



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 02:49 am GMT

PDB ID : 6ZQV  
EMDB ID : EMD-11371  
Title : Cryo-EM structure of mature Spondweni virus  
Authors : Renner, M.; Dejnirattisai, W.; Carrique, L.; Serna Martin, I.; Karia, D.; Ilca, S.L.; Ho, S.F.; Kotecha, A.; Keown, J.R.; Mongkolsapaya, J.; Screaton, G.R.; Grimes, J.M.  
Deposited on : 2020-07-10  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, 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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

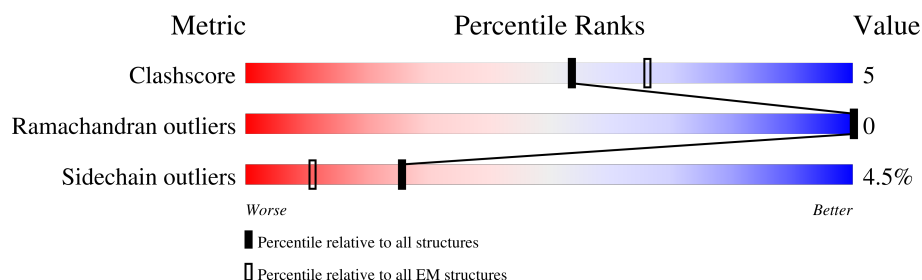
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	505	85% 15%
1	C	505	87% 12% .
1	E	505	83% 16% .
2	B	75	88% 11% .
2	D	75	85% 12% ..
2	F	75	79% 17% . .
3	G	3	67% 33%
3	H	3	100%
3	I	3	100%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13479 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3835	2408	676	719	32		
1	C	504	Total	C	N	O	S	0	0
			3835	2408	676	719	32		
1	E	504	Total	C	N	O	S	0	0
			3835	2408	676	719	32		

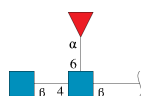
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASN	ASP	conflict	UNP C8XPB6
A	187	ILE	PHE	conflict	UNP C8XPB6
C	37	ASN	ASP	conflict	UNP C8XPB6
C	187	ILE	PHE	conflict	UNP C8XPB6
E	37	ASN	ASP	conflict	UNP C8XPB6
E	187	ILE	PHE	conflict	UNP C8XPB6

- Molecule 2 is a protein called Genome polypeptide.

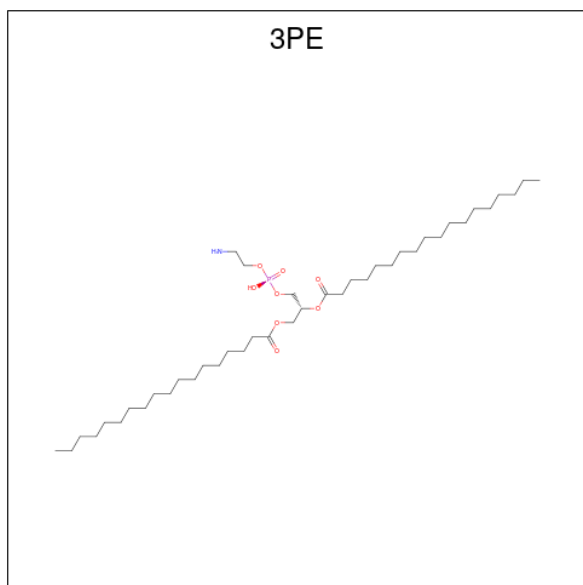
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	74	Total	C	N	O	S	0	0
			591	385	99	106	1		
2	D	74	Total	C	N	O	S	0	0
			591	385	99	106	1		
2	F	74	Total	C	N	O	S	0	0
			591	385	99	106	1		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			38	22	2	14		
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	I	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).

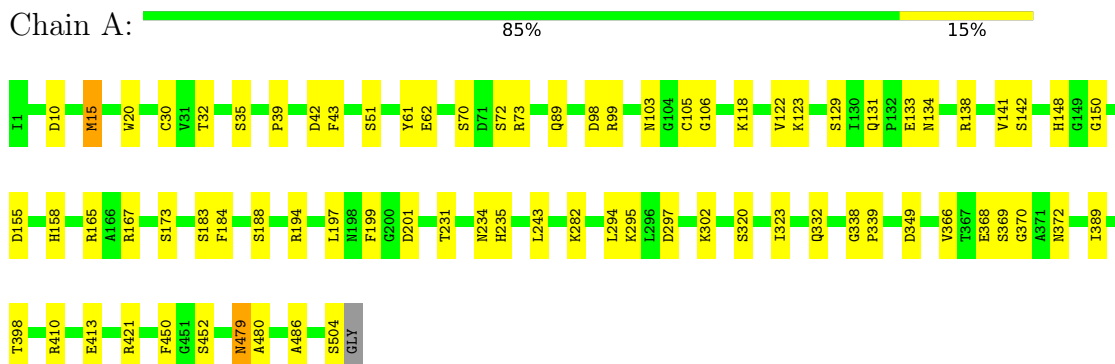


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
4	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
4	E	1	Total	C	N	O	P	0
			29	19	1	8	1	

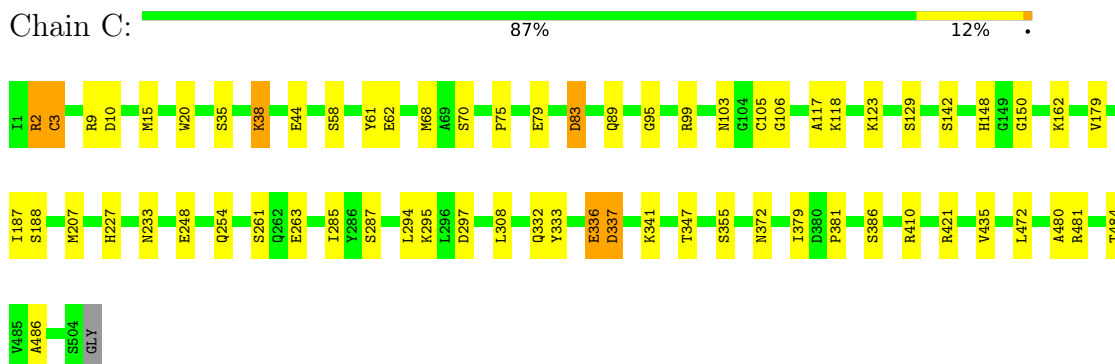
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

