



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 05:12 PM EDT

PDB ID : 6PXH  
Title : Crystal Structure of MERS-CoV S1-NTD bound with G2 Fab  
Authors : Wang, N.; McLellan, J.S.  
Deposited on : 2019-07-26  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

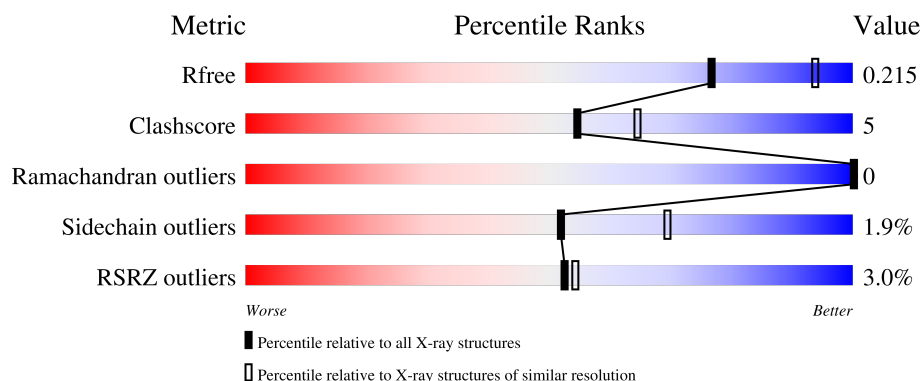
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div>0%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	B	342	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	C	229	<div> <div>2%</div> <div>85%</div> <div>7%</div> <div>7%</div> <div>.</div> </div>
2	H	229	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>.</div> </div>
3	D	218	<div> <div>6%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	218	
4	E	3	
4	F	3	
4	G	3	
4	M	3	
5	I	2	
5	K	2	
5	N	2	
5	P	2	
6	J	8	
7	O	5	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13170 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MERS-CoV S1-NTD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2647	1699	437	498	13			
1	B	341	Total	C	N	O	S	0	0	0
			2700	1735	444	508	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	expression tag	UNP V9TWK2
A	353	SER	-	expression tag	UNP V9TWK2
A	354	LEU	-	expression tag	UNP V9TWK2
A	355	GLU	-	expression tag	UNP V9TWK2
A	356	VAL	-	expression tag	UNP V9TWK2
A	357	LEU	-	expression tag	UNP V9TWK2
A	358	PHE	-	expression tag	UNP V9TWK2
A	359	GLN	-	expression tag	UNP V9TWK2
B	352	GLY	-	expression tag	UNP V9TWK2
B	353	SER	-	expression tag	UNP V9TWK2
B	354	LEU	-	expression tag	UNP V9TWK2
B	355	GLU	-	expression tag	UNP V9TWK2
B	356	VAL	-	expression tag	UNP V9TWK2
B	357	LEU	-	expression tag	UNP V9TWK2
B	358	PHE	-	expression tag	UNP V9TWK2
B	359	GLN	-	expression tag	UNP V9TWK2

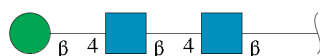
- Molecule 2 is a protein called G2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1593	1010	254	321	8			
2	H	220	Total	C	N	O	S	0	0	0
			1637	1034	263	332	8			

- Molecule 3 is a protein called G2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	218	Total	C	N	O	S	0	0	0
			1674	1038	285	343	8			
3	L	212	Total	C	N	O	S	0	0	0
			1627	1008	278	333	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

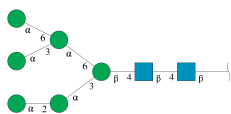
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

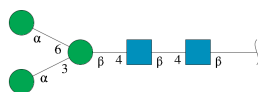
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyr

anose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



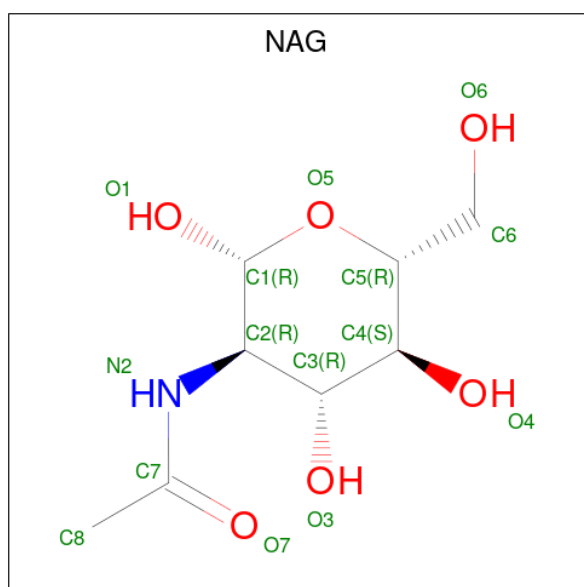
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



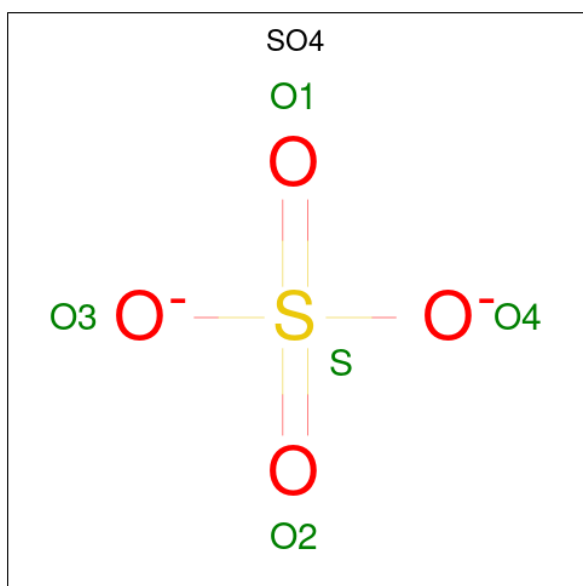
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	H	1	Total O S 5 4 1	0	0

- # DHF

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	216	Total O 216 216	0	0
11	B	152	Total O 152 152	0	0
11	C	109	Total O 109 109	0	0
11	D	80	Total O 80 80	0	0





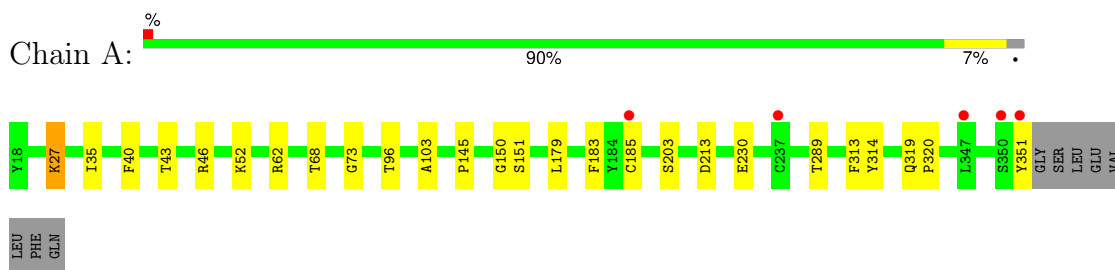
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	88	Total 88	O 88	0	0
11	L	40	Total 40	O 40	0	0

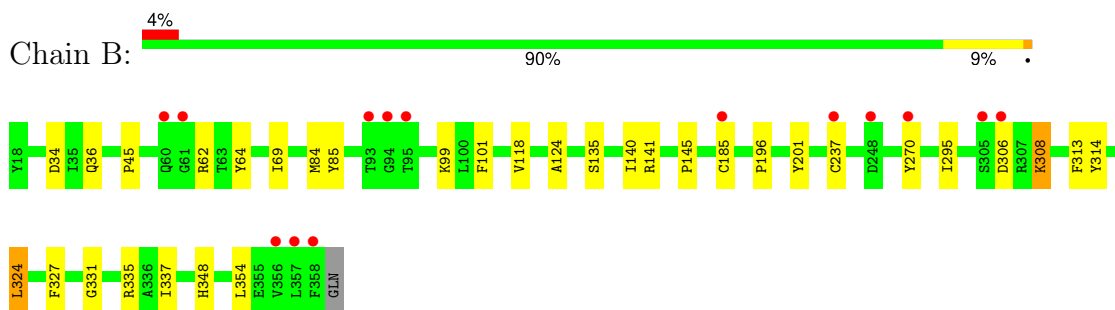
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

