



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 10:41 AM JST

PDB ID : 7XU2  
EMDB ID : EMD-33456  
Title : Structure of SARS-CoV-2 Spike Protein with Engineered x3 Disulfide (x3(D427C, V987C) and single Arg S1/S2 cleavage site), Locked-2 Conformation  
Authors : Qu, K.; Chen, Q.; Ciazynska, K.A.; Liu, B.; Zhang, X.; Wang, J.; He, Y.; Guan, J.; He, J.; Liu, T.; Zhang, X.; Carter, A.P.; Xiong, X.; Briggs, J.A.G.  
Deposited on : 2022-05-18  
Resolution : 3.20 Å(reported)  
Based on initial model : 6ZP2

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

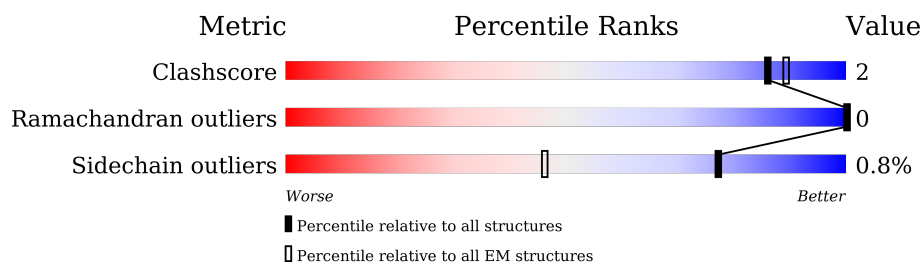
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.



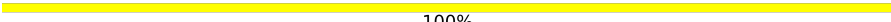
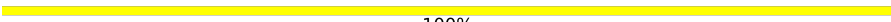






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1127	92% 6% •
1	B	1127	92% 6% •
1	C	1127	92% 6% •
2	D	2	100%
2	E	2	100%
2	F	2	50% 100%
2	G	2	50% 100%

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	I	2	 100%
2	J	2	 50% 100%
2	K	2	 50% 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 50% 100%
2	O	2	 50% 100%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 53175 atoms, of which 26205 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1107	Total	C	H	N	O	S	0	0
			17063	5511	8416	1447	1647	42		
1	C	1107	Total	C	H	N	O	S	0	0
			17063	5511	8416	1447	1647	42		
1	B	1107	Total	C	H	N	O	S	0	0
			17063	5511	8416	1447	1647	42		

There are 30 discrepancies between the modelled and reference sequences:

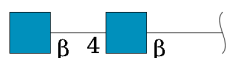
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	427	CYS	ASP	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	987	CYS	VAL	engineered mutation	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	427	CYS	ASP	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	987	CYS	VAL	engineered mutation	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	427	CYS	ASP	engineered mutation	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	987	CYS	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 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
2	D	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	E	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	F	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	G	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	H	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	I	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	J	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	K	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	L	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	M	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	N	2	Total 53	C 16	H 25	N 2	O 10	0	0
2	O	2	Total 53	C 16	H 25	N 2	O 10	0	0

- Molecule 3 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
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

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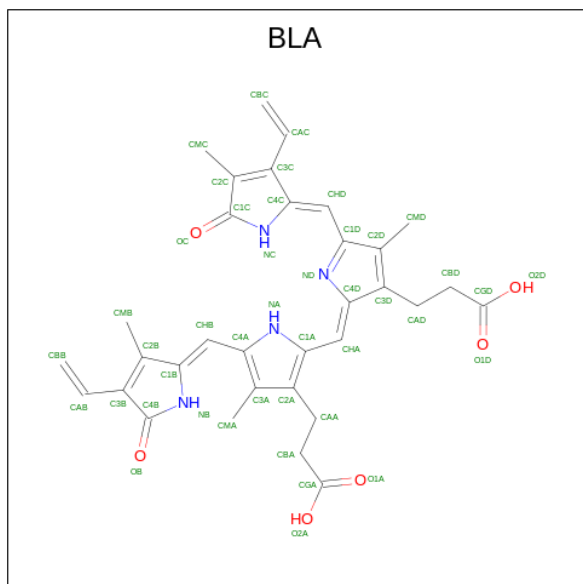
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

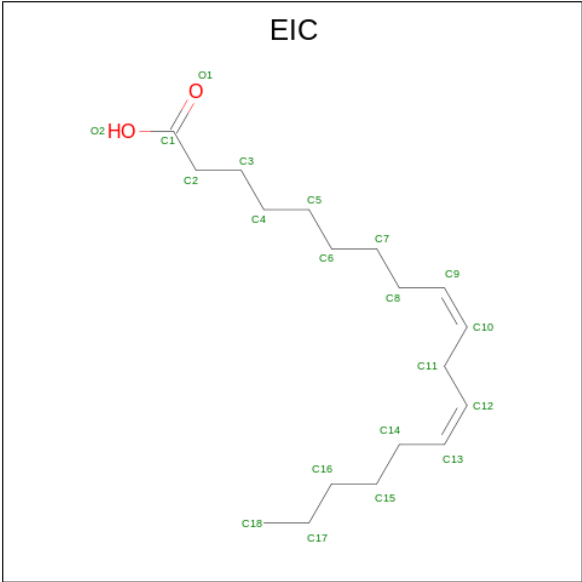
- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			75	33	32	4	6	
4	C	1	Total	C	H	N	O	0
			75	33	32	4	6	
4	B	1	Total	C	H	N	O	0
			75	33	32	4	6	

- Molecule 5 is LINOLEIC ACID (three-letter code: EIC) (formula:  $C_{18}H_{32}O_2$ ).



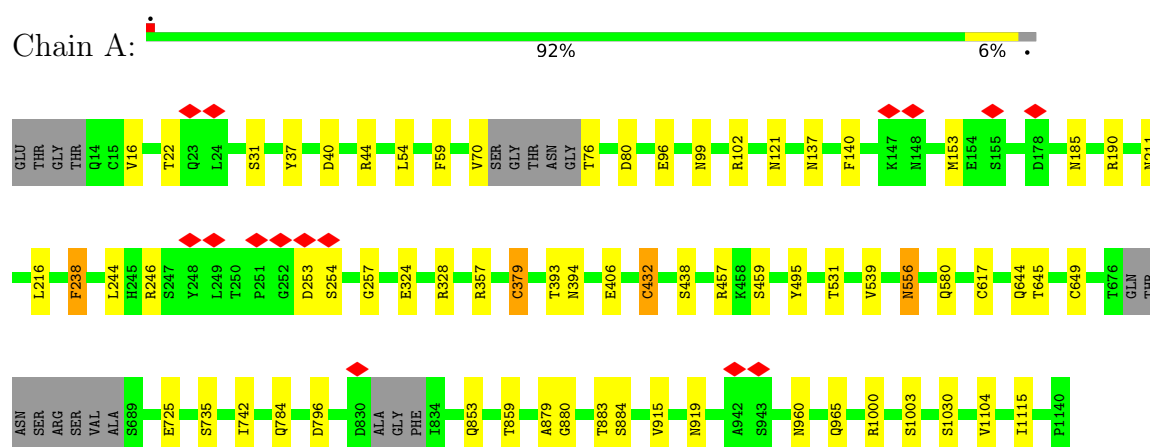


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			51	18	31	2	
5	C	1	Total	C	H	O	0
			51	18	31	2	
5	B	1	Total	C	H	O	0
			51	18	31	2	

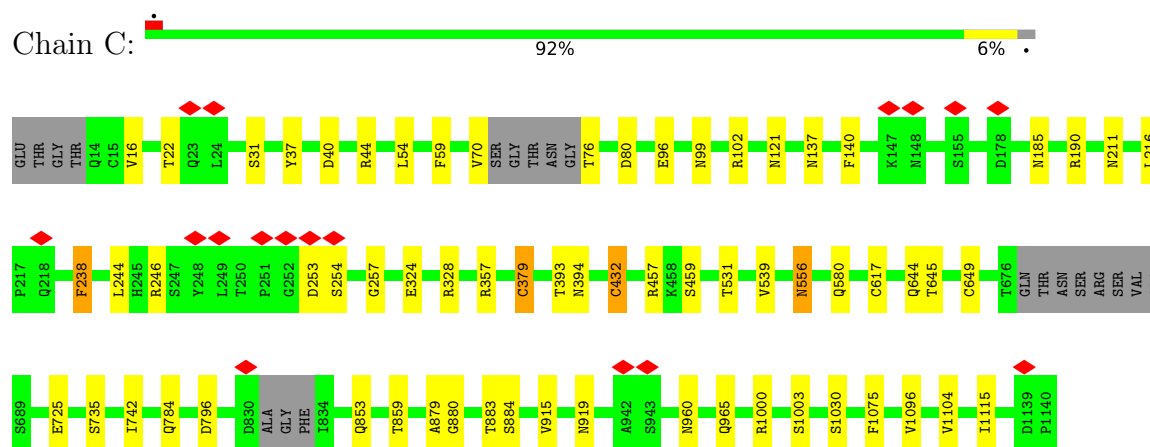
### 3 Residue-property plots

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.

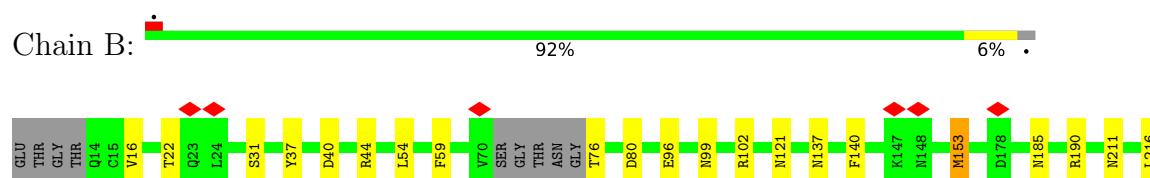
#### • Molecule 1: Spike glycoprotein

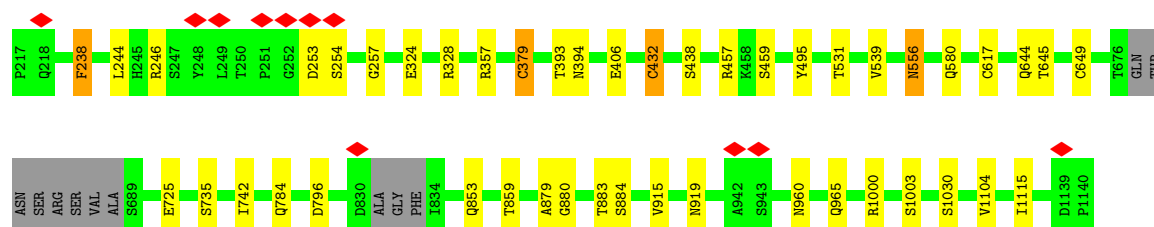


#### • Molecule 1: Spike glycoprotein



#### • Molecule 1: Spike glycoprotein





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

Chain D:  100%

NAG1  
NAG2

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

Chain E:  100%

NAG1  
NAG2

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

Chain F:  50% 100%

NAG1  
NAG2

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

Chain G:  50% 100%

NAG1  
NAG2

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

Chain H:  100%

NAG1  
NAG2

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

Chain I:  100%

NAG1  
NAG2

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

Chain J:  50%  
 100%

♦  
NAG1  
NAG2

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

Chain K:  50%  
 100%

♦  
NAG1  
NAG2

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

Chain L:  100%

NAG1  
NAG2

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

Chain M:  100%

NAG1  
NAG2

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

Chain N:  50%  
 100%

♦  
NAG1  
NAG2

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

Chain O:  50%  
 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	18364	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)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.33	2/8847 (0.0%)	0.59	3/12040 (0.0%)
1	B	0.33	2/8847 (0.0%)	0.60	4/12040 (0.0%)
1	C	0.33	2/8847 (0.0%)	0.59	3/12040 (0.0%)
All	All	0.33	6/26541 (0.0%)	0.59	10/36120 (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	B	1	0
1	C	1	0
All	All	2	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	432	CYS	CB-SG	-6.31	1.71	1.82
1	A	432	CYS	CB-SG	-6.28	1.71	1.82
1	C	432	CYS	CB-SG	-6.27	1.71	1.82
1	C	379	CYS	CB-SG	5.39	1.91	1.82
1	A	379	CYS	CB-SG	5.32	1.91	1.82
1	B	379	CYS	CB-SG	5.31	1.91	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	CYS	CA-CB-SG	11.46	134.62	114.00
1	C	432	CYS	CA-CB-SG	11.38	134.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	CYS	CA-CB-SG	11.34	134.42	114.00
1	B	238	PHE	CB-CG-CD1	7.85	126.29	120.80
1	C	238	PHE	CB-CG-CD1	7.79	126.25	120.80
1	A	238	PHE	CB-CG-CD1	7.77	126.24	120.80
1	B	153	MET	CA-CB-CG	6.78	124.82	113.30
1	B	238	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	C	238	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	238	PHE	CB-CG-CD2	-5.66	116.84	120.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	70	VAL	CA
1	B	70	VAL	CA

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8647	8416	8422	36	0
1	B	8647	8416	8422	36	0
1	C	8647	8416	8422	34	0
2	D	28	25	25	0	0
2	E	28	25	25	0	0
2	F	28	25	25	0	0
2	G	28	25	25	0	0
2	H	28	25	25	0	0
2	I	28	25	25	0	0
2	J	28	25	25	0	0
2	K	28	25	25	0	0
2	L	28	25	25	0	0
2	M	28	25	25	0	0
2	N	28	25	25	0	0
2	O	28	25	25	0	0
3	A	168	156	156	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	168	156	156	1	0
3	C	168	156	156	2	0
4	A	43	32	32	1	0
4	B	43	32	32	1	0
4	C	43	32	32	1	0
5	A	20	31	31	0	0
5	B	20	31	31	0	0
5	C	20	31	31	0	0
All	All	26970	26205	26223	108	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 2.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:NH1	1:C:394:ASN:OD1	2.20	0.75
1:B:357:ARG:NH1	1:B:394:ASN:OD1	2.20	0.75
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.20	0.74
1:A:253:ASP:O	1:A:257:GLY:N	2.20	0.74
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.72	0.72
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.73	0.71
1:B:253:ASP:O	1:B:257:GLY:N	2.19	0.70
1:B:735:SER:OG	1:B:859:THR:OG1	2.10	0.70
1:A:379:CYS:HA	1:A:432:CYS:HB3	1.73	0.69
1:A:735:SER:OG	1:A:859:THR:OG1	2.10	0.69
1:C:735:SER:OG	1:C:859:THR:OG1	2.10	0.69
1:C:253:ASP:O	1:C:257:GLY:N	2.19	0.67
1:C:879:ALA:O	1:C:883:THR:OG1	2.12	0.61
1:A:879:ALA:O	1:A:883:THR:OG1	2.11	0.61
1:B:185:ASN:ND2	1:B:211:ASN:OD1	2.35	0.60
1:C:185:ASN:ND2	1:C:211:ASN:OD1	2.35	0.59
1:C:915:VAL:O	1:C:919:ASN:ND2	2.35	0.58
1:B:22:THR:OG1	1:B:76:THR:O	2.15	0.58
1:B:915:VAL:O	1:B:919:ASN:ND2	2.37	0.57
1:A:185:ASN:ND2	1:A:211:ASN:OD1	2.37	0.57
1:B:879:ALA:O	1:B:883:THR:OG1	2.12	0.57
1:A:915:VAL:O	1:A:919:ASN:ND2	2.39	0.55
1:B:121:ASN:ND2	4:B:1814:BLA:OB	2.41	0.54
1:C:121:ASN:ND2	4:C:1313:BLA:OB	2.42	0.53
1:A:121:ASN:ND2	4:A:1313:BLA:OB	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:O	1:C:59:PHE:N	2.42	0.52
1:C:617:CYS:N	1:C:649:CYS:SG	2.82	0.52
1:B:617:CYS:N	1:B:649:CYS:SG	2.83	0.52
1:A:96:GLU:OE2	1:A:190:ARG:NH2	2.43	0.52
1:B:379:CYS:HA	1:B:432:CYS:CB	2.39	0.52
1:B:31:SER:O	1:B:59:PHE:N	2.42	0.51
1:A:31:SER:O	1:A:59:PHE:N	2.43	0.51
1:A:617:CYS:N	1:A:649:CYS:SG	2.83	0.51
1:B:96:GLU:OE2	1:B:190:ARG:NH2	2.43	0.51
1:B:784:GLN:OE1	1:B:1030:SER:OG	2.29	0.51
1:C:379:CYS:HA	1:C:432:CYS:CB	2.40	0.51
1:B:246:ARG:NH2	1:B:254:SER:OG	2.45	0.50
1:C:784:GLN:OE1	1:C:1030:SER:OG	2.27	0.50
3:C:1302:NAG:O7	3:C:1302:NAG:O3	2.29	0.49
1:C:96:GLU:OE2	1:C:190:ARG:NH2	2.45	0.49
1:A:246:ARG:NH2	1:A:254:SER:OG	2.45	0.49
1:B:37:TYR:OH	1:B:54:LEU:O	2.20	0.49
1:A:784:GLN:OE1	1:A:1030:SER:OG	2.27	0.48
1:A:22:THR:OG1	1:A:76:THR:O	2.22	0.48
1:A:40:ASP:OD2	1:A:44:ARG:NH1	2.48	0.47
1:C:1104:VAL:HG23	1:C:1115:ILE:HD13	1.95	0.47
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.48	0.47
1:B:324:GLU:HG3	1:B:539:VAL:HG23	1.96	0.47
1:A:328:ARG:NH2	1:A:531:THR:O	2.47	0.47
1:C:137:ASN:ND2	3:C:1312:NAG:O7	2.48	0.47
1:C:457:ARG:NH1	1:C:459:SER:O	2.46	0.47
1:A:880:GLY:O	1:A:884:SER:OG	2.30	0.47
1:C:22:THR:OG1	1:C:76:THR:O	2.23	0.47
1:C:324:GLU:HG3	1:C:539:VAL:HG23	1.96	0.47
1:C:328:ARG:NH2	1:C:531:THR:O	2.48	0.47
1:B:40:ASP:OD2	1:B:44:ARG:NH1	2.47	0.47
1:A:1104:VAL:HG23	1:A:1115:ILE:HD13	1.95	0.47
1:B:1104:VAL:HG23	1:B:1115:ILE:HD13	1.96	0.47
1:C:99:ASN:O	1:C:102:ARG:NH1	2.48	0.47
1:C:246:ARG:NH2	1:C:254:SER:OG	2.45	0.47
1:A:379:CYS:HA	1:A:432:CYS:CB	2.40	0.47
1:C:796:ASP:OD1	1:C:796:ASP:N	2.48	0.47
1:B:853:GLN:NE2	1:B:960:ASN:OD1	2.48	0.47
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.48	0.46
1:A:140:PHE:CD2	1:A:244:LEU:HD12	2.50	0.46
1:A:796:ASP:N	1:A:796:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:ASP:N	1:B:796:ASP:OD1	2.48	0.46
1:B:328:ARG:NH2	1:B:531:THR:O	2.48	0.46
1:A:324:GLU:HG3	1:A:539:VAL:HG23	1.96	0.46
3:A:1302:NAG:O7	3:A:1302:NAG:O3	2.29	0.46
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.49	0.46
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.45	0.46
1:B:438:SER:O	1:B:438:SER:OG	2.34	0.46
1:B:406:GLU:OE1	1:B:495:TYR:OH	2.30	0.45
1:C:140:PHE:CD2	1:C:244:LEU:HD12	2.51	0.45
1:B:140:PHE:CD2	1:B:244:LEU:HD12	2.51	0.45
1:C:37:TYR:OH	1:C:54:LEU:O	2.21	0.45
1:C:40:ASP:OD2	1:C:44:ARG:NH1	2.49	0.45
1:A:137:ASN:ND2	3:A:1312:NAG:O7	2.49	0.45
1:A:438:SER:OG	1:A:438:SER:O	2.35	0.45
1:A:965:GLN:OE1	1:A:1003:SER:OG	2.35	0.45
1:C:853:GLN:NE2	1:C:960:ASN:OD1	2.46	0.45
1:A:556:ASN:O	1:A:556:ASN:ND2	2.49	0.45
1:A:644:GLN:NE2	1:A:645:THR:O	2.50	0.45
1:C:644:GLN:NE2	1:C:645:THR:O	2.50	0.44
1:B:99:ASN:O	1:B:102:ARG:NH1	2.51	0.44
1:B:137:ASN:ND2	3:B:1813:NAG:O7	2.51	0.44
1:B:644:GLN:NE2	1:B:645:THR:O	2.50	0.44
1:C:965:GLN:OE1	1:C:1003:SER:OG	2.36	0.44
1:B:457:ARG:NH1	1:B:459:SER:O	2.48	0.44
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.47	0.43
1:A:457:ARG:NH1	1:A:459:SER:O	2.47	0.43
1:A:853:GLN:NE2	1:A:960:ASN:OD1	2.48	0.43
1:A:99:ASN:O	1:A:102:ARG:NH1	2.52	0.42
1:C:393:THR:OG1	1:C:394:ASN:N	2.52	0.42
1:B:880:GLY:O	1:B:884:SER:OG	2.32	0.42
1:B:965:GLN:OE1	1:B:1003:SER:OG	2.37	0.42
1:C:556:ASN:O	1:C:556:ASN:ND2	2.49	0.42
1:A:37:TYR:OH	1:A:54:LEU:O	2.21	0.42
1:A:140:PHE:CE2	1:A:244:LEU:HD12	2.55	0.41
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.33	0.41
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.51	0.41
1:C:880:GLY:O	1:C:884:SER:OG	2.32	0.41
1:B:140:PHE:CE2	1:B:244:LEU:HD12	2.55	0.41
1:B:393:THR:OG1	1:B:394:ASN:N	2.54	0.41
1:A:393:THR:OG1	1:A:394:ASN:N	2.54	0.41
1:C:1075:PHE:HB3	1:C:1096:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ASN:O	1:B:556:ASN:ND2	2.49	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	1099/1127 (98%)	1038 (94%)	61 (6%)	0	100	100
1	B	1099/1127 (98%)	1040 (95%)	59 (5%)	0	100	100
1	C	1099/1127 (98%)	1037 (94%)	62 (6%)	0	100	100
All	All	3297/3381 (98%)	3115 (94%)	182 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	964/978 (99%)	956 (99%)	8 (1%)	79	90
1	B	964/978 (99%)	957 (99%)	7 (1%)	81	92
1	C	964/978 (99%)	957 (99%)	7 (1%)	81	92
All	All	2892/2934 (99%)	2870 (99%)	22 (1%)	77	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	70	VAL
1	A	80	ASP
1	A	153	MET
1	A	216	LEU
1	A	238	PHE
1	A	556	ASN
1	A	725	GLU
1	C	16	VAL
1	C	70	VAL
1	C	80	ASP
1	C	216	LEU
1	C	238	PHE
1	C	556	ASN
1	C	725	GLU
1	B	16	VAL
1	B	80	ASP
1	B	153	MET
1	B	216	LEU
1	B	238	PHE
1	B	556	ASN
1	B	725	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	C	137	ASN
1	B	137	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 ⓘ