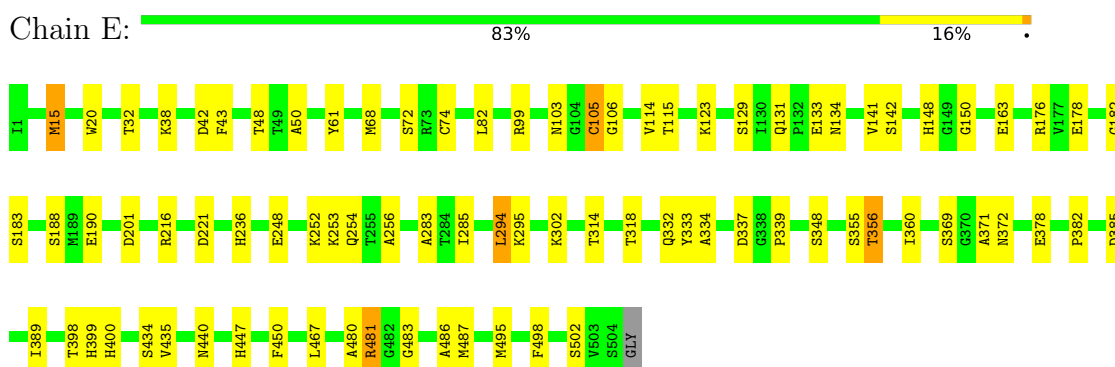
- Molecule 1: Genome polyprotein




- Molecule 1: Genome polyprotein



- Molecule 1: Genome polyprotein




- Molecule 2: Genome polyprotein

Chain B:  88% 11%




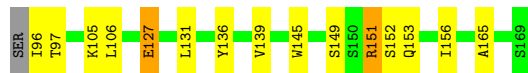
- Molecule 2: Genome polyprotein

Chain D:  85% 12%



- Molecule 2: Genome polyprotein

Chain F:  79% 17%



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

Chain G:  67% 33%



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

Chain H:  100%



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

Chain I:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	63222	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 3PE, 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	0.35	0/3919	0.46	0/5297
1	C	0.36	0/3919	0.46	0/5297
1	E	0.35	0/3919	0.46	0/5297
2	B	0.28	0/605	0.42	0/822
2	D	0.31	0/605	0.42	0/822
2	F	0.31	0/605	0.45	0/822
All	All	0.35	0/13572	0.46	0/18357

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3835	0	3738	38	0
1	C	3835	0	3738	32	0
1	E	3835	0	3738	50	0
2	B	591	0	612	3	0
2	D	591	0	612	5	0
2	F	591	0	612	11	0
3	G	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	38	0	34	0	0
3	I	38	0	34	0	0
4	A	29	0	32	1	0
4	C	29	0	32	1	0
4	E	29	0	32	4	0
All	All	13479	0	13248	133	0