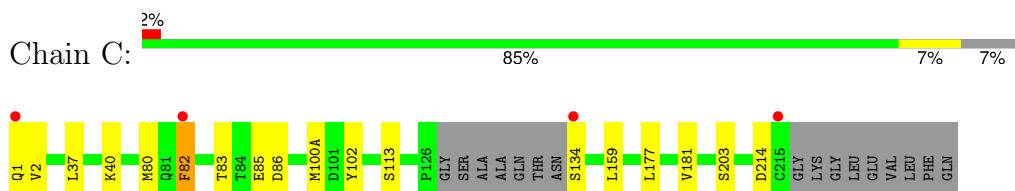
- Molecule 1: MERS-CoV S1-NTD



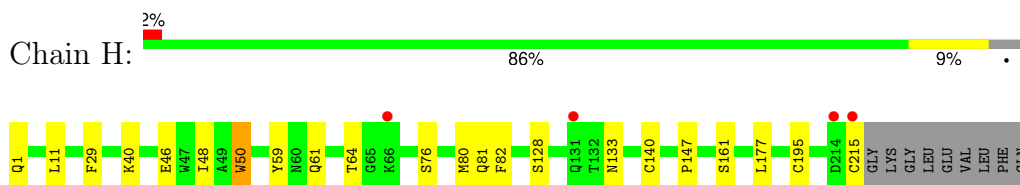
- Molecule 1: MERS-CoV S1-NTD



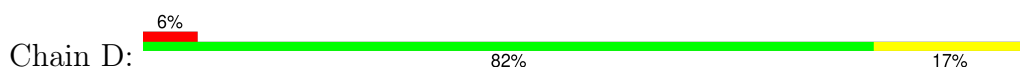
- Molecule 2: G2 heavy chain

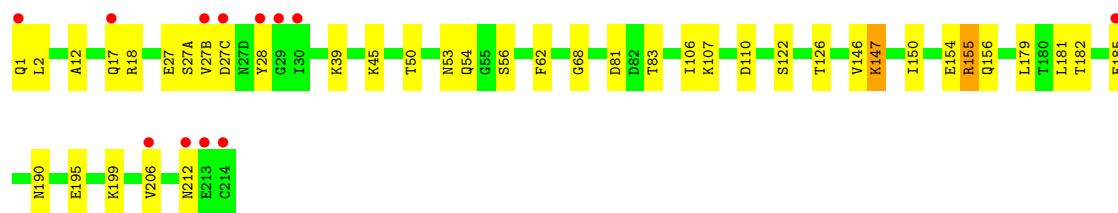


- Molecule 2: G2 heavy chain

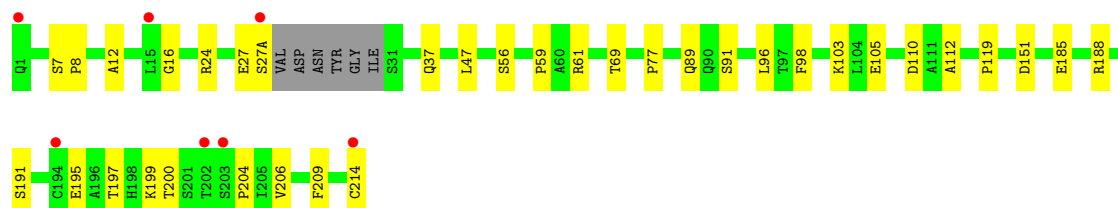
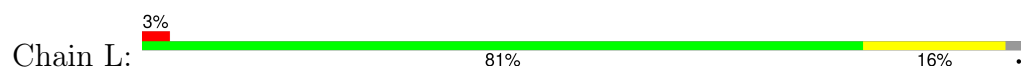


- Molecule 3: G2 light chain





● Molecule 3: G2 light chain



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



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



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



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



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

Chain I:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain N:  50% 50%


MAG1  
MAG2

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

Chain P:  50% 50%

MAG1  
MAG2

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

Chain J:  12% 62% 25%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  60% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.99Å 63.86Å 186.78Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	52.71 – 2.30 52.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (52.71-2.30) 97.9 (52.71-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.179 , 0.212 0.181 , 0.215	Depositor DCC
$R_{free}$ test set	4450 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: SO4, NAG, BMA, DHF, MAN

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	0.63	0/2723	0.58	0/3705
1	B	0.56	1/2777 (0.0%)	0.55	1/3778 (0.0%)
2	C	0.37	0/1635	0.56	1/2234 (0.0%)
2	H	0.36	0/1680	0.55	1/2297 (0.0%)
3	D	0.34	0/1711	0.55	1/2324 (0.0%)
3	L	0.30	0/1662	0.49	0/2255
All	All	0.48	1/12188 (0.0%)	0.55	4/16593 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	CYS	CB-SG	5.96	1.92	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	177	LEU	CA-CB-CG	6.00	129.10	115.30
1	B	185	CYS	CA-CB-SG	5.59	124.06	114.00
3	D	155	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	H	177	LEU	CA-CB-CG	5.20	127.25	115.30

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	A	2647	0	2506	12	0
1	B	2700	0	2561	19	0
2	C	1593	0	1543	12	0
2	H	1637	0	1583	14	0
3	D	1674	0	1597	29	0
3	L	1627	0	1554	20	0
4	E	39	0	34	2	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
4	M	39	0	34	1	0
5	I	28	0	25	0	0
5	K	28	0	25	0	0
5	N	28	0	25	3	0
5	P	28	0	25	1	0
6	J	94	0	79	2	0
7	O	61	0	52	0	0
8	A	28	0	26	0	0
8	B	42	0	39	0	0
9	A	20	0	0	0	0
9	B	15	0	0	1	0
9	C	10	0	0	1	0
9	H	5	0	0	0	0
10	A	32	0	19	0	0
10	B	32	0	19	1	0
11	A	216	0	0	3	1
11	B	152	0	0	4	0
11	C	109	0	0	5	0
11	D	80	0	0	5	0
11	H	88	0	0	3	1
11	L	40	0	0	2	0
All	All	13170	0	11814	114	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 114 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)
3:D:1:GLN:OE1	11:D:301:HOH:O	1.87	0.93
3:L:110:ASP:OD2	3:L:199:LYS:NZ	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:27(B):VAL:O	11:D:302:HOH:O	2.01	0.77
1:B:335:ARG:NH2	11:B:502:HOH:O	2.21	0.74
1:A:213:ASP:OD2	11:A:501:HOH:O	2.08	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:683:HOH:O	11:H:483:HOH:O[2_746]	2.15	0.05

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	332/342 (97%)	319 (96%)	13 (4%)	0	100	100
1	B	339/342 (99%)	328 (97%)	11 (3%)	0	100	100
2	C	209/229 (91%)	207 (99%)	2 (1%)	0	100	100
2	H	218/229 (95%)	217 (100%)	1 (0%)	0	100	100
3	D	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
3	L	208/218 (95%)	202 (97%)	6 (3%)	0	100	100
All	All	1522/1578 (96%)	1484 (98%)	38 (2%)	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 X-ray entries followed by that with respect to entries of similar resolution.



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	286/293 (98%)	280 (98%)	6 (2%)	48	66
1	B	292/293 (100%)	286 (98%)	6 (2%)	48	66
2	C	183/194 (94%)	181 (99%)	2 (1%)	70	83
2	H	187/194 (96%)	180 (96%)	7 (4%)	29	43
3	D	192/192 (100%)	190 (99%)	2 (1%)	73	85
3	L	187/192 (97%)	185 (99%)	2 (1%)	70	83
All	All	1327/1358 (98%)	1302 (98%)	25 (2%)	52	69

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	56	SER
2	H	81	GLN
3	L	56	SER
2	H	50	TRP
2	H	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	212	ASN
3	L	17	GLN
3	L	212	ASN
3	D	1	GLN
1	B	346	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

33 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	E	1	1,4	14,14,15	0.62	0	17,19,21	1.54	2 (11%)
4	NAG	E	2	4	14,14,15	0.64	1 (7%)	17,19,21	1.31	1 (5%)
4	BMA	E	3	4	11,11,12	0.88	0	15,15,17	0.66	0
4	NAG	F	1	1,4	14,14,15	0.39	0	17,19,21	0.72	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.72	1 (5%)
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.32	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.39	0	17,19,21	0.49	0
4	BMA	G	3	4	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.60	0	17,19,21	0.63	0
5	NAG	I	2	5	14,14,15	0.30	0	17,19,21	0.46	0
6	NAG	J	1	1,6	14,14,15	1.78	3 (21%)	17,19,21	1.24	1 (5%)
6	NAG	J	2	6	14,14,15	0.54	0	17,19,21	0.63	0
6	BMA	J	3	6	11,11,12	1.12	1 (9%)	15,15,17	0.78	0
6	MAN	J	4	6	11,11,12	0.57	0	15,15,17	1.07	1 (6%)
6	MAN	J	5	6	11,11,12	1.08	1 (9%)	15,15,17	1.16	1 (6%)
6	MAN	J	6	6	11,11,12	1.55	3 (27%)	15,15,17	1.39	2 (13%)
6	MAN	J	7	6	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
6	MAN	J	8	6	11,11,12	1.61	2 (18%)	15,15,17	1.71	3 (20%)
5	NAG	K	1	1,5	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	K	2	5	14,14,15	0.56	0	17,19,21	0.56	0
4	NAG	M	1	1,4	14,14,15	0.27	0	17,19,21	0.63	1 (5%)
4	NAG	M	2	4	14,14,15	0.45	0	17,19,21	0.50	0
4	BMA	M	3	4	11,11,12	0.82	0	15,15,17	0.98	1 (6%)
5	NAG	N	1	1,5	14,14,15	0.44	0	17,19,21	0.67	1 (5%)
5	NAG	N	2	5	14,14,15	0.48	0	17,19,21	0.49	0
7	NAG	O	1	1,7	14,14,15	0.62	0	17,19,21	0.57	0
7	NAG	O	2	7	14,14,15	0.43	0	17,19,21	0.55	0
7	BMA	O	3	7	11,11,12	0.75	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	O	4	7	11,11,12	0.84	0	15,15,17	1.16	2 (13%)
7	MAN	O	5	7	11,11,12	0.97	0	15,15,17	1.05	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.54	0
5	NAG	P	2	5	14,14,15	0.20	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	1/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	2/2/19/22	0/1/1/1
6	MAN	J	7	6	-	0/2/19/22	0/1/1/1
6	MAN	J	8	6	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
7	NAG	O	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	1/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	MAN	O	5	7	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	NAG	O5-C1	-4.72	1.35	1.43
6	J	1	NAG	C3-C2	3.01	1.58	1.52
6	J	6	MAN	C1-C2	2.97	1.59	1.52
6	J	6	MAN	C2-C3	2.93	1.57	1.52
6	J	8	MAN	O5-C5	2.91	1.49	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C2-N2-C7	4.67	129.16	122.90
4	E	2	NAG	C1-O5-C5	-4.49	106.17	112.19
6	J	8	MAN	C1-O5-C5	3.47	116.83	112.19
6	J	1	NAG	O5-C5-C6	-3.22	101.39	107.66
6	J	5	MAN	C1-O5-C5	3.09	116.33	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	4	MAN	C4-C5-C6-O6
6	J	4	MAN	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 9 short contacts:

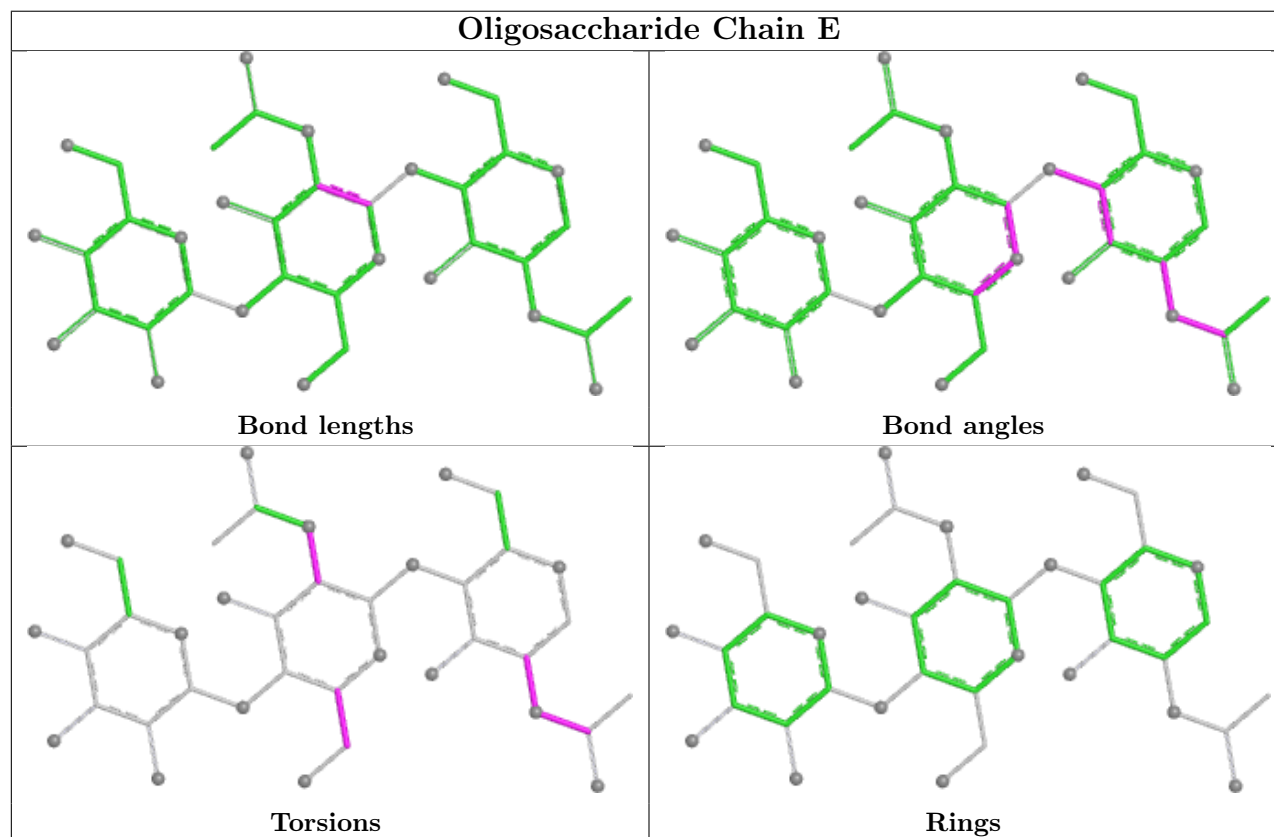
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1	NAG	1	0
5	N	2	NAG	3	0
5	P	2	NAG	1	0
6	J	3	BMA	2	0