24 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$
2	NAG	D	1	1,2	14,14,15	2.12	4 (28%)	17,19,21	1.09	0
2	NAG	D	2	2	14,14,15	2.15	4 (28%)	17,19,21	0.98	1 (5%)
2	NAG	E	1	1,2	14,14,15	2.09	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	E	2	2	14,14,15	2.18	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	F	1	1,2	14,14,15	2.19	4 (28%)	17,19,21	1.18	2 (11%)
2	NAG	F	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	G	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	0.87	1 (5%)
2	NAG	G	2	2	14,14,15	2.18	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	H	1	1,2	14,14,15	2.09	4 (28%)	17,19,21	1.07	0
2	NAG	H	2	2	14,14,15	2.17	4 (28%)	17,19,21	1.01	1 (5%)
2	NAG	I	1	1,2	14,14,15	2.10	4 (28%)	17,19,21	1.11	2 (11%)
2	NAG	I	2	2	14,14,15	2.17	4 (28%)	17,19,21	1.00	1 (5%)
2	NAG	J	1	1,2	14,14,15	2.20	4 (28%)	17,19,21	1.18	2 (11%)
2	NAG	J	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	K	1	1,2	14,14,15	2.18	4 (28%)	17,19,21	0.86	1 (5%)
2	NAG	K	2	2	14,14,15	2.18	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	L	1	1,2	14,14,15	2.10	4 (28%)	17,19,21	1.10	0
2	NAG	L	2	2	14,14,15	2.17	4 (28%)	17,19,21	0.99	1 (5%)
2	NAG	M	1	1,2	14,14,15	2.11	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	M	2	2	14,14,15	2.17	4 (28%)	17,19,21	1.00	1 (5%)
2	NAG	N	1	1,2	14,14,15	2.21	4 (28%)	17,19,21	1.17	2 (11%)
2	NAG	N	2	2	14,14,15	2.15	4 (28%)	17,19,21	1.02	1 (5%)
2	NAG	O	1	1,2	14,14,15	2.17	4 (28%)	17,19,21	0.87	1 (5%)
2	NAG	O	2	2	14,14,15	2.17	4 (28%)	17,19,21	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O5-C1	5.55	1.52	1.43
2	J	1	NAG	O5-C1	5.53	1.52	1.43
2	F	1	NAG	O5-C1	5.50	1.52	1.43
2	G	1	NAG	O5-C1	5.27	1.52	1.43
2	G	2	NAG	O5-C1	5.26	1.52	1.43
2	K	2	NAG	O5-C1	5.26	1.52	1.43
2	K	1	NAG	O5-C1	5.26	1.52	1.43
2	O	1	NAG	O5-C1	5.25	1.52	1.43
2	E	2	NAG	O5-C1	5.24	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	NAG	O5-C1	5.24	1.52	1.43
2	F	2	NAG	O5-C1	5.22	1.52	1.43
2	J	2	NAG	O5-C1	5.22	1.52	1.43
2	N	2	NAG	O5-C1	5.21	1.52	1.43
2	H	2	NAG	O5-C1	5.20	1.52	1.43
2	L	2	NAG	O5-C1	5.19	1.52	1.43
2	D	2	NAG	O5-C1	5.17	1.52	1.43
2	M	2	NAG	O5-C1	5.15	1.51	1.43
2	I	2	NAG	O5-C1	5.14	1.51	1.43
2	M	1	NAG	O5-C1	5.12	1.51	1.43
2	I	1	NAG	O5-C1	5.09	1.51	1.43
2	E	1	NAG	O5-C1	5.04	1.51	1.43
2	D	1	NAG	O5-C1	4.96	1.51	1.43
2	L	1	NAG	O5-C1	4.94	1.51	1.43
2	H	1	NAG	O5-C1	4.90	1.51	1.43
2	M	2	NAG	C7-N2	4.01	1.48	1.34
2	E	2	NAG	C7-N2	4.00	1.48	1.34
2	G	2	NAG	C7-N2	3.99	1.48	1.34
2	O	2	NAG	C7-N2	3.99	1.48	1.34
2	I	2	NAG	C7-N2	3.98	1.48	1.34
2	K	1	NAG	C7-N2	3.98	1.48	1.34
2	G	1	NAG	C7-N2	3.98	1.48	1.34
2	K	2	NAG	C7-N2	3.98	1.48	1.34
2	H	2	NAG	C7-N2	3.98	1.48	1.34
2	O	1	NAG	C7-N2	3.97	1.48	1.34
2	L	2	NAG	C7-N2	3.96	1.48	1.34
2	D	1	NAG	C7-N2	3.96	1.47	1.34
2	D	2	NAG	C7-N2	3.94	1.47	1.34
2	H	1	NAG	C7-N2	3.93	1.47	1.34
2	F	2	NAG	C7-N2	3.92	1.47	1.34
2	L	1	NAG	C7-N2	3.92	1.47	1.34
2	N	2	NAG	C7-N2	3.92	1.47	1.34
2	N	1	NAG	C7-N2	3.91	1.47	1.34
2	F	1	NAG	C7-N2	3.91	1.47	1.34
2	J	2	NAG	C7-N2	3.90	1.47	1.34
2	M	1	NAG	C7-N2	3.89	1.47	1.34
2	I	1	NAG	C7-N2	3.88	1.47	1.34
2	J	1	NAG	C7-N2	3.88	1.47	1.34
2	E	1	NAG	C7-N2	3.87	1.47	1.34
2	K	1	NAG	C2-N2	3.25	1.51	1.46
2	I	2	NAG	C2-N2	3.23	1.51	1.46
2	K	2	NAG	C2-N2	3.22	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	NAG	C2-N2	3.22	1.51	1.46
2	G	2	NAG	C2-N2	3.21	1.51	1.46
2	G	1	NAG	C2-N2	3.21	1.51	1.46
2	M	2	NAG	C2-N2	3.20	1.51	1.46
2	O	1	NAG	C2-N2	3.20	1.51	1.46
2	E	2	NAG	C2-N2	3.20	1.51	1.46
2	L	2	NAG	C2-N2	3.11	1.51	1.46
2	N	2	NAG	C2-N2	3.09	1.51	1.46
2	F	2	NAG	C2-N2	3.08	1.51	1.46
2	J	2	NAG	C2-N2	3.06	1.51	1.46
2	H	2	NAG	C2-N2	3.06	1.51	1.46
2	D	2	NAG	C2-N2	3.04	1.51	1.46
2	D	1	NAG	C2-N2	3.02	1.51	1.46
2	N	1	NAG	C2-N2	2.99	1.51	1.46
2	J	1	NAG	C2-N2	2.98	1.51	1.46
2	L	1	NAG	C2-N2	2.97	1.51	1.46
2	E	1	NAG	C2-N2	2.96	1.51	1.46
2	F	1	NAG	C2-N2	2.95	1.51	1.46
2	I	1	NAG	C2-N2	2.94	1.51	1.46
2	H	1	NAG	C2-N2	2.93	1.51	1.46
2	M	1	NAG	C2-N2	2.91	1.51	1.46
2	D	1	NAG	O7-C7	-2.19	1.18	1.23
2	L	1	NAG	O7-C7	-2.19	1.18	1.23
2	M	1	NAG	O7-C7	-2.19	1.18	1.23
2	O	1	NAG	O7-C7	-2.17	1.18	1.23
2	N	1	NAG	O7-C7	-2.17	1.18	1.23
2	H	1	NAG	O7-C7	-2.17	1.18	1.23
2	I	1	NAG	O7-C7	-2.17	1.18	1.23
2	M	2	NAG	O7-C7	-2.17	1.18	1.23
2	I	2	NAG	O7-C7	-2.16	1.18	1.23
2	F	1	NAG	O7-C7	-2.16	1.18	1.23
2	J	1	NAG	O7-C7	-2.15	1.18	1.23
2	K	1	NAG	O7-C7	-2.15	1.18	1.23
2	L	2	NAG	O7-C7	-2.14	1.18	1.23
2	E	2	NAG	O7-C7	-2.14	1.18	1.23
2	G	1	NAG	O7-C7	-2.14	1.18	1.23
2	E	1	NAG	O7-C7	-2.14	1.18	1.23
2	H	2	NAG	O7-C7	-2.13	1.18	1.23
2	G	2	NAG	O7-C7	-2.13	1.18	1.23
2	F	2	NAG	O7-C7	-2.13	1.18	1.23
2	D	2	NAG	O7-C7	-2.13	1.18	1.23
2	K	2	NAG	O7-C7	-2.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	NAG	O7-C7	-2.10	1.18	1.23
2	O	2	NAG	O7-C7	-2.10	1.18	1.23
2	N	2	NAG	O7-C7	-2.07	1.18	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	NAG	C8-C7-N2	2.27	119.95	116.10
2	I	1	NAG	C8-C7-N2	2.27	119.95	116.10
2	F	1	NAG	C8-C7-N2	2.27	119.95	116.10
2	E	1	NAG	C8-C7-N2	2.26	119.93	116.10
2	J	1	NAG	C8-C7-N2	2.26	119.93	116.10
2	G	2	NAG	C8-C7-N2	2.26	119.92	116.10
2	O	2	NAG	C8-C7-N2	2.25	119.91	116.10
2	M	1	NAG	C8-C7-N2	2.24	119.89	116.10
2	N	1	NAG	C8-C7-N2	2.23	119.87	116.10
2	N	2	NAG	C8-C7-N2	2.21	119.84	116.10
2	E	2	NAG	C8-C7-N2	2.21	119.83	116.10
2	G	1	NAG	C8-C7-N2	2.20	119.83	116.10
2	I	2	NAG	C8-C7-N2	2.20	119.83	116.10
2	O	1	NAG	C8-C7-N2	2.20	119.83	116.10
2	M	2	NAG	C8-C7-N2	2.20	119.83	116.10
2	K	1	NAG	C8-C7-N2	2.20	119.82	116.10
2	J	2	NAG	C8-C7-N2	2.19	119.80	116.10
2	F	2	NAG	C8-C7-N2	2.16	119.76	116.10
2	H	2	NAG	C8-C7-N2	2.14	119.72	116.10
2	D	2	NAG	C8-C7-N2	2.13	119.71	116.10
2	L	2	NAG	C8-C7-N2	2.13	119.71	116.10
2	J	1	NAG	C2-N2-C7	-2.10	119.91	122.90
2	N	1	NAG	C2-N2-C7	-2.10	119.92	122.90
2	E	1	NAG	C2-N2-C7	-2.08	119.94	122.90
2	I	1	NAG	C2-N2-C7	-2.05	119.98	122.90
2	F	1	NAG	C2-N2-C7	-2.05	119.98	122.90
2	M	1	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6

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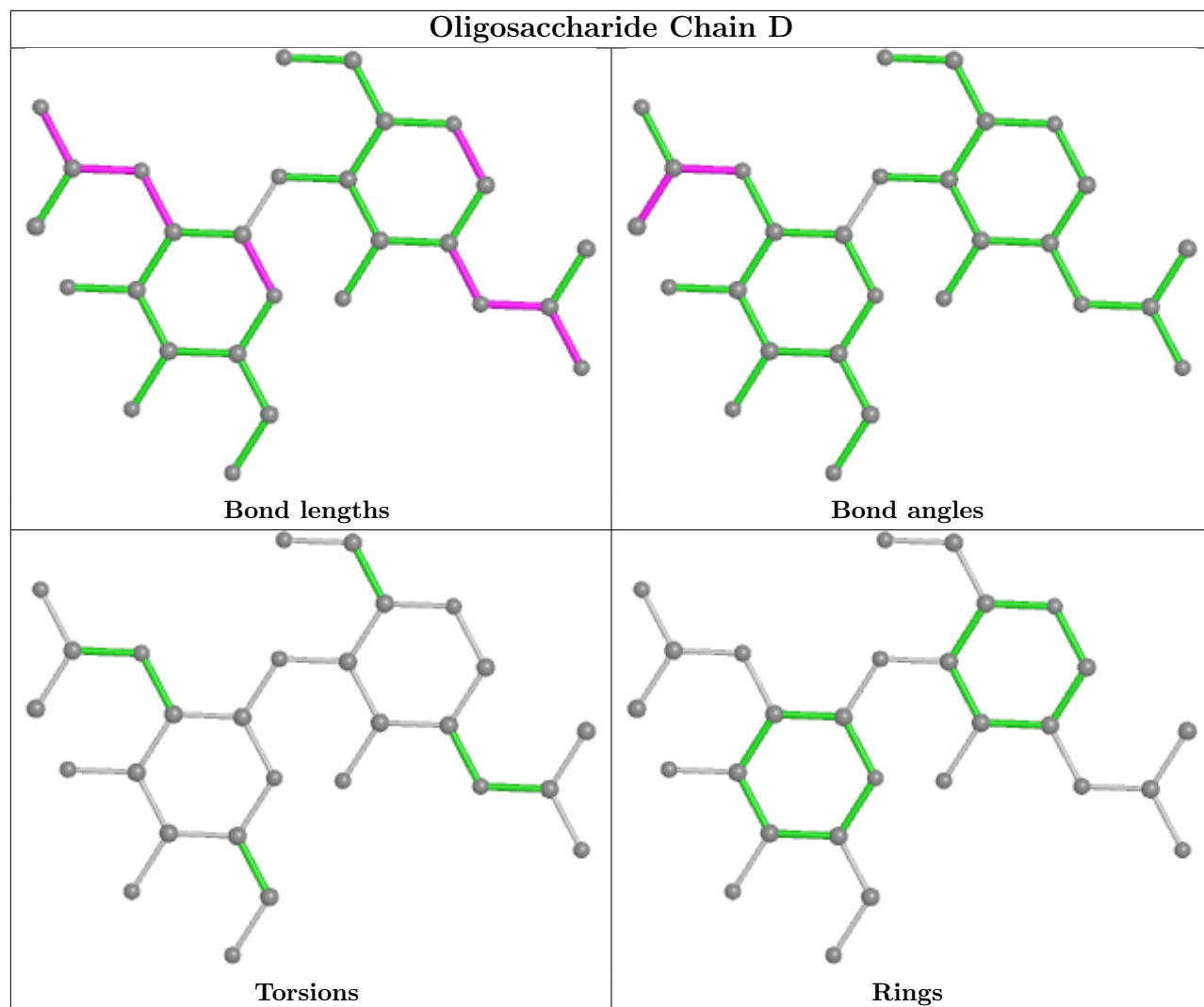
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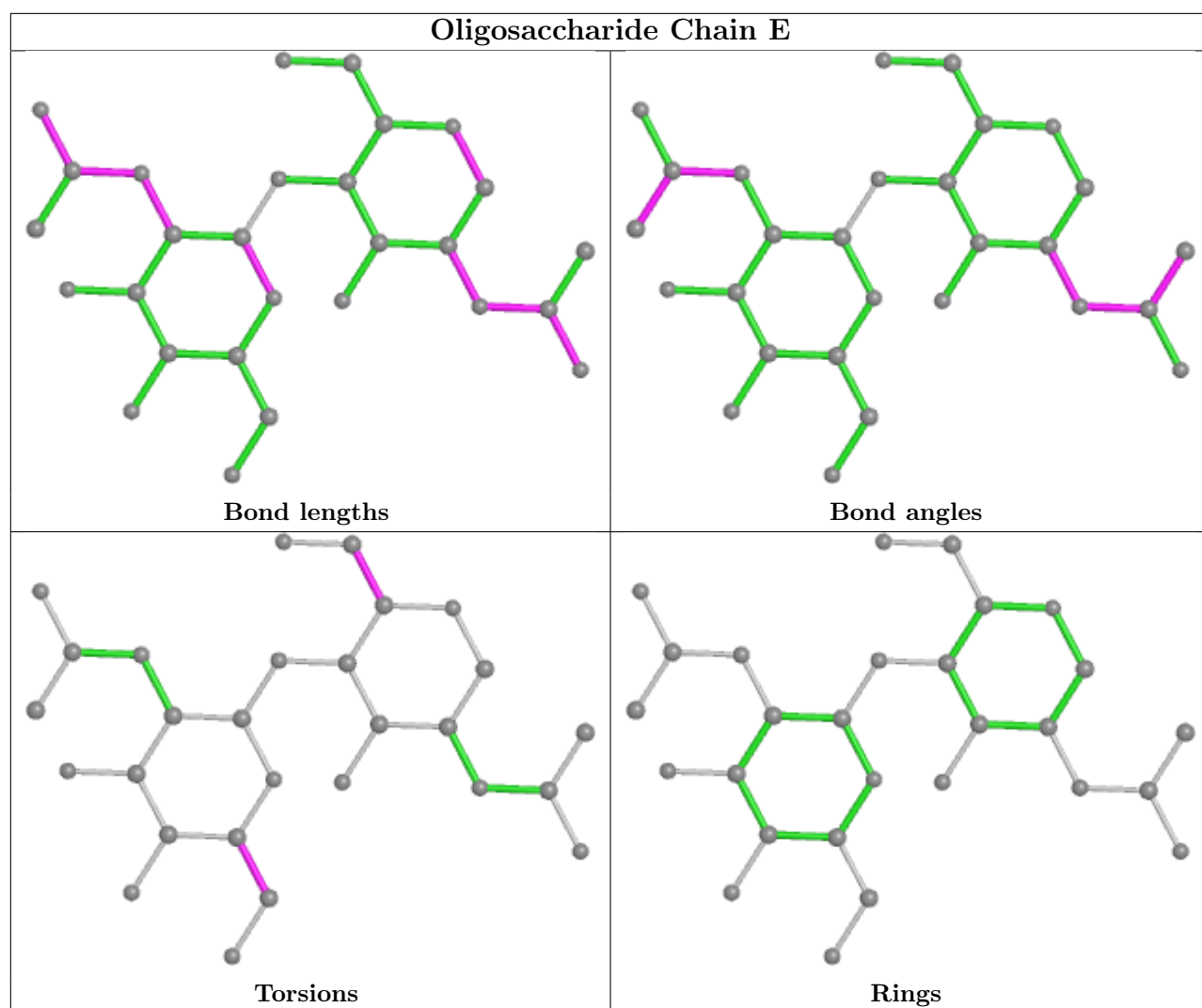
Mol	Chain	Res	Type	Atoms
2	N	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6

