



# Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:49 PM JST

PDB ID : 7Y75  
EMDB ID : EMD-33652  
Title : SIT1-ACE2-BA.2 RBD  
Authors : Shen, Y.P.; Li, Y.N.; Zhang, Y.Y.; Yan, R.H.  
Deposited on : 2022-06-21  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

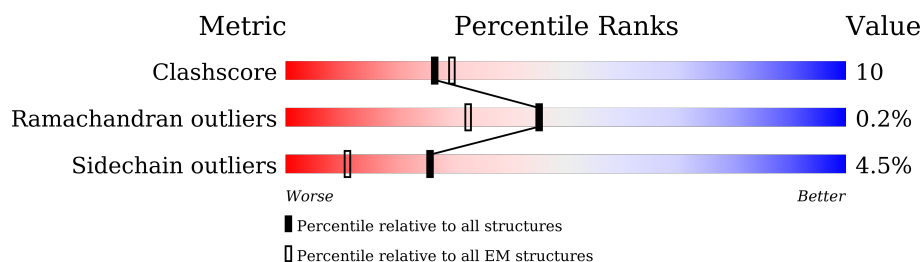
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	613	<div> <div>17%</div> <div>69%</div> <div>24%</div> <div>7%</div> </div>
1	D	613	<div> <div>17%</div> <div>69%</div> <div>24%</div> <div>7%</div> </div>
2	A	826	<div> <div>76%</div> <div>12%</div> <div>9%</div> </div>
2	C	826	<div> <div>77%</div> <div>12%</div> <div>9%</div> </div>
3	E	252	<div> <div>25%</div> <div>61%</div> <div>17%</div> <div>21%</div> </div>
3	F	252	<div> <div>24%</div> <div>60%</div> <div>17%</div> <div>21%</div> </div>
4	G	2	<div> <div>50%</div> <div>50%</div> </div>
4	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	I	2	
4	J	2	
4	K	2	
4	L	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25186 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 Sodium- and chloride-dependent transporter XTRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	573	Total	C	N	O	S	0	0
			4499	2972	696	800	31		
1	D	573	Total	C	N	O	S	0	0
			4499	2972	696	800	31		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q9NP91
B	-19	ALA	-	expression tag	UNP Q9NP91
B	-18	ASP	-	expression tag	UNP Q9NP91
B	-17	TYR	-	expression tag	UNP Q9NP91
B	-16	LYS	-	expression tag	UNP Q9NP91
B	-15	ASP	-	expression tag	UNP Q9NP91
B	-14	ASP	-	expression tag	UNP Q9NP91
B	-13	ASP	-	expression tag	UNP Q9NP91
B	-12	ASP	-	expression tag	UNP Q9NP91
B	-11	LYS	-	expression tag	UNP Q9NP91
B	-10	SER	-	expression tag	UNP Q9NP91
B	-9	GLY	-	expression tag	UNP Q9NP91
B	-8	PRO	-	expression tag	UNP Q9NP91
B	-7	ASP	-	expression tag	UNP Q9NP91
B	-6	GLU	-	expression tag	UNP Q9NP91
B	-5	VAL	-	expression tag	UNP Q9NP91
B	-4	ASP	-	expression tag	UNP Q9NP91
B	-3	ALA	-	expression tag	UNP Q9NP91
B	-2	SER	-	expression tag	UNP Q9NP91
B	-1	GLY	-	expression tag	UNP Q9NP91
B	0	ARG	-	expression tag	UNP Q9NP91
D	-20	MET	-	initiating methionine	UNP Q9NP91
D	-19	ALA	-	expression tag	UNP Q9NP91
D	-18	ASP	-	expression tag	UNP Q9NP91
D	-17	TYR	-	expression tag	UNP Q9NP91
D	-16	LYS	-	expression tag	UNP Q9NP91

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	ASP	-	expression tag	UNP Q9NP91
D	-14	ASP	-	expression tag	UNP Q9NP91
D	-13	ASP	-	expression tag	UNP Q9NP91
D	-12	ASP	-	expression tag	UNP Q9NP91
D	-11	LYS	-	expression tag	UNP Q9NP91
D	-10	SER	-	expression tag	UNP Q9NP91
D	-9	GLY	-	expression tag	UNP Q9NP91
D	-8	PRO	-	expression tag	UNP Q9NP91
D	-7	ASP	-	expression tag	UNP Q9NP91
D	-6	GLU	-	expression tag	UNP Q9NP91
D	-5	VAL	-	expression tag	UNP Q9NP91
D	-4	ASP	-	expression tag	UNP Q9NP91
D	-3	ALA	-	expression tag	UNP Q9NP91
D	-2	SER	-	expression tag	UNP Q9NP91
D	-1	GLY	-	expression tag	UNP Q9NP91
D	0	ARG	-	expression tag	UNP Q9NP91

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	750	Total	C	N	O	S	0	0
			6102	3913	1020	1135	34		
2	C	750	Total	C	N	O	S	0	0
			6102	3913	1020	1135	34		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9BYF1
A	-7	ARG	-	expression tag	UNP Q9BYF1
A	10	TRP	-	insertion	UNP Q9BYF1
A	11	SER	-	insertion	UNP Q9BYF1
A	12	HIS	-	insertion	UNP Q9BYF1
A	13	PRO	-	insertion	UNP Q9BYF1
A	14	GLN	-	insertion	UNP Q9BYF1
A	15	PHE	-	insertion	UNP Q9BYF1
A	16	GLU	-	insertion	UNP Q9BYF1
A	17	LYS	-	insertion	UNP Q9BYF1
A	806	LEU	-	expression tag	UNP Q9BYF1
A	807	GLU	-	expression tag	UNP Q9BYF1
A	808	HIS	-	expression tag	UNP Q9BYF1
A	809	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	810	HIS	-	expression tag	UNP Q9BYF1
A	811	HIS	-	expression tag	UNP Q9BYF1
A	812	HIS	-	expression tag	UNP Q9BYF1
A	813	HIS	-	expression tag	UNP Q9BYF1
A	814	HIS	-	expression tag	UNP Q9BYF1
A	815	HIS	-	expression tag	UNP Q9BYF1
A	816	HIS	-	expression tag	UNP Q9BYF1
A	817	HIS	-	expression tag	UNP Q9BYF1
C	-8	MET	-	initiating methionine	UNP Q9BYF1
C	-7	ARG	-	expression tag	UNP Q9BYF1
C	10	TRP	-	insertion	UNP Q9BYF1
C	11	SER	-	insertion	UNP Q9BYF1
C	12	HIS	-	insertion	UNP Q9BYF1
C	13	PRO	-	insertion	UNP Q9BYF1
C	14	GLN	-	insertion	UNP Q9BYF1
C	15	PHE	-	insertion	UNP Q9BYF1
C	16	GLU	-	insertion	UNP Q9BYF1
C	17	LYS	-	insertion	UNP Q9BYF1
C	806	LEU	-	expression tag	UNP Q9BYF1
C	807	GLU	-	expression tag	UNP Q9BYF1
C	808	HIS	-	expression tag	UNP Q9BYF1
C	809	HIS	-	expression tag	UNP Q9BYF1
C	810	HIS	-	expression tag	UNP Q9BYF1
C	811	HIS	-	expression tag	UNP Q9BYF1
C	812	HIS	-	expression tag	UNP Q9BYF1
C	813	HIS	-	expression tag	UNP Q9BYF1
C	814	HIS	-	expression tag	UNP Q9BYF1
C	815	HIS	-	expression tag	UNP Q9BYF1
C	816	HIS	-	expression tag	UNP Q9BYF1
C	817	HIS	-	expression tag	UNP Q9BYF1

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	198	Total	C	N	O	S	0	0
			1581	1021	267	285	8		
3	F	198	Total	C	N	O	S	0	0
			1581	1021	267	285	8		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	300	MET	-	initiating methionine	UNP P0DTC2
E	301	GLY	-	expression tag	UNP P0DTC2
E	302	VAL	-	expression tag	UNP P0DTC2
E	303	LYS	-	expression tag	UNP P0DTC2
E	304	VAL	-	expression tag	UNP P0DTC2
E	305	LEU	-	expression tag	UNP P0DTC2
E	306	PHE	-	expression tag	UNP P0DTC2
E	307	ALA	-	expression tag	UNP P0DTC2
E	308	LEU	-	expression tag	UNP P0DTC2
E	309	ILE	-	expression tag	UNP P0DTC2
E	310	CYS	-	expression tag	UNP P0DTC2
E	311	ILE	-	expression tag	UNP P0DTC2
E	312	ALA	-	expression tag	UNP P0DTC2
E	313	VAL	-	expression tag	UNP P0DTC2
E	314	ALA	-	expression tag	UNP P0DTC2
E	315	GLU	-	expression tag	UNP P0DTC2
E	316	ALA	-	expression tag	UNP P0DTC2
E	317	GLY	-	expression tag	UNP P0DTC2
E	318	THR	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	542	LEU	-	expression tag	UNP P0DTC2
E	543	GLU	-	expression tag	UNP P0DTC2
E	544	HIS	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2
E	548	HIS	-	expression tag	UNP P0DTC2
E	549	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	550	HIS	-	expression tag	UNP P0DTC2
E	551	HIS	-	expression tag	UNP P0DTC2
F	300	MET	-	initiating methionine	UNP P0DTC2
F	301	GLY	-	expression tag	UNP P0DTC2
F	302	VAL	-	expression tag	UNP P0DTC2
F	303	LYS	-	expression tag	UNP P0DTC2
F	304	VAL	-	expression tag	UNP P0DTC2
F	305	LEU	-	expression tag	UNP P0DTC2
F	306	PHE	-	expression tag	UNP P0DTC2
F	307	ALA	-	expression tag	UNP P0DTC2
F	308	LEU	-	expression tag	UNP P0DTC2
F	309	ILE	-	expression tag	UNP P0DTC2
F	310	CYS	-	expression tag	UNP P0DTC2
F	311	ILE	-	expression tag	UNP P0DTC2
F	312	ALA	-	expression tag	UNP P0DTC2
F	313	VAL	-	expression tag	UNP P0DTC2
F	314	ALA	-	expression tag	UNP P0DTC2
F	315	GLU	-	expression tag	UNP P0DTC2
F	316	ALA	-	expression tag	UNP P0DTC2
F	317	GLY	-	expression tag	UNP P0DTC2
F	318	THR	-	expression tag	UNP P0DTC2
F	339	ASP	GLY	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	493	ARG	GLN	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	542	LEU	-	expression tag	UNP P0DTC2
F	543	GLU	-	expression tag	UNP P0DTC2
F	544	HIS	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2
F	551	HIS	-	expression tag	UNP P0DTC2

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



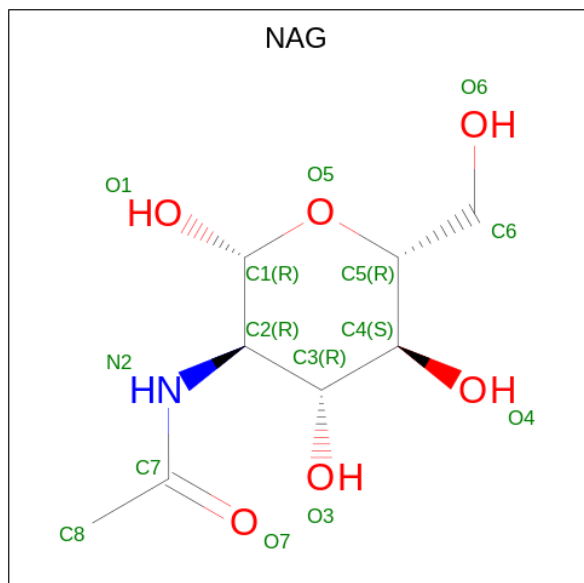
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		

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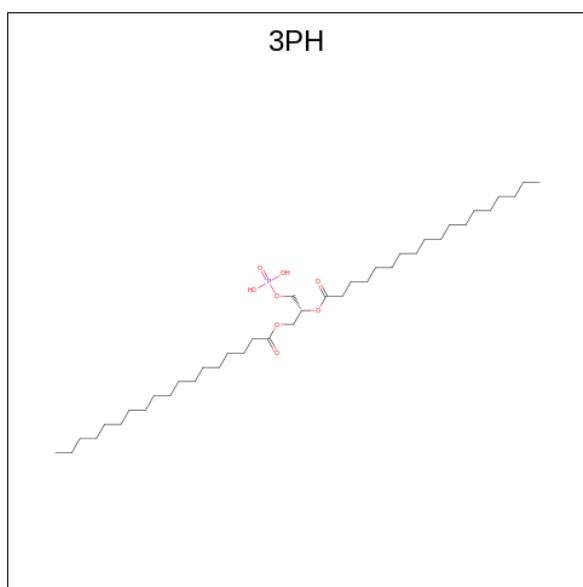
Mol	Chain	Residues	Atoms				AltConf	Trace
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	P	0
			48	39	8	1	
6	B	1	Total	C	O	P	0
			48	39	8	1	
6	B	1	Total	C	O	P	0
			48	39	8	1	
6	D	1	Total	C	O	P	0
			48	39	8	1	
6	D	1	Total	C	O	P	0
			48	39	8	1	
6	D	1	Total	C	O	P	0
			48	39	8	1	

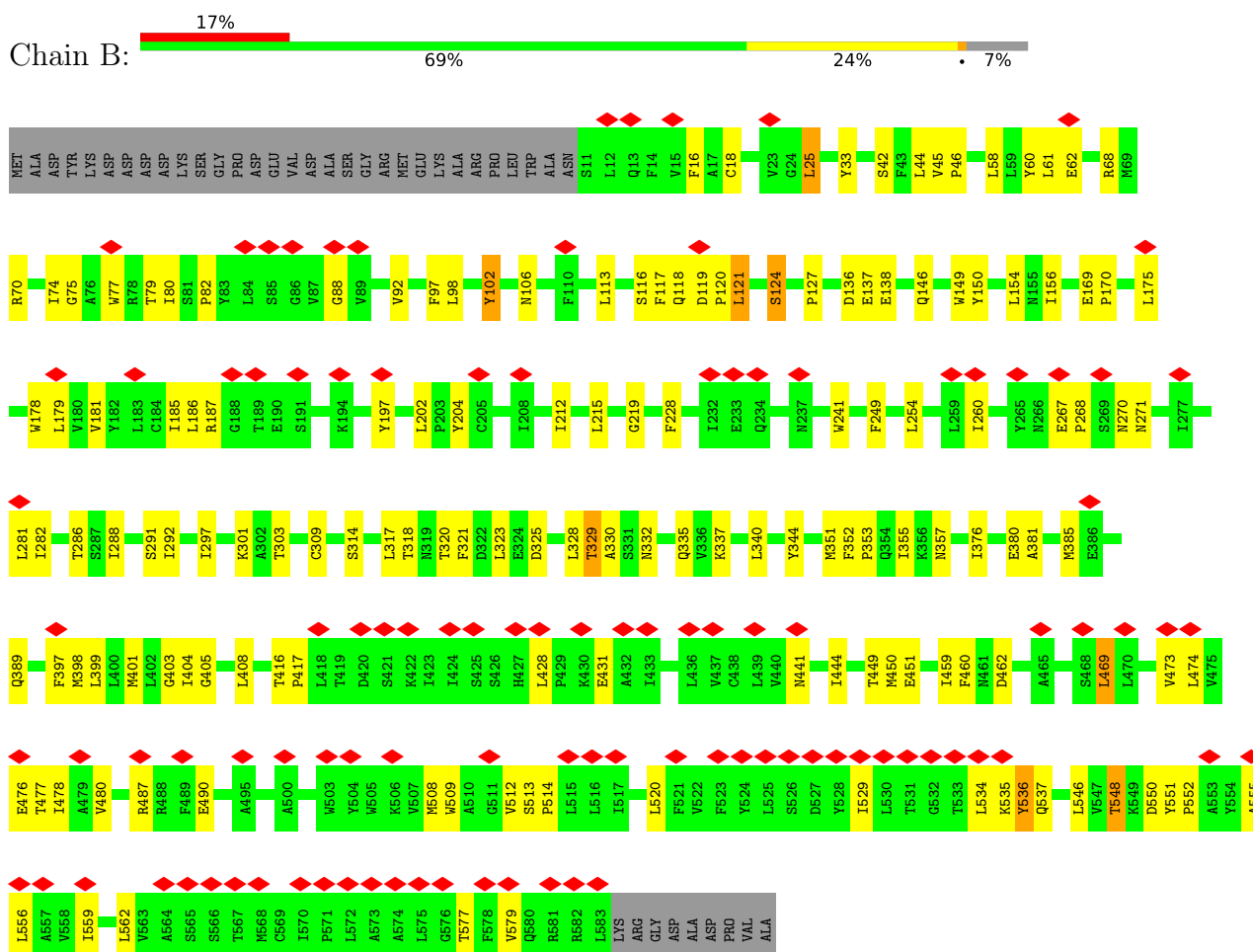
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	
7	C	1	Total	Zn	0
			1	1	

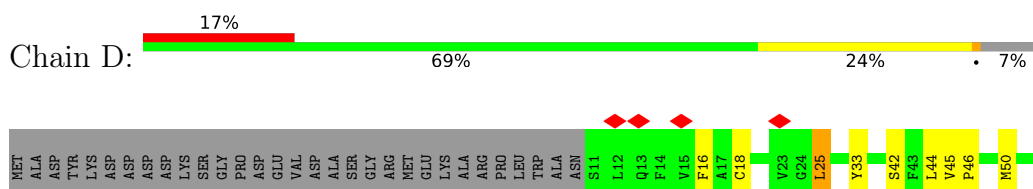
### 3 Residue-property plots

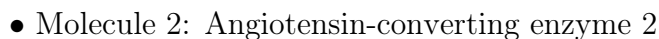
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Sodium- and chloride-dependent transporter XTRP3



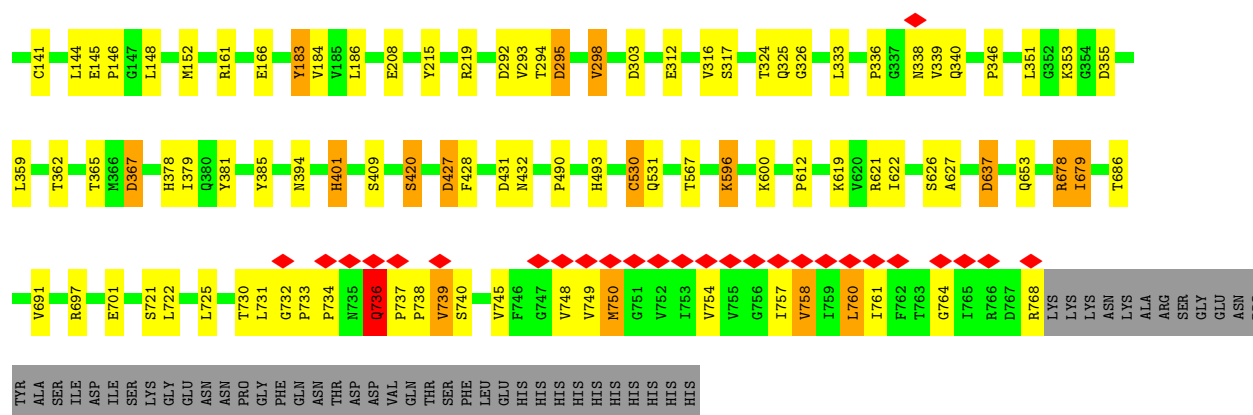
#### • Molecule 1: Sodium- and chloride-dependent transporter XTRP3



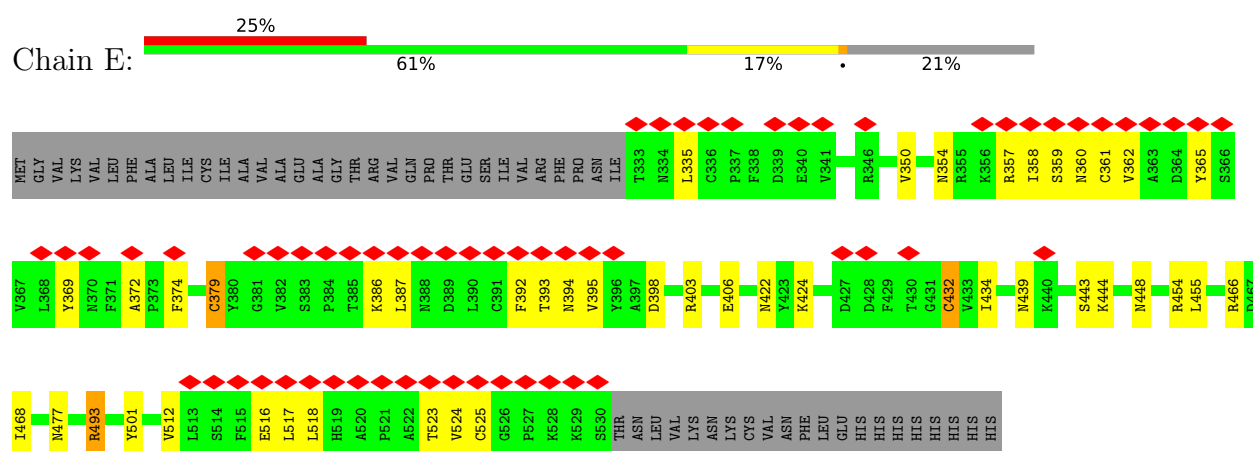
[illegible]

- Molecule 2: Angiotensin-converting enzyme 2

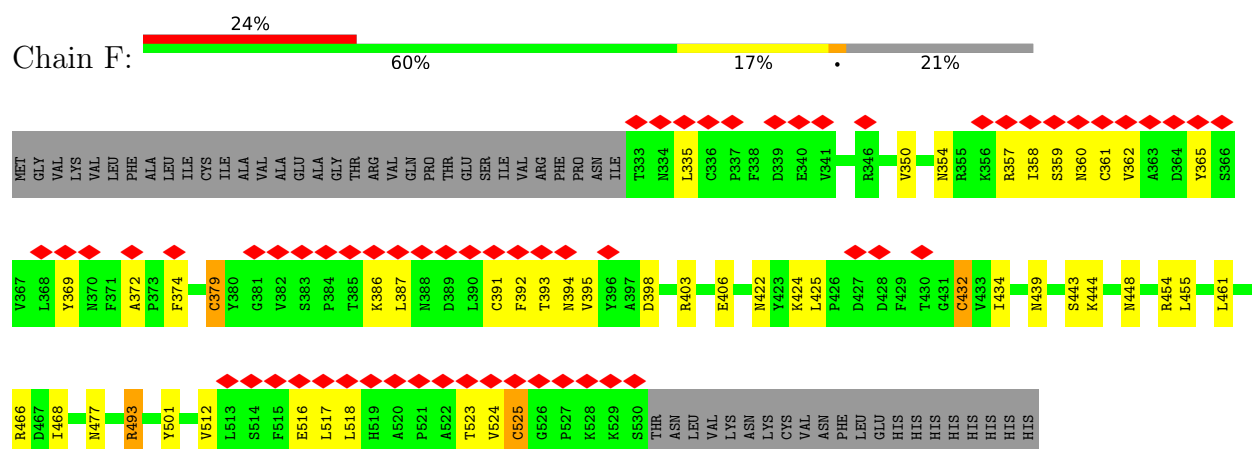
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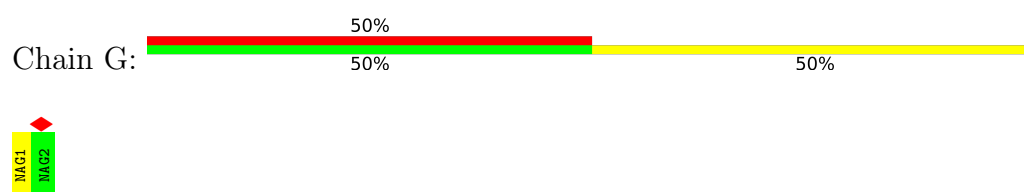
### • Molecule 3: Spike protein S1



### • Molecule 3: Spike protein S1



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



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

Chain H: 



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

Chain I: 



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

Chain J: 



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

Chain K: 



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

Chain L: 



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

Chain M: 



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



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



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



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



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



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



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



Chain T:  50% 50%

MAG1  
MAG2

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

Chain U:  50% 50%

MAG1  
MAG2

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

Chain V:  100% 100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518306	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.066	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: ZN, 3PH, 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	B	0.31	0/4622	0.44	0/6301
1	D	0.31	0/4622	0.44	0/6301
2	A	0.50	0/6265	0.48	0/8506
2	C	0.50	0/6265	0.47	0/8506
3	E	0.31	0/1629	0.46	0/2215
3	F	0.31	0/1629	0.46	0/2215
All	All	0.42	0/25032	0.46	0/34044

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	B	4499	0	4502	115	0
1	D	4499	0	4502	109	0
2	A	6102	0	5914	105	0
2	C	6102	0	5914	97	0
3	E	1581	0	1512	30	0
3	F	1581	0	1512	33	0
4	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	1	0
4	I	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	1	0
4	M	28	0	25	0	0
4	N	28	0	25	1	0
4	O	28	0	25	2	0
4	P	28	0	25	2	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	1	0
5	A	14	0	13	0	0
5	B	28	0	26	0	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
6	B	144	0	225	18	0
6	D	144	0	225	17	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
All	All	25186	0	24784	487	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 10.