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

All (133) 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:A:15:MET:SD	1:A:15:MET:N	2.52	0.83
1:E:15:MET:SD	1:E:15:MET:N	2.55	0.78
1:C:99:ARG:HA	1:C:103:ASN:HD22	1.50	0.74
1:A:368:GLU:HG3	1:A:370:GLY:H	1.51	0.74
1:A:99:ARG:HA	1:A:103:ASN:HD22	1.57	0.70
1:A:89:GLN:OE1	1:A:118:LYS:NZ	2.28	0.67
1:E:99:ARG:HA	1:E:103:ASN:HD22	1.60	0.66
1:A:10:ASP:OD2	1:A:421:ARG:NH2	2.29	0.65
1:E:148:HIS:HD2	1:E:150:GLY:H	1.45	0.65
1:A:131:GLN:HB2	1:A:134:ASN:HD22	1.61	0.64
1:E:332:GLN:HE21	1:E:372:ASN:HB2	1.62	0.64
1:A:323:ILE:HD12	1:A:323:ILE:H	1.63	0.63
1:C:148:HIS:HD2	1:C:150:GLY:H	1.45	0.63
4:C:601:3PE:N	2:D:106:LEU:O	2.32	0.62
1:E:15:MET:HB3	1:E:435:VAL:HG11	1.82	0.61
1:A:450:PHE:HB3	4:A:601:3PE:H222	1.83	0.60
1:C:20:TRP:HA	1:C:294:LEU:O	2.02	0.59
1:A:148:HIS:HD2	1:A:150:GLY:H	1.51	0.58
2:D:132:ARG:NH2	1:E:221:ASP:OD2	2.36	0.58
1:E:337:ASP:OD1	1:E:337:ASP:N	2.34	0.58
1:A:32:THR:OG1	1:A:42:ASP:OD1	2.17	0.58
1:E:385:ASP:OD1	1:E:400:HIS:NE2	2.36	0.57
1:E:356:THR:HB	1:E:382:PRO:HG3	1.87	0.57
1:E:32:THR:OG1	1:E:42:ASP:OD1	2.17	0.56
1:C:2:ARG:NH1	1:C:44:GLU:OE1	2.37	0.56
1:E:481:ARG:NH1	1:E:483:GLY:O	2.30	0.56
2:F:149:SER:H	2:F:153:GLN:HE21	1.53	0.56
1:E:163:GLU:HG3	1:E:182:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ASP:OD1	1:C:421:ARG:NH2	2.39	0.55
1:E:447:HIS:HE2	4:E:601:3PE:H32	1.72	0.55
1:A:188:SER:OG	1:A:295:LYS:HB2	2.07	0.55
1:C:89:GLN:OE1	1:C:118:LYS:NZ	2.41	0.54
1:A:62:GLU:HB3	1:A:123:LYS:HB2	1.88	0.54
1:E:360:ILE:HB	1:E:378:GLU:HG2	1.89	0.53
2:B:126:VAL:O	2:B:130:ILE:HG13	2.09	0.53
1:E:115:THR:OG1	1:E:254:GLN:OE1	2.20	0.52
1:E:480:ALA:HB3	1:E:486:ALA:HB2	1.92	0.52
1:A:105:CYS:SG	1:A:106:GLY:N	2.83	0.51
1:A:389:ILE:HG12	1:A:398:THR:HG23	1.93	0.51
1:C:480:ALA:HB3	1:C:486:ALA:HB2	1.92	0.51
2:F:127:GLU:O	2:F:131:LEU:HG	2.10	0.51
1:E:333:TYR:O	1:E:372:ASN:HA	2.09	0.51
1:A:62:GLU:HG2	1:A:122:VAL:HB	1.93	0.51
1:C:179:VAL:HB	1:C:187:ILE:HG13	1.93	0.51
1:E:20:TRP:HA	1:E:294:LEU:O	2.11	0.50
1:C:188:SER:OG	1:C:295:LYS:HB2	2.11	0.50
1:A:338:GLY:HA2	1:A:369:SER:HB2	1.92	0.49
1:A:20:TRP:HA	1:A:294:LEU:O	2.12	0.49
1:C:35:SER:OG	1:C:38:LYS:HB2	2.12	0.49
1:E:82:LEU:HD12	1:E:114:VAL:HG13	1.94	0.49
1:C:15:MET:HG2	1:C:435:VAL:HG11	1.94	0.49
1:C:337:ASP:N	1:C:337:ASP:OD1	2.46	0.49
2:F:151:ARG:HH11	2:F:152:SER:H	1.59	0.49
2:D:96:ILE:HG22	2:D:97:THR:H	1.77	0.48
1:E:389:ILE:HG12	1:E:398:THR:HG23	1.95	0.48
1:C:333:TYR:O	1:C:372:ASN:HA	2.13	0.48
4:E:601:3PE:N	2:F:106:LEU:O	2.46	0.48
2:F:136:TYR:CZ	2:F:165:ALA:HB2	2.49	0.47
1:E:498:PHE:O	1:E:502:SER:OG	2.31	0.47
1:C:379:ILE:HG13	1:C:381:PRO:HD3	1.96	0.47
1:A:155:ASP:OD1	1:A:165:ARG:NH1	2.45	0.47
1:A:61:TYR:CZ	1:A:123:LYS:HB3	2.50	0.47
1:C:83:ASP:N	1:C:83:ASP:OD1	2.48	0.47
1:E:447:HIS:NE2	4:E:601:3PE:H32	2.30	0.47
1:A:479:ASN:N	1:A:479:ASN:OD1	2.48	0.47
1:C:332:GLN:HE21	1:C:372:ASN:HB3	1.80	0.46
2:F:152:SER:O	2:F:156:ILE:HG13	2.15	0.46
1:C:58:SER:HB2	1:C:227:HIS:CE1	2.51	0.46
1:E:48:THR:HB	1:E:285:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:SER:OG	1:E:295:LYS:HB2	2.16	0.46
1:E:129:SER:OG	1:E:216:ARG:NH1	2.49	0.46
1:A:73:ARG:HA	1:A:73:ARG:HD3	1.69	0.46
1:C:308:LEU:HD23	1:C:341:LYS:HB3	1.97	0.46
1:A:133:GLU:HG3	1:E:318:THR:HG21	1.98	0.46
1:E:74:CYS:HB3	1:E:105:CYS:SG	2.56	0.46
1:A:332:GLN:HE21	1:A:372:ASN:HB3	1.80	0.45
1:C:105:CYS:SG	1:C:106:GLY:N	2.88	0.45
2:B:136:TYR:CZ	2:B:165:ALA:HB2	2.51	0.45
1:E:450:PHE:HB3	4:E:601:3PE:H222	1.98	0.45
1:A:194:ARG:HB2	1:E:400:HIS:ND1	2.30	0.45
1:C:61:TYR:CZ	1:C:123:LYS:HB3	2.51	0.45
1:E:176:ARG:HG2	1:E:190:GLU:HG2	1.98	0.45
1:A:194:ARG:HH21	1:E:399:HIS:HE1	1.64	0.45
1:C:68:MET:HG3	1:C:117:ALA:HB2	1.98	0.45
1:E:131:GLN:H	1:E:134:ASN:ND2	2.15	0.45
1:E:43:PHE:CE2	1:E:294:LEU:HD11	2.52	0.45
1:A:339:PRO:HA	1:A:366:VAL:O	2.17	0.44
1:C:3:CYS:SG	1:C:9:ARG:HG3	2.57	0.44
1:E:183:SER:HB2	1:E:302:LYS:HD2	2.00	0.44
1:A:51:SER:HB3	1:A:282:LYS:HG2	1.99	0.44
1:A:194:ARG:HB2	1:E:400:HIS:CE1	2.53	0.44
1:A:231:THR:HA	1:A:235:HIS:NE2	2.33	0.44
2:F:136:TYR:HA	2:F:139:VAL:HG12	1.98	0.44
1:C:207:MET:HE1	1:C:263:GLU:HA	2.00	0.44
1:E:105:CYS:SG	1:E:106:GLY:N	2.91	0.44
1:A:480:ALA:O	1:A:486:ALA:HB2	2.18	0.43
1:A:39:PRO:HG3	1:A:184:PHE:HD1	1.84	0.43
1:E:50:ALA:HB3	1:E:283:ALA:HB3	2.00	0.43
1:E:131:GLN:H	1:E:134:ASN:HD22	1.65	0.43
1:E:201:ASP:HA	1:E:216:ARG:HD2	2.00	0.43
1:E:434:SER:OG	1:E:440:ASN:ND2	2.51	0.43
1:E:61:TYR:CZ	1:E:123:LYS:HB3	2.54	0.43
1:C:336:GLU:OE1	1:C:336:GLU:N	2.52	0.42
1:C:248:GLU:HG3	1:C:254:GLN:HG3	2.02	0.42
1:E:252:LYS:HE3	1:E:252:LYS:HB2	1.61	0.42
2:F:149:SER:HB2	2:F:153:GLN:HE22	1.84	0.42
1:A:98:ASP:O	1:A:103:ASN:ND2	2.52	0.42
1:A:197:LEU:HB3	1:A:199:PHE:CE2	2.54	0.42
1:E:43:PHE:CZ	1:E:294:LEU:HD11	2.55	0.42
2:F:105:LYS:HB3	2:F:105:LYS:HE2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:HB3	1:C:123:LYS:HB2	2.02	0.42
1:C:472:LEU:HD23	1:C:472:LEU:HA	1.90	0.42
1:A:243:LEU:HD23	2:B:96:ILE:HD11	2.01	0.42
2:D:149:SER:OG	2:D:150:SER:N	2.53	0.42
1:E:467:LEU:HD12	1:E:467:LEU:HA	1.91	0.42
2:F:149:SER:H	2:F:153:GLN:NE2	2.17	0.42
1:C:308:LEU:HD23	1:C:308:LEU:HA	1.92	0.41
1:A:183:SER:HB2	1:A:302:LYS:HD2	2.02	0.41
1:A:43:PHE:CD1	1:A:141:VAL:HG22	2.55	0.41
1:C:15:MET:HE2	1:C:435:VAL:HB	2.03	0.41
1:E:248:GLU:HA	1:E:253:LYS:O	2.20	0.41
1:C:75:PRO:HD2	1:C:105:CYS:SG	2.60	0.41
1:A:138:ARG:CZ	1:A:167:ARG:HD3	2.50	0.41
2:D:136:TYR:CZ	2:D:165:ALA:HB2	2.55	0.41
1:C:285:ILE:HG22	1:C:287:SER:H	1.86	0.41
1:E:68:MET:SD	1:E:256:ALA:HB3	2.61	0.41
1:C:95:GLY:HA3	1:C:248:GLU:OE2	2.21	0.40
1:E:43:PHE:CD1	1:E:141:VAL:HG22	2.56	0.40
1:E:163:GLU:OE1	1:E:302:LYS:NZ	2.38	0.40
1:E:334:ALA:HA	1:E:371:ALA:O	2.21	0.40
2:F:96:ILE:HG22	2:F:97:THR:H	1.86	0.40
1:A:349:ASP:OD1	1:A:349:ASP:N	2.54	0.40
1:E:339:PRO:HD3	1:E:369:SER:OG	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/505 (99%)	481 (96%)	21 (4%)	0	100	100
1	C	502/505 (99%)	489 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	502/505 (99%)	482 (96%)	20 (4%)	0	100	100
2	B	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
2	D	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
2	F	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
All	All	1722/1740 (99%)	1661 (96%)	61 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	388 (96%)	18 (4%)	24	48
1	C	406/406 (100%)	386 (95%)	20 (5%)	21	43
1	E	406/406 (100%)	390 (96%)	16 (4%)	27	53
2	B	65/66 (98%)	62 (95%)	3 (5%)	23	46
2	D	65/66 (98%)	62 (95%)	3 (5%)	23	46
2	F	65/66 (98%)	62 (95%)	3 (5%)	23	46
All	All	1413/1416 (100%)	1350 (96%)	63 (4%)	26	47