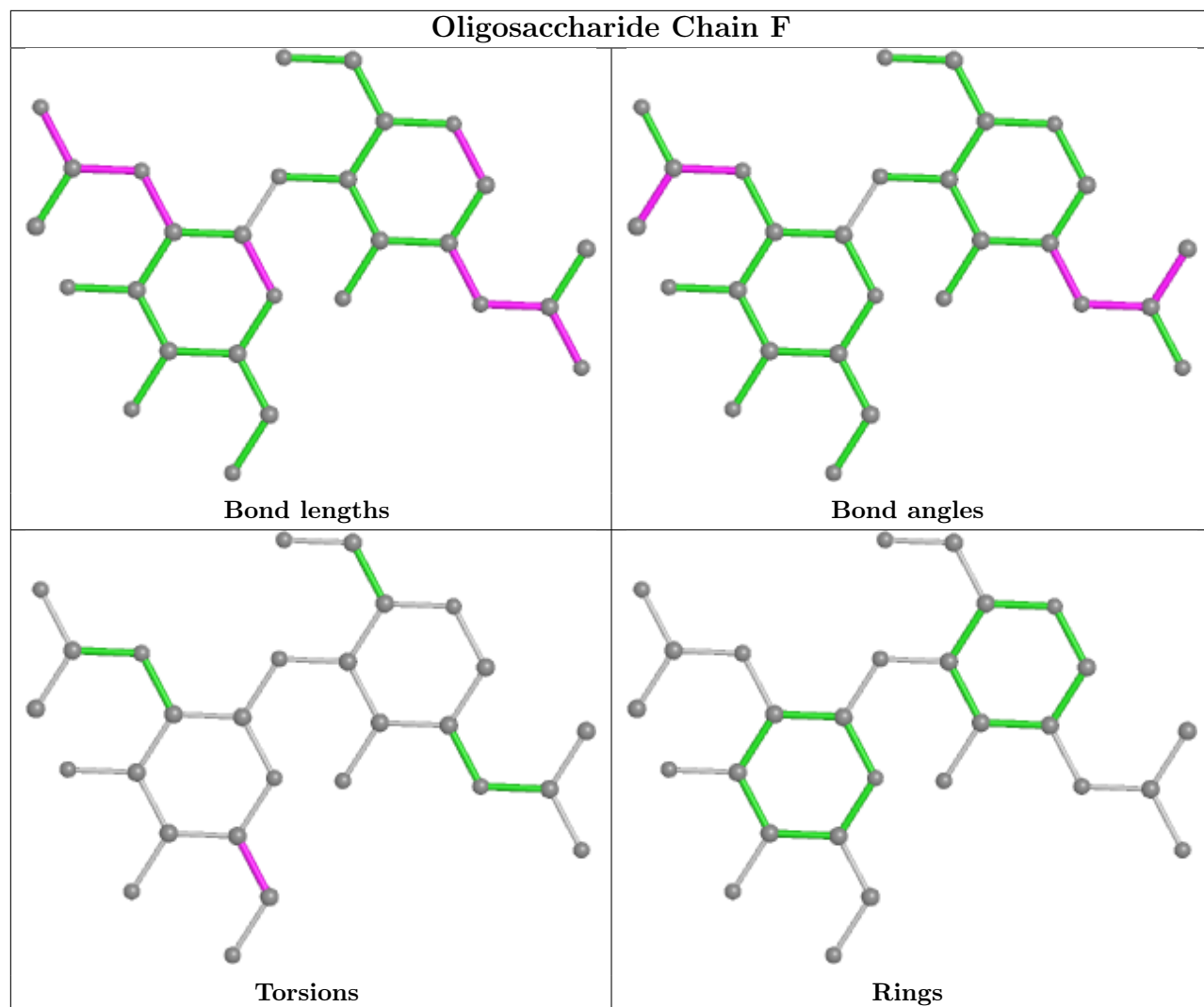
There are no ring outliers.

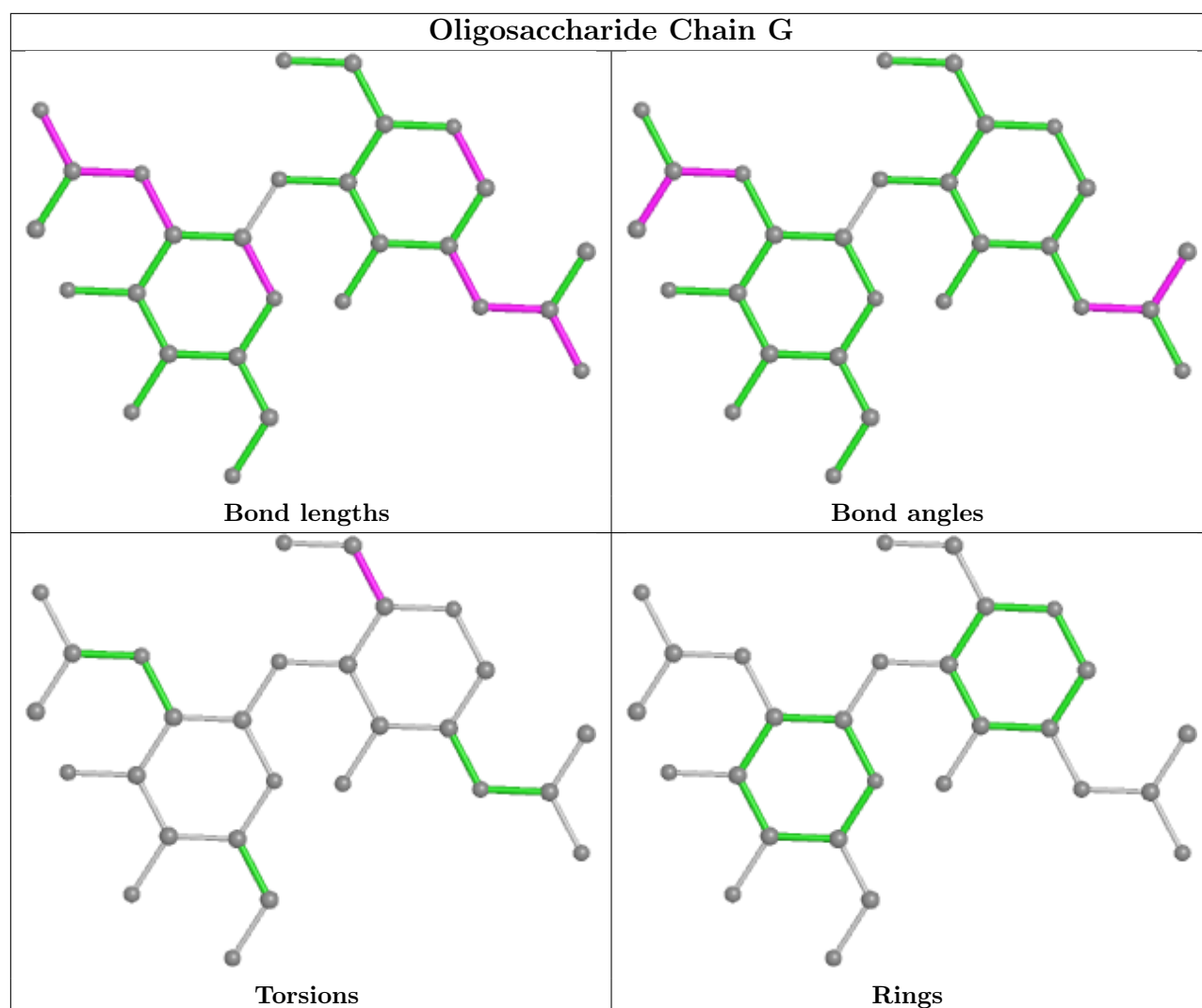
No monomer is involved in short contacts.

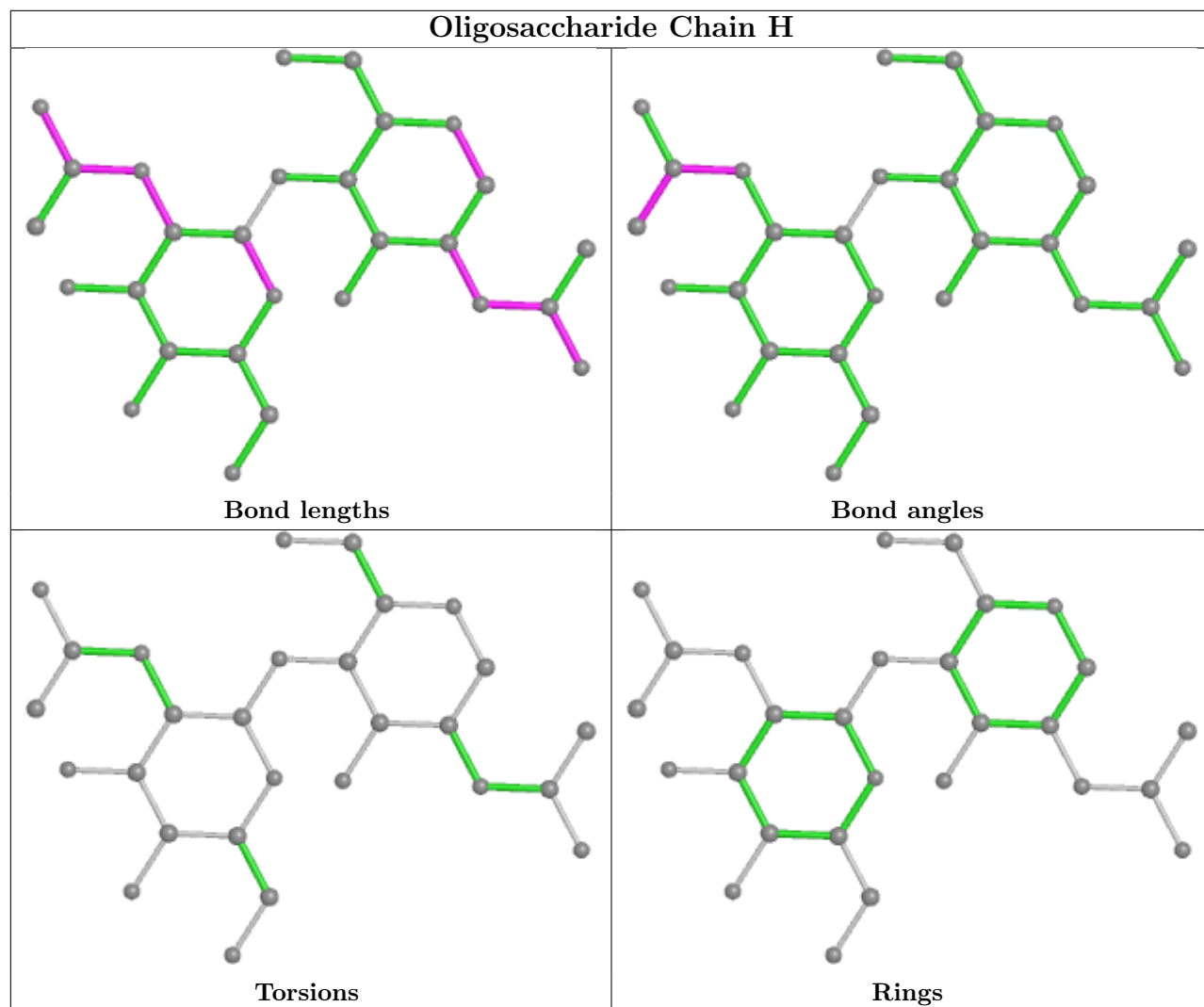
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