All (487) 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)
2:C:622:ILE:HB	2:C:679:ILE:CG2	1.29	1.57
2:A:622:ILE:HB	2:A:679:ILE:CG2	1.29	1.53
2:A:622:ILE:CB	2:A:679:ILE:HG21	1.50	1.40
2:C:622:ILE:CB	2:C:679:ILE:HG21	1.50	1.39
1:B:179:LEU:HD23	6:B:1005:3PH:C3I	1.71	1.20
6:B:1004:3PH:H291	6:B:1004:3PH:H251	1.28	1.12
1:D:179:LEU:HD23	6:D:1005:3PH:C3I	1.81	1.10
2:A:740:SER:HB2	2:A:743:LEU:HB2	1.34	1.08
1:B:179:LEU:CD2	6:B:1005:3PH:C3I	2.31	1.08
1:D:179:LEU:CD2	6:D:1005:3PH:H3I2	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1004:3PH:H251	6:D:1004:3PH:H291	1.28	1.04
1:B:179:LEU:HD23	6:B:1005:3PH:H3I3	1.45	0.98
1:B:179:LEU:CD2	6:B:1005:3PH:H3I2	1.93	0.98
2:C:736:GLN:H	2:C:737:PRO:CD	1.79	0.96
2:A:736:GLN:H	2:A:737:PRO:HD3	1.31	0.94
1:D:179:LEU:CD2	6:D:1005:3PH:C3I	2.43	0.93
2:A:622:ILE:CB	2:A:679:ILE:CG2	2.23	0.91
2:C:622:ILE:CB	2:C:679:ILE:CG2	2.23	0.91
2:A:739:VAL:HG22	2:A:740:SER:H	1.38	0.86
1:B:179:LEU:HD21	6:B:1005:3PH:H3I2	1.57	0.85
2:A:736:GLN:H	2:A:737:PRO:CD	1.91	0.82
1:B:179:LEU:CD2	6:B:1005:3PH:H3I3	2.07	0.80
1:B:118:GLN:HG2	2:A:741:ILE:HD12	1.66	0.78
3:F:379:CYS:HA	3:F:432:CYS:HB3	1.65	0.78
3:E:379:CYS:HA	3:E:432:CYS:HB3	1.66	0.77
3:E:422:ASN:HD21	3:E:454:ARG:H	1.32	0.77
1:D:179:LEU:HD21	6:D:1005:3PH:H3I2	1.67	0.77
6:D:1004:3PH:H291	6:D:1004:3PH:C25	2.12	0.75
2:C:736:GLN:H	2:C:737:PRO:HD2	1.50	0.75
6:B:1005:3PH:H291	6:B:1005:3PH:H2D2	1.69	0.75
6:B:1004:3PH:H251	6:B:1004:3PH:C29	2.14	0.74
3:F:422:ASN:HD21	3:F:454:ARG:H	1.32	0.74
6:D:1004:3PH:H251	6:D:1004:3PH:C29	2.14	0.73
2:C:133:CYS:HB3	2:C:141:CYS:HA	1.72	0.72
6:D:1005:3PH:H291	6:D:1005:3PH:H2D2	1.70	0.72
2:A:697:ARG:NH1	2:A:701:GLU:OE2	2.23	0.72
2:C:697:ARG:NH1	2:C:701:GLU:OE2	2.23	0.71
1:D:106:ASN:HD21	1:D:403:GLY:HA3	1.55	0.71
2:A:133:CYS:HB3	2:A:141:CYS:HA	1.71	0.71
1:B:106:ASN:HD21	1:B:403:GLY:HA3	1.55	0.70
1:B:301:LYS:HE2	1:B:380:GLU:HG3	1.74	0.69
1:B:556:LEU:HA	1:B:559:ILE:HD12	1.73	0.69
1:D:556:LEU:HA	1:D:559:ILE:HD12	1.73	0.69
1:B:357:ASN:HB2	4:G:1:NAG:HN2	1.58	0.69
1:D:301:LYS:HE2	1:D:380:GLU:HG3	1.74	0.68
1:D:357:ASN:HB2	4:O:1:NAG:HN2	1.59	0.68
2:A:739:VAL:HG13	2:A:740:SER:N	2.08	0.68
2:C:637:ASP:OD1	2:C:637:ASP:N	2.23	0.68
3:F:361:CYS:H	3:F:524:VAL:HB	1.59	0.67
3:E:361:CYS:H	3:E:524:VAL:HB	1.59	0.67
2:C:678:ARG:HH21	2:C:678:ARG:CG	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:739:VAL:HG22	2:A:740:SER:N	2.11	0.64
2:A:738:PRO:O	2:A:739:VAL:HB	1.97	0.64
2:A:678:ARG:HH21	2:A:678:ARG:CG	2.10	0.64
3:E:392:PHE:HA	3:E:517:LEU:HD13	1.80	0.64
2:C:622:ILE:H	2:C:679:ILE:HG22	1.62	0.64
2:C:678:ARG:HH21	2:C:678:ARG:HG3	1.62	0.64
2:C:736:GLN:H	2:C:737:PRO:HD3	1.63	0.64
3:F:392:PHE:HA	3:F:517:LEU:HD13	1.80	0.63
2:A:678:ARG:HH21	2:A:678:ARG:HG3	1.63	0.63
1:B:118:GLN:HE21	2:A:741:ILE:HG13	1.64	0.63
1:B:187:ARG:HG3	2:A:760:LEU:HD21	1.80	0.63
2:A:133:CYS:HB3	2:A:141:CYS:CA	2.29	0.63
2:A:622:ILE:CG2	2:A:679:ILE:HG21	2.27	0.63
1:B:154:LEU:HD13	1:B:156:ILE:HD11	1.80	0.63
2:A:622:ILE:H	2:A:679:ILE:HG22	1.63	0.62
1:D:154:LEU:HD13	1:D:156:ILE:HD11	1.80	0.62
2:C:133:CYS:HB3	2:C:141:CYS:CA	2.29	0.62
1:D:357:ASN:HB2	4:O:1:NAG:N2	2.15	0.62
2:C:622:ILE:CG2	2:C:679:ILE:HG21	2.27	0.62
2:C:622:ILE:N	2:C:679:ILE:HG22	2.15	0.61
2:A:622:ILE:N	2:A:679:ILE:HG22	2.15	0.61
1:D:187:ARG:HG3	2:C:760:LEU:HD21	1.80	0.61
1:B:219:GLY:HA3	1:B:303:THR:HG21	1.83	0.61
1:B:357:ASN:HB2	4:G:1:NAG:N2	2.14	0.61
1:D:219:GLY:HA3	1:D:303:THR:HG21	1.83	0.61
2:A:57:GLU:HG3	2:A:58:ASN:N	2.16	0.61
6:B:1004:3PH:H291	6:B:1004:3PH:C25	2.12	0.61
1:D:179:LEU:HD23	6:D:1005:3PH:H3I3	1.81	0.60
3:E:350:VAL:HG22	3:E:422:ASN:HB3	1.84	0.60
2:A:754:VAL:O	2:A:758:VAL:HG22	2.01	0.60
2:C:152:MET:O	2:C:161:ARG:NH2	2.35	0.59
2:C:754:VAL:O	2:C:758:VAL:HG22	2.01	0.59
2:C:134:ASN:ND2	2:C:136:ASP:OD1	2.35	0.59
1:B:321:PHE:HE2	1:B:340:LEU:HD13	1.67	0.59
3:E:360:ASN:HA	3:E:524:VAL:HB	1.84	0.59
2:C:736:GLN:N	2:C:737:PRO:CD	2.55	0.59
1:D:321:PHE:HE2	1:D:340:LEU:HD13	1.67	0.59
1:D:478:ILE:HD11	1:D:514:PRO:HB3	1.84	0.59
2:A:622:ILE:HB	2:A:679:ILE:HG21	0.61	0.58
2:A:152:MET:O	2:A:161:ARG:NH2	2.36	0.58
3:E:432:CYS:O	3:E:512:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:360:ASN:HA	3:F:524:VAL:HB	1.84	0.58
3:F:350:VAL:HG22	3:F:422:ASN:HB3	1.84	0.58
1:B:478:ILE:HD11	1:B:514:PRO:HB3	1.83	0.58
2:A:134:ASN:ND2	2:A:136:ASP:OD1	2.36	0.58
2:C:622:ILE:HB	2:C:679:ILE:HG21	0.61	0.58
3:F:432:CYS:O	3:F:512:VAL:HG23	2.03	0.58
2:A:336:PRO:HB2	2:A:340:GLN:HB2	1.85	0.58
1:B:204:TYR:HH	1:B:286:THR:HG1	1.47	0.58
4:J:2:NAG:H83	4:J:2:NAG:H3	1.86	0.58
1:B:186:LEU:HD22	1:B:431:GLU:HG3	1.86	0.57
3:F:357:ARG:HE	3:F:394:ASN:HD22	1.52	0.57
2:C:431:ASP:N	2:C:431:ASP:OD1	2.37	0.57
2:C:336:PRO:HB2	2:C:340:GLN:HB2	1.85	0.57
2:A:431:ASP:N	2:A:431:ASP:OD1	2.37	0.57
1:D:508:MET:HA	1:D:512:VAL:HG22	1.86	0.57
1:B:508:MET:HA	1:B:512:VAL:HG22	1.86	0.56
4:R:2:NAG:H3	4:R:2:NAG:H83	1.86	0.56
1:B:398:MET:HA	1:B:401:MET:HE2	1.87	0.56
2:A:622:ILE:HB	2:A:679:ILE:HG22	1.67	0.56
2:A:637:ASP:OD1	2:A:637:ASP:N	2.23	0.56
1:D:186:LEU:HD22	1:D:431:GLU:HG3	1.86	0.56
3:E:357:ARG:HE	3:E:394:ASN:HD22	1.52	0.55
1:B:74:ILE:HG12	1:B:88:GLY:HA3	1.88	0.55
3:E:358:ILE:HD13	3:E:395:VAL:HG13	1.89	0.55
3:F:455:LEU:HD22	3:F:493:ARG:HG3	1.89	0.55
3:E:455:LEU:HD22	3:E:493:ARG:HG3	1.89	0.55
1:D:121:LEU:O	1:D:124:SER:OG	2.21	0.55
6:B:1004:3PH:C2C	6:B:1004:3PH:C28	2.86	0.54
2:A:638:ASN:ND2	2:C:653:GLN:OE1	2.27	0.54
1:D:323:LEU:O	2:C:678:ARG:HG3	2.06	0.54
1:D:74:ILE:HG12	1:D:88:GLY:HA3	1.88	0.54
3:F:358:ILE:HD13	3:F:395:VAL:HG13	1.89	0.54
3:F:444:LYS:HG2	3:F:448:ASN:HB2	1.90	0.54
2:C:730:THR:O	2:C:730:THR:OG1	2.26	0.54
3:F:335:LEU:HD13	3:F:362:VAL:HG13	1.90	0.54
1:D:175:LEU:O	1:D:179:LEU:HG	2.08	0.53
2:A:736:GLN:N	2:A:737:PRO:CD	2.68	0.53
1:B:241:TRP:HB2	1:B:520:LEU:HD11	1.90	0.53
6:D:1004:3PH:C2C	6:D:1004:3PH:C28	2.86	0.53
1:B:121:LEU:O	1:B:124:SER:OG	2.21	0.53
3:E:357:ARG:HH12	3:E:359:SER:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:335:LEU:HD13	3:E:362:VAL:HG13	1.90	0.53
1:D:249:PHE:HB3	1:D:469:LEU:HD11	1.91	0.53
1:B:45:VAL:HB	1:B:46:PRO:HD3	1.91	0.53
2:C:294:THR:HG23	2:C:365:THR:HA	1.91	0.53
1:B:249:PHE:HB3	1:B:469:LEU:HD11	1.91	0.52
1:D:179:LEU:HD23	6:D:1005:3PH:H3I1	1.82	0.52
2:A:294:THR:HG23	2:A:365:THR:HA	1.91	0.52
3:E:444:LYS:HG2	3:E:448:ASN:HB2	1.90	0.52
1:D:45:VAL:HB	1:D:46:PRO:HD3	1.91	0.52
1:B:337:LYS:HE2	1:B:355:ILE:HG21	1.91	0.52
1:D:321:PHE:CE2	1:D:340:LEU:HD13	2.45	0.52
1:B:118:GLN:HG2	2:A:741:ILE:CD1	2.38	0.52
1:B:175:LEU:O	1:B:179:LEU:HG	2.08	0.52
2:C:622:ILE:HB	2:C:679:ILE:HG22	1.68	0.52
1:B:428:LEU:HD11	6:B:1005:3PH:H2I2	1.91	0.52
1:D:127:PRO:HG2	1:D:136:ASP:HB2	1.92	0.52
3:F:357:ARG:HH12	3:F:359:SER:HA	1.74	0.52
1:B:127:PRO:HG2	1:B:136:ASP:HB2	1.92	0.52
1:D:241:TRP:HB2	1:D:520:LEU:HD11	1.90	0.52
2:A:144:LEU:HA	2:A:148:LEU:HB2	1.93	0.51
1:D:337:LYS:HE2	1:D:355:ILE:HG21	1.91	0.51
3:F:392:PHE:HD1	3:F:517:LEU:HB2	1.75	0.51
2:A:338:ASN:ND2	2:A:339:VAL:H	2.08	0.51
2:A:432:ASN:OD1	2:A:432:ASN:N	2.43	0.51
1:B:321:PHE:CE2	1:B:340:LEU:HD13	2.45	0.51
1:B:323:LEU:O	2:A:678:ARG:HG3	2.10	0.51
1:B:462:ASP:OD1	1:B:462:ASP:N	2.43	0.51
2:C:338:ASN:ND2	2:C:339:VAL:H	2.08	0.51
3:E:392:PHE:HD1	3:E:517:LEU:HB2	1.75	0.51
2:C:144:LEU:HA	2:C:148:LEU:HB2	1.93	0.51
1:D:170:PRO:HB2	1:D:449:THR:HG22	1.93	0.51
2:C:757:ILE:O	2:C:761:ILE:HG13	2.11	0.51
2:C:346:PRO:HA	2:C:359:LEU:O	2.11	0.51
1:D:462:ASP:OD1	1:D:462:ASP:N	2.43	0.50
2:A:346:PRO:HA	2:A:359:LEU:O	2.11	0.50
2:A:730:THR:O	2:A:730:THR:OG1	2.26	0.50
2:A:31:LYS:HG2	2:A:35:GLU:OE1	2.11	0.50
2:A:757:ILE:O	2:A:761:ILE:HG13	2.11	0.50
2:C:31:LYS:HG2	2:C:35:GLU:OE1	2.11	0.50
2:A:303:ASP:OD1	2:A:303:ASP:N	2.44	0.50
3:F:392:PHE:CD1	3:F:517:LEU:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:439:ASN:O	3:E:443:SER:OG	2.30	0.50
1:B:170:PRO:HB2	1:B:449:THR:HG22	1.93	0.50
2:C:732:GLY:H	2:C:733:PRO:HD3	1.77	0.50
3:E:392:PHE:CD1	3:E:517:LEU:HB2	2.47	0.50
1:B:536:TYR:H	1:B:536:TYR:HD1	1.60	0.50
2:C:303:ASP:OD1	2:C:303:ASP:N	2.44	0.50
2:A:183:TYR:CD1	2:A:183:TYR:C	2.85	0.49
2:C:732:GLY:O	2:C:734:PRO:HD3	2.12	0.49
6:D:1004:3PH:C28	6:D:1004:3PH:H2C2	2.42	0.49
6:B:1004:3PH:C28	6:B:1004:3PH:H2C2	2.42	0.49
2:C:183:TYR:CD1	2:C:183:TYR:C	2.86	0.49
2:C:324:THR:HG23	2:C:326:GLY:H	1.78	0.49
2:C:351:LEU:HB2	2:C:355:ASP:HB3	1.94	0.49
2:A:351:LEU:HB2	2:A:355:ASP:HB3	1.94	0.49
2:C:622:ILE:CA	2:C:679:ILE:CG2	2.89	0.49
1:D:398:MET:HA	1:D:401:MET:HE2	1.95	0.49
1:D:474:LEU:HD11	1:D:514:PRO:HA	1.94	0.49
2:A:324:THR:HG23	2:A:326:GLY:H	1.78	0.49
3:E:393:THR:N	3:E:516:GLU:O	2.45	0.49
1:D:281:LEU:HD21	6:D:1004:3PH:H3C1	1.93	0.49
3:F:392:PHE:O	3:F:523:THR:OG1	2.24	0.49
1:B:474:LEU:HD11	1:B:514:PRO:HA	1.94	0.48
2:A:764:GLY:O	2:A:768:ARG:NH1	2.46	0.48
2:A:19:SER:N	2:A:23:GLU:OE2	2.46	0.48
1:B:42:SER:O	1:B:42:SER:OG	2.28	0.48
1:D:178:TRP:CZ2	1:D:441:ASN:HB3	2.49	0.48
1:D:320:THR:HG21	1:D:351:MET:SD	2.53	0.48
1:D:121:LEU:HD12	1:D:121:LEU:H	1.79	0.48
1:D:150:TYR:CD1	1:D:156:ILE:HD12	2.48	0.48
2:C:19:SER:N	2:C:23:GLU:OE2	2.47	0.48
2:C:622:ILE:CA	2:C:679:ILE:HG21	2.36	0.48
1:B:178:TRP:CZ2	1:B:441:ASN:HB3	2.49	0.48
1:B:320:THR:HG21	1:B:351:MET:SD	2.53	0.48
1:B:329:THR:HG23	1:B:330:ALA:H	1.78	0.48
1:B:113:LEU:O	1:B:116:SER:OG	2.21	0.48
2:C:736:GLN:O	2:C:738:PRO:HD3	2.13	0.48
1:B:117:PHE:HD2	2:A:745:VAL:HG21	1.79	0.48
1:D:113:LEU:O	1:D:116:SER:OG	2.21	0.48
1:B:121:LEU:HD12	1:B:121:LEU:H	1.79	0.48
1:B:150:TYR:CD1	1:B:156:ILE:HD12	2.48	0.48
1:D:106:ASN:ND2	1:D:403:GLY:HA3	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:ILE:HD11	2:C:186:LEU:HD12	1.96	0.48
1:B:552:PRO:HG2	1:B:555:ALA:HB2	1.96	0.47
1:B:118:GLN:O	1:B:389:GLN:NE2	2.27	0.47
2:A:353:LYS:HD2	3:E:501:TYR:CZ	2.49	0.47
1:D:513:SER:HB2	1:D:514:PRO:HD3	1.96	0.47
2:C:764:GLY:O	2:C:768:ARG:NH1	2.46	0.47
2:A:119:ILE:HD11	2:A:186:LEU:HD12	1.96	0.47
1:D:329:THR:HG23	1:D:330:ALA:H	1.78	0.47
2:A:20:THR:HG23	2:A:21:ILE:H	1.79	0.47
1:D:118:GLN:O	1:D:389:GLN:NE2	2.27	0.47
2:A:622:ILE:CA	2:A:679:ILE:CG2	2.90	0.47
1:D:552:PRO:HG2	1:D:555:ALA:HB2	1.96	0.47
2:C:353:LYS:HD2	3:F:501:TYR:CZ	2.49	0.47
1:B:513:SER:HB2	1:B:514:PRO:HD3	1.96	0.47
2:A:732:GLY:N	2:A:733:PRO:CD	2.78	0.47
1:D:61:LEU:HD11	1:D:480:VAL:HG11	1.97	0.47
2:A:596:LYS:HB2	2:A:596:LYS:HE2	1.69	0.47
1:B:228:PHE:HZ	1:B:292:ILE:HD11	1.80	0.46
1:D:77:TRP:HA	1:D:80:ILE:HG22	1.98	0.46
1:D:117:PHE:HD2	2:C:745:VAL:HG21	1.79	0.46
1:D:146:GLN:HG2	1:D:376:ILE:HG21	1.98	0.46
1:D:150:TYR:HD1	1:D:156:ILE:HD12	1.80	0.46
1:B:61:LEU:HD11	1:B:480:VAL:HG11	1.97	0.46
1:B:150:TYR:HD1	1:B:156:ILE:HD12	1.80	0.46
1:D:228:PHE:HZ	1:D:292:ILE:HD11	1.80	0.46
1:D:536:TYR:HD1	1:D:536:TYR:H	1.60	0.46
3:F:439:ASN:O	3:F:443:SER:OG	2.30	0.46
2:A:621:ARG:CG	2:A:678:ARG:HE	2.28	0.46
2:A:745:VAL:HA	2:A:748:VAL:HG12	1.98	0.46
2:C:20:THR:HG23	2:C:21:ILE:H	1.80	0.46
2:C:427:ASP:OD1	2:C:428:PHE:N	2.44	0.46
2:C:678:ARG:CG	2:C:678:ARG:NH2	2.73	0.46
1:D:314:SER:OG	1:D:328:LEU:O	2.34	0.46
2:A:760:LEU:HD12	2:A:760:LEU:HA	1.70	0.46
3:E:424:LYS:HA	3:E:424:LYS:HD2	1.81	0.46
1:B:314:SER:OG	1:B:328:LEU:O	2.34	0.46
2:C:367:ASP:OD1	2:C:367:ASP:N	2.48	0.46
2:C:622:ILE:CB	2:C:679:ILE:HG22	2.37	0.46
1:B:146:GLN:HG2	1:B:376:ILE:HG21	1.98	0.46
2:C:145:GLU:HB3	2:C:146:PRO:HD3	1.98	0.46
2:C:745:VAL:HA	2:C:748:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:ND2	1:B:403:GLY:HA3	2.26	0.46
1:B:450:MET:HG2	1:B:451:GLU:H	1.81	0.46
1:D:249:PHE:HB3	1:D:469:LEU:HD21	1.97	0.46
2:C:34:HIS:CE1	3:F:493:ARG:HD3	2.51	0.46
2:A:34:HIS:CE1	3:E:493:ARG:HD3	2.51	0.46
2:A:732:GLY:H	2:A:733:PRO:HD3	1.80	0.46
1:D:450:MET:HG2	1:D:451:GLU:H	1.81	0.46
3:F:466:ARG:HE	3:F:468:ILE:HD11	1.81	0.46
2:A:55:THR:HG21	4:H:1:NAG:H62	1.98	0.46
1:B:487:ARG:HA	1:B:490:GLU:HG3	1.98	0.45
2:A:367:ASP:OD1	2:A:367:ASP:N	2.48	0.45
2:C:750:MET:O	2:C:754:VAL:HG23	2.17	0.45
1:B:77:TRP:HA	1:B:80:ILE:HG22	1.98	0.45
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.79	0.45
1:B:249:PHE:HB3	1:B:469:LEU:HD21	1.97	0.45
6:B:1005:3PH:H2D2	6:B:1005:3PH:C29	2.44	0.45
1:D:297:ILE:HG21	1:D:381:ALA:HB2	1.99	0.45
1:D:428:LEU:HD11	6:D:1005:3PH:H2I2	1.98	0.45
1:D:536:TYR:HB3	1:D:551:TYR:CE2	2.51	0.45
2:C:48:TRP:O	2:C:52:THR:HG22	2.17	0.45
1:B:536:TYR:HB3	1:B:551:TYR:CE2	2.51	0.45
1:D:42:SER:O	1:D:42:SER:OG	2.28	0.45
1:D:401:MET:HE2	1:D:401:MET:HB2	1.82	0.45
2:C:148:LEU:HD23	2:C:148:LEU:HA	1.86	0.45
2:A:48:TRP:O	2:A:52:THR:HG22	2.17	0.45
3:E:466:ARG:HE	3:E:468:ILE:HD11	1.81	0.45
2:C:55:THR:HG21	4:P:1:NAG:H62	1.98	0.45
2:C:292:ASP:OD1	2:C:294:THR:OG1	2.22	0.45
2:A:145:GLU:HB3	2:A:146:PRO:HD3	1.98	0.45
1:D:291:SER:O	1:D:291:SER:OG	2.35	0.45
3:F:393:THR:N	3:F:516:GLU:O	2.44	0.45
1:B:212:ILE:HD13	1:B:212:ILE:HA	1.90	0.45
1:D:117:PHE:CD2	2:C:745:VAL:HG21	2.52	0.45
1:D:117:PHE:HE2	2:C:745:VAL:HG11	1.82	0.45
2:C:432:ASN:OD1	2:C:432:ASN:N	2.43	0.45
1:B:254:LEU:O	1:B:469:LEU:HD13	2.17	0.45
1:B:297:ILE:HG21	1:B:381:ALA:HB2	1.99	0.45
1:D:254:LEU:O	1:D:469:LEU:HD13	2.17	0.45
1:B:77:TRP:CZ2	1:B:476:GLU:HG2	2.52	0.45
1:D:75:GLY:O	1:D:79:THR:HG23	2.17	0.45
1:D:459:ILE:HD11	1:D:551:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:GLU:OE2	4:P:1:NAG:O6	2.33	0.45
1:B:117:PHE:HE2	2:A:745:VAL:HG11	1.82	0.44
1:B:270:ASN:OD1	1:B:271:ASN:N	2.49	0.44
1:B:548:THR:O	1:B:548:THR:OG1	2.32	0.44
2:A:750:MET:O	2:A:754:VAL:HG23	2.17	0.44
6:D:1004:3PH:H2C2	6:D:1004:3PH:H282	1.99	0.44
1:B:117:PHE:CD2	2:A:745:VAL:HG21	2.52	0.44
3:E:365:TYR:CD1	3:E:387:LEU:HB3	2.52	0.44
1:D:228:PHE:CZ	1:D:292:ILE:HD11	2.53	0.44
3:F:365:TYR:CD1	3:F:387:LEU:HB3	2.52	0.44
2:A:678:ARG:CG	2:A:678:ARG:NH2	2.72	0.44
1:B:228:PHE:CZ	1:B:292:ILE:HD11	2.53	0.44
2:C:378:HIS:CD2	2:C:401:HIS:HD2	2.36	0.44
1:B:169:GLU:HB2	1:B:170:PRO:HD3	2.00	0.44
1:B:536:TYR:HB3	1:B:551:TYR:CZ	2.53	0.44
2:A:378:HIS:CD2	2:A:401:HIS:HD2	2.36	0.44
1:D:60:TYR:CD2	1:D:509:TRP:HZ2	2.36	0.44
1:B:60:TYR:CD2	1:B:509:TRP:HZ2	2.36	0.44
1:B:537:GLN:NE2	1:B:546:LEU:HD23	2.33	0.44
2:A:622:ILE:CB	2:A:679:ILE:HG22	2.37	0.44
3:E:392:PHE:O	3:E:523:THR:OG1	2.24	0.44
2:C:183:TYR:CD1	2:C:184:VAL:N	2.86	0.44
1:D:487:ARG:HA	1:D:490:GLU:HG3	1.98	0.44
1:B:281:LEU:HD21	6:B:1004:3PH:H3C1	2.00	0.44
1:B:459:ILE:HD11	1:B:551:TYR:CE1	2.52	0.44
2:A:732:GLY:H	2:A:733:PRO:CD	2.31	0.44
1:D:182:TYR:HE2	6:D:1005:3PH:H3E2	1.83	0.44
1:D:536:TYR:HB3	1:D:551:TYR:CZ	2.53	0.43
1:D:474:LEU:O	1:D:478:ILE:HG12	2.18	0.43
2:C:295:ASP:HA	2:C:298:VAL:HG13	2.01	0.43
2:A:295:ASP:HA	2:A:298:VAL:HG13	2.01	0.43
1:D:70:ARG:HH22	1:D:268:PRO:HA	1.84	0.43
1:D:77:TRP:CZ2	1:D:476:GLU:HG2	2.52	0.43
1:B:75:GLY:O	1:B:79:THR:HG23	2.17	0.43
2:A:619:LYS:HD3	2:A:725:LEU:HD22	2.01	0.43
1:D:548:THR:O	1:D:548:THR:OG1	2.31	0.43
6:B:1004:3PH:H2C2	6:B:1004:3PH:H282	1.99	0.43
2:A:148:LEU:HD23	2:A:148:LEU:HA	1.86	0.43
2:A:740:SER:O	2:A:743:LEU:N	2.52	0.43
2:C:730:THR:O	2:C:731:LEU:HD23	2.19	0.43
2:C:739:VAL:O	2:C:740:SER:OG	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:THR:HG22	2:A:678:ARG:NH2	2.34	0.43
2:A:166:GLU:OE1	2:A:493:HIS:HE1	2.01	0.43
3:E:372:ALA:HB3	3:E:374:PHE:CE1	2.54	0.43
2:C:31:LYS:HE2	2:C:31:LYS:HB3	1.87	0.43
1:B:535:LYS:HD3	1:B:550:ASP:HA	2.01	0.43
2:A:530:CYS:SG	2:A:531:GLN:N	2.92	0.43
3:F:391:CYS:HB3	3:F:525:CYS:HB3	1.82	0.43
1:B:44:LEU:HD23	1:B:288:ILE:HD12	2.00	0.43
2:C:621:ARG:CG	2:C:678:ARG:HE	2.31	0.43
1:B:404:ILE:HD12	1:B:404:ILE:HA	1.87	0.43
1:B:474:LEU:O	1:B:478:ILE:HG12	2.18	0.43
2:A:215:TYR:HB3	2:A:567:THR:OG1	2.19	0.43
2:A:292:ASP:OD1	2:A:294:THR:OG1	2.22	0.43
1:D:44:LEU:HD23	1:D:288:ILE:HD12	2.00	0.43
1:D:397:PHE:O	1:D:401:MET:HG3	2.19	0.43
2:C:490:PRO:HA	2:C:612:PRO:HG2	2.00	0.43
2:C:686:THR:HG21	2:C:691:VAL:HA	2.01	0.43
2:A:490:PRO:HA	2:A:612:PRO:HG2	2.00	0.42
1:D:202:LEU:HD23	1:D:401:MET:HE1	2.01	0.42
1:B:118:GLN:NE2	2:A:741:ILE:HG13	2.31	0.42
2:A:21:ILE:HD12	2:A:87:GLU:HG3	2.01	0.42
2:C:166:GLU:OE1	2:C:493:HIS:HE1	2.01	0.42
2:C:760:LEU:HD12	2:C:760:LEU:HA	1.70	0.42
2:A:325:GLN:O	2:A:325:GLN:NE2	2.52	0.42
2:C:73:LEU:HD12	2:C:73:LEU:HA	1.89	0.42
2:C:530:CYS:SG	2:C:531:GLN:N	2.92	0.42
3:F:398:ASP:HB2	3:F:512:VAL:CG1	2.49	0.42
1:B:70:ARG:HH22	1:B:268:PRO:HA	1.84	0.42
2:A:312:GLU:O	2:A:316:VAL:HG23	2.20	0.42
2:A:333:LEU:O	2:A:362:THR:HG23	2.19	0.42
1:D:318:THR:HG22	2:C:678:ARG:NH2	2.34	0.42
1:D:537:GLN:NE2	1:D:546:LEU:HD23	2.33	0.42
1:B:98:LEU:O	1:B:102:TYR:HB2	2.19	0.42
1:B:291:SER:O	1:B:291:SER:OG	2.35	0.42
2:A:427:ASP:OD1	2:A:428:PHE:N	2.44	0.42
2:A:678:ARG:O	2:A:679:ILE:O	2.37	0.42
2:A:732:GLY:N	2:A:733:PRO:HD3	2.34	0.42
1:D:169:GLU:HB2	1:D:170:PRO:HD3	2.00	0.42
1:D:215:LEU:HD23	1:D:215:LEU:HA	1.79	0.42
6:D:1005:3PH:H2D2	6:D:1005:3PH:C29	2.45	0.42
2:C:333:LEU:O	2:C:362:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:PHE:O	1:B:401:MET:HG3	2.19	0.42
1:B:416:THR:OG1	1:B:417:PRO:HD3	2.19	0.42
3:E:398:ASP:HB2	3:E:512:VAL:CG1	2.49	0.42
2:C:600:LYS:HE3	2:C:600:LYS:HB2	1.81	0.42
1:D:535:LYS:HD3	1:D:550:ASP:HA	2.01	0.42
2:C:21:ILE:HD12	2:C:87:GLU:HG3	2.01	0.42
2:C:619:LYS:HD3	2:C:725:LEU:HD22	2.01	0.42
3:F:461:LEU:HD23	3:F:461:LEU:HA	1.88	0.42
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.92	0.42
2:A:420:SER:OG	4:L:1:NAG:H83	2.20	0.42
3:E:403:ARG:HB3	3:E:406:GLU:HG3	2.02	0.42
1:D:98:LEU:O	1:D:102:TYR:HB2	2.19	0.42
1:D:178:TRP:O	1:D:181:VAL:HG12	2.20	0.42
1:D:352:PHE:N	1:D:353:PRO:HD2	2.35	0.42
2:C:208:GLU:HB2	2:C:219:ARG:HG2	2.02	0.42
2:C:420:SER:OG	4:T:1:NAG:H83	2.20	0.42
2:A:627:ALA:HB2	2:A:721:SER:OG	2.20	0.42
1:D:44:LEU:HD12	1:D:44:LEU:H	1.85	0.42
1:D:82:PRO:O	1:D:577:THR:HG21	2.20	0.42
1:B:381:ALA:O	1:B:385:MET:HG3	2.19	0.42
1:B:405:GLY:O	1:B:408:LEU:HG	2.20	0.42
1:D:400:LEU:HD23	1:D:400:LEU:HA	1.84	0.42
1:D:460:PHE:CE2	1:D:562:LEU:HD21	2.55	0.42
3:F:372:ALA:HB3	3:F:374:PHE:CE1	2.54	0.42
2:A:208:GLU:HB2	2:A:219:ARG:HG2	2.02	0.41
2:A:450:LEU:HD23	2:A:450:LEU:HA	1.88	0.41
1:D:270:ASN:OD1	1:D:271:ASN:N	2.49	0.41
1:D:318:THR:CG2	2:C:678:ARG:NH2	2.83	0.41
1:D:381:ALA:O	1:D:385:MET:HG3	2.20	0.41
1:D:405:GLY:O	1:D:408:LEU:HG	2.20	0.41
3:F:357:ARG:NE	3:F:394:ASN:HD22	2.17	0.41
1:B:178:TRP:O	1:B:181:VAL:HG12	2.20	0.41
1:B:460:PHE:CE2	1:B:562:LEU:HD21	2.55	0.41
2:A:730:THR:O	2:A:731:LEU:HD23	2.19	0.41
2:A:743:LEU:HD23	2:A:743:LEU:HA	1.91	0.41
2:A:753:ILE:HD13	2:A:753:ILE:HA	1.85	0.41
2:C:325:GLN:O	2:C:325:GLN:NE2	2.52	0.41
4:N:1:NAG:H61	4:N:2:NAG:N2	2.35	0.41
1:B:82:PRO:O	1:B:577:THR:HG21	2.20	0.41
1:B:179:LEU:HD23	6:B:1005:3PH:H3I1	1.83	0.41
1:B:477:THR:HA	1:B:480:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:97:LEU:HD23	2:A:97:LEU:HA	1.87	0.41
1:D:16:PHE:CD2	1:D:197:TYR:HA	2.56	0.41
1:D:536:TYR:CG	1:D:537:GLN:N	2.88	0.41
3:F:403:ARG:HB3	3:F:406:GLU:HG3	2.01	0.41
1:B:25:LEU:HD11	1:B:403:GLY:HA2	2.03	0.41
1:B:202:LEU:HD23	1:B:401:MET:HE1	2.02	0.41
2:A:622:ILE:CA	2:A:679:ILE:HG21	2.37	0.41
2:A:686:THR:HG21	2:A:691:VAL:HA	2.01	0.41
3:E:354:ASN:O	3:E:398:ASP:HA	2.21	0.41
1:D:477:THR:HA	1:D:480:VAL:HG12	2.01	0.41
2:C:215:TYR:HB3	2:C:567:THR:OG1	2.19	0.41
3:E:398:ASP:HB2	3:E:512:VAL:HG13	2.03	0.41
1:D:416:THR:OG1	1:D:417:PRO:HD3	2.19	0.41
3:F:354:ASN:O	3:F:398:ASP:HA	2.21	0.41
3:F:468:ILE:HG22	3:F:468:ILE:O	2.20	0.41
4:V:1:NAG:H61	4:V:2:NAG:N2	2.35	0.41
1:B:352:PHE:N	1:B:353:PRO:HD2	2.35	0.41
1:D:137:GLU:HG2	1:D:138:GLU:N	2.36	0.41
2:C:678:ARG:O	2:C:679:ILE:O	2.39	0.41
3:F:398:ASP:HB2	3:F:512:VAL:HG13	2.03	0.41
1:B:181:VAL:O	1:B:185:ILE:HG12	2.21	0.41
1:B:536:TYR:CG	1:B:537:GLN:N	2.88	0.41
3:E:357:ARG:NE	3:E:394:ASN:HD22	2.17	0.41
2:C:293:VAL:HG23	2:C:293:VAL:O	2.21	0.41
2:C:627:ALA:HB2	2:C:721:SER:OG	2.20	0.41
1:B:332:ASN:HA	1:B:335:GLN:OE1	2.21	0.41
2:C:379:ILE:HD13	2:C:379:ILE:HA	1.95	0.41
2:C:736:GLN:N	2:C:737:PRO:HD2	2.27	0.41
3:F:424:LYS:HD2	3:F:424:LYS:HA	1.81	0.41
1:B:92:VAL:CG1	6:B:1003:3PH:H3G2	2.51	0.41
1:B:137:GLU:HG2	1:B:138:GLU:N	2.36	0.41
1:B:149:TRP:HD1	1:B:150:TYR:CD2	2.38	0.41
1:B:441:ASN:HA	1:B:444:ILE:HG22	2.03	0.41
2:A:493:HIS:HD2	2:A:499:ASP:OD2	2.04	0.41
2:A:622:ILE:HG12	2:A:722:LEU:HD13	2.03	0.41
2:A:678:ARG:CG	2:A:678:ARG:O	2.69	0.41
1:D:25:LEU:HD11	1:D:403:GLY:HA2	2.03	0.41
2:C:312:GLU:O	2:C:316:VAL:HG23	2.20	0.41
1:B:401:MET:HE2	1:B:401:MET:HB2	1.92	0.41
1:B:469:LEU:O	1:B:473:VAL:HG23	2.21	0.41
2:A:513:ILE:HD12	2:A:513:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:MET:HA	1:D:53:VAL:HG22	2.03	0.41
1:D:246:THR:HA	1:D:249:PHE:HB2	2.03	0.41
1:D:267:GLU:HG3	1:D:270:ASN:HB3	2.03	0.41
2:A:379:ILE:HD13	2:A:379:ILE:HA	1.95	0.40
1:B:44:LEU:H	1:B:44:LEU:HD12	1.85	0.40
1:D:149:TRP:HD1	1:D:150:TYR:CD2	2.38	0.40
1:D:298:TYR:CE2	1:D:368:VAL:HG12	2.56	0.40
1:D:503:TRP:HA	1:D:506:LYS:HD2	2.03	0.40
1:B:16:PHE:HD2	1:B:197:TYR:HA	1.86	0.40
1:B:267:GLU:HG3	1:B:270:ASN:HB3	2.03	0.40
1:D:332:ASN:HA	1:D:335:GLN:OE1	2.21	0.40
1:D:375:PHE:O	1:D:379:THR:HG22	2.21	0.40
1:D:464:ALA:HB2	1:D:562:LEU:HD22	2.03	0.40
1:B:16:PHE:CD2	1:B:197:TYR:HA	2.56	0.40
1:B:62:GLU:HG3	1:B:260:ILE:HG13	2.04	0.40
1:D:181:VAL:O	1:D:185:ILE:HG12	2.21	0.40
1:D:469:LEU:O	1:D:473:VAL:HG23	2.21	0.40
2:C:183:TYR:HD1	2:C:184:VAL:N	2.19	0.40
2:C:596:LYS:HB2	2:C:596:LYS:HE2	1.69	0.40
2:C:622:ILE:HG12	2:C:722:LEU:HD13	2.03	0.40
1:B:58:LEU:HD22	1:B:473:VAL:HG12	2.04	0.40
1:B:119:ASP:HA	1:B:120:PRO:HA	1.94	0.40
2:A:293:VAL:HG23	2:A:293:VAL:O	2.21	0.40
3:E:468:ILE:HG22	3:E:468:ILE:O	2.20	0.40
2:C:678:ARG:CG	2:C:678:ARG:O	2.69	0.40
3:F:425:LEU:HD23	3:F:425:LEU:HA	1.90	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	B	571/613 (93%)	527 (92%)	44 (8%)	0	100	100
1	D	571/613 (93%)	527 (92%)	44 (8%)	0	100	100
2	A	748/826 (91%)	697 (93%)	48 (6%)	3 (0%)	30	63
2	C	748/826 (91%)	693 (93%)	53 (7%)	2 (0%)	37	68
3	E	196/252 (78%)	183 (93%)	13 (7%)	0	100	100
3	F	196/252 (78%)	183 (93%)	13 (7%)	0	100	100
All	All	3030/3382 (90%)	2810 (93%)	215 (7%)	5 (0%)	45	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	736	GLN
2	A	739	VAL
2	C	736	GLN
2	A	679	ILE
2	C	679	ILE