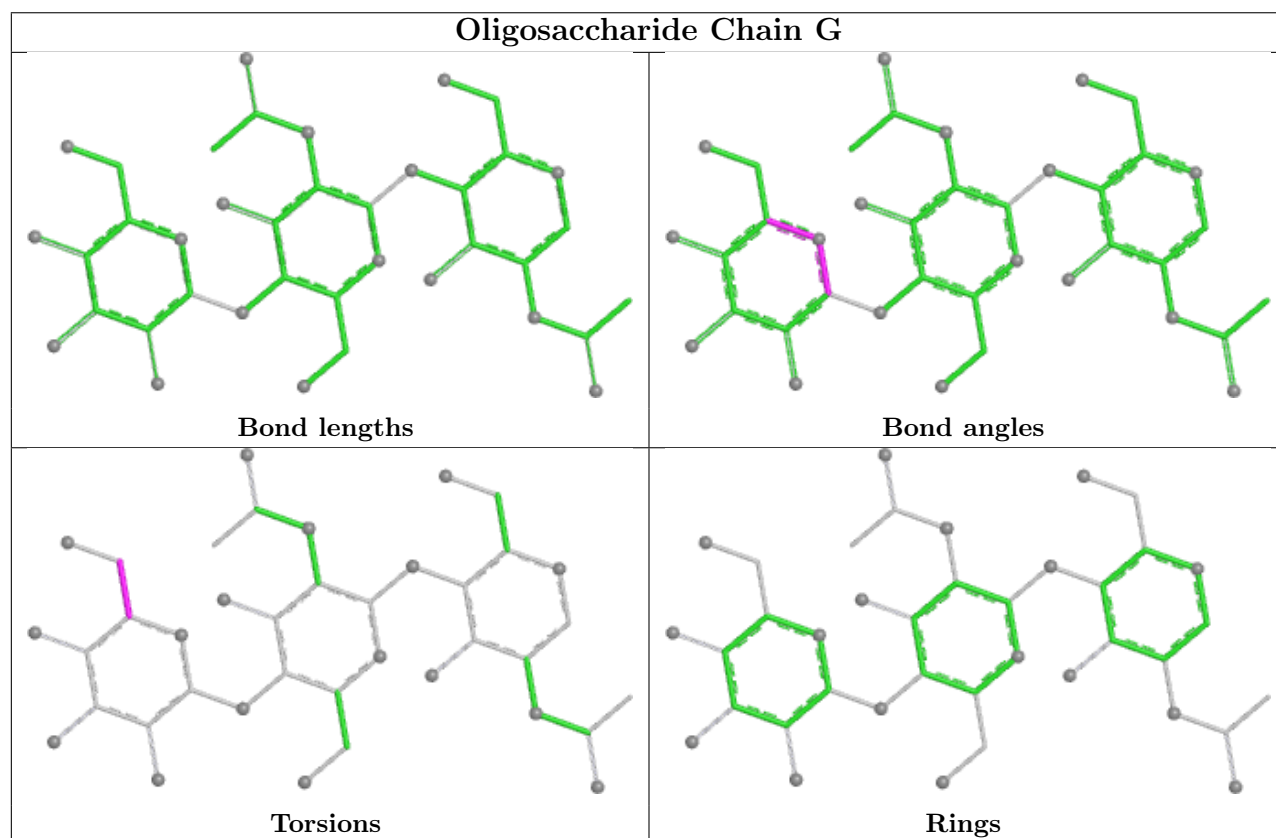
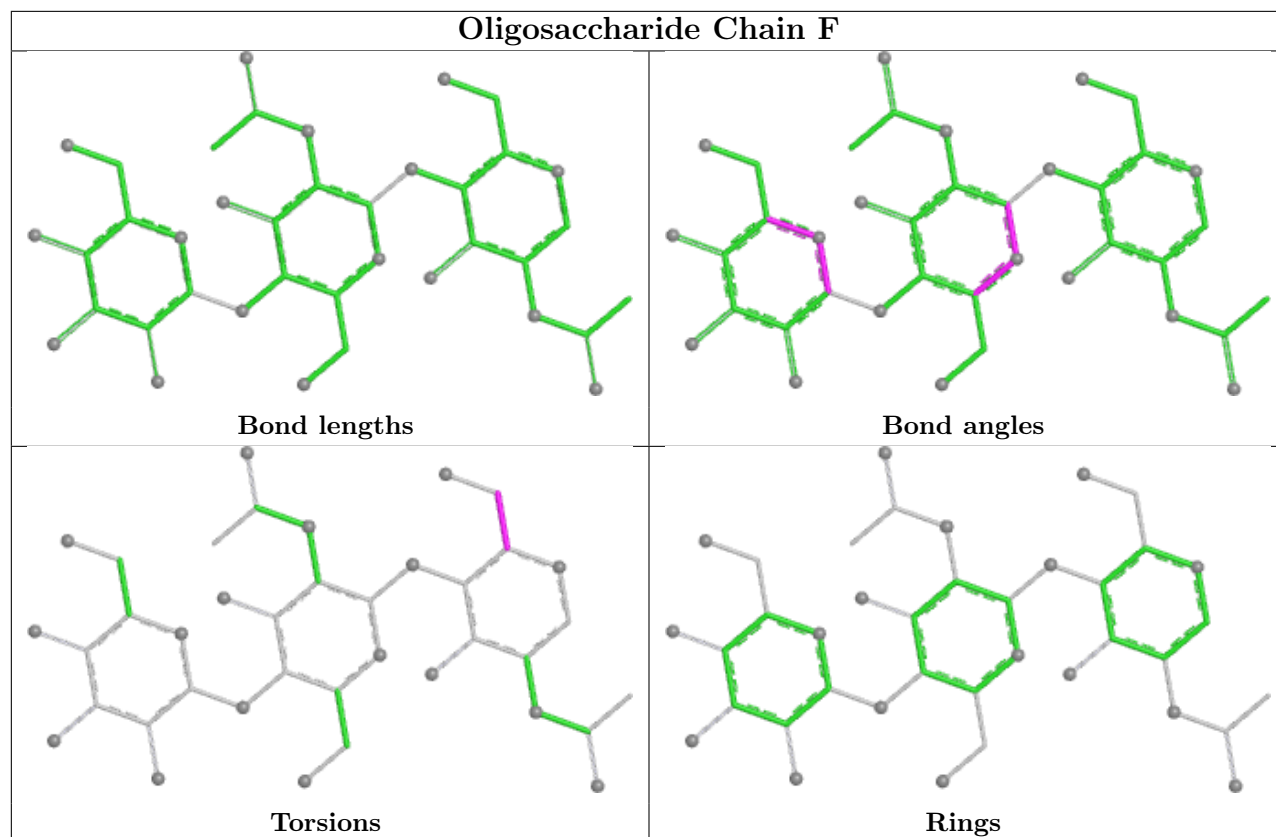
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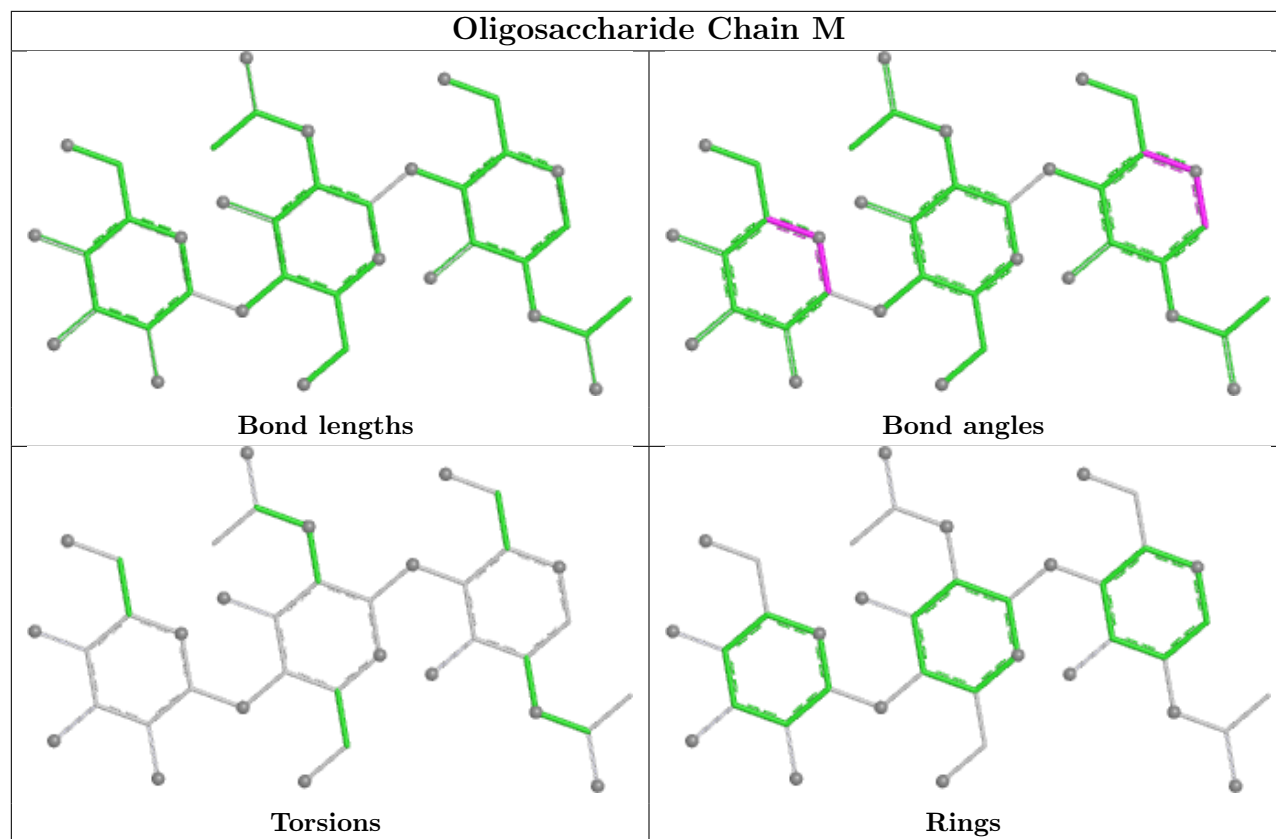
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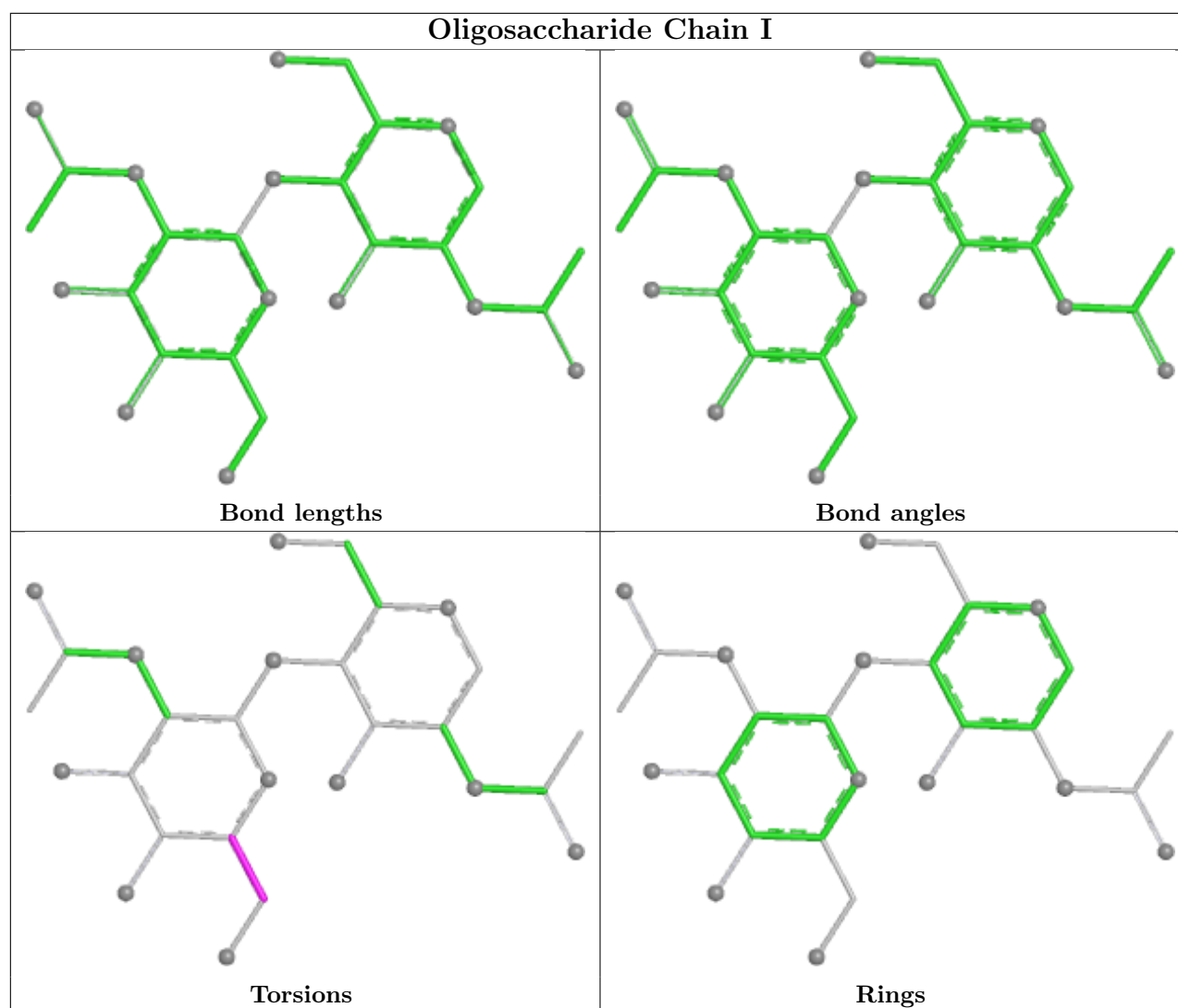
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	6	MAN	2	0
4	M	3	BMA	1	0
4	E	1	NAG	2	0
5	N	1	NAG	2	0