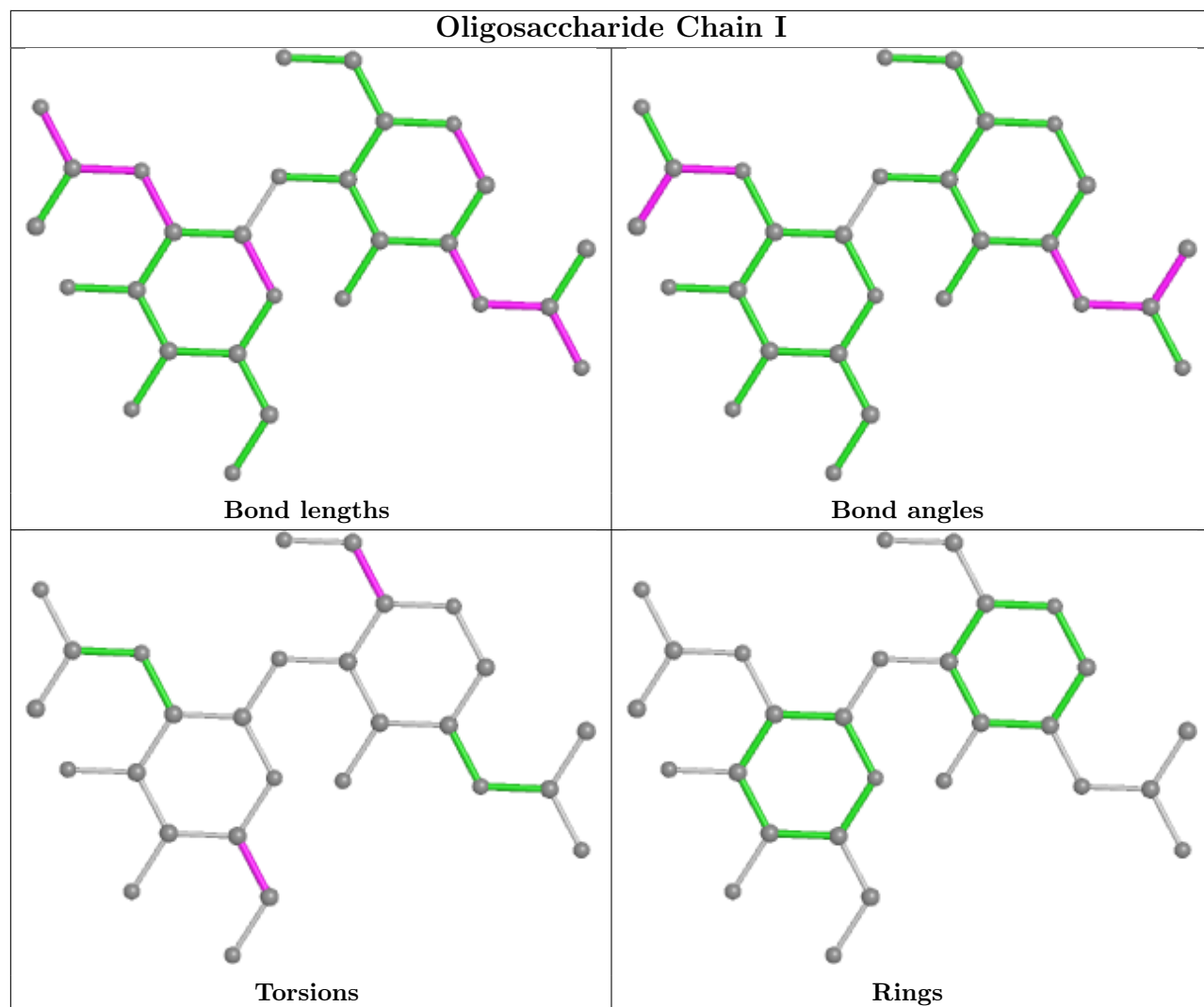


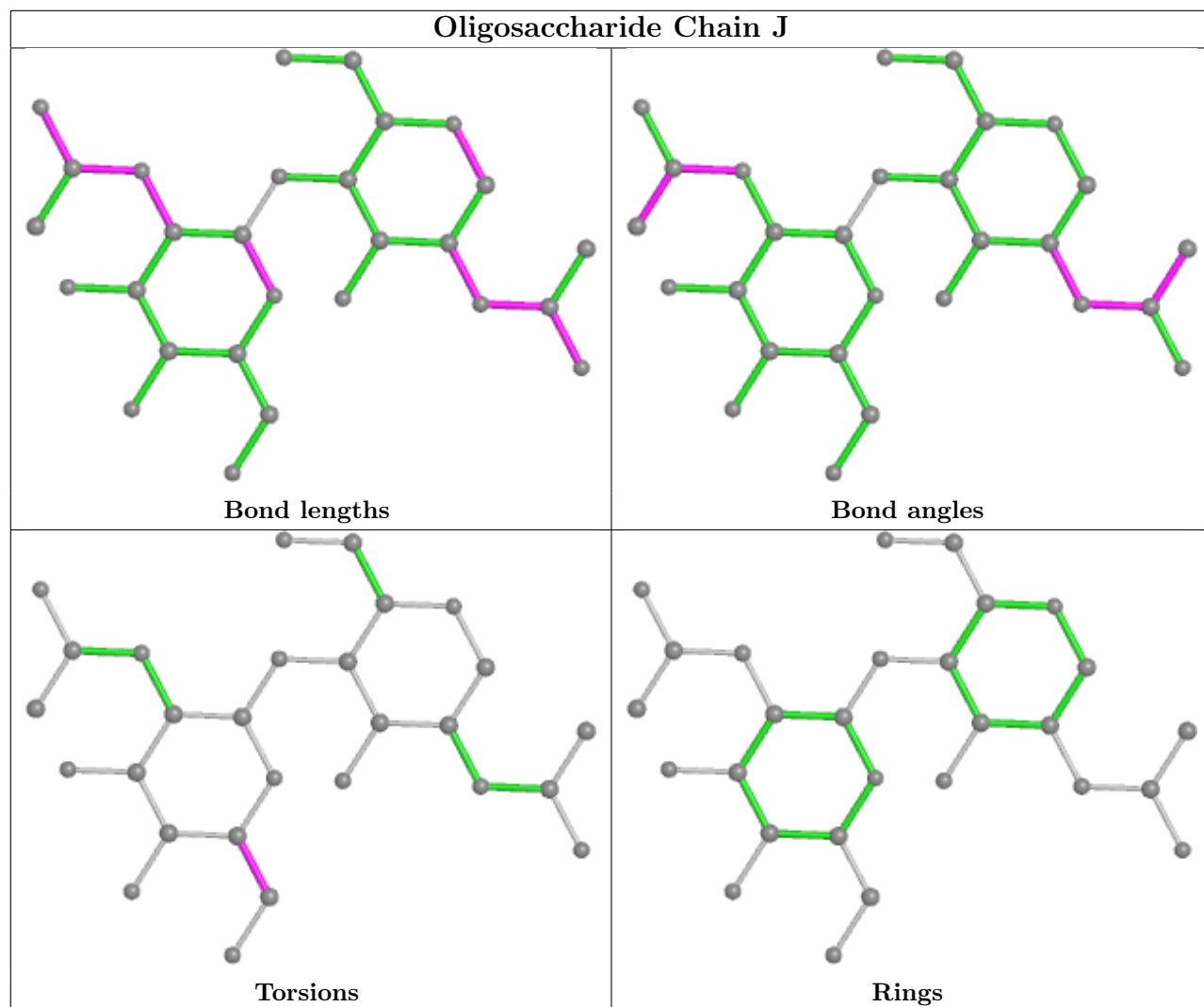


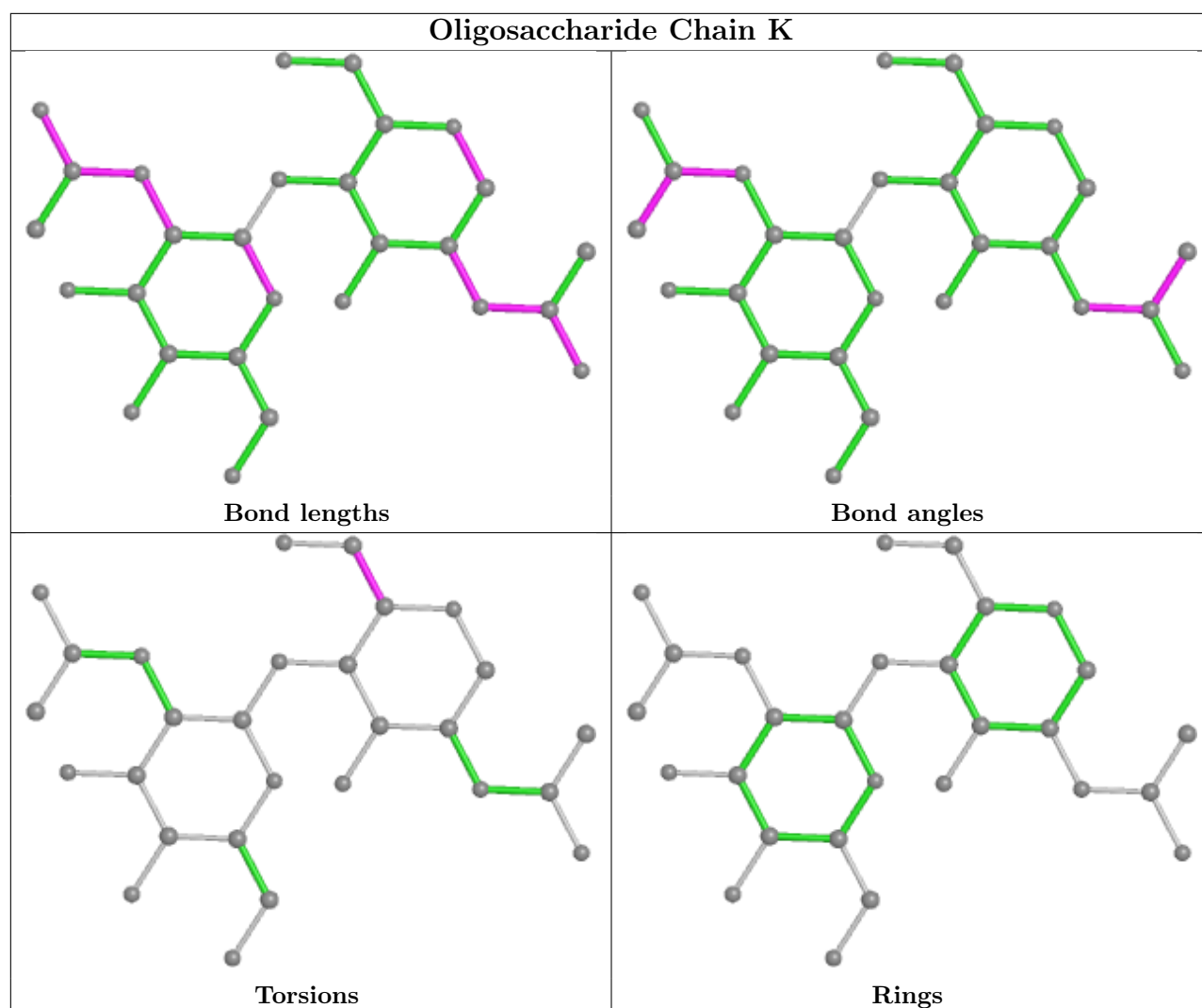


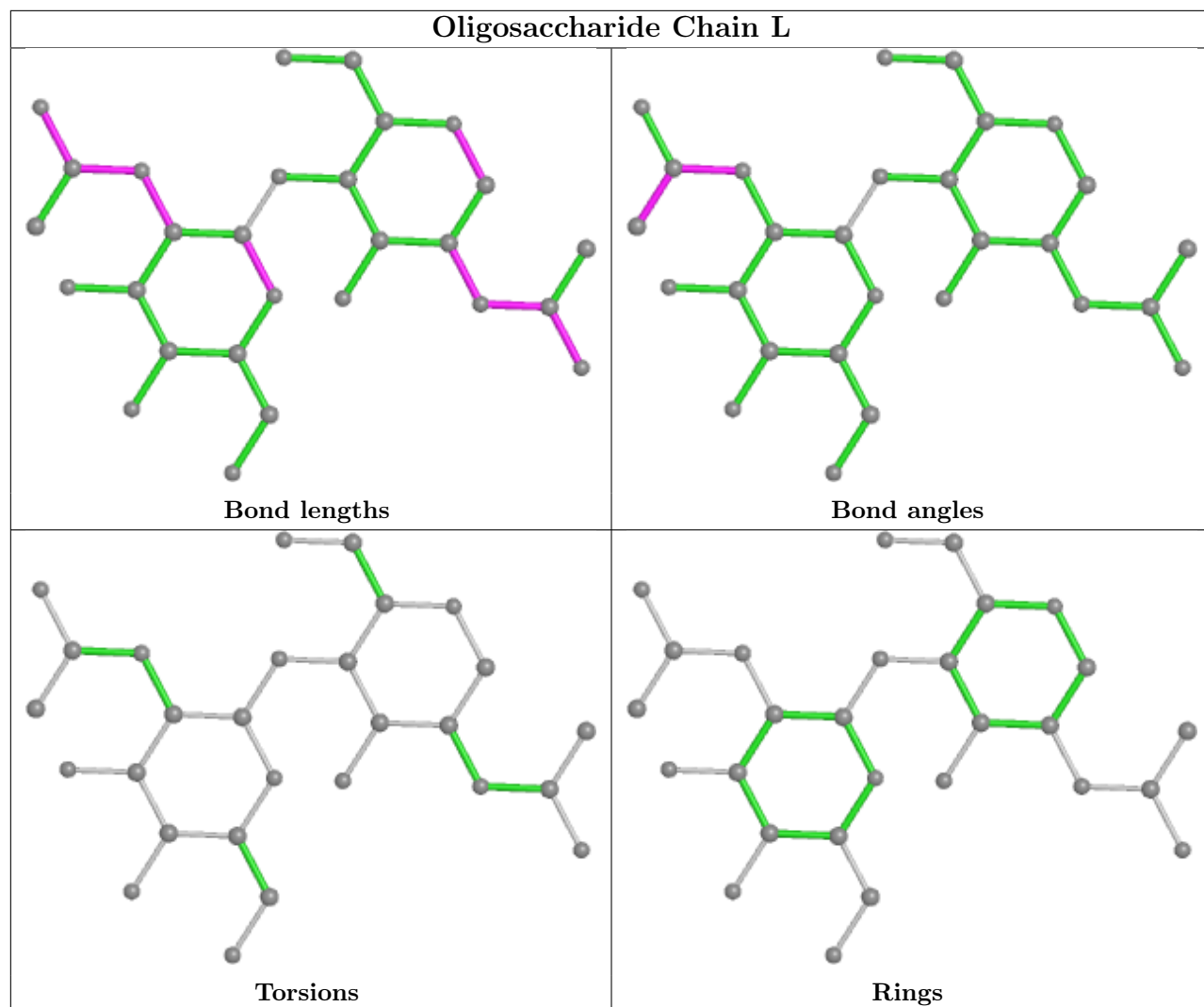


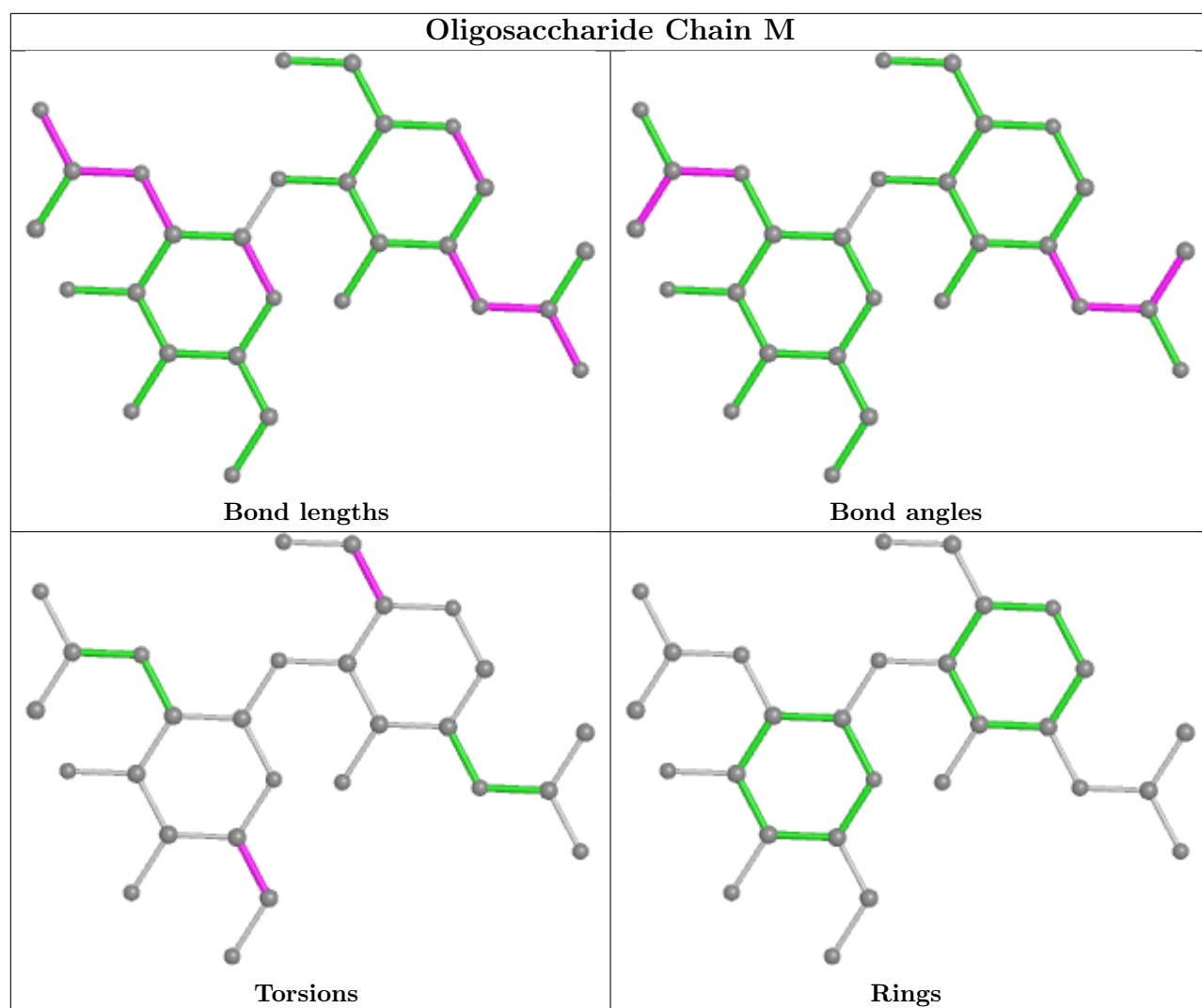


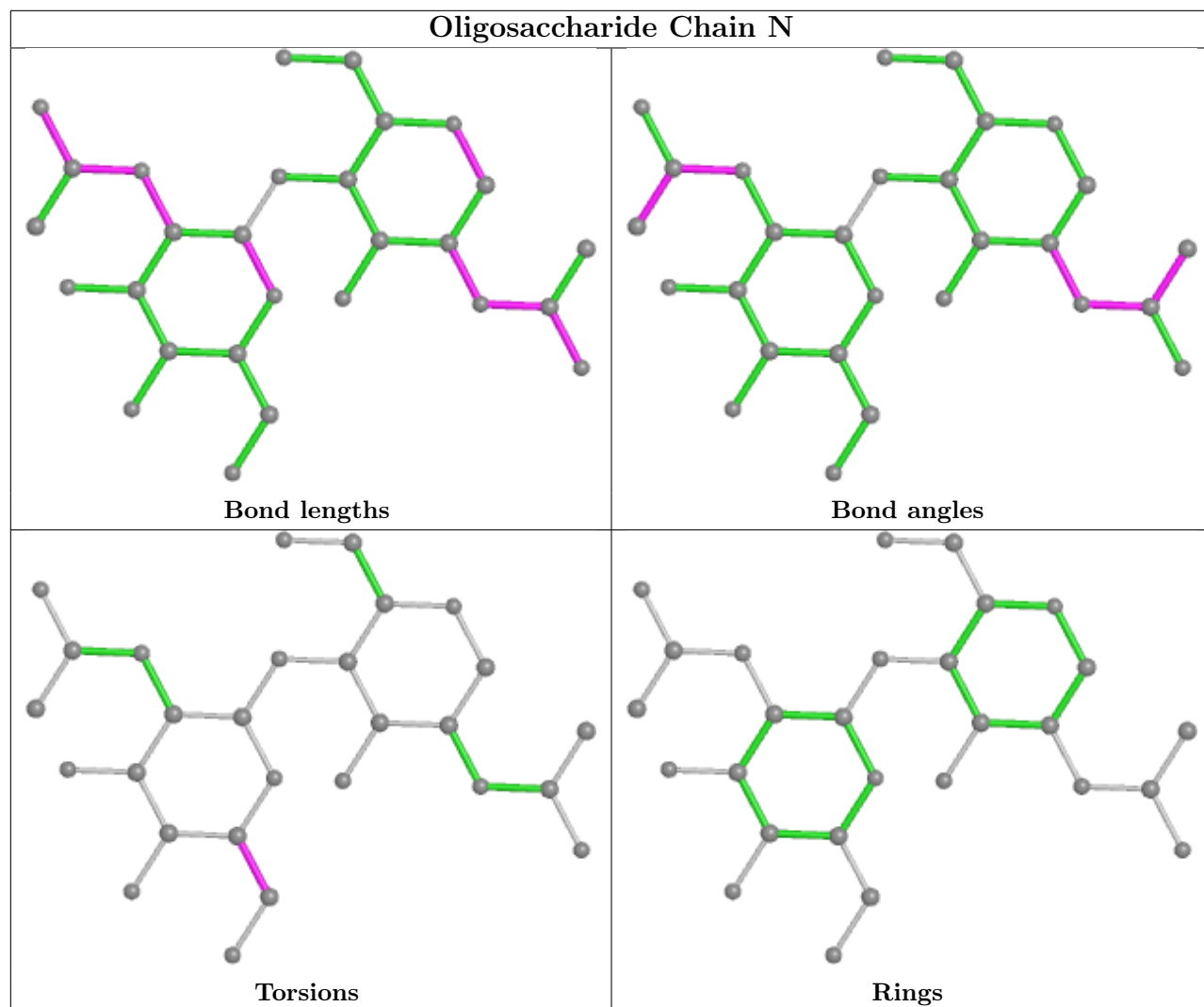


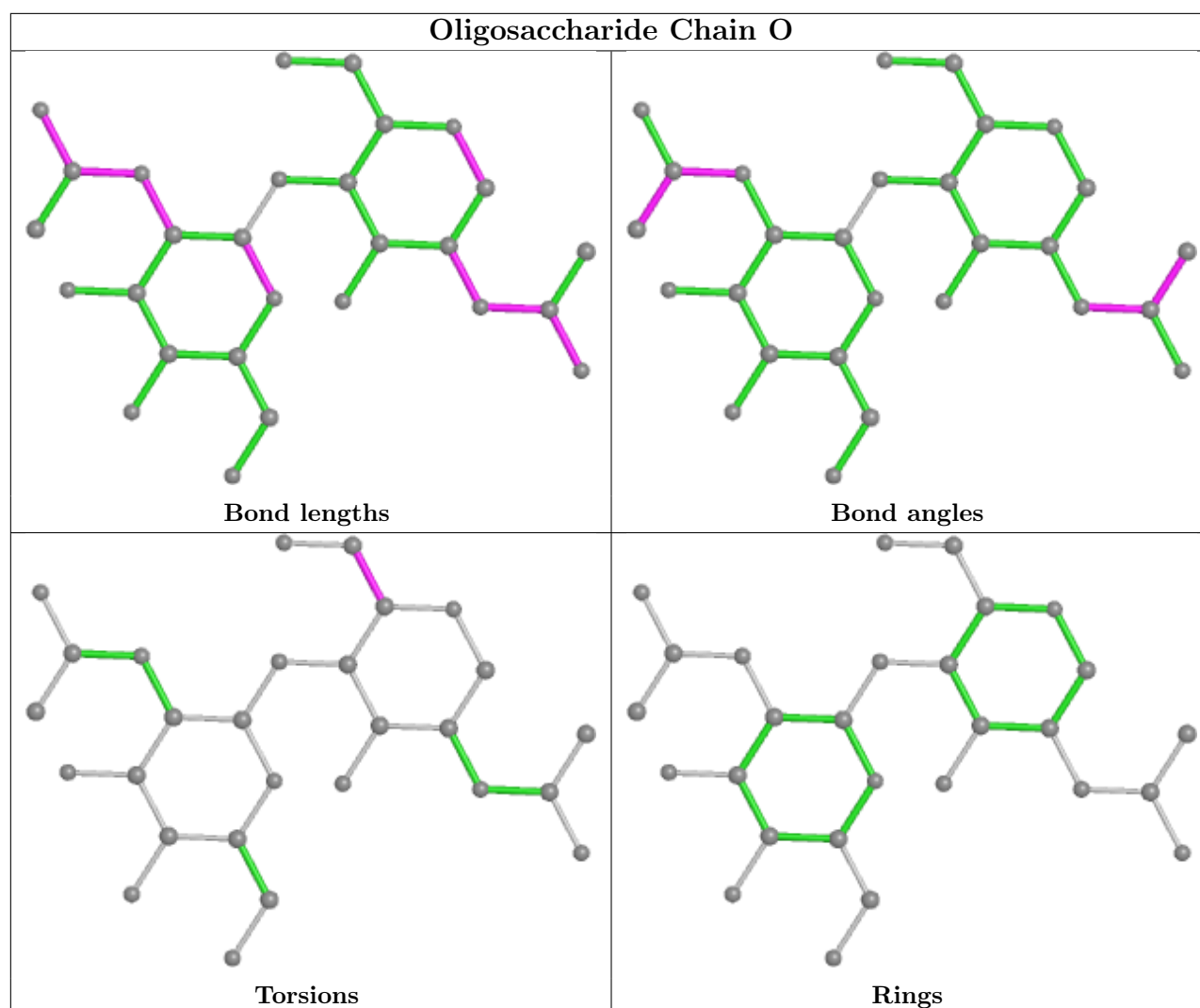












## 5.6 Ligand geometry [i](#)

42 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
3	NAG	B	1804	1	14,14,15	2.20	4 (28%)	17,19,21	0.84	0
3	NAG	C	1312	1	14,14,15	2.22	4 (28%)	17,19,21	0.99	1 (5%)
4	BLA	A	1313	-	42,46,46	3.59	19 (45%)	53,67,67	1.80	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1303	1	14,14,15	2.21	4 (28%)	17,19,21	0.84	0
3	NAG	A	1303	1	14,14,15	2.19	4 (28%)	17,19,21	0.85	0
3	NAG	C	1306	1	14,14,15	2.14	4 (28%)	17,19,21	0.94	1 (5%)
5	EIC	C	1314	-	19,19,19	0.82	0	19,19,19	1.03	0
3	NAG	B	1813	1	14,14,15	2.23	4 (28%)	17,19,21	1.00	1 (5%)
3	NAG	C	1308	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	C	1305	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	A	1304	1	14,14,15	2.18	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	B	1809	1	14,14,15	2.15	4 (28%)	17,19,21	1.00	1 (5%)
3	NAG	C	1310	1	14,14,15	2.15	4 (28%)	17,19,21	1.09	1 (5%)
5	EIC	A	1314	-	19,19,19	0.83	0	19,19,19	1.01	0
3	NAG	A	1305	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
4	BLA	C	1313	-	42,46,46	3.59	19 (45%)	53,67,67	1.80	12 (22%)
3	NAG	A	1307	1	14,14,15	2.16	4 (28%)	17,19,21	1.08	1 (5%)
3	NAG	A	1302	1	14,14,15	2.13	4 (28%)	17,19,21	1.49	3 (17%)
3	NAG	B	1805	1	14,14,15	2.19	4 (28%)	17,19,21	1.03	1 (5%)
4	BLA	B	1814	-	42,46,46	3.60	19 (45%)	53,67,67	1.80	11 (20%)
3	NAG	C	1304	1	14,14,15	2.19	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	C	1309	1	14,14,15	2.17	4 (28%)	17,19,21	1.05	1 (5%)
3	NAG	B	1812	1	14,14,15	2.15	4 (28%)	17,19,21	1.10	1 (5%)
3	NAG	C	1307	1	14,14,15	2.16	4 (28%)	17,19,21	1.08	1 (5%)
3	NAG	B	1807	1	14,14,15	2.15	4 (28%)	17,19,21	0.94	1 (5%)
5	EIC	B	1801	-	19,19,19	0.82	0	19,19,19	1.03	1 (5%)
3	NAG	A	1312	1	14,14,15	2.21	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	C	1302	1	14,14,15	2.11	4 (28%)	17,19,21	1.49	3 (17%)
3	NAG	A	1301	1	14,14,15	2.16	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	B	1808	1	14,14,15	2.17	4 (28%)	17,19,21	1.08	1 (5%)
3	NAG	B	1811	1	14,14,15	2.15	4 (28%)	17,19,21	1.10	1 (5%)
3	NAG	B	1803	1	14,14,15	2.13	4 (28%)	17,19,21	1.50	4 (23%)
3	NAG	B	1810	1	14,14,15	2.17	4 (28%)	17,19,21	1.04	1 (5%)
3	NAG	B	1802	1	14,14,15	2.17	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	B	1806	1	14,14,15	2.16	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	A	1311	1	14,14,15	2.16	4 (28%)	17,19,21	1.12	1 (5%)
3	NAG	A	1306	1	14,14,15	2.15	4 (28%)	17,19,21	0.94	1 (5%)
3	NAG	C	1301	1	14,14,15	2.17	4 (28%)	17,19,21	1.02	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1311	1	14,14,15	2.15	4 (28%)	17,19,21	1.13	1 (5%)
3	NAG	A	1308	1	14,14,15	2.15	4 (28%)	17,19,21	1.01	1 (5%)
3	NAG	A	1310	1	14,14,15	2.15	4 (28%)	17,19,21	1.10	2 (11%)
3	NAG	A	1309	1	14,14,15	2.17	4 (28%)	17,19,21	1.03	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
3	NAG	B	1804	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
4	BLA	A	1313	-	-	6/26/74/74	0/4/4/4
3	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	EIC	C	1314	-	-	6/17/17/17	-
3	NAG	B	1813	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1809	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	EIC	A	1314	-	-	6/17/17/17	-
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	BLA	C	1313	-	-	6/26/74/74	0/4/4/4
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1805	1	-	2/6/23/26	0/1/1/1
4	BLA	B	1814	-	-	6/26/74/74	0/4/4/4
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1812	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1807	1	-	2/6/23/26	0/1/1/1
5	EIC	B	1801	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1808	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1811	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1803	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1810	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1814	BLA	C4C-NC	10.08	1.54	1.37
4	C	1313	BLA	C4C-NC	10.06	1.54	1.37
4	A	1313	BLA	C4C-NC	10.04	1.54	1.37
4	A	1313	BLA	C1B-NB	9.82	1.54	1.37
4	C	1313	BLA	C1B-NB	9.76	1.54	1.37
4	B	1814	BLA	C1B-NB	9.74	1.54	1.37
4	B	1814	BLA	C4B-NB	7.47	1.53	1.38
4	C	1313	BLA	C4B-NB	7.45	1.53	1.38
4	A	1313	BLA	C4B-NB	7.43	1.53	1.38
4	A	1313	BLA	C1C-NC	7.22	1.53	1.38
4	C	1313	BLA	C1C-NC	7.18	1.53	1.38
4	B	1814	BLA	C1C-NC	7.17	1.53	1.38
4	A	1313	BLA	CHD-C1D	5.63	1.53	1.40
4	B	1814	BLA	CHD-C1D	5.62	1.53	1.40
4	C	1313	BLA	CHD-C1D	5.60	1.53	1.40
4	B	1814	BLA	C3D-C2D	5.57	1.48	1.36
4	C	1313	BLA	C3D-C2D	5.54	1.48	1.36
4	A	1313	BLA	C3D-C2D	5.53	1.48	1.36
3	B	1813	NAG	O5-C1	5.45	1.52	1.43
3	C	1312	NAG	O5-C1	5.42	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	NAG	O5-C1	5.39	1.52	1.43
3	A	1312	NAG	O5-C1	5.38	1.52	1.43
4	A	1313	BLA	C4D-ND	5.35	1.50	1.38
3	B	1804	NAG	O5-C1	5.34	1.52	1.43
3	B	1805	NAG	O5-C1	5.34	1.52	1.43
4	C	1313	BLA	C4D-ND	5.34	1.50	1.38
4	B	1814	BLA	C4D-ND	5.33	1.49	1.38
3	A	1303	NAG	O5-C1	5.31	1.52	1.43
3	B	1806	NAG	O5-C1	5.31	1.52	1.43
3	C	1304	NAG	O5-C1	5.31	1.52	1.43
3	C	1309	NAG	O5-C1	5.31	1.52	1.43
3	A	1309	NAG	O5-C1	5.30	1.52	1.43
3	A	1305	NAG	O5-C1	5.30	1.52	1.43
3	B	1810	NAG	O5-C1	5.29	1.52	1.43
3	A	1307	NAG	O5-C1	5.29	1.52	1.43
3	B	1808	NAG	O5-C1	5.29	1.52	1.43
3	C	1308	NAG	O5-C1	5.28	1.52	1.43
3	C	1311	NAG	O5-C1	5.28	1.52	1.43
3	C	1307	NAG	O5-C1	5.27	1.52	1.43
3	A	1301	NAG	O5-C1	5.27	1.52	1.43
3	B	1809	NAG	O5-C1	5.27	1.52	1.43
3	A	1306	NAG	O5-C1	5.27	1.52	1.43
3	A	1311	NAG	O5-C1	5.26	1.52	1.43
3	A	1304	NAG	O5-C1	5.25	1.52	1.43
3	A	1310	NAG	O5-C1	5.25	1.52	1.43
3	B	1802	NAG	O5-C1	5.25	1.52	1.43
3	C	1310	NAG	O5-C1	5.25	1.52	1.43
3	C	1305	NAG	O5-C1	5.25	1.52	1.43
3	B	1811	NAG	O5-C1	5.24	1.52	1.43
3	B	1812	NAG	O5-C1	5.24	1.52	1.43
3	C	1301	NAG	O5-C1	5.24	1.52	1.43
3	C	1306	NAG	O5-C1	5.24	1.52	1.43
3	A	1308	NAG	O5-C1	5.23	1.52	1.43
3	B	1807	NAG	O5-C1	5.23	1.52	1.43
4	B	1814	BLA	C4D-C3D	5.19	1.54	1.45
3	A	1302	NAG	O5-C1	5.18	1.52	1.43
3	B	1803	NAG	O5-C1	5.15	1.51	1.43
4	A	1313	BLA	C4D-C3D	5.13	1.53	1.45
4	C	1313	BLA	C4D-C3D	5.13	1.53	1.45
3	C	1302	NAG	O5-C1	5.10	1.51	1.43
4	B	1814	BLA	C1D-ND	4.58	1.47	1.36
4	C	1313	BLA	C1D-ND	4.57	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1313	BLA	C1D-ND	4.55	1.47	1.36
3	B	1813	NAG	C7-N2	4.01	1.48	1.34
3	A	1312	NAG	C7-N2	3.99	1.48	1.34
3	B	1805	NAG	C7-N2	3.99	1.48	1.34
3	C	1312	NAG	C7-N2	3.97	1.48	1.34
3	A	1304	NAG	C7-N2	3.97	1.48	1.34
3	C	1303	NAG	C7-N2	3.97	1.48	1.34
3	C	1304	NAG	C7-N2	3.96	1.48	1.34
3	A	1309	NAG	C7-N2	3.96	1.48	1.34
3	B	1804	NAG	C7-N2	3.95	1.47	1.34
3	C	1309	NAG	C7-N2	3.95	1.47	1.34
3	B	1810	NAG	C7-N2	3.94	1.47	1.34
3	B	1808	NAG	C7-N2	3.94	1.47	1.34
3	A	1302	NAG	C7-N2	3.94	1.47	1.34
3	B	1803	NAG	C7-N2	3.93	1.47	1.34
3	A	1303	NAG	C7-N2	3.93	1.47	1.34
3	A	1305	NAG	C7-N2	3.93	1.47	1.34
3	B	1809	NAG	C7-N2	3.93	1.47	1.34
3	B	1802	NAG	C7-N2	3.92	1.47	1.34
3	C	1308	NAG	C7-N2	3.92	1.47	1.34
3	A	1307	NAG	C7-N2	3.92	1.47	1.34
3	A	1308	NAG	C7-N2	3.92	1.47	1.34
3	C	1305	NAG	C7-N2	3.91	1.47	1.34
3	B	1806	NAG	C7-N2	3.91	1.47	1.34
3	C	1302	NAG	C7-N2	3.91	1.47	1.34
3	A	1301	NAG	C7-N2	3.91	1.47	1.34
3	C	1301	NAG	C7-N2	3.91	1.47	1.34
3	C	1307	NAG	C7-N2	3.91	1.47	1.34
3	A	1310	NAG	C7-N2	3.90	1.47	1.34
3	A	1306	NAG	C7-N2	3.90	1.47	1.34
3	C	1306	NAG	C7-N2	3.89	1.47	1.34