### 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	B	486/517 (94%)	466 (96%)	20 (4%)	26	57
1	D	486/517 (94%)	466 (96%)	20 (4%)	26	57
2	A	664/732 (91%)	632 (95%)	32 (5%)	21	51
2	C	664/732 (91%)	636 (96%)	28 (4%)	25	56
3	E	170/218 (78%)	161 (95%)	9 (5%)	19	48
3	F	170/218 (78%)	161 (95%)	9 (5%)	19	48
All	All	2640/2934 (90%)	2522 (96%)	118 (4%)	26	53

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	CYS
1	B	25	LEU
1	B	33	TYR
1	B	68	ARG
1	B	97	PHE
1	B	102	TYR
1	B	121	LEU
1	B	124	SER
1	B	282	ILE
1	B	309	CYS
1	B	325	ASP
1	B	329	THR
1	B	344	TYR
1	B	399	LEU
1	B	469	LEU
1	B	529	ILE
1	B	534	LEU
1	B	536	TYR
1	B	548	THR
1	B	579	VAL
2	A	20	THR
2	A	57	GLU
2	A	62	MET
2	A	87	GLU
2	A	131	LYS
2	A	133	CYS
2	A	183	TYR
2	A	295	ASP
2	A	298	VAL
2	A	317	SER
2	A	331	SER
2	A	362	THR
2	A	367	ASP
2	A	381	TYR
2	A	385	TYR
2	A	394	ASN
2	A	401	HIS
2	A	409	SER
2	A	420	SER
2	A	427	ASP
2	A	530	CYS
2	A	596	LYS
2	A	626	SER

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Mol	Chain	Res	Type
2	A	637	ASP
2	A	678	ARG
2	A	735	ASN
2	A	740	SER
2	A	741	ILE
2	A	749	VAL
2	A	750	MET
2	A	758	VAL
2	A	760	LEU
3	E	369	TYR
3	E	379	CYS
3	E	386	LYS
3	E	432	CYS
3	E	434	ILE
3	E	477	ASN
3	E	493	ARG
3	E	518	LEU
3	E	525	CYS
1	D	18	CYS
1	D	25	LEU
1	D	33	TYR
1	D	68	ARG
1	D	97	PHE
1	D	102	TYR
1	D	121	LEU
1	D	124	SER
1	D	282	ILE
1	D	309	CYS
1	D	325	ASP
1	D	329	THR
1	D	344	TYR
1	D	399	LEU
1	D	469	LEU
1	D	529	ILE
1	D	534	LEU
1	D	536	TYR
1	D	548	THR
1	D	579	VAL
2	C	20	THR
2	C	62	MET
2	C	87	GLU
2	C	131	LYS

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Mol	Chain	Res	Type
2	C	133	CYS
2	C	183	TYR
2	C	295	ASP
2	C	298	VAL
2	C	317	SER
2	C	367	ASP
2	C	381	TYR
2	C	385	TYR
2	C	394	ASN
2	C	401	HIS
2	C	409	SER
2	C	420	SER
2	C	427	ASP
2	C	530	CYS
2	C	596	LYS
2	C	626	SER
2	C	637	ASP
2	C	678	ARG
2	C	736	GLN
2	C	739	VAL
2	C	749	VAL
2	C	750	MET
2	C	758	VAL
2	C	760	LEU
3	F	369	TYR
3	F	379	CYS
3	F	386	LYS
3	F	432	CYS
3	F	434	ILE
3	F	477	ASN
3	F	493	ARG
3	F	518	LEU
3	F	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	71	GLN
1	B	106	ASN
1	B	115	HIS
1	B	118	GLN
1	B	237	ASN

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Mol	Chain	Res	Type
1	B	369	GLN
1	B	543	GLN
1	B	545	GLN
2	A	58	ASN
2	A	98	GLN
2	A	102	GLN
2	A	137	ASN
2	A	139	GLN
2	A	159	ASN
2	A	210	ASN
2	A	239	HIS
2	A	277	ASN
2	A	325	GLN
2	A	378	HIS
2	A	401	HIS
2	A	437	ASN
2	A	472	GLN
2	A	493	HIS
2	A	505	HIS
3	E	422	ASN
1	D	71	GLN
1	D	106	ASN
1	D	115	HIS
1	D	237	ASN
1	D	369	GLN
1	D	543	GLN
1	D	545	GLN
2	C	58	ASN
2	C	98	GLN
2	C	102	GLN
2	C	137	ASN
2	C	159	ASN
2	C	210	ASN
2	C	239	HIS
2	C	277	ASN
2	C	325	GLN
2	C	378	HIS
2	C	401	HIS
2	C	437	ASN
2	C	472	GLN
2	C	493	HIS
2	C	505	HIS

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Mol	Chain	Res	Type
3	F	422	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

32 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	$\# Z  > 2$
4	NAG	G	1	4,1	14,14,15	0.51	0	17,19,21	0.63	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	H	1	4,2	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	H	2	4	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	I	1	4,2	14,14,15	0.39	0	17,19,21	0.45	0
4	NAG	I	2	4	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	J	1	4,2	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	1.31	2 (11%)
4	NAG	K	1	4,2	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	K	2	4	14,14,15	0.16	0	17,19,21	0.47	0
4	NAG	L	1	4,2	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	L	2	4	14,14,15	0.20	0	17,19,21	0.36	0
4	NAG	M	1	4,2	14,14,15	0.62	1 (7%)	17,19,21	0.51	0
4	NAG	M	2	4	14,14,15	0.37	0	17,19,21	0.53	0
4	NAG	N	1	4,3	14,14,15	0.15	0	17,19,21	0.56	0
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	O	1	4,1	14,14,15	0.51	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	O	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	P	1	4,2	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	Q	1	4,2	14,14,15	0.40	0	17,19,21	0.44	0
4	NAG	Q	2	4	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	R	1	4,2	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
4	NAG	R	2	4	14,14,15	0.40	0	17,19,21	1.31	2 (11%)
4	NAG	S	1	4,2	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	S	2	4	14,14,15	0.15	0	17,19,21	0.46	0
4	NAG	T	1	4,2	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	T	2	4	14,14,15	0.18	0	17,19,21	0.36	0
4	NAG	U	1	4,2	14,14,15	0.62	1 (7%)	17,19,21	0.52	0
4	NAG	U	2	4	14,14,15	0.37	0	17,19,21	0.55	0
4	NAG	V	1	4,3	14,14,15	0.16	0	17,19,21	0.56	0
4	NAG	V	2	4	14,14,15	0.25	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
4	NAG	S	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C1	-2.19	1.40	1.43
4	U	1	NAG	O5-C1	-2.16	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	J	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	R	1	NAG	C1-O5-C5	2.48	115.56	112.19
4	J	1	NAG	C1-O5-C5	2.47	115.54	112.19
4	J	2	NAG	C1-C2-N2	2.07	114.03	110.49
4	R	2	NAG	C1-C2-N2	2.07	114.03	110.49

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	M	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	H	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 13 short contacts:

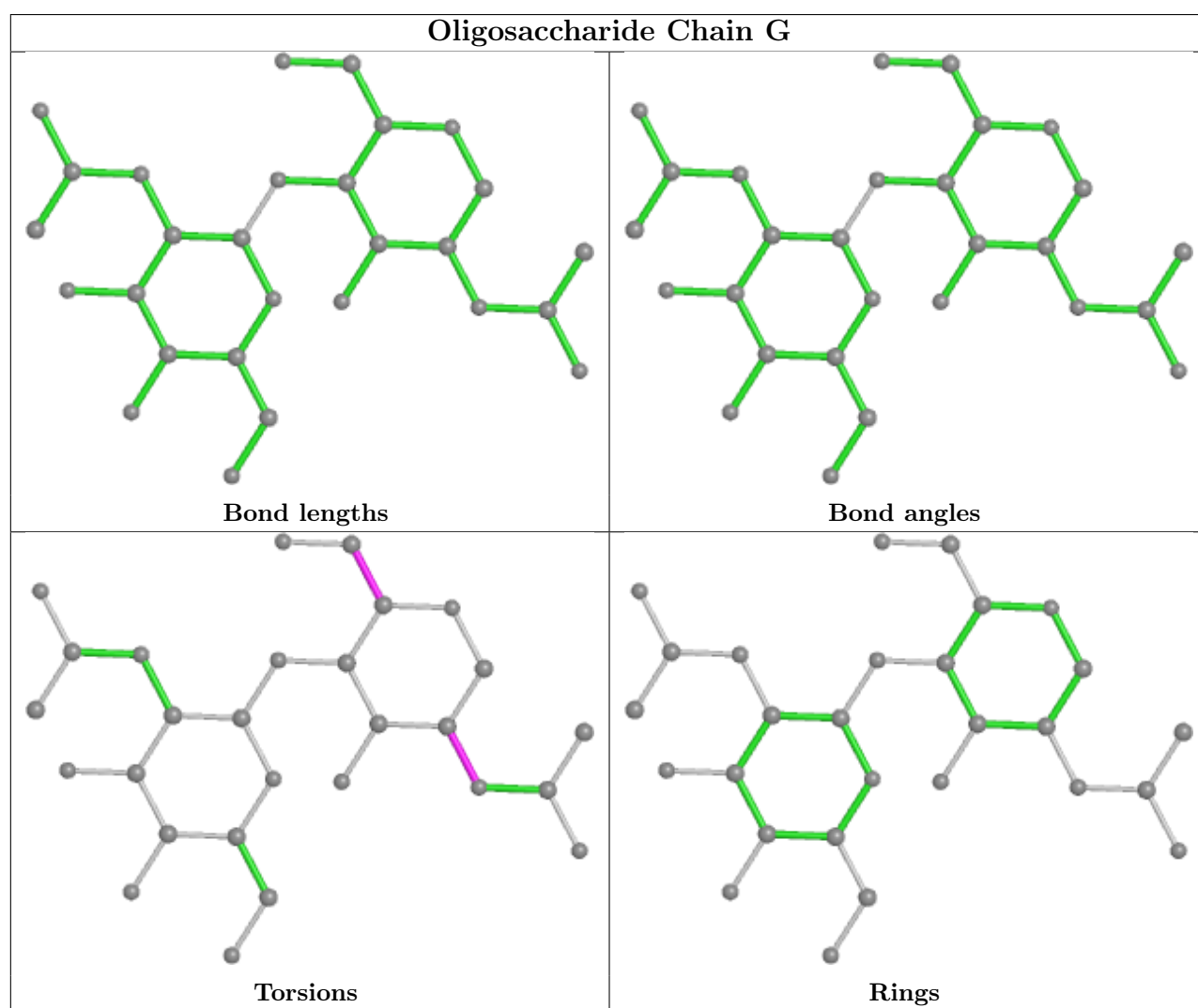
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	1	NAG	1	0
4	P	1	NAG	2	0
4	G	1	NAG	2	0
4	R	2	NAG	1	0