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

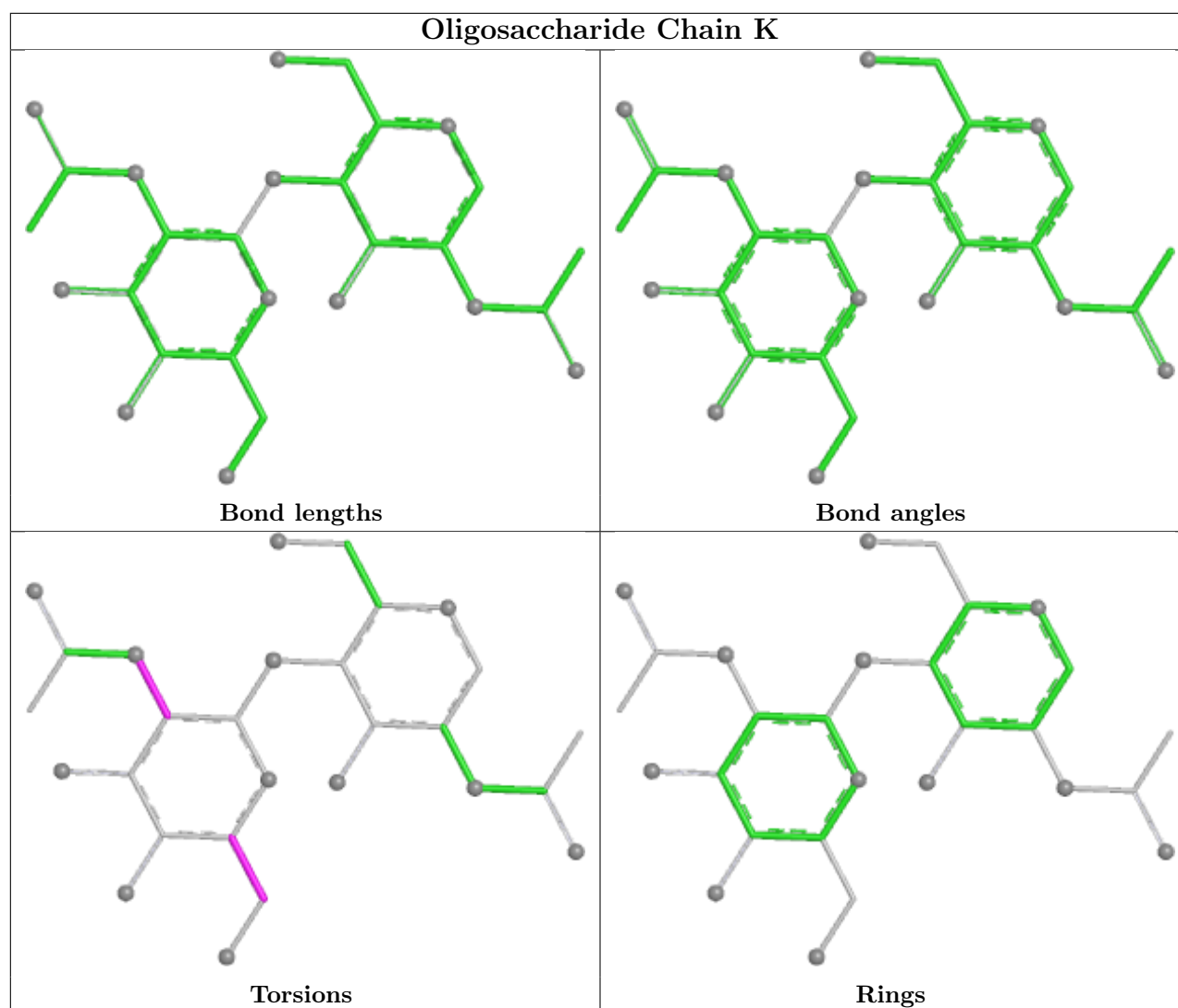


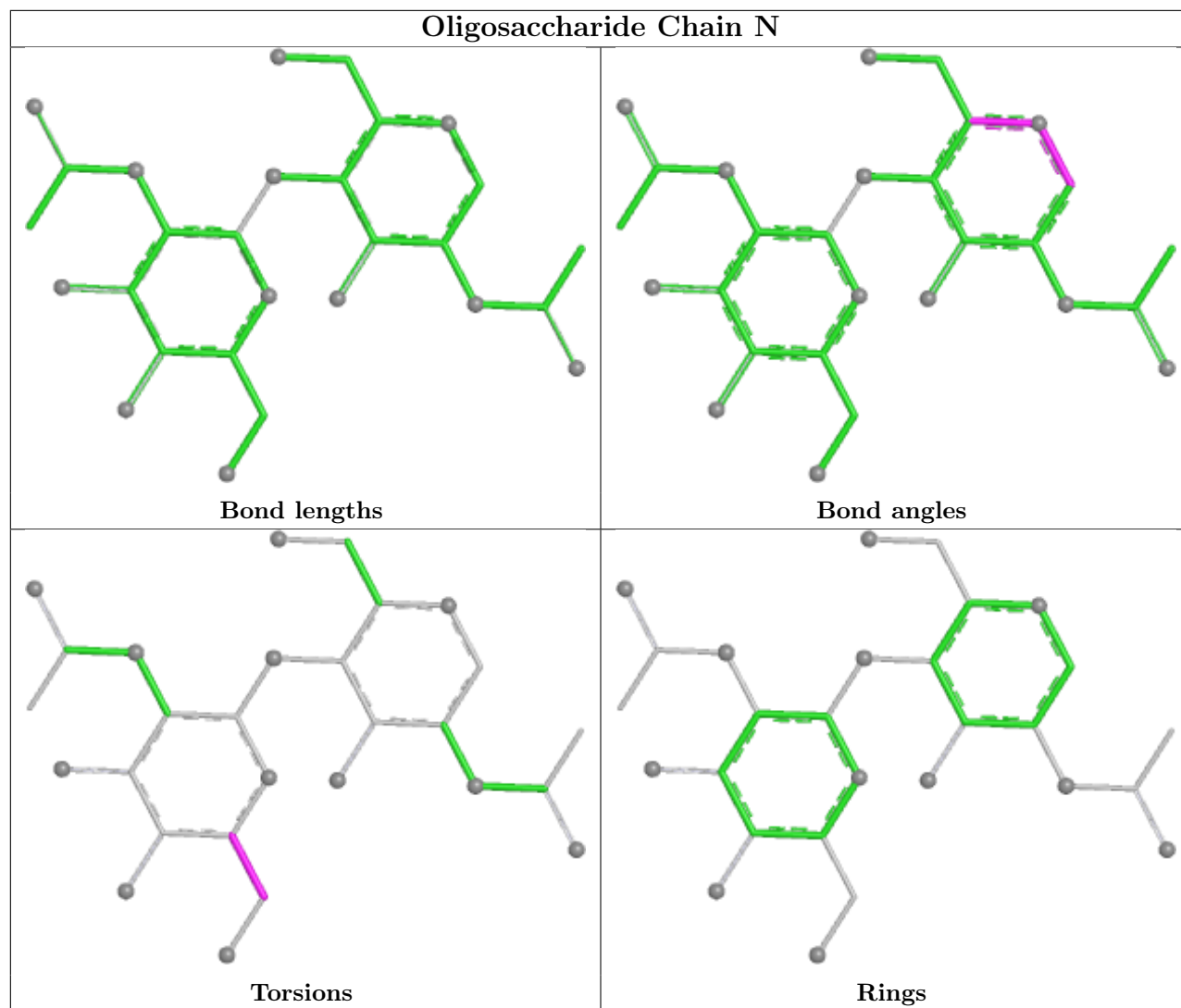


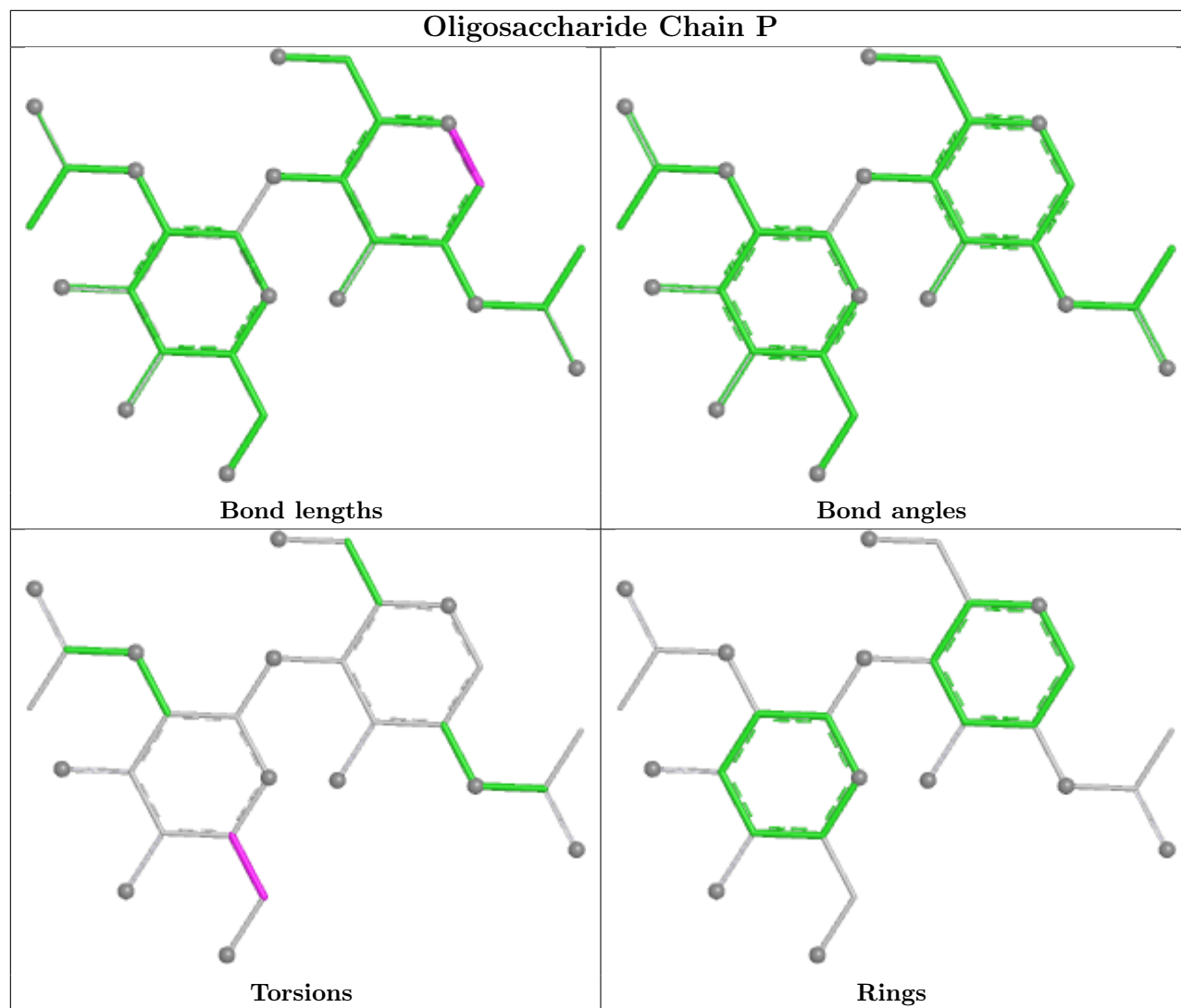


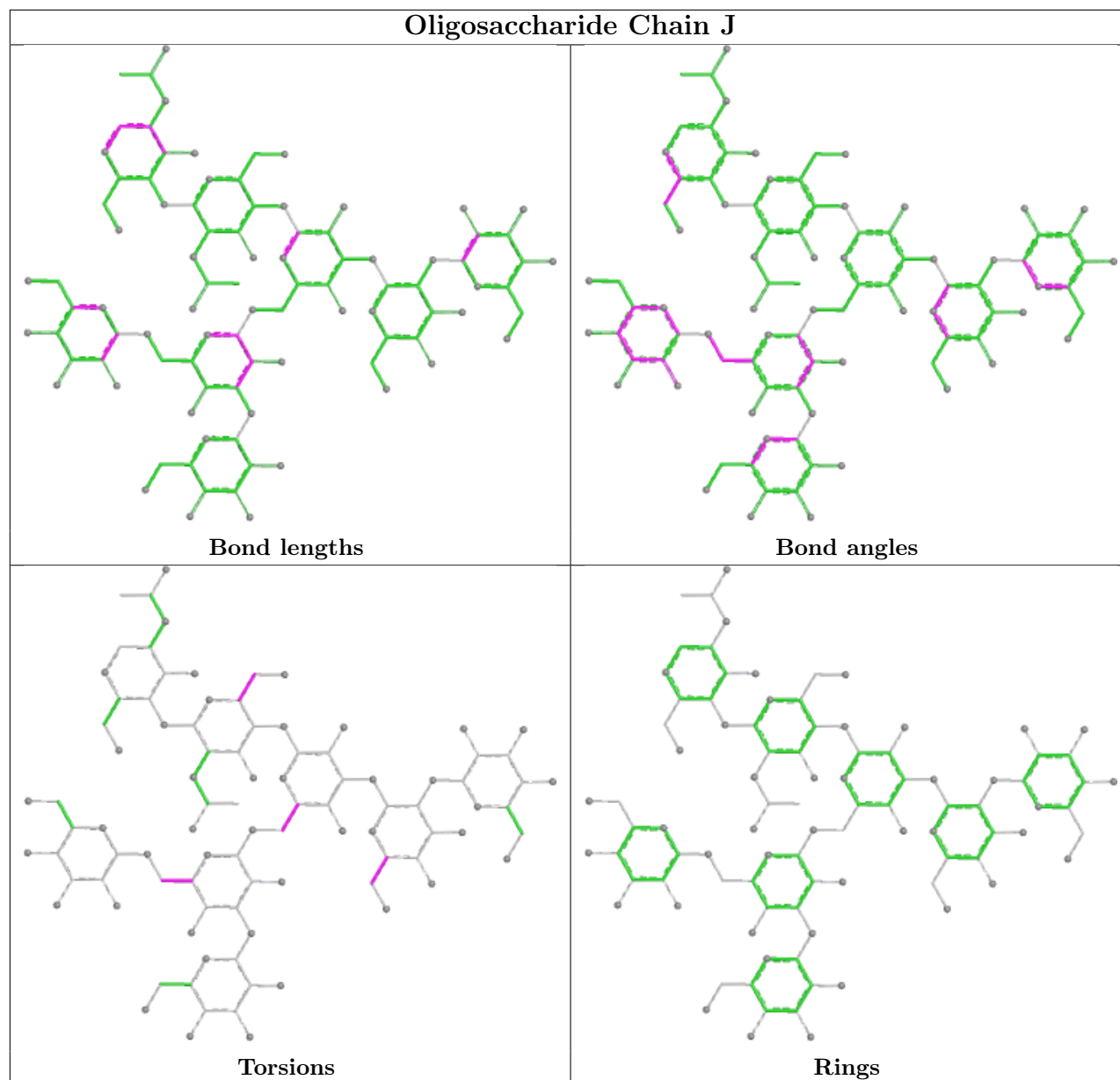


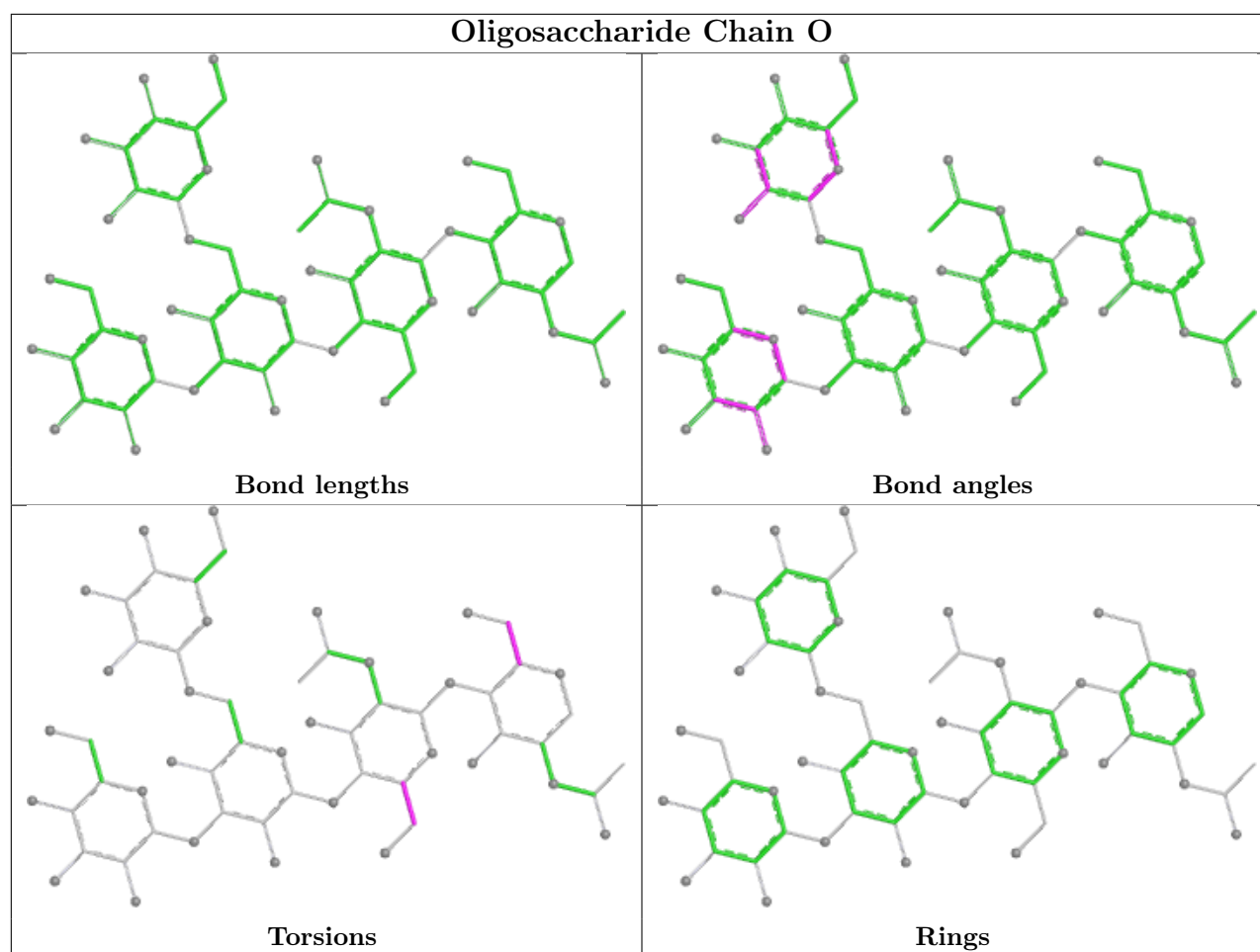












## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
9	SO4	H	301	-	4,4,4	0.25	0	6,6,6	0.07	0
9	SO4	A	427	-	4,4,4	0.29	0	6,6,6	0.19	0
8	NAG	B	405	1	14,14,15	0.36	0	17,19,21	0.48	0
8	NAG	A	410	1	14,14,15	0.34	0	17,19,21	0.40	0
9	SO4	A	425	-	4,4,4	0.24	0	6,6,6	0.22	0
9	SO4	B	416	-	4,4,4	0.23	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SO4	A	426	-	4,4,4	0.22	0	6,6,6	0.17	0
9	SO4	B	417	-	4,4,4	0.24	0	6,6,6	0.06	0
8	NAG	A	423	1	14,14,15	0.56	0	17,19,21	0.59	0