3	A	1311	NAG	C7-N2	3.89	1.47	1.34
3	B	1811	NAG	C7-N2	3.89	1.47	1.34
3	B	1807	NAG	C7-N2	3.89	1.47	1.34
3	B	1812	NAG	C7-N2	3.89	1.47	1.34
3	C	1310	NAG	C7-N2	3.89	1.47	1.34
3	C	1311	NAG	C7-N2	3.88	1.47	1.34
4	B	1814	BLA	C1A-CHA	3.57	1.55	1.41
4	C	1313	BLA	C1A-CHA	3.57	1.55	1.41
4	A	1313	BLA	C1A-CHA	3.55	1.54	1.41
3	C	1303	NAG	C2-N2	3.32	1.52	1.46
3	A	1303	NAG	C2-N2	3.29	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1804	NAG	C2-N2	3.28	1.51	1.46
4	B	1814	BLA	C4A-CHB	3.24	1.53	1.41
3	C	1312	NAG	C2-N2	3.23	1.51	1.46
4	A	1313	BLA	C4A-CHB	3.23	1.53	1.41
4	C	1313	BLA	C4A-CHB	3.21	1.53	1.41
3	B	1813	NAG	C2-N2	3.21	1.51	1.46
3	C	1304	NAG	C2-N2	3.21	1.51	1.46
3	A	1312	NAG	C2-N2	3.20	1.51	1.46
3	A	1304	NAG	C2-N2	3.17	1.51	1.46
3	B	1805	NAG	C2-N2	3.13	1.51	1.46
3	C	1305	NAG	C2-N2	3.11	1.51	1.46
3	C	1307	NAG	C2-N2	3.11	1.51	1.46
3	B	1803	NAG	C2-N2	3.11	1.51	1.46
3	B	1808	NAG	C2-N2	3.10	1.51	1.46
3	C	1301	NAG	C2-N2	3.10	1.51	1.46
3	C	1308	NAG	C2-N2	3.09	1.51	1.46
3	C	1311	NAG	C2-N2	3.09	1.51	1.46
3	A	1302	NAG	C2-N2	3.09	1.51	1.46
3	B	1812	NAG	C2-N2	3.07	1.51	1.46
3	B	1810	NAG	C2-N2	3.07	1.51	1.46
3	B	1802	NAG	C2-N2	3.07	1.51	1.46
3	A	1305	NAG	C2-N2	3.06	1.51	1.46
3	B	1807	NAG	C2-N2	3.06	1.51	1.46
3	C	1309	NAG	C2-N2	3.06	1.51	1.46
3	A	1311	NAG	C2-N2	3.06	1.51	1.46
3	C	1302	NAG	C2-N2	3.05	1.51	1.46
3	A	1307	NAG	C2-N2	3.04	1.51	1.46
3	A	1309	NAG	C2-N2	3.04	1.51	1.46
3	A	1308	NAG	C2-N2	3.04	1.51	1.46
3	B	1811	NAG	C2-N2	3.02	1.51	1.46
3	B	1806	NAG	C2-N2	3.02	1.51	1.46
3	C	1310	NAG	C2-N2	3.01	1.51	1.46
3	B	1809	NAG	C2-N2	3.01	1.51	1.46
3	C	1306	NAG	C2-N2	3.01	1.51	1.46
3	A	1301	NAG	C2-N2	3.01	1.51	1.46
3	A	1306	NAG	C2-N2	3.00	1.51	1.46
3	A	1310	NAG	C2-N2	3.00	1.51	1.46
4	C	1313	BLA	OC-C1C	-2.77	1.18	1.23
4	A	1313	BLA	OC-C1C	-2.76	1.18	1.23
4	B	1814	BLA	C3C-C2C	2.75	1.42	1.37
4	A	1313	BLA	C3C-C2C	2.74	1.42	1.37
4	B	1814	BLA	OC-C1C	-2.73	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1313	BLA	C3C-C2C	2.73	1.42	1.37
4	B	1814	BLA	C1B-C2B	2.63	1.49	1.45
4	A	1313	BLA	C3C-C4C	2.63	1.49	1.45
4	C	1313	BLA	C3B-C2B	2.62	1.42	1.37
4	C	1313	BLA	C1B-C2B	2.61	1.49	1.45
4	A	1313	BLA	C3B-C2B	2.59	1.42	1.37
4	B	1814	BLA	C3B-C2B	2.59	1.42	1.37
4	B	1814	BLA	C3C-C4C	2.58	1.49	1.45
4	A	1313	BLA	C1B-C2B	2.56	1.49	1.45
4	B	1814	BLA	CHA-C4D	-2.56	1.33	1.35
4	C	1313	BLA	C3C-C4C	2.54	1.49	1.45
4	C	1313	BLA	OB-C4B	-2.54	1.18	1.23
4	C	1313	BLA	CHA-C4D	-2.53	1.33	1.35
4	B	1814	BLA	OB-C4B	-2.53	1.18	1.23
4	A	1313	BLA	OB-C4B	-2.50	1.18	1.23
4	A	1313	BLA	CHA-C4D	-2.49	1.33	1.35
3	B	1804	NAG	O7-C7	-2.19	1.18	1.23
3	B	1808	NAG	O7-C7	-2.17	1.18	1.23
3	A	1306	NAG	O7-C7	-2.17	1.18	1.23
3	A	1308	NAG	O7-C7	-2.17	1.18	1.23
3	A	1311	NAG	O7-C7	-2.16	1.18	1.23
3	C	1309	NAG	O7-C7	-2.16	1.18	1.23
3	B	1802	NAG	O7-C7	-2.16	1.18	1.23
3	C	1308	NAG	O7-C7	-2.15	1.18	1.23
3	C	1304	NAG	O7-C7	-2.15	1.18	1.23
3	C	1301	NAG	O7-C7	-2.14	1.18	1.23
3	A	1309	NAG	O7-C7	-2.14	1.18	1.23
3	B	1806	NAG	O7-C7	-2.14	1.18	1.23
3	C	1303	NAG	O7-C7	-2.14	1.18	1.23
3	B	1811	NAG	O7-C7	-2.14	1.18	1.23
3	B	1807	NAG	O7-C7	-2.14	1.18	1.23
3	C	1306	NAG	O7-C7	-2.14	1.18	1.23
3	C	1311	NAG	O7-C7	-2.14	1.18	1.23
3	A	1307	NAG	O7-C7	-2.14	1.18	1.23
3	B	1812	NAG	O7-C7	-2.14	1.18	1.23
3	A	1304	NAG	O7-C7	-2.13	1.18	1.23
3	A	1310	NAG	O7-C7	-2.13	1.18	1.23
3	C	1310	NAG	O7-C7	-2.13	1.18	1.23
3	A	1301	NAG	O7-C7	-2.13	1.18	1.23
3	B	1803	NAG	O7-C7	-2.13	1.18	1.23
3	A	1303	NAG	O7-C7	-2.13	1.18	1.23
3	C	1312	NAG	O7-C7	-2.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	NAG	O7-C7	-2.12	1.18	1.23
3	B	1810	NAG	O7-C7	-2.11	1.18	1.23
3	B	1805	NAG	O7-C7	-2.11	1.18	1.23
3	C	1302	NAG	O7-C7	-2.11	1.18	1.23
3	C	1305	NAG	O7-C7	-2.11	1.18	1.23
3	A	1305	NAG	O7-C7	-2.11	1.18	1.23
3	A	1312	NAG	O7-C7	-2.10	1.18	1.23
3	C	1307	NAG	O7-C7	-2.10	1.18	1.23
3	B	1813	NAG	O7-C7	-2.10	1.18	1.23
3	B	1809	NAG	O7-C7	-2.10	1.18	1.23
4	B	1814	BLA	CAB-C3B	2.08	1.53	1.47
4	C	1313	BLA	CAB-C3B	2.04	1.53	1.47
4	A	1313	BLA	CAB-C3B	2.04	1.53	1.47

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1814	BLA	C1A-CHA-C4D	-6.43	121.12	128.81
4	C	1313	BLA	C1A-CHA-C4D	-6.43	121.13	128.81
4	A	1313	BLA	C1A-CHA-C4D	-6.41	121.15	128.81
4	A	1313	BLA	C3D-C4D-ND	-4.45	103.58	110.05
4	C	1313	BLA	C3D-C4D-ND	-4.44	103.59	110.05
4	B	1814	BLA	C3D-C4D-ND	-4.44	103.59	110.05
4	A	1313	BLA	C4C-CHD-C1D	-3.29	120.05	128.08
4	B	1814	BLA	C4C-CHD-C1D	-3.27	120.10	128.08
4	C	1313	BLA	C4C-CHD-C1D	-3.25	120.14	128.08
3	A	1302	NAG	C1-O5-C5	-3.18	107.88	112.19
3	C	1302	NAG	C1-O5-C5	-3.15	107.93	112.19
3	B	1803	NAG	C1-O5-C5	-3.13	107.95	112.19
4	A	1313	BLA	C4D-ND-C1D	2.68	111.56	106.51
4	C	1313	BLA	C4D-ND-C1D	2.68	111.56	106.51
4	B	1814	BLA	C4D-ND-C1D	2.68	111.56	106.51
4	C	1313	BLA	C4D-C3D-C2D	2.55	109.60	106.78
4	A	1313	BLA	C4D-C3D-C2D	2.53	109.58	106.78
4	B	1814	BLA	C4D-C3D-C2D	2.49	109.54	106.78
4	A	1313	BLA	C1B-NB-C4B	-2.42	107.58	110.67
4	B	1814	BLA	C1B-NB-C4B	-2.42	107.59	110.67
4	C	1313	BLA	C1B-NB-C4B	-2.40	107.61	110.67
3	C	1311	NAG	C8-C7-N2	2.38	120.12	116.10
4	A	1313	BLA	CHA-C4D-C3D	2.35	130.75	125.32
4	C	1313	BLA	CHA-C4D-C3D	2.35	130.74	125.32
4	A	1313	BLA	C3B-C2B-C1B	2.34	110.85	108.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1814	BLA	CHA-C4D-C3D	2.33	130.70	125.32
3	B	1812	NAG	C8-C7-N2	2.33	120.04	116.10
3	B	1811	NAG	C8-C7-N2	2.31	120.01	116.10
3	C	1307	NAG	C8-C7-N2	2.30	120.00	116.10
4	C	1313	BLA	C3B-C2B-C1B	2.30	110.81	108.03
3	A	1307	NAG	C8-C7-N2	2.30	120.00	116.10
3	B	1808	NAG	C8-C7-N2	2.29	119.98	116.10
3	B	1809	NAG	C8-C7-N2	2.29	119.98	116.10
3	A	1310	NAG	C8-C7-N2	2.29	119.98	116.10
3	A	1311	NAG	C8-C7-N2	2.29	119.98	116.10
3	C	1308	NAG	C8-C7-N2	2.28	119.96	116.10
3	A	1308	NAG	C8-C7-N2	2.28	119.96	116.10
3	C	1310	NAG	C8-C7-N2	2.28	119.95	116.10
4	A	1313	BLA	CHA-C4D-ND	-2.28	125.67	128.83
4	C	1313	BLA	CHA-C4D-ND	-2.28	125.67	128.83
4	B	1814	BLA	C3B-C2B-C1B	2.27	110.77	108.03
3	C	1305	NAG	C8-C7-N2	2.26	119.92	116.10
4	B	1814	BLA	CHA-C4D-ND	-2.25	125.70	128.83
3	B	1806	NAG	C8-C7-N2	2.25	119.91	116.10
3	A	1305	NAG	C8-C7-N2	2.24	119.90	116.10
3	B	1810	NAG	C8-C7-N2	2.24	119.90	116.10
3	C	1301	NAG	C8-C7-N2	2.23	119.88	116.10
3	C	1309	NAG	C8-C7-N2	2.23	119.88	116.10
3	B	1802	NAG	C8-C7-N2	2.23	119.87	116.10
3	C	1302	NAG	C8-C7-N2	2.22	119.86	116.10
3	A	1301	NAG	C8-C7-N2	2.21	119.85	116.10
3	A	1309	NAG	C8-C7-N2	2.21	119.84	116.10
3	B	1805	NAG	C8-C7-N2	2.21	119.84	116.10
4	C	1313	BLA	C4C-NC-C1C	-2.18	107.90	110.67
4	B	1814	BLA	C4B-C3B-C2B	2.18	110.72	107.92
3	C	1304	NAG	C8-C7-N2	2.18	119.78	116.10
4	B	1814	BLA	C4C-NC-C1C	-2.17	107.90	110.67
3	A	1304	NAG	C8-C7-N2	2.17	119.77	116.10
3	A	1312	NAG	C8-C7-N2	2.17	119.77	116.10
3	A	1302	NAG	C8-C7-N2	2.17	119.77	116.10
3	C	1312	NAG	C8-C7-N2	2.16	119.76	116.10
4	A	1313	BLA	C4C-NC-C1C	-2.16	107.92	110.67
3	B	1813	NAG	C8-C7-N2	2.14	119.72	116.10
4	C	1313	BLA	C4B-C3B-C2B	2.14	110.67	107.92
3	B	1807	NAG	C8-C7-N2	2.12	119.69	116.10
4	A	1313	BLA	C4B-C3B-C2B	2.12	110.65	107.92
3	B	1803	NAG	C8-C7-N2	2.12	119.69	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1306	NAG	C8-C7-N2	2.12	119.68	116.10
3	C	1306	NAG	C8-C7-N2	2.11	119.67	116.10
3	B	1803	NAG	C1-C2-N2	-2.07	106.95	110.49
3	A	1302	NAG	C4-C3-C2	2.05	114.03	111.02
3	B	1803	NAG	C4-C3-C2	2.05	114.02	111.02
3	C	1302	NAG	C4-C3-C2	2.03	113.99	111.02
3	A	1310	NAG	C2-N2-C7	-2.03	120.02	122.90
4	C	1313	BLA	CBA-CAA-C2A	-2.02	109.17	112.62
5	B	1801	EIC	C3-C2-C1	-2.02	109.38	114.47
4	A	1313	BLA	CBA-CAA-C2A	-2.01	109.19	112.62