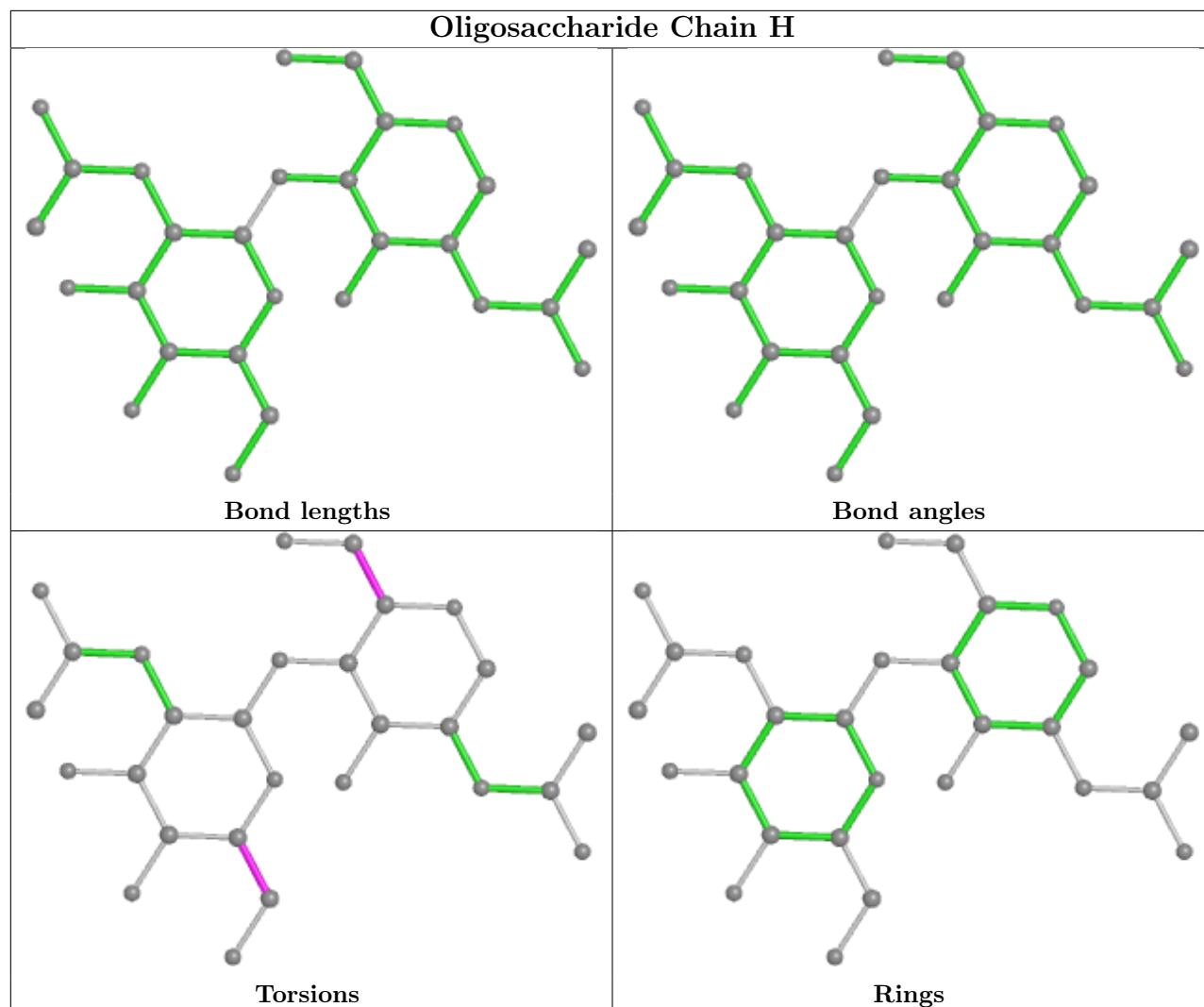
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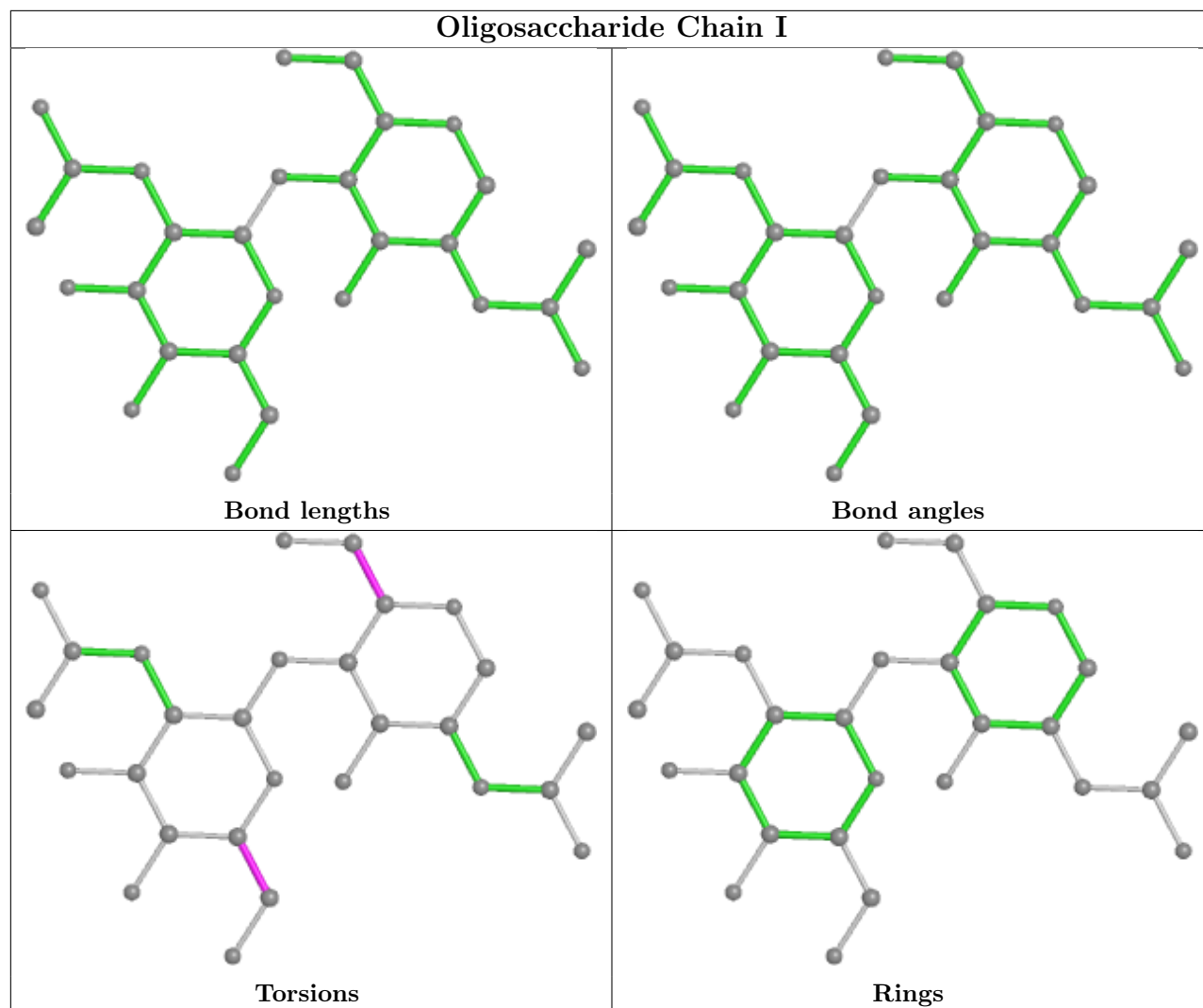
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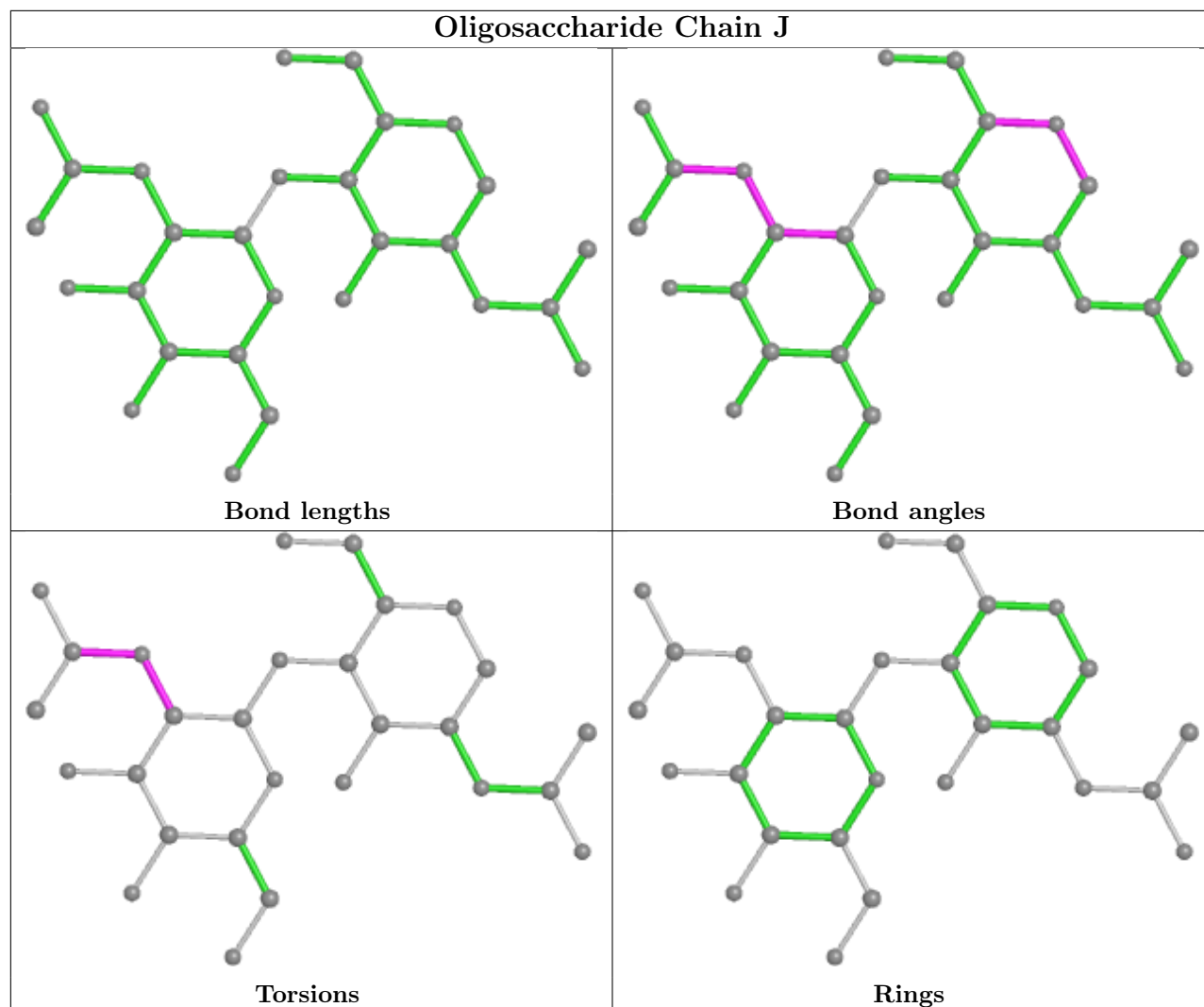
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	2	NAG	1	0
4	V	1	NAG	1	0
4	L	1	NAG	1	0
4	N	2	NAG	1	0
4	N	1	NAG	1	0
4	J	2	NAG	1	0
4	H	1	NAG	1	0
4	O	1	NAG	2	0

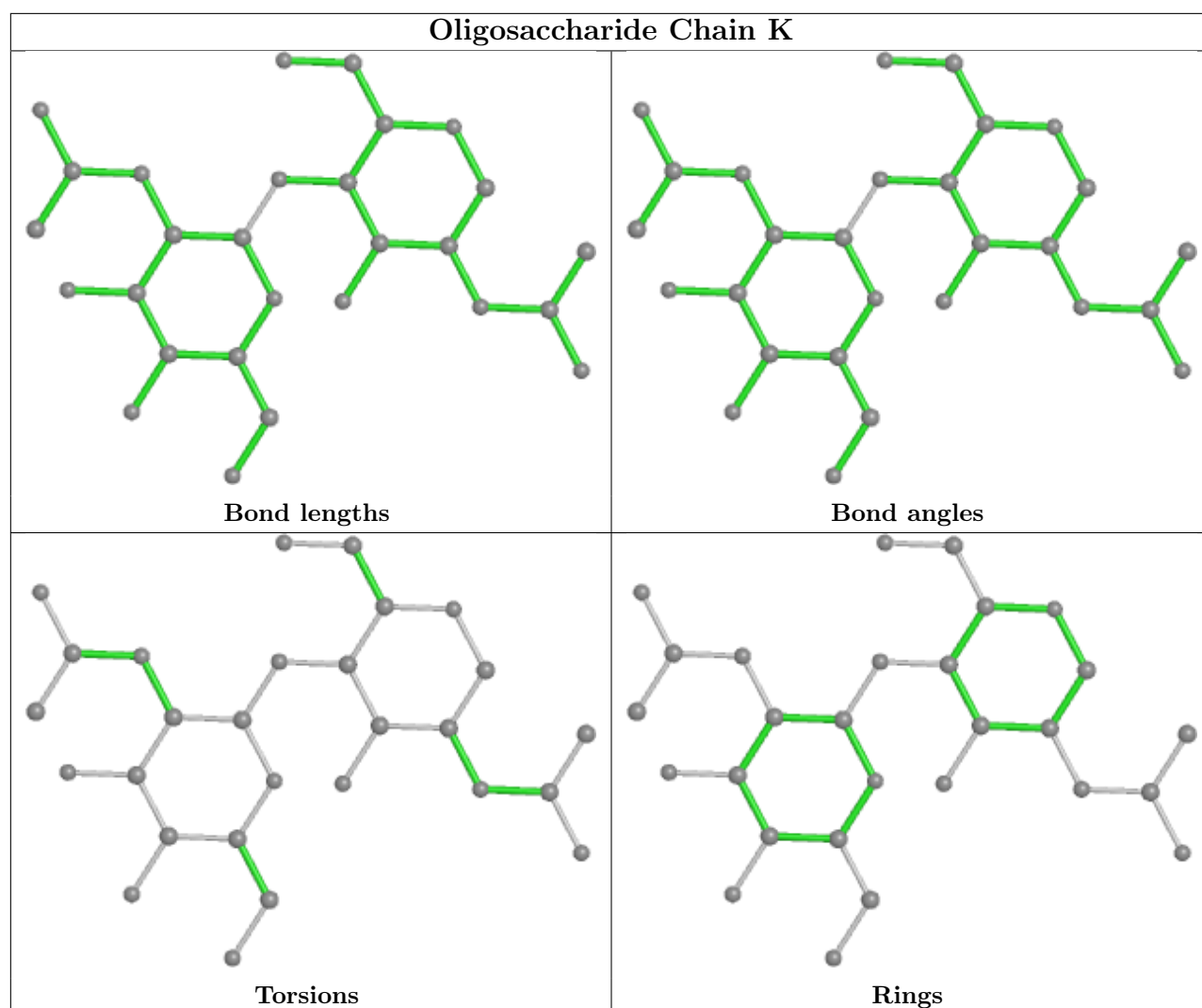
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