9	SO4	A	424	-	4,4,4	0.25	0	6,6,6	0.09	0
9	SO4	C	301	-	4,4,4	0.27	0	6,6,6	0.20	0
9	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.21	0
10	DHF	B	419	-	30,34,34	2.73	3 (10%)	36,47,47	1.72	7 (19%)
8	NAG	B	401	1	14,14,15	0.37	0	17,19,21	0.38	0
9	SO4	B	418	-	4,4,4	0.23	0	6,6,6	0.18	0
8	NAG	B	415	1	14,14,15	0.19	0	17,19,21	0.72	0
10	DHF	A	428	-	30,34,34	2.72	3 (10%)	36,47,47	1.71	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	405	1	-	0/6/23/26	0/1/1/1
8	NAG	A	410	1	-	2/6/23/26	0/1/1/1
8	NAG	A	423	1	-	1/6/23/26	0/1/1/1
10	DHF	B	419	-	-	3/20/31/31	0/3/3/3
8	NAG	B	401	1	-	2/6/23/26	0/1/1/1
8	NAG	B	415	1	-	4/6/23/26	0/1/1/1
10	DHF	A	428	-	-	10/20/31/31	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	419	DHF	C7-C6	-10.48	1.37	1.49
10	A	428	DHF	C7-C6	-10.47	1.37	1.49
10	B	419	DHF	C7-N8	-8.23	1.31	1.45
10	A	428	DHF	C7-N8	-8.22	1.31	1.45
10	A	428	DHF	C4A-N5	-3.42	1.31	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	419	DHF	C2-N3-C4	4.92	122.81	115.96
10	A	428	DHF	C2-N3-C4	4.89	122.76	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	419	DHF	C4A-C4-N3	-4.61	117.25	123.42
10	A	428	DHF	C4A-C4-N3	-4.41	117.52	123.42
10	B	419	DHF	C9-N10-C14	-3.61	115.42	122.42

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

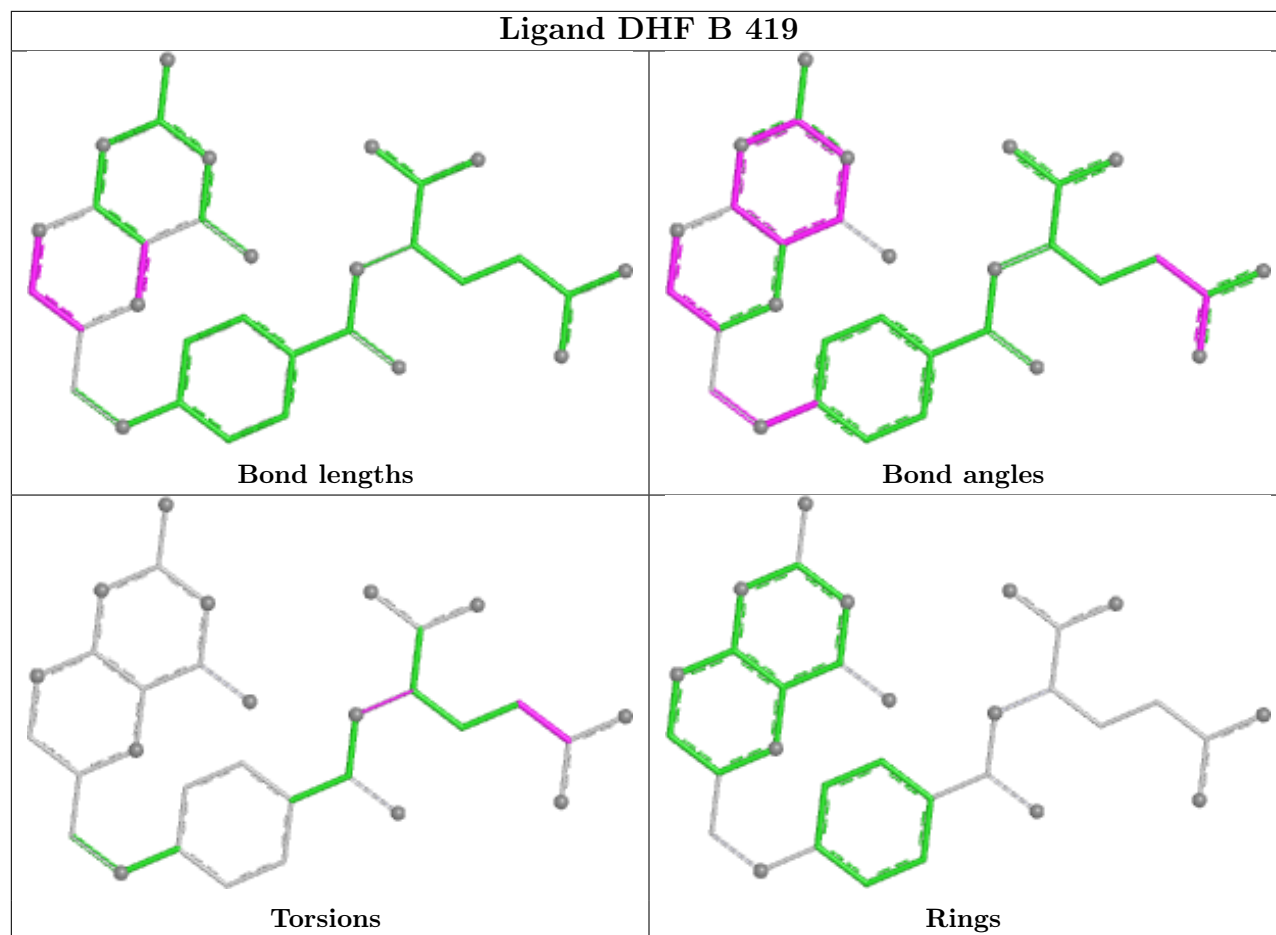
Mol	Chain	Res	Type	Atoms
10	A	428	DHF	C11-C-N-CA
10	A	428	DHF	O-C-N-CA
10	A	428	DHF	N-CA-CB-CG
8	B	401	NAG	O5-C5-C6-O6
8	B	415	NAG	O5-C5-C6-O6

There are no ring outliers.