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	30	CYS
1	A	35	SER
1	A	70	SER
1	A	72	SER
1	A	129	SER
1	A	142	SER
1	A	158	HIS
1	A	173	SER

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Mol	Chain	Res	Type
1	A	201	ASP
1	A	234	ASN
1	A	297	ASP
1	A	320	SER
1	A	410	ARG
1	A	413	GLU
1	A	452	SER
1	A	479	ASN
1	A	504	SER
2	B	120	SER
2	B	145	TRP
2	B	151	ARG
1	C	2	ARG
1	C	3	CYS
1	C	38	LYS
1	C	70	SER
1	C	79	GLU
1	C	83	ASP
1	C	129	SER
1	C	142	SER
1	C	162	LYS
1	C	233	ASN
1	C	261	SER
1	C	297	ASP
1	C	336	GLU
1	C	337	ASP
1	C	347	THR
1	C	355	SER
1	C	386	SER
1	C	410	ARG
1	C	481	ARG
1	C	484	THR
2	D	145	TRP
2	D	149	SER
2	D	151	ARG
1	E	15	MET
1	E	38	LYS
1	E	72	SER
1	E	105	CYS
1	E	133	GLU
1	E	142	SER
1	E	178	GLU

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Mol	Chain	Res	Type
1	E	236	HIS
1	E	294	LEU
1	E	314	THR
1	E	348	SER
1	E	355	SER
1	E	356	THR
1	E	481	ARG
1	E	487	MET
1	E	495	MET
2	F	127	GLU
2	F	145	TRP
2	F	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	134	ASN
1	A	148	HIS
1	A	209	ASN
1	A	233	ASN
1	A	234	ASN
1	A	332	GLN
1	A	440	ASN
2	B	153	GLN
1	C	103	ASN
1	C	148	HIS
1	C	157	ASN
1	C	233	ASN
1	C	332	GLN
1	C	440	ASN
1	C	448	GLN
1	C	479	ASN
2	D	153	GLN
1	E	103	ASN
1	E	134	ASN
1	E	148	HIS
1	E	153	ASN
1	E	157	ASN
1	E	332	GLN
1	E	372	ASN
1	E	399	HIS

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Mol	Chain	Res	Type
1	E	440	ASN
2	F	104	GLN
2	F	133	ASN
2	F	153	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 ⓘ

9 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	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	FUC	G	3	3	10,10,11	0.74	1 (10%)	14,14,16	0.74	0
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.49	0
3	NAG	H	2	3	14,14,15	0.20	0	17,19,21	0.38	0
3	FUC	H	3	3	10,10,11	0.61	0	14,14,16	0.83	0
3	NAG	I	1	1,3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.41	0
3	FUC	I	3	3	10,10,11	0.68	0	14,14,16	0.70	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	FUC	O5-C1	-2.02	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