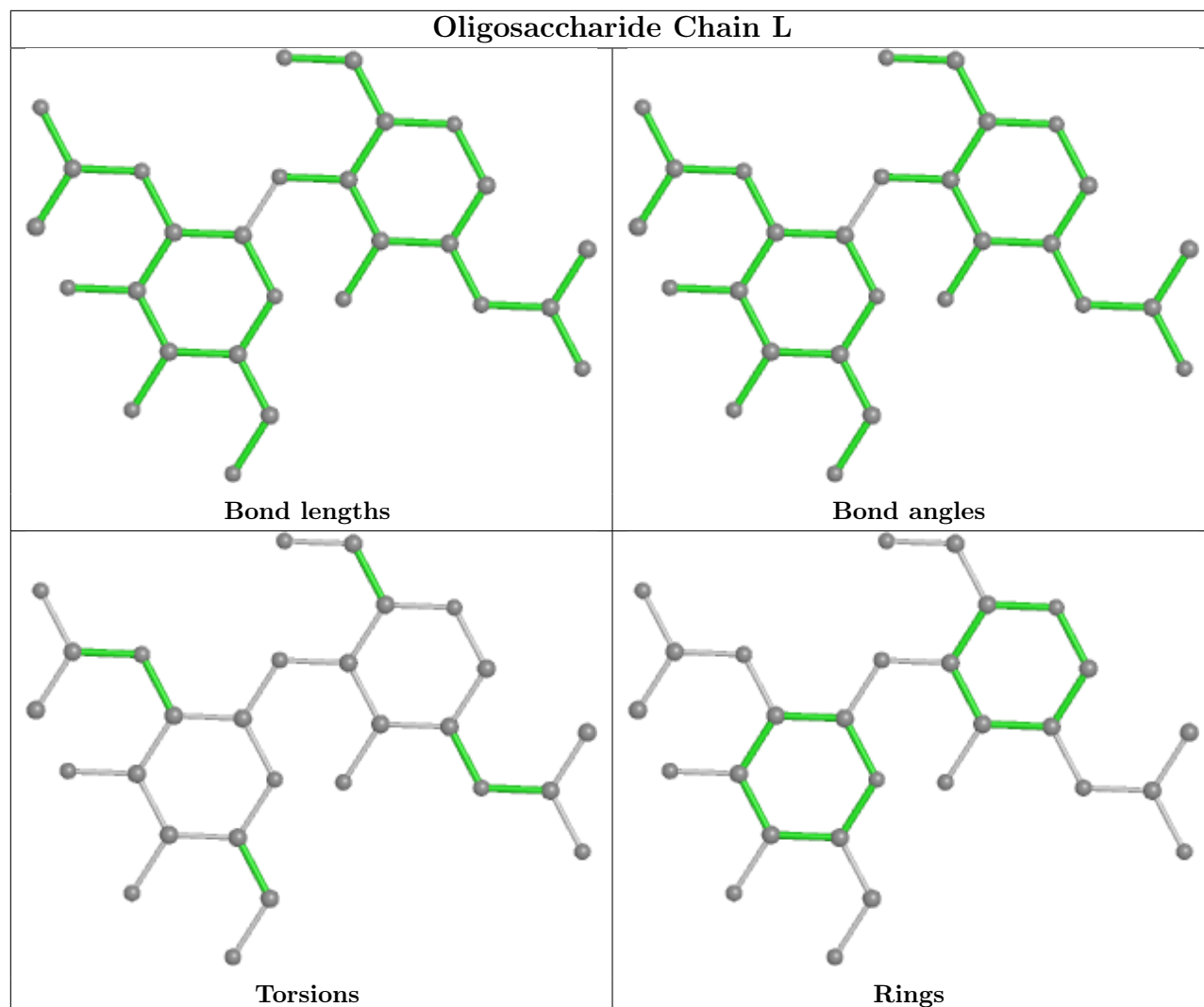


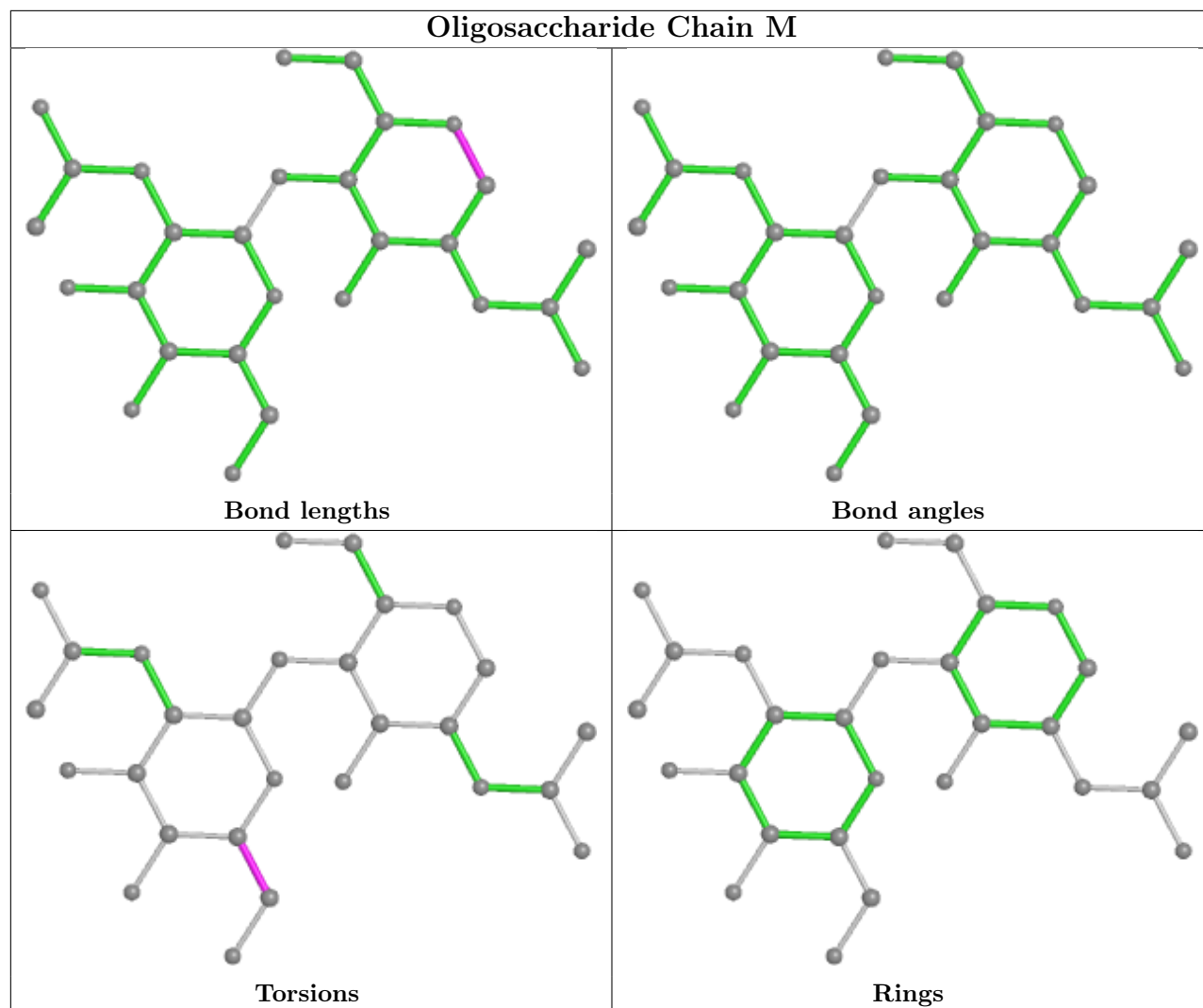




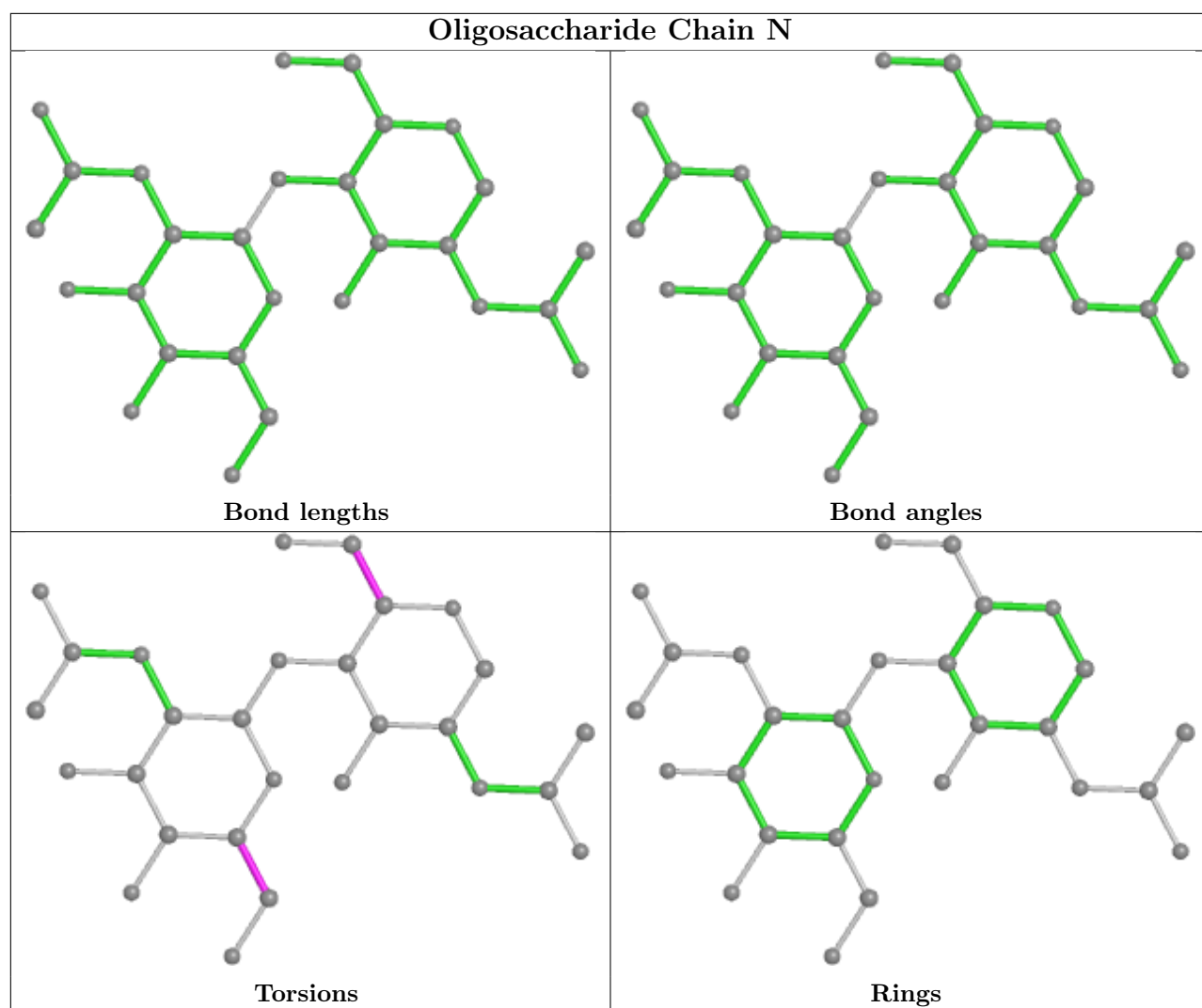


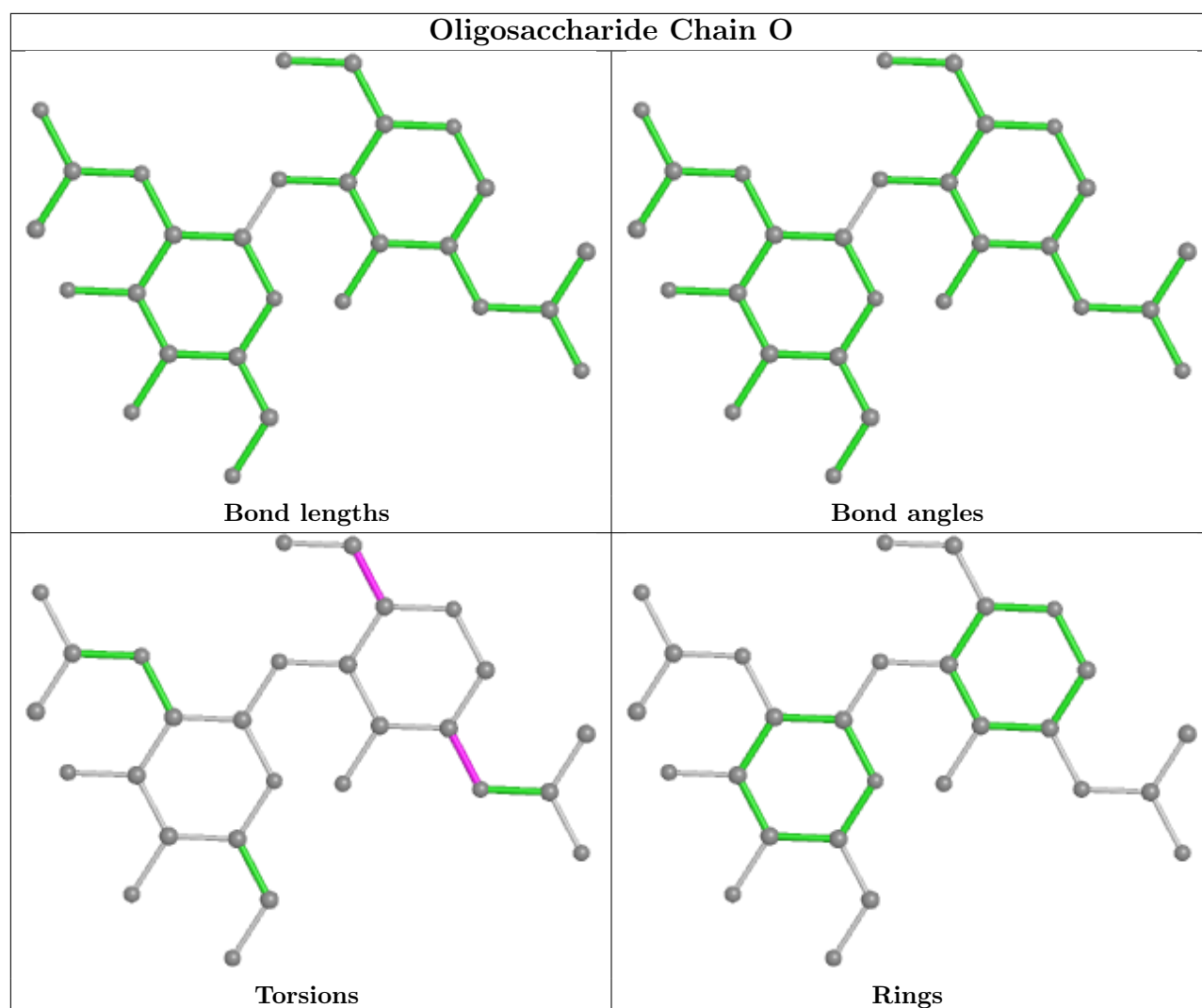


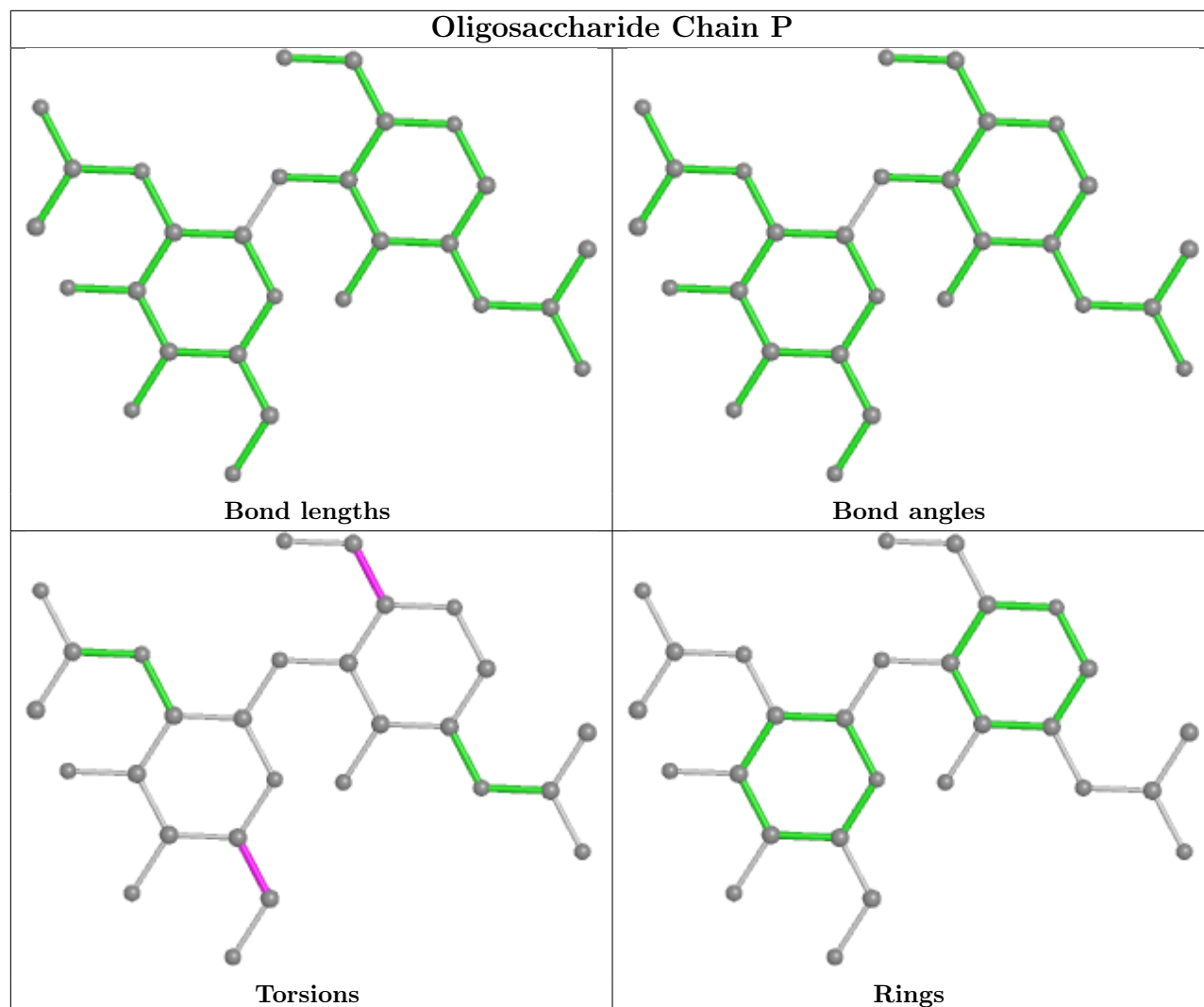


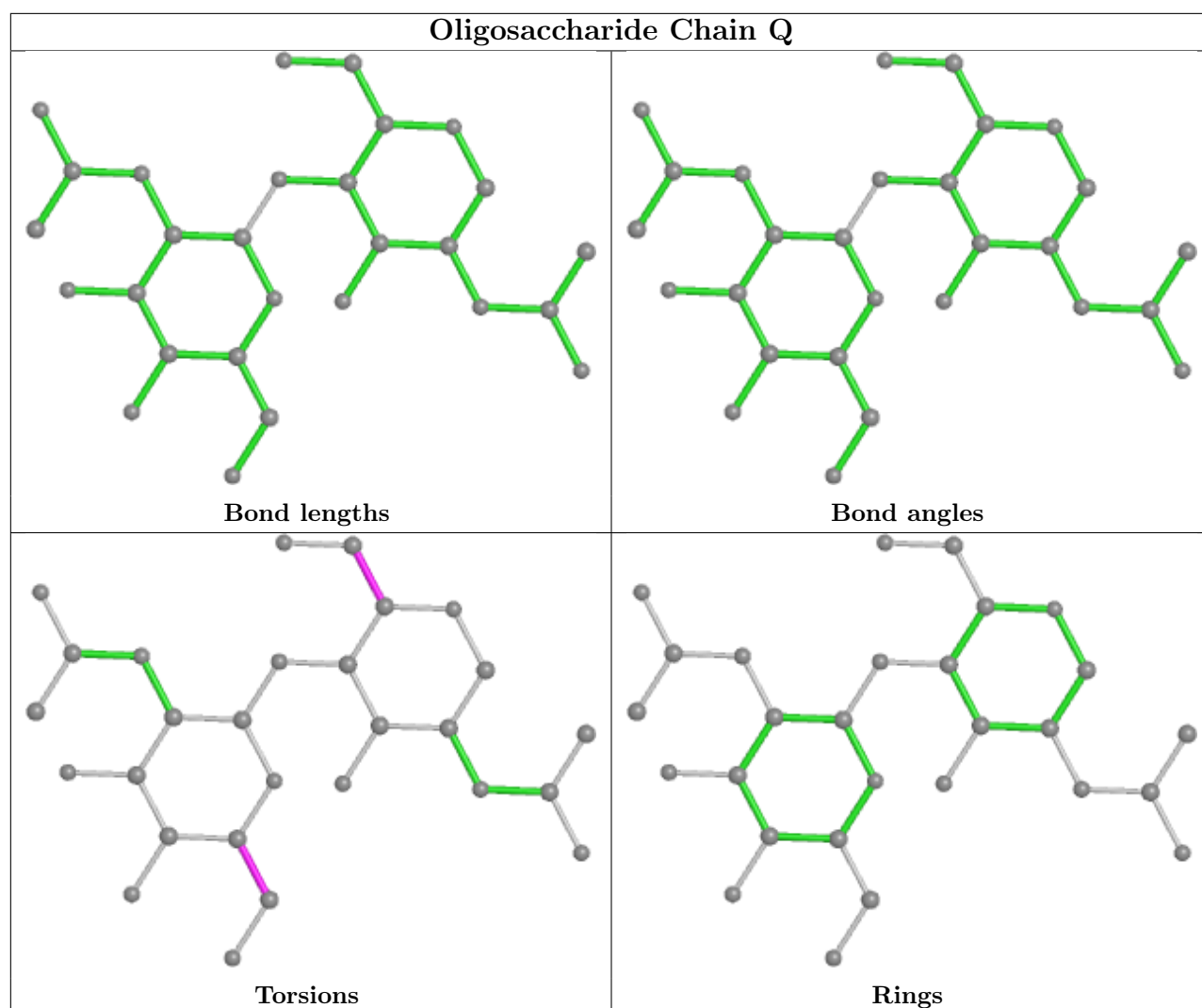


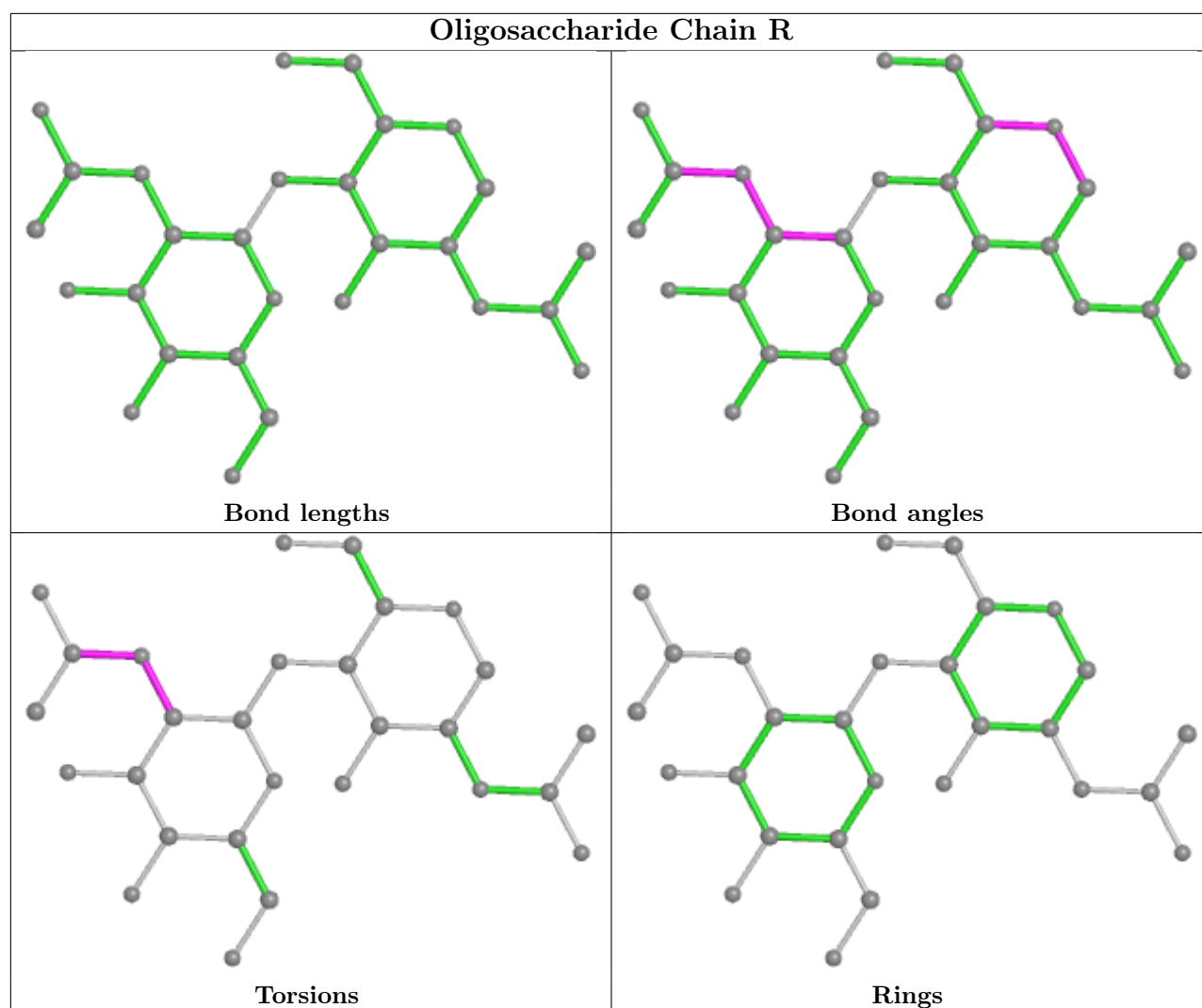


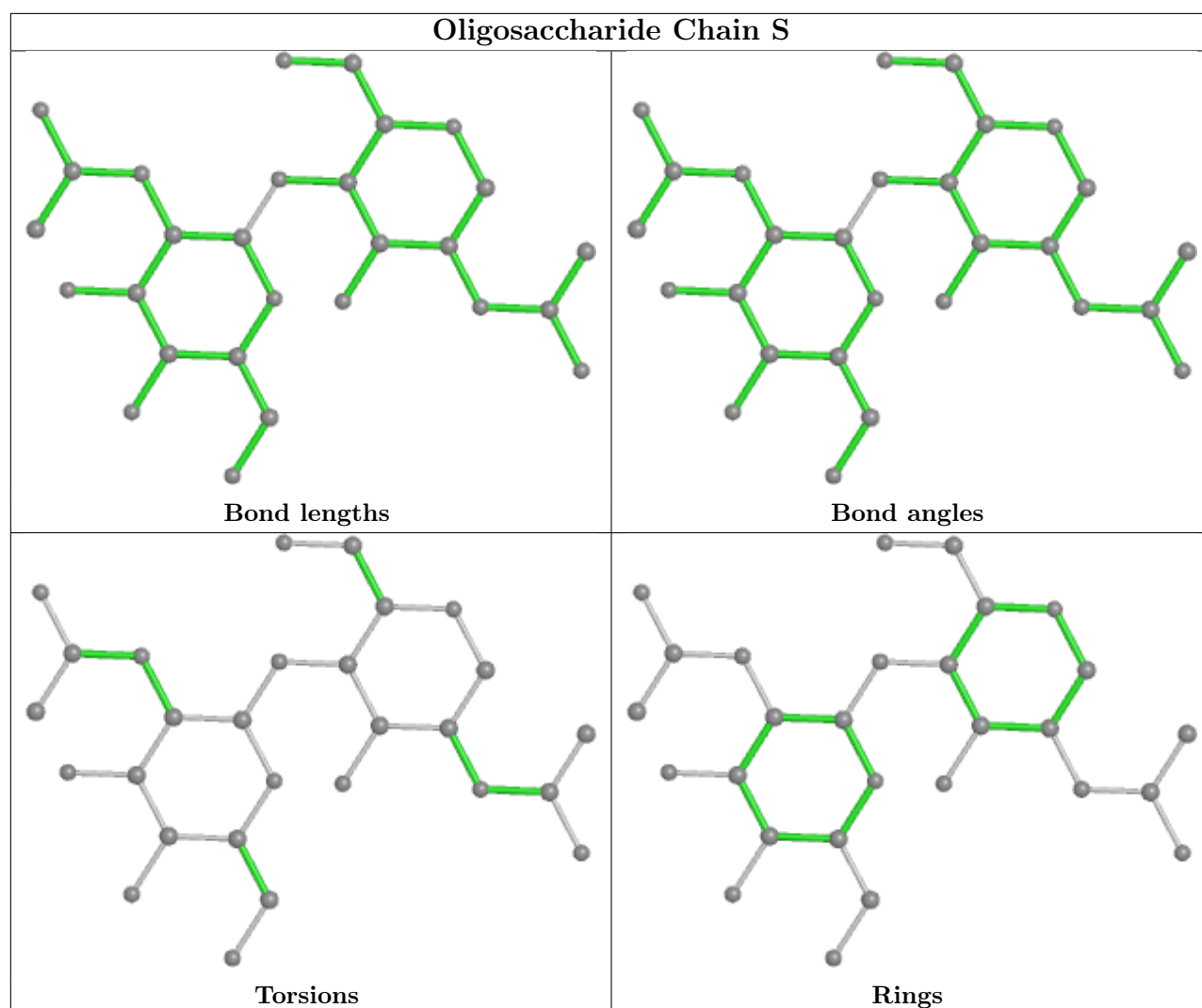


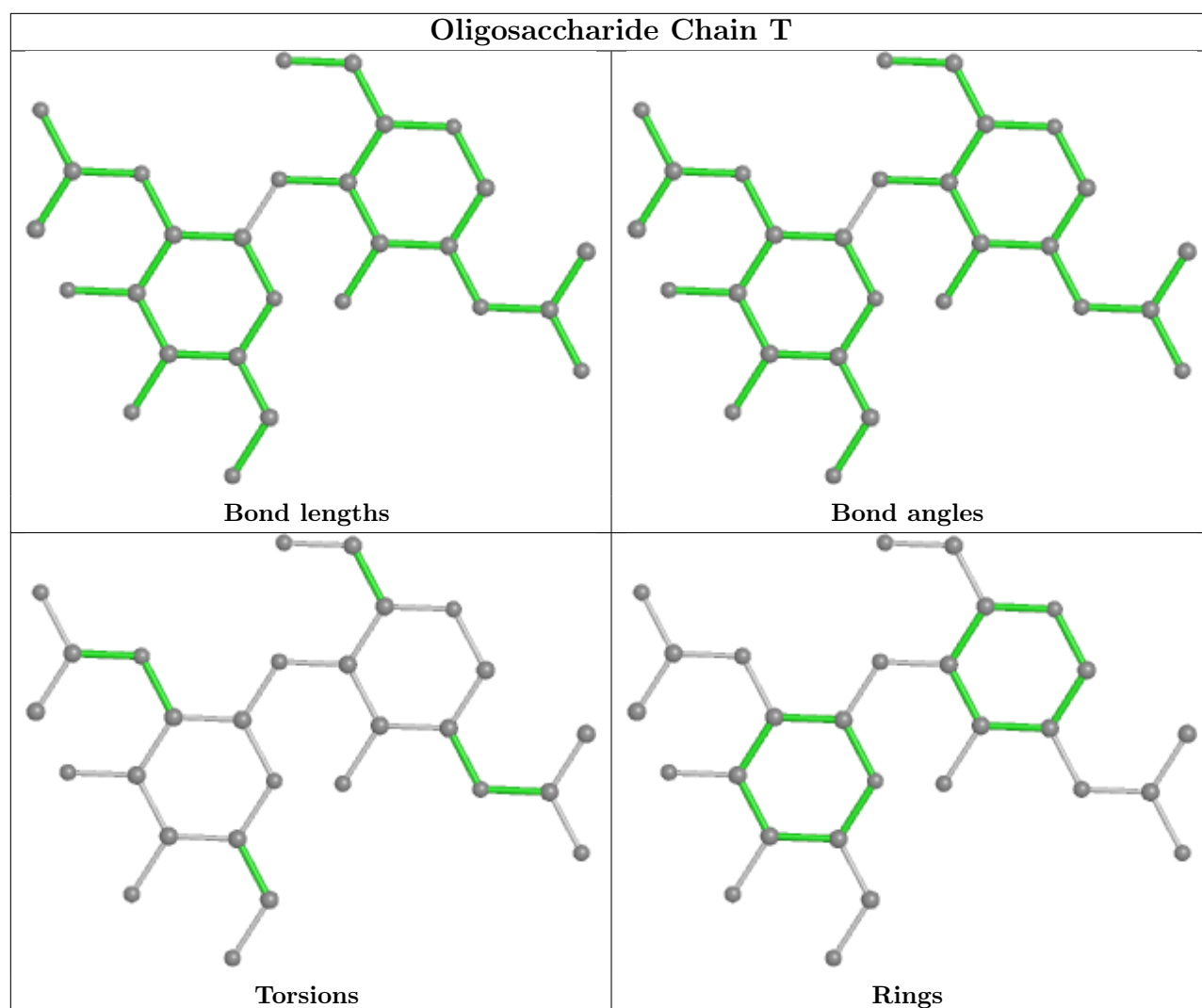


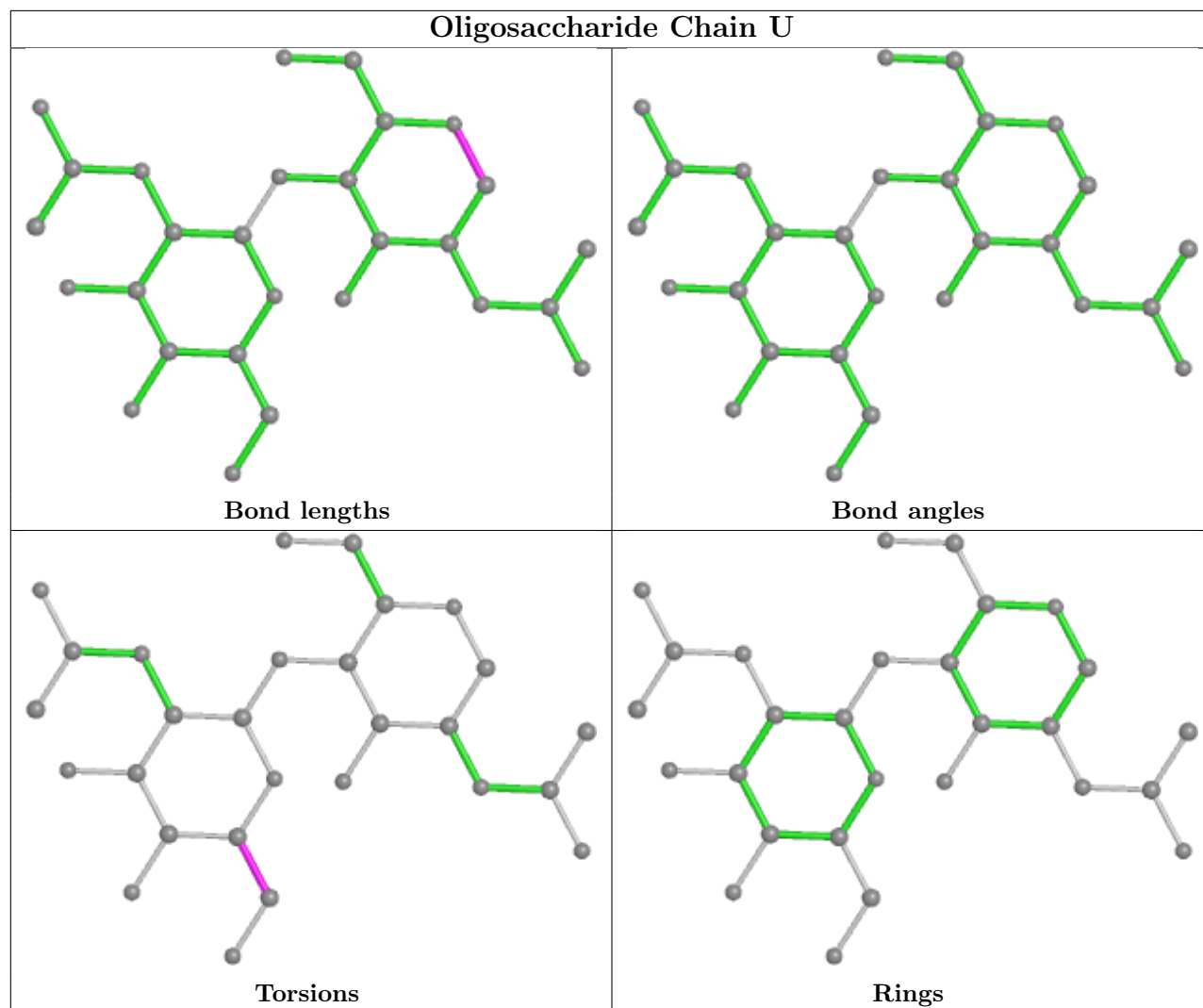




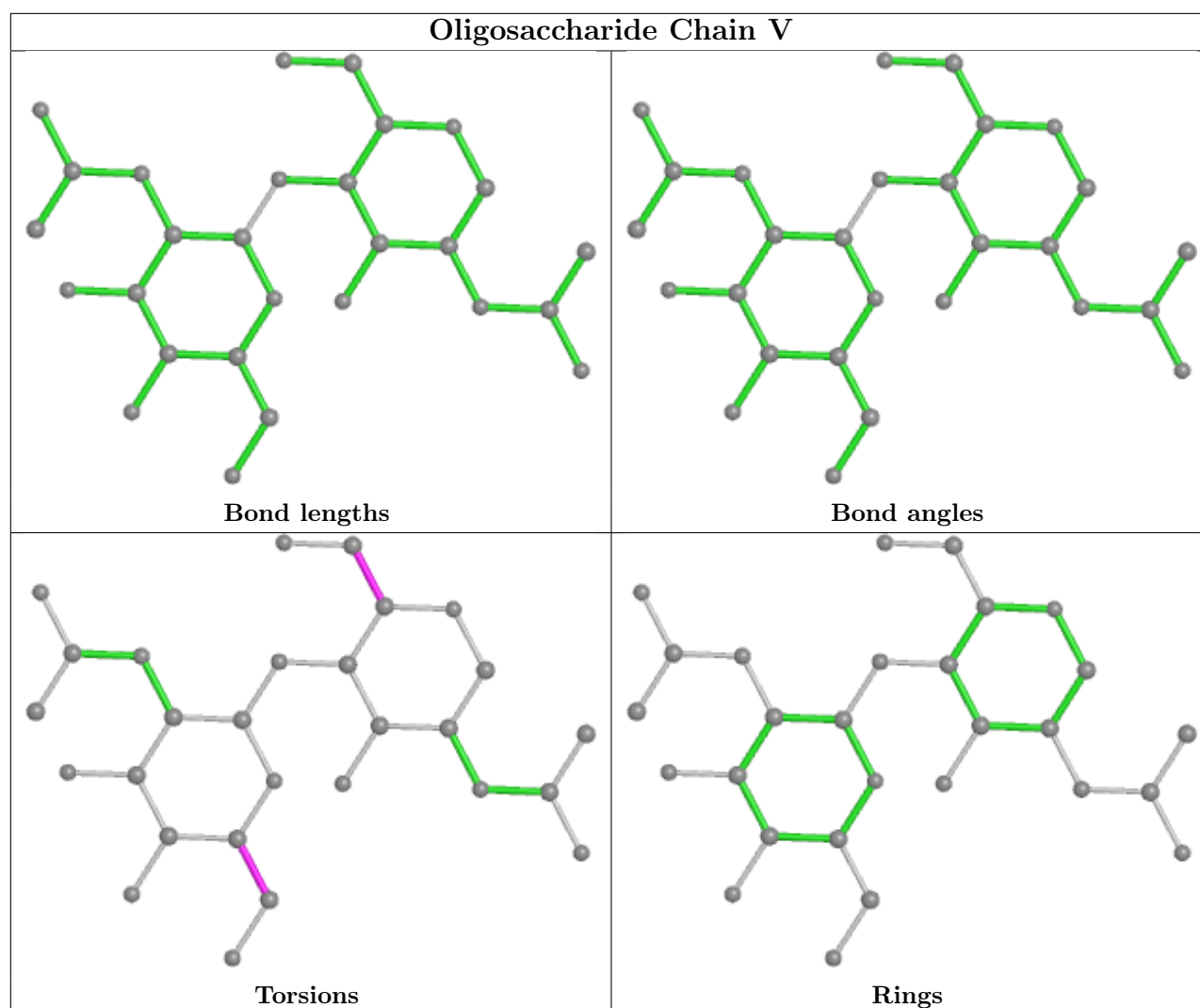












## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z  > 2$
6	3PH	B	1005	-	47,47,47	0.95	2 (4%)	51,52,52	1.10	3 (5%)
5	NAG	B	1002	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	D	1002	1	14,14,15	0.26	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	1001	1	14,14,15	0.28	0	17,19,21	0.35	0
6	3PH	B	1003	-	47,47,47	0.96	2 (4%)	51,52,52	1.09	2 (3%)
6	3PH	D	1003	-	47,47,47	0.96	2 (4%)	51,52,52	1.10	2 (3%)
5	NAG	A	901	2	14,14,15	0.21	0	17,19,21	0.53	0
6	3PH	D	1005	-	47,47,47	0.96	2 (4%)	51,52,52	1.10	3 (5%)
6	3PH	D	1004	-	47,47,47	0.95	2 (4%)	51,52,52	1.11	3 (5%)
5	NAG	B	1001	1	14,14,15	0.28	0	17,19,21	0.35	0
5	NAG	C	901	2	14,14,15	0.20	0	17,19,21	0.53	0
6	3PH	B	1004	-	47,47,47	0.95	2 (4%)	51,52,52	1.11	3 (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
6	3PH	B	1005	-	-	29/49/49/49	-
5	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
6	3PH	B	1003	-	-	32/49/49/49	-
6	3PH	D	1003	-	-	32/49/49/49	-
5	NAG	A	901	2	-	0/6/23/26	0/1/1/1
6	3PH	D	1005	-	-	31/49/49/49	-
6	3PH	D	1004	-	-	33/49/49/49	-
5	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
5	NAG	C	901	2	-	0/6/23/26	0/1/1/1
6	3PH	B	1004	-	-	33/49/49/49	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1003	3PH	O31-C31	4.33	1.46	1.33
6	D	1003	3PH	O31-C31	4.32	1.46	1.33
6	D	1005	3PH	O31-C31	4.31	1.45	1.33
6	B	1005	3PH	O31-C31	4.30	1.45	1.33
6	B	1004	3PH	O31-C31	4.24	1.45	1.33
6	D	1004	3PH	O31-C31	4.22	1.45	1.33
6	D	1003	3PH	O21-C21	4.17	1.46	1.34
6	B	1003	3PH	O21-C21	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1004	3PH	O21-C21	4.13	1.46	1.34
6	B	1004	3PH	O21-C21	4.10	1.45	1.34
6	D	1005	3PH	O21-C21	4.10	1.45	1.34
6	B	1005	3PH	O21-C21	4.06	1.45	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1003	3PH	O21-C21-C22	4.26	120.68	111.50
6	B	1003	3PH	O21-C21-C22	4.25	120.65	111.50
6	D	1004	3PH	O21-C21-C22	4.18	120.50	111.50
6	B	1004	3PH	O21-C21-C22	4.16	120.47	111.50
6	B	1005	3PH	O21-C21-C22	4.03	120.18	111.50
6	D	1005	3PH	O21-C21-C22	4.00	120.13	111.50
6	D	1003	3PH	O31-C31-C32	2.72	120.43	111.91
6	B	1004	3PH	O31-C31-C32	2.69	120.36	111.91
6	B	1003	3PH	O31-C31-C32	2.69	120.35	111.91
6	D	1004	3PH	O31-C31-C32	2.69	120.35	111.91
6	D	1005	3PH	O31-C31-C32	2.63	120.16	111.91
6	B	1005	3PH	O31-C31-C32	2.62	120.14	111.91
6	D	1005	3PH	C2-O21-C21	-2.45	111.76	117.79
6	B	1005	3PH	C2-O21-C21	-2.44	111.79	117.79
6	D	1004	3PH	C2-O21-C21	-2.12	112.58	117.79
6	B	1004	3PH	C2-O21-C21	-2.11	112.58	117.79