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C1-C2-N2-C7
3	B	1803	NAG	C1-C2-N2-C7
4	A	1313	BLA	NA-C4A-CHB-C1B
4	A	1313	BLA	C3A-C4A-CHB-C1B
4	C	1313	BLA	NA-C4A-CHB-C1B
4	C	1313	BLA	C3A-C4A-CHB-C1B
4	B	1814	BLA	NA-C4A-CHB-C1B
4	B	1814	BLA	C3A-C4A-CHB-C1B
3	B	1804	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	B	1806	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1805	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	B	1810	NAG	C4-C5-C6-O6
3	B	1810	NAG	O5-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1804	NAG	C4-C5-C6-O6

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
3	B	1807	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1806	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1805	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	B	1807	NAG	C4-C5-C6-O6
5	A	1314	EIC	C1-C2-C3-C4
5	C	1314	EIC	C1-C2-C3-C4
5	B	1801	EIC	C1-C2-C3-C4
3	B	1811	NAG	O5-C5-C6-O6
3	B	1811	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1808	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	B	1803	NAG	O5-C5-C6-O6
5	B	1801	EIC	C4-C5-C6-C7
5	A	1314	EIC	C4-C5-C6-C7
5	C	1314	EIC	C4-C5-C6-C7
3	A	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	B	1808	NAG	O5-C5-C6-O6
4	A	1313	BLA	C2C-C3C-CAC-CBC
4	C	1313	BLA	C2C-C3C-CAC-CBC
4	B	1814	BLA	C2C-C3C-CAC-CBC
3	A	1303	NAG	C1-C2-N2-C7
3	B	1804	NAG	C1-C2-N2-C7
3	C	1303	NAG	C1-C2-N2-C7
5	B	1801	EIC	C7-C8-C9-C10
5	A	1314	EIC	C7-C8-C9-C10
5	C	1314	EIC	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	1314	EIC	C6-C7-C8-C9
5	C	1314	EIC	C6-C7-C8-C9
3	A	1302	NAG	C3-C2-N2-C7
3	C	1302	NAG	C3-C2-N2-C7
3	B	1803	NAG	C3-C2-N2-C7
5	B	1801	EIC	C6-C7-C8-C9
5	A	1314	EIC	O2-C1-C2-C3
5	C	1314	EIC	O2-C1-C2-C3
5	B	1801	EIC	O2-C1-C2-C3
4	A	1313	BLA	C4C-C3C-CAC-CBC
4	C	1313	BLA	C4C-C3C-CAC-CBC
4	B	1814	BLA	C4C-C3C-CAC-CBC
5	A	1314	EIC	O1-C1-C2-C3
5	C	1314	EIC	O1-C1-C2-C3
5	B	1801	EIC	O1-C1-C2-C3
4	A	1313	BLA	CAA-CBA-CGA-O2A
4	C	1313	BLA	CAA-CBA-CGA-O2A
4	B	1814	BLA	CAA-CBA-CGA-O2A
3	A	1303	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7
3	B	1804	NAG	C3-C2-N2-C7
4	A	1313	BLA	CAA-CBA-CGA-O1A
4	C	1313	BLA	CAA-CBA-CGA-O1A
4	B	1814	BLA	CAA-CBA-CGA-O1A

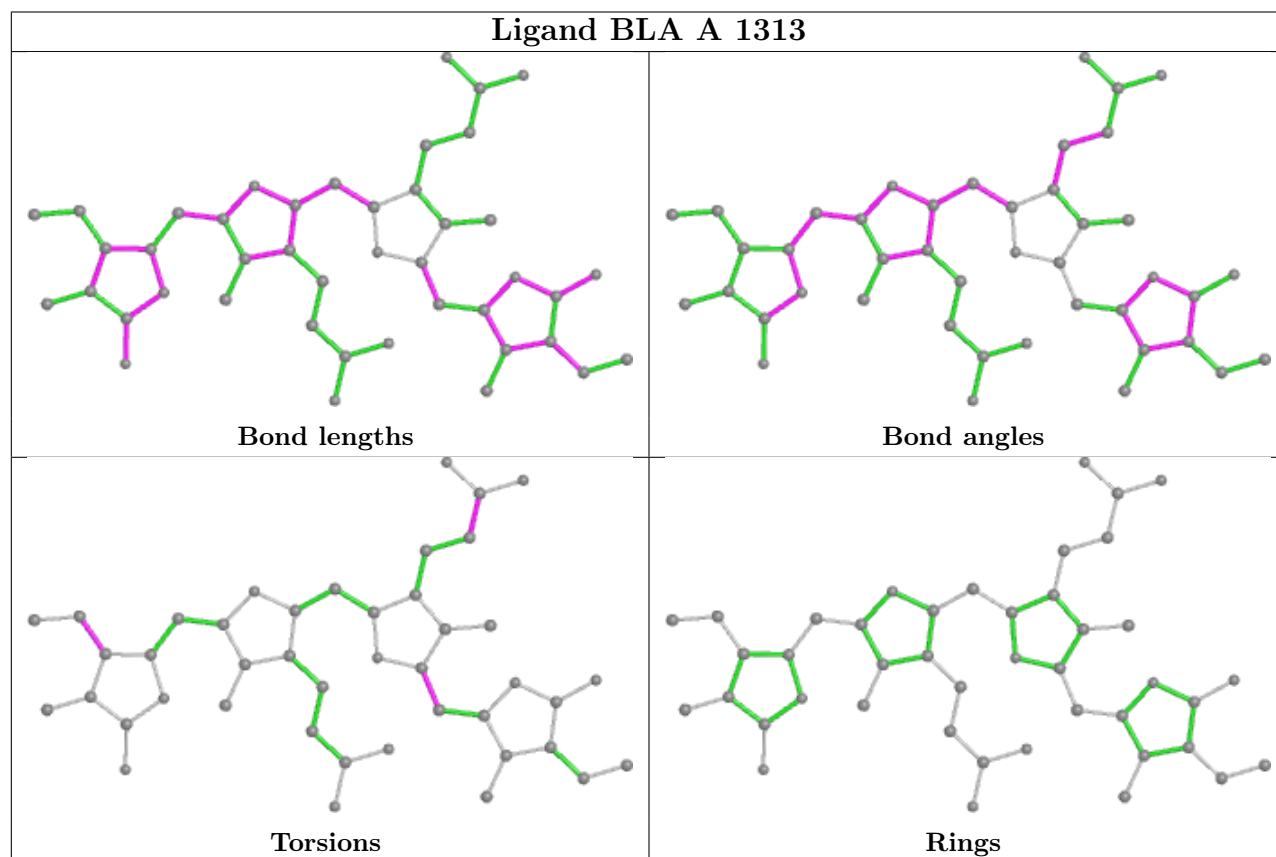
There are no ring outliers.

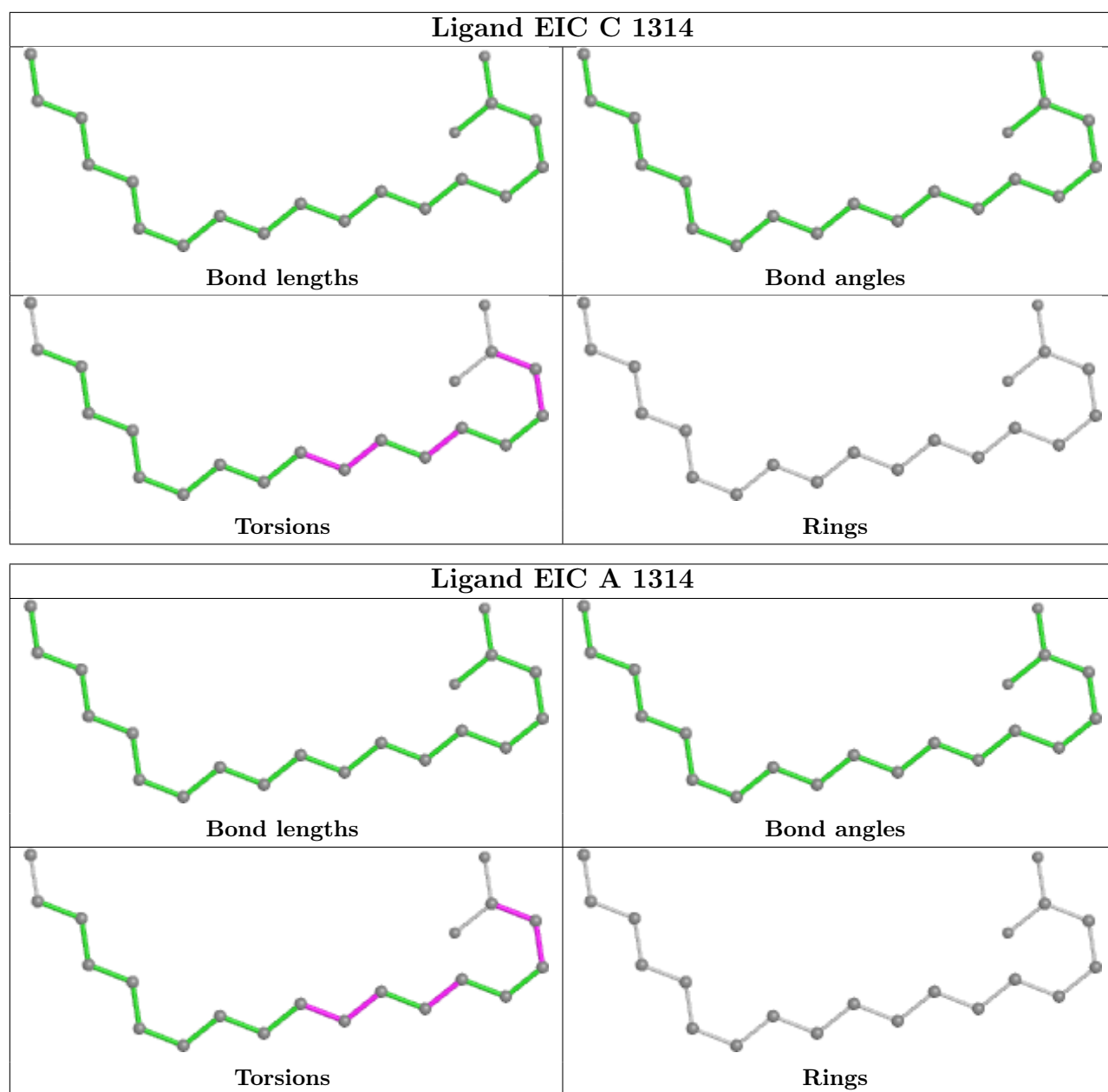
8 monomers are involved in 8 short contacts:

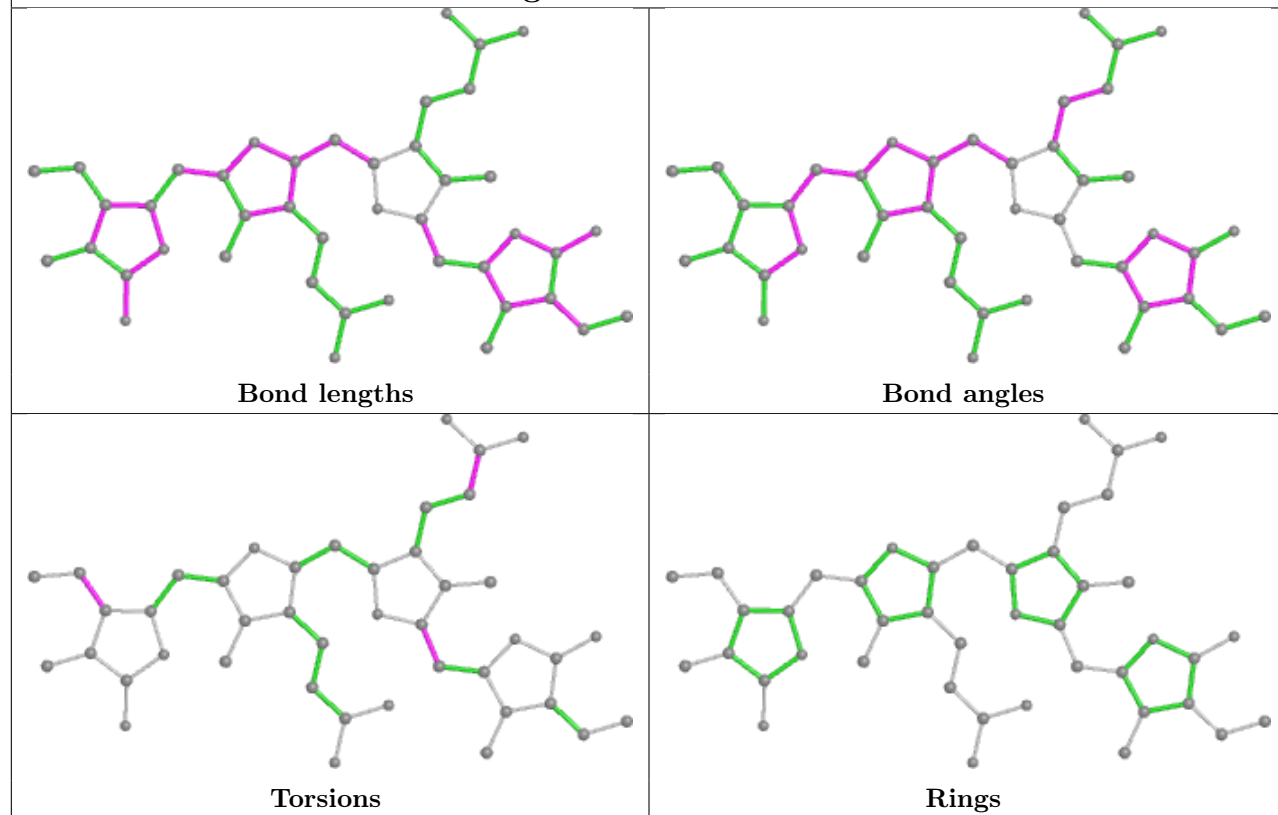
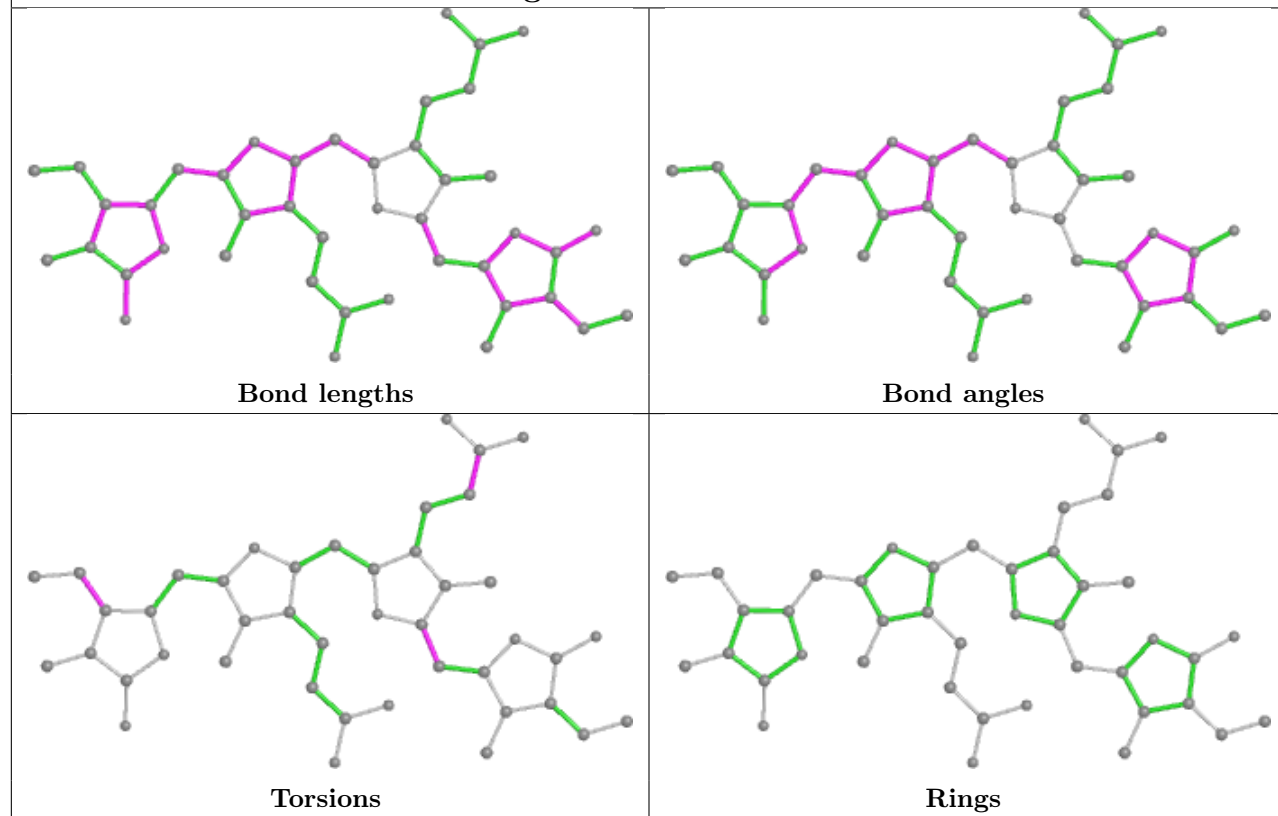
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1312	NAG	1	0
4	A	1313	BLA	1	0
3	B	1813	NAG	1	0
4	C	1313	BLA	1	0
3	A	1302	NAG	1	0
4	B	1814	BLA	1	0
3	A	1312	NAG	1	0
3	C	1302	NAG	1	0

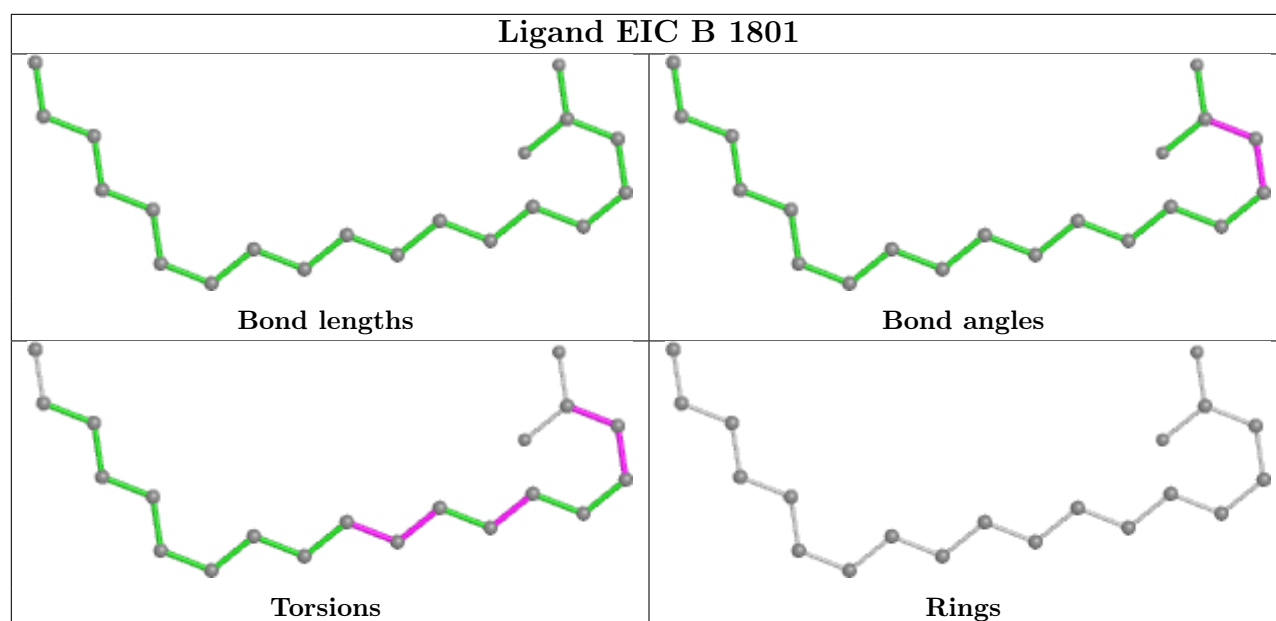
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.