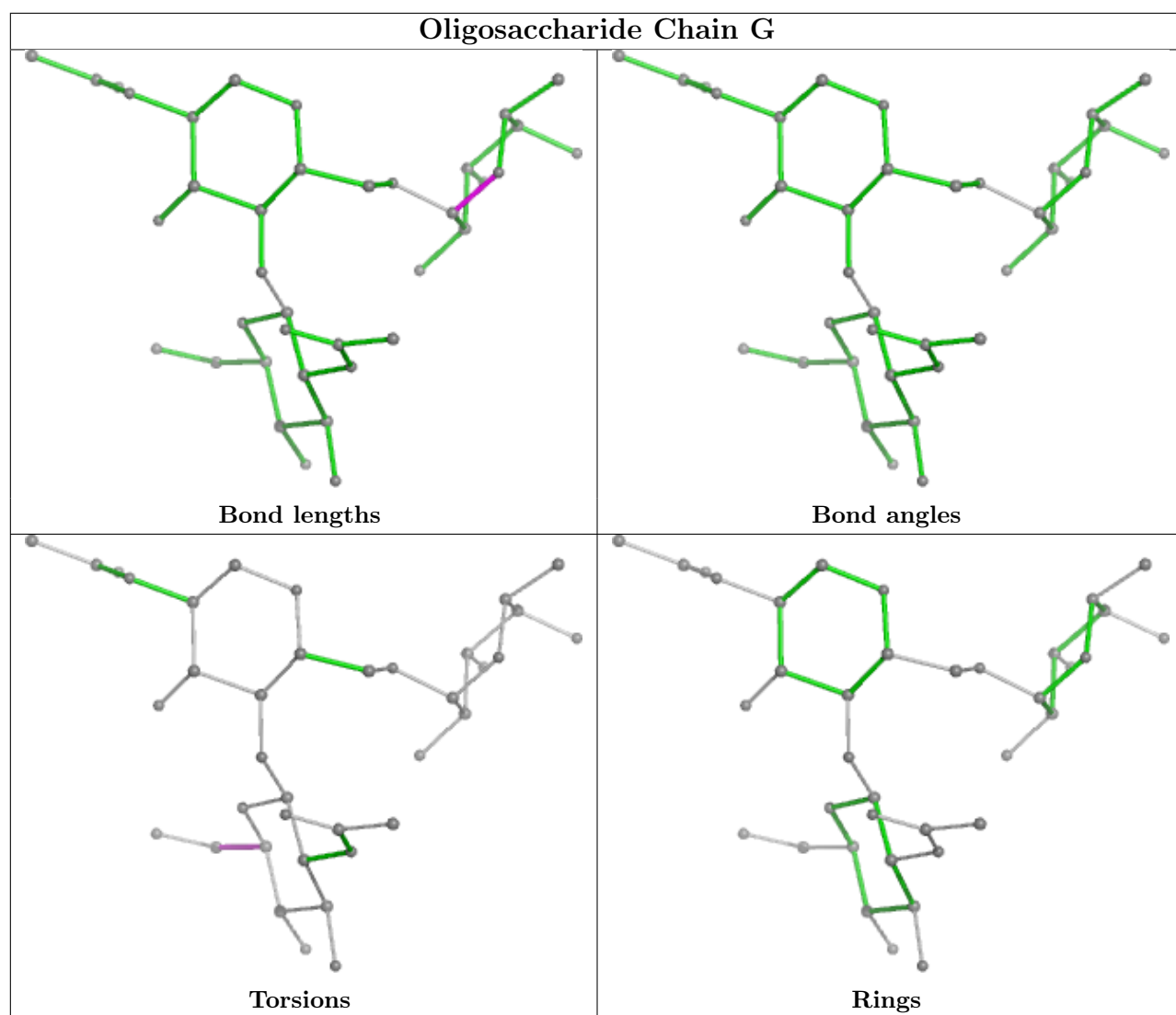
All (4) torsion outliers are listed below:

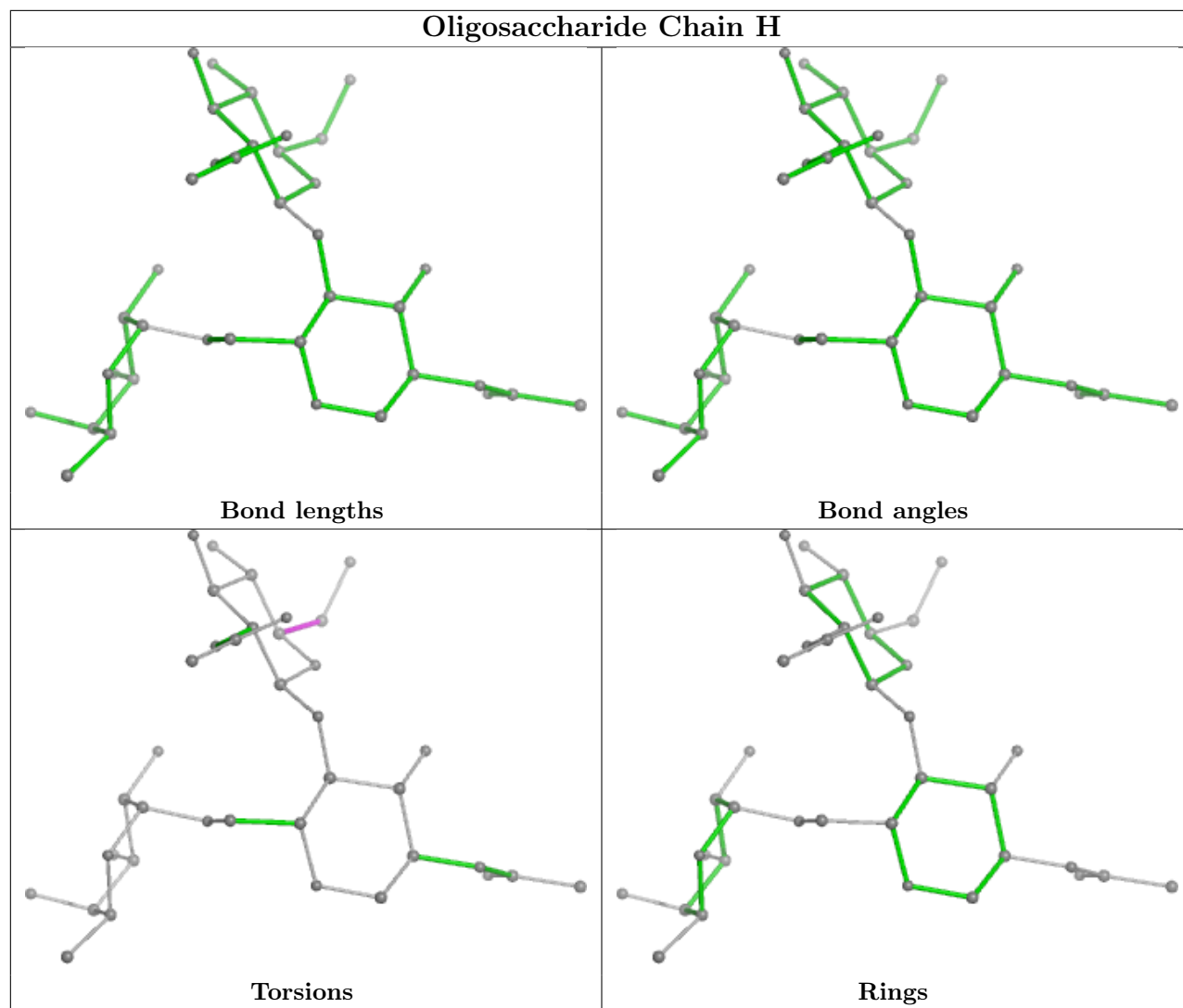
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