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1003	3PH	C1-O11-P-O13
6	B	1003	3PH	C1-O11-P-O14
6	B	1003	3PH	O22-C21-O21-C2
6	B	1004	3PH	C1-O11-P-O13
6	B	1004	3PH	C1-O11-P-O14
6	B	1004	3PH	C1-O11-P-O12
6	B	1004	3PH	C22-C21-O21-C2
6	B	1005	3PH	C1-O11-P-O13
6	B	1005	3PH	C1-O11-P-O14
6	B	1005	3PH	C1-O11-P-O12
6	D	1003	3PH	C1-O11-P-O13
6	D	1003	3PH	C1-O11-P-O14
6	D	1003	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
6	D	1004	3PH	C1-O11-P-O13
6	D	1004	3PH	C1-O11-P-O14
6	D	1004	3PH	C1-O11-P-O12
6	D	1004	3PH	C22-C21-O21-C2
6	D	1005	3PH	C1-O11-P-O13
6	D	1005	3PH	C1-O11-P-O14
6	D	1005	3PH	C1-O11-P-O12
6	B	1004	3PH	O22-C21-O21-C2
6	D	1004	3PH	O22-C21-O21-C2
6	B	1003	3PH	C22-C21-O21-C2
6	D	1003	3PH	C22-C21-O21-C2
6	B	1003	3PH	C32-C31-O31-C3
6	D	1003	3PH	C32-C31-O31-C3
6	B	1003	3PH	C21-C22-C23-C24
6	D	1003	3PH	C21-C22-C23-C24
6	B	1003	3PH	C31-C32-C33-C34
6	B	1005	3PH	C31-C32-C33-C34
6	D	1005	3PH	C31-C32-C33-C34
6	B	1004	3PH	C31-C32-C33-C34
6	D	1003	3PH	C31-C32-C33-C34
6	D	1004	3PH	C31-C32-C33-C34
6	B	1003	3PH	O32-C31-O31-C3
6	D	1003	3PH	O32-C31-O31-C3
6	B	1005	3PH	C22-C21-O21-C2
6	D	1005	3PH	C22-C21-O21-C2
6	B	1005	3PH	O22-C21-O21-C2
6	B	1003	3PH	C29-C2A-C2B-C2C
6	D	1003	3PH	C29-C2A-C2B-C2C
6	D	1005	3PH	C3B-C3C-C3D-C3E
6	B	1004	3PH	C38-C39-C3A-C3B
6	D	1004	3PH	C38-C39-C3A-C3B
6	D	1005	3PH	O22-C21-O21-C2
6	B	1005	3PH	C3B-C3C-C3D-C3E
6	B	1004	3PH	C2D-C2E-C2F-C2G
6	D	1004	3PH	C2D-C2E-C2F-C2G
6	B	1005	3PH	C2C-C2D-C2E-C2F
6	B	1005	3PH	C3A-C3B-C3C-C3D
6	D	1003	3PH	C24-C25-C26-C27
6	D	1005	3PH	C3A-C3B-C3C-C3D
6	D	1005	3PH	C21-C22-C23-C24
6	B	1003	3PH	C24-C25-C26-C27
6	D	1005	3PH	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
6	B	1003	3PH	C22-C23-C24-C25
6	B	1004	3PH	C32-C33-C34-C35
6	D	1004	3PH	C32-C33-C34-C35
6	D	1003	3PH	C22-C23-C24-C25
6	B	1005	3PH	C21-C22-C23-C24
6	D	1004	3PH	C36-C37-C38-C39
6	B	1004	3PH	C33-C34-C35-C36
6	B	1004	3PH	C36-C37-C38-C39
6	D	1004	3PH	C33-C34-C35-C36
6	B	1003	3PH	C2A-C2B-C2C-C2D
6	B	1003	3PH	C33-C34-C35-C36
6	D	1003	3PH	C2A-C2B-C2C-C2D
6	D	1003	3PH	C33-C34-C35-C36
6	D	1005	3PH	C2E-C2F-C2G-C2H
6	B	1003	3PH	C32-C33-C34-C35
6	B	1003	3PH	C35-C36-C37-C38
6	B	1004	3PH	C37-C38-C39-C3A
6	B	1005	3PH	C2E-C2F-C2G-C2H
6	D	1003	3PH	C32-C33-C34-C35
6	D	1004	3PH	C37-C38-C39-C3A
6	D	1003	3PH	C35-C36-C37-C38
6	D	1005	3PH	C25-C26-C27-C28
6	B	1005	3PH	C25-C26-C27-C28
6	B	1003	3PH	C36-C37-C38-C39
6	D	1003	3PH	C36-C37-C38-C39
6	D	1003	3PH	C3C-C3D-C3E-C3F
6	B	1003	3PH	C3C-C3D-C3E-C3F
6	D	1003	3PH	C28-C29-C2A-C2B
6	B	1003	3PH	C28-C29-C2A-C2B
6	D	1005	3PH	C39-C3A-C3B-C3C
6	B	1005	3PH	C2-C1-O11-P
6	D	1005	3PH	C2-C1-O11-P
6	B	1003	3PH	C2D-C2E-C2F-C2G
6	D	1003	3PH	C2D-C2E-C2F-C2G
6	B	1004	3PH	C2C-C2D-C2E-C2F
6	D	1004	3PH	C2C-C2D-C2E-C2F
6	B	1003	3PH	C27-C28-C29-C2A
6	B	1004	3PH	C3D-C3E-C3F-C3G
6	D	1003	3PH	C27-C28-C29-C2A
6	B	1005	3PH	C39-C3A-C3B-C3C
6	D	1004	3PH	C3D-C3E-C3F-C3G
6	B	1003	3PH	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
6	B	1004	3PH	C1-C2-C3-O31
6	D	1003	3PH	C1-C2-C3-O31
6	D	1004	3PH	C1-C2-C3-O31
6	B	1003	3PH	C2F-C2G-C2H-C2I
6	D	1003	3PH	C2F-C2G-C2H-C2I
6	B	1004	3PH	C27-C28-C29-C2A
6	D	1004	3PH	C27-C28-C29-C2A
6	D	1003	3PH	C2B-C2C-C2D-C2E
6	B	1003	3PH	C2B-C2C-C2D-C2E
6	B	1003	3PH	C37-C38-C39-C3A
6	D	1003	3PH	C37-C38-C39-C3A
6	B	1003	3PH	C1-O11-P-O12
6	D	1003	3PH	C1-O11-P-O12
6	B	1003	3PH	C3A-C3B-C3C-C3D
6	D	1003	3PH	C3A-C3B-C3C-C3D
6	D	1005	3PH	C2A-C2B-C2C-C2D
6	B	1004	3PH	C23-C24-C25-C26
6	B	1005	3PH	C2A-C2B-C2C-C2D
6	D	1004	3PH	C23-C24-C25-C26
6	B	1005	3PH	C26-C27-C28-C29
6	D	1005	3PH	C26-C27-C28-C29
6	B	1004	3PH	C22-C23-C24-C25
6	D	1004	3PH	C22-C23-C24-C25
6	D	1004	3PH	C3B-C3C-C3D-C3E
6	B	1004	3PH	C3B-C3C-C3D-C3E
6	B	1003	3PH	C26-C27-C28-C29
6	D	1003	3PH	C26-C27-C28-C29
6	B	1003	3PH	O21-C2-C3-O31
6	D	1003	3PH	O21-C2-C3-O31
6	D	1004	3PH	C26-C27-C28-C29
6	B	1004	3PH	C26-C27-C28-C29
6	D	1003	3PH	C2C-C2D-C2E-C2F
6	B	1003	3PH	C2C-C2D-C2E-C2F
6	D	1005	3PH	C36-C37-C38-C39
6	D	1005	3PH	C22-C23-C24-C25
6	B	1005	3PH	C22-C23-C24-C25
6	B	1004	3PH	C34-C35-C36-C37
6	D	1004	3PH	C34-C35-C36-C37
6	B	1004	3PH	O21-C2-C3-O31
6	D	1004	3PH	O21-C2-C3-O31
6	D	1004	3PH	C2B-C2C-C2D-C2E
6	D	1005	3PH	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
6	B	1004	3PH	C2B-C2C-C2D-C2E
6	B	1005	3PH	C29-C2A-C2B-C2C
6	D	1005	3PH	C2F-C2G-C2H-C2I
6	B	1005	3PH	C2F-C2G-C2H-C2I
6	D	1005	3PH	C34-C35-C36-C37
6	B	1003	3PH	C3D-C3E-C3F-C3G
6	D	1003	3PH	C3D-C3E-C3F-C3G
6	B	1005	3PH	C34-C35-C36-C37
6	D	1005	3PH	C32-C33-C34-C35
6	B	1005	3PH	C24-C25-C26-C27
6	D	1005	3PH	C24-C25-C26-C27
6	D	1005	3PH	C3F-C3G-C3H-C3I
6	B	1004	3PH	C3F-C3G-C3H-C3I
6	D	1004	3PH	C3F-C3G-C3H-C3I
6	B	1003	3PH	C2E-C2F-C2G-C2H
6	D	1003	3PH	C2E-C2F-C2G-C2H
6	D	1004	3PH	C3C-C3D-C3E-C3F
6	B	1004	3PH	C3C-C3D-C3E-C3F
6	B	1004	3PH	C39-C3A-C3B-C3C
6	D	1004	3PH	C39-C3A-C3B-C3C
6	B	1005	3PH	C32-C33-C34-C35
6	D	1005	3PH	C27-C28-C29-C2A
6	B	1005	3PH	C27-C28-C29-C2A
6	D	1005	3PH	C2B-C2C-C2D-C2E
6	B	1005	3PH	C36-C37-C38-C39
6	B	1004	3PH	C3E-C3F-C3G-C3H
6	D	1004	3PH	C3E-C3F-C3G-C3H
6	B	1005	3PH	C2B-C2C-C2D-C2E
6	D	1003	3PH	C3F-C3G-C3H-C3I
6	B	1003	3PH	C3F-C3G-C3H-C3I
6	B	1004	3PH	C25-C26-C27-C28
6	D	1004	3PH	C25-C26-C27-C28
6	D	1005	3PH	C35-C36-C37-C38
6	D	1004	3PH	C28-C29-C2A-C2B
6	B	1004	3PH	C28-C29-C2A-C2B
6	B	1004	3PH	O21-C21-C22-C23
6	D	1004	3PH	O21-C21-C22-C23
6	D	1005	3PH	C23-C24-C25-C26
6	B	1005	3PH	C23-C24-C25-C26
6	D	1005	3PH	C28-C29-C2A-C2B
6	B	1004	3PH	C2A-C2B-C2C-C2D
6	B	1005	3PH	C28-C29-C2A-C2B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	1004	3PH	C2A-C2B-C2C-C2D
6	B	1004	3PH	O22-C21-C22-C23
6	D	1004	3PH	O22-C21-C22-C23
6	B	1005	3PH	O21-C21-C22-C23
6	D	1005	3PH	O21-C21-C22-C23
6	B	1004	3PH	C29-C2A-C2B-C2C
6	B	1005	3PH	O22-C21-C22-C23
6	D	1004	3PH	C29-C2A-C2B-C2C
6	D	1005	3PH	O22-C21-C22-C23

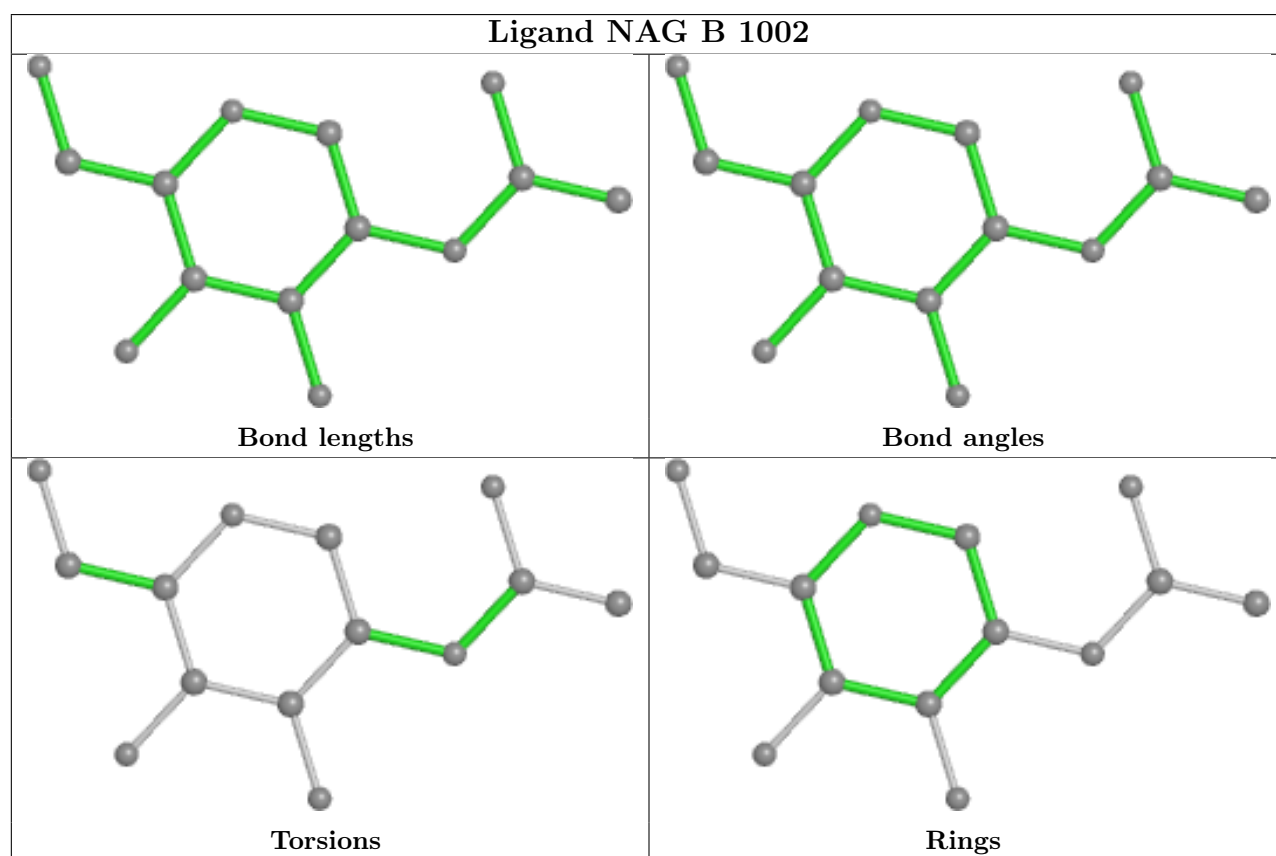
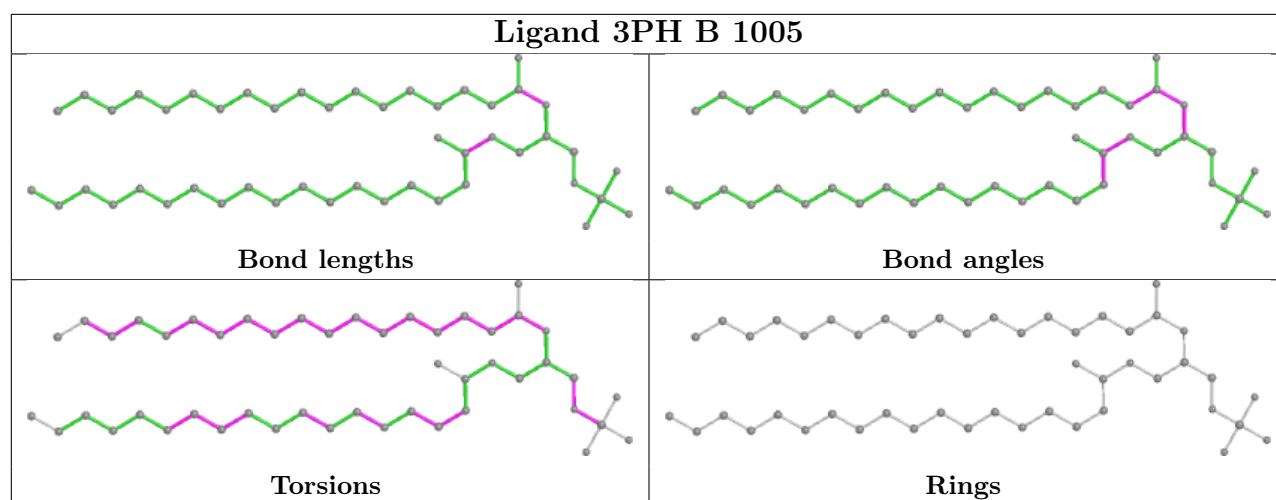
There are no ring outliers.

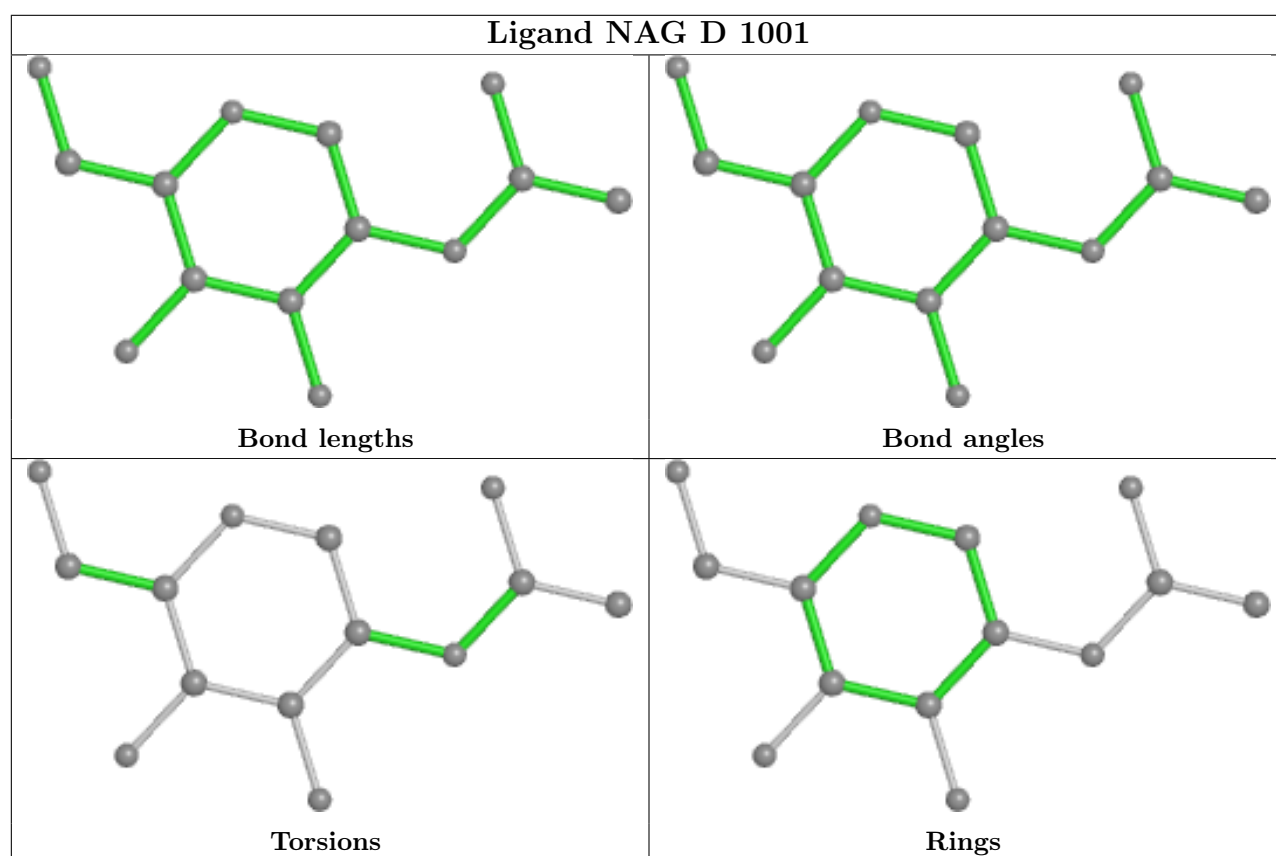
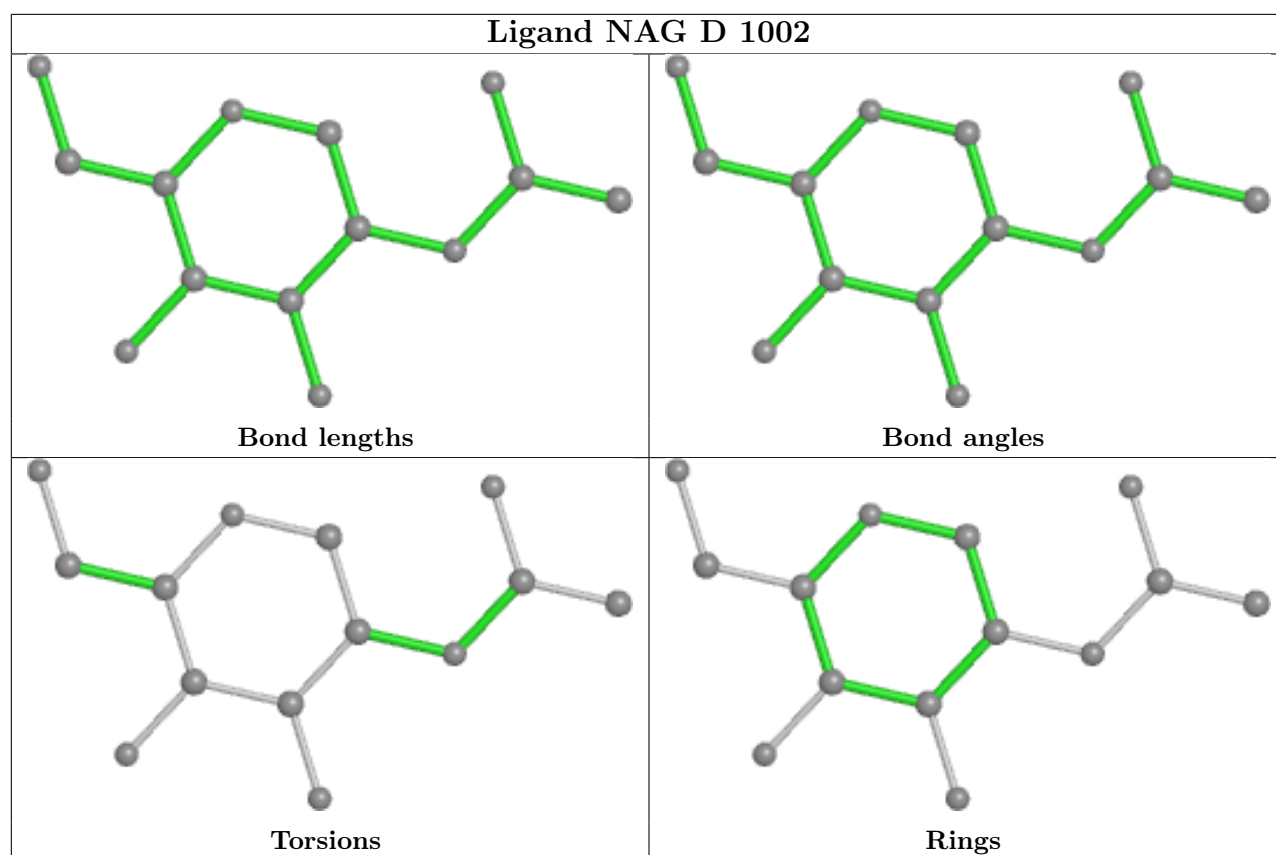
5 monomers are involved in 35 short contacts:

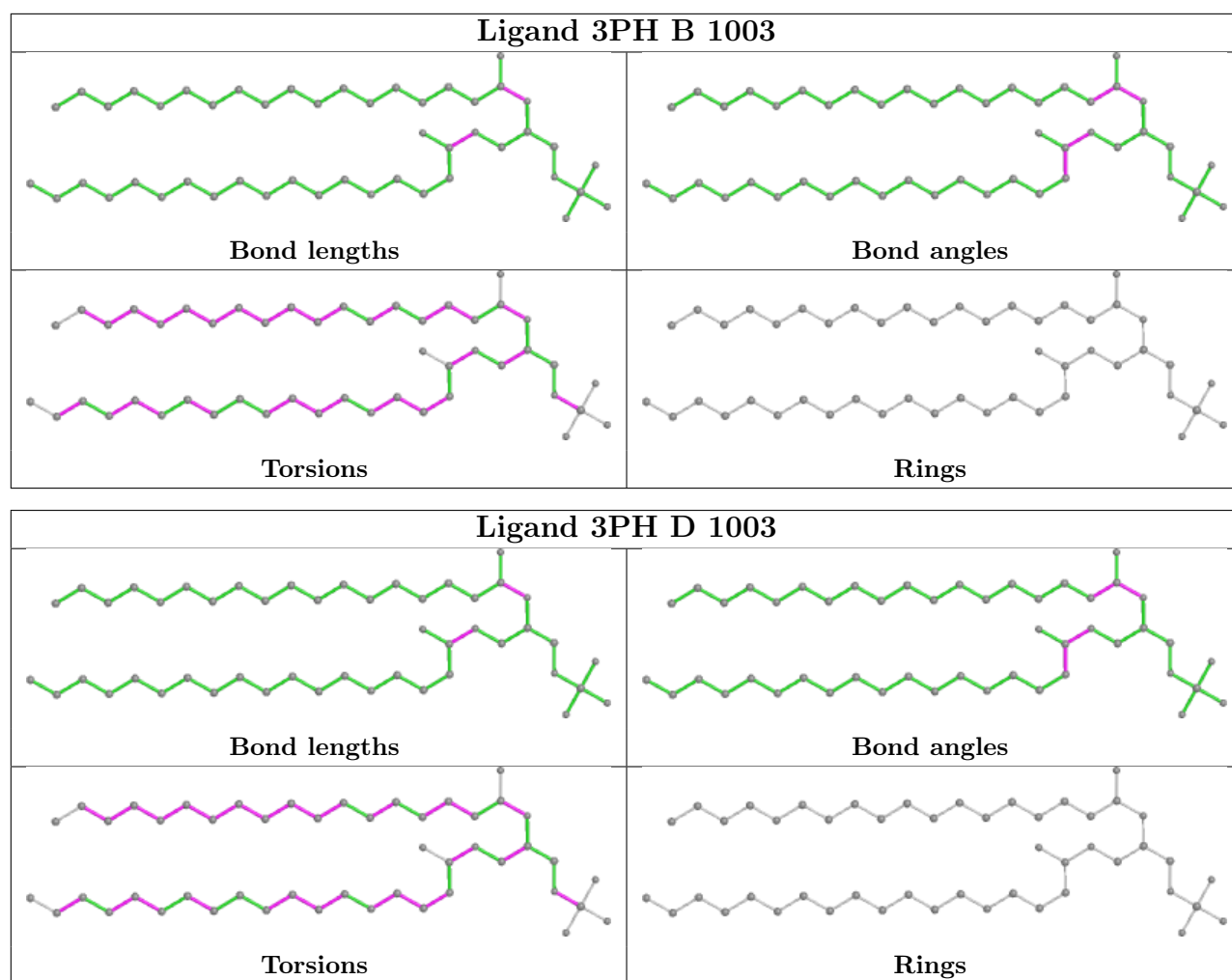
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1005	3PH	10	0
6	B	1003	3PH	1	0
6	D	1005	3PH	10	0
6	D	1004	3PH	7	0
6	B	1004	3PH	7	0