**Ligand BLA C 1313****Ligand BLA B 1814**



## 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.

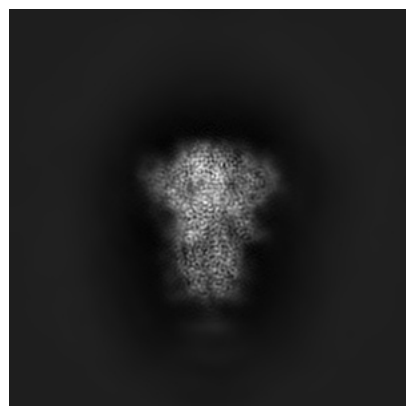
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33456. These allow visual inspection of the internal detail of the map and identification of artifacts.

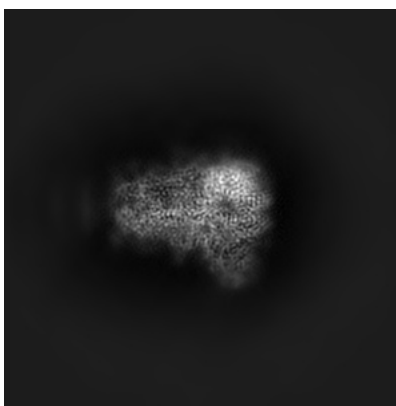
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

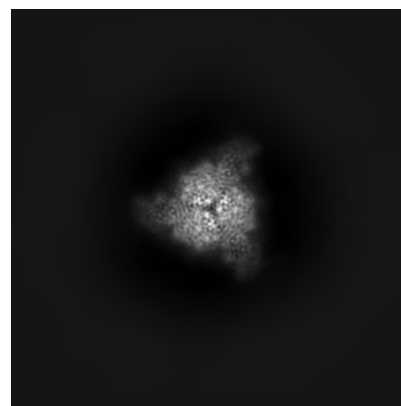
#### 6.1.1 Primary map



X

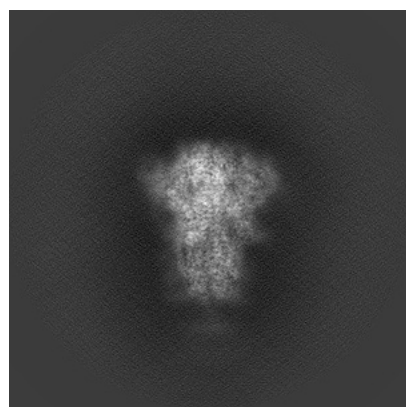


Y

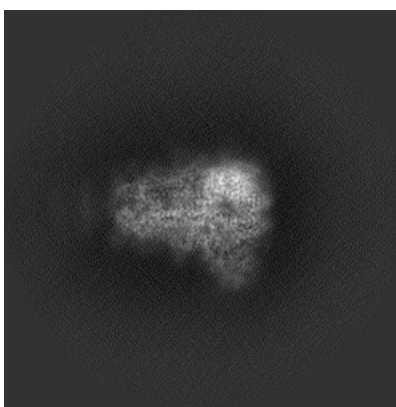


Z

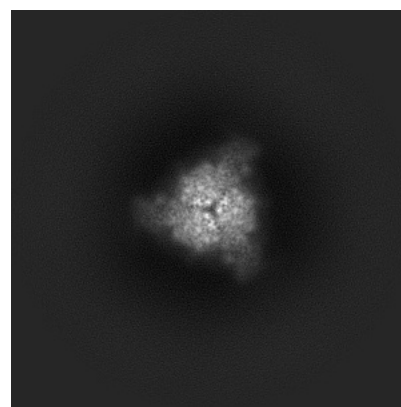
#### 6.1.2 Raw map



X



Y



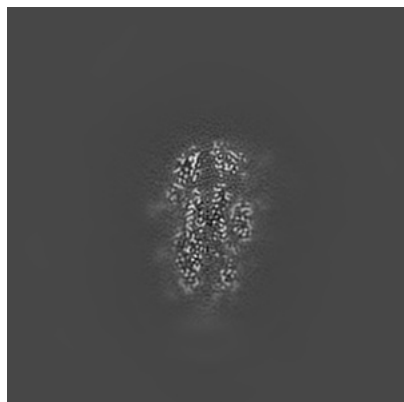
Z

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

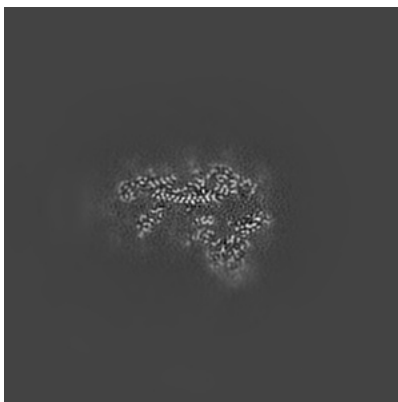


## 6.2 Central slices [i](#)

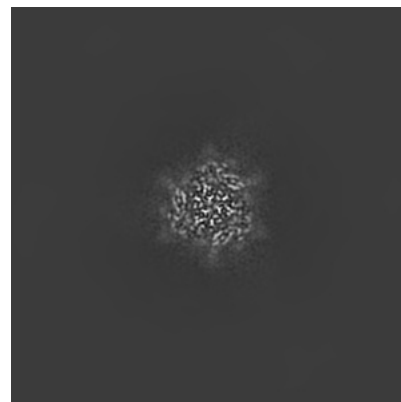
### 6.2.1 Primary map



X Index: 180

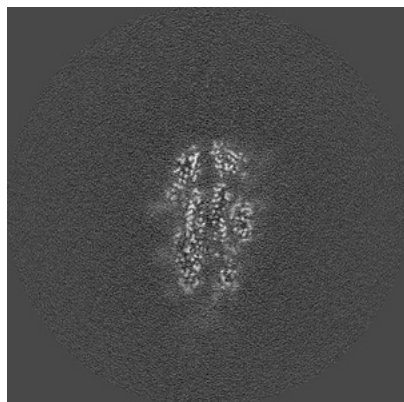


Y Index: 180

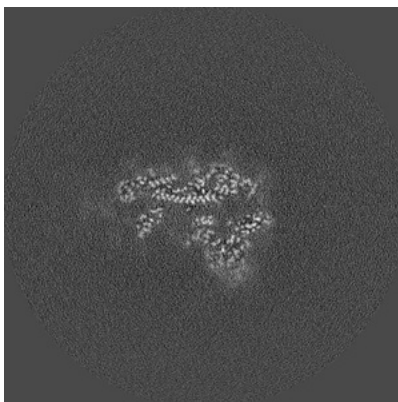


Z Index: 180

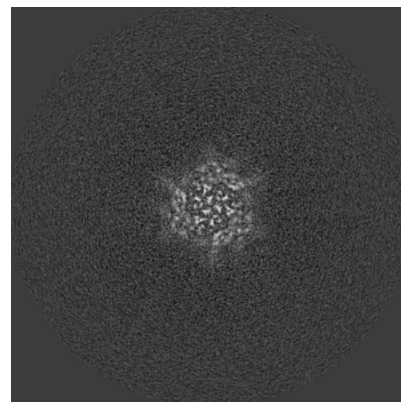
### 6.2.2 Raw map



X Index: 180



Y Index: 180

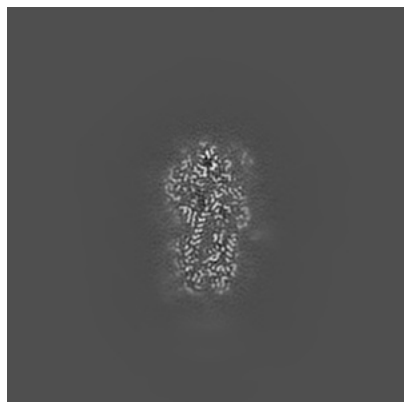


Z Index: 180

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

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

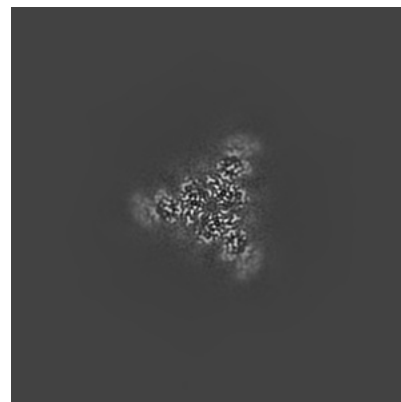
### 6.3.1 Primary map



X Index: 169

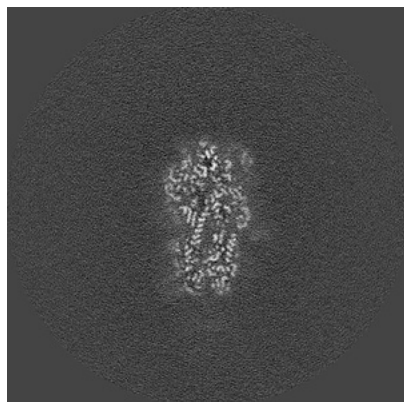


Y Index: 186

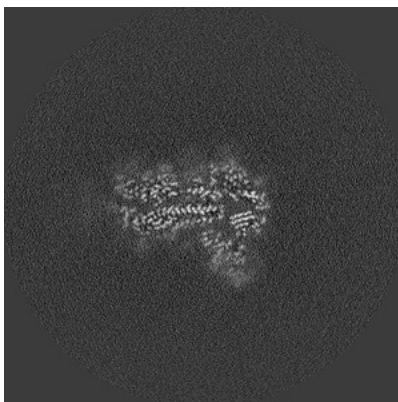


Z Index: 211

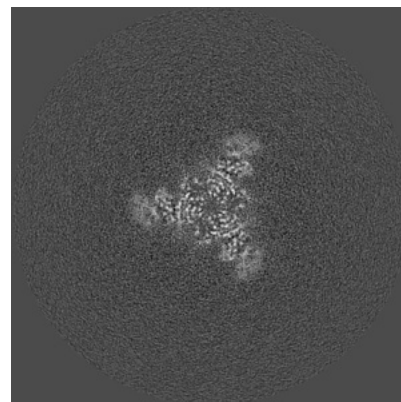
### 6.3.2 Raw map



X Index: 169



Y Index: 186

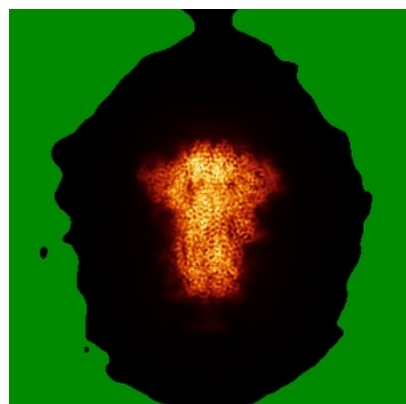


Z Index: 210

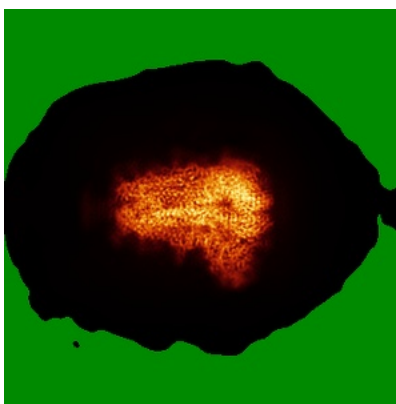
The images above show the largest variance slices of the map in three orthogonal directions.

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

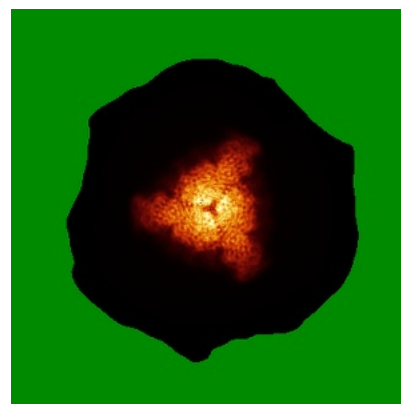
### 6.4.1 Primary map



X

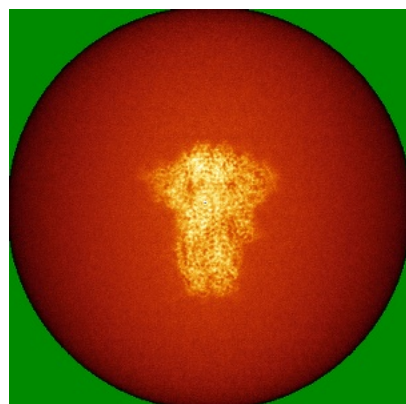


Y

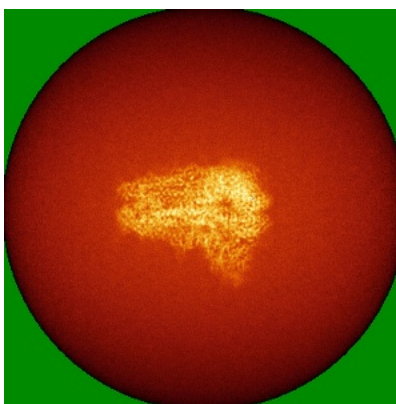


Z

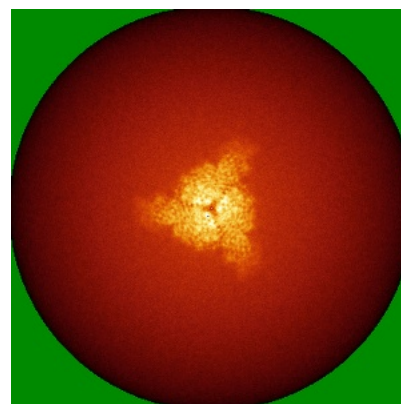
### 6.4.2 Raw map



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.

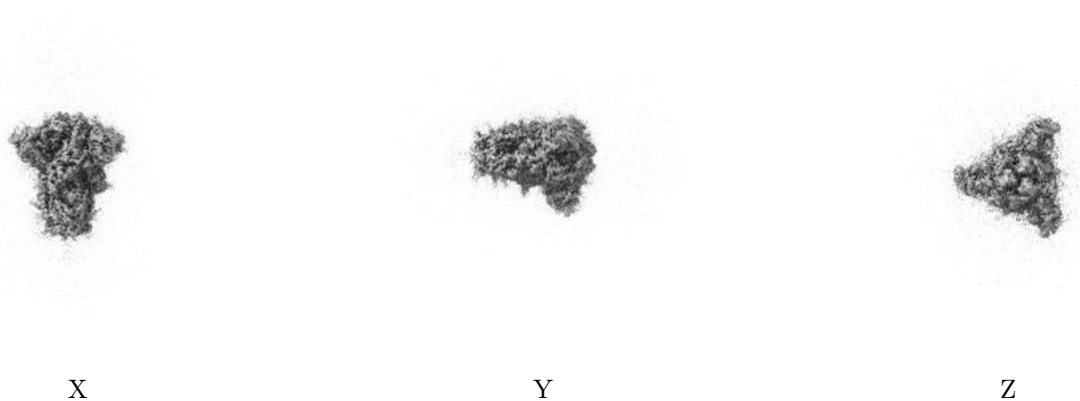
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

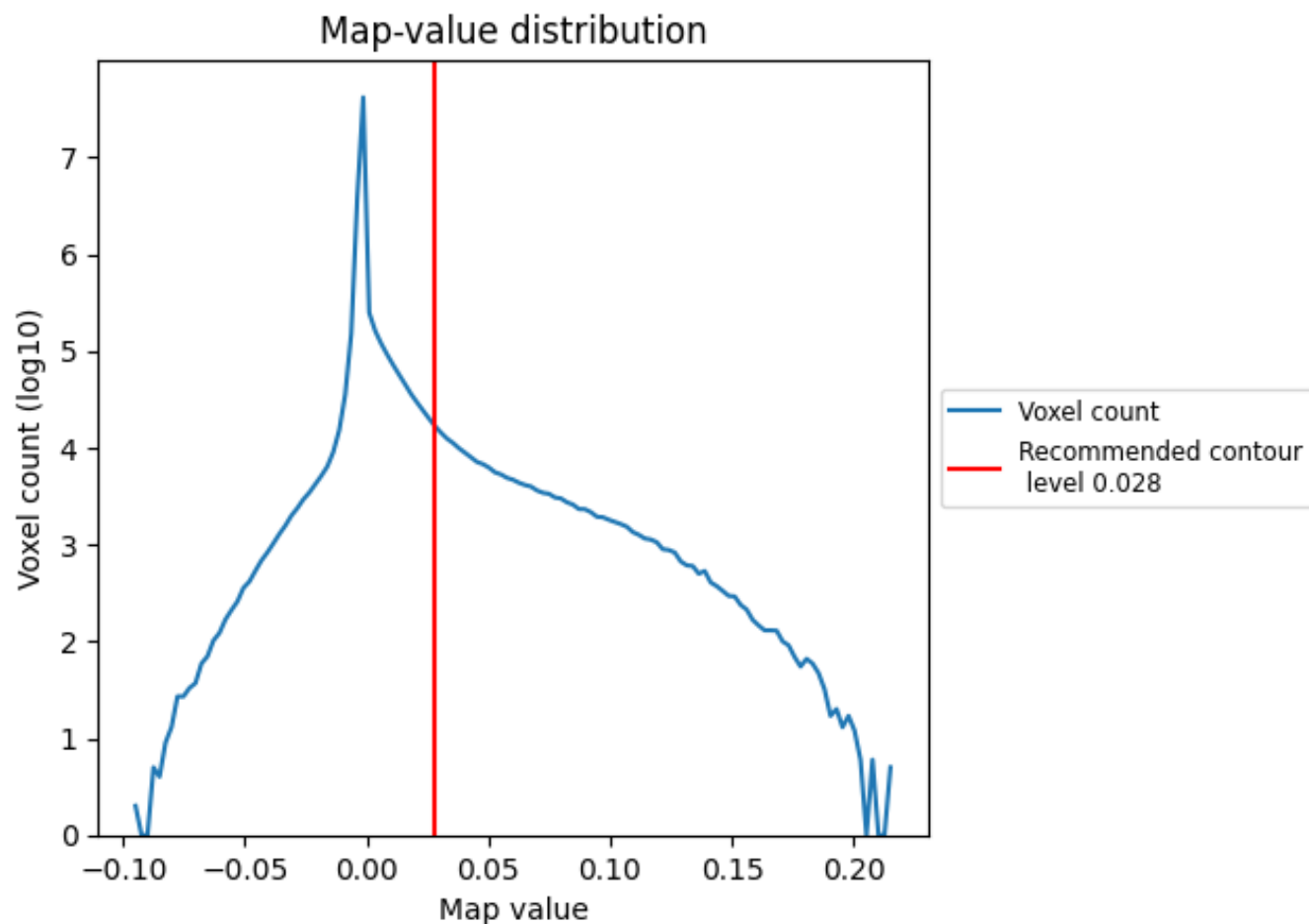
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

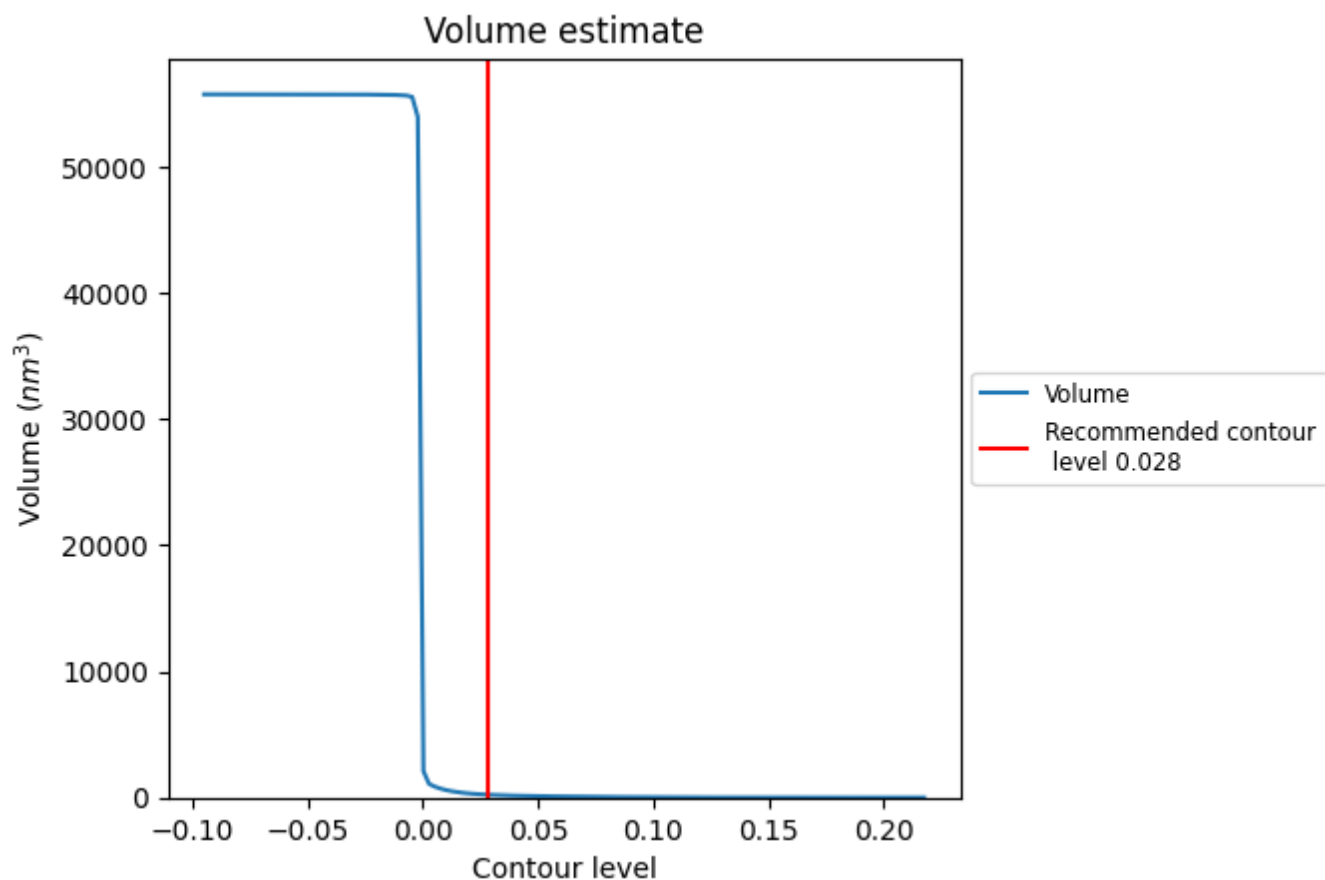
This section contains the results of statistical analysis of the map.