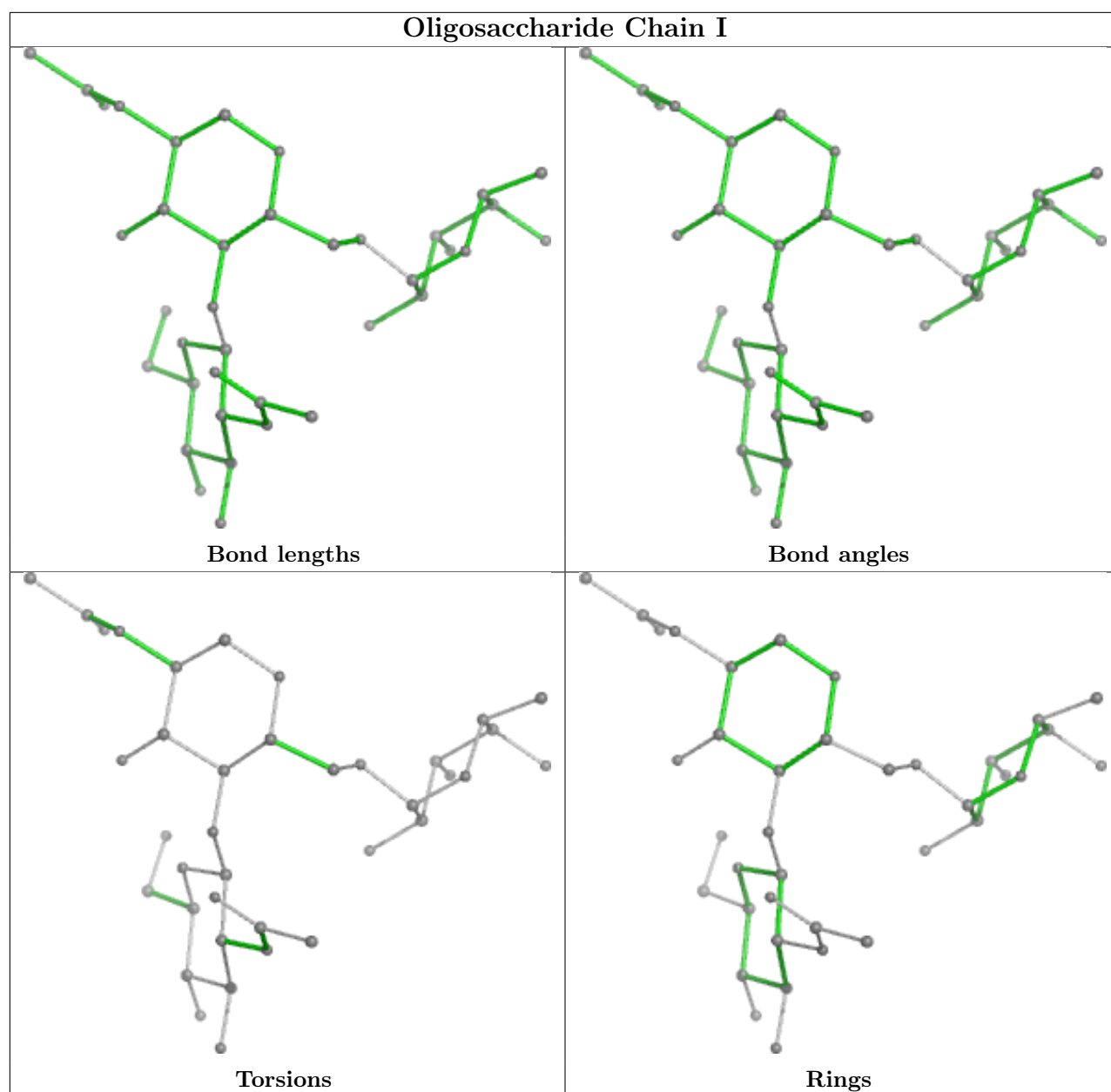
There are no ring outliers.

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 ⓘ

3 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
4	3PE	C	601	-	28,28,50	1.35	3 (10%)	31,33,55	1.05	3 (9%)
4	3PE	E	601	-	28,28,50	1.35	3 (10%)	31,33,55	1.06	3 (9%)
4	3PE	A	601	-	28,28,50	1.36	3 (10%)	31,33,55	1.06	3 (9%)

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	3PE	C	601	-	-	17/32/32/54	-
4	3PE	E	601	-	-	14/32/32/54	-
4	3PE	A	601	-	-	14/32/32/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	3PE	P-O11	3.60	1.73	1.59
4	C	601	3PE	P-O11	3.52	1.73	1.59
4	E	601	3PE	P-O11	3.50	1.73	1.59
4	A	601	3PE	C3-C2	2.75	1.59	1.50
4	C	601	3PE	C3-C2	2.69	1.59	1.50
4	C	601	3PE	P-O13	2.69	1.70	1.59
4	E	601	3PE	P-O13	2.67	1.70	1.59
4	E	601	3PE	C3-C2	2.63	1.58	1.50
4	A	601	3PE	P-O13	2.62	1.69	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	3PE	O12-P-O14	2.93	126.74	112.24
4	A	601	3PE	O12-P-O14	2.92	126.69	112.24
4	C	601	3PE	O12-P-O14	2.92	126.66	112.24
4	A	601	3PE	O21-C21-C22	2.84	117.62	111.50
4	E	601	3PE	O21-C21-C22	2.78	117.50	111.50
4	C	601	3PE	O21-C21-C22	2.76	117.46	111.50
4	E	601	3PE	O31-C3-C2	2.25	114.97	108.43
4	A	601	3PE	O31-C3-C2	2.21	114.85	108.43
4	C	601	3PE	O31-C3-C2	2.13	114.62	108.43