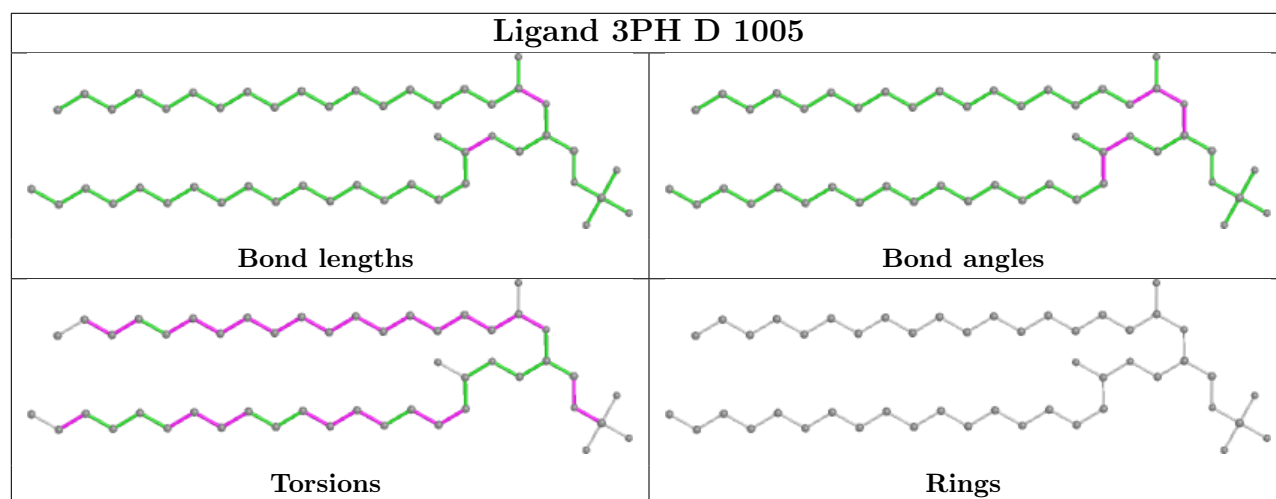
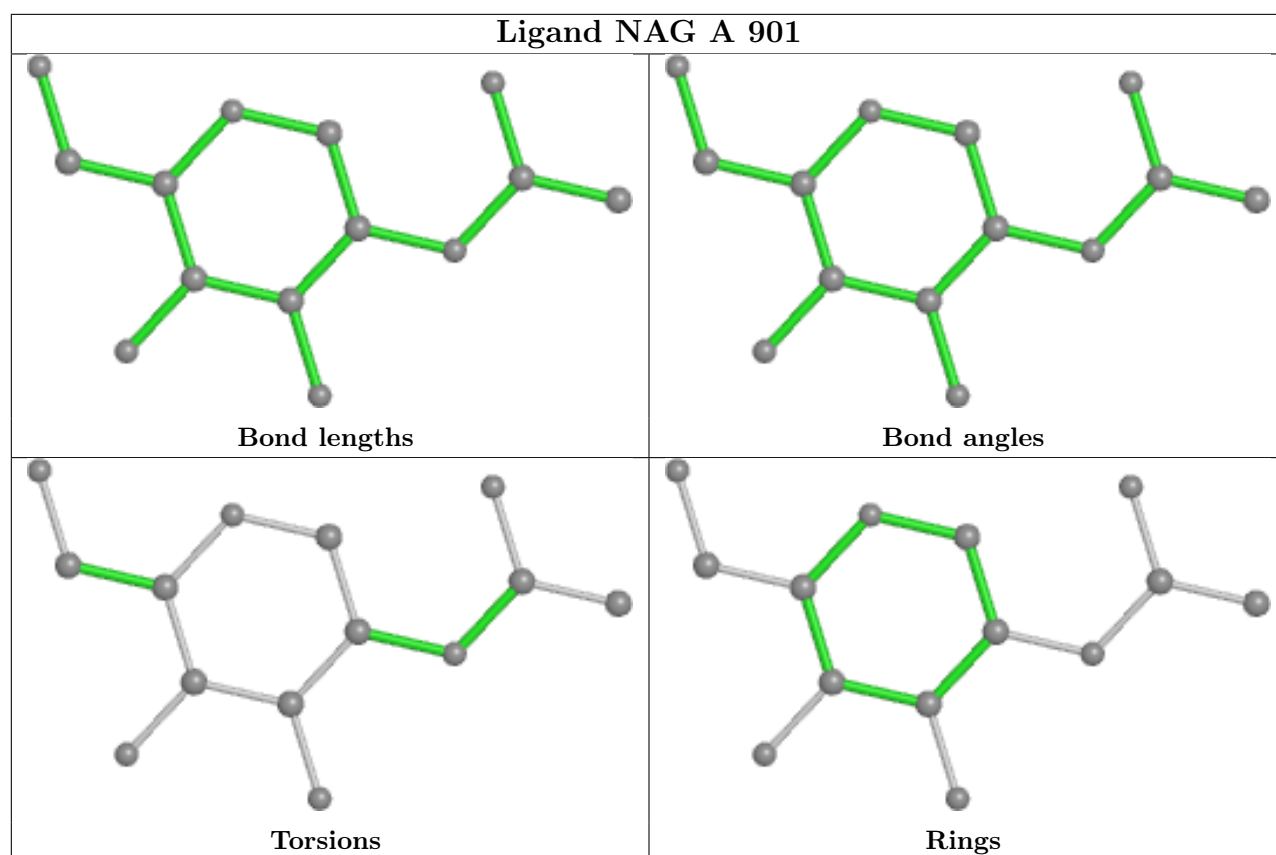
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

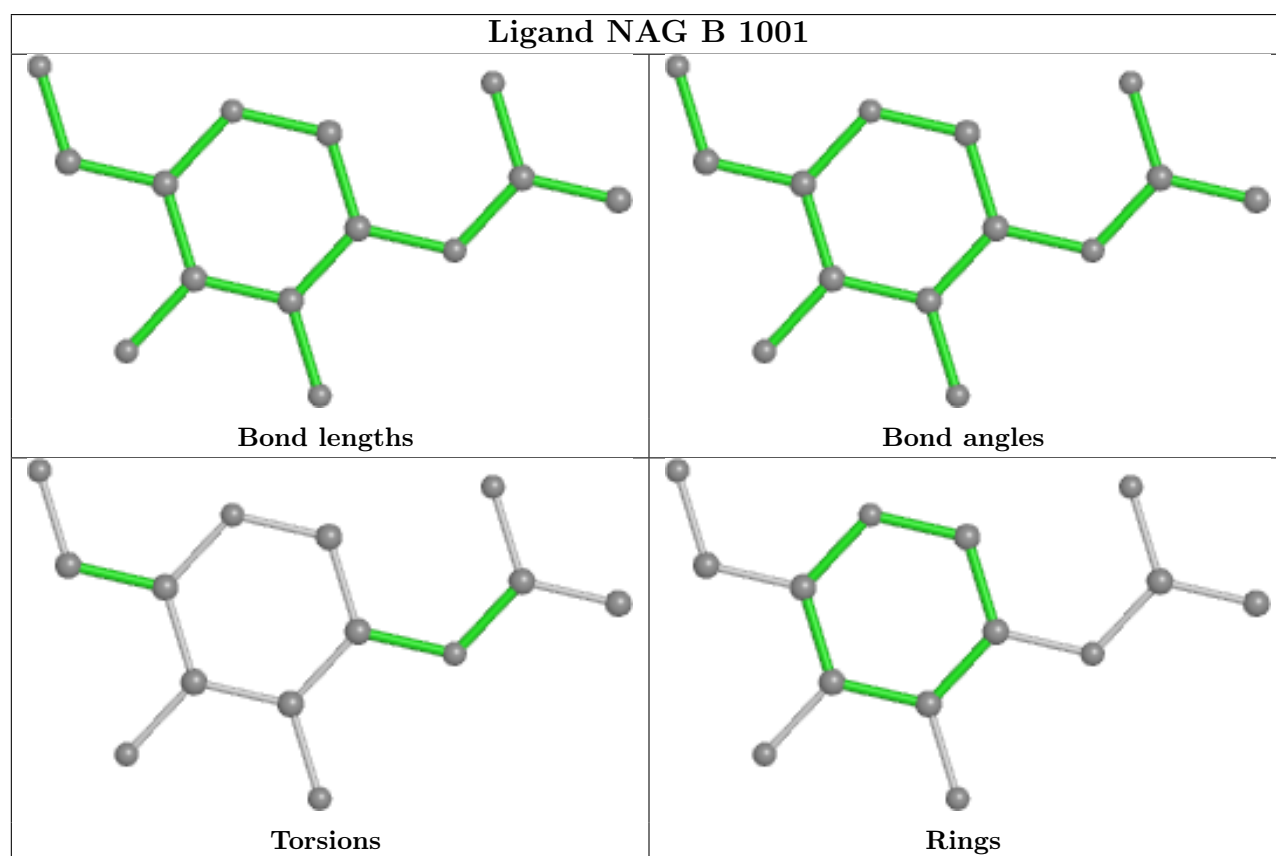
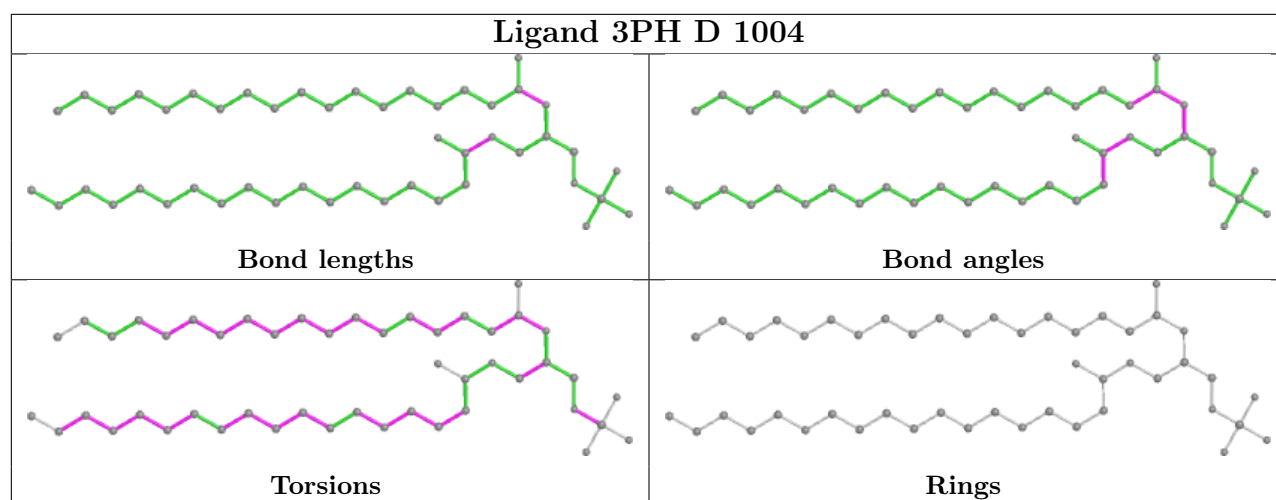


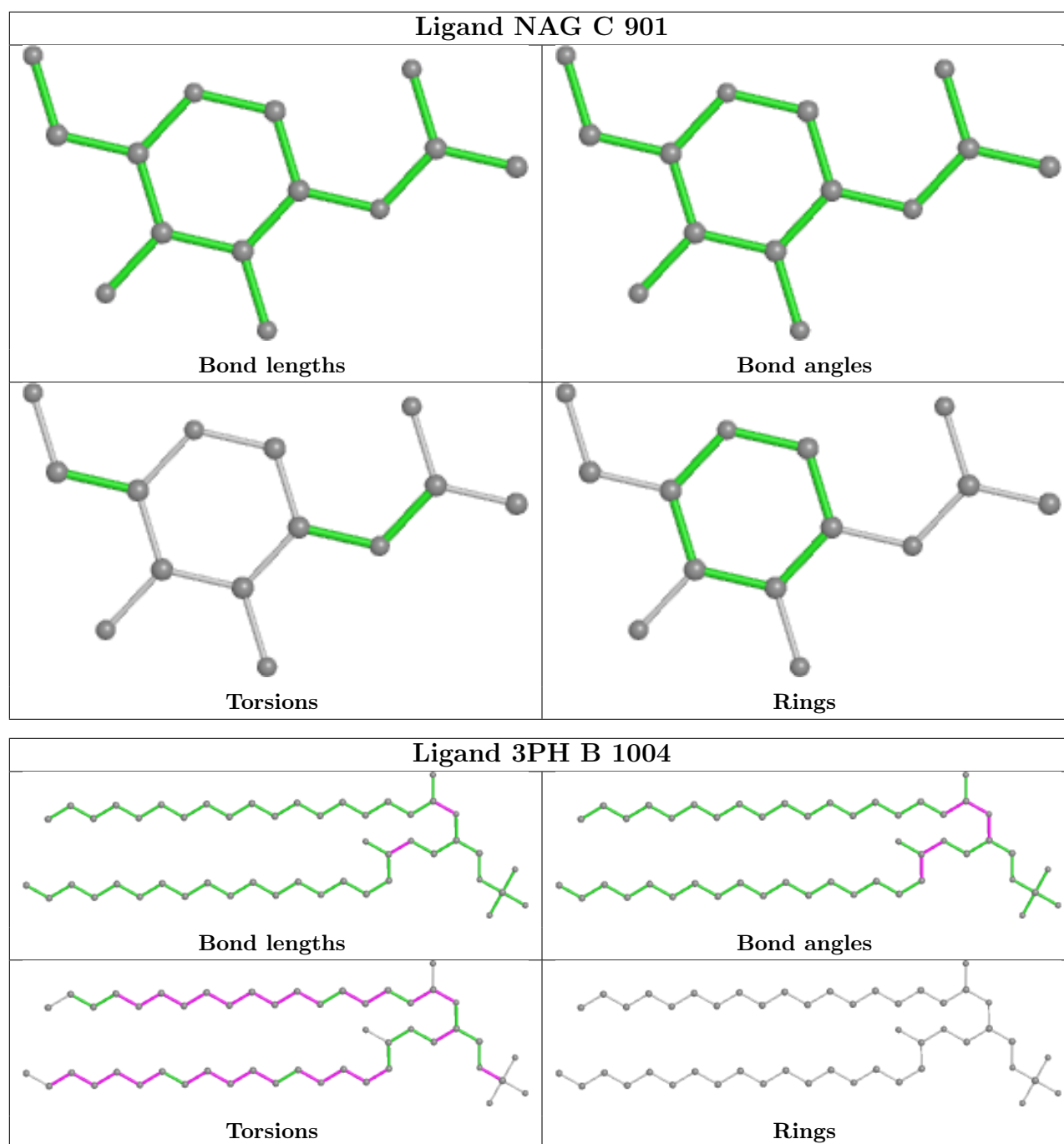












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

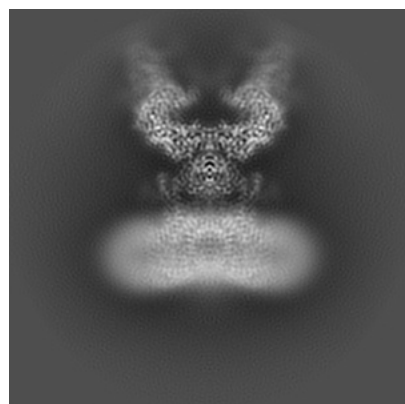
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33652. These allow visual inspection of the internal detail of the map and identification of artifacts.

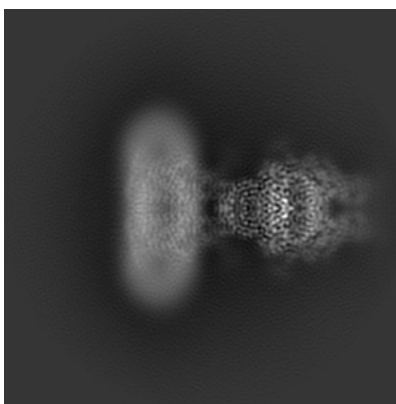
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

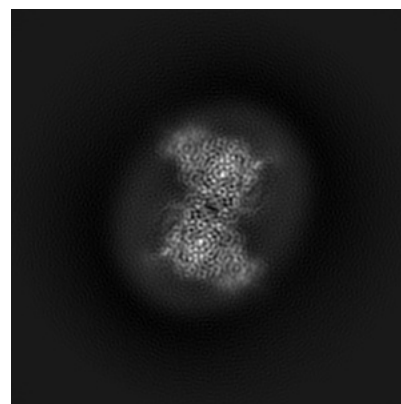
#### 6.1.1 Primary map



X

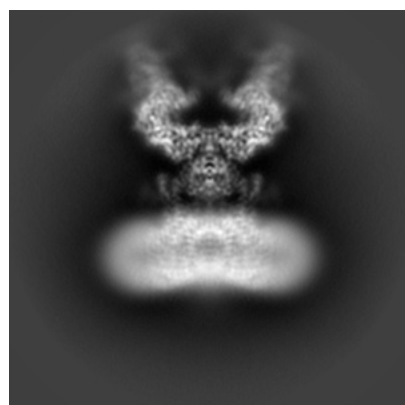


Y

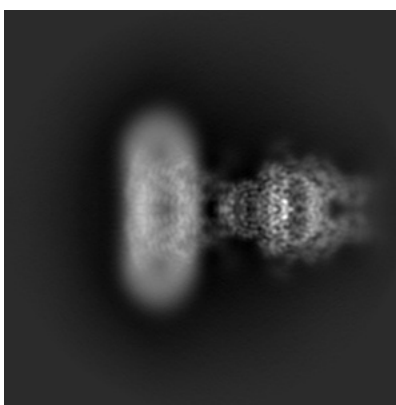


Z

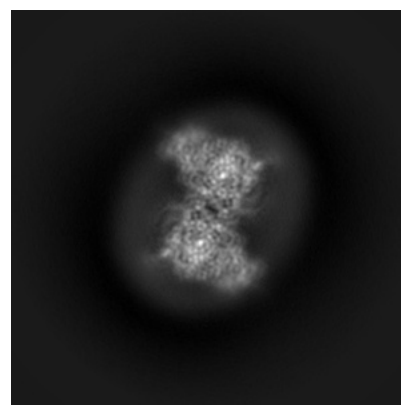
#### 6.1.2 Raw map



X



Y

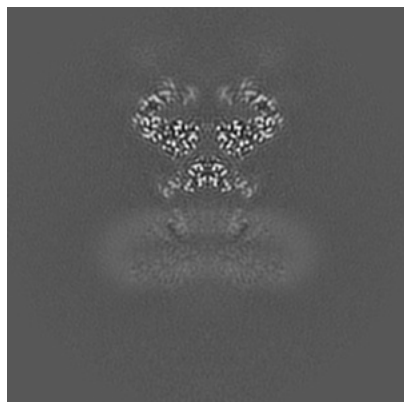


Z

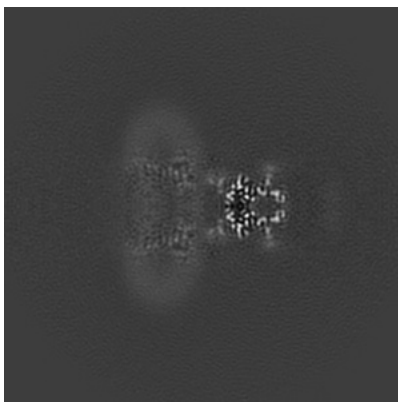
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

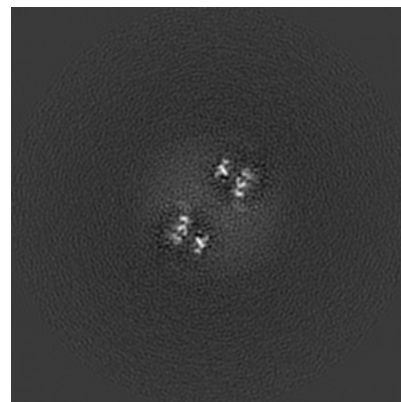
### 6.2.1 Primary map



X Index: 144

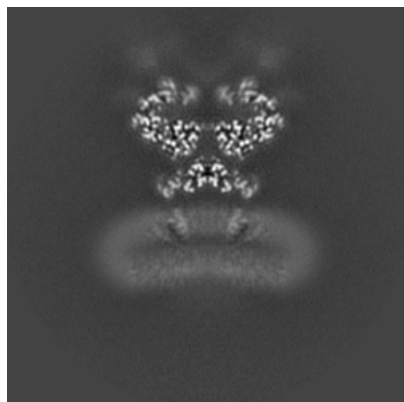


Y Index: 144

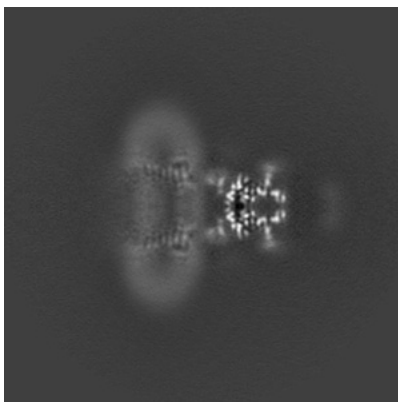


Z Index: 144

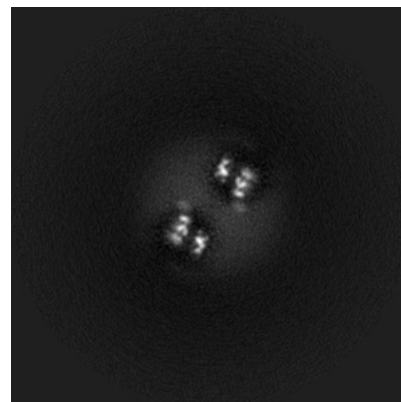
### 6.2.2 Raw map



X Index: 144



Y Index: 144



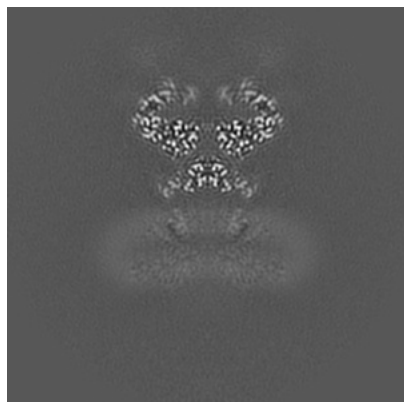
Z Index: 144

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

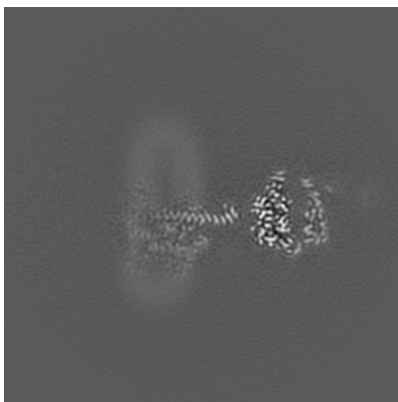


## 6.3 Largest variance slices [i](#)

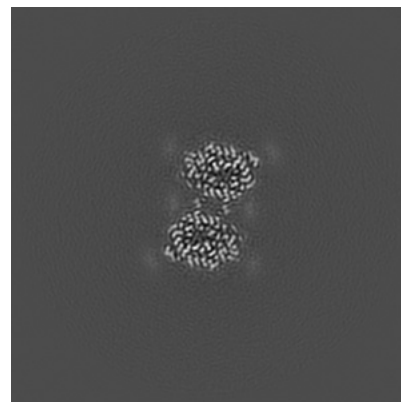
### 6.3.1 Primary map



X Index: 144

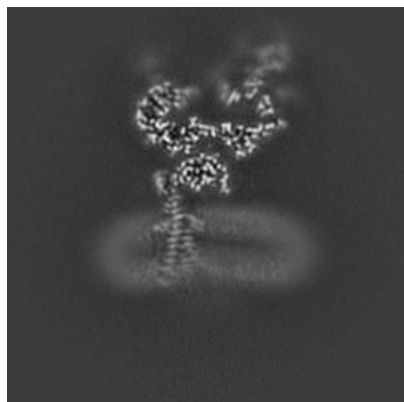


Y Index: 121

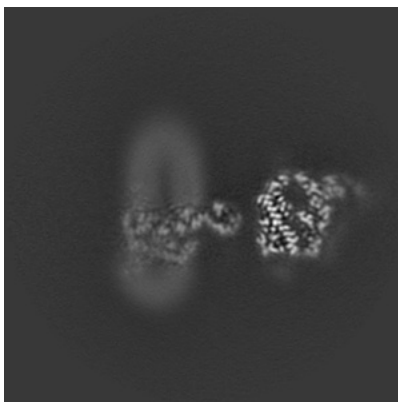


Z Index: 194

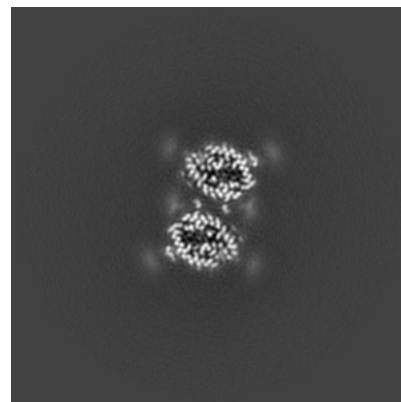
### 6.3.2 Raw map



X Index: 138



Y Index: 114

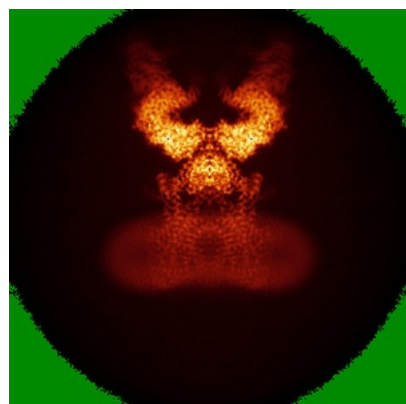


Z Index: 193

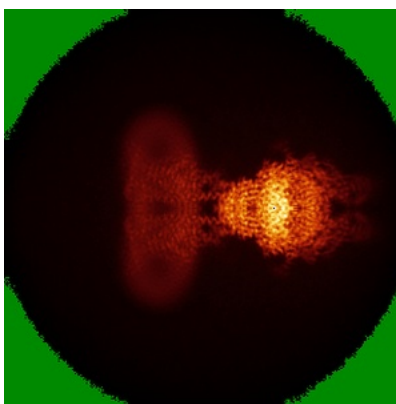
The images above show the largest variance slices of the map in three orthogonal directions.

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

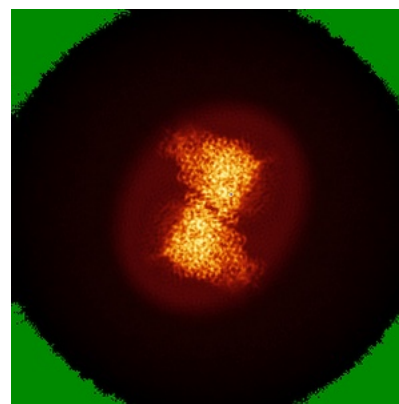
### 6.4.1 Primary map



X



Y

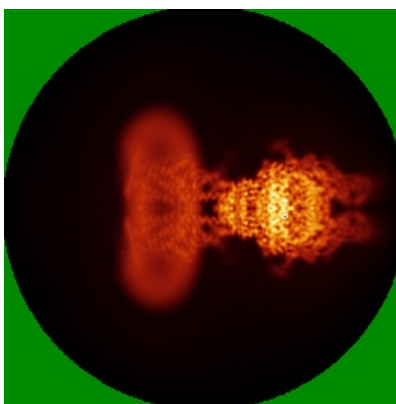


Z

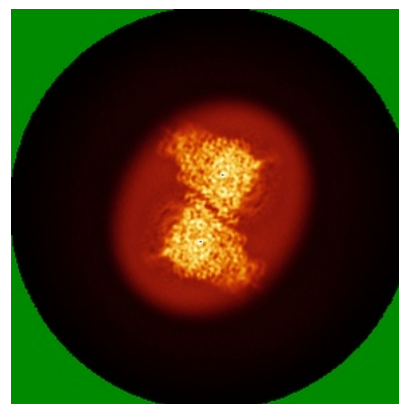
### 6.4.2 Raw map



X



Y

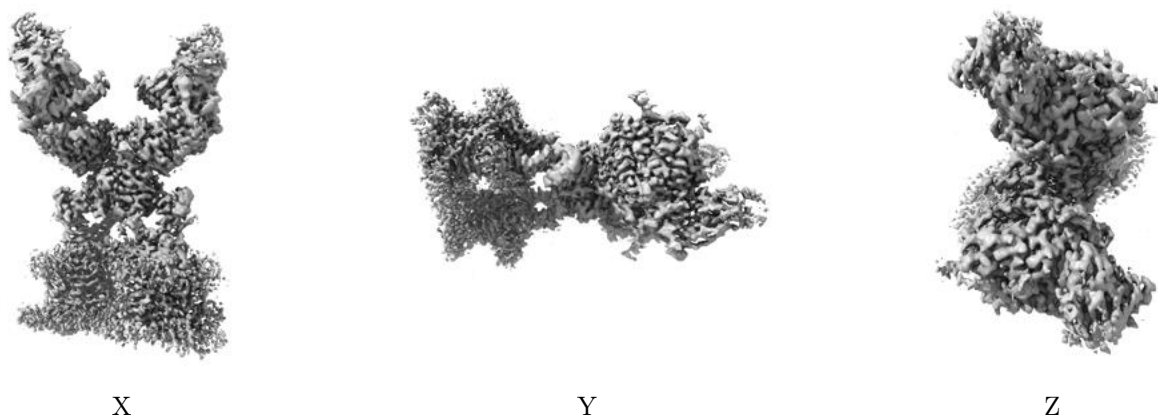


Z

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.

