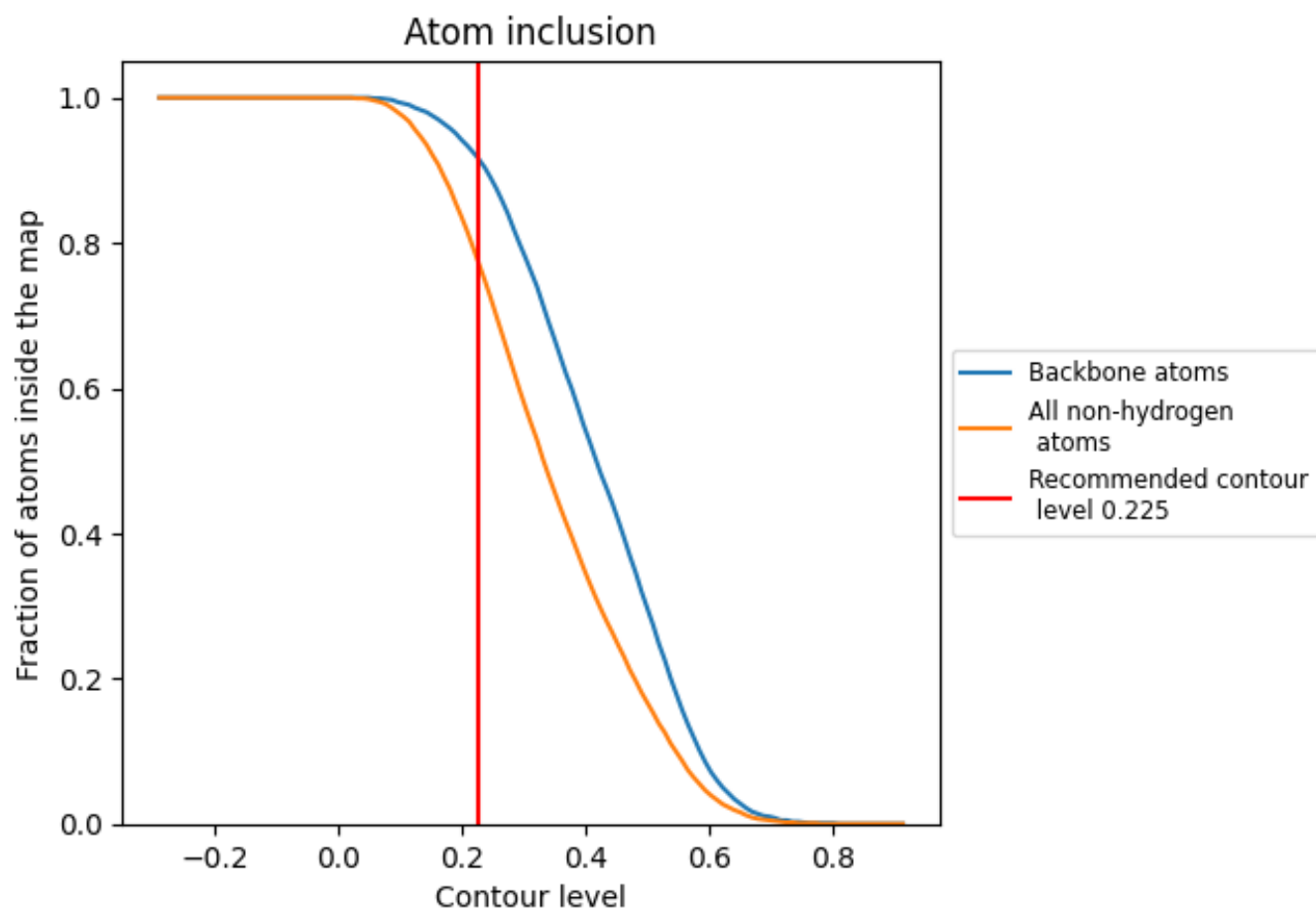
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.225).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.3910
A	 0.8280	 0.4330
B	 0.7820	 0.3640
C	 0.8330	 0.4330
D	 0.7920	 0.3660
E	 0.8320	 0.4370
F	 0.8110	 0.3860
G	 0.7500	 0.3950
H	 0.6910	 0.3940
I	 0.6960	 0.4020
J	 0.5930	 0.2650
K	 0.5710	 0.3720
L	 0.8460	 0.4450
M	 0.7140	 0.3540
N	 0.8570	 0.4750
O	 0.8970	 0.4060
P	 0.7860	 0.3680
Q	 0.6070	 0.3680
R	 0.7400	 0.4490
S	 0.6790	 0.4030
T	 0.8930	 0.4520
U	 0.8570	 0.4690
V	 0.7140	 0.4130
W	 0.8970	 0.4650
X	 0.5710	 0.1820
Y	 0.8970	 0.4850
Z	 0.8570	 0.4230
a	 0.8210	 0.4270