### 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.

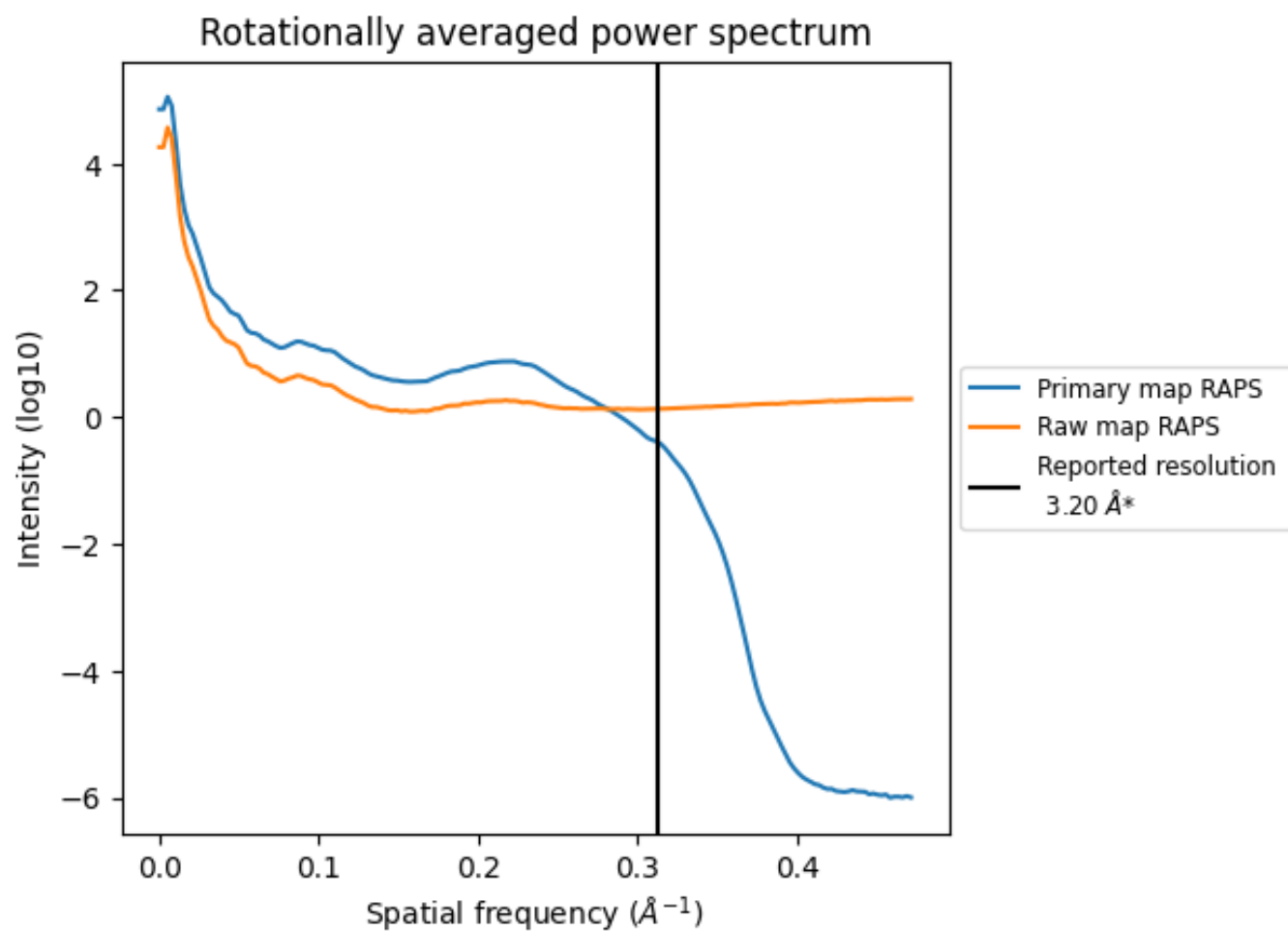
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm<sup>3</sup>; this corresponds to an approximate mass of 204 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 ⓘ

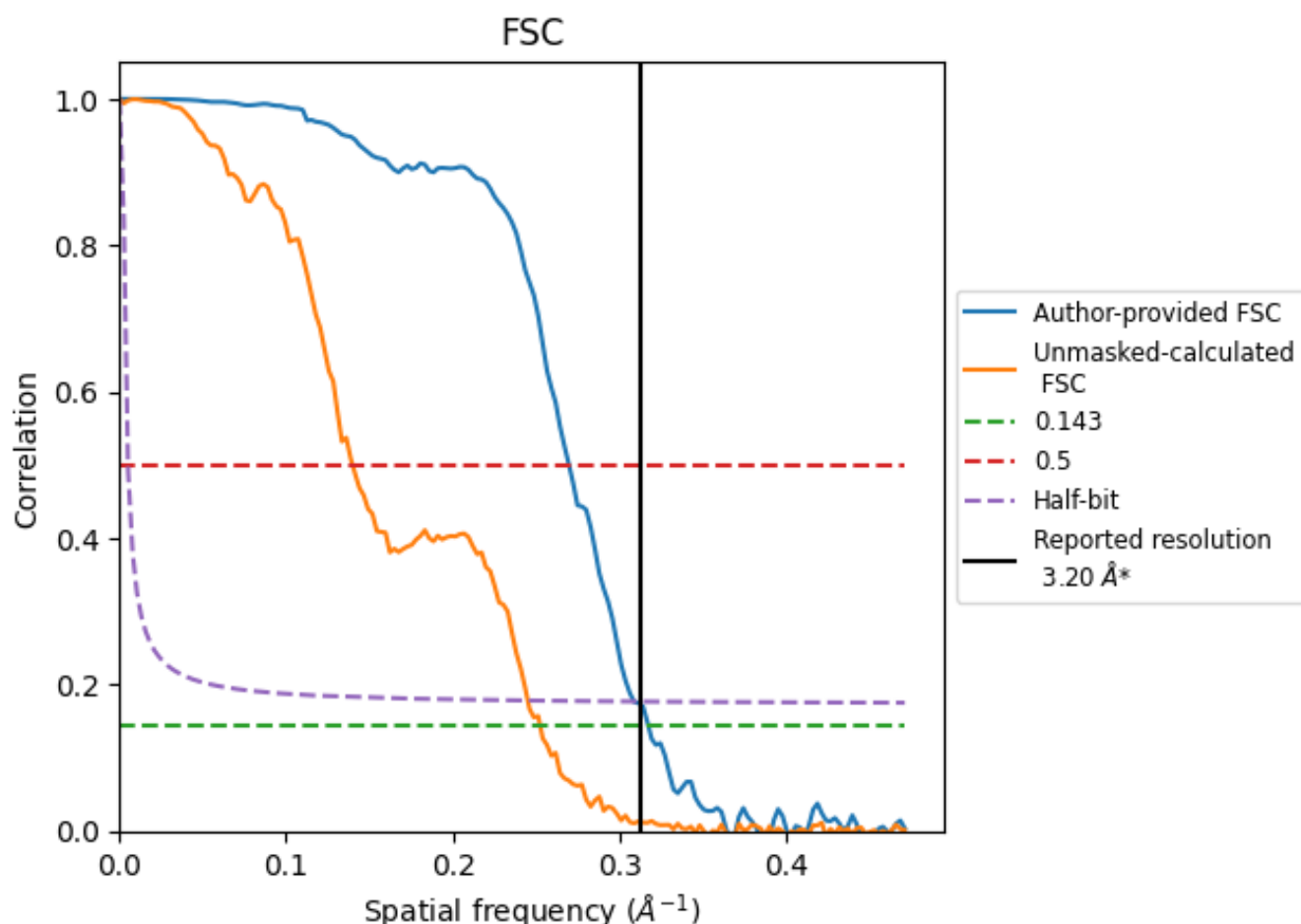


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

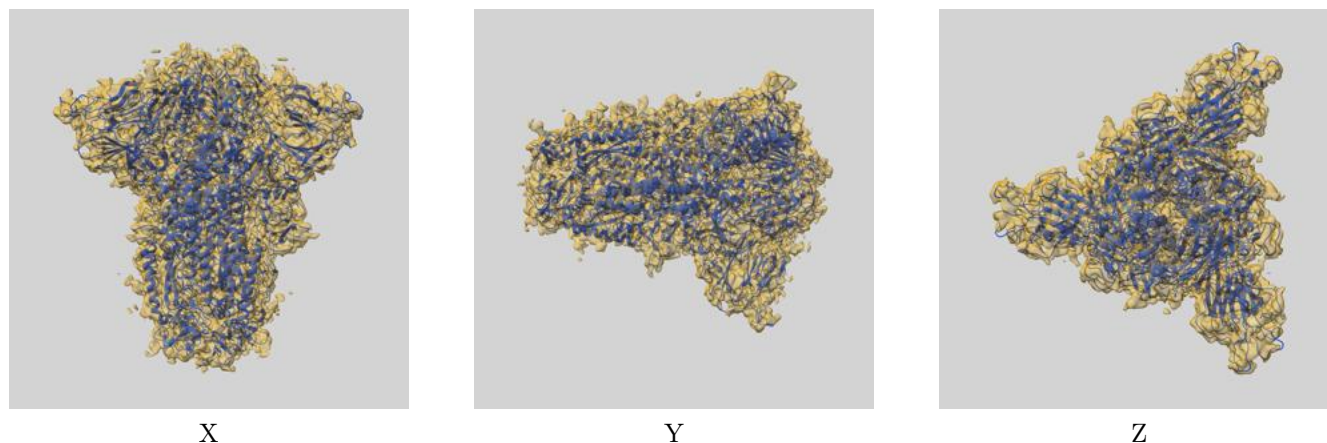
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.71	3.24
Unmasked-calculated*	3.96	7.15	4.08

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.2 by more than 10 %

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

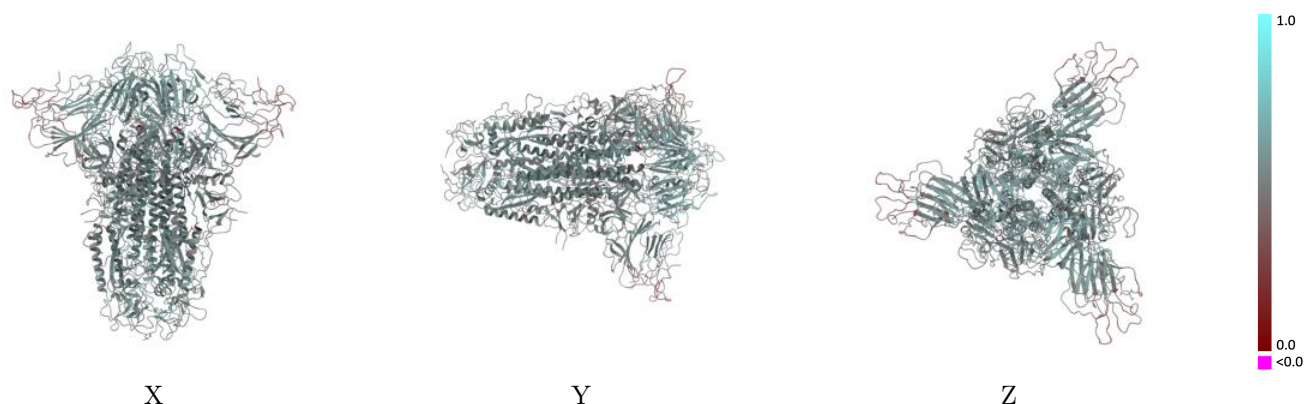
This section contains information regarding the fit between EMDB map EMD-33456 and PDB model 7XU2. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



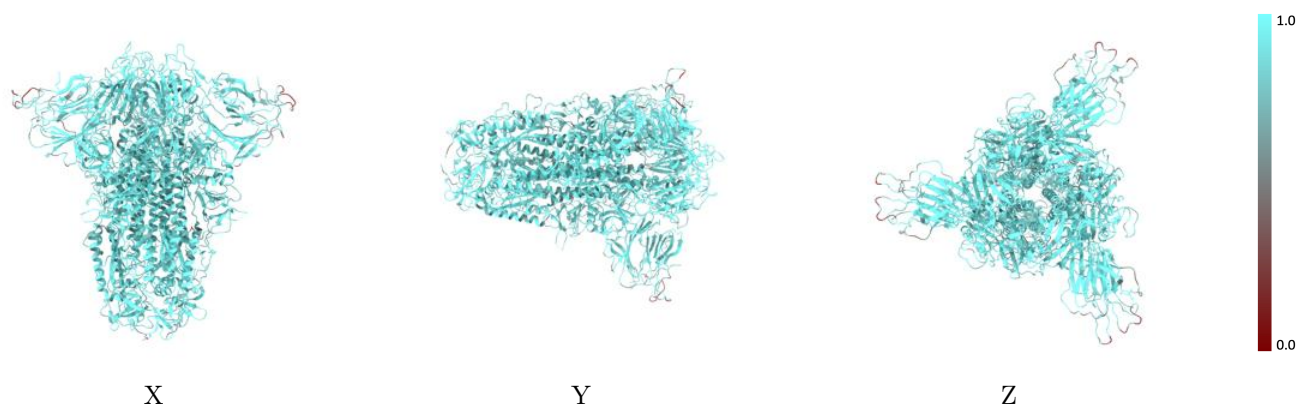
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



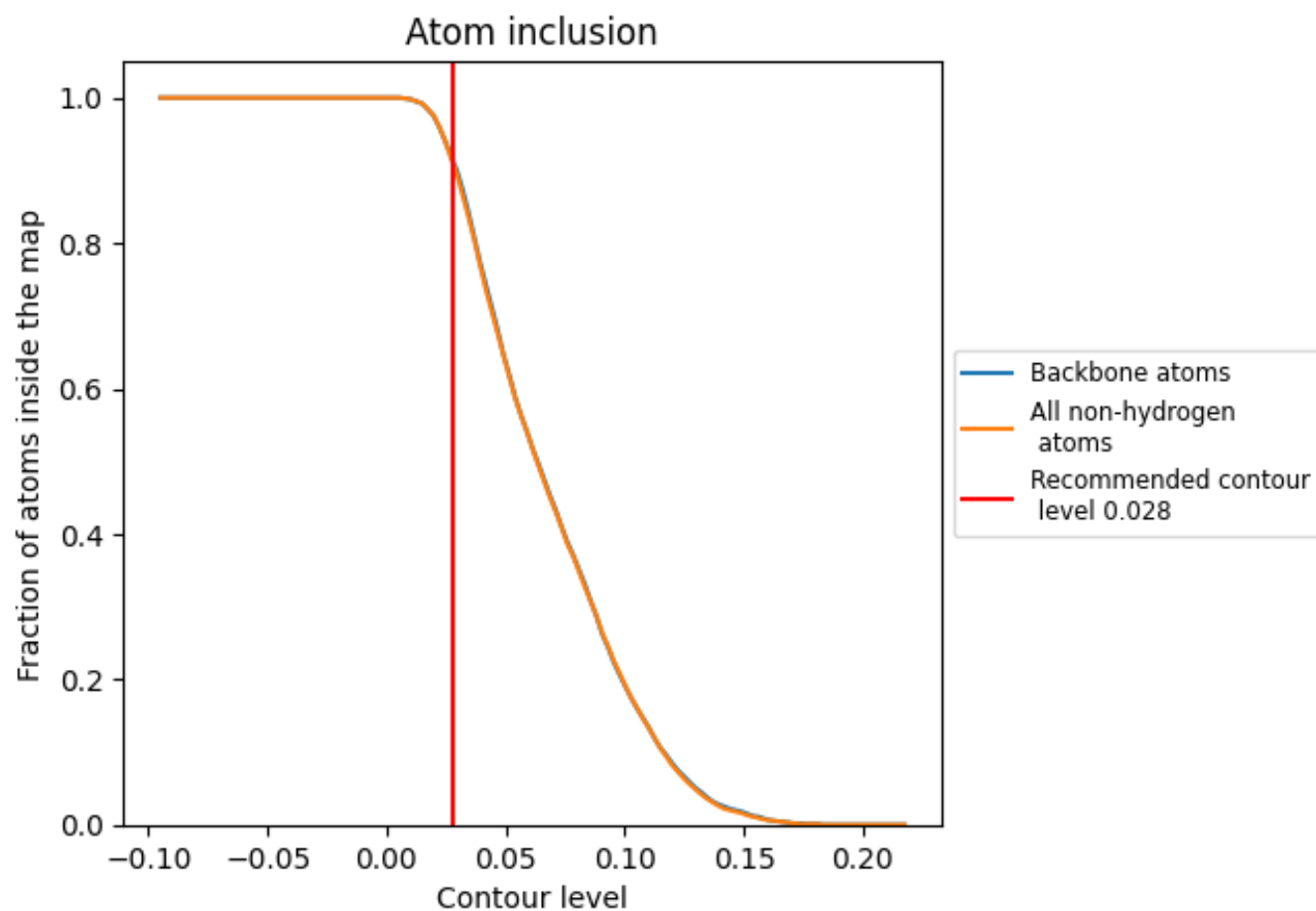
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9080	<div></div> 0.5230
A	<div></div> 0.9150	<div></div> 0.5240
B	<div></div> 0.9160	<div></div> 0.5240
C	<div></div> 0.9150	<div></div> 0.5250
D	<div></div> 0.8570	<div></div> 0.4840
E	<div></div> 0.7140	<div></div> 0.4470
F	<div></div> 0.6070	<div></div> 0.4390
G	<div></div> 0.3210	<div></div> 0.3630
H	<div></div> 0.8570	<div></div> 0.5170
I	<div></div> 0.6790	<div></div> 0.4520
J	<div></div> 0.6070	<div></div> 0.4260
K	<div></div> 0.3210	<div></div> 0.3590
L	<div></div> 0.8570	<div></div> 0.4850
M	<div></div> 0.6790	<div></div> 0.4380
N	<div></div> 0.6070	<div></div> 0.4380
O	<div></div> 0.2860	<div></div> 0.3790

1.0

0.0

<0.0