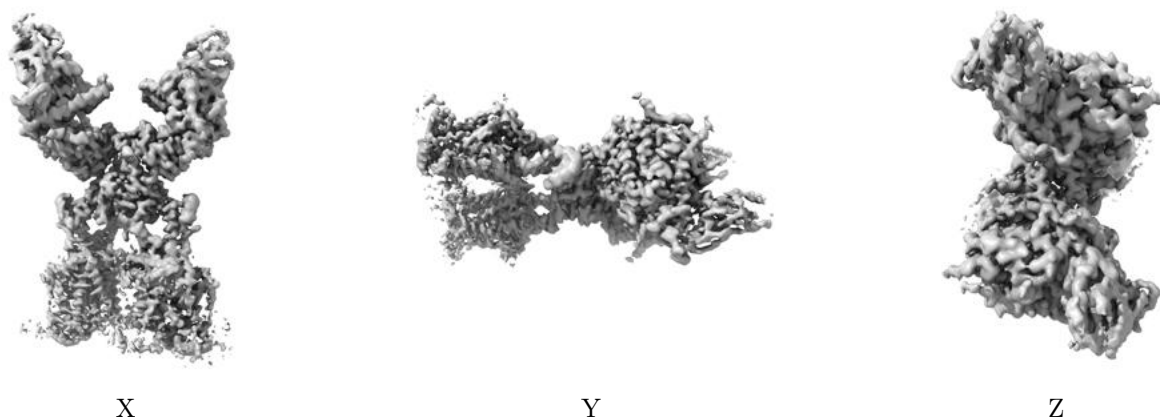
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

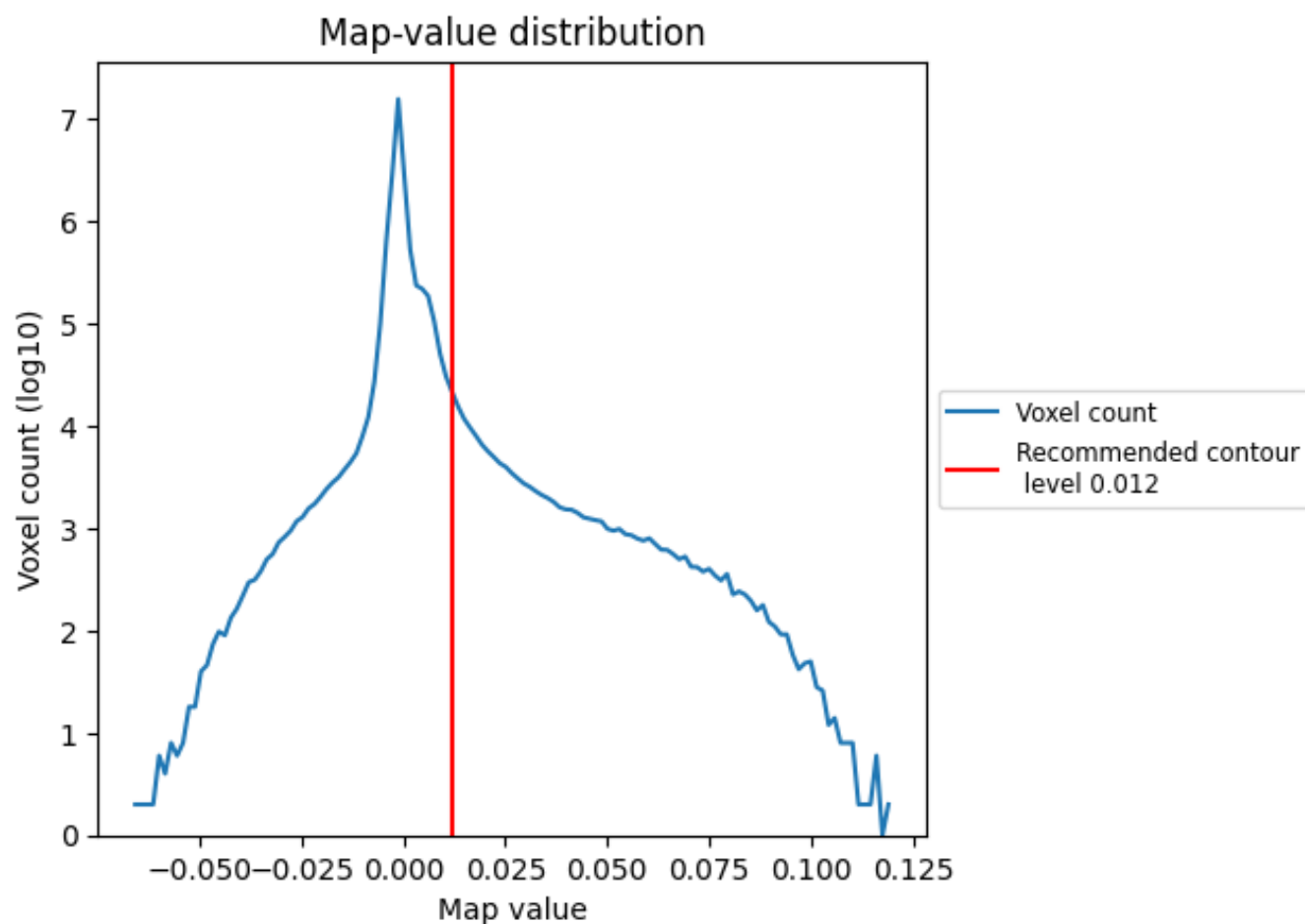
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

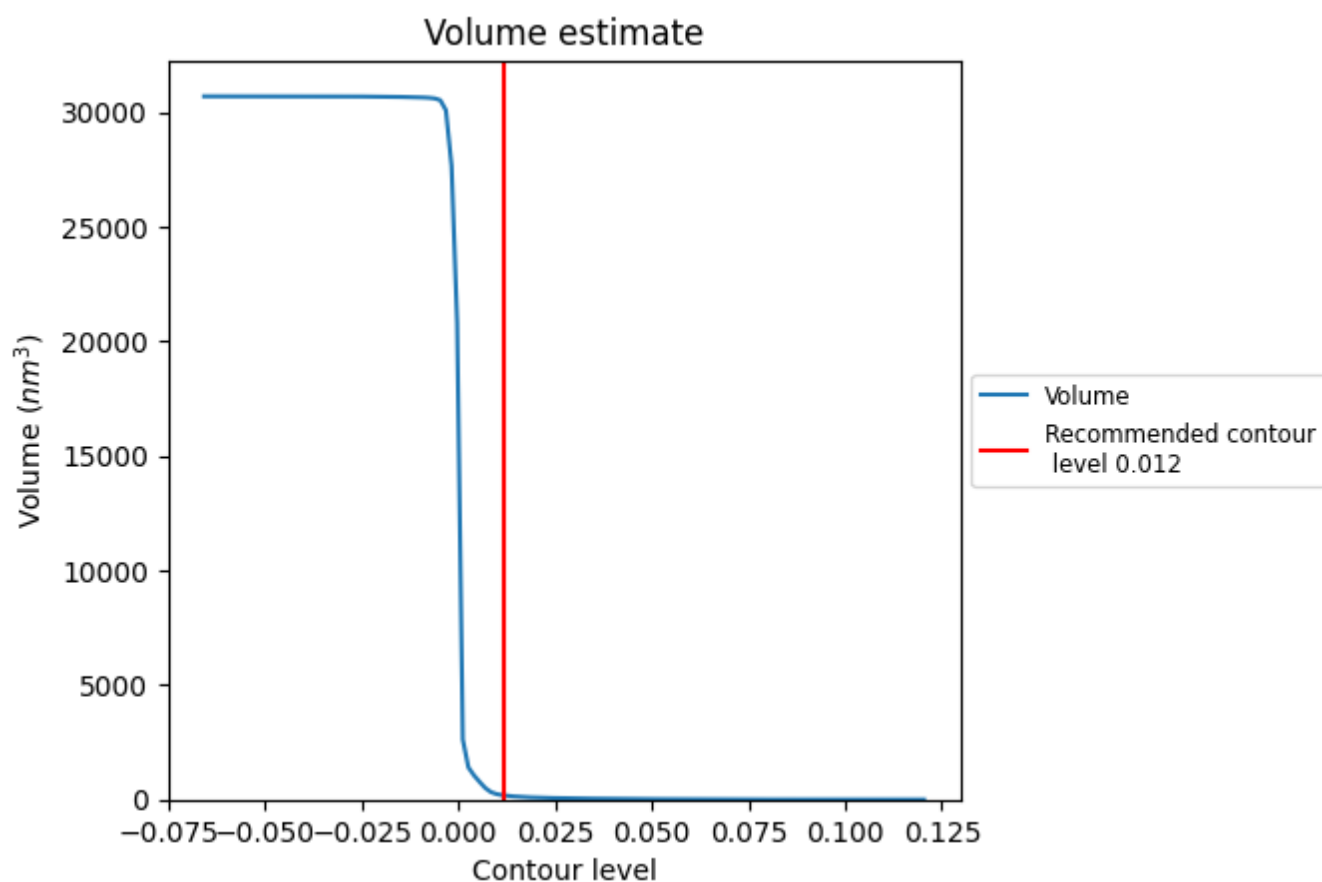
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

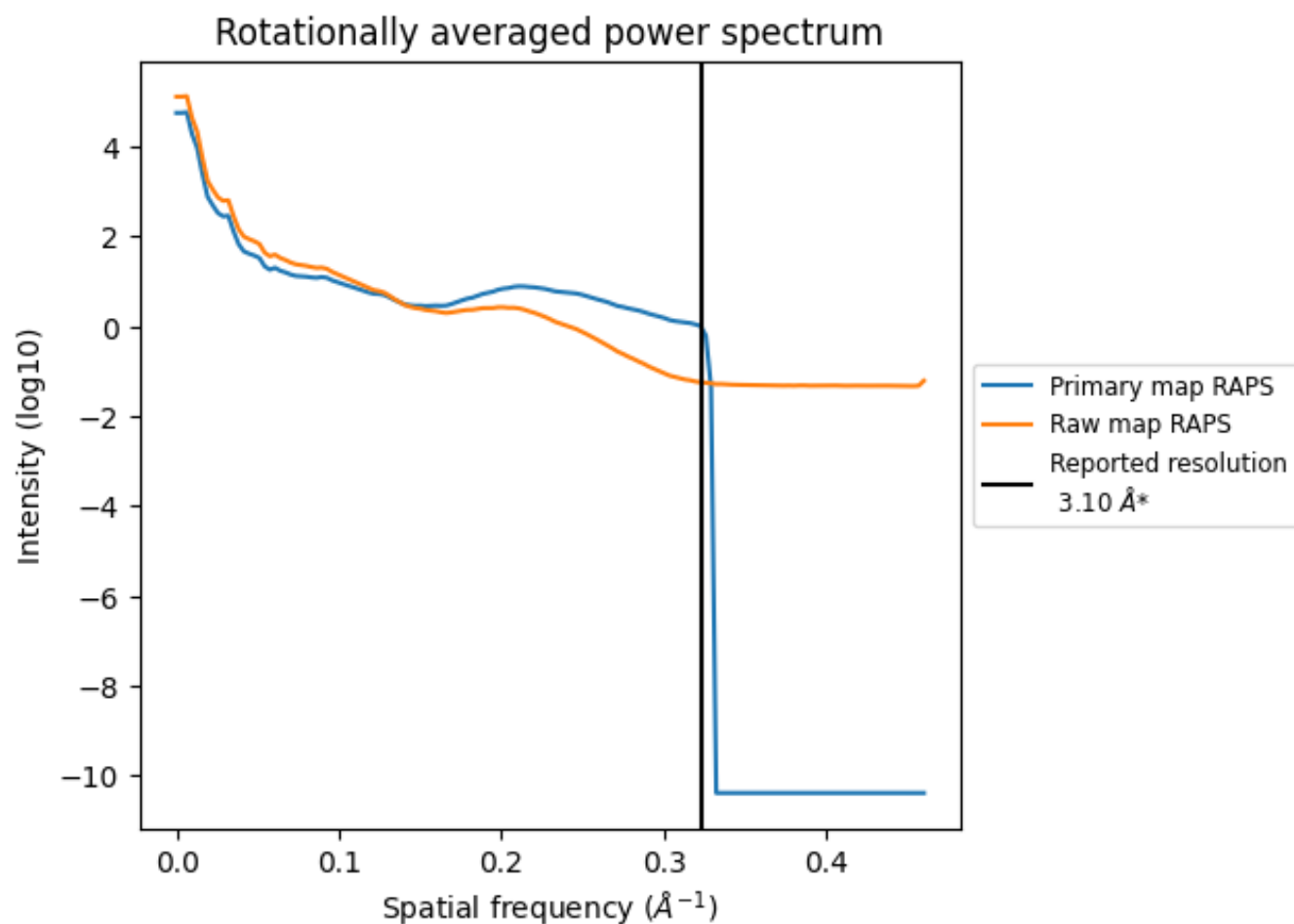
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178  $\text{nm}^3$ ; this corresponds to an approximate mass of 161 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 ⓘ

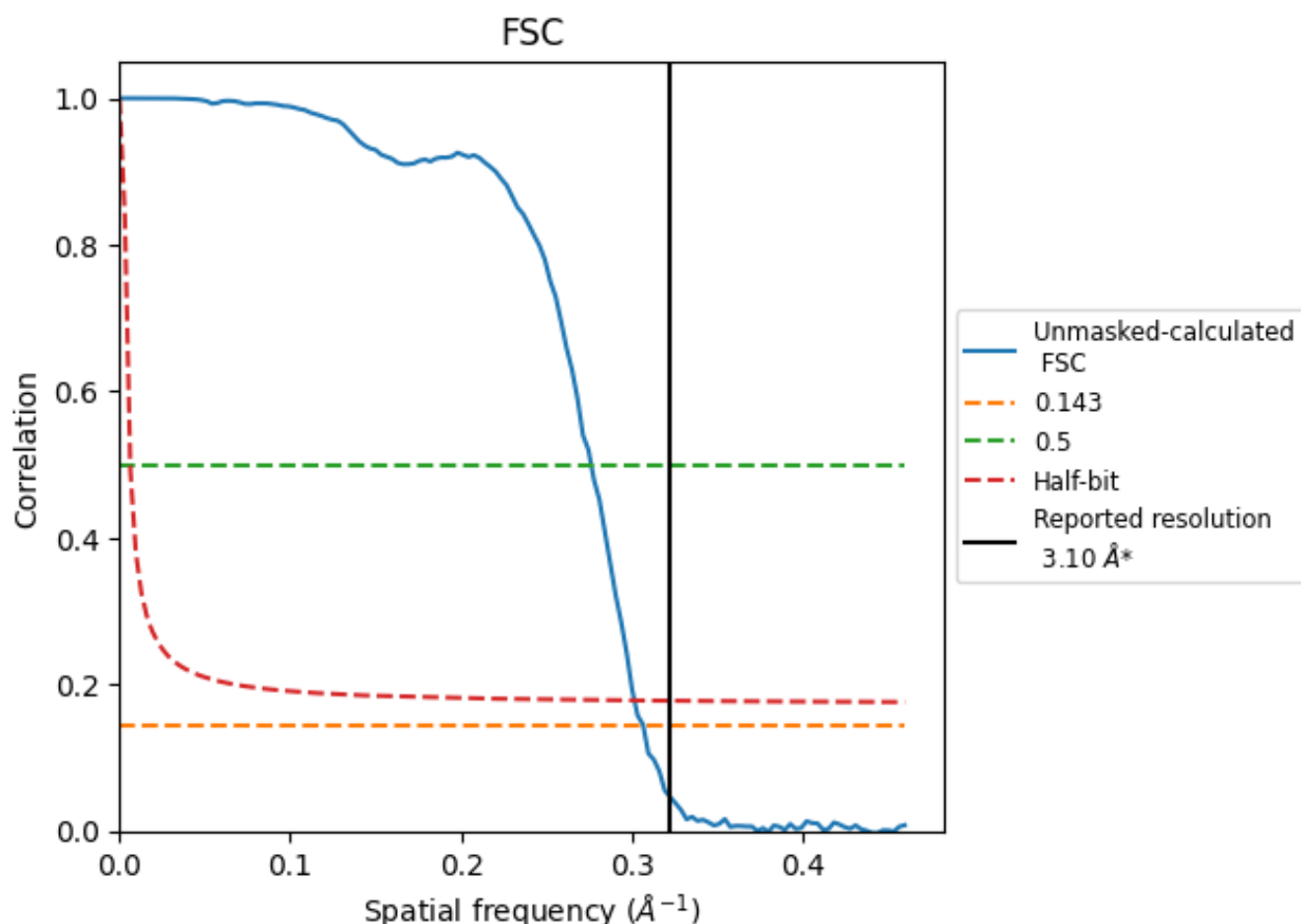


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.62	3.32

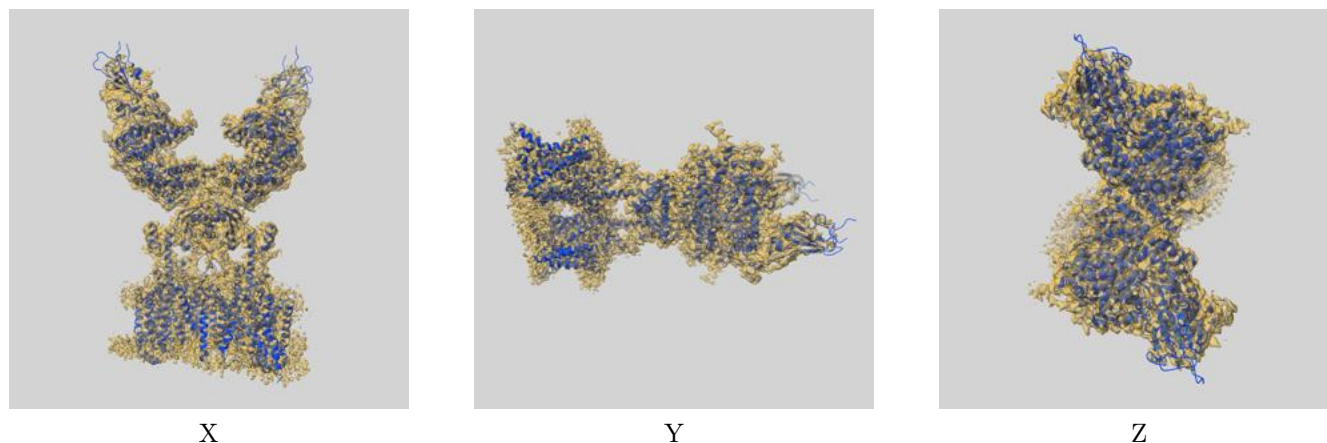
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

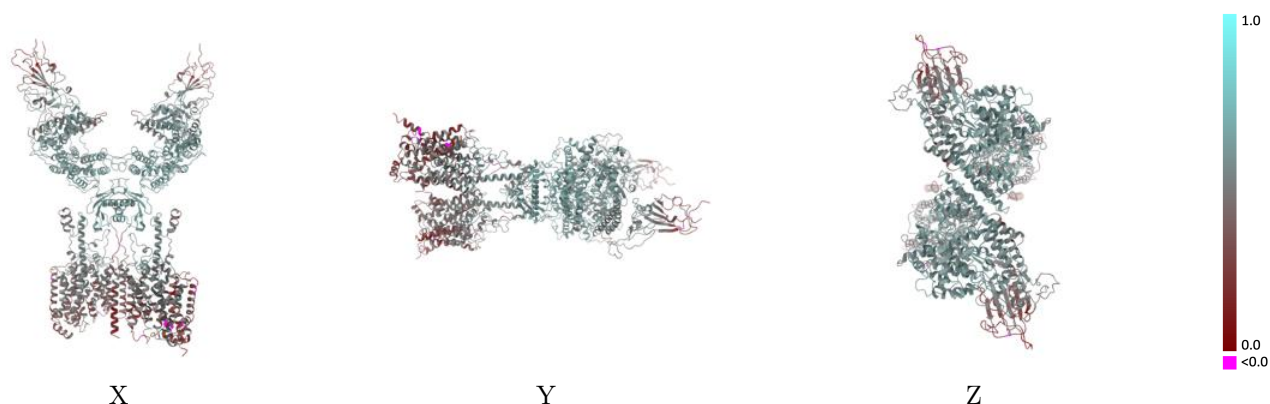
This section contains information regarding the fit between EMDB map EMD-33652 and PDB model 7Y75. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



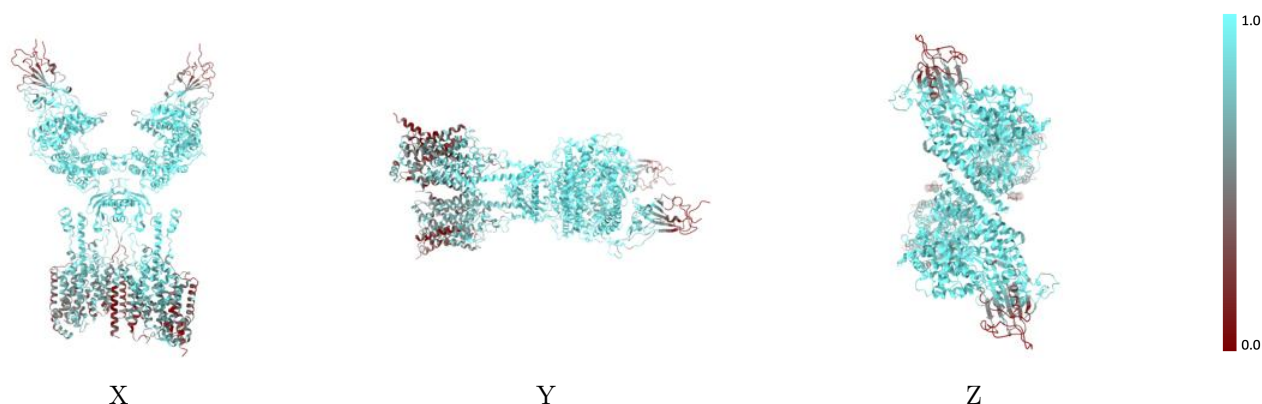
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



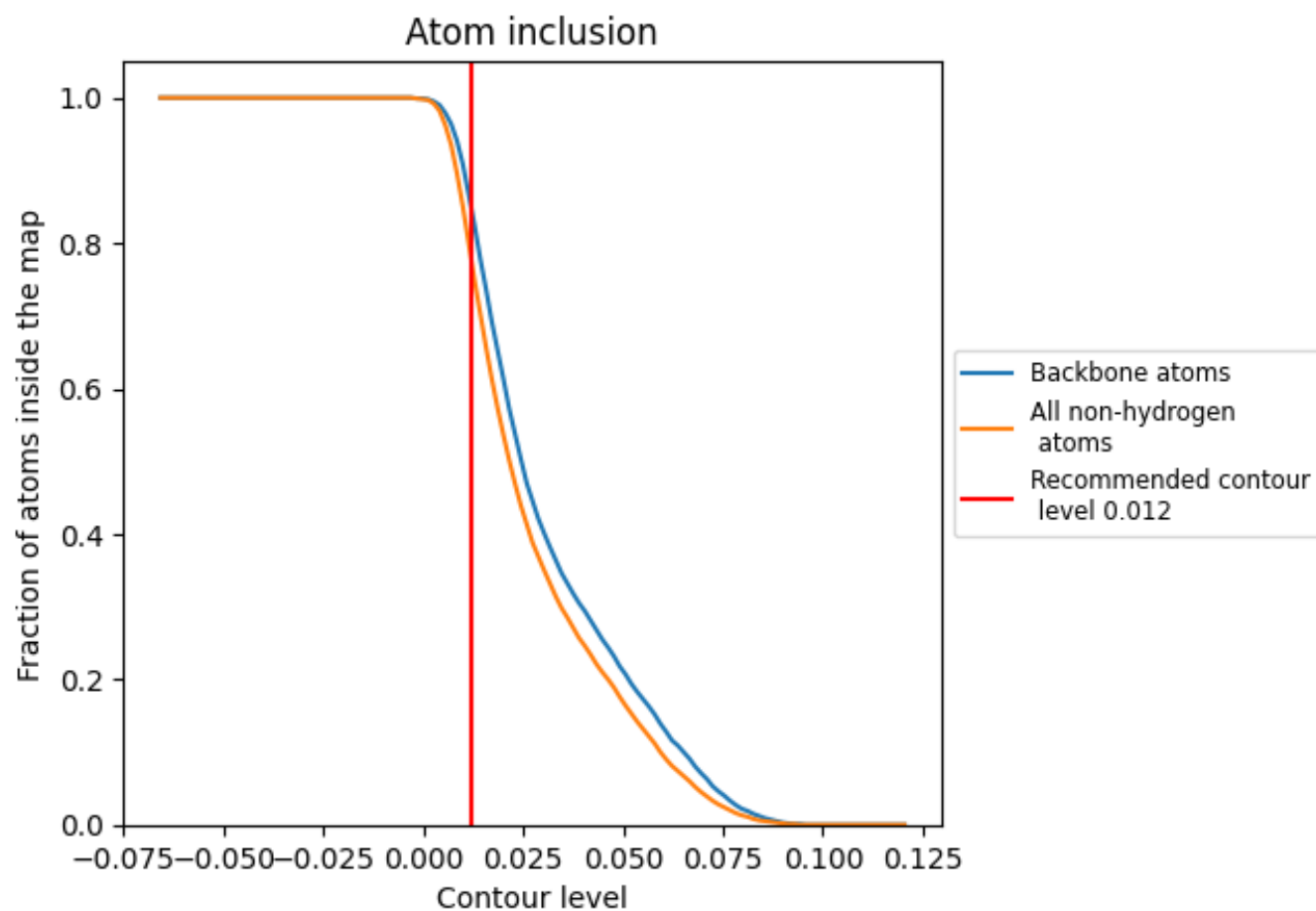
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.4880
A	 0.9330	 0.5670
B	 0.6500	 0.4090
C	 0.9340	 0.5680
D	 0.6540	 0.4100
E	 0.5760	 0.4210
F	 0.5770	 0.4220
G	 0.3570	 0.3490
H	 0.5000	 0.4350
I	 0.6070	 0.3370
J	 0.7500	 0.4060
K	 0.7500	 0.4640
L	 0.7860	 0.4530
M	 0.9640	 0.5650
N	 0.0000	 0.1670
O	 0.3570	 0.3490
P	 0.4290	 0.4170
Q	 0.6070	 0.3300
R	 0.7500	 0.3970
S	 0.7500	 0.4610
T	 0.7860	 0.4460
U	 0.9640	 0.5550
V	 0.0000	 0.1720