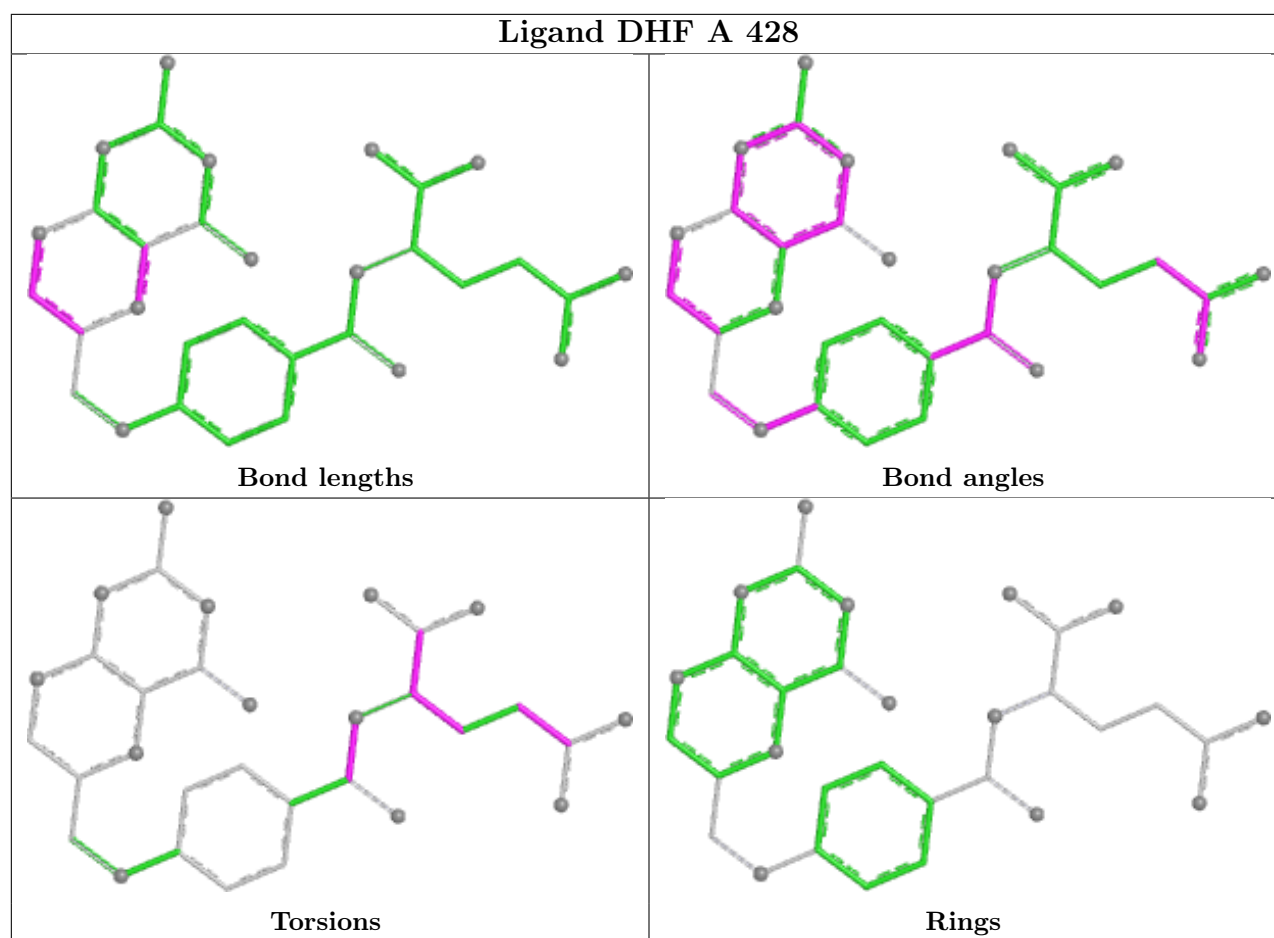
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	416	SO4	1	0
9	C	302	SO4	1	0
10	B	419	DHF	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.







## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/342 (97%)	-0.35	5 (1%) 71 72	19, 34, 60, 97	0
1	B	341/342 (99%)	-0.02	14 (4%) 42 43	29, 45, 69, 84	0
2	C	213/229 (93%)	-0.27	4 (1%) 66 67	20, 33, 54, 93	0
2	H	220/229 (96%)	-0.11	4 (1%) 67 68	24, 39, 71, 97	0
3	D	218/218 (100%)	-0.07	12 (5%) 32 33	23, 38, 69, 97	0
3	L	212/218 (97%)	0.33	7 (3%) 49 51	28, 54, 82, 105	0
All	All	1538/1578 (97%)	-0.10	46 (2%) 52 54	19, 40, 71, 105	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	TYR	4.5
3	L	27(A)	SER	4.0
3	D	214	CYS	3.7
2	C	134	SER	3.6
1	B	237	CYS	3.5

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

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

### 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands ⓘ

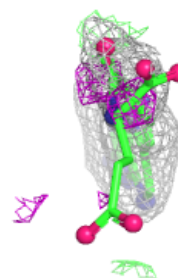
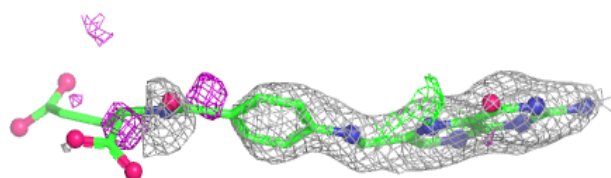
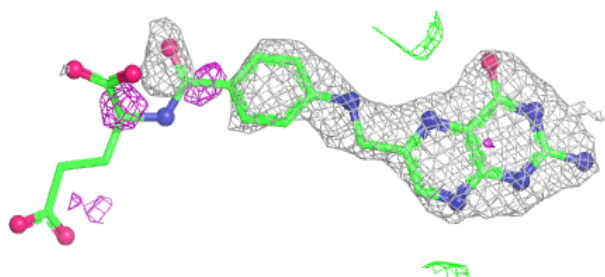
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	B	415	14/15	0.67	0.18	66,76,79,80	0
8	NAG	B	405	14/15	0.74	0.14	52,60,64,65	0
8	NAG	A	423	14/15	0.77	0.15	47,60,63,64	0
8	NAG	B	401	14/15	0.77	0.14	62,69,73,74	0
9	SO4	B	418	5/5	0.78	0.14	93,93,94,94	0
9	SO4	A	426	5/5	0.80	0.16	85,85,85,87	0
10	DHF	B	419	32/32	0.80	0.15	69,92,110,110	0
8	NAG	A	410	14/15	0.81	0.12	48,57,61,63	0
10	DHF	A	428	32/32	0.86	0.17	37,78,115,116	0
9	SO4	A	427	5/5	0.88	0.13	95,95,96,96	0
9	SO4	B	417	5/5	0.89	0.11	98,98,99,99	0
9	SO4	B	416	5/5	0.89	0.12	71,72,72,73	0
9	SO4	H	301	5/5	0.90	0.14	68,70,72,72	0
9	SO4	A	425	5/5	0.94	0.10	61,61,63,64	0
9	SO4	C	302	5/5	0.95	0.09	63,63,64,66	0
9	SO4	A	424	5/5	0.95	0.08	61,63,65,65	0
9	SO4	C	301	5/5	0.99	0.04	32,32,36,36	0

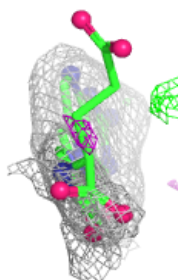
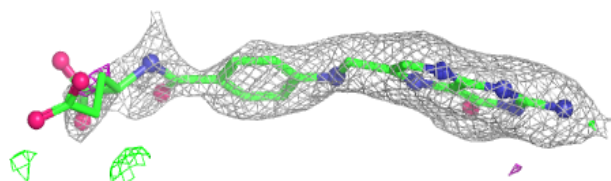
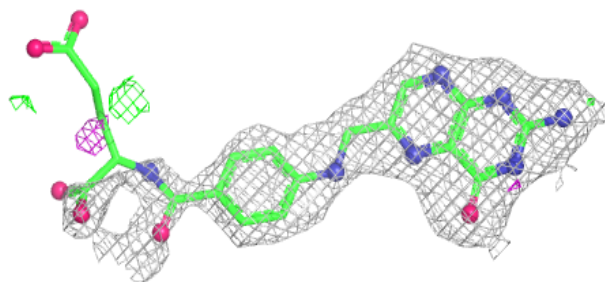
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around DHF B 419:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DHF A 428:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.