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	3PE	O22-C21-O21-C2
4	A	601	3PE	C22-C21-O21-C2
4	C	601	3PE	O21-C2-C3-O31
4	C	601	3PE	O22-C21-O21-C2
4	C	601	3PE	C22-C21-O21-C2
4	E	601	3PE	O22-C21-O21-C2
4	E	601	3PE	C22-C21-O21-C2
4	A	601	3PE	C31-C32-C33-C34
4	C	601	3PE	C11-O13-P-O11
4	A	601	3PE	O21-C2-C3-O31
4	E	601	3PE	O21-C2-C3-O31
4	E	601	3PE	C22-C23-C24-C25
4	A	601	3PE	C1-C2-C3-O31
4	E	601	3PE	C1-C2-C3-O31
4	C	601	3PE	C32-C33-C34-C35
4	A	601	3PE	C26-C27-C28-C29
4	E	601	3PE	C32-C31-O31-C3
4	C	601	3PE	C26-C27-C28-C29
4	A	601	3PE	O13-C11-C12-N
4	C	601	3PE	C31-C32-C33-C34
4	C	601	3PE	C2-C1-O11-P
4	E	601	3PE	C2-C1-O11-P
4	A	601	3PE	O11-C1-C2-O21
4	E	601	3PE	O32-C31-O31-C3
4	A	601	3PE	C2-C1-O11-P
4	A	601	3PE	O11-C1-C2-C3
4	C	601	3PE	C21-C22-C23-C24
4	E	601	3PE	C26-C27-C28-C29
4	C	601	3PE	C1-C2-C3-O31
4	C	601	3PE	C11-O13-P-O12
4	C	601	3PE	C11-O13-P-O14
4	C	601	3PE	C24-C25-C26-C27
4	A	601	3PE	C32-C33-C34-C35
4	E	601	3PE	C21-C22-C23-C24
4	A	601	3PE	C1-O11-P-O13
4	C	601	3PE	C1-O11-P-O13
4	E	601	3PE	C1-O11-P-O13
4	A	601	3PE	C24-C25-C26-C27
4	E	601	3PE	O13-C11-C12-N
4	C	601	3PE	O11-C1-C2-O21
4	E	601	3PE	O31-C31-C32-C33
4	E	601	3PE	O11-C1-C2-O21

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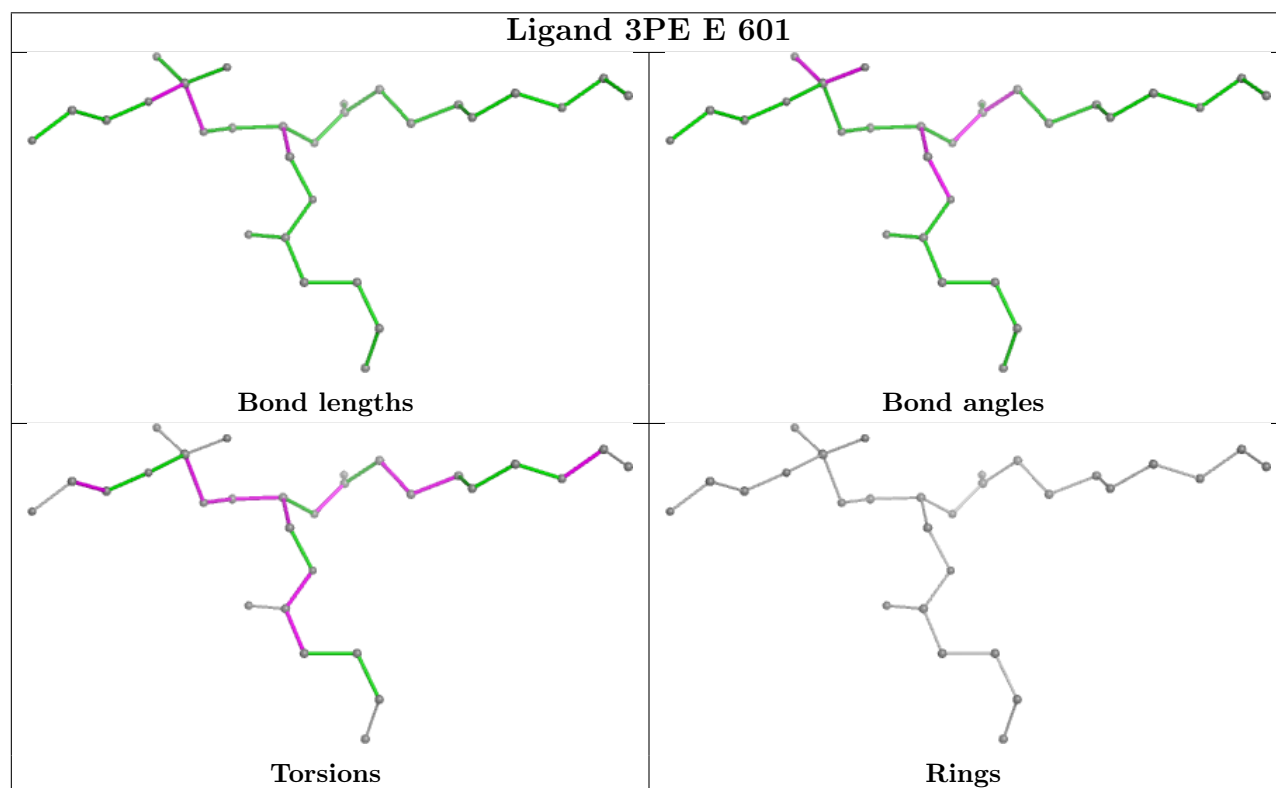
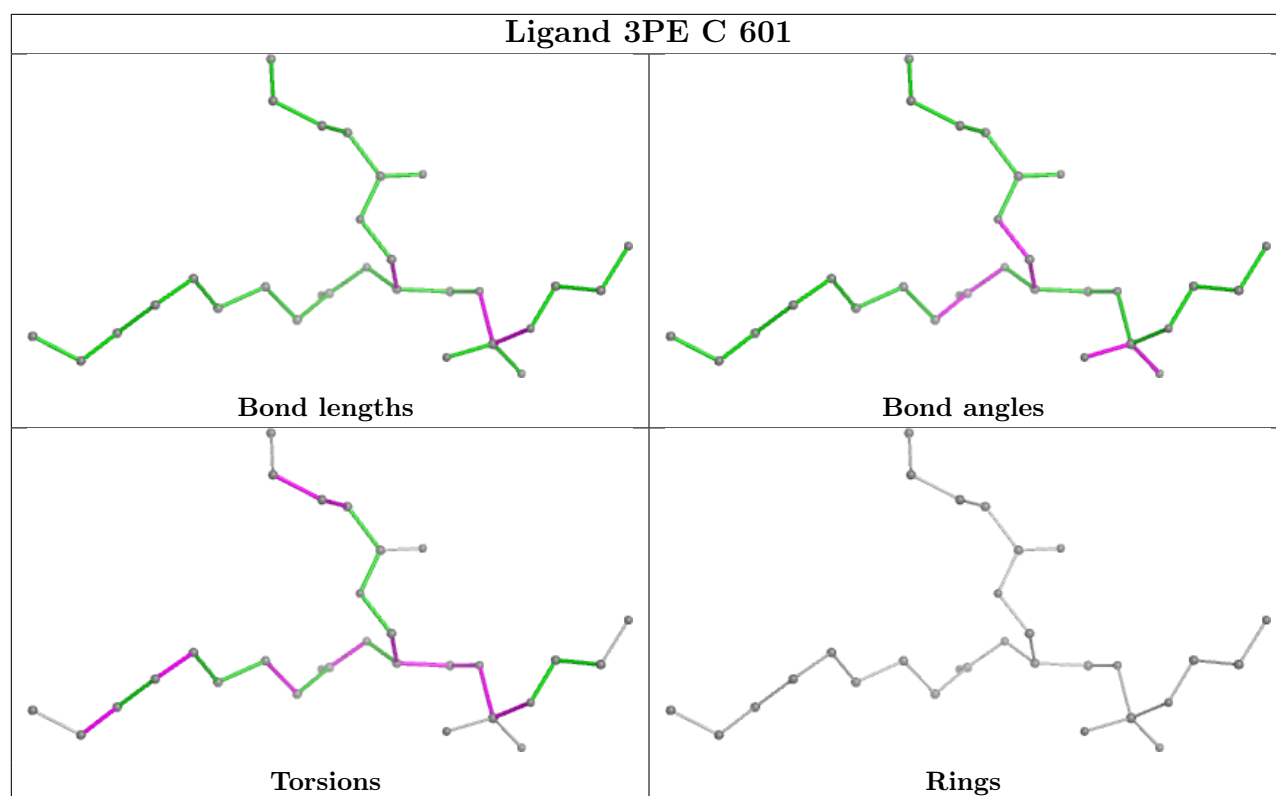
Mol	Chain	Res	Type	Atoms
4	C	601	3PE	O11-C1-C2-C3
4	A	601	3PE	C1-O11-P-O14
4	C	601	3PE	C1-O11-P-O14

There are no ring outliers.

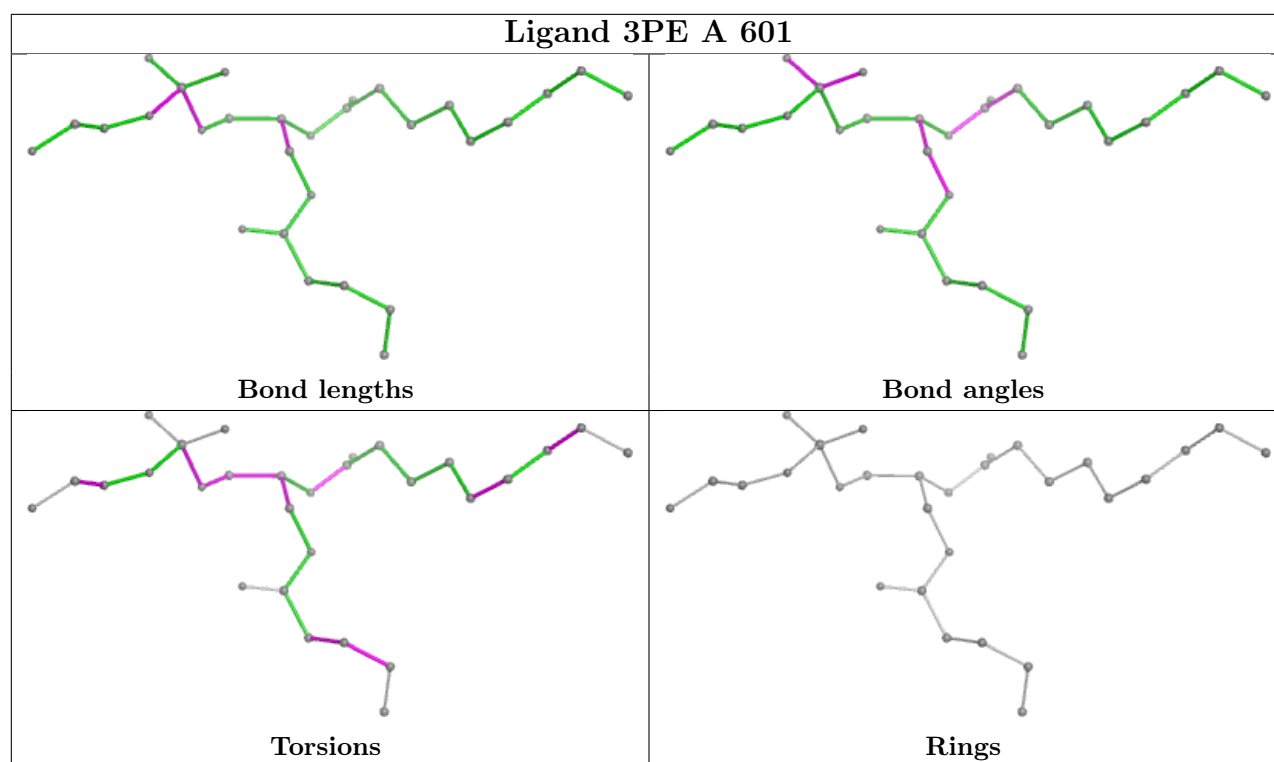
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	3PE	1	0
4	E	601	3PE	4	0
4	A	601	3PE	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.